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From Schrödinger to Feynman: A Hands-On Guide to Quantum Field Theory[1]

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Abstract: Quantum field theory is the framework for describing quantum mechanical processes that can change the number of particles. Such a framework proves to be useful pretty much everywhere in physics (even if you don't want to change the number of particles), but turns out to be compulsory when describing the quantum mechanics of relativistic systems. These notes present an introduction to quantum field theory (both nonrelativistic and relativistic) and are meant to provide a bridge between standard undergraduate topics – nonrelativistic Schrödinger quantum mechanics and introductory electromagnetism (with background material reviewed as needed) – and introductory graduate-level subjects like path integrals and Quantum Electrodynamics (QED). More sophisticated topics (notably nonabelian gauge theories and Fadeev-Popov-DeWitt ghosts) are not covered, though a master of these notes has all of the background needed for their study. The development starts with nonrelativistic processes that change the number of particles, building up the foundations needed to describe how special relativity is incorporated into quantum mechanics (including the need for antiparticles and the spin-statistics connection), covering topics usually omitted in introductory treatments. The utility of – and so motivation for – more advanced tools like canonical and path-integral methods is not assumed, but is built up along the way.

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Contents

1 Preliminaries

In a nutshell, quantum field theory (or QFT for short) is the application of quantum mechanics to systems for which the number of particles can change. This in itself seems not that big a deal and might lead one to believe that quantum field theory is not useful for areas of physics where the number of particles does not change.

Yet it happens that quantum field theory is perhaps the most central theoretical tool in use in physics today, across almost all subdisciplines of study. The reasons for this are two-fold. First, quantum field theory turns out to provide an extremely efficient way of describing physical laws that build in important properties shared by much of nature: things like unitarity and cluster decomposition (more about which in these notes below). Second, once combined with relativity it happens that quantum mechanics *forbids* the existence of interactions that strictly preserve the number of particles. For this reason use of quantum field theory is compulsory for relativistic quantum applications (and in particular to our understanding of nature's laws at their most fundamental level).

Before diving in it is useful to all be on the same page, so the first few sections review some useful material likely to be familiar to you from your other courses.

1.1 Fundamental units

It is common to use specific units adapted to specific problems so that numerical values are not too far from one (such as using the Angstrom or Rydberg for atomic electrons, femtometres or MeV for nuclear processes,[1] astronomical units for the solar system or megaparsecs in cosmology). Such choices are mostly not made here, since one of the points of this book is to emphasize the broad utility of QFT methods across many different areas in physics.

Instead, these notes use *fundamental units*, for which the constants $\hbar$, c and k_B (Planck's constant, the speed of light and Boltzmann's constant) equal 1. For instance $c = 1$ is ensured by measuring time and distances both in seconds (where a second of distance means a light-second; the distance light travels in a second). Similarly, $\hbar = 1$ if $(\text{energy})^{-1}$ and time are both measured in seconds — where an inverse-second of energy means the amount $\hbar/(1\text{sec}) = 6.58211 \times 10^{-16}$ eV — and so on.

In fundamental units basic units can be expressed as a power of length (or a power of energy, or time, if either of these is preferred). This has the very useful benefit of boiling equations down to relations between physical quantities without cluttering them up with

[1] An eV is the amount of energy acquired by a particle with charge e falling through a potential difference of 1 Volt, so 1 erg is close to 624 GeV.

symbols purely to do with units. This is a particularly good virtue when identifying which scales are relevant to any given problem, as is central to any physical analysis. Electromagnetic units are set by using the proton charge e as the unit of charge rather than the Coulomb. Ordinary units may always be retrieved by putting in any missing factors of $\hbar$, c or k_B as required by dimensional analysis.

In these notes the basic unit is taken to be energy, given in eV or multiples thereof. The utility of this choice is that a proton and neutron rest masses in these units are (respectively) 0.938 GeV and 0.940 GeV (which is to say, the energy tied up in the rest mass of a proton, for example, is 0.938 GeV). This is useful because once told that the mass of the earth is $M_\oplus \simeq 3.35 \times 10^{51}$ GeV you also know roughly how many nucleons are in it, since the biggest contributor to an object's mass usually comes from the mass of each nucleon residing in its constituent nuclei. In many ways this is more useful than knowing that $M_\oplus \simeq 5.97 \times 10^{24}$ kg.

Useful rules of thumb when converting between eV and other units are:

$$1 \text{ fm} \simeq (0.2 \text{ GeV})^{-1} \simeq 3 \times 10^{-24} \text{ sec} \quad \text{and} \quad 1 \text{ K} \simeq 9 \times 10^{-5} \text{ eV} \,. \tag{1.1.1}$$

The conversions of many other units are summarized in the tables of Appendix A.1.

1.2 Review of Dirac notation

A very convenient notation in quantum mechanics was provided by Dirac, which emphasizes physical states as vectors in an abstract Hilbert space, as opposed to specifically as wavefunctions, as is often first encountered in introductory courses in quantum mechanics.

1.2.1 Bras and kets

In the Dirac language a physical quantum state ψ is represented by a vector, denoted $|\psi\rangle$. In this notation suppose $|n\rangle$ represent a basis of states that span the quantum Hilbert space for a choice of labels 'n'. Then any other vector can be represented as a linear combination of the form

$$|\psi\rangle = \sum_n \psi_n |n\rangle \,, \tag{1.2.1}$$

for some labels 'n'.

In Dirac notation the inner product of two states – what in wavefunctions might have been written $\int \mathrm{d}x\, \psi^*(x)\phi(x)$ – is written $\langle\psi|\phi\rangle$ and so is a complex number satisfying

$$\langle\psi|\phi\rangle^* = \langle\phi|\psi\rangle \,. \tag{1.2.2}$$

In this sense the quantity $\langle\psi|$ (called a 'bra') is the adjoint of the quantity $|\psi\rangle$ (called a 'ket').[2]

In this notation a basis of states is orthonormal if its elements satisfy

$$\langle n|m\rangle = \delta_{nm} \,, \tag{1.2.3}$$

[2]The nomenclature is chosen so that $\langle\psi|\phi\rangle$ is a 'bra-ket' or bracket.

and when a basis is orthonormal then the expansion coefficients, ψ_n, for the expansion of any state – such as in (1.2.1) – is found by multiplying through on the left by $\langle m|$ to get

$$\langle m|\psi\rangle = \sum_n \psi_n \langle m|n\rangle = \sum_n \psi_n \delta_{mn} = \psi_m \,. \tag{1.2.4}$$

1.2.2 Representations

What is useful about this representation is that it separates the abstract state vector, $|\psi\rangle$, from its *representation* in terms of any particular basis, the ψ_n's. For instance, the usual wave-function representation $\psi(x)$ in this language is obtained by referring states to the specific 'position' basis $|x\rangle$ of states that diagonalize the position operator X, with $\psi(x) = \langle x|\psi\rangle$. That is, defining

$$X|x\rangle = x|x\rangle \,, \tag{1.2.5}$$

implies the states are orthonormal (because X is hermitian). Because x runs over a continuous range of values (rather than a denumerable set, like the integers, say), the orthonormality condition is usually taken to be

$$\langle x|y\rangle = \delta(x-y) \,, \tag{1.2.6}$$

where $\delta(x-y)$ is the usual Dirac delta-function defined by the condition $\int \mathrm{d}y\, f(y)\delta(x-y) = f(x)$ for a class of functions f.

If there is a second orthonormal basis of states, $|a\rangle$, labelled by some quantities 'a' then ψ would instead be represented by

$$|\psi\rangle = \sum_a \psi_a |a\rangle \quad \text{with} \quad \psi_a = \langle a|\psi\rangle \,, \tag{1.2.7}$$

To convert between two bases use the completeness of either basis to expand the elements of one in terms of the other:

$$|n\rangle = \sum_a c_{an}|a\rangle \quad \text{with} \quad c_{an} = \langle a|n\rangle \,, \tag{1.2.8}$$

so that

$$|\psi\rangle = \sum_n \psi_n |n\rangle = \sum_n \sum_a \psi_n c_{an}|a\rangle \tag{1.2.9}$$

which compared with (1.2.7) implies the coefficients ψ_n and ψ_a are related by matrix multiplication:

$$\psi_a = \sum_n c_{an}\psi_n \quad \text{or} \quad \langle a|\psi\rangle = \sum_n \langle a|n\rangle\langle n|\psi\rangle \,. \tag{1.2.10}$$

Since this last formula holds for any state $|\psi\rangle$ and any bases $|a\rangle$ and $|n\rangle$ it shows that the completeness of the basis states can be expressed as the following operator expression

$$\sum_n |n\rangle\langle n| = 1 \,, \tag{1.2.11}$$

called a 'resolution of the identity', for any orthonormal basis. For a continuous basis like $|x\rangle$ this completeness relation becomes

$$\int \mathrm{d}x\ |x\rangle\langle x| = 1\,, \tag{1.2.12}$$

whose consistency with $\langle x|y\rangle = \delta(x-y)$ is seen by multiplying through on the right by $|y\rangle$.

The action of any operator, $\mathcal{O}$ say, on a state can be written as matrix multiplication within any particular representation. That is, the expansion of the state $|\phi\rangle := \mathcal{O}|\psi\rangle$ in terms of a basis is given by $\mathcal{O}|\psi\rangle = \sum_n \phi_n|n\rangle$ for coefficients

$$\phi_n = \langle n|\phi\rangle = \langle n|\mathcal{O}|\psi\rangle = \sum_m \langle n|\mathcal{O}|m\rangle\psi_m = \sum_m \mathcal{O}_{nm}\psi_m\,, \tag{1.2.13}$$

where the second-last equality expands $|\psi\rangle$ in terms of the basis $|m\rangle$ and the last equality defines the *matrix elements* $\mathcal{O}_{nm} := \langle n|\mathcal{O}|m\rangle$. The upshot of (1.2.13) is that the action of linear operators in the Hilbert space is equivalent to ordinary matrix multiplication once both the operators and state vectors are referred to a specific basis. The matrix multiplication way to write (1.2.13) is :

$$\begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} (\mathcal{O}\psi)_1 \\ (\mathcal{O}\psi)_2 \\ \vdots \\ (\mathcal{O}\psi)_n \end{pmatrix} = \begin{pmatrix} \mathcal{O}_{11} & \mathcal{O}_{12} & \cdots & \mathcal{O}_{1n} \\ \mathcal{O}_{21} & \mathcal{O}_{22} & \cdots & \mathcal{O}_{2n} \\ \vdots & & \ddots & \vdots \\ \mathcal{O}_{n1} & \mathcal{O}_{n2} & \cdots & \mathcal{O}_{nn} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix}. \tag{1.2.14}$$

1.2.3 Position representation

In this language the wave-function representation (or Schrödinger representation) of a state ψ is defined as the coefficient 'ψ_n' that appears when $|\psi\rangle$ is expanded in the position basis:

$$\psi(x) := \langle x|\psi\rangle\,. \tag{1.2.15}$$

The action of the position operator X on ψ in this basis is then fairly simple

$$\langle x|X|\psi\rangle = x\langle x|\psi\rangle = x\,\psi(x)\,, \tag{1.2.16}$$

as is usually taken in the Schrödinger representation.

In this basis the same arguments that led to (1.2.13) show that in a continuous basis it is instead written

$$\langle x|\mathcal{O}|\psi\rangle = \int \mathrm{d}y\ \langle x|\mathcal{O}|y\rangle\langle y|\psi\rangle = \int \mathrm{d}y\ \langle x|\mathcal{O}|y\rangle\psi(y)\,, \tag{1.2.17}$$

so the action of operators on states look like a continuous version of matrix multiplication, *i.e.* like an integral transformation,

$$\phi(x) = \int \mathrm{d}y\ K(x,y)\,\psi(y)\,, \tag{1.2.18}$$

with kernel $K(x,y) = \langle x|\mathcal{O}|y\rangle$.

In particular, the matrix element (or kernel) of the position operator in this language is

$$\langle x|X|y\rangle = y\,\langle x|y\rangle = y\,\delta(x-y) = x\,\delta(x-y)\,, \tag{1.2.19}$$

which when used in (1.2.17) gives the usual Schrödinger-representation action

$$\mathcal{X}\,\psi(x) := \langle x|X|\psi\rangle = \int \mathrm{d}y\;\langle x|X|y\rangle\langle y|\psi\rangle = \int \mathrm{d}y\; x\,\delta(x-y)\,\psi(y) = x\,\psi(x)\,. \tag{1.2.20}$$

That is, the operator $\mathcal{X}$ representing X in the Schrödinger representation just amounts to multiplication by x.

The action of momentum in this language can also be worked out given the canonical commutation relation $[P,X] = -i$ which also implies

$$\langle x|P|y\rangle = -i\partial_x\delta(x-y) \tag{1.2.21}$$

so that the action of P on a state is

$$\mathcal{P}\,\psi(x) := \langle x|P|\psi\rangle = \int \mathrm{d}y\;\langle x|P|y\rangle\,\langle y|\psi\rangle = -i\partial_x\int \mathrm{d}y\;\delta(x-y)\psi(y) = -i\partial_x\psi(x)\,, \tag{1.2.22}$$

as usual. That this is the right representation can be seen by verifying it reproduces the commutation relation $[\mathcal{P},\mathcal{X}]f = -if$ for any function $f(x) = \langle x|f\rangle$ in the Hilbert space.

1.2.4 Momentum representation

Even more useful is the momentum representation since momentum is often conserved. Defining the states $|p\rangle$ by the eigenvalue condition $P|p\rangle = p|p\rangle$ implies the overlap $\langle x|p\rangle$ satisfies

$$p\langle x|p\rangle = \langle x|P|p\rangle = \int \mathrm{d}y\;\langle x|P|y\rangle\langle y|p\rangle = -i\partial_x\langle x|p\rangle \tag{1.2.23}$$

which is a differential equation whose solution is

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}}\,e^{ipx}\,, \tag{1.2.24}$$

where the normalization is chosen so that

$$\langle p|q\rangle = \int \mathrm{d}x\;\langle p|x\rangle\langle x|q\rangle = \frac{1}{2\pi}\int \mathrm{d}x\;e^{i(q-p)x} = \delta(p-q)\,. \tag{1.2.25}$$

Using this to change from position to momentum representation reveals the transformation as the usual Fourier transform:

$$\psi(x) = \langle x|\psi\rangle = \int \mathrm{d}p\;\langle x|p\rangle\langle p|\psi\rangle = \int \frac{\mathrm{d}p}{\sqrt{2\pi}}\,e^{ipx}\langle p|\psi\rangle = \int \frac{\mathrm{d}p}{\sqrt{2\pi}}\,e^{ipx}\psi(p)\,, \tag{1.2.26}$$

and so on.

1.3 Continuum and discrete momentum eigenstates

This review is taken from an Appendix of [1].

There are three different conventions often used for momentum eigenstates: discrete normalization, continuum normalization, and relativistic continuum normalization. All three types arise in these notes, so this section furnishes a brief reminder of how to convert from one to another. For simplicity this is done here for one spatial dimension, though identical arguments also work in other choices for the number of dimensions.

Discrete normalization corresponds to situations where momentum takes a denumerably infinite set of values, such as occurs if spatial dimensions have finite length, L say, perhaps satisfying periodic boundary conditions so functions satisfy $\psi(x+L) = \psi(x)$ for any x. For momentum eigenstates, $\psi(x) = L^{-1/2}\exp[ipx]$, this condition implies $p = 2\pi n/L$ for integer n, making p denumerable as required. Normalization and completeness relations for states then take the usual quantum form, such as

$$(p\,|\,q) = \delta_{pq} \qquad \text{and} \qquad \sum_p |p)(p\,| = 1\,, \tag{1.3.1}$$

where the sum over p is really a sum over the integer n. Here the 'rounded ket' notation, $|p)$, is used to distinguish states normalized this way from non-denumerable situations normalized in the continuum.

1.3.1 Continuum normalization

Continuum-normalized states $|p\rangle$ are obtained from discrete-normalized states in the infinite-volume limit $L \to \infty$. In this limit the spacing, $2\pi/L$, between adjacent levels goes to zero so the denumerable label p goes over to a continuum one. For L very large but still finite there are $\mathrm{d}N = \mathrm{d}p/(2\pi/L)$ states in a small continuous interval $\mathrm{d}p$, and so the density of states is $\mathrm{d}N/\mathrm{d}p = L/(2\pi)$. Therefore any sum over p goes over to an integral in the large-L limit according to the rule

$$\sum_p F(p) = \int \mathrm{d}p\, F(p)\, \frac{\mathrm{d}N}{\mathrm{d}p} = L \int \frac{\mathrm{d}p}{2\pi}\, F(p)\,, \tag{1.3.2}$$

where $F(p)$ is *any* function that varies negligibly over scales of order $2\pi/L$.

Using this conversion, for very large L the completeness relation for $|p)$ becomes

$$1 = \sum_p |p)(p| = L \int \frac{\mathrm{d}p}{2\pi}\, |p)(p| =: \int \mathrm{d}p\, |p\rangle\langle p|\,, \tag{1.3.3}$$

where the last equality suggests the definition of the continuum-normalized state $|p\rangle := [L/(2\pi)]^{1/2}|p)$. Multiplying (1.3.3) through on the right by $|q\rangle$ shows that consistency requires the continuum state must satisfy the normalization condition

$$\langle p\,|\,q\rangle = \delta(p-q)\,, \tag{1.3.4}$$

which can also be inferred directly from the definitions using

$$\langle p \,|\, q \rangle = \frac{L}{2\pi}(p \,|\, q) = \frac{L}{2\pi}\, \delta_{pq}\,. \tag{1.3.5}$$

The right-hand side of this expression is zero if $p \neq q$ and if $p = q$ it goes to infinity as $L \to \infty$. It is therefore a Dirac delta function, $\delta(p-q)$, up to normalization. To get the normalization notice that the integral over p of (1.3.5) in this limit is given by

$$\int \mathrm{d}p\, \langle p \,|\, q \rangle = \frac{2\pi}{L} \sum_p \langle p \,|\, q \rangle = \sum_p (p \,|\, q) = 1\,, \tag{1.3.6}$$

and so the right-hand side of (1.3.5) goes to $\delta(p-q)$ as $L \to \infty$, as claimed.

A useful relation when converting between discrete and continuum normalizations is

$$\sum_p |p)(p| = \frac{2\pi}{L} \sum_p \left[\frac{L}{2\pi}\, |p)(p|\right] \to \int \mathrm{d}p\, |p\rangle\langle p| \quad (\text{as } L \to \infty)\,, \tag{1.3.7}$$

showing that completeness sums are the same, regardless of whether momenta are normalized discretely or in the continuum. Often these kinds of sums arise weighted by quantities like an initial probability distribution for $P(p)$ for finding the system in the state $|p)$, and when this is so $P(p)$ goes over in the continuum limit to a phase-space distribution as follows. If $P(p)$ is the probability of having any one value for p, and varies slowly enough to be regarded as being constant in a short interval $\mathrm{d}p$, then the density of probability, $\mathrm{d}\mathcal{P}(p)$, for finding the particle in the interval between p and $p + \mathrm{d}p$ is:

$$\mathrm{d}\mathcal{P}(p) = \frac{\mathrm{d}N}{\mathrm{d}p}\, P(p)\, \mathrm{d}p = \frac{L}{2\pi}\, P(p)\, \mathrm{d}p\,. \tag{1.3.8}$$

and so the differential probability per-unit-spatial-volume of finding the particle in this momentum region (*i.e.* the phase-space probability density) becomes

$$\mathfrak{p} := \frac{1}{L}\left(\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}p}\right) = \frac{P(p)}{2\pi}\,. \tag{1.3.9}$$

The normalization $\sum_p P(p) = 1$ then implies $\int \mathrm{d}x\, \mathrm{d}p\; \mathfrak{p} = 1$. With this normalization the average of a single-particle observable $\mathcal{O}$ is

$$\overline{\mathcal{O}} = \sum_p P(p)\, (p|\mathcal{O}|p) = \int \mathrm{d}p\, P(p)\, \langle p|\mathcal{O}|p\rangle\,. \tag{1.3.10}$$

For three spatial dimensions identical arguments show that the density of states is $\mathrm{d}N/\mathrm{d}^3p = \mathcal{V}/(2\pi)^3$ where $\mathrm{d}^3p := \mathrm{d}p_x\, \mathrm{d}p_y\, \mathrm{d}p_z$ and $\mathcal{V} := L^3$ is the system's large spatial volume. This means discrete sums go over into 3D integrals according to

$$\sum_{\mathbf{p}} \to \mathcal{V} \int \frac{\mathrm{d}^3p}{(2\pi)^3} = \mathcal{V} \int \frac{\mathrm{d}p_x \mathrm{d}p_y \mathrm{d}p_z}{(2\pi)^3}\,, \tag{1.3.11}$$

so if $|\mathbf{p}\rangle = [\mathcal{V}/(2\pi)^3]^{1/2}|\mathbf{p})$ then as $\mathcal{V} \to \infty$ the completeness formula (1.3.7) becomes

$$1 = \sum_{\mathbf{p}} |\mathbf{p})(\mathbf{p}| \to \int \mathrm{d}^3p \, |\mathbf{p}\rangle\langle\mathbf{p}| \,, \tag{1.3.12}$$

while orthogonality goes over to

$$\langle\mathbf{p}|\mathbf{q}\rangle = \delta^3(\mathbf{p}-\mathbf{q}) = \delta(p_x - q_x)\,\delta(p_y - q_y)\,\delta(p_z - q_z)\,. \tag{1.3.13}$$

A sum weighted by an initial probability distribution similarly goes over to

$$\sum_{\mathbf{p}} P(\mathbf{p})\,|\mathbf{p})(\mathbf{p}\,| \to \int \mathrm{d}^3p\, P(\mathbf{p})\,|\mathbf{p}\rangle\langle\mathbf{p}\,|\,, \tag{1.3.14}$$

where the continuum phase-space probability distribution is given in terms of $P(\mathbf{p})$ by

$$\mathfrak{p} := \frac{1}{\mathcal{V}}\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}^3p} = \frac{P(\mathbf{p})}{(2\pi)^3}\,. \tag{1.3.15}$$

1.4 Multiparticle quantum mechanics

The first step towards formulating the quantum mechanics of processes that change the number of particles (the *raison d'etre* of quantum field theory) is formulating how multiparticle states are different in quantum mechanics from single-particle ones.

At first blush adding more particles is no big deal. Consider a non-interacting particle type whose single-particle states are labelled by $|p\,\sigma\rangle$, where p is momentum and σ denotes all of the other labels — charge, baryon number, spin (in 2 or more dimensions) and so on — required to uniquely specify a given particle state. The Hilbert space of ordinary single-particle quantum mechanics is the span of all such basis states:

$$\mathfrak{H}_1 = \left\{ |\psi\rangle = \sum_{p\sigma} c(p,\sigma)\;|p\,\sigma\rangle \right\}, \tag{1.4.1}$$

for some complex coefficients $c(p,\sigma)$, with the 'sum' over all allowed values for p and σ.

The two-particle Hilbert space similarly contains the span of all possible two-particle states and so is the product of two copies of $\mathfrak{H}_1$, spanned by all possible states of the form

$$\mathfrak{H}_2 = \left\{ |\psi\rangle = \sum_{p_1\sigma_1}\sum_{p_2\sigma_2} c(p_1,\sigma_1;p_2,\sigma_2)\;|p_1\,\sigma_1\,;p_2\,\sigma_2\rangle \right\}. \tag{1.4.2}$$

$\mathfrak{H}_3$ is similarly spanned by all three-particle states, and so on for $\mathfrak{H}_N$ for all integers $N \geq 0$.

Operators act on these states in a straightforward way. Single-particle operators (like momentum or position) can be defined using the tensor product of the usual operators used in single-particle quantum mechanics. For instance, the momentum of particle '1' would be $P_1 = P \otimes I$, the momentum of particle two would be $P_2 = I \otimes P$ and the total momentum

would be $P_{\rm tot} = P_1 + P_2 = P \otimes I + I \otimes P$ where P is the operator used for single-particle systems above and I is the unit operator in the single-particle Hilbert space.

Concretely, in the Schrödinger (or position) representation a two-particle state $|\psi\rangle$ can be written in terms of a wave-function $\langle x_1, x_2|\psi\rangle = \psi(x_1, x_2)$ in terms of which the operation of position and momentum are (in the absence of other quantum numbers, such as spin)

$$\begin{aligned} \mathcal{X}_1\psi(x_1,x_2) &= x_1\,\psi(x_1,x_2)\,, \quad \mathcal{X}_2\psi(x_1,x_2) = x_2\,\psi(x_1,x_2) \\ \mathcal{P}_1\psi(x_1,x_2) &= -i\frac{\partial\psi}{\partial x_1}\,, \quad \mathcal{P}_2\psi(x_1,x_2) = -i\frac{\partial\psi}{\partial x_2} \end{aligned} \tag{1.4.3}$$

since these satisfy $[\mathcal{P}_k\,, \mathcal{X}_j] = -i\delta_{kj}$ and $[\mathcal{X}_k\,, \mathcal{X}_j] = [\mathcal{P}_k\,, \mathcal{P}_j] = 0$.

Not all operators must have this single-particle form, however. The total momentum is a simple example, represented by

$$\mathcal{P}_{\rm tot}\psi(x_1,x_2) = (\mathcal{P}_1 + \mathcal{P}_2)\psi(x_1,x_2) = -i\frac{\partial\psi}{\partial x_1} - i\frac{\partial\psi}{\partial x_2}\,. \tag{1.4.4}$$

Another is an interaction potential which could be a more general function of both positions: $V(X_1, X_2)$, which in Schrödinger picture acts as

$$V(X_1,X_2)\psi(x_1,x_2) = V(x_1,x_2)\psi(x_1,x_2)\,, \tag{1.4.5}$$

and so on.

A similar story goes through in three dimensions, with the Schrödinger representation of a two-particle state being $\langle \mathbf{x}_1, \mathbf{x}_2|\psi\rangle = \psi(\mathbf{x}_1, \mathbf{x}_2)$ in terms of which the operation of position and momentum are

$$\begin{aligned} \mathbf{X}_1\psi(\mathbf{x}_1,\mathbf{x}_2) &= \mathbf{x}_1\,\psi(\mathbf{x}_1,\mathbf{x}_2)\,, \quad \mathbf{X}_2\psi(\mathbf{x}_1,\mathbf{x}_2) = \mathbf{x}_2\,\psi(\mathbf{x}_1,\mathbf{x}_2) \\ \mathbf{P}_1\psi(\mathbf{x}_1,\mathbf{x}_2) &= -i\nabla_1\psi(\mathbf{x}_1,\mathbf{x}_2)\,, \quad \mathbf{P}_2\psi(\mathbf{x}_1,\mathbf{x}_2) = -i\nabla_2\psi(\mathbf{x}_1,\mathbf{x}_2) \end{aligned} \tag{1.4.6}$$

since these satisfy $[P_{ka}\,, \mathcal{X}_{jb}] = -i\delta_{kj}\delta_{ab}$ and $[\mathcal{X}_{ka}\,, \mathcal{X}_{jb}] = [\mathcal{P}_{ka}\,, \mathcal{P}_{jb}] = 0$ where $k, j = x, y, z$ label the spatial components of the vectors and $a, b = 1, 2$ label which particle is involved. The total momentum is similarly

$$\mathbf{P}_{\rm tot}\psi(\mathbf{x}_1,\mathbf{x}_2) = (\mathbf{P}_1 + \mathbf{P}_2)\psi(\mathbf{x}_1,\mathbf{x}_2) = -i\nabla_1\psi(\mathbf{x}_1,\mathbf{x}_2) - i\nabla_2\psi(\mathbf{x}_1,\mathbf{x}_2)\,, \tag{1.4.7}$$

while a three-dimensional interaction potential which could be written $V(\mathbf{X}_1, \mathbf{X}_2)$, with

$$V(\mathbf{X}_1,\mathbf{X}_2)\psi(\mathbf{x}_1,\mathbf{x}_2) = V(\mathbf{x}_1,\mathbf{x}_2)\psi(\mathbf{x}_1,\mathbf{x}_2)\,. \tag{1.4.8}$$

A concrete example of this form in 3D is the case of two nonrelativistic particles that mutually interact through a potential that depends only on the relative separation, $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$, for which the Hamiltonian in the Schrödinger representation would be

$$\langle \mathbf{x}_1, \mathbf{x}_2|H|\psi\rangle = \mathcal{H}\psi(\mathbf{x}_1,\mathbf{x}_2) = \left[-\frac{1}{2m_1}\nabla_1^2 - \frac{1}{2m_2}\nabla_2^2 + V(\mathbf{x}_1 - \mathbf{x}_2)\right]\psi(\mathbf{x}_1,\mathbf{x}_2)\,. \tag{1.4.9}$$

1.5 Indistinguishable particles

For the present descriptive purposes the main new conceptual issue that arises with more than one particle concerns their indistinguishability: all evidence indicates that particles of a specific species (*e.g.* all electrons or all photons, say) are absolutely idistinguishable from one another. That is to say, there is no evidence for a 'hidden' property carried by each electron or photon that allows one to distinguish "electron 1 is in state A and electron 2 is in state B" from "electron 2 is in state A and electron 1 is in state B".

The notation being used to this point tends to obscure this indistinguishability because when writing a two-particle state (say) as $|\mathbf{p}_1\,;\mathbf{p}_2\rangle$ the labels '1' and '2' make it seem as if $|\mathbf{p}_2\,;\mathbf{p}_1\rangle$ would be a different state. Although this might be true if particle 1 were a proton and particle 2 an electron, it is definitely not true if both particles are the same type.

Physics remains invariant if identical particles are permuted into one another, and because physical predictions always involve squares of amplitudes like $|\langle\phi|\psi\rangle|^2$ there are two logically distinct ways (in three spatial dimensions) that these permutations can be realized on a state. If we define $\mathrm{Perm}_{12}|\mathbf{p}_1\,;\mathbf{p}_2\rangle := |\mathbf{p}_2\,;\mathbf{p}_1\rangle$ then

$$\mathrm{Perm}_{12}|\mathbf{p}_1\,;\mathbf{p}_2\rangle = \pm|\mathbf{p}_1\,;\mathbf{p}_2\rangle\,. \tag{1.5.1}$$

The sign on the right-most side is a characteristic property of each particle type, with particles satisfying (1.5.1) with the upper sign called *bosons* and those that satisfy it with the lower sign called *fermions*.

Condition (1.5.1) restricts the kinds of states that can be entertained. For example a two particle state of the form $\psi(\mathbf{x}_1,\mathbf{x}_2) = f(\mathbf{x}_1)g(\mathbf{x}_2)$ for specific (and distinct) single-particle functions f and g is not allowed if the particles involved are indistinguishable. The closest to this factorized form that is allowed for identical particles would be

$$\psi_\pm(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{\sqrt{2}}\Big[f(\mathbf{x}_1)g(\mathbf{x}_2) \pm f(\mathbf{x}_2)g(\mathbf{x}_1)\Big]\,, \tag{1.5.2}$$

with the sign here being the same one that appears in (1.5.1). In particular two fermions can never be in precisely the same state since in this limit the corresponding wave-function must vanish (an observation that is at the root of the Pauli exclusion principle for fermions).

It happens to be an experimental fact that all known particles (elementary or otherwise) are either bosons or fermions. Furthermore, it is also experimentally true that a particle is a boson if and only if it also has integer spin (such as photons, gravitons, Higgs bosons, Deuterium nuclei and so on). All particles with half-integer spin are fermions (such as protons, neutrons, electrons, Tritium nuclei and so on). This spin-statistics connection turns out to be a consistency condition for special relativity and quantum mechanics to co-exist (see §11.4.4), and so is now also theoretically well-understood.

1.6 Occupation-number representation

In general it is useful to use the 'occupation number' basis, where we label a given state by the quantum number of the single-particle states that are occupied, as well as with the number of particles occupying the state. For instance

$$|n_1(\mathbf{p}_1, \sigma_1); \cdots ; n_r(\mathbf{p}_r, \sigma_r)\rangle \,, \tag{1.6.1}$$

represents a state in which (for each $j = 1, 2, ..., r$) the single-particle state, $|\mathbf{p}_j\, \sigma_j\rangle$, is occupied by n_j particles, so the total number of particles present is

$$N = \sum_{j=1}^{r} n_j \,. \tag{1.6.2}$$

This simplifies the description of states where a specific label is multiply occupied since a state with (say) two particles with labels $(\mathbf{p}, \sigma)$ and three particles with label $(\mathbf{q}, \lambda)$ would be written

$$|n(\mathbf{p}, \sigma) = 2; n(\mathbf{q}, \lambda) = 3\rangle \quad \text{rather than} \quad |\mathbf{p}, \sigma; \mathbf{p}, \sigma; \mathbf{q}, \lambda; \mathbf{q}, \lambda; \mathbf{q}, \lambda\rangle \,. \tag{1.6.3}$$

The simplification becomes particularly important once the occupation numbers become large – imagine having an Avogadro's number of particles in the same state!

In what follows it is sometimes useful to write this type of state using the alternative notation $|n(\mathbf{q}, \lambda) = 4; n(\mathbf{k}, \sigma) = 90; \cdots\rangle = |(\mathbf{p}, \lambda)_4; (\mathbf{k}, \sigma)_{90}; \cdots\rangle$, and so on.

1.6.1 Quantum grand canonical ensembles

As a simple application of the use of the occupation-number representation imagine computing the partition function,

$$Z := \text{tr}\, \left[e^{-\beta(H - \mu N)} \right] \,, \tag{1.6.4}$$

for the grand-canonical ensemble of statistical mechanics, where H is the system's Hamiltonian and N is the number operator (whose eigenvalues give the number of particles in any given state).

As a brief reminder recall that in quantum statistical mechanics the state of the system is not precisely known and so one imagines that there is a basis of states, $|r\rangle$, (where r is a complete set of state labels) and the system has some probability p_r to be found in any one of these basis states (so $0 \leq p_r \leq 1$ and $\sum_r p_r = 1$). Only the case $p_{r_0} = 1$ (for some $r = r_0$) and all others zero corresponds to complete system knowledge, and is called a 'pure' state.

In this case expectation values for observables have a statistical average in addition to the quantum one, and so for a hermitian operator $\mathcal{O}$ describing an observable the expectation value is

$$\overline{\mathcal{O}} = \sum_r p_r \langle r|\mathcal{O}|r\rangle = \text{tr}\, (\rho\, \mathcal{O}) \tag{1.6.5}$$

where the final equality is written in a basis-independent way. The hermitian operator ρ describes what is known about the system's state (and is called its density matrix) and is defined by

$$\rho = \sum_r p_r |r\rangle\langle r| \,. \tag{1.6.6}$$

The normalization condition on the probabilities implies ρ satisfies the property

$$\mathrm{tr}\,\rho = \sum_r p_r = 1 \,. \tag{1.6.7}$$

In the grand-canonical ensemble the probability is assumed to depend only on a state's energy and the number of particles present, with

$$p_r = \frac{e^{-\beta(E_r - \mu N_r)}}{Z} \,, \tag{1.6.8}$$

and μ and β are parameters (the chemical potential and inverse temperature, respectively). The normalization Z is the determined by the normalization condition, (1.6.7), and so is given by (1.6.4). For free particles the trace can be evaluated explicitly using the occupation-number representation, wherein the label 'r' corresponds to the occupation number n_p for each single-particle mode, whose labels are generically denoted by 'p'. In terms of these occupation numbers the state's total energy, E, and particle number, N, are given by

$$N = \sum_p n_p \quad \text{and} \quad E = \sum_p n_p \, E_p \,, \tag{1.6.9}$$

where E_p is the energy per particle with mode label p.

To start the evaluation proceeds in precisely the same way for bosons and fermions, which only differ on the allowed values taken by the n_p. Denoting the partitions of N particles amongst modes as $\{n_p\}_N$, the expression for Z becomes

$$\begin{aligned} Z &= \mathrm{tr}\,\left(e^{-\beta(H-\mu N)}\right) = \sum_{N=0}^{\infty} \sum_{\{n_p\}_N} \exp\left[-\beta \sum_p (E_p - \mu) n_p\right] \\ &= \sum_{N=0}^{\infty} \sum_{\{n_p\}_N} \prod_p \left[e^{-\beta(E_p-\mu)}\right]^{n_p} = \prod_p \sum_{n_p=0}^{n_{\max}} \left[e^{-\beta(E_p-\mu)}\right]^{n_p} . \end{aligned} \tag{1.6.10}$$

The final equality is obtained by reversing the order of the product and sum, and is most directly proven by induction, starting by evaluating both sides directly for a small number of states p.

Here the only difference between bosons and fermions lies in the upper range of the mode-number sum, which is $n_{\max} = \infty$ for bosons and $n_{\max} = 1$ for fermions. The sum over n_p can be evaluated in both cases, with the bosonic result being

$$Z_B = \prod_p \sum_{n_p=0}^{\infty} \left[e^{-\beta(E_p-\mu)}\right]^{n_p} = \prod_p \frac{1}{1 - e^{-\beta(E_p-\mu)}} \,. \tag{1.6.11}$$

The fermionic result is similarly given by

$$Z_F = \prod_p \sum_{n_p=0}^{1} \Big[e^{-\beta(E_p-\mu)}\Big]^{n_p} = \prod_p \Big[1 + e^{-\beta(E_p-\mu)}\Big]\,. \tag{1.6.12}$$

The utility of computing $Z(\mu,\beta)$ is that useful physical averages can be computed from it by differentiating with respect to its arguments. For instance, defining the Grand canonical potential Ξ by $Z = e^{-\beta\Xi}$ then allows physical averages to be evaluated by differentiating with respect to β and μ. For instance

$$-\frac{\partial\Xi}{\partial\mu} = \frac{1}{\beta Z}\left(\frac{\partial Z}{\partial\mu}\right)_\beta = \text{tr }(\rho\, N) = \overline{N}\,, \tag{1.6.13}$$

gives the average number of particles, where the subscript 'β' on the partial derivative of Z indicates that β is held fixed as μ is varied. Similarly

$$\frac{\partial(\beta\Xi)}{\partial\beta} = -\frac{1}{Z}\left(\frac{\partial Z}{\partial\beta}\right)_\mu = \text{tr }[\rho\,(H-\mu N)] = \overline{U} - \mu\overline{N}\,, \tag{1.6.14}$$

where $\overline{U}$ denotes the average energy.

Using the above calculation of Z_B and Z_F gives the results

$$\Xi(\beta,\mu) = -\frac{1}{\beta}\,\ln Z = \pm\frac{1}{\beta}\sum_p \ln\Big[1 \mp e^{-\beta(E_p-\mu)}\Big]\,, \tag{1.6.15}$$

where the upper (lower) sign applies for bosons (fermions). Differentiating with respect to μ then gives

$$\overline{N} = -\frac{\partial\Xi}{\partial\mu} = \sum_p \frac{1}{e^{\beta(E_p-\mu)} \mp 1} = \mathcal{V}\int \frac{\mathrm{d}^3p}{(2\pi)^3}\,\frac{1}{e^{\beta(E_p-\mu)}\mp 1}\,, \tag{1.6.16}$$

which reveals the average phase-space density for bosons and fermions to be given by the Bose-Einstein or Fermi-Dirac distributions, respectively:

$$f_B(p) = \frac{1}{e^{\beta(E_p-\mu)}-1} \quad \text{and} \quad f_F(p) = \frac{1}{e^{\beta(E_p-\mu)}+1}\,, \tag{1.6.17}$$

where f is related to the particle density by

$$\frac{\overline{N}}{\mathcal{V}} = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\, f(p)\,. \tag{1.6.18}$$

2 Creation and annihilation operators

This section aims to define the main work-horses of quantum field theory: creation and annihilation operators. These operators provide a convenient basis of operators in terms of which any observable of interest (such as Hamiltonians or particle densities) can be expressed.

Before defining them in detail, however, it is useful to do a short prelude to do with the Heisenberg treatment of the harmonic oscillator. This is useful to review because the harmonic oscillator shares the spectrum of the quantum field theory of non-interacting many-particle systems. Both systems involve energy levels that are precisely equally spaced and, unlike the more commonly encountered Schrödinger formalism, the Heisenberg treatment is not narrowly cast in terms of position-dependent wave-functions $\psi_n(x)$.

2.1 Heisenberg's Harmonic oscillator

The single-particle 1D harmonic oscillator can be defined by the time-independent Schrödinger equation

$$H\psi_n(x) = \left[-\frac{1}{2m}\,\frac{\partial^2}{\partial x^2} + \frac{1}{2}\,m\omega^2\,x^2\right]\psi_n(x) = E_n\;\psi_n(x)\,, \tag{2.1.1}$$

where m is the particle mass and ω is the oscillator frequency. This Hamiltonian has eigenvalues

$$E_n = \left(n + \frac{1}{2}\right)\omega\,, \tag{2.1.2}$$

with eigenfunctions

$$\psi_n(x) = \sqrt{\frac{m\,\omega}{\pi 2^n n!}}\;\mathcal{H}_n(x)\,e^{-\frac{1}{2}\,m\omega x^2}\,, \tag{2.1.3}$$

where $n = 0, 1, 2, \ldots$ and $\mathcal{H}_n(x)$ are the (order n) Hermite polynomials.

Heisenberg's treatment of this problem focusses on the *ladder* operator

$$A := \frac{1}{\sqrt{2m\omega}}\;(m\omega\,X + i\,P) = \frac{1}{\sqrt{2m\omega}}\;\left(m\omega\,x + \frac{\partial}{\partial x}\right)\,, \tag{2.1.4}$$

and its adjoint,

$$A^\star := \frac{1}{\sqrt{2m\omega}}\;(m\omega\,X - i\,P) = \frac{1}{\sqrt{2m\omega}}\;\left(m\omega\,x - \frac{\partial}{\partial x}\right)\,, \tag{2.1.5}$$

rather than the position and momentum operators X and P. The commutation relation $[X, P] = i$ implies A satisfies the commutation relation

$$\left[A, A^\star\right] = A\,A^\star - A^\star A = 1\,, \tag{2.1.6}$$

as can be checked by acting on an arbitrary function, $\psi(x)$, and performing the differentiations explicitly.

Since X and P can be rewritten in terms of A and $A^\star$,

$$X = \frac{1}{\sqrt{2m\omega}}\Big(A^\star + A\Big) \quad \text{and} \quad P = i\sqrt{\frac{m\omega}{2}}\Big(A^\star - A\Big)\,, \tag{2.1.7}$$

the same is true of any other observable for the harmonic oscillator, making A, $A^\star$ an equivalent basis of operators to X and P when describing harmonic oscillator observables. In particular, the Hamiltonian itself is given by

$$H = \frac{P^2}{2m} + \frac{1}{2}\, m\,\omega^2\, X^2 = \frac{\omega}{2}\,(A^\star A + A\,A^\star) = \omega\left(A^\star A + \frac{1}{2}\right)\,, \tag{2.1.8}$$

and the last equality uses the commutation relation (2.1.6). This expression for H is also easily verified by directly writing out the right-hand side in terms of the explicit derivatives given in (2.1.4) and (2.1.5).

The above formula for H shows in particular that the combination $N := A^\star A$ is diagonal in the energy eigenbasis with eigenvalue n. That is, if $\psi_n(x) = \langle x|n\rangle$ for the energy eigenstates $|n\rangle$, then

$$A^\star A\,|n\rangle = n\,|n\rangle \quad \text{so that} \quad H\,|n\rangle = \left(n + \frac{1}{2}\right)\omega\,|n\rangle\,. \tag{2.1.9}$$

This last equation implies in particular that $A^\star A$ gives zero when acting on the ground state, and this is easily verified by applying A directly to $\psi_0(x)$:

$$\langle x|A|0\rangle = \frac{1}{\sqrt{2m\omega}}\left(m\omega\, x + \frac{\partial}{\partial x}\right)\psi_0(x) = 0\,, \tag{2.1.10}$$

where the last equality uses $\psi_0(x) = C\,\exp\left(-\frac{1}{2}\,m\omega\,x^2\right)$ where C is a normalization constant (recall $\mathcal{H}_0(x)$ is an order-0 polynomial and so is a constant).

More generally A and $A^\star$ are *ladder operators*, in the sense that they take one energy eigenstate and give the next one, with n shifted by one. That is, we now show

$$A^\star\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad \text{and} \qquad A\,|n\rangle = \sqrt{n}\,|n-1\rangle\,. \tag{2.1.11}$$

Notice that taking the inner product of the second of these with itself gives

$$\langle n|A^\star A|n\rangle = (\sqrt{n})^2\langle n-1|n-1\rangle = n \tag{2.1.12}$$

and so agrees with (2.1.9). Eq. (2.1.11) can be proven by direct application of the definitions together with the definition of the Hermite polynomials. But an easier way to show it is to instead start from the easily proven commutation relation $[H, A^\star] = HA^\star - A^\star H = \omega\, A^\star$, together with its adjoint $[H, A] = HA - AH = -\omega\, A$. This commutation relation implies

$$\begin{aligned} H\,(A^\star\,|n\rangle) &= HA^\star\,|n\rangle = (A^\star H + \omega\, A^\star)\,|n\rangle \\ &= \left[\left(n+\frac{1}{2}\right)\omega + \omega\right]A^\star\,|n\rangle = \left[(n+1) + \frac{1}{2}\right]\omega\;\left(A^\star|n\rangle\right)\,, \end{aligned} \tag{2.1.13}$$

which uses $H\,|n\rangle = \left(n+\frac{1}{2}\right)\omega\,|n\rangle$. The above manipulations show $A^\star|n\rangle$ is also an eigenstate of H with eigenvalue $\left[(n+1)+\frac{1}{2}\right]\omega$ and so $A^\star\,|n\rangle$ must be proportional to $|n+1\rangle$, as required. The proportionality constants in (2.1.11) then follow from the orthogonality and normalization conditions $\langle n|m\rangle = \delta_{mn}$. (Prove this.)

2.2 Creation and annihilation operators

The reason for the above digression on harmonic oscillators is that it is very similar to the quantum system of many noninteracting particles. The similarity arises because of the observation that harmonic oscillator energy levels are equally spaced:

$$E_{n+1} - E_n = \omega \qquad \text{for any } n. \tag{2.2.1}$$

This is very similar to the energy difference between states containing n identical non-interacting particles all having mass (*i.e.* rest energy) M. The energy of n such particles is then simply n times M plus whatever energy, E_0, the no-particle state (or vacuum) may have: $E_n = E_0 + n\,M$, and so $E_{n+1} - E_n = M$ for any n. It is crucial for this that the particles involved be strictly *noninteracting* since interactions allow energy differences to depend on the number of particles that are present.

2.2.1 Creation and annihilation for bosons

We now formalise this resemblance more explicitly. To this end suppose we consider a non-interacting particle whose single-particle states are labelled by momentum and a collection of other labels, $|\mathbf{p}\,\sigma\rangle$, where σ denotes all of the other labels (spin, charge, baryon number, and so on) required to uniquely specify a given particle state. Then the Hilbert space of ordinary single-particle quantum mechanics is the span of these basis states: $\mathfrak{H}_1$ is the set of all states of the generic form $|\psi\rangle = \sum c(\mathbf{p},\sigma)\,|\mathbf{p}\,\sigma\rangle$ for some complex coefficients $c(\mathbf{p},\sigma)$, with the 'sum' running over all allowed values for $\mathbf{p}$ and σ.

The Hilbert space of quantum field theory is *much* larger than just the space of states in $\mathfrak{H}_1$. For instance, it also includes the space of no-particle states, spanned by the single state $|0\rangle$, so $\mathfrak{H}_0 = \{|0\rangle\}$. It also contains the space of all possible two-particle states: $\mathfrak{H}_2$, spanned by all possible states of the form $|\mathbf{p}_1\,\sigma_1\,;\mathbf{p}_2\,\sigma_2\rangle$, as well as $\mathfrak{H}_3$, spanned by all three-particle states, and so on for $\mathfrak{H}_n$ for all integers $n \geq 0$. In general it is useful to use the 'occupation number' basis, where we label a given state by the quantum number of the single-particle states that are occupied, as well as with the number of particles occupying the state. For instance

$$|n_1(\mathbf{p}_1,\sigma_1);\cdots;n_r(\mathbf{p}_r,\sigma_r)\rangle\,, \tag{2.2.2}$$

represents a state in which (for each $j = 1, 2, ..., r$) the single-particle state, $|\mathbf{p}_j\,\sigma_j\rangle$, is occupied by n_j particles, so the total number of particles present is

$$N = \sum_{j=1}^{r} n_j\,. \tag{2.2.3}$$

Using the operator $A^\star$ for the harmonic oscillator as a guide, we define the *creation operator* $a^\star_{p\sigma}$ as the operator that adds one particle with quantum numbers $\mathbf{p}\,\sigma$ to any given

state. That is, when acting on an N-particle state we have

$$a^\star_{p\sigma}|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle = |n(\mathbf{p}\,\sigma)=1;n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle\,, \tag{2.2.4}$$

if $\mathbf{p}\,\sigma$ is not already present, while

$$a^\star_{p\sigma}|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle = \sqrt{n_j+1}\;|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_j(\mathbf{q}_j\,\sigma_j)+1;\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle \tag{2.2.5}$$

if $\mathbf{p}\,\sigma = \mathbf{q}_j\,\zeta_j$ for one of the particles already present (whose label is j).

Similarly, the *annihilation operator* $a_{p\sigma}$ is defined to remove one particle with quantum number $\mathbf{p}\,\sigma$ if such a particle is present, and to give zero if no such particle is present. That is

$$a_{p\sigma}|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle = \sum_{j=1}^{r}\delta^3(\mathbf{p}-\mathbf{q}_j)\delta_{\sigma\zeta_j}\sqrt{n_j}\;|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_j(\mathbf{q}_j\,\sigma_j)-1;n_r(\mathbf{q}_r\,\zeta_r)\rangle\,. \tag{2.2.6}$$

In particular, acting on zero- and single-particle states the above specializes to

$$a_{p\sigma}|0\rangle = 0\,,\quad a^\star_{p\sigma}|0\rangle = |\mathbf{p}\,\sigma\rangle\quad\text{and}\quad a_{p\sigma}|\mathbf{q}\,\zeta\rangle = \delta^3(\mathbf{p}-\mathbf{q})\,\delta_{\sigma\zeta}|0\rangle\,, \tag{2.2.7}$$

while any multiple-particle state can be regarded as being obtained by applying an appropriate combination of creation operators to the vacuum:

$$|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle \propto \left(a^\star_{q_1\zeta_1}\right)^{n_1}\cdots\left(a^\star_{q_r\zeta_r}\right)^{n_r}|0\rangle\,. \tag{2.2.8}$$

Repeated application of these operators shows (not surprisingly) that they satisfy the same commutation relations as did[3] A and $A^\star$:

$$\left[a_{p\sigma},a^\star_{q\zeta}\right] = a_{p\sigma}a^\star_{q\zeta} - a^\star_{q\zeta}a_{p\sigma} = \delta^3(\mathbf{p}-\mathbf{q})\,\delta_{\sigma\zeta}\,. \tag{2.2.9}$$

Notice that this algebra only applies to bosons since only bosons can have multiply occupied states. Because a multi-particle bose state must be completely symmetric under particle interchange (this is the definition of a boson), $|\mathbf{q}_1\,\zeta_1;\mathbf{q}_2\,\zeta_2\rangle = |\mathbf{q}_2\,\zeta_2;\mathbf{q}_1\,\zeta_1\rangle$, and because $|\mathbf{q}_1\,\zeta_1;\mathbf{q}_2\,\zeta_2\rangle = a^\star_{q_1\zeta_1}a^\star_{q_2\zeta_2}|0\rangle$, it follows that we can choose $a_{p\sigma}a_{q\zeta} = a_{q\zeta}a_{p\sigma}$ and so

$$\left[a_{p\sigma},a_{q\zeta}\right] = a_{p\sigma}a_{q\zeta} - a_{q\zeta}a_{p\sigma} = 0\,. \tag{2.2.10}$$

Just as is true for the harmonic oscillator, the algebra defined by (2.2.9) and (2.2.10) ensures that the operator $N_{p\sigma} = a^\star_{p\sigma}a_{p\sigma}$ is diagonal in the occupation number representation. Keeping track of the density of states associated with the switch from discrete to continuum normalization, its eigenvalues count the number of particles in the following precise sense:

$$a^\star_{p\sigma}a_{p\sigma}|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle = \sum_{j=1}^{r}n_j\;\delta^3(\mathbf{p}-\mathbf{q}_j)\delta_{\sigma\zeta_j}\;|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle\,, \tag{2.2.11}$$

[3] This is the same up to normalization, since we normalize momentum eigenstates differently than we do harmonic oscillator states.

and so it is the operator $N = \sum_\sigma \int \mathrm{d}^3p\; a^\star_{p\sigma} a_{p\sigma}$ that counts the number of particles present in a state:

$$\begin{aligned} N|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle &= \sum_\sigma \int \mathrm{d}^3p\; a^\star_{p\sigma} a_{p\sigma} |n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle \\ &= \sum_{j=1}^{r} n_j\; |n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle\,. \end{aligned} \tag{2.2.12}$$

Consequently the Hamiltonian for free particles can be written

$$H_{\text{free}} = E_0 + \sum_\sigma \int \mathrm{d}^3\mathbf{p}\; \varepsilon(\mathbf{p}\,\sigma)\, a^\star_{p\sigma} a_{p\sigma}\,, \tag{2.2.13}$$

with $\varepsilon(\mathbf{p}\,\sigma)$ the single-particle energy for a state labelled by $(\mathbf{p}\,\sigma)$. For relativistic systems the single-particle energy is $\varepsilon(\mathbf{p}\,\sigma) = \sqrt{\mathbf{p}^2 + M^2(\sigma)}$, but for nonrelativistic systems it can be more complicated. The above manipulations show that H does what it should do:

$$H_{\text{free}}|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle = E_{\text{free}}\,(\mathbf{q}_1\,\zeta_1\,n_1;\ldots;\mathbf{q}_r\,\zeta_r\,n_r)\,|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle\,, \tag{2.2.14}$$

with

$$E_{\text{free}}\,(\mathbf{q}_1\,\zeta_1\,n_1;\ldots;\mathbf{q}_r\,\zeta_r\,n_r) = E_0 + \sum_{j=1}^{r} n_j\,\varepsilon(\mathbf{q}_j\,\sigma_j)\,. \tag{2.2.15}$$

In particular, the ground state is the state with the lowest-energy eigenvalue which — assuming[4] $\varepsilon(\mathbf{p}\,\sigma) > 0$ — is given by the no-particle state, $|0\rangle$, with

$$H_{\text{free}}\,|0\rangle = E_0\,|0\rangle\,. \tag{2.2.16}$$

Usually this *vacuum energy* is not measurable in experiments in the laboratory, because such measurements usually are sensitive only to energy differences in which E_0 cancels out. The vacuum energy density can be measured, however, through its gravitational effects since gravity responds to all energies, regardless of their origin. The evidence for the existence of *Dark Energy* in cosmology can be interpreted as the detection of the gravitational influence of the vacuum energy.

2.3 Fermions and anticommutation relations

As mentioned earlier, the above discussion necessarily involves particles that can multiply occupy a state, since nothing stops applying a creation operator $a^\star_{p\sigma}$ as often as one wishes to a state like $|\mathbf{p}\,\sigma\rangle$ already containing the particle in question. Consequently the formalism as described so far necessarily only applies to bosons.

[4]Notice that if $\varepsilon(\mathbf{p}\,\sigma) < 0$ for any $(\mathbf{p}\,\sigma)$ then the spectrum of H_{free} is not bounded from below, since the energy can be lowered arbitrarily far just by multiply occupying any negative-energy particle states. For this reason systems with negative-energy single-particle states are usually regarded as being sick.

How do creation and annihilation operators for fermions differ from the previous discussion? Since a fermionic state is either occupied or not, it is essentially a two-level system, rather than the infinite tower of states described above. Suppose, then, we denote the unoccupied and occupied states as follows

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{(unoccupied)} \qquad \text{and} \qquad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{(occupied)}\,. \tag{2.3.1}$$

In this case the creation and annihilation operators are defined by the four conditions $c|0\rangle = 0$, $c|1\rangle = |0\rangle$, $c^\star|0\rangle = |1\rangle$ and $c^\star|1\rangle = 0$. This corresponds to the following explicit two-by-two matrices

$$c = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \text{and} \qquad c^\star = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\,. \tag{2.3.2}$$

Explicit matrix multiplication then shows that c (and $c^\star$) is *nilpotent* — that is, $c^2 = 0$ and $(c^\star)^2 = 0$ — and furthermore that c and $c^\star$ satisfy the *anticommutator* relation

$$\Big\{c^\star, c\Big\} := c^\star\, c + c\, c^\star = 1\,. \tag{2.3.3}$$

Furthermore direct multiplication also shows that

$$c^\star c = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\,, \tag{2.3.4}$$

and so

$$c^\star c|n\rangle = n|n\rangle \qquad (\text{for } n = 0, 1)\,. \tag{2.3.5}$$

Fermi statistics also determines how the creation and destruction operators for different particles or different momenta commute or anticommute. That is, fermionic states are antisymmetric under particle interchange, $|\mathbf{q}_1\,\sigma_1; \mathbf{q}_2\,\sigma_2\rangle = -|\mathbf{q}_2\,\sigma_2; \mathbf{q}_1\,\sigma_1\rangle$ (and similarly for states with more particles). Consequently, because $|\mathbf{q}_1\,\zeta_1; \mathbf{q}_2\,\zeta_2\rangle = c^\star_{q_1\zeta_1} c^\star_{q_2\zeta_2}|0\rangle$ we impose the following anticommutation relations for fermionic operators

$$\Big\{c^\star_{q_1\zeta_1}, c_{q_2\zeta_2}\Big\} := c^\star_{q_1\zeta_1}\, c_{q_2\zeta_2} + c_{q_2\zeta_2}\, c^\star_{q_1\zeta_1} = \delta^3(\mathbf{q}_1 - \mathbf{q}_2)\,\delta_{\zeta_1\zeta_2}\,, \tag{2.3.6}$$

and

$$\Big\{c_{q_1\zeta_1}, c_{q_2\zeta_2}\Big\} := c_{q_1\zeta_1}\, c_{q_2\zeta_2} + c_{q_2\zeta_2}\, c_{q_1\zeta_1} = 0\,. \tag{2.3.7}$$

The upshot is that the Hamiltonian for free fermions can also be written in precisely the same way as for bosons:

$$H_{\text{free}} = E_0 + \sum_\sigma \int \mathrm{d}^3\mathbf{p}\; \varepsilon(\mathbf{p}\,\sigma)\, c^\star_{p\sigma} c_{p\sigma}\,, \tag{2.3.8}$$

with $\varepsilon(\mathbf{p}\,\sigma)$ the single-particle energy for a state labelled by $(\mathbf{p}\,\sigma)$. This again does what it should do:

$$H_{\rm free}|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle = E_{\rm free}\left(\mathbf{q}_1\,\zeta_1\,n_1;\ldots;\mathbf{q}_r\,\zeta_r\,n_r\right)|n_1(\mathbf{q}_1\,\zeta_1);\ldots;n_r(\mathbf{q}_r\,\zeta_r)\rangle\,, \tag{2.3.9}$$

with

$$E_{\rm free}\left(\mathbf{q}_1\,\zeta_1\,n_1;\ldots;\mathbf{q}_r\,\zeta_r\,n_r\right) = E_0 + \sum_{j=1}^{r} n_j\,\varepsilon(\mathbf{q}_j\,\sigma_j)\,, \tag{2.3.10}$$

with the only new feature (relative to bosons) being that relations (2.3.6) and (2.3.7) replace (2.2.9) and (2.2.10) in order to ensure that the occupation numbers, n_j, always equal zero or one.

Notice that both bosonic and fermionic creation and destruction operators therefore satisfy

$$\begin{aligned} a_q|n_{p_1},\cdots,n_q,\cdots\rangle &= \sqrt{n_q}|n_{p_1},\cdots,n_q-1,\cdots\rangle \\ \text{and}\quad c_q|n_{p_1},\cdots,n_q,\cdots\rangle &= \pm\sqrt{n_q}|n_{p_1},\cdots,n_q-1,\cdots\rangle\,, \end{aligned} \tag{2.3.11}$$

where the sign corresponds to the number of times $c_q^\star$ must be brought past another fermionic operator. Similarly

$$\begin{aligned} a_q^\star|n_{p_1},\cdots,n_q,\cdots\rangle &= \sqrt{1+n_q}|n_{p_1},\cdots,n_q+1,\cdots\rangle \\ \text{and}\quad c_q^\star|n_{p_1},\cdots,n_q,\cdots\rangle &= \pm\sqrt{1-n_q}|n_{p_1},\cdots,n_q+1,\cdots\rangle\,. \end{aligned} \tag{2.3.12}$$

2.4 Completeness of operators

Before moving on to interactions, it is worth emphasizing that *any* operator can be decomposed as a sum of products of a_p and $a_p^\star$, for all particle types. For instance consider an operator $\mathcal{O}$ that is specified by its matrix elements in the 'Fock' basis consisting of single-particle states: $\langle\{n_p\}|\mathcal{O}|\{n_q\}\rangle$. That is, all matrix elements of this form are regarded as known, and any two operators that share precisely the same matrix elements are the same operator.

The expansion of $\mathcal{O}$ in terms of creation and annihilation operators has the form

$$\begin{aligned} \mathcal{O} = N_{0,0} &+ \sum_p \left\{N_{0,1}(p)a_p + N_{1,0}(p)\,a_p^\star\right\} \\ &+ \sum_{pq}\left\{N_{0,2}(p;q)a_pa_q + N_{2,0}(p;q)a_p^\star a_q^\star + N_{1,1}(p;q)a_p^\star a_q\right\} + \cdots\,, \end{aligned} \tag{2.4.1}$$

for some choice of constant $N_{0,0}$ and coefficient functions $N_{i,j}(p_1,\cdots,p_i;q_1,\cdots,q_j)$. The notation is such that 'i' counts the number of $a_p^\star$'s appearing while 'j' counts the number of a_q's. The convention is that all operators are written with all $a_p^\star$'s appearing to the left of the a_q's, a convention called 'normal ordering'. There is no loss in demanding terms to be

normal ordered because any term not normal ordered can be put into normal-ordered form through repeated use of the condition $a_p a_q^\star \mp a_q^\star a_p = \delta_{pq}$ to trade $a_q a_p^\star$ for $a_p^\star a_q$ plus terms involving fewer operators.

The main point is that the coefficient functions are in one-to-one relation to the operator's matrix elements in an occupation number basis, and so *any* operator can be written as in (2.4.1). To see this one works recursively by taking matrix elements between states involving more and more particles, using $a_p|0\rangle = 0$ and $\langle 0|a_p^\star = 0$ repeatedly:

$$\begin{aligned}
\langle 0|\mathcal{O}|0\rangle &= N_{0,0} \\
\langle 0|\mathcal{O}|k\rangle &= \sum_p N_{1,0}(p)\langle 0|a_p|k\rangle = N_{0,1}(k) \\
\langle k|\mathcal{O}|0\rangle &= \sum_p N_{0,1}(p)\langle k|a_p^\star|0\rangle = N_{1,0}(k) \\
\langle l|\mathcal{O}|k\rangle &= \sum_{pq} N_{1,1}(p;q)\langle l|a_p^\star a_q|k\rangle = N_{1,1}(l;k)\,,
\end{aligned} \tag{2.4.2}$$

and so on. Continuing in this way shows that it is always possible to read off the coefficients $N_{i,j}$ for any choice of matrix elements, with different choices for $N_{i,j}$ leading to different matrix elements. So any operator at all can be expanded in the form (2.4.1). It will turn out that this expansion is also a very efficient one when writing interaction terms in a Hamiltonian, though the reasons for this need not be clear at this stage.

3 Perturbation theory and scattering

So far the concrete examples all involve free (non-interacting) particles, defined as those whose multiple-particle energies are simply the sum of the independent single-particle energies (plus the energy of the no-particle state). This section begins the process of extending this discussion to include Hamiltonians that describe interactions amongst the various particles.

To develop intuition for what interactions might look like it is useful to start off with interactions that are weak enough to allow use of perturbative methods. That is, the system Hamiltonian is written

$$H = H_{\text{free}} + H_{\text{int}}\,, \tag{3.0.1}$$

where H_{free} is the free-particle Hamiltonian given in eq. (2.2.13) or (2.3.8). The assumption is that H_{int} is proportional to a small dimensionless parameter — typically a coupling constant, call it g, so $H_{\text{int}} = gV$ for some operator V — with $|g| \ll 1$ small enough that it is fruitful to compute observables as a Taylor expansion in powers of g.

3.1 Time-independent perturbation theory

Under the perturbative assumption the energy levels of H are not that different from those of H_{free}, since these by assumption agree when $g = 0$. In general all the energy eigenvalues

are functions of g which can be written as a series

$$E_n = E_n^{(0)} + gE_n^{(1)} + g^2 E_n^{(2)} + \cdots , \tag{3.1.1}$$

with calculable coefficients.

To see what these coeffiicents are, imagine solving the energy eigenvalue condition for the energy eigenstates, $|n\rangle$, and eigenvalues, E_n:

$$H|n\rangle = (H_{\text{free}} + gV)|n\rangle = E_n|n\rangle \,, \tag{3.1.2}$$

and expanding E_n in powers of g – (as in (3.1.1) – and expanding the state $|n\rangle$ using

$$|n\rangle = |n\rangle_0 + g|n\rangle_1 + g^2|n\rangle_2 + \cdots . \tag{3.1.3}$$

In this last expansion there is no loss in generality to assume ${}_0\langle n|n\rangle_k = 0$ for all n and for all $k > 0$.

Inserting these into (3.1.2) gives an equation that equates two series in powers of g:

$$(H_{\text{free}} + gV)\left(|n\rangle_0 + g|n\rangle_1 + \cdots\right) = \left(E_n^{(0)} + gE_n^{(1)} + \cdots\right)\left(|n\rangle_0 + g|n\rangle_1 + \cdots\right) , \tag{3.1.4}$$

which is meant to be true for all g.

Since the equation is true for all g it can only hold if the coefficient of each power of g on both sides are separately equal to one another. This leads to the following equations

$$\begin{aligned} H_{\text{free}}|n\rangle_0 &= E_n^{(0)}|n\rangle_0 \\ H_{\text{free}}|n\rangle_1 + V|n\rangle_0 &= E_n^{(1)}|n\rangle_0 + E_n^{(0)}|n\rangle_1 \\ H_{\text{free}}|n\rangle_2 + V|n\rangle_1 &= E_n^{(2)}|n\rangle_0 + E_n^{(1)}|n\rangle_1 + E_n^{(0)}|n\rangle_2 \,, \end{aligned} \tag{3.1.5}$$

and so on. The first of these is easily solved because it just says that $|n\rangle_0$ and $E_n^{(0)}$ are the eigenstates and eigenvalues of H_{free}, which for non-interacting particles means the states are occupation-number representation states and the energies are given by expressions like (2.3.10). In particular, these zeroth order states are orthonormal, so ${}_0\langle m|n\rangle_0 = \delta_{mn}$.

To solve the second equation in (3.1.5) take its inner product with ${}_0\langle n|$ and with ${}_0\langle m|$ where $m \neq n$, using ${}_0\langle n|n\rangle_k = 0$ for $k > 0$ and ${}_0\langle m|n\rangle_0 = \delta_{mn}$. This leads to the following two equations

$$\begin{aligned} E_n^{(1)} &= {}_0\langle n|V|n\rangle_0 \\ {}_0\langle m|n\rangle_1 &= \frac{{}_0\langle m|V|n\rangle_0}{E_n^{(0)} - E_m^{(0)}} \,, \end{aligned} \tag{3.1.6}$$

so to linear order in g the eigenvalues and eigenvectors are

$$E_n = E_n^{(0)} + g\,{}_0\langle n|V|n\rangle_0 + \mathcal{O}(g^2) = E_n^{(0)} + {}_0\langle n|H_{\text{int}}|n\rangle_0 + \mathcal{O}(g^2) \,, \tag{3.1.7}$$

and

$$|n\rangle = |n\rangle_0 + \sum_{m\neq n} \left(\frac{{}_0\langle m|H_{\rm int}|n\rangle_0}{E_n^{(0)} - E_m^{(0)}} \right) |m\rangle_0 + \mathcal{O}(g^2)\,. \tag{3.1.8}$$

Proceeding iteratively in this way gives a general solution to the energy spectrum, including any shifts in energy associated with the interactions. In particular, including also the second-order energy shift gives the result

$$E_n = E_n^{(0)} + {}_0\langle n|H_{\rm int}|n\rangle_0 + \sum_{m\neq n} \frac{|{}_0\langle m|H_{\rm int}|n\rangle_0|^2}{E_n^{(0)} - E_m^{(0)}} + \mathcal{O}(g^3)\,. \tag{3.1.9}$$

Clearly both (3.1.8) and (3.1.9) must be rethought if there exists a state $|m\rangle_0$ that shares the same energy as does the state $|n\rangle_0$ whose perturbed energy is to be calculated – a situation that is quite common for single-particle states, such as when the single-particle energy $\varepsilon(|\mathbf{p}|)$ depends only on the magnitude (and not the direction) of particle momentum.

3.2 Time-dependent perturbation theory

Besides shifting energy levels interactions can also cause transitions between states initially prepared as eigenstates of $H_{\rm free}$. These transitions occur because such states are no longer really energy eigenstates and so are no longer guaranteed to evolve simply by the multiplication by a phase e^{-iE_nt}.

A similar kind of perturbative procedure can also be used to compute such time-dependent processes, including transition rates or scattering, in powers of g. This culminates in particular to a very simple and useful expression for the leading part of a transition rate in terms of matrix elements of $H_{\rm int}$, called Fermi's Golden Rule.

3.2.1 Schrödinger, Heisenberg and Interaction pictures

For time-dependent problems it is useful to use what is called the 'interaction picture' or the 'interaction representation', so first a brief aside to describe what this is. Recall that in the Schrödinger way of thinking about time-evolution it is the system's state that evolves, and it does so according to the Schrödinger evolution equation

$$i\partial_t|\psi(t)\rangle_s = H|\psi(t)\rangle_s\,, \tag{3.2.1}$$

which has formal solution

$$|\psi(t)\rangle_s = e^{-iH(t-t_0)}|\psi(t_0)\rangle_s\,. \tag{3.2.2}$$

In particular, states prepared as energy eigenstates evolve very simply. If $H|\psi\rangle_s = E|\psi\rangle_s$ then $|\psi(t)\rangle_s = e^{-iE(t-t_0)}|\psi(t_0)\rangle_s$. In this 'Schrödinger picture' operators do not evolve with time at all: operators like H or P or X or A and $A^\star$ (collectively called $\mathcal{O}$) are time-independent and all time-evolution occurs because of the time-dependence of the system's state vector, $\psi(t)$.

A different way to frame questions about time-evolution is called the 'Heisenberg picture', in which it is the operators that evolve in time while the system's state vector remains time-independent. The Heisenberg picture is obtained from the Schrödinger picture by performing a time-dependent basis change in the quantum Hilbert space:

$$|\psi\rangle_h := e^{+iHt}|\psi(t)\rangle_s = |\psi(0)\rangle_s \quad \text{and} \quad \mathcal{O}_h(t) := e^{iHt}\mathcal{O}_s e^{-iHt}\,. \tag{3.2.3}$$

In this picture a system's state is described by a time-independent vector, $|\psi\rangle_h$, that is conventionally chosen to agree with the Schrödinger picture description at $t = 0$. Eqs. (3.2.3) imply operators now evolve in time, in a way that satisfies the differential evolution equation

$$\partial_t \mathcal{O}_h = i\Big[H, \mathcal{O}_h\Big]\,. \tag{3.2.4}$$

For instance for the harmonic oscillator, where $H = \omega(A^\star A + \frac{1}{2})$ and so $[H, A] = \omega[A^\star, A]A = -\omega A$ this implies the Heisenberg-representation evolution equation

$$\partial_t A = i\Big[H, A\Big] = -i\omega A\,, \tag{3.2.5}$$

and so $A_h(t) = A_h(t_0)e^{-i\omega(t-t_0)}$.

Eqs. (3.2.3) also ensure the Heisenberg and Schrödinger pictures are physically equivalent because (for hermitian H) all matrix elements are the same in the two pictures for all time:

$${}_h\langle\psi|\mathcal{O}_h(t)|\psi\rangle_h = \Big({}_s\langle\psi(t)|e^{-iHt}\Big)e^{iHt}\mathcal{O}_s e^{-iHt}\Big(e^{iHt}|\psi(t)\rangle_s\Big) = {}_s\langle\psi(t)|\mathcal{O}_s|\psi(t)\rangle_s\,. \tag{3.2.6}$$

As mentioned above, these two pictures are defined conventionally to agree with one another at $t = 0$, though in principle this time of agreement could be chosen arbitrarily.

A more convenient picture when using perturbation theory is the a third equivalent option, called the 'interaction picture'. In the interaction picture the operators evolve in time governed by $H_{\rm free}$ while the states evolve with an evolution governed by $H_{\rm int}$. That is, starting from the Schrödinger picture define:

$$|\psi\rangle_I := e^{+iH_{\rm free}t}|\psi(t)\rangle_s \quad \text{and} \quad \mathcal{O}_h(t) := e^{iH_{\rm free}t}\mathcal{O}_s e^{-iH_{\rm free}t}\,. \tag{3.2.7}$$

In this picture the evolution of operators is fairly simple, since they satisfy

$$\partial_t \mathcal{O}_I = i\Big[H_{\rm free}, \mathcal{O}_I\Big]\,, \tag{3.2.8}$$

and so evolve as they would in the absence of the interaction Hamiltonian.

The evolution of states is similarly given by

$$\begin{aligned} i\partial_t|\psi(t)\rangle_I &= i\partial_t\left[e^{iH_{\rm free}t}|\psi(t)\rangle_s\right] = -e^{iH_{\rm free}t}H_{\rm free}|\psi(t)\rangle_s + e^{iH_{\rm free}t}i\partial_t|\psi(t)\rangle_s \\ &= e^{iH_{\rm free}t}(H - H_{\rm free})|\psi(t)\rangle_s = H_{{\rm int},I}(t)|\psi(t)\rangle_I\,, \end{aligned} \tag{3.2.9}$$

where the interaction-picture interaction Hamiltonian is defined as in (3.2.7):

$$H_{\text{int},I}(t) := e^{iH_{\text{free}}t}(H - H_{\text{free}})e^{-iH_{\text{free}}t}\,. \tag{3.2.10}$$

Eq. (3.2.9) says that the interaction-picture evolution of states is controlled by the interaction Hamiltonian, itself evaluated in the interaction picture (which is, in particular, time-dependent).

3.2.2 Scattering and time-dependent perturbation theory

With these definitions in place the problem of evolving states perturbatively in g can be set up and solved, once and for all.

To this end, imagine that in the remote past the system is prepared in an energy eigenstate, $|\alpha\rangle_0$, of the unperturbed Hamiltonian, H_{free}. After evolving forward in time using the full Hamiltonian the goal is to find the likelihood of finding the system in a different unperturbed energy eigenstate, $|\beta\rangle_0$. To set this problem up we choose the full system state to have the initial condition $|\psi(t_0)\rangle = |\alpha\rangle_0$ in the remote past, and then evolve $|\psi(t)\rangle$ forward in time, eventually asking for the overlap at time t with measured final state:

$$P_t(\alpha \to \beta) = |{}_0\langle\beta|\psi(t)\rangle|^2 = |{}_0\langle\beta|U(t,t_0)|\alpha\rangle_0|^2\,, \tag{3.2.11}$$

where the interaction-picture time-evolution operator is defined by

$$|\psi(t)\rangle_I = U(t,t_0)|\psi(t_0)\rangle_I\,, \tag{3.2.12}$$

and so, given (3.2.9), must satisfy

$$i\partial_t U(t,t_0) = H_{\text{int},I}(t)U(t,t_0)\,, \tag{3.2.13}$$

with initial condition

$$U(t_0,t_0) = I\,. \tag{3.2.14}$$

The problem becomes how to integrate (3.2.13) explicitly, order by order in g. This can be done by directly integrating and iterating, leading to

$$\begin{aligned} U(t,t_0) &= I + (-i)\int_{t_0}^{t} \mathrm{d}\tau\; H_{\text{int},I}(\tau)U(\tau,t_0) \qquad (3.2.15)\\ &= I + (-i)\int_{t_0}^{t} \mathrm{d}\tau\; H_{\text{int},I}(\tau) + (-i)^2\int_{t_0}^{t}\mathrm{d}\tau_1\int_{t_0}^{\tau_1}\mathrm{d}\tau_2\; H_{\text{int},I}(\tau_1)H_{\text{int},I}(\tau_2)U(\tau_2,t_0)\,. \end{aligned}$$

Continuing in this way generates an infinite series for $U(t,t_0)$, of the form

$$\begin{aligned} U(t,t_0) &= I + \sum_{n=1}^{\infty}(-i)^n\int_{t_0}^{t}\mathrm{d}\tau_1\int_{t_0}^{\tau_1}\mathrm{d}\tau_2\cdots\int_{t_0}^{\tau_{n-1}}\mathrm{d}\tau_n\; H_{\text{int},I}(\tau_1)H_{\text{int},I}(\tau_2)\cdots H_{\text{int},I}(\tau_n)\\ &= I + \sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\int_{t_0}^{t}\mathrm{d}\tau_1\int_{t_0}^{t}\mathrm{d}\tau_2\cdots\int_{t_0}^{t}\mathrm{d}\tau_n\; T\Big[H_{\text{int},I}(\tau_1)H_{\text{int},I}(\tau_2)\cdots H_{\text{int},I}(\tau_n)\Big]\,, \end{aligned} \tag{3.2.16}$$

where the second line introduces the time-ordering operator

$$T[\mathcal{O}(t_1)\cdots\mathcal{O}(t_n)] = \mathcal{O}(t_{\text{latest}})\cdots\mathcal{O}(t_{\text{earliest}})\,. \tag{3.2.17}$$

The equivalence of the two ways of writing (3.2.16) can be seen by writing the time ordering as a sum over all possible permutations of the n times t_i, with Heaviside step functions included to give zero unless the operators are listed in increasing order of time:

$$T[\mathcal{O}(t_1)\cdots\mathcal{O}(t_n)] = \sum_{\text{permutations}} \mathcal{O}(P(t_1))\cdots\mathcal{O}(P(t_n))\Theta[P(t_1)-P(t_2)]\cdots\Theta[P(t_{n-1})-P(t_n)]\,, \tag{3.2.18}$$

and then changing integration variables from τ_i to $P(\tau_i)$. This makes the integral in the second line of (3.2.16) $n!$ times the integral in the first line, and so establishes the result.

The upshot is an expression for $U(t,t_0)$ in which every term in the sum over n carries an additional power of g. The leading nontrivial contribution for small g stops the sum at linear order in H_{int} and so gives

$$U(t,t_0) \simeq I - i\int_{t_0}^{t} \mathrm{d}\tau\, H_{\text{int},I}(\tau)\,, \tag{3.2.19}$$

and so using this the transition probability (3.2.11) becomes (for $\alpha \neq \beta$)

$$P_t(\alpha\to\beta) = |{}_0\langle\beta|U(t,t_0)|\alpha\rangle_0|^2 \simeq \left|\int_{t_0}^{t} \mathrm{d}\tau_0\langle\beta|H_{\text{int},I}(\tau)|\alpha\rangle_0\right|^2 . \tag{3.2.20}$$

More can be said about this transition probability for time-translation invariant systems, for which H_{int} is time-independent in the Schrödinger picture, and so the τ-dependence of the matrix element can be made explicit when the initial and final states are eigenstates of H_{free}:

$$\begin{aligned} {}_0\langle\beta|H_{\text{int},I}(\tau)|\alpha\rangle_0 &= {}_0\langle\beta|e^{iH_{\text{free}}\tau}H_{\text{int}}e^{-iH_{\text{free}}\tau}|\alpha\rangle_0 \\ &= {}_0\langle\beta|H_{\text{int}}|\alpha\rangle_0\, e^{i(E_\beta-E_\alpha)\tau}\,. \end{aligned} \tag{3.2.21}$$

The τ integral can be evaluated most simply in the long-time limit, $t\to\infty$ and $t_0\to-\infty$, in which case the evolution operator is called the S-matrix,

$$\mathcal{S} := U(\infty,-\infty) \simeq I + \sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}\mathrm{d}\tau_1\cdots\int_{-\infty}^{\infty}\mathrm{d}\tau_n\; T\Big[H_{\text{int},I}(\tau_1)\cdots H_{\text{int},I}(\tau_n)\Big]\,. \tag{3.2.22}$$

At lowest nontrivial order this becomes

$$\mathcal{S} \simeq I - i\int_{-\infty}^{\infty}\mathrm{d}\tau\; H_{\text{int},I}(\tau)\,, \tag{3.2.23}$$

and so predicts the matrix elements

$$\begin{aligned} {}_0\langle\beta|\mathcal{S}|\alpha\rangle_0 &\simeq -i\int_{-\infty}^{\infty}\mathrm{d}\tau\; {}_0\langle\beta|H_{\text{int},I}(\tau)|\alpha\rangle_0 = -i\;{}_0\langle\beta|H_{\text{int}}|\alpha\rangle_0\int_{-\infty}^{\infty}\mathrm{d}\tau\; e^{i(E_\beta-E_\alpha)\tau} \\ &= -2\pi i\;{}_0\langle\beta|H_{\text{int}}|\alpha\rangle_0\;\delta(E_\beta-E_\alpha)\,, \end{aligned} \tag{3.2.24}$$

which (assuming energy eigenvalues to be continuous rather than discrete) shows how energy conservation emerges in the late-time limit as a consequence of the time-translation invariance of the Schrödinger-picture interaction Hamiltonian.

But energy conservation makes the late-time transition probability poorly defined because $P_t(\alpha \to \beta) = |{}_0\langle\beta|\mathcal{S}|\alpha\rangle_0|^2$ involves the square of $\delta(E_\beta - E_\alpha)$, and so always involves a divergent factor of $\delta(E)$ evaluated at $E = 0$. This problem partly arises because if the system is time-translation invariant then it is the transition rate (probability per unit time) that is well-defined and independent of time. This makes the integrated probability diverge at late times, a symptom of which is the factor of $\delta(E)$ evaluated at $E = 0$. But it is also clear that the limit $t - t_0 \to \infty$ and the continuum limit for the energy spectrum must also be subtle, since a transition rate really cannot remain constant for infinite times and still have the integrated probability remain in the interval $0 \le P_t \le 1$.

Because of this it is better to go back to the finite-time expression, whose evaluation leads to

$$\begin{aligned} {}_0\langle\beta|\mathcal{S}|\alpha\rangle_0 &\simeq -i\int_{t_0}^{t} \mathrm{d}\tau\ {}_0\langle\beta|H_{\mathrm{int},I}(\tau)|\alpha\rangle_0 = -i\ {}_0\langle\beta|H_{\mathrm{int}}|\alpha\rangle_0 \int_{t_0}^{t} \mathrm{d}\tau\ e^{i(E_\beta - E_\alpha)\tau} \\ &= {}_0\langle\beta|H_{\mathrm{int}}|\alpha\rangle_0 \left[\frac{1 - e^{i(E_\beta - E_\alpha)(t-t_0)}}{E_\beta - E_\alpha}\right] e^{i(E_\beta - E_\alpha)t_0}\,, \end{aligned} \tag{3.2.25}$$

and so

$$\left|{}_0\langle\beta|\mathcal{S}|\alpha\rangle_0\right|^2 \simeq 4\left|\frac{{}_0\langle\beta|H_{\mathrm{int}}|\alpha\rangle_0}{E_\beta - E_\alpha}\right|^2 \sin^2\left[\frac{1}{2}(E_\beta - E_\alpha)(t - t_0)\right]. \tag{3.2.26}$$

So far nothing is assumed about the spectrum of energies (*i.e.* whether they take discrete or continuous values). The case of most practical interest is when the energy spectrum is continuous, as is appropriate for most scattering transitions. In this case the physical question to ask is for the probability of having a transition into a small range of energies within an interval $\mathrm{d}E$ of the final state energy E_β. Figure 1 plots the envelope of energies appearing in (3.2.26) relative to the spacing of discrete energy levels, and the continuum approximation works if the levels are densely spaced relative to the shape of the envelope: $\mathrm{d}E/\mathrm{d}n \ll 2\pi/(t - t_0)$. In this case assuming that the density of final states for this interval is $\mathrm{d}n/\mathrm{d}E(E_\beta)$ the transition rate can therefore be written

$$\mathrm{d}P_t(\alpha \to \beta) = 4|{}_0\langle\beta|H_{\mathrm{int}}|\alpha\rangle_0|^2\ \frac{\sin^2\left[\frac{1}{2}(E_\beta - E_\alpha)(t - t_0)\right]}{(E_\beta - E_\alpha)^2}\ \frac{\mathrm{d}n}{\mathrm{d}E_\beta}\,\mathrm{d}E_\beta\,. \tag{3.2.27}$$

Provided that the integration range for E_β is wider than the width of the peaks in the envelope shown in Figure 1, most of the contribution comes from the central peak, which becomes more and more sharply peaked around $E_\beta = E_\alpha$ as $t - t_0$ gets larger. Using the limit

$$\frac{\sin^2(xt/2)}{x^2 t/2} \to \pi\delta(x)\,, \tag{3.2.28}$$

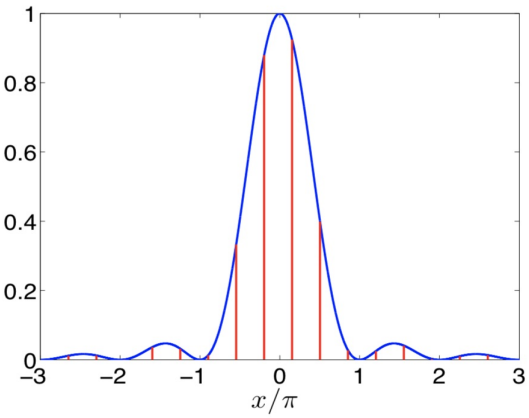


Figure 1. A plot of the envelope $\sin^2 x/x^2$ showing discrete energy levels within the envelope. (Figure source: `arXiv:1604.06916`).

for sufficiently large t implies the transition rate becomes

$$\mathrm{d}\Gamma(\alpha \to \beta) = \frac{\mathrm{d}P_t(\alpha \to \beta)}{t - t_0} \simeq 2\pi |{}_0\langle\beta|H_{\mathrm{int}}|\alpha\rangle_0|^2 \, \delta(E_\beta - E_\alpha) \, \frac{\mathrm{d}n}{\mathrm{d}E_\beta} \, \mathrm{d}E_\beta \,. \tag{3.2.29}$$

This last result is known as Fermi's Golden rule (though apparently first written down by Dirac). Notice that the result (3.2.29) could also have been derived slightly more sloppily by directly squaring (3.2.24) to find

$$|{}_0\langle\beta|S|\alpha\rangle_0|^2 \simeq (2\pi)^2 |{}_0\langle\beta|H_{\mathrm{int}}|\alpha\rangle_0|^2 \, \delta(E_\beta - E_\alpha)\delta(E = 0) \,, \tag{3.2.30}$$

and using

$$\delta(E) = \lim_{T\to\infty} \int_{-T/2}^{T/2} \frac{\mathrm{d}t}{2\pi} \, e^{iEt} \tag{3.2.31}$$

to conclude $\delta(E = 0) = T/(2\pi)$ while defining $\Gamma(\alpha \to \beta) := P(\alpha \to \beta)/T$.

The limit of large $t - t_0$ used in (3.2.28) corresponds to choosing $2\pi/(t - t_0)$ much smaller than the integration region for the final states E_β. Eventually (3.2.29) breaks down because it cannot be true that $P_t(\alpha \to \beta)$ continues to grow linearly with time indefinitely. This breakdown is a reflection of a general fact: no matter how small an interaction Hamiltonian H_{int} might be, there is always eventually a time for which $H_{\mathrm{int}}(t - t_0)$ is no longer small, invalidating a naive perturbative calculation of time evolution.

3.3 Operator matrix elements

For some purposes it can be useful to work with the matrix elements of Heisenberg-picture operators, $A_h(t)$, since it is sometimes possible to derive exact properties for these. It is

usually then also useful to have explicit expressions for these matrix elements in perturbation theory, since this allows exact arguments to interface with explicit perturbative calculations. A derivation of this connection is what this section aims to provide.

First a few useful preliminaries. Consider a Heisenberg-picture operator $A_h(t)$ that is constructed from a time-independent Schrödinger-picture operator A_s in the usual way

$$A_h(t) = e^{iHt} A_s e^{-iHt} \tag{3.3.1}$$

and so $A_h(0) = A_s$. The corresponding interaction-picture operator is simply denoted by $A(t)$, where

$$A(t) = e^{iH_0 t} A_s e^{-iH_0 t}\,, \tag{3.3.2}$$

relative to some split $H = H_0 + H_{\rm int}$ of the Hamiltonian into free and interacting parts.

The time-evolution of the Heisenberg- and interaction-picture operators is related by

$$A_h(t) = e^{iHt} A_s e^{-Ht} = e^{iHt} e^{-iH_0 t} A(t) e^{iH_0 t} e^{-iHt} =: \Omega(t) A(t) \Omega^{-1}(t)\,, \tag{3.3.3}$$

where the last equality defines the operator $\Omega(t) = e^{iHt} e^{-iH_0 t}$. In terms of this the evolution operator $U(t, t_0)$ for interaction-picture states defined in (3.2.12) is formally given by

$$U(t, t_0) = \Omega^{-1}(t)\Omega(t_0) = e^{iH_0 t} e^{-iH(t-t_0)} e^{-iH_0 t_0}\,, \tag{3.3.4}$$

since this transforms to Schrödinger picture at t_0, evolves forward in time using Schrödinger evolution, and then transforms back to interaction picture at time t.

Consider now a system that is prepared in an eigenstate $|\alpha\rangle$ of H_0 in the remote past. This is a typical starting point for a scattering calculation. In the interaction picture we evolve this state forward using $U(t, t_0)$ and ask for its overlap with a different free eigenstate $|\beta\rangle$ in the remote future. As $t \to \infty$ and $t_0 \to -\infty$ the operator $U(t, t_0) \to \mathcal{S}$ and this leads to the matrix element $\langle\beta|\mathcal{S}|\alpha\rangle$ whose form in perturbation theory is given in (3.2.22).

A slightly different way to formulate scattering asks instead what state does $|\alpha\rangle$ evolve into at $t = 0$? This is the state in Heisenberg picture that describes the scattering, and this should be time-independent (as are all states in Heisenberg picture). Denoting the resulting state by $|\alpha, \text{in}\rangle\!\rangle$, chasing through the definitions shows that that it is given explicitly by

$$|\alpha, \text{in}\rangle\!\rangle = \lim_{t \to -\infty} \Omega(t) |\alpha\rangle\,, \tag{3.3.5}$$

since this converts to Schrödinger picture and then evolves to $t = 0$ using standard Schrödinger evolution. A similar construction can be made for a state $|\beta\rangle$ that satisfies $H_0|\beta\rangle = E_\beta|\beta\rangle$ at very late times, leading to the definition

$$|\alpha, \text{out}\rangle\!\rangle = \lim_{t \to +\infty} \Omega(t) |\alpha\rangle\,. \tag{3.3.6}$$

In this language the description of scattering in Heisenberg picture is given by the overlaps between these 'in' and 'out' states:

$$\langle\!\langle \beta, \text{out}|\alpha\,\text{in}\rangle\!\rangle = \langle\beta|\Omega^{-1}(\infty)\Omega(-\infty)|\alpha\rangle = \langle\beta|\mathcal{S}|\alpha\rangle\,. \tag{3.3.7}$$

Because interactions are formally treated as being turned on and turned off infinitely adiabatically when deriving scattering amplitudes we can regard the states $|\alpha, \text{in}\rangle\!\rangle$ and $|\alpha, \text{out}\rangle\!\rangle$ as being eigenstates of the full Hamiltonian with the same eigenvalues as were asymptotically used at infinity. That is, if $H_0|\alpha\rangle = E_\alpha|\alpha\rangle$ then

$$H|\alpha, \text{in}\rangle\!\rangle = E_\alpha|\alpha, \text{in}\rangle\!\rangle \quad \text{and} \quad H|\alpha, \text{out}\rangle\!\rangle = E_\alpha|\alpha, \text{out}\rangle\!\rangle\,. \tag{3.3.8}$$

These states are known as scattering eigenstates of the full Hamiltonian H.

3.3.1 Low's Theorem

With these definitions we can state the main result that expresses the matrix elements of Heisenberg-picture operators as an explicit perturbative series in interaction picture:

$$\begin{aligned}&\langle\!\langle \beta, \text{out}|T\Big[A_{h\,1}(t_1)\cdots A_{h\,k}(t_k)\Big]|\alpha, \text{in}\rangle\!\rangle \\ &\qquad = \sum_{N=0}^{\infty}\frac{(-i)^N}{N!}\int_{-\infty}^{\infty}\mathrm{d}\tau_1\cdots\mathrm{d}\tau_N\;\langle\beta|T\Big[A_1(t_1)\cdots A_k(t_k)H_{\text{int},I}(\tau_1)\cdots H_{\text{int},I}(\tau_N)\Big]|\alpha\rangle\,,\end{aligned} \tag{3.3.9}$$

where, as usual, T denotes time ordering and $H_{\text{int},I}(t)$ is the interaction Hamilton in the interaction picture. In the special case $k = 0$ (*i.e.* when the left-hand side has no operators) this – together with (3.3.7) – reduces to the previous perturbative result (3.2.22) for S-matrix elements.

The proof of (3.3.9) starts by using the definitions (3.3.3), (3.3.5) and (3.3.6) to convert the Heisenberg-picture states and operators to interaction-picture quantities, then combines the Ω's into $U(t_1, t_2)$ using (3.3.4). Since the left-hand side is time-ordered anyway, we are free to choose the labelling so that $t_1 > t_2 > \cdots > t_k$, and with this choice the left-hand side of (3.3.9) can be rewritten as

$$\text{LHS} = \langle\beta|U(\infty, t_1)A_1(t_1)U(t_1, t_2)A_2(t_2)\cdots U(t_{k-1}, t_k)A_k(t_k)U(t_k, -\infty)|\alpha\rangle\,, \tag{3.3.10}$$

Next we use the perturbative expansion (3.2.16) for the U's to get the lengthy expression

$$\begin{aligned}\text{LHS} = \sum_{N_1=0}^{\infty}\cdots\sum_{N_{k+1}=0}^{\infty}\frac{(-i)^{N_1+\cdots+N_{k+1}}}{N_1!\cdots N_{k+1}!}\int_{t_1}^{\infty}\mathrm{d}\tau_{11}\cdots\mathrm{d}\tau_{1N_1}\int_{t_2}^{t_1}\mathrm{d}\tau_{21}\cdots\mathrm{d}\tau_{2N_2}\cdots \\ \times\langle\beta|T\Big[H_{\text{int}}(\tau_{11})\cdots H_{\text{int}}(\tau_{1N_1})\Big]A_1(t_1)T\Big[\Big[H_{\text{int}}(\tau_{21})\cdots H_{\text{int}}(\tau_{2N_2})\Big]A_2(t_2)\cdots|\alpha\rangle\,.\end{aligned} \tag{3.3.11}$$

Because the A_i's are already ordered chronologically the limits on the integrations allow the time-ordering to be pulled out to act on all operators at once, so the matrix element in the previous expression becomes

$$\langle\beta|T\Big[H_{\rm int}(\tau_{11})\cdots H_{\rm int}(\tau_{1N_1})\,A_1(t_1)\,H_{\rm int}(\tau_{21})\cdots H_{\rm int}(\tau_{2N_2})\,A_2(t_2)\cdots\Big]|\alpha\rangle\,. \tag{3.3.12}$$

Finally comes some combinatorial gymnastics. Define $N = N_1 + N_2 + \cdots N_{k+1}$. For fixed N the matrix element partitions the N interaction Hamiltonians into $k+1$ groups for which the ordering of the $H_{\rm int}$'s within each group does not matter. There are

$$C_{N,k} = \frac{N!}{N_1!N_2!\cdots N_{k+1}!} \tag{3.3.13}$$

ways to perform such a partition. The left-hand side of (3.3.9) tells us to sum over all such partitions. Next consider the right-hand side of (3.3.9). This states one must simply sum over all possible ways of distributing the N interaction Hamiltonians and divide the result by $N!$. But this is equivalent to first putting them into a specific set of partitions of $k+1$ operators between each of the A_i's so

$$\begin{aligned}\frac{1}{N!}&(\text{sum over all arrangements of } N\ H_{\rm int}\text{'s}) \\ &= \frac{1}{N!}C_{N,k}(\text{sum over all ways of partitioning the } H_{\rm int}\text{'s into } k+1 \text{ sets})\end{aligned} \tag{3.3.14}$$

and so the sum performed on the left-hand side agrees with the sum performed on the right-hand side.

3.3.2 Expectation values

Although (3.3.9) gives an explicit perturbative expression for the 'in-out' matrix elements of time-ordered products of operators, it is not always true that this is the class of operators needed in physical applications. Often in quantum mechanics one instead wishes to prepare the system in a particular state and then compute the expectation value of different operators in that state.

Since $|\alpha, {\rm in}\rangle\!\rangle$ is the Heisenberg-picture state that corresponds to a state prepared in the remote past to look like a non-interacting eigenstate $|\alpha\rangle$, the natural Heisenberg-picture expectation values to evaluate in these situations is an 'in-in' matrix element like

$$M(t) := \langle\!\langle\alpha, {\rm in}|A_h(t)|\alpha, {\rm in}\rangle\!\rangle\,. \tag{3.3.15}$$

The interaction-picture version of this result is the one useful when using perturbation

theory is obtained in the same way as before, using (3.3.3), (3.3.4) and (3.3.5), leading to

$$\begin{aligned} M(t) &= \langle\alpha|\Omega^{-1}(-\infty)\,\Omega(t)A(t)\Omega^{-1}(t)\,\Omega(-\infty)|\alpha\rangle \\ &= \langle\alpha|U^{-1}(t,-\infty)A(t)U(t,-\infty)|\alpha\rangle \\ &= \sum_{M=0}^{\infty}\sum_{N=0}^{\infty}\frac{(-i)^{N-M}}{M!N!}\int_{-\infty}^{t}\mathrm{d}\sigma_1\cdots\mathrm{d}\sigma_M\mathrm{d}\tau_1\cdots\mathrm{d}\tau_N \\ &\qquad\times\langle\alpha|\overline{T}\Big[H_{\rm int}(\sigma_1)\cdots H_{\rm int}(\sigma_M)\Big]A(t)\,T\Big[H_{\rm int}(\tau_1)\cdots H_{\rm int}(\tau_N)\Big]|\alpha\rangle\,, \end{aligned} \tag{3.3.16}$$

which uses $U(t_0,t) = U^{-1}(t,t_0) = U^\star(t,t_0)$ and defines $\overline{T}$ to denote *anti-time-ordering* so (compare (3.2.17))

$$\overline{T}[\mathcal{O}(t_1)\cdots\mathcal{O}(t_n)] = \mathcal{O}(t_{\rm earliest})\cdots\mathcal{O}(t_{\rm latest})\,. \tag{3.3.17}$$

Although not directly used in these notes, such matrix elements are useful for many kinds of physical questions.

4 Simple interactions

With these perturbative tools in hand we can now transition to a discussion of several interaction Hamiltonians and their use in physical situations.

4.1 Emission and absorption

Consider first a process of emitting or absorbing a particle, such as the decay of an excited atom or nucleus by emitting a particle, or its inverse process wherein a particle is absorbed. What kind of interaction Hamiltonian might describe this process?

Given that transition amplitudes are proportional to $\langle\beta|H_{\rm int}|\alpha\rangle$ a simple suggestion is to choose $H = H_{\rm free} + H_{\rm int}$ with

$$\begin{aligned} H_{\rm free} &= E_0 + \sum_p\Big[\varepsilon_{\scriptscriptstyle A}(p)\,a_p^\star a_p + \varepsilon_{\scriptscriptstyle B}(p)\,b_p^\star b_p + \varepsilon_{\scriptscriptstyle C}(p)\,c_p^\star c_p\Big] \qquad (4.1.1)\\ &= E_0 + \int \mathrm{d}^3p\Big[\varepsilon_{\scriptscriptstyle A}(p)\,\mathfrak{a}_p^\star\mathfrak{a}_p + \varepsilon_{\scriptscriptstyle B}(p)\,\mathfrak{b}_p^\star\mathfrak{b}_p + \varepsilon_{\scriptscriptstyle C}(p)\,\mathfrak{c}_p^\star\mathfrak{c}_p\Big] \\ \text{and}\quad H_{\rm int} &= \sum_{pqk}\Big[g(p,q,k)c_p^\star b_q a_k + g^*(p,q,k)a_k^\star b_q^\star c_p\Big]\delta_{p-q-k} \qquad (4.1.2)\\ &= \int \mathrm{d}^3p\,\mathrm{d}^3q\,\mathrm{d}^3k\Big[\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})\mathfrak{c}_p^\star\mathfrak{b}_q\mathfrak{a}_k + \mathfrak{g}^*(\mathbf{p},\mathbf{q},\mathbf{k})\mathfrak{a}_k^\star\mathfrak{b}_q^\star\mathfrak{c}_p\Big]\delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k})\,, \end{aligned}$$

where the expression is given for both discrete and continuum normalized states (recall the discussion surrounding eq. (1.3.5)), with continuum and discrete destruction operators related by

$$\mathfrak{a}_p := \left[\frac{\mathcal{V}}{(2\pi)^3}\right]^{1/2} a_p\,,\quad \mathfrak{b}_p := \left[\frac{\mathcal{V}}{(2\pi)^3}\right]^{1/2} b_p \quad\text{and}\quad \mathfrak{c}_p := \left[\frac{\mathcal{V}}{(2\pi)^3}\right]^{1/2} c_p\,, \tag{4.1.3}$$

while the continuum coefficient function is defined by

$$\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k}) := \left[\frac{\mathcal{V}}{(2\pi)^3}\right]^{1/2} g(p,q,k)\,. \tag{4.1.4}$$

The second term in $H_{\rm int}$ is required to ensure $H_{\rm int}$ remains hermitian. Here the single-particle energies, $\varepsilon_A(p)$, $\varepsilon_B(p)$, $\varepsilon_C(p)$ and complex coupling function $g(p,q,k)$ are regarded as known functions in terms of which physical observables can be calculated.

This form for $H_{\rm int}$ describes the reactions $C \leftrightarrow A + B$ where A, B and C are the three species of particles corresponding to the three types of destruction operators. This can be seen by asking what the creation and destruction operators in $H_{\rm int}$ do when acting on a free-particle state. In what follows A, B and C are all imagined to be bosons (perhaps with A an internally excited atom, B representing an atom in the ground state and C being the emitted particle). But any two of these could instead be fermions without changing the discussion of this section.[5]

With this Hamiltonian the emission rate for the reaction $C(p) \to A(q) + B(k)$ obtained using (3.2.29) involves the matrix element[6]

$$\begin{aligned}
(A(q),B(k)|H_{\rm int}|C(p)) &= g^*(p,q,k)\,\delta_{p-q-k} \qquad \text{(discrete norm.)} \\
\langle A(\mathbf{q}),B(\mathbf{k})|H_{\rm int}|C(\mathbf{p})\rangle &= \mathfrak{g}^*(\mathbf{p},\mathbf{q},\mathbf{k})\,\delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k}) \quad \text{(continuum norm.)}\,,
\end{aligned} \tag{4.1.5}$$

which helps understand how one guesses the form of $H_{\rm int}$ when trying to understand a particular type of process. The hermitian conjugate term similarly gives a nonzero matrix element for absorption, $A(q) + B(k) \to C(p)$, with

$$\begin{aligned}
(C(p)|H_{\rm int}|A(q),B(k)) &= g(p,q,k)\,\delta_{p-q-k} \qquad \text{(discrete norm.)} \\
\langle C(\mathbf{p})|H_{\rm int}|A(\mathbf{q}),B(\mathbf{k})\rangle &= \mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})\,\delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k}) \quad \text{(continuum norm.)}\,.
\end{aligned} \tag{4.1.6}$$

For discrete normalization the arguments of §3.2.2 show that this matrix element implies the transition rate between specific momentum eigenstates is given by

$$\Gamma[C(p) \to A(q) + B(k)] \simeq 2\pi |g(p,q,k)|^2 \delta[\varepsilon_C(p) - \varepsilon_A(q) - \varepsilon_B(k)]\,\delta_{p-q-k}\,, \tag{4.1.7}$$

which uses $[\delta_{p-k-q}]^2 = \delta_{p-q-k}$. Of more practical interest in the continuum limit is the rate for the transition to occur with the final momenta living in a small range of values. Recalling that the quantum mechanical prediction for the probability of two mutually exclusive and distinguishable outcomes $A \to B$ or $A \to C$ is

$$P(A \to B \text{ or } C) = P(A \to B) + P(A \to C) \tag{4.1.8}$$

[5] Since the energy density satisfies Bose statistics only an even number of the destruction operators appearing in $H_{\rm int}$ can be fermions.

[6] Round brackets are used here rather than bras and kets to emphasize that the state labels p, q and k are discrete variables and not continuum normalized.

the transition rate into a range of final momenta is obtained by summing (4.1.7) over the final momenta of interest. Assuming the range of final momenta is small enough that the matrix element does not vary much, this rate is given by

$$\mathrm{d}\Gamma[C(p) \to A(q) + B(k)] \simeq 2\pi |g(p,q,k)|^2 \delta[\varepsilon_C(p) - \varepsilon_A(q) - \varepsilon_B(k)]\, \delta_{p-q-k}\, \mathrm{d}n\,, \tag{4.1.9}$$

where $\mathrm{d}n$ denotes the number of states contained in the range of final momenta being summed.

If the range of final states is defined as those whose energies lie in a small range $\mathrm{d}E$ then $\mathrm{d}n = (\mathrm{d}n/\mathrm{d}E)\,\mathrm{d}E$, where $\mathrm{d}n/\mathrm{d}E$ is the final configuration's density of states. It is this result summed over a narrow range of final momenta that lends itself to the continuum limit, since the arguments around eq. (1.3.7) show that the number of states in a small volume in momentum space of size d^3q and d^3k around specific final momenta $\mathbf{q}$ and $\mathbf{k}$ is

$$\mathrm{d}n = \frac{\mathrm{d}n}{\mathrm{d}E}\,\mathrm{d}E = \left[\frac{\mathcal{V}}{(2\pi)^3}\,\mathrm{d}^3q\right]\,\left[\frac{\mathcal{V}}{(2\pi)^3}\,\mathrm{d}^3k\right]\,. \tag{4.1.10}$$

But if we use continuous momenta care must also be taken with the normalization of states, and so we must also use $g(p,q,k) = [(2\pi)^3/\mathcal{V}]^{1/2}\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})$ and $\delta_{p-q-k} = [(2\pi)^3/\mathcal{V}]\,\delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k})$ in (4.1.9) leading to the useful result

$$\mathrm{d}\Gamma[C(p) \to A(q) + B(k)] \simeq 2\pi |\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})|^2 \delta[\varepsilon_C(p) - \varepsilon_A(q) - \varepsilon_B(k)]\, \delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k})\, \mathrm{d}^3q\, \mathrm{d}^3k\,. \tag{4.1.11}$$

This same result can also be obtained by starting again with (3.2.29), and converting immediately to continuum normalization

$$\begin{aligned}
\mathrm{d}\Gamma[C \to A + B] &= 2\pi |(A(k), B(q)|H_{\text{int}}|C(p))|^2\, \delta(\varepsilon_C - \varepsilon_B - \varepsilon_A)\, \mathrm{d}n \\
&= 2\pi \left|\left[\frac{(2\pi)^3}{\mathcal{V}}\right]^{3/2} \langle A(\mathbf{q}), B(\mathbf{k})|H_{\text{int}}|C(\mathbf{p})\rangle\right|^2\, \delta(\varepsilon_C - \varepsilon_B - \varepsilon_A)\, \mathrm{d}n \\
&= 2\pi \left[\frac{(2\pi)^3}{\mathcal{V}}\right] \left|\langle A(\mathbf{q}), B(\mathbf{k})|H_{\text{int}}|C(\mathbf{p})\rangle\right|^2\, \delta(\varepsilon_C - \varepsilon_B - \varepsilon_A)\, \mathrm{d}^3q\, \mathrm{d}^3k
\end{aligned} \tag{4.1.12}$$

in which we use

$$\begin{aligned}
|\langle A(\mathbf{k}), B(\mathbf{q})|H_{\text{int}}|C(\mathbf{p})\rangle|^2 &= \left|\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})\, \delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k})\right|^2 \\
&= |\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})|^2\, \delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k})\, \delta^3(\mathbf{0})\,,
\end{aligned} \tag{4.1.13}$$

where

$$\delta^3(\mathbf{p}) = \int \frac{\mathrm{d}^3x}{(2\pi)^3}\, e^{i\mathbf{p}\cdot\mathbf{x}} \quad \text{implies} \quad \delta^3(\mathbf{0}) = \frac{\mathcal{V}}{(2\pi)^3}\,, \tag{4.1.14}$$

again leading to (4.1.11).

An *inclusive* emission rate is defined to be the total rate summed over a range of final momenta that are not measured (such as if the momentum $\mathbf{q}$ of the outgoing particle $B(\mathbf{q})$

is not measured and the differential decay rate is required only as a function of $\mathbf{k}$). This is obtained by integrating over the range of final momenta of interest, and if this range is large it need not be true that the matrix element is a constant over the entire range. For instance consider integrating over $\mathbf{q}$ in the above expression, as appropriate if $\mathbf{q}$ is not measured. Then the differential decay rate as a function of $\mathbf{k}$ only is obtained by integrating over all possible values of $\mathbf{q}$. Using the momentum-conserving δ-function to perform this integration then gives

$$\begin{aligned}\mathrm{d}\Gamma[C \to A + B] &\simeq 2\pi \int \mathrm{d}^3q\, |\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})|^2 \delta[-\varepsilon_C(p) + \varepsilon_A(q) + \varepsilon_B(k)]\, \delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k}) \\ &= 2\pi\, |\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})|^2 \delta[-\varepsilon_C(p) + \varepsilon_A(q) + \varepsilon_B(k)]\big|_{\mathbf{q}=\mathbf{p}-\mathbf{k}}\,. \end{aligned} \tag{4.1.15}$$

Further progress requires knowing the functional form of $\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})$ and the single-particle energies. For simplicity take the example

$$\mathfrak{g} = \mathfrak{g}(|\mathbf{k}|)\,, \quad \varepsilon_C(p) = \frac{|\mathbf{p}|^2}{2m} + \Delta\,, \quad \varepsilon_B(p) = \frac{|\mathbf{p}|^2}{2m} \quad \text{and} \quad \varepsilon_A(k) = c_s|\mathbf{k}|\,, \tag{4.1.16}$$

where $0 < \Delta \ll m$ is the internal energy difference between the excited and ground states of an atom, and use of non-relativistic expressions for kinetic energy requires both $|\mathbf{p}|$ and $|\mathbf{q}|$ to be much smaller than m (as is usually true for real atoms in the lab). The parameter c_s has the interpretation of the phase speed of the emitted particle and so $c_s = 1$ for something like a photon that moves at the speed of light, while $0 < c_s \leq 1$ (say) for a particle moving more slowly than light, such as a phonon (quantum of a sound wave – more about which later – for which c_s is the speed of sound) or a photon moving with speed $c_s = 1/n_s$ in a medium with index of refraction n_s.

Using these and writing the integration measure d^3k in polar coordinates – $\mathrm{d}^3k = k^2 \sin\theta\, \mathrm{d}k\, \mathrm{d}\theta\, \mathrm{d}\phi$ (with θ chosen to be the angle between $\mathbf{p}$ and $\mathbf{k}$) – shows that the differential rate per unit solid angle, $\mathrm{d}\Omega = \sin\theta\, \mathrm{d}\theta\mathrm{d}\phi$, is:

$$\begin{aligned}\frac{\mathrm{d}\Gamma}{\mathrm{d}\Omega}[C \to A + B] &\simeq 2\pi \int_0^\infty k^2 \mathrm{d}k\, |\mathfrak{g}|^2 \delta\left[-\frac{\mathbf{p}^2}{2m} - \Delta + \frac{(\mathbf{p}-\mathbf{k})^2}{2m} + c_s|\mathbf{k}|\right] \\ &= 2\pi \int_0^\infty k^2 \mathrm{d}k\, |\mathfrak{g}|^2 \delta\left[-\Delta + c_s k + \frac{(k^2 - 2|\mathbf{p}|k\cos\theta)}{2m}\right] \\ &= 2\pi \int_0^\infty k^2 \mathrm{d}k\, |\mathfrak{g}|^2 \delta\Big[-\Delta + k(c_s - v\cos\theta) + (k^2/2m)\Big]\,, \end{aligned} \tag{4.1.17}$$

where the last line defines the initial particle's speed as $v = |\mathbf{p}|/m$.

Rest-frame decay

Consider first the emission rate in the rest frame of the initial particle (for which $\mathbf{p} = 0$ and so also $v = 0$), and denote the value of k in this frame by k_0. In this case the energy-conservation

delta function implies that k_0 is given by solving a quadratic equation with root

$$k_0 = mc_s \left[\sqrt{1 + \frac{2\Delta}{mc_s^2}} - 1 \right] \simeq \frac{\Delta}{c_s} \qquad \text{(rest frame)}\,, \tag{4.1.18}$$

chosen so that k is positive. The approximate equality applies in the limit of practical interest: $\Delta \ll mc_s^2$, for which the emitted particle energy is $\omega_0 = \varepsilon_A(k_0) = c_s k_0 \simeq \Delta$. In this limit the $k_0^2/2m$ term can be dropped in the delta function in comparison to Δ. Performing the integration over k using $\delta(ax - b) = \delta(x - b/a)/|a|$ then gives the rest-frame result for the differential decay rate:

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}\Omega}[C \to A + B] \simeq \frac{2\pi |\mathfrak{g}_0|^2 \Delta^2}{c_s^3} \qquad \text{(rest frame)}\,, \tag{4.1.19}$$

which is isotropic in the sense that it is independent of the direction (θ, ϕ) of $\mathbf{k}$. Here $\mathfrak{g}_0$ denotes the evaluation of $\mathfrak{g}(k)$ at the expression for k dictated by energy conservation.

The total decay rate is found by performing the remaining angular integrations, which is particularly simple in the decaying particle's rest frame, with the final result

$$\Gamma_{\text{rest}} \simeq \frac{8\pi^2 |\mathfrak{g}_0|^2 \Delta^2}{c_s^3} \qquad \text{(rest frame)}\,. \tag{4.1.20}$$

Fermi's Golden Rule makes the various factors in this result easy to estimate without working as hard as was done above. In particular, the power of $\mathfrak{g}_0$ appears because of the proportionality of H_{int} to $\mathfrak{g}_0$ and the result that Γ is proportional to $|\langle\beta|H_{\text{int}}|\alpha\rangle|^2$. The factor of Δ^2 comes on dimensional grounds because $\mathfrak{g}_0$ has dimension $(\text{mass})^{-1/2}$ and Γ has dimension of mass (in fundamental units). The rest of the dimensions come from the integration over d^3k and the scale for this is set (because of energy conservation) by Δ, since this is the maximum allowed value for $|\mathbf{k}|$. The powers of 2π can also be tracked by counting the factors of $\mathcal{V}/(2\pi)^3$ and the angular integrations. In the end the detailed calculation is just used to establish that the numerical factor in (4.1.20) is 2.

This calculation captures in particular the special case of a photon emitted as an atom de-excites in the vacuum, if we take m to be the atomic mass and $c_s = 1$. The theory of Quantum Electrodynamics – see Chapter §9.4 below – in this case predicts

$$\mathfrak{g} \simeq \left(\frac{ie}{m_e}\right) \frac{\boldsymbol{\epsilon} \cdot \mathbf{d}_{fi}}{\sqrt{(2\pi)^3 2\varepsilon_A(k)}}\,, \quad \text{where} \quad \mathbf{d}_{fi} = \int \mathrm{d}^3x\, \psi_f^* \nabla \psi_i \tag{4.1.21}$$

is the transition dipole moment matrix element for the initial and final electronic wavefunctions $\psi_i(x)$ and $\psi_f(x)$, while m_e and $-e$ are the electron's mass and charge, and $\boldsymbol{\epsilon}$ is the polarization vector of the emitted photon. Much of what follows is devoted to identifying how to figure out what the right choices are for couplings like $\mathfrak{g}$ in particular situations.

Decay in flight

In the 'lab' frame (in which the initial particle moves with momentum $\mathbf{p}$) energy and momentum conservation imply that k depends on the direction of emission relative to the velocity of the initial particle,

$$k = m(c_s - v\cos\theta)\left[\sqrt{1 + \frac{2\Delta}{m(c_s - v\cos\theta)^2}} - 1\right] \qquad \text{(lab frame)}\,, \tag{4.1.22}$$

and so the emitted particle has lab-frame energy $\omega = \varepsilon_A(k) = c_s k \simeq \Delta/[1 - (v/c_s)\cos\theta]$ if Δ is much smaller than $m(c_s - v\cos\theta)^2$. The angular dependence here is precisely what is expected from the Doppler effect because the lab-frame and rest-frame energies are related by

$$\omega_0 = k_0 c_s \simeq \omega\left(1 - \frac{v}{c_s}\cos\theta\right) = \omega - \mathbf{v}\cdot\mathbf{k}\,. \tag{4.1.23}$$

Not surprisingly, particles emitted in the direction of the decaying particle's initial motion (for which $\cos\theta > 0$) carry more energy than they would in the rest frame, and those emitted in the opposite direction (with $\cos\theta < 0$) have less energy.

The differential rate in the lab frame in the limit $\Delta \ll m(c_s - v\cos\theta)^2$ is now

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}\Omega}[C \to A + B] \simeq \frac{2\pi|\mathfrak{g}_0|^2\Delta^2}{(c_s - v\cos\theta)^3}\,, \tag{4.1.24}$$

which depends on θ but not on ϕ. The total decay rate is found by performing the remaining angular integrations and gives

$$\Gamma[C \to A + B] = 2\pi\int_0^\pi \mathrm{d}\theta\left(\frac{\mathrm{d}\Gamma}{\mathrm{d}\Omega}\right)\sin\theta \simeq \frac{8\pi^2|\mathfrak{g}_0|^2\Delta^2 c_s}{(c_s^2 - v^2)^2} \qquad \text{(lab frame)}\,. \tag{4.1.25}$$

If the emitted particle moves at the speed of light (so $c_s = 1$) then $c_s - v\cos\theta > 0$ for all θ (because for non-relativistic B and C particles $0 \le v \ll 1$) and so the denominator of (4.1.24) is always positive. But if $c_s < 1$ (such as for sound waves or photons moving in a medium with index of refraction) there can be angles for which $c_s - v\cos\theta$ can pass through zero and become negative and the above formulae must break down. What happens in this case?

Čerenkov radiation and sonic booms

When $v\cos\theta \to c_s$ the solution for k predicted by (4.1.22) remains bounded, with

$$k = m(c_s - v\cos\theta)\left[\sqrt{1 + \frac{2\Delta}{m(c_s - v\cos\theta)^2}} - 1\right] \to \sqrt{2m\Delta}\,. \tag{4.1.26}$$

Once $c_s < v\cos\theta$ the root of the quadratic formula for k that is positive is

$$k = m(v\cos\theta - c_s)\left[\sqrt{1 + \frac{2\Delta}{m(v\cos\theta - c_s)^2}} + 1\right]. \tag{4.1.27}$$

In particular, notice that this does *not* approach zero as $\Delta \to 0$ and instead approaches

$$\lim_{\Delta\to 0} k = 2m(v\cos\theta - c_s)\,, \tag{4.1.28}$$

showing that when $v > c_s$ emission can occur *without* the emitting particle having to lose internal energy through a transition involving internal degrees of freedom. As a consequence *any* particle is energetically capable of emitting particles regardless of whether it has any internal energy levels, with the energy for the emitted particle instead being extracted from the energy of motion until v falls below c_s. It is similarly true that k can remain positive even when $\Delta < 0$, showing that during supersonic/superluminal motion a phonon/photon can be radiated with the atom simultaneously *absorbing* energy rather than losing it.

To compute the rate for this decay in the limit $\Delta \to 0$ with $v > c_s$ we must return and use the root (4.1.28) for k in (4.1.17), leading to

$$\lim_{\Delta\to 0} \frac{\mathrm{d}\Gamma}{\mathrm{d}\Omega}[C \to A + B] \simeq \frac{2\pi|\mathfrak{g}_0|^2 k^2}{J} = 8\pi|\mathfrak{g}_0|^2 m^2 (v\cos\theta - c_s)\,, \tag{4.1.29}$$

where $J = (\mathrm{d}/\mathrm{d}k)[-\Delta + k(c_s - v\cos\theta) + (k^2/2m)] = c_s - v\cos\theta + (k/m)$ is the Jacobian encountered when using the delta function to perform the k integration. Unlike (4.1.24) this remains nonzero as $\Delta \to 0$, although it does vanish as $v\cos\theta \to c_s$. The total emission rate is obtained by integrating this over all angles satisfying $v\cos\theta \geq c_s$ and so

$$\lim_{\Delta\to 0} \Gamma[C \to A + B] = \frac{8\pi^2 m^2}{v}|\mathfrak{g}_0|^2 (v - c_s)^2\,. \tag{4.1.30}$$

Notice that the locus of directions that mark the transition between the two regimes satisfies $v\cos\theta = c_s$ and this defines a cone in space that is centred about the direction of the initial particle's motion (see Fig. 2). The opening angle of this cone satisfies $\Theta = \frac{\pi}{2} - \theta$ and so $\sin\Theta = c_s/v$. This is the expression for the opening angle of the Čerenkov cone of light emitted by relativistic particles in a dielectric medium (and, in the case of sound waves, for the Mach cone of the sonic boom produced by supersonic motion through a compressible medium). This cone arises in practice because the production of particles at different times accumulates for this particular direction, allowing the cumulative strength of the radiation in this direction to become large.

4.2 Bosons and stimulated emission

It is instructive to consider the same emission process $C \to A + B$ but start with a state that contains N_A of the A particles multiply occupying a state with momentum $\mathbf{l}$ and N_C of the C particles multiply occupying momentum $\mathbf{p}$. We ask what is the likelihood that one of the C particles emits an A particle in the presence of all of the others. That is, suppose the initial state is

$$|\alpha) = \Big|[C(\mathbf{p})]_{N_C}, [A(\mathbf{l})]_{N_A}\Big) = \Big|n[C(p)] = N_C, n[A(l)] = N_A\Big)\,, \tag{4.2.1}$$

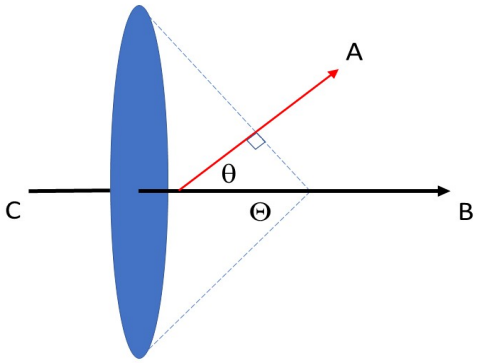


Figure 2. A sketch of the kinematics of particle emission in the case $v > c_s$. The angle θ is defined by $v\cos\theta = c_s$ while $\Theta = \frac{\pi}{2} - \theta$ denotes the opening angle of the cone defined by θ.

and the final state is either

$$\begin{aligned} |\beta) &= \Big|[C(\mathbf{p})]_{N_C-1}, [A(\mathbf{l})]_{N_A+1}, [B(\mathbf{q})]_1\Big) \\ \text{or} \quad |\beta) &= \Big|[C(\mathbf{p})]_{N_C-1}, [A(\mathbf{l})]_{N_A}, [A(\mathbf{k})]_1, [B(\mathbf{q})]_1\Big)\,, \end{aligned} \tag{4.2.2}$$

where the round bracket emphasizes the state is assumed to be discretely normalized so we can count the occupation number of specific states.

Fermi's Golden Rule says that the main change arises in this case when taking the matrix element, particularly when the emission is into the final state with momentum $\mathbf{k} = \mathbf{l}$:

$$\Big([C(\mathbf{q})]_{N_C-1}, [A(\mathbf{l})]_{N_A+1}, [B(\mathbf{q})]_1\Big|H_{\text{int}}\Big|[C(\mathbf{p})]_{N_C}, [A(\mathbf{l})]_{N_A}\Big) = g^*(\mathbf{p},\mathbf{q},\mathbf{l})\,\sqrt{N_C(N_A+1)}\,\delta_{\mathbf{p}-\mathbf{q}-\mathbf{l}}\,, \tag{4.2.3}$$

which uses the results

$$(N+1|a^\star|N) = \sqrt{N+1} \quad \text{and} \quad (N-1|a|N) = \sqrt{N}\,, \tag{4.2.4}$$

(see *e.g.* eq. (2.3.12)). This is to be compared with the amplitude for producing particle A with a momentum different than $\mathbf{l}$, which is given by

$$\Big([C(\mathbf{q})]_{N_C-1}, [A(\mathbf{l})]_{N_A}, [A(\mathbf{k})]_1, [B(\mathbf{q})]_1\Big|H_{\text{int}}\Big|[C(\mathbf{p})]_{N_C}, [A(\mathbf{l})]_{N_A}\Big) = g^*(\mathbf{p},\mathbf{q},\mathbf{k})\,\sqrt{N_C}\,\delta_{\mathbf{p}-\mathbf{q}-\mathbf{k}}\,, \tag{4.2.5}$$

which agrees with (4.1.5) when $N_C = 1$. Because of the relative factor of $\sqrt{N_A+1}$ between (4.2.3) and (4.2.5), if it is kinematically possible for emission to occur at momentum $\mathbf{l}$ it will preferentially do so, and the larger N_A is the larger the preference is.

Applying Fermi's Golden Rule to a specific discretely normalized final state then gives

$$\begin{aligned}\Gamma[N_A A(\mathbf{l}) + N_C C(\mathbf{p}) \to (N_A+1)A(\mathbf{l}) + (N_C-1)C(\mathbf{p}) + B(\mathbf{q})] \\ = 2\pi\Big|g(\mathbf{p},\mathbf{q},\mathbf{l})\Big|^2 N_C(N_A+1)\delta_{\mathbf{p}-\mathbf{q}-\mathbf{l}}\delta\Big[\varepsilon_B(q)+\varepsilon_A(l)-\varepsilon_C(p)\Big]\,.\end{aligned} \tag{4.2.6}$$

This is proportional to the number N_C of decaying particles simply because the more particles there are the more likely that a decay will happen in any given small time window. (This is why people search for very rare decays by watching for them within very large samples of decaying particles.) The decay rate *per particle* is obtained by dividing (4.2.6) by N_C (or by setting $N_C = 1$) and so is

$$\begin{aligned}\Gamma[N_A A(\mathbf{l}) + C(\mathbf{p}) \to NA(\mathbf{l}) + A(\mathbf{k}) + B(\mathbf{q})] \\ = 2\pi\Big|g(\mathbf{p},\mathbf{q},\mathbf{k})\Big|^2 (N_A\delta_{\mathbf{kl}}+1)\delta_{\mathbf{p}-\mathbf{q}-\mathbf{k}}\delta\Big[\varepsilon_B(q)+\varepsilon_A(k)-\varepsilon_C(p)\Big]\,.\end{aligned} \tag{4.2.7}$$

In the continuum limit we cannot specify that the initially occupied A states have a specific momentum $\mathbf{l}$, but instead say that the initial state is described by a phase-space distribution function $f(\mathbf{l})$ where we conventionally normalize things so that $\mathrm{d}N = f(\mathbf{l})\mathcal{V}\,\mathrm{d}^3l/(2\pi)^3$ is the number of particles in a volume d^3l around the momentum $\mathbf{l}$. This is the same normalization as used in §1.6.1 – see the discussion around (1.6.18) – for the grand canonical distribution, for which the distribution is given by $f_{\mathbf{p}} = 1/(\exp[\beta(\varepsilon_{\mathbf{p}}-\mu)]-1)$. Since the number of particles, $N_{\mathbf{l}}$, at momentum $\mathbf{l}$ must sum to the total number of particles, $\sum_{\mathbf{l}} N_{\mathbf{l}} = N_{\mathrm{tot}}$, in the continuum limit one finds

$$N_{\mathrm{tot}} = \sum_{\mathbf{l}} N_{\mathbf{l}} = \frac{\mathcal{V}}{(2\pi)^3}\int \mathrm{d}^3l\, N_{\mathbf{l}}\,, \tag{4.2.8}$$

showing that $N_{\mathbf{l}} \to f(\mathbf{l})$ for infinite volume. In the differential rate the statistics factor therefore becomes

$$1 + N_A\,\delta_{\mathbf{kl}} \to 1 + f_A(\mathbf{k})\,, \tag{4.2.9}$$

where $f_A(\mathbf{k})$ vanishes if $\mathbf{k}$ does not lie within d^3l of the momenta $\mathbf{l}$ that are occupied in the initial state.

This leads to the following differential rate for the final particles lying within a small volume d^3q and d^3k of the momenta $\mathbf{q}$ and $\mathbf{k}$,

$$\begin{aligned}\mathrm{d}\Gamma[NA + C \to (N+1)A + B] &= 2\pi\Big|g(\mathbf{p},\mathbf{q},\mathbf{k})\Big|^2\Big[f_A(\mathbf{k})+1\Big]\,\delta_{\mathbf{p}-\mathbf{q}-\mathbf{k}}\delta\Big[\varepsilon_B(q)+\varepsilon_A(k)-\varepsilon_C(p)\Big]\,\mathrm{d}n \\ &= 2\pi\left|\left[\frac{(2\pi)^3}{\mathcal{V}}\right]^{1/2}\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k})\right|^2 (f_A+1)\left[\frac{(2\pi)^3}{\mathcal{V}}\delta^3(\mathbf{p}-\mathbf{q}-\mathbf{l})\right] \\ &\qquad \times\delta\Big[\varepsilon_B(q)+\varepsilon_A(l)-\varepsilon_C(p)\Big]\left[\frac{\mathcal{V}}{(2\pi)^3}\mathrm{d}^3q\right]\left[\frac{\mathcal{V}}{(2\pi)^3}\mathrm{d}^3l\right] \\ &= 2\pi|\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{l})|^2(f_A+1)\,\delta^4(p-q-l)\,\mathrm{d}^3q\,\mathrm{d}^3l\,,\end{aligned} \tag{4.2.10}$$

where in the last line the 4D delta function is a short form for joint momentum and energy conservation:

$$\delta^4(p-q-k) := \delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k})\,\delta[\varepsilon_C(p)-\varepsilon_B(q)-\varepsilon_A(k)]\,. \tag{4.2.11}$$

Repeating this exercise when there is a distribution of $N_C(\mathbf{p})$ particles in the initial state shows and using $\sum_{\mathbf{p}} = [\mathcal{V}/(2\pi)^3]\int \mathrm{d}^3p$ when summing over the *initial* momentum $\mathbf{p}$ in

$$\begin{aligned}\mathrm{d}\Gamma[N_A A + N_C C \to (N_A+1)A + B + (N_C-1)C] \\ = 2\pi \sum_{\mathbf{p}} \Big|g(\mathbf{p},\mathbf{q},\mathbf{k})\Big|^2 N_C(\mathbf{p})\Big[N_A(\mathbf{l})\,\delta_{\mathbf{lk}}+1\Big]\delta_{\mathbf{p}-\mathbf{q}-\mathbf{l}}\delta\Big[\varepsilon_B(q)+\varepsilon_A(l)-\varepsilon_C(p)\Big]\,.\end{aligned} \tag{4.2.12}$$

shows that the differential rate is proportional to the volume. This is because our choice of initial momentum eigenstates means that the initial C particles are uniformly distributed throughout space and so can decay everywhere. Realistically the proportionality to volume gets cut off by the wave-packets that in practice localize the initial C particles within a smaller volume. But for large packets the rate-per-unit-volume is both packet-independent and well-defined in the limit $\mathcal{V}\to\infty$ and so can be written

$$\begin{aligned}\mathrm{d}\mathcal{R}[N_A A + N_C C \to (N_A+1)A + B + (N_C-1)C] &:= \frac{\mathrm{d}\Gamma[NA + C \to (N+1)A + B]}{\mathcal{V}} \\ &= 2\pi|\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{l})|^2 f_C(\mathbf{p})\Big[f_A(\mathbf{l})+1\Big]\,\delta^4(p-q-l)\frac{\mathrm{d}^3q}{(2\pi)^3}\,\frac{\mathrm{d}^3l}{(2\pi)^3}\,\frac{\mathrm{d}^3p}{(2\pi)^3}\,.\end{aligned} \tag{4.2.13}$$

Notice that this reduces to (4.2.10) after integrating over d^3p if $f_C(\mathbf{p}) = [(2\pi)^3/\mathcal{V}]\delta^3(\mathbf{p}-\mathbf{p}_0)$ is chosen, as the normalization (4.2.8) requires if there were only a single initial C particle with momentum $\mathbf{p}_0$.

The upshot for continuum-normalized states is the same as for discrete-normalized states: transitions $C \to B + A$ are enhanced (when A is a boson) by factors of $f+1$ if they take place in an environment where A particles already are present with phase-space distribution f. The phenomenon where boson emission is enhanced by already-present bosons of the same type is called *stimulated emission*, and is the principle that underlies the ability of lasers to deposit macroscopic amounts of energy into a few quantum states.

4.3 Fermions and Pauli blocking

A very similar phenomenon occurs for final-state fermions if reactions are performed in an environment with some final-state particles already present. The main difference is that Fermi statistics suppress rather than enhance reactions when a final-state particle is already occupied. The reason for this is identical to the argument given above, with the bosonic expression (4.2.4) replaced by its fermionic counterpart (see (2.3.12)):

$$(N+1|a^\star|N) = \sqrt{1-N}\,, \tag{4.3.1}$$

which is always real because for fermions N is restricted to 0 or 1. For continuum normalized momentum eigenstates the same arguments as given above for bosons imply (4.3.1) becomes replaced by

$$\langle N+1|\mathfrak{a}^\star|N\rangle = \sqrt{1-f}\,, \tag{4.3.2}$$

where $f(\mathbf{p})/(2\pi)^3$ is the phase-space density of fermionic particles.

Worked example: fermion scattering

To see what the implications of this kind of factor are (and to introduce scattering calculations in their own right) consider a scattering process $A(\mathbf{p}) + B(\mathbf{q}) \to A(\tilde{\mathbf{p}}) + B(\tilde{\mathbf{q}})$, mediated by a Hamiltonian $H = H_{\text{free}} + H_{\text{int}}$ with

$$\begin{aligned} H_{\text{free}} &= E_0 + \sum_p \Big[\varepsilon_{\scriptscriptstyle A}(p)\, a_p^\star a_p + \varepsilon_{\scriptscriptstyle B}(p)\, b_p^\star b_p\Big] \\ \text{and}\quad H_{\text{int}} &= \sum_{pqkl} \Big[h(p,q,\tilde{p},\tilde{q})\, a_{\tilde{p}}^\star a_p\, b_{\tilde{q}}^\star b_q + h^*(p,q,\tilde{p},\tilde{q}) a_p^\star a_{\tilde{p}}\, b_q^\star b_{\tilde{q}}\Big]\delta_{p+q-\tilde{p}-\tilde{q}}\,. \end{aligned} \tag{4.3.3}$$

which for continuum-normalized states becomes

$$\begin{aligned} H_{\text{free}} &= E_0 + \int \mathrm{d}^3p \Big[\varepsilon_{\scriptscriptstyle A}(p)\, \mathfrak{a}_p^\star \mathfrak{a}_p + \varepsilon_{\scriptscriptstyle B}(p)\, \mathfrak{b}_p^\star \mathfrak{b}_p\Big] \\ \text{and}\quad H_{\text{int}} &= \int \mathrm{d}^3p\, \mathrm{d}^3q\, \mathrm{d}^3\tilde{p}\, \mathrm{d}^3\tilde{q}\, \Big[\mathfrak{h}(p,q,\tilde{p},\tilde{q})\, \mathfrak{a}_{\tilde{p}}^\star \mathfrak{a}_p\, \mathfrak{b}_{\tilde{q}}^\star \mathfrak{b}_q \\ &\qquad + \mathfrak{h}^*(p,q,\tilde{p},\tilde{q}) \mathfrak{a}_p^\star \mathfrak{a}_{\tilde{p}}\, \mathfrak{b}_q^\star \mathfrak{b}_{\tilde{q}}\Big]\, \delta^3(\mathbf{p}+\mathbf{q}-\tilde{\mathbf{p}}-\tilde{\mathbf{q}})\,, \end{aligned} \tag{4.3.4}$$

where

$$h(p,q,\tilde{p},\tilde{q}) = \left[\frac{(2\pi)^3}{\mathcal{V}}\right] \mathfrak{h}(p,q,\tilde{p},\tilde{q})\,. \tag{4.3.5}$$

Consider now a two-body scattering process, $A+B \to A+B$, that occurs when $N_{\scriptscriptstyle A}$ particles of type A encounter $N_{\scriptscriptstyle B}$ particles of type B. When switching to continuum normalization the initial particles A and B will be assumed to have phase-space densities $f_{\scriptscriptstyle A}(\mathbf{p})/(2\pi)^3$ and $f_{\scriptscriptstyle B}(\mathbf{p})/(2\pi)^3$, normalized as in (1.6.18). The relevant matrix element that appears in Fermi's Golden Rule for discretely normalized states is

$$\begin{aligned} (A(\tilde{\mathbf{p}}), B(\tilde{\mathbf{q}}), \cdots |H_{\text{int}}| A(\mathbf{p}), B(\mathbf{q}), \cdots) &= h(p,q,\tilde{p},\tilde{q})\, \delta_{p+q-\tilde{p}-\tilde{q}} \\ &\quad \times \sqrt{N_{\scriptscriptstyle A}(p) N_{\scriptscriptstyle B}(q) [1-N_{\scriptscriptstyle A}(\tilde{p})][1-N_{\scriptscriptstyle B}(\tilde{q})]}\,, \end{aligned} \tag{4.3.6}$$

where the square-root factors come from repeated use of the relations $(N-1|a|N) = \sqrt{N}$ and $(N+1|a^\star|N) = \sqrt{1-N}$ (for fermions). (For bosons the final-state factors would instead be $\sqrt{1+N}$.)

The rate predicted by Fermi's Golden Rule for the transition for specific initial and final states (assuming discrete normalization) is then

$$\begin{aligned} \Gamma[A+B\to A+B] &= 2\pi \Big|(A(\tilde{\mathbf{p}}), B(\tilde{\mathbf{q}}), \cdots |H_{\text{int}}| A(\mathbf{p}), B(\mathbf{q}), \cdots)\Big|^2 \\ &\qquad \times \delta[\varepsilon_{\scriptscriptstyle A}(p) + \varepsilon_{\scriptscriptstyle B}(q) - \varepsilon_{\scriptscriptstyle A}(\tilde{p}) - \varepsilon_{\scriptscriptstyle B}(\tilde{q})] \\ &= 2\pi |h(p,q,\tilde{p},\tilde{q})|^2\, N_{\scriptscriptstyle A}(p) N_{\scriptscriptstyle B}(q) [1-N_{\scriptscriptstyle A}(\tilde{p})][1-N_{\scriptscriptstyle B}(\tilde{q})] \\ &\qquad \times \delta_{p+q-\tilde{p}-\tilde{q}} \delta[\varepsilon_{\scriptscriptstyle A}(p) + \varepsilon_{\scriptscriptstyle B}(q) - \varepsilon_{\scriptscriptstyle A}(\tilde{p}) - \varepsilon_{\scriptscriptstyle B}(\tilde{q})]\,. \end{aligned} \tag{4.3.7}$$

The proportionality of the result to $N_A(p)$ and $N_B(q)$ simply reflects that the number of scatterings is proportional to the number of initial particles that are present to scatter. More specific to fermions is the factor of $1-N$ for each type of fermion in the final state. This has the effect of turning off any transition that would have produced a final-state fermion if that fermion is already present, since having two fermions in the same state is forbidden by Fermi-Dirac statistics; a phenomenon called *Pauli blocking*. (The previous section showed that boson scattering comes with a similar factor, $1+N$, describing stimulated emission.)

An analogous result goes through for continuum-normalized states, with N replaced by f where the phase-space density is $f_p/(2\pi)^3$. To see this in detail, notice in this case the differential transition to final-state particles within a small momentum-space volume $\mathrm{d}^3\tilde{p}$ and $\mathrm{d}^3\tilde{q}$ of two specific momenta $\tilde{\mathbf{p}}$ and $\tilde{\mathbf{q}}$ is given by

$$\begin{aligned}
\mathrm{d}\Gamma[A+B\to A+B] &= 2\pi \left|\left[\frac{(2\pi)^3}{\mathcal{V}}\right]\mathfrak{h}(p,q,\tilde{p},\tilde{q})\right|^2 f_A(p)f_B(q)[1-f_A(\tilde{p})][1-f_B(\tilde{q})] \\
&\qquad\times\left[\frac{(2\pi)^3}{\mathcal{V}}\delta^3(\mathbf{p}+\mathbf{q}-\tilde{\mathbf{p}}-\tilde{\mathbf{q}})\right]\delta[\varepsilon_A(p)+\varepsilon_B(q)-\varepsilon_A(\tilde{p})-\varepsilon_B(\tilde{q})]\,. \\
&\qquad\times\left[\frac{\mathcal{V}}{(2\pi)^3}\mathrm{d}^3p\right]\left[\frac{\mathcal{V}}{(2\pi)^3}\mathrm{d}^3q\right]\left[\frac{\mathcal{V}}{(2\pi)^3}\mathrm{d}^3\tilde{p}\right]\left[\frac{\mathcal{V}}{(2\pi)^3}\mathrm{d}^3\tilde{q}\right] \\
&= \frac{\mathcal{V}}{(2\pi)^2}\,|\mathfrak{h}(p,q,\tilde{p},\tilde{q})|^2\;\delta^4(p+q-\tilde{p}-\tilde{q}) \\
&\qquad\times f_A(p)f_B(q)[1-f_A(\tilde{p})][1-f_B(\tilde{q})]\,\mathrm{d}^3p\,\mathrm{d}^3q\,\mathrm{d}^3\tilde{p}\,\mathrm{d}^3\tilde{q}\,,
\end{aligned} \tag{4.3.8}$$

where the final form uses the definition (4.2.11) and the factors of d^3p and d^3q for the initial state momenta must be included because these momenta are weighted with an initial distribution $f_A(p)$ and $f_B(q)$.

As before it is the transition rate per unit volume that is well-behaved in the $\mathcal{V}\to\infty$ limit,[7] so

$$\begin{aligned}
\mathrm{d}\mathcal{R}[A+B\to A+B] &= \frac{\mathrm{d}\Gamma[A+B\to A+B]}{\mathcal{V}} \\
&= \frac{1}{(2\pi)^2}\,|\mathfrak{h}(p,q,\tilde{p},\tilde{q})|^2\;\delta^4(p+q-\tilde{p}-\tilde{q}) \\
&\qquad\times f_A(p)f_B(q)[1-f_A(\tilde{p})][1-f_B(\tilde{q})]\,\mathrm{d}^3p\,\mathrm{d}^3q\,\mathrm{d}^3\tilde{p}\,\mathrm{d}^3\tilde{q}\,.
\end{aligned} \tag{4.3.9}$$

For bosons the final-state factors of $1-f$ get replaced by factors of $1+f$.

Often one is interested in the transition rate per particle in an initial beam. This is obtained by dividing the rate-per-unit-volume, $\mathrm{d}\mathcal{R}$, by the density of one of the initial species of particles, *e.g.* $\mathrm{d}n_A = \mathrm{d}N_A/\mathcal{V} = [f_A/(2\pi)^3]\,\mathrm{d}^3p$. This leads to the scattering rate per initial A particle being

$$\begin{aligned}
\mathrm{d}\mathcal{R}_A[A+B\to A+B] &= \frac{\mathrm{d}\mathcal{R}[A+B\to A+B]}{[f_A(p)/(2\pi)^3]\,\mathrm{d}^3p} \\
&= 2\pi\,|\mathfrak{h}(p,q,\tilde{p},\tilde{q})|^2\;\delta^4(p+q-\tilde{p}-\tilde{q}) \\
&\qquad\times f_B(q)[1-f_A(\tilde{p})][1-f_B(\tilde{q})]\,\mathrm{d}^3q\,\mathrm{d}^3\tilde{p}\,\mathrm{d}^3\tilde{q}\,.
\end{aligned} \tag{4.3.10}$$

The reaction cross-section is similarly defined by dividing out the scattering rate per incident particle A by the flux of particle B that this particle sees. Since the flux is $\mathrm{d}n_B\,v_{\rm rel} = [f_B(q)/(2\pi)^3]\,v_{\rm rel}\,\mathrm{d}^3q$,

[7] This is not an accident of two-body scattering, and the rate is proportional to $\mathcal{V}$ also for an N-body scattering process.

where $v_{\rm rel}$ is the relative speed of approach of the two initial particles, the cross section is

$$\begin{aligned} \mathrm{d}\sigma[A+B\to A+B] &= \frac{\mathrm{d}\mathcal{R}_{A}[A+B\to A+B]}{[f_{B}(p)/(2\pi)^3]\,v_{\rm rel}\,\mathrm{d}^3q} \\ &= \frac{(2\pi)^4}{v_{\rm rel}}\,|\mathfrak{h}(p,q,\tilde{p},\tilde{q})|^2\;\delta^4(p+q-\tilde{p}-\tilde{q}) \\ &\qquad\qquad \times[1-f_{A}(\tilde{p})][1-f_{B}(\tilde{q})]\,\mathrm{d}^3\tilde{p}\,\mathrm{d}^3\tilde{q}\,. \end{aligned} \tag{4.3.11}$$

For scattering where final-state statistics are not important simply take the limits $f_{A}(\tilde{p})\to 0$ and $f_{B}(\tilde{q})\to 0$ in this expression. The utility of the cross section is that it removes all of the factors that are specific to the details of the experimental setup (the initial particles and their relative motion) and zeros in on the physics responsible for the transition itself.

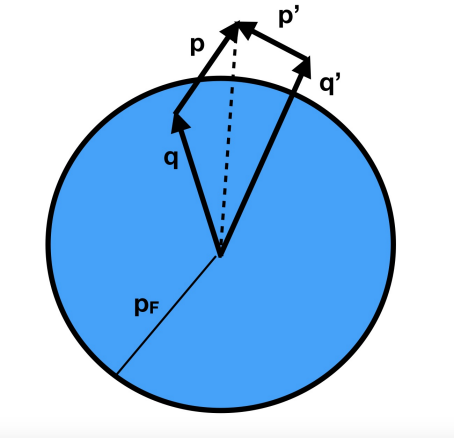


Figure 3. A sketch of the kinematics of scattering near the Fermi surface (represented here by the shaded blue circle). Pauli blocking ensures the vector $\mathbf{q}$ must lie within the surface and the vector $\tilde{\mathbf{q}}=\mathbf{q}'$ must be outside it. In the example examined in the text energy conservation requires $|\mathbf{p}|^2+|\mathbf{q}|^2=|\mathbf{p}'|^2+|\mathbf{q}'|^2$.

As a concrete example consider the special case of the above where $\mathfrak{h}=\mathfrak{h}_0$ is momentum-independent, and the single-particle energies are simply $\varepsilon_{A}(p)=\mathbf{p}^2/(2m)$ and $\varepsilon_{B}(q)=\mathbf{q}^2/(2m)$. Finally suppose a single A particle is scattered from a collection of $N_{\rm tot}$ B particles who singly occupy all of the energy levels up to the minimum required to contain all the particles. This gives rise to a spherical Fermi sea whose radius in momentum space, p_{F}, satisfies

$$n_{B}:=\frac{N_{B}}{\mathcal{V}}=\frac{1}{\mathcal{V}}\sum_{p<p_{F}}1=\int_{0}^{p_{F}}\frac{\mathrm{d}^3p}{(2\pi)^3}=\frac{p_{F}^3}{6\pi^2}\,. \tag{4.3.12}$$

The phase-space distribution for this is a step function,

$$f_{B}(\mathbf{p})=\Theta(p_{F}-|\mathbf{p}|)\,, \tag{4.3.13}$$

where $\Theta(x) = 0$ if $x < 0$ and $\Theta(x) = 1$ if $x > 0$, and so $1 - \Theta(x) = \Theta(-x)$. The scattering rate for the incident A particle of momentum $\mathbf{p}$ then is

$$\begin{aligned} \mathrm{d}\mathcal{R}_A[A + B \to A + B] \;=\; 2\pi\,|\mathfrak{h}_0|^2\;\delta^4(p + q - \tilde{p} - \tilde{q}) \\ \times\Theta(p_F - |\mathbf{q}|)\,\Theta(|\tilde{\mathbf{q}}| - p_F)\,\mathrm{d}^3q\,\mathrm{d}^3\tilde{p}\,\mathrm{d}^3\tilde{q}\,. \end{aligned} \tag{4.3.14}$$

The momenta in this problem must satisfy the four conditions

$$\begin{aligned} \mathbf{p} + \mathbf{q} = \tilde{\mathbf{p}} + \tilde{\mathbf{q}}\,, \qquad \mathbf{p}^2 + \mathbf{q}^2 = \tilde{\mathbf{p}}^2 + \tilde{\mathbf{q}}^2 \\ |\mathbf{q}| < p_F \qquad \text{and} \qquad |\tilde{\mathbf{q}}| > p_F\,, \end{aligned} \tag{4.3.15}$$

of which the first two express energy and momentum conservation and the second two are the constraints of Pauli blocking. These are shown pictorially in Figure 3. The first two conditions together also imply $\mathbf{p} \cdot \mathbf{q} = \tilde{\mathbf{p}} \cdot \tilde{\mathbf{q}}$, so momentum conservation automatically implies energy conservation if $\mathbf{q}$ within the Fermi sea can be chosen orthogonal to $\mathbf{p}$. Call this the 'pythagorean' solution.

A pythagorean solution always exists for a spherical Fermi surface, as may be seen by choosing $\mathbf{p}$ to be tangent to the Fermi surface with $\mathbf{q}$ therefore orthogonal to $\mathbf{p}$, as in Figure 4. With this choice $\mathbf{p} + \mathbf{q}$ lies outside the Fermi sea and by choosing $\tilde{\mathbf{p}}$ sufficiently small it is always possible to find $\tilde{\mathbf{q}}$ orthogonal to $\tilde{\mathbf{p}}$ such that $\tilde{\mathbf{p}} + \tilde{\mathbf{q}} = \mathbf{p} + \mathbf{q}$ and $|\tilde{\mathbf{q}}| > p_F$.

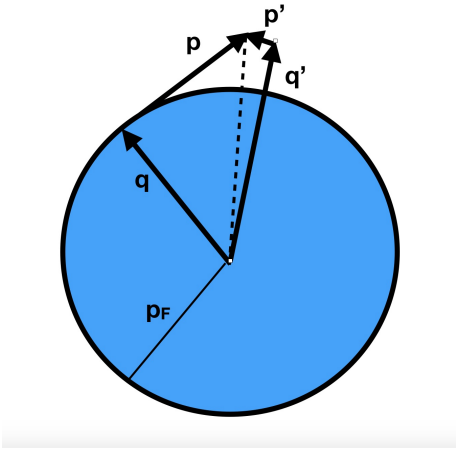


Figure 4. A sketch of the 'pythagorean' choice for $\mathbf{q}$ with $|\mathbf{q}| \le p_F$ that for any $\mathbf{p}$ ensures $\mathbf{q} \cdot \mathbf{p} = 0$ and so always allows a solution where $\tilde{\mathbf{p}} \cdot \tilde{\mathbf{q}} = 0$ and $\tilde{\mathbf{q}} + \tilde{\mathbf{p}} = \mathbf{q} + \mathbf{p}$ with $|\tilde{\mathbf{q}}| \ge p_F$. For equal mass nonrelativistic particles this solution always exists. For $|\mathbf{p}| \ll p_F$ only states very near the Fermi surface are accessible in this way.

The total rate is obtained by integrating over the initial and final momenta, and this integration can be tricky due to the interlacing constraints of conservation and Pauli blocking. An approximate result in the particular limit $|\mathbf{p}| \ll p_F$ can be done fairly straightforwardly, however, as follows.

For $|\mathbf{p}| \ll p_{\scriptscriptstyle F}$ it is also true that $|\mathbf{p}|, |\tilde{\mathbf{p}}| \ll |\mathbf{q}|, |\tilde{\mathbf{q}}|$ and so energy conservation becomes

$$\begin{aligned}\delta\Big[\varepsilon_{\scriptscriptstyle A}(\tilde{p}) + \varepsilon_{\scriptscriptstyle B}(\tilde{q}) - \varepsilon_{\scriptscriptstyle A}(p) - \varepsilon_{\scriptscriptstyle B}(q)\Big] &= \delta\left[\frac{|\tilde{\mathbf{p}}|^2}{2m} + \frac{|\mathbf{p}+\mathbf{q}-\tilde{\mathbf{p}}|^2}{2m} - \frac{|\mathbf{p}|^2}{2m} - \frac{|\mathbf{q}|^2}{2m}\right] \\ &= \delta\left[\frac{(\tilde{p})^2}{m} + \frac{pq\cos\theta_{pq} - p\tilde{p}\cos\theta_{p\tilde{p}} - q\tilde{p}\cos\theta_{q\tilde{p}}}{m}\right], \\ &\simeq \delta\left[\frac{pq\cos\theta_{pq} - q\tilde{p}\cos\theta_{q\tilde{p}}}{m}\right] \end{aligned} \tag{4.3.16}$$

which uses the momentum-conserving delta function to impose $\tilde{\mathbf{q}} = \mathbf{p} + \mathbf{q} - \tilde{\mathbf{p}}$. When performing the remaining integrations choose coordinates so the momentum $\mathbf{q}$ points along the z-axis:

$$\mathbf{q} = q\,\mathbf{e}_z\,. \tag{4.3.17}$$

The x-axis can then be chosen so that

$$\mathbf{p} = p\cos\theta_{pq}\,\mathbf{e}_z + p\sin\theta_{pq}\,\mathbf{e}_x\,, \tag{4.3.18}$$

so that $\mathbf{p}+\mathbf{q}$ lies in the x-z plane. Then the momentum $\tilde{\mathbf{p}}$ can be written

$$\tilde{\mathbf{p}} = \tilde{p}\cos\theta_{q\tilde{p}}\,\mathbf{e}_z + \tilde{p}\sin\theta_{q\tilde{p}}\cos\phi_{\tilde{p}}\,\mathbf{e}_x + \tilde{p}\sin\theta_{q\tilde{p}}\sin\phi_{\tilde{p}}\,\mathbf{e}_y\,. \tag{4.3.19}$$

Writing d^3q in polar coordinates, $\mathrm{d}^3q = q^2\sin\theta_q\,\mathrm{d}q\,\mathrm{d}\theta_q\,\mathrm{d}\phi_q$, the integration over ϕ_q gives a factor of 2π since it appears nowhere in the integrand. Pauli blocking ensures the integral over q then runs over $0 < q < p_{\scriptscriptstyle F}$ and angle $0 < \theta_q < \pi$, so

$$\int \mathrm{d}^3q\,\Theta(p_{\scriptscriptstyle F} - |\mathbf{q}|) = 2\pi\int_0^{p_{\scriptscriptstyle F}} \mathrm{d}q\,q^2\int_{-1}^{1}\mathrm{d}\cos\theta_{qp}\,. \tag{4.3.20}$$

The integral over $\tilde{\mathbf{p}}$ in polar coordinates is performed similarly, with

$$\begin{aligned}&\int \mathrm{d}^3\tilde{p}\,\delta\Big[\varepsilon_{\scriptscriptstyle A}(\tilde{p}) + \varepsilon_{\scriptscriptstyle B}(\tilde{q}) - \varepsilon_{\scriptscriptstyle A}(p) - \varepsilon_{\scriptscriptstyle B}(q)\Big] \\ &\qquad= \int_0^{2\pi}\mathrm{d}\phi_{\tilde{p}}\int_{-1}^{1}\mathrm{d}\cos\theta_{q\tilde{p}}\int_0^{\infty}\mathrm{d}\tilde{p}\,\tilde{p}^2\;\delta\left[\frac{|\tilde{\mathbf{p}}|^2}{2m} + \frac{|\mathbf{p}+\mathbf{q}-\tilde{\mathbf{p}}|^2}{2m} - \frac{|\mathbf{p}|^2}{2m} - \frac{|\mathbf{q}|^2}{2m}\right] \\ &\qquad= \int_0^{2\pi}\mathrm{d}\phi_{\tilde{p}}\int_{-1}^{1}\mathrm{d}\cos\theta_{q\tilde{p}}\int_0^{\infty}\mathrm{d}\tilde{p}\,\tilde{p}^2 \\ &\qquad\qquad\times\delta\left[\frac{\tilde{p}^2}{m} + \frac{pq\cos\theta_{qp} - p\tilde{p}\cos\theta_{p\tilde{p}} - q\tilde{p}\cos\theta_{q\tilde{p}}}{m}\right], \end{aligned} \tag{4.3.21}$$

which in general depends on $\phi_{\tilde{p}}$ because $\theta_{p\tilde{p}}$ does, as can be seen by taking the dot product $\mathbf{p}\cdot\tilde{\mathbf{p}} = p\tilde{p}\cos\theta_{p\tilde{p}}$ using the explicit representations (4.3.18) and (4.3.19), leading to

$$\cos\theta_{p\tilde{p}} = \cos\theta_{qp}\cos\theta_{q\tilde{p}} + \sin\theta_{qp}\sin\theta_{q\tilde{p}}\cos\phi_{\tilde{p}}\,. \tag{4.3.22}$$

This complication goes away in the limit $|\mathbf{p}|, |\tilde{\mathbf{p}}| \ll |\mathbf{q}|, |\tilde{\mathbf{q}}|$, in which case (4.3.16) gives

$$\begin{aligned}
&\int \mathrm{d}^3\tilde{p}\,\delta\Big[\varepsilon_{A}(\tilde{p}) + \varepsilon_{B}(\tilde{q}) - \varepsilon_{A}(p) - \varepsilon_{B}(q)\Big] \\
&\qquad \simeq \int_0^{2\pi} \mathrm{d}\phi_{\tilde{p}} \int_{-1}^{1} \mathrm{d}\cos\theta_{q\tilde{p}} \int_0^{\infty} \mathrm{d}\tilde{p}\,\tilde{p}^2\;\delta\left[\frac{pq\cos\theta_{qp} - q\tilde{p}\cos\theta_{q\tilde{p}}}{m}\right] \\
&\qquad = 2\pi \int_{-1}^{1} \mathrm{d}\cos\theta_{q\tilde{p}} \int_0^{\infty} \mathrm{d}\tilde{p}\,\tilde{p}^2\;\delta\left[\frac{pq\cos\theta_{qp} - q\tilde{p}\cos\theta_{q\tilde{p}}}{m}\right], \\
&\qquad = \frac{2\pi m}{q} \int_0^{\infty} \mathrm{d}\tilde{p}\,\tilde{p}\,,
\end{aligned} \tag{4.3.23}$$

which uses the delta function to do the $\mathrm{d}\cos\theta_{q\tilde{p}}$ integral, giving a nonzero result provided $\cos\theta_{q\tilde{p}} = (p/\tilde{p})\cos\theta_{qp}$ lies in the interval $(-1, 1)$. If $\tilde{p} > p$ then this is always true, but if $\tilde{p} < p$ then this requires $\cos\theta_{qp} < \tilde{p}/p$.

Combining everything, eq. (4.3.14) evaluates to

$$\begin{aligned}
\mathcal{R}_{A}[A + B \to A + B] \;&=\; 2\pi\,|\mathfrak{h}_0|^2 \int \mathrm{d}^3q\,\mathrm{d}^3\tilde{p}\,\mathrm{d}^3\tilde{q}\;\delta^4(p + q - \tilde{p} - \tilde{q}) \\
&\qquad\qquad \times\Theta(p_{F} - |\mathbf{q}|)\,\Theta(|\tilde{\mathbf{q}}| - p_{F}) \\
&\simeq\; 2\pi\,|\mathfrak{h}_0|^2 \int \mathrm{d}^3q\,\mathrm{d}^3\tilde{p}\;\delta\left[\frac{pq\cos\theta_{qp} - q\tilde{p}\cos\theta_{q\tilde{p}}}{m}\right] \\
&\qquad\qquad \times\Theta(p_{F} - |\mathbf{q}|)\,\Theta\Big[q + \frac{1}{2}(p^2 - \tilde{p}^2) - p_{F}\Big] \\
&=\; (2\pi)^3 m\,|\mathfrak{h}_0|^2 \int_0^{\infty} \mathrm{d}\tilde{p}\,\tilde{p} \int \mathrm{d}\cos\theta_{qp} \int_{p_{L}}^{p_{F}} \mathrm{d}q\,q\,,
\end{aligned} \tag{4.3.24}$$

which evaluates the step function $\Theta(|\tilde{\mathbf{q}}| - p_{F})$ using energy conservation, so

$$|\tilde{\mathbf{q}}| = \sqrt{\mathbf{q}^2 + \mathbf{p}^2 - \tilde{\mathbf{p}}^2} \simeq q + \frac{\mathbf{p}^2 - \tilde{\mathbf{p}}^2}{2q} + \cdots \tag{4.3.25}$$

and arrives at the following lower limit for the q integration

$$p_{L} \simeq p_{F} - \frac{p^2 - \tilde{p}^2}{2p_{F}} \tag{4.3.26}$$

which is only smaller than p_{F} if $\tilde{p} < p$, making this an upper limit for the $\tilde{p}$ integral. In this regime the discussion above also says the limits of integration over $\cos\theta_{qp}$ are $\pm\tilde{p}/p$, in which case this integral needs to be performed before the integral over $\tilde{p}$.

The q integration therefore gives

$$\int_{p_{L}}^{p_{F}} \mathrm{d}q\,q = \frac{1}{2}(p_{F}^2 - p_{L}^2) \simeq p_{F}(p_{F} - p_{L}) = \frac{1}{2}\left(p^2 - \tilde{p}^2\right), \tag{4.3.27}$$

and the angular integration becomes

$$\int_{-\tilde{p}/p}^{\tilde{p}/p} \mathrm{d}\cos\theta_{qp} = \frac{2\tilde{p}}{p}\,. \tag{4.3.28}$$

Finally, the integral over $\tilde{p}$ then gives

$$\int_0^{p} \mathrm{d}\tilde{p}\,\tilde{p}\left[\frac{1}{2}\left(p^2 - \tilde{p}^2\right)\right]\frac{2\tilde{p}}{p} = \left[\frac{p^4}{3} - \frac{p^4}{5}\right] = \frac{2p^4}{15}\,. \tag{4.3.29}$$

leading to the complete result

$$\mathcal{R}_{A}[A+B\to A+B]\simeq\frac{16\pi^{3}m}{15}\left|\mathfrak{h}_{0}\right|^{2}p^{4}\,,$$

for $p\ll p_{F}$.

By way of comparison, it is instructive to contrast the above exercise with the result from a similar calculation in the absence of the Fermi sea suppose a statistically nondegenerate initial distribution of particles were assumed which corresponds to the same particle density as did the Fermi sea in the previous example: $\int \mathrm{d}^3q\, f_B(q)/(2\pi)^3 = n_B = p_F^3/(6\pi^2)$. Given a typical momentum of order $q\sim p_F$, a typical centre-of-mass momentum for a two-body collision is of order p_F even if p is small. So on dimensional grounds one expects $\mathcal{R}_A\sim m|\mathfrak{h}_0|^2p_F^4$. This is much larger than the result found above because it lacks the suppression by p^4/p_F^4. This suppression entered the calculation using the Fermi sea through the squeezing of the q range of integration into the narrow window $p_L<q<p_F$, which does not happen in the absence of Pauli blocking.

4.4 Equilibrium and detailed balance

For initial and final states characterized by single-particle distribution functions the transition rate has the general form

$$\Gamma(\alpha\to\beta)=\int\Xi(\alpha\to\beta)\prod_{i\in\alpha}\mathrm{d}^{3}p_{i}\,f_{i}\prod_{j\in\beta}\mathrm{d}^{3}p_{j}\,(1\pm f_{j})\,,\tag{4.4.1}$$

where $\Xi(\alpha\to\beta)\propto|M(\alpha\to\beta)|^2\delta^4(P_\alpha-P_\beta)$ is the basic underlying squared amplitude for scattering from multiparticle state α to state β and the upper sign applying for bosons and the lower sign for fermions. The rate for the reaction in the opposite direction similarly is

$$\Gamma(\beta\to\alpha)=\int\Xi(\beta\to\alpha)\prod_{j\in\beta}\mathrm{d}^{3}p_{j}\,f_{j}\prod_{i\in\alpha}\mathrm{d}^{3}p_{i}\,(1\pm f_{i})\,,\tag{4.4.2}$$

where $\Xi(\beta\to\alpha)\propto|M(\beta\to\alpha)|^2\delta^4(P_\alpha-P_\beta)$.

Macroscopic systems with many particles tend to evolve towards equilibrium states characterized by 'detailed balance', a condition that says that the distribution functions adjust themselves so that on average every possible reaction runs equally fast in both directions. The idea is that if this were not true then the distribution functions would start to evolve due to some reactions proceeding faster than their reverse reactions. The process continues until there is a balance in all reactions running in either direction.

One might think that the resulting detailed balance condition depends on the details of the reactions because of the appearance in the above of the factors $\Xi(\alpha\to\beta)$ and $\Xi(\beta\to\alpha)$,

but it turns out that the unitarity of the $\mathcal{S}$-matrix relates these in such a way that the difference in rates can be written

$$\Gamma(\alpha \to \beta) - \Gamma(\beta \to \alpha) = \int \Xi(\alpha \to \beta) \prod_{i\in\alpha} \mathrm{d}^3 p_i \prod_{j\in\beta} \mathrm{d}^3 p_j \Big[f_i(1 \pm f_j) - f_j(1 \pm f_i) \Big] , \qquad (4.4.3)$$

for all choices for $|\alpha\rangle$ and $|\beta\rangle$. (Notice that this relies only on unitarity and does *not* rely on assuming the underlying interactions are time-reversal invariant.)

The condition of detailed balance for arbitrary initial and final states therefore requires the distribution functions to satisfy

$$\prod_{i\in\alpha} f_i \prod_{j\in\beta} (1 \pm f_j) = \prod_{i\in\alpha} (1 \pm f_i) \prod_{j\in\beta} f_j \,, \qquad (4.4.4)$$

for all possible collision processes. This can also be written as the condition

$$\prod_{i\in\alpha} \frac{f_i}{1 \pm f_i} = \prod_{j\in\beta} \frac{f_j}{1 \pm f_j} \,, \qquad (4.4.5)$$

which is a kind of conservation law: it states that the quantity $\prod_i f_i/(1 \pm f_i)$ should always remain unchanged in all of the possible kinds of scattering processes that can occur. This conservation law can be written in a more familiar, additive, form by taking the logarithm, since then it says

$$\sum_{i\in\alpha} \log\left(\frac{f_i}{1 \pm f_i}\right) = \sum_{j\in\beta} \log\left(\frac{f_j}{1 \pm f_j}\right) . \qquad (4.4.6)$$

The basic idea of statistical mechanics is that the general solution to condition (4.4.6) is to ask the summand on each side to be a linear combination of all of the additively conserved quantities — *e.g.* energy, E, momentum, $\mathbf{P}$, electric charge, Q, and so on — that hold microscopically for each collision:

$$\log\left(\frac{f_i}{1 \pm f_i}\right) = \beta(-E_p + \mathbf{u}\cdot\mathbf{p} + \mu_Q q_p + \cdots) \,, \qquad (4.4.7)$$

where E_p, $\mathbf{p}$ and q_p are the eigenvalues taken by the conserved quantities E, $\mathbf{P}$ and Q for the single-particle states. β, $\mathbf{u}$ and μ_Q are parameters that are characteristic of the equilibrium state that detailed balance determines.

Solving (4.4.7) for f_i gives the result

$$f_i = \frac{e^{-\beta(E_p - \mathbf{u}\cdot\mathbf{p} - \mu_Q q_p)}}{1 \mp e^{-\beta(E_p - \mathbf{u}\cdot\mathbf{p} - \mu_Q q_p)}} = \frac{1}{e^{\beta(E_p - \mathbf{u}\cdot\mathbf{p} - \mu_Q q_p)} \mp 1} \qquad (4.4.8)$$

which is recognized as the usual thermodynamic distributions — see eqs. (1.6.17) — for bosons and fermions. The quantity $\mathbf{u}$ represents the centre-of-mass velocity of the bath and is usually set to zero by working in the bath's rest frame. Comparison with the thermodynamic result

reveals the interpretation that $\beta = 1/T$ is related to the temperature and μ_Q is the chemical potential for the conserved charge Q (and there can be a separate chemical potential for any additive conserved charge in the system).

Using a chemical potential for the total number of particles, N, is seen in this way to be consistent only if the total number of particles is conserved. This observation plays an important role in later sections, where it is shown for relativistic systems that it is *never* true that interactions exactly preserve the total number of particles.

5 Emergence of classical fields

When discussing fundamental physics an important distinction is often made between elementary particles and fundamental forces. On one hand elementary particles — such as electrons, quarks or neutrinos, say — are normally regarded as the building blocks of matter. On the other hand fundamental forces — such as electromagnetism, gravity or the weak and strong interactions — are regarded as the medium through which the particles interact.

This section argues that this dichotomy is not quite right, however. The more useful split is between bosons and fermions rather than elementary particles and fundamental forces. The above notion of a fundamental force is often built around experience with classical fields, particularly for electromagnetism and gravity since for these the classical theory was discovered first. The present section argues that classical fields are simply a particularly useful limit that arises when particle states become multiply occupied. Because of this the main distinction is between bosons (for which multiply occupied states are possible) and fermions (for which they are not).

To see what is involved, return to the Hamiltonian of (4.1.1) and (4.1.2), but with particles B and C identified so that the process mediated by $H_{\rm int}$ does not change the intial particle's type when particle A is emitted or absorbed, leading to $H = H_{\rm free} + H_{\rm int}$ with:

$$H_{\rm free} = E_0 + \sum_p \Big[\varepsilon_{\scriptscriptstyle A}(p)\, a_p^\star a_p + \varepsilon_{\scriptscriptstyle C}(p)\, c_p^\star c_p\Big] = E_0 + \int \mathrm{d}^3p \Big[\varepsilon_{\scriptscriptstyle A}(p)\, \mathfrak{a}_p^\star \mathfrak{a}_p + \varepsilon_{\scriptscriptstyle C}(p)\, \mathfrak{c}_p^\star \mathfrak{c}_p\Big]\,, \quad (5.0.1)$$

and

$$\begin{aligned} H_{\rm int} &= \sum_{pqk} \Big[g(\mathbf{p},\mathbf{q},\mathbf{k}) a_k^\star c_q^\star c_p + g^*(\mathbf{p},\mathbf{q},\mathbf{k}) c_p^\star c_q a_k\Big]\delta_{p-q-k} \\ &= \int \mathrm{d}^3p\, \mathrm{d}^3q\, \mathrm{d}^3k\, \Big[\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k}) \mathfrak{a}_k^\star \mathfrak{c}_q^\star \mathfrak{c}_p + \mathfrak{g}^*(\mathbf{p},\mathbf{q},\mathbf{k}) \mathfrak{c}_p^\star \mathfrak{c}_q \mathfrak{a}_k\Big]\delta^3(\mathbf{p}-\mathbf{q}-\mathbf{k})\,, \end{aligned} \quad (5.0.2)$$

which uses (4.1.4) when taking the continuum limit. Recall this implies $\mathfrak{g}$ has dimension $(\text{length})^{1/2}$. We ask how the presence of this interaction modifies the energy of states involving multiple C particles.

5.1 Self-energy, UV divergences and renormalization

The goal is to compute the interaction energy the Hamiltonian (5.0.2) implies for states involving two C particles, since this might be expected to reveal a contribution that depends on the presence of more than one particle. We do so using (time-independent) perturbation theory since that is the one general tool at our disposal at this point.

Before doing so this section first provides a preliminary result: the *self-energy* that interactions imply for single-particle states. This is useful as a point of comparison for the two-particle result, since our interest below in §5.2 is on energy shifts whose existence relies on the presence of more than one particle. Along the way the self-energy calculation also provides a first encounter with the phenomenon of ultraviolet (UV) divergences and how they can be dealt with through a process called *renormalization*.

Worked example: single-particle energy shift

To start use the expression for energy shifts coming from time-independent perturbation theory, (3.1.9), which when applied to the (discretely normalized) state $|C(\mathbf{p})\rangle$ gives

$$E(\mathbf{p}) = E^{(0)}(\mathbf{p}) + \delta E^{(1)}(\mathbf{p}) + \delta E^{(2)}(\mathbf{p}) + \cdots \tag{5.1.1}$$

with

$$E^{(0)}(\mathbf{p}) = \varepsilon_C(\mathbf{p})\,, \tag{5.1.2}$$

while

$$\delta E^{(1)}(\mathbf{q}) = (C(\mathbf{p})|H_{\rm int}|C(\mathbf{p})) = 0\,, \tag{5.1.3}$$

because of the particle-A contribution: $\langle 0|a_k|0\rangle = 0$. The leading interaction-induced energy shift therefore comes from the second-order contribution,

$$\delta E^{(2)}(\mathbf{p}) = \sum_N \frac{|(N|H_{\rm int}|C(\mathbf{p}))|^2}{\varepsilon_C(\mathbf{p}) - E^{(0)}_N} = \sum_{k\,\tilde{p}}{}' \frac{|(A(\mathbf{k}), C(\tilde{\mathbf{p}})|H_{\rm int}|C(\mathbf{p}))|^2}{\varepsilon_C(\mathbf{p}) - \varepsilon_C(\tilde{\mathbf{p}}) - \varepsilon_A(\mathbf{k})}\,, \tag{5.1.4}$$

where the prime on the sum indicates the omission of the term with $\mathbf{k} = 0$.

The required matrix element is

$$(A(\mathbf{k}), C(\tilde{\mathbf{p}})|H_{\rm int}|C(\mathbf{p})) = g(\mathbf{p}, \tilde{\mathbf{p}}, \mathbf{k})\, \delta_{p-\tilde{p}-k}\,, \tag{5.1.5}$$

and so

$$\begin{aligned}
\delta E^{(2)}(\mathbf{p}) &= \sum_{k\,\tilde{p}}{}' \frac{|g(\mathbf{p}, \tilde{\mathbf{p}}, \mathbf{k})|^2}{\varepsilon_C(\mathbf{p}) - \varepsilon_C(\tilde{\mathbf{p}}) - \varepsilon_A(\mathbf{k})}\, \delta_{p-\tilde{p}-k} \\
&= \sum_{\tilde{p}}{}' \frac{|g(\mathbf{p}, \tilde{\mathbf{p}}, \mathbf{p}-\tilde{\mathbf{p}})|^2}{\varepsilon_C(\mathbf{p}) - \varepsilon_C(\tilde{\mathbf{p}}) - \varepsilon_A(\mathbf{p}-\tilde{\mathbf{p}})} \\
&= \int \mathrm{d}^3\tilde{p}\, \frac{|\mathfrak{g}(\mathbf{p}, \tilde{\mathbf{p}}, \mathbf{p}-\tilde{\mathbf{p}})|^2}{\varepsilon_C(\mathbf{p}) - \varepsilon_C(\tilde{\mathbf{p}}) - \varepsilon_A(\mathbf{p}-\tilde{\mathbf{p}})}\,,
\end{aligned} \tag{5.1.6}$$

where the last line takes the continuum limit, again using (4.1.4).

To get a feeling for what this expression means, consider the special case where

$$\varepsilon_{C}(\mathbf{p}) \simeq \varepsilon_0 + \frac{\mathbf{p}^2}{2m}\,, \quad \varepsilon_{A}(\mathbf{p}) \simeq |\mathbf{p}| \quad \text{and} \quad \mathfrak{g}(\mathbf{p},\tilde{\mathbf{p}},\mathbf{k}) \simeq \frac{\mathfrak{g}_0}{\sqrt{|\mathbf{k}|}}\,, \tag{5.1.7}$$

which is what actually arises when a_k destroys a relativistic particle like a photon. Then the integral evaluates to

$$\begin{aligned}
\delta E^{(2)}(\mathbf{p}) &= |\mathfrak{g}_{\circ}|^2 \int \frac{\mathrm{d}^3k}{|\mathbf{k}|}\, \frac{1}{\mathbf{p}^2/2m - (\mathbf{p}-\mathbf{k})^2/2m - |\mathbf{k}|} \\
&= 2\pi|\mathfrak{g}_{\circ}|^2 \int_0^\infty k\mathrm{d}k \int_0^\pi \mathrm{d}\theta\, \sin\theta\, \frac{1}{(2pk\cos\theta - k^2)/2m - k} \\
&= 2\pi|\mathfrak{g}_{\circ}|^2 \int_0^\infty \mathrm{d}k \int_{-1}^1 \mathrm{d}x\, \frac{1}{(2px-k)/2m - 1} \\
&= \frac{2\pi m|\mathfrak{g}_{\circ}|^2}{p} \int_0^\infty \mathrm{d}k\, \log\left[\frac{k+2(m-p)}{k+2(m+p)}\right]\,.
\end{aligned} \tag{5.1.8}$$

This last integral diverges at the upper end. But we really do not imagine that we understand everything at all energies, so it is useful to cut off this integral at an upper limit $k = K$, keeping in mind that we should not trust results that depend strongly on K.

Taylor expanding in powers of $\mathbf{p}$ then gives

$$\begin{aligned}
\delta E^{(2)}(p) &= \frac{2\pi m|\mathfrak{g}_{\circ}|^2}{p} \int_0^K \mathrm{d}k\, \log\left[\frac{k+2(m-p)}{k+2(m+p)}\right] \\
&\simeq -2\pi|\mathfrak{g}_{\circ}|^2 \left[4m\log\left(\frac{K+2m}{2m}\right) + \frac{2p^2}{3m} + \frac{p^4}{5m^3} + \mathcal{O}(p^6)\right]\,.
\end{aligned} \tag{5.1.9}$$

Combining this with $\varepsilon_{C}(p)$ allows a physical interpretation:

$$E(p) \simeq \varepsilon_{C}(p) + \delta E^{(2)}(p) \tag{5.1.10}$$

$$\begin{aligned}
&= \left[\varepsilon_0 - 8\pi m|\mathfrak{g}_{\circ}|^2 \log\left(\frac{K+2m}{2m}\right)\right] + \frac{p^2}{2m}\left(1 - \frac{8\pi|\mathfrak{g}_{\circ}|^2}{3}\right) - \frac{2\pi|\mathfrak{g}_{\circ}|^2 p^4}{5m^3} + \mathcal{O}(p^6) \\
&= \varepsilon_{0\,\mathrm{phys}} + \frac{p^2}{2m_{\mathrm{phys}}} - \frac{2\pi|\mathfrak{g}_{\circ}|^2 p^4}{5m^3} + \mathcal{O}(p^6)\,.
\end{aligned} \tag{5.1.11}$$

The physical single-particle energy 'gap' is

$$E(0) = \varepsilon_{0\,\mathrm{phys}} \simeq \varepsilon_0 - 4m\log\left(\frac{K+2m}{2m}\right)\,, \tag{5.1.12}$$

which shows how the dependence on the unknown scale K can be absorbed (or renormalized) into the value of the unknown parameter ε_0. The physical particle mass similarly is given by

$$\frac{1}{m_{\mathrm{phys}}} = \frac{1}{m}\left(1 - \frac{8\pi|\mathfrak{g}_{\circ}|^2}{3}\right)\,, \tag{5.1.13}$$

so m is no longer directly the mass parameter once corrections are included. The real content of the corrections is therefore to add a more complicated momentum-dependence to the single-particle energies, starting for low p with the order p^4/m^3 contribution.

5.2 Two-particle interaction energy

Now back to the main event. Imagine now computing (using time-independent perturbation theory) the energy shift this interaction implies for the energy of two C particles.

Worked example: Two-particle shift

The main result needed from perturbation theory in this case is (3.1.9), which when applied to the (discretely normalized) state $|C(\mathbf{p})C(\mathbf{q})\rangle$ implies

$$E(\mathbf{p},\mathbf{q}) = E^{(0)}(\mathbf{p},\mathbf{q}) + \delta E^{(1)}(\mathbf{p},\mathbf{q}) + \delta E^{(2)}(\mathbf{p},\mathbf{q}) + \cdots \tag{5.2.1}$$

with

$$E^{(0)}(\mathbf{p},\mathbf{q}) = \varepsilon_C(\mathbf{p}) + \varepsilon_C(\mathbf{q})\,, \tag{5.2.2}$$

while

$$\delta E^{(1)}(\mathbf{q},\mathbf{q}) = (C(\mathbf{p}),C(\mathbf{q})|H_{\rm int}|C(\mathbf{p}),C(\mathbf{q})) = 0\,, \tag{5.2.3}$$

because of the particle-A contribution: $\langle 0|a_k|0\rangle = 0$. The leading shift therefore comes from the second-order contribution,

$$\begin{aligned}\delta E^{(2)}(\mathbf{p},\mathbf{q}) &= \sum_N \frac{|(N|H_{\rm int}|C(\mathbf{p}),C(\mathbf{q}))|^2}{\varepsilon_C(\mathbf{p})+\varepsilon_C(\mathbf{q})-E^{(0)}_N} \\ &= \sum_{k,\tilde{p},\tilde{q}}{}' \frac{|(A(\mathbf{k}),C(\tilde{\mathbf{p}}),C(\tilde{\mathbf{q}})|H_{\rm int}|C(\mathbf{p}),C(\mathbf{q}))|^2}{\varepsilon_C(\mathbf{p})+\varepsilon_C(\mathbf{q})-[\varepsilon_C(\tilde{\mathbf{p}})+\varepsilon_C(\tilde{\mathbf{q}})+\varepsilon_A(\mathbf{k})]}\,,\end{aligned} \tag{5.2.4}$$

where the prime on the sum indicates the omission of the term with $(\tilde{\mathbf{p}},\tilde{\mathbf{q}}) = (\mathbf{p},\mathbf{q})$ or – because the particles are indistinguishable – the term with $(\tilde{\mathbf{p}},\tilde{\mathbf{q}}) = (\mathbf{q},\mathbf{p})$.

Assuming all particles are bosons the relevant matrix element is

$$\begin{aligned}(A(\mathbf{k}),C(\tilde{\mathbf{p}}),C(\tilde{\mathbf{q}})|H_{\rm int}|C(\mathbf{p}),C(\mathbf{q})) &= g(p,\tilde{p},k)\,(C(\tilde{\mathbf{q}})|C(\mathbf{q}))\,\delta_{p-\tilde{p}-k} \\ &+g(p,\tilde{q},k)\,(C(\tilde{\mathbf{p}})|C(\mathbf{q}))\,\delta_{p-\tilde{q}-k} + g(q,\tilde{q},k)\,(C(\tilde{\mathbf{p}})|C(\mathbf{p}))\,\delta_{q-\tilde{q}-k} \\ &+g(q,\tilde{p},k)\,(C(\tilde{\mathbf{q}})|C(\mathbf{p}))\,\delta_{q-\tilde{p}-k}\,,\end{aligned} \tag{5.2.5}$$

and so using $(C(\tilde{\mathbf{q}})|C(\mathbf{p})) = \delta_{p\tilde{q}}$ gives

$$\begin{aligned}(A(\mathbf{k}),C(\tilde{\mathbf{p}}),C(\tilde{\mathbf{q}})|H_{\rm int}|C(\mathbf{p}),C(\mathbf{q})) &= g(p,\tilde{p},k)\,\delta_{p-\tilde{p}-k}\,\delta_{q\tilde{q}} \\ &+g(p,\tilde{q},k)\,\delta_{p-\tilde{q}-k}\,\delta_{q\tilde{p}} + g(q,\tilde{q},k)\,\delta_{q-\tilde{q}-k}\,\delta_{p\tilde{p}} + g(q,\tilde{p},k)\,\delta_{q-\tilde{p}-k}\,\delta_{p\tilde{q}}\,.\end{aligned} \tag{5.2.6}$$

Consequently

$$\begin{aligned}|(A(\mathbf{k}),C(\tilde{\mathbf{p}}),C(\tilde{\mathbf{q}})|H_{\rm int}|C(\mathbf{p}),C(\mathbf{q}))|^2 &= |g(p,\tilde{p},k)|^2\,\delta_{p-\tilde{p}-k}\,\delta_{q\tilde{q}} \\ &+|g(p,\tilde{q},k)|^2\,\delta_{p-\tilde{q}-k}\,\delta_{q\tilde{p}} + |g(q,\tilde{q},k)|^2\,\delta_{q-\tilde{q}-k}\,\delta_{p\tilde{p}} + |g(q,\tilde{p},k)|^2\,\delta_{q-\tilde{p}-k}\,\delta_{p\tilde{q}} \\ &+2\mathrm{Re}\Big\{g^*(p,\tilde{p},k)\delta_{p-\tilde{p}-k}\,\delta_{q\tilde{q}}\Big[g(p,\tilde{q},k)\,\delta_{p-\tilde{q}-k}\,\delta_{q\tilde{p}} + g(q,\tilde{q},k)\,\delta_{q-\tilde{q}-k}\,\delta_{p\tilde{p}} + g(q,\tilde{p},k)\,\delta_{q-\tilde{p}-k}\,\delta_{p\tilde{q}}\Big] \\ &+g^*(p,\tilde{q},k)\delta_{p-\tilde{q}-k}\,\delta_{q\tilde{p}}\Big[g(q,\tilde{q},k)\,\delta_{q-\tilde{q}-k}\,\delta_{p\tilde{p}} + g(q,\tilde{p},k)\,\delta_{q-\tilde{p}-k}\,\delta_{p\tilde{q}}\Big] \\ &+g^*(q,\tilde{q},k)\delta_{q-\tilde{q}-k}\,\delta_{p\tilde{p}}\,g(q,\tilde{p},k)\,\delta_{q-\tilde{p}-k}\,\delta_{p\tilde{q}}\Big\}\,.\end{aligned} \tag{5.2.7}$$

Notice that in the cross terms (*i.e.* the last three lines) of this expression there are more deltas than there are sums in eq. (5.2.4), meaning that a delta survives after the sum is performed over $\tilde{p}$, $\tilde{q}$ and k.

When $p = q$ the first cross term vanishes (because $\tilde{p} = \tilde{q} = q$ and the sum omits the cases $(\tilde{p}, \tilde{q}) = (p, q)$ and $(\tilde{p}, \tilde{q}) = (q, p)$). When $p \neq q$ it instead becomes

$$\sum_{k\tilde{p}\,\tilde{q}}{}' \frac{g^*(p,\tilde{p},k)\, g(p,\tilde{q},k)}{\varepsilon_C(p) + \varepsilon_C(q) - \varepsilon_C(\tilde{p}) - \varepsilon_C(\tilde{q}) - \varepsilon_A(k)}\, \delta_{p-\tilde{p}-k}\, \delta_{q\tilde{q}}\, \delta_{p-\tilde{q}-k}\, \delta_{q\tilde{p}} \tag{5.2.8}$$

$$= \frac{|g(p,q,p-q)|^2}{\varepsilon_C(p) - \varepsilon_C(q) - \varepsilon_A(p-q)} \qquad \text{(1st cross term)}\,.$$

The second cross term is

$$\sum_{k\tilde{p}\,\tilde{q}}{}' \frac{g^*(p,\tilde{p},k)\, g(q,\tilde{q},k)}{\varepsilon_C(p) + \varepsilon_C(q) - \varepsilon_C(\tilde{p}) - \varepsilon_C(\tilde{q}) - \varepsilon_A(k)}\, \delta_{p-\tilde{p}-k}\, \delta_{q\tilde{q}}\, \delta_{q-\tilde{q}-k}\, \delta_{p\tilde{p}} \tag{5.2.9}$$

$$= 0 \qquad \text{(2nd cross term)}$$

because $\tilde{p} = p$ and $\tilde{q} = q$ means the only contribution comes from the terms omitted in the sum. Similarly, the third term gives

$$\sum_{k\tilde{p}\,\tilde{q}}{}' \frac{g^*(p,\tilde{p},k)\, g(q,\tilde{p},k)}{\varepsilon_C(p) + \varepsilon_C(q) - \varepsilon_C(\tilde{p}) - \varepsilon_C(\tilde{q}) - \varepsilon_A(k)}\, \delta_{p-\tilde{p}-k}\, \delta_{q\tilde{q}}\, \delta_{q-\tilde{p}-k}\, \delta_{p\tilde{q}} \tag{5.2.10}$$

$$= \sum_{\tilde{p}}{}' \frac{|g(p,\tilde{p},p-\tilde{p})|^2}{\varepsilon_C(p) - \varepsilon_C(\tilde{p}) - \varepsilon_A(p-\tilde{p})}\, \delta_{pq} \qquad \text{(3rd cross term)}$$

while the fourth term is

$$\sum_{k\tilde{p}\,\tilde{q}}{}' \frac{g^*(p,\tilde{q},k)\, g(q,\tilde{q},k)}{\varepsilon_C(p) + \varepsilon_C(q) - \varepsilon_C(\tilde{p}) - \varepsilon_C(\tilde{q}) - \varepsilon_A(k)}\, \delta_{p-\tilde{q}-k}\, \delta_{q\tilde{p}}\, \delta_{q-\tilde{q}-k}\, \delta_{p\tilde{p}} \tag{5.2.11}$$

$$= \sum_{\tilde{q}}{}' \frac{|g(p,\tilde{q},p-\tilde{q})|^2}{\varepsilon_C(q) - \varepsilon_C(\tilde{q}) - \varepsilon_A(p-\tilde{q})}\, \delta_{pq} \qquad \text{(4th cross term)}$$

and

$$\sum_{k\tilde{p}\,\tilde{q}}{}' \frac{g^*(p,\tilde{q},k)\, g(q,\tilde{p},k)}{\varepsilon_C(p) + \varepsilon_C(q) - \varepsilon_C(\tilde{p}) - \varepsilon_C(\tilde{q}) - \varepsilon_A(k)}\, \delta_{p-\tilde{q}-k}\, \delta_{q\tilde{p}}\, \delta_{q-\tilde{p}-k}\, \delta_{p\tilde{q}}$$

$$= 0 \qquad \text{(5th cross term)}$$

because $\tilde{p} = q$ and $\tilde{q} = p$ is excluded in the sum. Finally the sixth cross term is

$$\sum_{k\tilde{p}\,\tilde{q}}{}' \frac{g^*(q,\tilde{q},k)\, g(q,\tilde{p},k)}{\varepsilon_C(p) + \varepsilon_C(q) - \varepsilon_C(\tilde{p}) - \varepsilon_C(\tilde{q}) - \varepsilon_A(k)}\, \delta_{q-\tilde{q}-k}\, \delta_{p\tilde{p}}\, \delta_{q-\tilde{p}-k}\, \delta_{p\tilde{q}}$$

$$= \frac{|g(q,p,q-p)|^2}{\varepsilon_C(q) - \varepsilon_C(p) - \varepsilon_A(q-p)} \qquad \text{(6th cross term).} \tag{5.2.12}$$

Using these in (5.2.4) then gives

$$\begin{aligned}\delta E^{(2)}(\mathbf{p},\mathbf{q}) &= \sum_{k\tilde{p}\,\tilde{q}}{}' \frac{|(A(k),C(\tilde{p}),C(\tilde{q})|H_{\rm int}|C(p),C(q))|^2}{\varepsilon_C(p)+\varepsilon_C(q)-[\varepsilon_C(\tilde{p})+\varepsilon_C(\tilde{q})+\varepsilon_A(k)]} \\ &= \sum_{\tilde{p}}{}' \frac{|g(p,\tilde{p},p-\tilde{p})|^2}{\varepsilon_C(p)-\varepsilon_C(\tilde{p})-\varepsilon_A(p-\tilde{p})} + \sum_{\tilde{q}}{}' \frac{|g(p,\tilde{q},p-\tilde{q})|^2}{\varepsilon_C(p)-\varepsilon_C(\tilde{q})-\varepsilon_A(p-\tilde{q})} \\ &\quad + \sum_{\tilde{q}}{}' \frac{|g(q,\tilde{q},q-\tilde{q})|^2}{\varepsilon_C(q)-\varepsilon_C(\tilde{q})-\varepsilon_A(q-\tilde{q})} + \sum_{\tilde{p}}{}' \frac{|g(q,\tilde{p},q-\tilde{p})|^2}{\varepsilon_C(q)-\varepsilon_C(\tilde{p})-\varepsilon_A(q-\tilde{p})} \\ &\quad + 2\mathrm{Re}\left\{ \frac{|g(p,q,p-q)|^2}{\varepsilon_C(p)-\varepsilon_C(q)-\varepsilon_A(p-q)} + \frac{|g(q,p,q-p)|^2}{\varepsilon_C(q)-\varepsilon_C(p)-\varepsilon_A(q-p)} \right. \\ &\quad \left. + \sum_{\tilde{p}}{}' \frac{|g(p,\tilde{p},p-\tilde{p})|^2}{\varepsilon_C(p)-\varepsilon_C(\tilde{p})-\varepsilon_A(p-\tilde{p})}\,\delta_{pq} + \sum_{\tilde{q}}{}' \frac{|g(p,\tilde{q},p-\tilde{q})|^2}{\varepsilon_C(q)-\varepsilon_C(\tilde{q})-\varepsilon_A(p-\tilde{q})}\,\delta_{pq} \right\},\end{aligned} \tag{5.2.13}$$

which after grouping terms becomes

$$\begin{aligned}\delta E^{(2)}(\mathbf{p},\mathbf{q}) &= \sum_{\tilde{p}}{}' \frac{2|g(p,\tilde{p},p-\tilde{p})|^2}{\varepsilon_C(p)-\varepsilon_C(\tilde{p})-\varepsilon_A(p-\tilde{p})}(1+\delta_{pq}) + \sum_{\tilde{q}}{}' \frac{2|g(q,\tilde{q},q-\tilde{q})|^2}{\varepsilon_C(q)-\varepsilon_C(\tilde{q})-\varepsilon_A(q-\tilde{q})}(1+\delta_{pq}) \\ &\quad + \frac{2|g(p,q,p-q)|^2}{\varepsilon_C(p)-\varepsilon_C(q)-\varepsilon_A(p-q)} + \frac{2|g(q,p,q-p)|^2}{\varepsilon_C(q)-\varepsilon_C(p)-\varepsilon_A(q-p)}\,,\end{aligned} \tag{5.2.14}$$

where the prime on the sum excludes the case $\tilde{p}=p$.

Comparing (5.2.14) with (5.1.6) shows that the first line consists of the single-particle energy shift for each particle, with the δ_{pq} contribution reproducing the additional factor of $1+N=2$ expected for identical bosons with a doubly occupied ($N=2$) initial state. This reveals the interaction energy to be the second line of (5.2.14):

$$\begin{aligned}\delta E^{(2)}_{\rm int}(\mathbf{p},\mathbf{q}) &= \frac{2|g(p,q,p-q)|^2}{\varepsilon_C(p)-\varepsilon_C(q)-\varepsilon_A(p-q)} + \frac{2|g(q,p,q-p)|^2}{\varepsilon_C(q)-\varepsilon_C(p)-\varepsilon_A(q-p)} \\ &= \frac{(2\pi)^3}{\mathcal{V}}\left[\frac{2|\mathfrak{g}(p,q,p-q)|^2}{\varepsilon_C(p)-\varepsilon_C(q)-\varepsilon_A(p-q)} + \frac{2|\mathfrak{g}(q,p,q-p)|^2}{\varepsilon_C(q)-\varepsilon_C(p)-\varepsilon_A(q-p)}\right].\end{aligned} \tag{5.2.15}$$

This is the main result of the two-particle energy-shift calculation.

Now comes the point: in some circumstances eq. (5.2.15) turns out to resemble the energy shift produced if the C particles were to couple to a classical field. Consider, for example, the situation where the A particle is gapless, such as if it has a photon-like single-particle energy $\varepsilon_A(\mathbf{p})=|\mathbf{p}|$. In this case low-momentum modes cost arbitrarily little energy. Relativistic descriptions of massless particles (like photons) often have this dispersion relation, and in addition typically have emission amplitudes that satisfy $\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k}) \propto 1/\sqrt{\varepsilon_A(\mathbf{k})} = 1/\sqrt{|\mathbf{k}|}$. Suppose also the recoil of the emitting particle in response to the emission of an A particle can be neglected. This is ensured if $\varepsilon_C(\mathbf{p}) \simeq \varepsilon_0 + \mathbf{p}^2/2m$ with m very large.

Using $\mathfrak{g}(\mathbf{p},\mathbf{q},\mathbf{k}) \simeq \mathfrak{g}_0/\sqrt{|\mathbf{k}|}$ in eq. (5.2.15) gives

$$\begin{aligned}\delta E^{(2)}_{\rm int}(\mathbf{p},\mathbf{q}) &\simeq \frac{(2\pi)^3}{\mathcal{V}}\,\frac{2|\mathfrak{g}_0|^2}{|\mathbf{p}-\mathbf{q}|}\left[\frac{1}{(\mathbf{p}^2-\mathbf{q}^2)/2m-|\mathbf{p}-\mathbf{q}|}+\frac{1}{(\mathbf{q}^2-\mathbf{p}^2)/2m-|\mathbf{p}-\mathbf{q}|}\right]\\ &\simeq -\frac{(2\pi)^3}{\mathcal{V}}\,\frac{4|\mathfrak{g}_0|^2}{|\mathbf{p}-\mathbf{q}|^2}\,,\end{aligned} \tag{5.2.16}$$

where the last line assumes m is so large that $\mathbf{p}^2/2m$ and $\mathbf{q}^2/2m$ are negligible compared with $|\mathbf{p}-\mathbf{q}|$. It is this result that has the same form as would the energy shift due to the interaction of C particles with a classical field.

To see why, suppose a classical field $\Phi(\mathbf{x})$ satisfies the Poisson equation, such as does the electrostatic potential:

$$\nabla^2\Phi = g\,n(\mathbf{x})\,, \tag{5.2.17}$$

for some constant g, where $n(\mathbf{x})$ is the number density of particles of type C. Following the same steps as in electrostatics, this has solution

$$\Phi(\mathbf{x}) = \frac{g}{4\pi}\int \mathrm{d}^3y\,\frac{n(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,, \tag{5.2.18}$$

and so leads to an interaction energy of the form

$$\delta E_{\rm field} = -\frac{g^2}{8\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\frac{n(\mathbf{x})\,n(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} = -\frac{g^2}{2}\int\frac{\mathrm{d}^3p}{(2\pi)^3}\,\frac{n(\mathbf{p})\,n(-\mathbf{p})}{\mathbf{p}^2}\,. \tag{5.2.19}$$

Here the last equality converts to momentum space using

$$n(\mathbf{x}) = \int\frac{\mathrm{d}^3p}{(2\pi)^3}\,n(\mathbf{p})\,\exp[i\mathbf{p}\cdot\mathbf{x}]\,. \tag{5.2.20}$$

To make contact with (5.2.16) use the usual Schrödinger expression for probability density $n(\mathbf{x}) = \psi^*(\mathbf{x})\psi(\mathbf{x})$ (rederived below) to write $n(\mathbf{x})$ for two momentum eigenstates $\psi_{\mathbf{p}}(\mathbf{x})$ as

$$n(\mathbf{x}) = \psi^*_{\mathbf{p}}(\mathbf{x})\psi_{\mathbf{q}}(\mathbf{x}) = \frac{1}{\mathcal{V}}\,\exp[i(\mathbf{q}-\mathbf{p})\cdot\mathbf{x}] \tag{5.2.21}$$

and so

$$n(\mathbf{k}) = \int \mathrm{d}^3x\,n(\mathbf{x})\exp[-i\mathbf{k}\cdot\mathbf{x}] = \frac{(2\pi)^3}{\mathcal{V}}\,\delta^3(\mathbf{k}-\mathbf{q}+\mathbf{p})\,. \tag{5.2.22}$$

Using this in the second of eqs. (5.2.19) then gives – using $\delta^3(\mathbf{0}) = \mathcal{V}/(2\pi)^3$,

$$\delta E_{\rm field} = -\frac{g^2}{2}\left[\frac{(2\pi)^3}{\mathcal{V}}\right]^2\frac{\delta^3(\mathbf{0})}{|\mathbf{p}-\mathbf{q}|^2} = -\frac{1}{2}\,\frac{(2\pi)^3}{\mathcal{V}}\,\frac{g^2}{|\mathbf{p}-\mathbf{q}|^2}\,, \tag{5.2.23}$$

in agreement with (5.2.16).

Why should interacting quantum systems sometimes resemble interactions mediated by classical fields? The next section explores this in more detail, arguing that classical fields

provide approximate descriptions of states containing a very large number of particles. This is only possible for bosons because multiple occupation of states is impossible for fermions. Furthermore, we saw in §4.2 that for bosons the phenomenon of stimulated emission favours multiply occupied states when interactions allow the emission of a boson since then emitted particles prefer to pile into states that are already occupied. Getting a large number of emitted quanta from a static source requires the energy cost for producing each boson should be very low (as can be the case if they are gapless). The source, on the other hand, should also not dramatically recoil when the bosons are emitted, so that it can just sit there long enough for enormous numbers of quanta to accumulate.

5.3 Coherent states and classical fields

We next quantify more carefully the kinds of states to which repeated emission of gapless bosons might lead. For a boson dispersion relation of the form $\varepsilon_{A}(\mathbf{p}) = |\mathbf{p}|$ the gapless bosons have zero momentum: $\varepsilon_{A}(0) = 0$. To study how gapless bosons respond when multiply emitted we focus on that part of the interaction (5.0.2) involving only gapless bosons:

$$H_{\rm int} \ni \sum_{p} \Big[g(\mathbf{p},\mathbf{p},0) a_0^\star c_p^\star c_p + g^*(\mathbf{p},\mathbf{p},0) c_p^\star c_p a_0 \Big] \,. \tag{5.3.1}$$

Up to this point the implications of the interactions in $H = H_{\rm free} + H_{\rm int}$ have been worked out by perturbing in $H_{\rm int}$. Can one do better than perturbation theory?

It turns out you can. To see how, for simplicity temporarily suppress the mode index 'p' in c_p and consider a Hamiltonian of the form $H = H_0 + H_1$ with

$$H_0 = \omega\, a^\star a + \varepsilon\, c^\star c \quad \text{and} \quad H_1 = g\, c^\star c\, a + g^*\, c^\star c\, a^\star \,, \tag{5.3.2}$$

where all particles are bosons and g, ω and ε are regarded as known couplings and single-particle energies, respectively. We assume (as usual) both ω and ε are real and positive and seek the exact energy eigenstates of H, which are generically denoted $|\Psi\rangle$.

Because H only involves c through the combination $c^\star c$ in the C-particle sector the eigenstates are the usual Fock states obtained by acting with $(c^\star)^N$ on a ground state and contain a definite number of particles:

$$|\Psi\rangle = |N\,, \alpha_{N}\rangle \,, \quad \text{where} \quad c^\star c |N\,, \alpha_{N}\rangle = N |N\,, \alpha_{N}\rangle \,, \tag{5.3.3}$$

where the number of C particles is given by the occupation number N. As usual $N = 0, 1, 2, \cdots$ and states with different values of N are related by

$$c|N\,, \alpha_{N}\rangle = \sqrt{N}\, |N-1\,, \alpha_{N}\rangle \quad \text{and} \quad c^\star |N\,, \alpha_{N}\rangle = \sqrt{N+1}\, |N+1\,, \alpha_{N}\rangle \,. \tag{5.3.4}$$

What is the structure of $|\Psi\rangle$ in the sector of A particles? Consider now the action of H *without* assuming H_1 is negligible relative to H_0:

$$H|N\,, \alpha_{N}\rangle = \Big[N\,\varepsilon + \omega\, a^\star a + N(g\, a + g^* a^\star \rangle \Big] |N\,, \alpha_{N}\rangle \,. \tag{5.3.5}$$

Because a does not commute with $a^\star a$ the eigenstates cannot be Fock states with a definite number of A particles.

To identify the eigenstates and eigenvalues define a new operator $b := a - \alpha_N$ where α_N is a constant whose value is to be determined. Because α_N is a constant this new operator satisfies the same algebra as does a, so

$$[b\,,b^\star] = [a\,,a^\star] = 1\,, \tag{5.3.6}$$

and so is a new type of destruction operator. In terms of b the Hamiltonian acting on $|\Psi\rangle$ is

$$\begin{aligned} H|N\,,\alpha_N\rangle &= \Big[N\,\varepsilon + \omega\, a^\star a + N(g\,a + g^* a^\star)\Big]|N\,,\alpha_N\rangle \\ &= \Big[N\,\varepsilon + \omega\,(b^\star + \alpha_N^*)(b+\alpha_N) + N(g\,b + g^* b^\star + g\alpha_N + g^*\alpha_N^*)\Big]|N\,,\alpha_N\rangle \\ &= \Big[N\,\varepsilon + \omega\, b^\star b + (\omega\alpha_N + g^* N)b^\star + (\omega\alpha_N^* + gN)b \\ &\qquad\qquad +\omega\alpha_N^*\alpha_N + N(g\alpha_N + g^*\alpha_N^*)\Big]|N\,,\alpha_N\rangle\,. \end{aligned} \tag{5.3.7}$$

Here comes the main point: if we choose

$$\alpha_N = -\frac{g^* N}{\omega}\,, \tag{5.3.8}$$

(we assume $\omega > 0$) then the action of H on $|N\,,\alpha_N\rangle$ simplifies to

$$\begin{aligned} H|N\,,\alpha_N\rangle &= \Big[N\,\varepsilon + \omega\, b^\star b + \omega\alpha_N^*\alpha_N + N(g\alpha_N + g^*\alpha_N^*)\Big]|N\,,\alpha_N\rangle \\ &= \left[N\,\varepsilon + \omega\, b^\star b - \frac{N^2|g|^2}{\omega}\right]|N\,,\alpha_N\rangle\,, \end{aligned} \tag{5.3.9}$$

which has the usual harmonic oscillator form (since b satisfies (5.3.6) and there are no longer any terms linear in the creation or destruction operators).

For any fixed N the ground state in the A-particle sector therefore is the state satisfying

$$b|N\,,\alpha_N\rangle = 0 \quad \text{and so} \quad a|N\,,\alpha_N\rangle = \alpha_N|N\,,\alpha_N\rangle\,. \tag{5.3.10}$$

Excited states in the A-particle sector are found (as usual) by acting repeatedly with $b^\star$: that is, if $|N\,,(\alpha_N,n)\rangle := (b^\star)^n|N\,,\alpha_N\rangle$ then

$$H|N\,,(\alpha_N,n)\rangle = \left[N\,\varepsilon + \omega\, n - \frac{N^2|g|^2}{\omega}\right]|N\,,(\alpha_N,n)\rangle\,. \tag{5.3.11}$$

The state $|(\alpha_N,n)\rangle$ is sometimes called an 'Agarwal' state.

This shows that the excited states involve a spectrum of two types of non-interacting particles with single-particle energies ε and ω, whose occupation numbers are respectively given by N and n. When $N \neq 0$ the ground state in the A-particle sector has acquired an energy

$$E_N = -\frac{N^2|g|^2}{\omega}\,, \tag{5.3.12}$$

which because of its N-dependence can be regarded as a type of interaction energy for the C-type particles.

Although the A-particle sector has an interpretation in terms of particles created by $b^\star$, the eigenstates in this sector do not have a definite number of the original A-particles created by $a^\star$. This is simplest to see for the ground state defined by (5.3.10), which is an eigenstate of the destruction operator a with complex eigenvalue α_N. The properties of these states are worth exploring because they provide a good approximation to a classical field configuration within quantum field theory (a connection that is made more explicitly in the section on quantum electrodynamics below). In this way of thinking the energy shift found in (5.3.12) is the two-body interaction energy of the source particles (whose number is counted by N) that arises due to the intervening A-particle field.

An eigenstate of a destruction operator with a nonzero eigenvalue is called a *coherent state*, and the above argument shows that they can be expected to arise whenever bosons can be emitted and absorbed by a large number of sources. Properties of coherent states can be explicitly computed by relating them to the basis of original Fock states, $|n\rangle$, created and destroyed by $a^\star$ and a. Given that $a|n\rangle = \sqrt{n}|n-1\rangle$ it follows that the state

$$|\alpha\rangle := e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \tag{5.3.13}$$

does the job, since

$$a|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{(n-1)!}} |n-1\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^{n+1}}{\sqrt{n!}} |n\rangle = \alpha|\alpha\rangle \,. \tag{5.3.14}$$

The prefactor ensures the normalization of the state is

$$\langle\alpha|\alpha\rangle = e^{-|\alpha|^2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\alpha^n (\alpha^*)^m}{\sqrt{n!\, m!}} \langle m|n\rangle = e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} = 1 \,, \tag{5.3.15}$$

which uses $\langle m|n\rangle = \delta_{mn}$ and $\sum_{n=0}^{\infty} x^n/n! = e^x$.

States with different values of α are *not* orthogonal, since

$$\begin{aligned} \langle\beta|\alpha\rangle &= e^{-(|\alpha|^2+|\beta|^2)/2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\alpha^n (\beta^*)^m}{\sqrt{n!\, m!}} \langle m|n\rangle = e^{-(|\alpha|^2+|\beta|^2)/2} \sum_{n=0}^{\infty} \frac{(\alpha\beta^*)^n}{n!} \\ &= e^{-(|\alpha|^2+|\beta|^2-2\alpha\beta^*)/2} \,, \end{aligned} \tag{5.3.16}$$

but they do satisfy a completeness relation,

$$\frac{1}{\pi} \int \mathrm{d}\alpha \mathrm{d}\alpha^* |\alpha\rangle\langle\alpha| = 1 \,, \tag{5.3.17}$$

and so are called *over-complete*.

The probability of finding a specific number of the original A particles in a coherent state $|\alpha\rangle$ is given by

$$P_n = \Big|\langle n|\alpha\rangle\Big|^2 = e^{-|\alpha|^2}\,\frac{|\alpha|^{2n}}{n!}\,, \tag{5.3.18}$$

which is a Poisson distribution, with mean

$$\overline{n} := \langle\alpha|\,a^\star a\,|\alpha\rangle = \sum_{n=0}^{\infty} n\Big|\langle n|\alpha\rangle\Big|^2 = \sum_{n=0}^{\infty} nP_n = e^{-|\alpha|^2}\sum_{n=1}^{\infty}\frac{|\alpha|^{2n}}{(n-1)!} = |\alpha|^2\,. \tag{5.3.19}$$

The variance of this distribution is

$$\begin{aligned}(\Delta n)^2 \,:=\, \overline{(n-\overline{n})^2} = \overline{n^2} - \overline{n}^2 &= -|\alpha|^4 + e^{-|\alpha|^2}\sum_{n=1}^{\infty}\frac{n|\alpha|^{2n}}{(n-1)!}\\ &=\, -|\alpha|^4 + e^{-|\alpha|^2}\sum_{n=1}^{\infty}\frac{|\alpha|^{2n}}{(n-1)!} + e^{-|\alpha|^2}\sum_{n=2}^{\infty}\frac{|\alpha|^{2n}}{(n-2)!}\\ &=\, |\alpha|^2 = \overline{n}\,,\end{aligned} \tag{5.3.20}$$

where the second line follows from the first by writing $n = 1 + (n-1)$. This shows that although a coherent state does not contain a fixed number of A particles (since it is not an eigenstate of $a^\star a$) the uncertainty in the number of A-particles is $\Delta n = \sqrt{\overline{n}}$, and so for $\overline{n} \gg 1$ the fractional uncertainty $\Delta n/\overline{n} = 1/\sqrt{\overline{n}}$ tends to zero.

This variance calculation also illustrates the sense with which coherent states describe 'classical' field configurations. They are classical inasmuch as the failure of $a^\star$ and a to commute can be regarded as an effect suppressed by a power of $1/\overline{n}$. To make this more precise consider the expectation values of $aa^\star$ and $a^\star a$ in a coherent state. Since $[\,a\,,a^\star] = 1$ it follows that

$$\langle\alpha|\,a\,a^\star|\alpha\rangle = \langle\alpha|\,a^\star a\,+1\,|\alpha\rangle = |\alpha|^2 + 1 = \overline{n} + 1\,, \tag{5.3.21}$$

and so

$$\langle\alpha|\,a\,a^\star|\alpha\rangle = \langle\alpha|\,a^\star a\,|\alpha\rangle\left[1 + \mathcal{O}\left(\frac{1}{\overline{n}}\right)\right]. \tag{5.3.22}$$

Once $\overline{n} \gg 1$ the cost of replacing the quantum operators a and $a^\star$ with the classical numbers α and α^* is only a relative error of order $1/\overline{n}$. In particular, coherent states for specific momentum eigenstates

$$a_p|\alpha_q) = e^{-|\alpha|^2/2}\sum_{n_q=0}^{\infty}\frac{\alpha^{n_q}}{\sqrt{n_q!}}\,a_p\,|n_q) = \alpha_q|\alpha_q\rangle\,\delta_{pq} \tag{5.3.23}$$

are related to classical plane waves inasmuch as $(\alpha_q|a_p|\alpha_q) = \alpha_q\,\delta_{pq}$ implies

$$\sum_p\,(\alpha_q|a_p|\alpha_q)\,\exp[i\mathbf{p}\cdot\mathbf{x}] = \alpha_q\,\exp[i\mathbf{q}\cdot\mathbf{x}]\,. \tag{5.3.24}$$

If having large $\bar{n}$ is the classical limit, how does one arrange $\bar{n}$ to become large? The answer to this comes from $\bar{n} = |\alpha_N|^2$, where α_N is given in terms of parameters in the Hamiltonian by eq. (5.3.8), which states $|\alpha_N| = |g|N/\omega$. This shows that large $\bar{n}$ is driven by large N, large g and/or small ω. Large g makes each C particle more efficient at producing A particles, and more C particles (large N) produce more A particles. Because ω gives the energy cost of producing each A particle, making ω small increases $\bar{n}$ by making each A quantum cheaper to produce.

6 Locality

So far all example Hamiltonians considered have been built from small numbers of creation and annihilation operators that are labelled by particle quantum numbers like $\mathbf{p}$. This section describes the special role played by a fields defined as functions of position, and why they are encountered so frequently when describing physical systems.

6.1 Factorization and cluster decomposition

Position-space fields are useful because they allow the systematic incorporation of a fundamental physical property when formulating the Hamiltonian for particular systems. The property in question is locality (which is closely related to another property called 'cluster decomposition').

A basic property of probability states that the joint probability of statistically independent events is the product of the probability for each of the events separately. That is if a coin has a probability p (with $0 \leq p \leq 1$) of coming up heads in any one flip, then when flipped twice the probability of getting heads twice is p^2; of getting tails twice is $(1-p)^2$; and the probability of getting heads followed by tails is $p(1-p)$. The probability of getting heads in every one of a sequence of N flips is p^N.

It happens that this same property is usually also true for quantum systems that are widely separated in space at a given time.[8] That is, if a reaction $A \to A'$ happens in a system prepared on earth and $B \to B'$ for a system simultaneously prepared on the Andromeda galaxy, the amplitude for the transitions for these regarded as a joint system factorizes:

$$\mathcal{A}(A \to A' \text{ and } B \to B') = \mathcal{A}(A \to A')\,\mathcal{A}(B \to B') \tag{6.1.1}$$

This factorization ensures that the probability of simultaneous events in A and B also factorize, as they would if they were statistically independent:

$$\begin{aligned} P(A \to A' \text{ and } B \to B') &= \Big|\mathcal{A}(A \to A' \text{ and } B \to B')\Big|^2 = |\mathcal{A}(A \to A')|^2\,|\mathcal{A}(B \to B')|^2 \\ &= P(A \to A')\,P(B \to B')\,. \end{aligned} \tag{6.1.2}$$

[8] Here widely separated means too far apart for signals moving at most at the speed of light to get from one to the other.

This factorization condition has two logical components. First, the initial wave-function for the states themselves should come as a product, $\Psi(A \text{ and } B) = \psi_A(A)\,\psi_B(B)$, and (second) this factorized form should be maintained as time evolves (at least so long as signals cannot propagate between A and B to allow them to begin to correlate with one another).

Consider each of these conditions in turn. The factorization of the initial state itself can clearly be thwarted, such as by preparing the two systems in a correlated state, such as the state produced by an earlier EPR (Einstein-Podolsky-Rosen) experiment. In such an experiment a pair of spinning particles might be produced by the decay of a spinless particle, say, ensuring that the spins of the two particles are correlated with one another (since angular-momentum conservation ensures they must sum to zero). This correlation can persist even after the daughter particles separate to enormous distances, such as between earth and the Andromeda galaxy.

The content of cluster decomposition is that it is an experimental fact that the ground state of most systems are observed to factorize in the way required by cluster decomposition unless correlations are painstakingly arranged for the initial state. This point proves to be important for phenomena like spontaneous symmetry breaking described in later sections.

It is the second condition — preservation of any initial factorization as time evolves — that is the main focus of this section, because it imposes conditions on the form that is allowed by any system's Hamiltonian. To see how this works recall that within quantum mechanics time evolution is accomplished by a unitary transformation of the form

$$U(t,t_0) = \exp\Big[-iH(t-t_0)\Big]\,. \tag{6.1.3}$$

Preservation of factorization of states with time evolution basically requires this evolution operator should also factorize. Because clustering requires factorization for systems separated in space this schematically means $U(t,t_0)$ should arise as a product:

$$U(t,t_0) = \prod_{\mathbf{x}} U_{\mathbf{x}}(t,t_0)\,, \tag{6.1.4}$$

and because of (6.1.3) this becomes a condition for the Hamiltonian, which should schematically come as a sum of terms for each spatial position:

$$H = \int \mathrm{d}^3x\; \mathcal{H}(\mathbf{x})\,, \tag{6.1.5}$$

a condition called 'locality'.

Because locality plays such a central role in what follows, we record for future use what it implies for the useful expressions (3.2.22) for the perturbative expression for the S-matrix. This now becomes

$$\mathcal{S} \simeq I + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} \mathrm{d}^4x_1 \cdots \int_{-\infty}^{\infty} \mathrm{d}^4x_n\; T\Big[\mathcal{H}_{\mathrm{int},I}(x_1)\cdots\mathcal{H}_{\mathrm{int},I}(x_n)\Big]\,. \tag{6.1.6}$$

Having integrals over all four coordinates helps immensely when trying to identify circumstances where expressions like (6.1.6) are consistent with special relativity.

The locality condition (6.1.5) makes it convenient to work with fields defined in position space rather than using creation operators defined in momentum space:

$$\Phi(\mathbf{x}) = \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\, \mathfrak{a}_{\mathbf{p}}\, e^{i\mathbf{p}\cdot\mathbf{x}} \quad \text{and} \quad \Phi^\star(\mathbf{x}) = \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\, \mathfrak{a}^\star_{\mathbf{p}}\, e^{-i\mathbf{p}\cdot\mathbf{x}}\,. \tag{6.1.7}$$

The normalization of these last expressions is chosen so that the commutation relations $[\mathfrak{a}_{\mathbf{p}}\,,\mathfrak{a}_{\mathbf{q}}] = 0$ and $[\mathfrak{a}_{\mathbf{p}}\,,\mathfrak{a}^\star_{\mathbf{q}}] = \delta^3(\mathbf{p}-\mathbf{q})$ imply

$$\Big[\Phi(\mathbf{x})\,,\Phi(\mathbf{y})\Big] = 0\,, \tag{6.1.8}$$

and

$$\Big[\Phi(\mathbf{x})\,,\Phi^\star(\mathbf{y})\Big] = \frac{1}{(2\pi)^3}\int \mathrm{d}^3p\,\mathrm{d}^3q\,\Big[\mathfrak{a}_{\mathbf{p}}\,,\mathfrak{a}^\star_{\mathbf{q}}\Big] e^{i(\mathbf{p}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{y})} = \delta^3(\mathbf{x}-\mathbf{y})\,. \tag{6.1.9}$$

Locality can then be built in from the get-go by building $\mathcal{H}(\mathbf{x})$ from polynomials of $\Phi(\mathbf{x})$, $\Phi^\star(\mathbf{x})$ and their derivatives, such as

$$\mathcal{H}(\mathbf{x}) = f(\mathbf{x})\Phi^\star(\mathbf{x})\Phi(\mathbf{x}) + g(\mathbf{x})\nabla\Phi^\star\cdot\nabla\Phi + \cdots\,, \tag{6.1.10}$$

for some coefficients $f(\mathbf{x})$ and $g(\mathbf{x})$ and so on. (For translation-invariant systems these coefficients must be $\mathbf{x}$-independent, but not otherwise.) With this kind of construction the Hamiltonian becomes

$$\begin{aligned} H &= \int \mathrm{d}^3x\, \mathcal{H}(\mathbf{x}) \\ &= \int \mathrm{d}^3x\, \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\,\frac{\mathrm{d}^3q}{(2\pi)^{3/2}}\,\frac{\mathrm{d}^3k}{(2\pi)^3}\,\Big[\mathfrak{f}(\mathbf{k}) + \mathbf{p}\cdot\mathbf{q}\,\mathfrak{g}(\mathbf{k})\Big]\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{q}} e^{i(\mathbf{k}+\mathbf{q}-\mathbf{p})\cdot\mathbf{x}} + \cdots \\ &= \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\,\frac{\mathrm{d}^3q}{(2\pi)^{3/2}}\Big[\mathfrak{f}(\mathbf{p}-\mathbf{q}) + \mathbf{p}\cdot\mathbf{q}\,\mathfrak{g}(\mathbf{p}-\mathbf{q})\Big]\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{q}} + \cdots\,, \end{aligned} \tag{6.1.11}$$

where

$$f(\mathbf{x}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\,\mathfrak{f}(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}} \quad \text{and} \quad g(\mathbf{x}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\,\mathfrak{g}(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}}\,. \tag{6.1.12}$$

The special case of a translation-invariant system corresponds to $f(\mathbf{x}) = f_0$ independent of $\mathbf{x}$ and so $\mathfrak{f}(\mathbf{k}) = (2\pi)^3 f_0\,\delta^3(\mathbf{k})$ and $\mathfrak{g}(\mathbf{k}) = (2\pi)^3 g_0\,\delta^3(\mathbf{k})$, in which case

$$H = \int \mathrm{d}^3p\,\Big[f_0 + g_0\,\mathbf{p}^2\Big]\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{p}} + \cdots\,. \tag{6.1.13}$$

As usual, the signature of translation invariance in Fourier space is the presence of only momentum-conserving interactions and spatial derivatives appear as powers of momenta.

With these observations in hand we have the tools to write down the Hamiltonians appropriate for various well-known physical systems.

6.2 The Schrödinger field and second quantization

To start with consider a system of non-interacting non-relativistic particles having single-particle energy $\varepsilon(\mathbf{p}) = \varepsilon_0 + \mathbf{p}^2/(2m)$. The Hamiltonian for this system is the one discussed earlier,

$$H_{\rm free} = E_0 + \int \mathrm{d}^3p \left[\varepsilon_0 + \frac{\mathbf{p}^2}{2m}\right] \mathfrak{a}^\star_{\mathbf{p}} \mathfrak{a}_{\mathbf{p}} \,. \tag{6.2.1}$$

Is this Hamiltonian a local Hamiltonian? If so, what is the Hamiltonian density, $\mathcal{H}$, as a function of $\Phi(\mathbf{x})$ defined in (6.1.7)? Comparing with (6.1.13) shows that (6.2.1) is indeed a special case of a local form, with Hamiltonian density given by

$$\mathcal{H} = \rho_0 + \varepsilon_0 \, \Phi^\star \Phi + \frac{1}{2m} \nabla\Phi^\star \cdot \nabla\Phi \,, \tag{6.2.2}$$

where ρ_0 is the ground-state energy density defined in terms of E_0 by[9]

$$E_0 = \int \mathrm{d}^3x \; \rho_0 \,. \tag{6.2.3}$$

Clearly using an expansion $\varepsilon(\mathbf{p})$ in powers of $\mathbf{p}$ in $H_{\rm free}$ corresponds to performing a derivative expansion in $\mathcal{H}$ (but restricting to terms bilinear in $\Phi^\star$ and Φ). Interaction terms involving more than one creation and one annihilation operator similarly correspond to terms in $\mathcal{H}$ that involve more powers of either Φ or $\Phi^\star$ (or both).

The Hamiltonian obtained from (6.2.2) is often called the free Schrödinger Hamiltonian, for reasons that become clearer once H is written after an integration by parts:

$$H = \int \mathrm{d}^3x \; \mathcal{H} = \int \mathrm{d}^3x \left[\rho_0 + \Phi^\star \left(\varepsilon_0 - \frac{\nabla^2}{2m}\right) \Phi\right] \,. \tag{6.2.4}$$

To see why this is called the Schrödinger Hamiltonian, consider using it to compute how the field evolves within the Heisenberg picture. Recall that although $\Phi(\mathbf{x})$ is time-independent in the Schrödinger picture, within the Heisenberg picture one can ask how the field

$$\Phi_h(\mathbf{x}, t) := e^{iH(t-t_0)} \Phi(\mathbf{x}) e^{-iH(t-t_0)} \tag{6.2.5}$$

evolves in time. This satisfies – see (3.2.4) – the differential equation

$$i\partial_t \Phi_h(\mathbf{x}, t) = \Big[\Phi_h(\mathbf{x}, t) \,, H\Big] = \left(\varepsilon_0 - \frac{\nabla^2}{2m}\right) \Phi(\mathbf{x}, t) \tag{6.2.6}$$

which uses the commutation relations – *c.f.* eq. (6.1.9), which in Heisenberg picture become the equal-time commutation relations $[\Phi_h(\mathbf{x}, t) \,, \Phi_h(\mathbf{y}, t)] = 0$ and

$$\Big[\Phi_h(\mathbf{x}, t) \,, \Phi^\star_h(\mathbf{y}, t)\Big] = \delta^3(\mathbf{x} - \mathbf{y}) \,. \tag{6.2.7}$$

[9] Since ρ_0 is a constant for translationally invariant systems, for such systems if $\rho_0 \neq 0$ the total ground-state energy satisfies $E_0 = \rho_0 \, \mathcal{V}$ and so diverges in the infinite-volume limit.

Equation (6.2.6) is recognized as the Schrödinger equation in the presence of a constant potential ε_0. But the quantity $\Phi(\mathbf{x},t)$ that satisfies it is an operator-valued field and not a wave-function. Because this is as if the quantum Schrödinger equation itself has been quantized by promoting the wave-function to an operator, quantum field theory in position space is sometimes called 'second quantization'.

6.3 Interaction with an external potential

The connection with the Schrödinger equation is even more explicit if the single-particle gap term $\varepsilon_0\,\Phi^\star(\mathbf{x})\Phi(\mathbf{x})$ is replaced by a more general position-dependent interaction of the form $V(\mathbf{x})\Phi^\star(\mathbf{x})\Phi(\mathbf{x})$, by writing

$$H = \int \mathrm{d}^3x \left\{ \rho_0 + \Phi^\star \left[-\frac{\nabla^2}{2m} + V(\mathbf{x}) \right] \Phi \right\} . \tag{6.3.1}$$

Because the potential $V(\mathbf{x})$ breaks translation invariance momentum is not conserved and so is no longer a useful label for single-particle states. As a result the relation (6.1.7) must be generalized to allow (6.3.1) to be expressed in the free-particle form (6.2.1).

This can be remedied by replacing (6.1.7) by the more general expression

$$\Phi(\mathbf{x}) = \sum_n a_n\, u_n(\mathbf{x}) \quad \text{and} \quad \Phi^\star(\mathbf{x}) = \sum_n a_n^\star\, u_n^*(\mathbf{x}) \,, \tag{6.3.2}$$

with (as usual)

$$[a_n \,, a_m^\star] = \delta_{mn} \tag{6.3.3}$$

and the basis functions $u_n(\mathbf{x})$ to be determined. Inserting this into (6.3.1) gives

$$H = E_0 + \sum_{nm} \int \mathrm{d}^3x\; u_n^\star(\mathbf{x}) \left[-\frac{\nabla^2}{2m} + V(\mathbf{x}) \right] u_m(\mathbf{x})\; a_n^\star a_m \,, \tag{6.3.4}$$

which suggests asking the functions $u_n(\mathbf{x})$ to satisfy the time-independent Schrödinger equation[10]

$$\left[-\frac{\nabla^2}{2m} + V(\mathbf{x}) \right] u_n(\mathbf{x}) = \epsilon_n\, u_n(\mathbf{x}) \,. \tag{6.3.5}$$

Eq. (6.3.5) states that $u_n(\mathbf{x})$ are eigenfunctions (with eigenvalue ϵ_n) of the Schrödinger operator, and because this operator is hermitian these eigenvalues are real and the eigenfunctions can be chosen to be orthonormal

$$\int \mathrm{d}^3x\; u_n^*(\mathbf{x})\, u_m(\mathbf{x}) = \delta_{nm} \,. \tag{6.3.6}$$

The corresponding completeness relation

$$\sum_n u_n(\mathbf{x})\, u_n^*(\mathbf{y}) = \delta^3(\mathbf{x}-\mathbf{y}) \,, \tag{6.3.7}$$

[10] Notice that, despite the similarity to single-particle Schrödinger quantum mechanics, the mode-functions $u_n(\mathbf{x})$ are *not* wave-functions. They are instead matrix elements $u_n(\mathbf{x}) = \langle 0|\Phi(\mathbf{x})|n\rangle$ where $|n\rangle = a_n^\star|0\rangle$.

when combined with (6.3.3) ensures the field operator again satisfies (6.1.9):

$$\Big[\Phi(\mathbf{x})\,,\Phi^\star(\mathbf{y})\Big] = \sum_{nm}\Big[a_n\,,a_m^\star\Big]u_n(\mathbf{x})\,u_m^*(\mathbf{y}) = \sum_n u_n(\mathbf{x})\,u_n^*(\mathbf{y}) = \delta^3(\mathbf{x}-\mathbf{y})\,. \tag{6.3.8}$$

Using (6.3.5) and (6.3.6) in (6.3.4) then leads to

$$H = E_0 + \sum_n \epsilon_n\, a_n^\star a_n\,, \tag{6.3.9}$$

revealing the free-particle form with single-particle labels 'n' and single-particle energies ϵ_n. This last equation shows the advantage of using the mode functions $u_n(\mathbf{x})$ – as in (6.3.2) – rather than plane waves – as in (6.1.7) – when expanding $\Phi(\mathbf{x})$ in terms of creation and annihilation operators. The advantage is that (6.3.9) is *diagonal* in that it involves only $a_n^\star$ and a_n (with the same n) rather than $a_p^\star$ and a_q with $p \neq q$ (compare (6.3.9) with (6.1.11)).

Because a_n and $a_n^\star$ satisfy the usual creation-annihilation operator algebra (6.3.3) the energy eigenstates are given by the usual Fock states labelled by the occupation numbers $\{N_n\}$:

$$H|\{N_m\}\rangle = \left[E_0 + \sum_n N_n\epsilon_n\right]|\{N_m\}\rangle\,, \tag{6.3.10}$$

describing N_m particles that occupy state 'm' and do not interact with one another – although they do interact with the potential $V(\mathbf{x})$. If, for instance, the potential is $V(\mathbf{x}) = -Z\alpha/|\mathbf{x}|$ and the particles are fermions, then this system describes multiple electrons interacting with the Coulomb potential of a nucleus situated at the origin (but neglecting the mutual Coulomb repulsion of the electrons with one another). In this example the $u_n(\mathbf{x}) \to u_{n\ell\mu}(\mathbf{x})$ would be the usual single-particle electron wave-functions in the presence of a Coulomb potential, with quantum numbers $\{n,\ell,\mu\}$, with $n = 1, 2, \cdots$ while $\mu = -\ell, -\ell+1, \cdots, \ell-1, \ell$ with $\ell = 0, 1, \cdots, n-1$. The corresponding energy eigenvalues then are $\epsilon_{n\ell\mu} = -m_e(Z\alpha)^2/(2n^2)$.

6.4 Interacting Schrödinger particles

Interactions between the Schrödinger particles just described are also easily included in position space. When written in terms of creation and annihilation operators interactions were described by terms in H involving more than two creation and annihilation operators, so in position space they involve terms in $\mathcal{H}$ that are more than bilinear in $\Phi(\mathbf{x})$ and $\Phi^\star(\mathbf{y})$.

Furthermore, interactions involving equal numbers of creation and destruction operators do not change the total number of particles, so these correspond in position to interactions involving the same number of Φ fields as $\Phi^\star$ fields. For example an instance of a local interaction that does not change the total number of Schrödinger particles might be

$$H_{\rm int} = g\int \mathrm{d}^3x\,\left[\Phi^\star(\mathbf{x})\Phi(\mathbf{x})\right]^2\,. \tag{6.4.1}$$

Written in terms of creation and annihilation operators using (6.3.2) this becomes

$$H_{\rm int} = \sum_{nmrs} h_{nmrs}\, a_n^\star a_m a_r^\star a_s\,, \tag{6.4.2}$$

with

$$h_{nmrs} = g \int \mathrm{d}^3x\; u_n^*(\mathbf{x}) u_m(\mathbf{x})\, u_r^*(\mathbf{x}) u_s(\mathbf{x})\,. \tag{6.4.3}$$

In the absence of a potential we can use momentum eigenstates, $u_{\mathbf{p}}(\mathbf{x}) = \mathcal{V}^{-1/2}\, e^{i\mathbf{p}\cdot\mathbf{x}}$, and so

$$h_{pqkl} = \frac{g}{\mathcal{V}^2} \int \mathrm{d}^3x\; e^{i(\mathbf{p}-\mathbf{q}+\mathbf{k}-\mathbf{l})\cdot\mathbf{x}} = \frac{g}{\mathcal{V}}\, \delta_{\mathbf{p}+\mathbf{k}-\mathbf{q}-\mathbf{l}}\,, \tag{6.4.4}$$

and so in the continuum limit

$$\begin{aligned} H_{\rm int} &= \frac{g}{\mathcal{V}} \sum_{pqkl} \delta_{\mathbf{p}+\mathbf{k}-\mathbf{q}-\mathbf{l}}\; a_{\mathbf{p}}^\star a_{\mathbf{q}} a_{\mathbf{k}}^\star a_{\mathbf{l}} \\ &= \frac{g}{\mathcal{V}} \left[\frac{\mathcal{V}}{(2\pi)^3}\right]^4 \int \mathrm{d}^3\mathbf{p}\, \mathrm{d}^3\mathbf{q}\, \mathrm{d}^3\mathbf{k}\, \mathrm{d}^3\mathbf{l} \left[\frac{(2\pi)^3}{\mathcal{V}} \delta^3(\mathbf{p}+\mathbf{k}-\mathbf{q}-\mathbf{l})\right] \left[\frac{(2\pi)^3}{\mathcal{V}}\right]^2 \mathfrak{a}_{\mathbf{p}}^\star \mathfrak{a}_{\mathbf{q}} \mathfrak{a}_{\mathbf{k}}^\star \mathfrak{a}_{\mathbf{l}} \\ &= \frac{g}{(2\pi)^3} \int \mathrm{d}^3\mathbf{p}\, \mathrm{d}^3\mathbf{q}\, \mathrm{d}^3\mathbf{k}\, \mathrm{d}^3\mathbf{l}\; \delta^3(\mathbf{p}+\mathbf{k}-\mathbf{q}-\mathbf{l})\; \mathfrak{a}_{\mathbf{p}}^\star \mathfrak{a}_{\mathbf{q}} \mathfrak{a}_{\mathbf{k}}^\star \mathfrak{a}_{\mathbf{l}}\,, \end{aligned}$$

corresponding to $\mathfrak{h}(\mathbf{p},\mathbf{q},\mathbf{k},\mathbf{l}) = g/(2\pi)^3$ in the notation of the quartic interactions of earlier sections.

By contrast, a nonlocal interaction is given by an interaction at a distance through a potential, which in second-quantized language looks like

$$H_U = \frac{1}{2} \int \mathrm{d}^3x\; \mathrm{d}^3y\; U(\mathbf{x},\mathbf{y})\, \Phi^\star(\mathbf{x})\Phi(\mathbf{x})\; \Phi^\star(\mathbf{y})\Phi(\mathbf{y})\,, \tag{6.4.5}$$

where the factor of $\frac{1}{2}$ keeps from double counting as $\mathbf{x}$ and $\mathbf{y}$ range over all of space. For instance, an example of this type is given by the Coulomb interaction, which in second-quantized language looks like

$$H_C = \frac{\alpha}{2} \int \mathrm{d}^3x\; \mathrm{d}^3y\; \frac{\Phi^\star(\mathbf{x})\Phi(\mathbf{x})\; \Phi^\star(\mathbf{y})\Phi(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,, \tag{6.4.6}$$

where $\alpha = e^2/4\pi$ is the electromagnetic fine-structure constant. Although at face value nonlocal interactions like the Coulomb interaction might seem to contradict the clustering (or locality) principle, later sections show that in reality they do not because they can be regarded as local once written in terms of the electromagnetic fields that are responsible for their origins.

The above form for the Coulomb interaction (and more general potential interactions) is motivated by the observation that the quantity $n(\mathbf{x}) := \Phi^\star(\mathbf{x})\Phi(\mathbf{x})$ is the position-space

number-density operator in the sense that its integral gives the operator that counts the total number of particles:

$$N = \int \mathrm{d}^3x\ \Phi^\star(\mathbf{x})\Phi(\mathbf{x}) = \int \mathrm{d}^3x\ \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\ \frac{\mathrm{d}^3q}{(2\pi)^{3/2}}\ \mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{q}}\, e^{i(\mathbf{q}-\mathbf{p})\cdot\mathbf{x}} = \int \mathrm{d}^3p\ \mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{p}}\,. \tag{6.4.7}$$

If a specific pair of particles situated at positions $\mathbf{x}$ and $\mathbf{y}$ interact with one another with potential energy $U(\mathbf{x},\mathbf{y})$ then for a distribution of particles the interaction energy per unit volume is obtained by convoluting $U(\mathbf{x},\mathbf{y})$ with the number of particles per unit volume, $n(\mathbf{x})$, at position $\mathbf{x}$ with the same at $\mathbf{y}$, as in (6.4.5). From this point of view the contact interaction of (6.4.1) corresponds to inter-particle interactions through a δ-function potential $U(\mathbf{x},\mathbf{y}) = g\,\delta^3(\mathbf{x}-\mathbf{y})$ (which is indeed why this is called a 'contact' interaction).

The message of this section is that it is easy to guess the Hamiltonian that describes the many-particle behaviour of any system for which the single-particle system is described by a Schrödinger equation of the form

$$i\partial_t\psi = \mathfrak{H}\,\psi\,, \tag{6.4.8}$$

where $\mathfrak{H}$ is the single-particle Hamiltonian — such as $\mathfrak{H} = -(\nabla^2/2m) + V(\mathbf{x})$ in the example given above. For any such a system the many-particle quantum field theory hamilton is simply

$$H = \int \mathrm{d}^3x\ \Big[\rho_0 + \Phi^\star(\mathbf{x})\,\mathfrak{H}\,\Phi(\mathbf{x})\Big]\,, \tag{6.4.9}$$

where the differential operator $\mathfrak{H}$ acts on the field to its right. This Hamiltonian is diagonalized – *i.e.* put into the form (6.3.9) – by writing $\Phi(\mathbf{x}) = \sum_n a_n\,u_n(\mathbf{x})$ with mode functions, $u_n(\mathbf{x})$, defined to satisfy

$$\mathfrak{H}\,u_n = \epsilon_n\,u_n\,. \tag{6.4.10}$$

Although the Hamiltonian (6.4.9) properly captures the single-particle energies as well as the statistics of multiply occupying single-particle states, it does not contain interactions between the particles (should more than one particle exist). These are captured by supplementing (6.4.9) by terms that need not be bilinear in Φ and $\Phi^\star$, such as those given by (6.4.5) or (6.4.6) (whose origins are discussed in more detail in §9.5).

6.5 Spin and exchange interactions

This section uses the interaction of (6.4.5) and (6.4.6) to compute the energy shift of two charged fermions, such as would apply to electrons in the atomic energy levels of the Helium atom. Besides illustrating the use of perturbation theory in field theory, this example also introduces the notion of exchange interactions that arise due to particle statistics.

Exchange interactions can be important in practice because they show how nominally spin-independent interactions (like electrostatic forces) can give rise to spin-dependent effects, such as those that underpin the understanding of most magnetic materials. To illustrate this

consider spin-half electrons, with single-particle states created by $c^\star_{n\sigma}$, where $\sigma = \pm\frac{1}{2}$ denotes the two spin states available to a spin-half electron. Because electrons are fermions the commutation relations in this case are

$$\left\{ c_{n\sigma}\,, c^\star_{m\xi} \right\} = \delta_{\sigma\xi}\,\delta_{nm}\,. \tag{6.5.1}$$

We again write $H = H_0 + H_{\rm int}$, with the unperturbed Hamiltonian H_0 describing non-relativistic electrons interacting with the Coulomb potential of a nucleus with electric charge Ze, given by

$$H_0 = \int \mathrm{d}^3x \, \left\{ \Phi^\star \left[-\frac{\nabla^2}{2\mu} + \varepsilon_g + V(\mathbf{x}) \right] \Phi \right\} = \sum_{\sigma=\pm 1/2} \sum_n \varepsilon_n \, c^\star_{n\sigma} c_{n\sigma}\,, \tag{6.5.2}$$

where ε_g denotes the single-particle 'gap' energy – or energy cost for producing a single particle at rest in the absence of the potential – and the last equality uses the field expansion (6.3.2) in the form

$$\Phi(\mathbf{x},t) = \sum_{\sigma=\pm 1/2} \sum_n u_{n\sigma}(\mathbf{x},t)\, c_{n\sigma} =: \sum_N u_N(\mathbf{x}.t)\, c_N\,, \tag{6.5.3}$$

where to simplify notation a single letter is used for the quantum-number pairs $N = \{n\,, \sigma\}$.

The potential $V(\mathbf{x})$ is assumed to be spin-independent, and when required for practical applications to the He atom is taken to be the attractive Coulomb potential of the nucleus

$$V(\mathbf{x}) = -\frac{Z\alpha}{r} = -\frac{Ze^2}{4\pi r}\,, \tag{6.5.4}$$

where Z is the nuclear charge in units of the proton charge e (so $Z = 2$ for He). For non-relativistic electrons spin-independence of the potential means that to leading approximation the energy is independent of spin label, so $\varepsilon_{n\sigma} = \varepsilon_n$ where $u_{n\sigma}(x)$ solves – *c.f.* (6.3.5):

$$\left[-\frac{\nabla^2}{2\mu} + V(\mathbf{x}) \right] u_{n\sigma}(\mathbf{x},t) = \varepsilon_n\, u_{n\sigma}(\mathbf{x},t) \quad \text{and} \quad \partial_t u_{n\sigma}(\mathbf{x},t) = -i\varepsilon_n\, u_{n\sigma}(\mathbf{x},t)\,. \tag{6.5.5}$$

Explicitly, for the Coulomb potential (6.5.4) the index 'n' is a shorthand for the quantum numbers $\{n, \ell, \ell_z\}$ that label the eigenstates for this potential, and the bound-state[11] energy eigenvalues found by solving the Schrödinger equation would be independent of the angular-momentum quantum numbers ℓ and ℓ_z, with

$$\varepsilon_{n\ell\ell_z} = \varepsilon_g - \frac{(Z\alpha)^2\mu}{2n^2}\,. \tag{6.5.6}$$

Given this spin-independence it is convenient to write the spin and position dependent parts of the mode functions separately, $u_{n\sigma}(\mathbf{x},t) = \psi_n(\mathbf{x},t)\,\chi_\sigma$ where the basis vectors in 2-dimensional spin space are written as

$$\chi_{+\frac{1}{2}} = \chi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \chi_{-\frac{1}{2}} = \chi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\,. \tag{6.5.7}$$

[11] Here 'bound state' means any states with single-particle energy $\varepsilon < \varepsilon_g$.

In this notation the field expansion (6.5.3) becomes

$$\Phi(\mathbf{x},t) = \sum_n \begin{pmatrix} u_{n\uparrow}(\mathbf{x},t)\, c_{n\uparrow} \\ u_{n\downarrow}(\mathbf{x},t)\, c_{n\downarrow} \end{pmatrix} = \sum_n \psi_n(\mathbf{x},t) \begin{pmatrix} c_{n\uparrow} \\ c_{n\downarrow} \end{pmatrix} , \tag{6.5.8}$$

In what follows we take the interaction Hamiltonian to consist of the mutual Coulomb repulsion of the two electrons, as described by the interaction Hamiltonian

$$H_{\rm int} = \frac{1}{8\pi} \int \mathrm{d}^3x\, \mathrm{d}^3y\, \frac{\rho(\mathbf{x},t)\, \rho(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|} , \tag{6.5.9}$$

where (for electrons) the charge density is given by

$$\rho(\mathbf{x},t) := -e\, \Phi^\star \Phi = -e \sum_{PQ} u_P^\dagger(\mathbf{x},t) u_Q(\mathbf{x},t)\, c_P^\star\, c_Q \, . \tag{6.5.10}$$

This form for the interaction Hamiltonian is intuitive from classical electromagnetism, and is derived explicitly for quantum electromagnetism in §9.6 below. We compute here the effects of this interaction perturbatively.

The goal is to compute in particular the contribution of $H_{\rm int}$ to the energy for both one- and a two-particle energy eigenstates

$$|N\rangle = c_N^\star |0\rangle \, , \quad \text{and} \quad |N\,,M\rangle = c_N^\star c_M^\star |0\rangle = -c_M^\star c_N^\star |0\rangle \, . \tag{6.5.11}$$

Although in practice our interest at the end is in the ground state, $\psi_0(x)$, the quantum numbers n and m are kept general for most of the calculation. The leading energy shift of a state predicted by time-independent perturbation theory is given – *c.f.* §3.1 – by

$$\delta E_\psi = \langle \psi | H_{\rm int} | \psi \rangle \, , \tag{6.5.12}$$

so we evaluate $\langle N | H_{\rm Coul} | N \rangle$ and $\langle N, M | H_{\rm Coul} | N, M \rangle$ using (6.5.9).

The calculation starts by evaluating

$$\langle N | \rho(\mathbf{x},t)\, \rho(\mathbf{y},t) | N \rangle = \sum_R \langle N | \rho(\mathbf{x},t) | R \rangle \, \langle R | \rho(\mathbf{y},t) | N \rangle \tag{6.5.13}$$

where a sum over a complete set of states is inserted, and only single-particle states are necessary because (6.5.10) contains precisely one factor of c and one factor of $c^\star$ and so does not change the total number of particles.

First some intermediate steps. For single-particle states direct evaluation gives the following off-diagonal matrix element

$$\langle R | \rho(\mathbf{x},t) | N \rangle = -e \sum_{PQ} u_P^\dagger(\mathbf{x},t) u_Q(\mathbf{x},t)\, \langle R | c_P^\star\, c_Q | N \rangle = -e\, u_R^\dagger(\mathbf{x},t) u_N(\mathbf{x},t) \tag{6.5.14}$$

which uses $c_Q|N\rangle = \delta_{QN}|0\rangle$, together with its adjoint. Using this in (6.5.13) then gives

$$\begin{aligned}\langle N|\rho(\mathbf{x},t)\,\rho(\mathbf{y},t)|N\rangle &= \sum_R \langle N|\rho(\mathbf{x},t)|R\rangle\,\langle R|\rho(\mathbf{y},t)|N\rangle \\ &= e^2 \sum_R \left[u_N^\dagger(\mathbf{x},t)u_R(\mathbf{x},t)\right]\,\left[u_R^\dagger(\mathbf{y},t)u_N(\mathbf{y},t)\right] \\ &= e^2\, u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)\;\delta^3(\mathbf{x}-\mathbf{y})\,. \end{aligned} \tag{6.5.15}$$

Here the last equality uses mode-function completeness in the form

$$\sum_R u_R(\mathbf{x},t)\,u_R^\dagger(\mathbf{y},t) = \sum_n \psi_n(\mathbf{x},t)\psi_n^*(\mathbf{y},t)\sum_\sigma \chi_\sigma\chi_\sigma^\dagger = \delta^3(\mathbf{x}-\mathbf{y})\,\mathbb{I}_2\,, \tag{6.5.16}$$

where $\mathbb{I}_2$ denotes the 2×2 unit matrix in spin space.

The two-particle expectation value is found through similar steps, though with one subtlety. Inserting a complete set of states between the two charge-density operators gives

$$\langle N,M|\rho(\mathbf{x},t)\,\rho(\mathbf{y},t)|N,M\rangle = {\sum_{PR}}'\langle N,M|\rho(\mathbf{x},t)|P,R\rangle\,\langle P,R|\rho(\mathbf{y},t)|N,M\rangle \tag{6.5.17}$$

where the sum need only include two-particle states because $\rho(\mathbf{x},t)$ does not change the total number of particles. The subtlety arises when specifying the limits of the summation over P and Q, since for identical particles this should only run over *half* the naive range or else one ends up double counting intermediate states (see exercise), and this is what the prime in the sum over P,R denotes.

Exercise: Suppose $\Phi(\mathbf{x}) = \sum_n u_n(\mathbf{x})\,c_n$ and $\Phi(\mathbf{x}) = \sum_a v_\alpha(\mathbf{x})\,b_\beta$ for two different orthonormal bases of mode functions with $u_n(\mathbf{x}) = \sum_\alpha U_{n\alpha}v_\alpha(\mathbf{x})$. Show that $\int \mathrm{d}^3x\; v_\alpha^* v_\beta = \delta_{\alpha\beta}$ implies $\int \mathrm{d}^3x\; u_n^* u_m = \delta_{mn}$ if $U_{n\alpha}$ is unitary: $\sum_\alpha U_{n\alpha}^* U_{m\alpha} = \delta_{nm}$ and $\sum_n U_{n\alpha}^* U_{n\beta} = \delta_{\alpha\beta}$. Express c_n in terms of b_α and show that $\{b_\alpha\,, b_\beta^\star\} = \delta_{\alpha\beta}$ implies both $\{c_n\,, c_m^\star\} = \delta_{nm}$ and $\{\Phi(\mathbf{x})\,, \Phi^\star(\mathbf{y})\} = \delta^3(\mathbf{x}-\mathbf{y})$.

Assuming $c_n|0\rangle = b_\alpha|0\rangle = 0$ show that the creation and annihilation algebra implies the two-particle states $|n,m\rangle = c_n^\star c_m^\star|0\rangle$ and $|\alpha,\beta\rangle = b_\alpha^\star b_\beta^\star|0\rangle$ (with $n\neq m$ and $\alpha\neq\beta$ for fermions) are normalized inasmuch as $\langle n,m|n,m\rangle = \langle\alpha,\beta|\alpha,\beta\rangle = 1$. Finally, explicitly insert a compete set of states to write

$$\langle n,m|n,m\rangle = \sum_{\alpha\beta}\langle n,m|\alpha,\beta\rangle\,\langle\alpha,\beta|n,m\rangle$$

and use this to show that the above sum evaluates to 2 rather than 1 if α and β are allowed to run jointly over their complete range.

The required two-particle matrix element of $\rho(\mathbf{x},t)$ is found using

$$\begin{aligned} c_R|N,M\rangle &= c_R c_N^\star c_M^\star|0\rangle = \delta_{RN}|M\rangle - \delta_{RM}|N\rangle \\ \text{and so}\quad \langle N,M|c_R^\star &= (c_R|N,M\rangle)^\star = \delta_{RN}\langle M| - \delta_{RM}\langle N|\,, \end{aligned} \tag{6.5.18}$$

and is given by

$$\begin{aligned} \langle P,R|\rho(\mathbf{x},t)|N,M\rangle &= -e\sum_{TQ}\Big[u_T^\dagger(\mathbf{x},t)u_Q(\mathbf{x},t)\Big]\,\langle P,R|c_T^\star\,c_Q|N,M\rangle \\ &= -e\sum_{TQ}\Big[u_T^\dagger(\mathbf{x},t)u_Q(\mathbf{x},t)\Big]\,\Big[\delta_{TP}\langle R| - \delta_{TR}\langle P|\Big]\Big[\delta_{QN}|M\rangle - \delta_{QM}|N\rangle\Big] \\ &= -e\Big\{\Big[u_P^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)\Big]\,\delta_{MR} - \Big[u_P^\dagger(\mathbf{x},t)u_M(\mathbf{x},t)\Big]\,\delta_{NR} \\ &\qquad + \Big[u_R^\dagger(\mathbf{x},t)u_M(\mathbf{x},t)\Big]\,\delta_{NP} - \Big[u_R^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)\Big]\,\delta_{MP}\Big\}\,. \end{aligned} \tag{6.5.19}$$

The diagonal part of this result provides a check on the calculation, because it predicts the charge distribution within the two-particle state to be

$$\langle N,M|\rho(\mathbf{x},t)|N,M\rangle = -e\Big\{u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t) + u_M^\dagger(\mathbf{x},t)u_M(\mathbf{x},t)\Big\}\,, \tag{6.5.20}$$

(which uses $M\neq N$ for fermions). This shows that the mode functions capture the electron's position distribution as would a wave-function in single-particle quantum mechanics.

The matrix element needed for the energy shift is found by using (6.5.19) in (6.5.17). The algebra is a bit tedious but simplifies a bit given that Fermi-Dirac statistics imply $N\neq M$ and so $\delta_{NR}\delta_{MR}=0$ for any R. In particular only 12 of the possible 16 terms that could arise in the product of $\langle N,M|\rho|P,R\rangle$ and $\langle P,R|\rho|N,M\rangle$ are actually nonzero. The result for these potentially nonzero terms is

$$\begin{aligned} \langle N,M|\rho(\mathbf{x},t)\,\rho(\mathbf{y},t)|N,M\rangle &= {\sum_{PR}}'\langle N,M|\rho(\mathbf{x},t)|P,R\rangle\,\langle P,R|\rho(\mathbf{y},t)|N,M\rangle \\ &= \frac{1}{2}\sum_{PR}\langle N,M|\rho(\mathbf{x},t)|P,R\rangle\,\langle P,R|\rho(\mathbf{y},t)|N,M\rangle \\ &= e^2\Big\{\Big[u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t) + u_M^\dagger(\mathbf{y},t)u_M(\mathbf{y},t)\Big]\delta^3(\mathbf{x}-\mathbf{y}) \\ &\qquad + \Big[u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)\;u_M^\dagger(\mathbf{y},t)u_M(\mathbf{y},t) + (\mathbf{x}\leftrightarrow\mathbf{y})\Big] \\ &\qquad - \Big[u_N^\dagger(\mathbf{x},t)u_M(\mathbf{x},t)\;u_M^\dagger(\mathbf{y},t)u_N(\mathbf{y},t) + (\mathbf{x}\leftrightarrow\mathbf{y})\Big]\Big\}\,. \end{aligned} \tag{6.5.21}$$

A check on the normalization of this expression comes from integrating over $\mathbf{x}$ and $\mathbf{y}$ using the orthonormality of the mode functions, and comparing the result to what is found from the total charge $Q=\int \mathrm{d}^3x\;\rho(\mathbf{x})$ and the knowledge that $Q|N,M\rangle = -2e|N,M\rangle$:

$$\begin{aligned} \langle N,M|Q^2|N,M\rangle &= \int \mathrm{d}^3x\,\mathrm{d}^3y\;\langle N,M|\rho(\mathbf{x},t)\,\rho(\mathbf{y},t)|N,M\rangle \\ &= 2e^2\int \mathrm{d}^3x\Big[u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t) + u_M^\dagger(\mathbf{x},t)u_M(\mathbf{x},t)\Big] = 4e^2\,. \end{aligned} \tag{6.5.22}$$

Single-particle energy shift

We can now use the above intermediate results to compute the leading Coulomb energy shifts. For single-particle states the corrected single-particle electron energy is

$$\mathcal{E}_N \simeq \varepsilon_N + \delta\mathcal{E}_N \tag{6.5.23}$$

where ε_N is the lowest-order energy eigenvalue obtained by solving (6.5.5) – such as, for instance, (6.5.6).

The leading Coulomb contribution is $\delta\mathcal{E}_N = \langle N|H_{\rm Coul}|N\rangle$ and so

$$\begin{aligned}\delta\mathcal{E}_N &= \frac{1}{8\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\frac{\langle N|\rho(\mathbf{x},t)\,\rho(\mathbf{y},t)|N\rangle}{|\mathbf{x}-\mathbf{y}|}\\ &= \frac{e^2}{8\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\frac{u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)}{|\mathbf{x}-\mathbf{y}|}\;\delta^3(\mathbf{x}-\mathbf{y})\\ &= \frac{e^2\Lambda_C}{8\pi}\int \mathrm{d}^3x\;u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t) = \frac{e^2\Lambda_C}{8\pi}\,.\end{aligned} \tag{6.5.24}$$

Here Λ_C is an N-independent divergent quantity with dimensions of energy that arises because the delta function performs the integration over d^3y by evaluating the denominator at $\mathbf{y}=\mathbf{x}$.

This is not the only divergent contribution to single-particle energy shifts, since other electromagnetic interactions also give divergent contributions. For instance, the leading contribution to $\delta\mathcal{E}_N$ from the term H_{PAA} of (9.6.7) similarly gives $\delta\tilde{\mathcal{E}}_N = \langle N|H_{PAA}|N\rangle$ and so

$$\begin{aligned}\delta\tilde{\mathcal{E}}_N &= \frac{e^2}{2\mu}\int \mathrm{d}^3x\;\langle N|\Phi^\star\Phi\,\mathbf{A}\cdot\mathbf{A}|N\rangle\\ &= \frac{e^2}{2\mu}\int \mathrm{d}^3x\;\Big[u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)\Big]\\ &\qquad\qquad\times\sum_{\lambda\zeta}\int\frac{\mathrm{d}^3k\,\mathrm{d}^3l}{(2\pi)^3 2\sqrt{|\mathbf{k}||\mathbf{l}|}}\;\boldsymbol{\epsilon}_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}_\zeta^*(\mathbf{l})\,\langle 0|\mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}^\star_{\mathbf{l}\zeta}|0\rangle\,e^{i(\mathbf{k}-\mathbf{l})\cdot\mathbf{x}-i(|\mathbf{k}|-|\mathbf{l}|)t}\\ &= \frac{e^2}{2\mu}\int \mathrm{d}^3x\;\Big[u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)\Big]\sum_\lambda\int\frac{\mathrm{d}^3k}{(2\pi)^3 2|\mathbf{k}|}\;\boldsymbol{\epsilon}_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}_\lambda^*(\mathbf{k})\\ &= \frac{e^2}{2\mu}\int\frac{\mathrm{d}^3k}{(2\pi)^3|\mathbf{k}|} =: \frac{e^2\Lambda_S^2}{2\mu}\end{aligned} \tag{6.5.25}$$

where the last equality defines the divergent parameter Λ_S that again has dimensions of energy. What is important about both this result and (6.5.24) is that they are state-independent and so can be absorbed into a redefinition of the gap energy parameter ε_g to get the physical gap energy:

$$\varepsilon_g^{\rm phys} := \varepsilon_g + \frac{e^2\Lambda_C}{8\pi} + \frac{e^2\Lambda_S^2}{2\mu}\,, \tag{6.5.26}$$

with physical quantities becoming UV-insensitive once they are expressed in terms of $\varepsilon_g^{\rm phys}$ rather than ε_g. A concrete example of this occurs when computing the Coulomb energy shift of a two-particle state, $|N,M\rangle$, as is now shown.

Two-particle energy shift

For two-fermion states the energy (above the energy of the no-particle state) is

$$\mathcal{E}_{N,M} \simeq \varepsilon_N + \varepsilon_M + \delta\mathcal{E}_{N,M}\,, \tag{6.5.27}$$

with

$$\delta\mathcal{E}_{N,M} = \langle N,M|H_{\rm Coul}|N,M\rangle = \frac{1}{8\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\frac{\langle N,M|\rho(\mathbf{x},t)\,\rho(\mathbf{y},t)|N,M\rangle}{|\mathbf{x}-\mathbf{y}|}\,. \tag{6.5.28}$$

Using (6.5.21) in this expression gives

$$\begin{aligned}\delta\mathcal{E}_{N,M} &= \frac{e^2}{8\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\left\{\frac{u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)+u_M^\dagger(\mathbf{y},t)u_M(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\,\delta^3(\mathbf{x}-\mathbf{y})\right.\\ &\qquad +\frac{2u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)\;u_M^\dagger(\mathbf{y},t)u_M(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\\ &\qquad \left.-\frac{2u_N^\dagger(\mathbf{x},t)u_M(\mathbf{x},t)\;u_M^\dagger(\mathbf{y},t)u_N(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\right\}\\ &= \frac{e^2\Lambda_C}{4\pi}+\frac{e^2}{4\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\left\{\frac{u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)\;u_M^\dagger(\mathbf{y},t)u_M(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\right.\\ &\qquad \left.-\frac{u_N^\dagger(\mathbf{x},t)u_M(\mathbf{x},t)\;u_M^\dagger(\mathbf{y},t)u_N(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\right\}.\end{aligned} \tag{6.5.29}$$

The first term (that diverges, proportional to Λ_C) is precisely the single-particle energy shift for each of the two particles in the state. It therefore cancels in the total energy (6.5.27) once ε_g is traded for $\varepsilon_g^{\rm phys}$, as described above. It is the remaining terms inside the integral in (6.5.29) that describe the interaction energy for each particle due to the presence of the other. The first of these is precisely what one would naively expect for the $N-M$ cross terms in the Coulomb interaction for a classical charge distribution $\varrho(\mathbf{x}) = -e[u_M^\dagger(\mathbf{x},t)u_M(\mathbf{x},t) + u_N^\dagger(\mathbf{x},t)u_N(\mathbf{x},t)]$, once the $N-N$ and $M-M$ self-interactions were subtracted.

It is the last of the terms in (6.5.29) that does not have a simple counterpart for classical charge distributions. This term arises because electrons are indistinguishable fermions, due to the requirement that this makes their states antisymmetric under the interchange of any two fermions. This contribution to the energy is called the Coulomb 'exchange' energy. One of its novel features is that it can generate spin-dependent energies from nominally spin-independent interactions (like the Coulomb interaction).

Exchange interactions also arise in ordinary two-particle quantum mechanics. There they arise due to the need to symmetrize or antisymmetrize the two-particle wave-function, where (dropping the spin label temporarily)

$$\Psi(\mathbf{x}_1,\mathbf{x}_2) = \frac{\mathcal{N}}{\sqrt{2}}\Big[\psi_n(\mathbf{x}_1)\,\psi_m(\mathbf{x}_2)\pm\psi_n(\mathbf{x}_2)\,\psi_m(\mathbf{x}_1)\Big]\,, \tag{6.5.30}$$

and $\mathcal{N}$ is a normalization factor (more about which below). With this wavefunction the average Coulomb energy is

$$\frac{e^2}{4\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\frac{|\Psi(\mathbf{x},\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|} = \frac{e^2}{4\pi}|\mathcal{N}|^2\int \mathrm{d}^3y\,\frac{|\psi_n(\mathbf{x})|^2|\psi_m(\mathbf{y})|^2 \pm \psi_n^*(\mathbf{x})\psi_m(\mathbf{x})\,\psi_m^*(\mathbf{y})\psi_n(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,, \tag{6.5.31}$$

which has the same form as (6.5.29) if $|\mathcal{N}|^2 = 1$. Indeed, the normalization condition is

$$\begin{aligned} 1 = \int \mathrm{d}^3x\,\mathrm{d}^3y\,|\Psi(\mathbf{x},\mathbf{y})|^2 &= \frac{|\mathcal{N}|^2}{2}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\Big[|\psi_n(\mathbf{x})|^2|\psi_m(\mathbf{y})|^2 + |\psi_m(\mathbf{x})|^2|\psi_n(\mathbf{y})|^2 \\ &\qquad \pm\psi_n^*(\mathbf{x})\psi_m(\mathbf{x})\,\psi_m^*(\mathbf{y})\psi_n(\mathbf{y}) \pm \psi_m^*(\mathbf{x})\psi_n(\mathbf{x})\,\psi_n^*(\mathbf{y})\psi_m(\mathbf{y})\Big] \\ &= \frac{|\mathcal{N}|^2}{2}\int \mathrm{d}^3x\,\Big[|\psi_n(\mathbf{x})|^2 + |\psi_m(\mathbf{x})|^2\Big](1\pm\delta_{mn}) = |\mathcal{N}|^2(1\pm\delta_{mn})\,, \end{aligned} \tag{6.5.32}$$

and so $|\mathcal{N}|^2 = 1$ *unless* the wave-function is symmetrized and $m = n$, in which case $|\mathcal{N}|^2 = \frac{1}{2}$. This extra factor of $\frac{1}{2}$ when $n = m$ is related to Exercise 6.5, since in this case the complete range of the $\mathrm{d}^3x\,\mathrm{d}^3y$ joint integral for intermediate position states double-counts unless it only runs over half of the naive joint volume.

Spin-dependence of exchange interactions

There is also interesting physics associated with the spin-dependence of (6.5.29). To see why, restore the full particle labels by replacing $N = \{n,\sigma\}$ and $M = \{m,\xi\}$. Then $u_{n\sigma}(\mathbf{x},t) = \psi_n(\mathbf{x},t)\,\chi_\sigma(t)$ we have $u_N^\dagger u_M = \psi_n^*\psi_m\,\chi_\sigma^\dagger\chi_\xi = \psi_n^*\psi_m\,\delta_{\sigma\xi}$ and using these in eq. (6.5.29) allows the inter-particle interaction energy to be rewritten as

$$\delta\mathcal{E}^{\rm int}_{n\sigma,m\xi} = \frac{e^2}{4\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\left\{\frac{\psi_n^*(\mathbf{x},t)\psi_n(\mathbf{x},t)\;\psi_m^*(\mathbf{y},t)\psi_m(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|} - \frac{\psi_n^*(\mathbf{x},t)\psi_m(\mathbf{x},t)\;\psi_m^*(\mathbf{y},t)\psi_n(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\,\delta_{\sigma\xi}\right\}, \tag{6.5.33}$$

and so

$$\delta\mathcal{E}^{\rm int}_{n\uparrow,m\downarrow} = \delta\mathcal{E}^{\rm int}_{n\downarrow,m\uparrow} = U_c \quad\text{and}\quad \delta\mathcal{E}^{\rm int}_{n\uparrow,m\uparrow} = \delta\mathcal{E}^{\rm int}_{n\downarrow,m\downarrow} = U_c - U_e\,, \tag{6.5.34}$$

where

$$\begin{aligned} U_c &:= \frac{e^2}{4\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\frac{\psi_n^*(\mathbf{x},t)\psi_n(\mathbf{x},t)\;\psi_m^*(\mathbf{y},t)\psi_m(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|} \\ \text{and}\quad U_e &:= \frac{e^2}{4\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\frac{\psi_n^*(\mathbf{x},t)\psi_m(\mathbf{x},t)\;\psi_m^*(\mathbf{y},t)\psi_n(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\,, \end{aligned} \tag{6.5.35}$$

and so $U_c = U_e$ in the special case where $n = m$.

These expressions explicitly show that the Coulomb energy shifts depend on the fermion spins when the exchange energy is nonzero, $U_e \neq 0$, despite the Coulomb interaction naively being spin-independent. This spin-dependence is important in practice because it is typically

much larger than the spin-dependence associated with intrinsic particle magnetic moments, and so provides the dominant source of spin-dependent couplings in most magnetic materials.

To find the energy eigenstates in spin space requires constructing the interaction Hamiltonian regarded as a matrix in spin-space: $\langle n\sigma, m\xi|H_{\rm Coul}|n\sigma', m\xi'\rangle$, with rows and columns labelled by the pairs $(\sigma\xi)$ and $(\sigma'\xi')$. The real energy shifts[12] are the eigenvalues (as opposed to the diagonal elements computed above) of the matrix $\langle\sigma, \xi|H_{\rm Coul}|\sigma', \xi'\rangle$ where the row and column labels are $\{\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow\}$, with the first spin in a pair like $\uparrow\downarrow$ denoting the spin associated with spatial state $\psi_n(\mathbf{x}, t)$ and the second being the spin associate with state $\psi_m(\mathbf{x}, t)$. In terms of the quantities U_c and U_e the extension of (6.5.34) to include off-diagonal terms in spin-space leads to the 4×4 spin-space interaction matrix

$$\langle n\sigma, m\xi|H_{\rm Coul}|n\sigma', m\xi'\rangle = \begin{pmatrix} U_c - U_e & 0 & 0 & 0 \\ 0 & U_c & -U_e & 0 \\ 0 & -U_e & U_c & 0 \\ 0 & 0 & 0 & U_c - U_e \end{pmatrix} . \tag{6.5.36}$$

This matrix has two distinct eigenvalues with different degeneracies. The three eigenstates $\uparrow\uparrow$, $\downarrow\downarrow$ and $\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$ that are symmetric under the interchange of the two spins share a common energy, and so form a triplet of degenerate energy eigenstates for which the two fermion spins combine into total spin $S = 1$. The one remaining eigenstate that is antisymmetric under the exchange of the two spins, $\frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$, has total spin $S = 0$ and in general has a different eigenvalue. Inspection of (6.5.36) shows that the corresponding energy eigenvalues are

$$\delta\mathcal{E}_{S=1} = U_c - U_e \quad \text{and} \quad \delta\mathcal{E}_{S=0} = U_c + U_e \, . \tag{6.5.37}$$

Notice that Fermi-Dirac statistics imply that the state $c^\star_{n\sigma}c^\star_{m\xi}|0\rangle$ must be antisymmetric under the interchange of fermion labels $(n, \sigma) \leftrightarrow (m, \xi)$ and so a state with $S = 1$ must necessarily be odd under the interchange $n \leftrightarrow m$ while a state with $S = 0$ must be even under this interchange. The corresponding position-space wave functions are therefore (for $m \neq n$)

$$\begin{aligned} \Psi_{S=1}(\mathbf{x}_1, \mathbf{x}_2) &= \frac{1}{\sqrt{2}}\Big[\psi_n(\mathbf{x}_1)\,\psi_m(\mathbf{x}_2) - \psi_n(\mathbf{x}_2)\,\psi_m(\mathbf{x}_1)\Big] \\ \text{and} \quad \Psi_{S=0}(\mathbf{x}_1, \mathbf{x}_2) &= \frac{1}{\sqrt{2}}\Big[\psi_n(\mathbf{x}_1)\,\psi_m(\mathbf{x}_2) + \psi_n(\mathbf{x}_2)\,\psi_m(\mathbf{x}_1)\Big] , \end{aligned} \tag{6.5.38}$$

and it is this antisymmetry under interchange of position that allows the $S = 1$ state to lower its energy relative to the $S = 0$ state. It does so because the antisymmetry keeps the two electrons further apart from one another on average, thereby reducing their mutual Coulomb repulsion.

[12] Strictly speaking this is a result from *degenerate* time-independent perturbation theory, rather than the non-degenerate case discussed in §3. In degenerate perturbation theory the leading energy shift is given by the eigenvalues of the matrix appearing in (6.5.36).

In the specific case that the two fermions are prepared in the same spatial state, with $n = m$, the spatial wave-function is necessarily symmetric and so antisymmetry of the 2-particle state under $M \leftrightarrow N$ only allows the antisymmetric combination of spins with $S = 0$. This is true in particular if both fermions are put into the ground state $\psi_0(\mathbf{x})$, and so the 2-particle ground state is necessarily a spin singlet. Since $U_c = U_e$ when $n = m$ — and keeping in mind the additional factor of $\frac{1}{2}$ discussed in (6.5.32) — the energy of the $S = 0$ case when $n = m$ becomes

$$\delta\mathcal{E}_{n=m,S=0} = \frac{1}{2}(U_c + U_e) = U_c\,. \tag{6.5.39}$$

Worked example: He energy levels

To get an idea of the size of the result consider the special case of atomic energy levels in atomic Helium. We can perform the integrals in U_c and U_e explicitly when the background potential is given by $V(r) = -Z\alpha/r$, and where both ψ_n and ψ_m are the single-particle ground state for $V(r)$ (for which both electrons have $n = 1$ and $\ell = \ell_z = 0$) and so

$$|\psi_0(r)|^2 = \frac{1}{\pi a_z^3}\, e^{-2r/a_z} \tag{6.5.40}$$

where $1/a_z = Z\alpha\mu = Z/a_0$ is the Bohr radius for a nucleus of charge Z (and a_0 is the corresponding quantity for Hydrogen). As a check of normalization the average nuclear Coulomb energy in this state is

$$\left\langle \frac{Z\alpha}{r} \right\rangle = \frac{4\pi Z\alpha}{\pi a_z^3} \int_0^\infty \mathrm{d}r\, r\, e^{-2r/a_z} = \frac{4\pi Z\alpha}{\pi a_z^3} \left(\frac{a_z}{2}\right)^2 = \frac{Z\alpha}{a_z} = (Z\alpha)^2\mu \tag{6.5.41}$$

as expected, which uses the integrals

$$\int_a^b \mathrm{d}x\, e^{-\lambda x} = \frac{1}{\lambda}\Big(e^{-\lambda a} - e^{-\lambda b}\Big)\,, \tag{6.5.42}$$

$$\int_a^b \mathrm{d}x\, x\, e^{-\lambda x} = \frac{1}{\lambda^2}\Big(e^{-\lambda a} - e^{-\lambda b}\Big) + \frac{1}{\lambda}\Big(a\, e^{-\lambda a} - b\, e^{-\lambda b}\Big)\,, \tag{6.5.43}$$

and

$$\int_a^b \mathrm{d}x\, x^2\, e^{-\lambda x} = \frac{2}{\lambda^3}\Big(e^{-\lambda a} - e^{-\lambda b}\Big) + \frac{2}{\lambda^2}\Big(a\, e^{-\lambda a} - b\, e^{-\lambda b}\Big) + \frac{1}{\lambda}\Big(a^2\, e^{-\lambda a} - b^2\, e^{-\lambda b}\Big)\,. \tag{6.5.44}$$

With this state the integrals appearing in the inter-electron Coulomb energy are (using $\alpha = e^2/4\pi$)

$$\begin{aligned} U_c = U_e &= \alpha \int \mathrm{d}^3x\, \mathrm{d}^3y\, \frac{|\psi_0(x)|^2 |\psi_0(y)|^2}{|\mathbf{x}-\mathbf{y}|} \\ &= \frac{4\pi\alpha}{(\pi a_z^3)^2} \int_0^\infty \mathrm{d}x\, x^2 \left\{ 2\pi \int_0^\infty \mathrm{d}y\, y^2 \int_{-1}^1 \mathrm{d}u\, \frac{e^{-2x/a_z - 2y/a_z}}{\sqrt{x^2+y^2-2xyu}} \right\}\,, \end{aligned} \tag{6.5.45}$$

which evaluates the two volume integrals in spherical polar coordinates, using the $\mathbf{x}$ direction to define the z-axis when performing the $\mathrm{d}^3y = y^2 \sin\theta\, \mathrm{d}y\, \mathrm{d}\theta\, \mathrm{d}\phi$ integration. The variables $x = |\mathbf{x}|$ and $y = |\mathbf{y}|$

are the radial coordinates in the two integrations, and the integral over the direction of $\mathbf{x}$ is trivial (leading to the overall factor of 4π). The integral over $u = \cos\theta$ is an elementary one

$$\int \frac{\mathrm{d}u}{\sqrt{A - Bu}} = -\frac{2}{B}\sqrt{A - Bu}\,, \tag{6.5.46}$$

and so

$$\begin{aligned}\int_{-1}^{1} \frac{\mathrm{d}u}{\sqrt{x^2 + y^2 - 2xyu}} &= \frac{1}{xy}\Big[\sqrt{x^2 + y^2 + 2xy} - \sqrt{x^2 + y^2 - 2xy}\Big] \\ &= \frac{1}{xy}\Big(x + y - |x - y|\Big) = \begin{cases} 2/x & \text{if } x > y \\ 2/y & \text{if } x < y \end{cases}\end{aligned} \tag{6.5.47}$$

leading to the result

$$\begin{aligned} U_c = U_e &= \frac{16\alpha}{a_z^6}\int_0^\infty \mathrm{d}x\, x^2 e^{-2x/a_z}\left\{\frac{1}{x}\int_0^x \mathrm{d}y\, y^2 e^{-2y/a_z} + \int_x^\infty \mathrm{d}y\, y\, e^{-2y/a_z}\right\} \\ &= \frac{5\alpha}{8a_z} = \frac{5}{8}(Z\alpha^2)\mu\,. \end{aligned} \tag{6.5.48}$$

Putting everything together, keeping in mind the $S = 0$ energy shift is given by $\frac{1}{2}(U_c + U_e) = U_c$ — *c.f.* (6.5.39) — in this approximation the He ground state energy is

$$\mathcal{E}_0 \simeq 2\varepsilon_0 + \delta\mathcal{E}_0 = 2\left[-\frac{(Z\alpha)^2\mu}{2}\right] + \frac{5}{8}(Z\alpha^2)\mu = \left(-2Z^2 + \frac{5Z}{4}\right)\frac{\alpha^2\mu}{2}\,, \tag{6.5.49}$$

where the combination $R_\infty := \frac{1}{2}\mu\alpha^2 \simeq 13.6$ eV is the binding energy of Hydrogen (a unit called the Rydberg). Using $Z = 2$ then gives $\mathcal{E}_0 \simeq (-8 + \frac{5}{2})R_\infty = (-109 + 34)\,\mathrm{eV} = -75$ eV. For comparison, the energy of a single electron orbiting a He nucleus would have been $\mathcal{E}_0^{\text{ion}} \simeq \varepsilon_0 = -Z^2 R_\infty \simeq -54.4$ eV. These imply the energy cost for stripping off the first electron is predicted to be $75 - 54 = 21$ eV and energy cost to remove both is 75 eV. The experimental values for these two ionization energies are 24.587387936(25) eV for the first electron and 54.41776311(2) eV for the second one, showing that the simple perturbative result works to within about 3 eV out of 75 eV, or about 4%.

The fact that perturbation theory works this well might come as a surprise, given that the ratio of the inter-electron-repulsion correction to the Hydrogen-like leading term has relative size $5/(8Z)$ and so is only truly small if the nuclear charge Z is very large. However this is not the relevant comparison, because using the Hydrogen-like solutions treats the interaction with the nucleus exactly[13] in $Z\alpha$. What counts for the validity of perturbation theory is the size of higher powers of H_{Coul} compared with the basic Hydrogen-like energy shift and the interplay of the Coulomb interaction with other atomic effects, like magnetic moments and relativistic corrections. These can be much smaller since each factor of H_{Coul} comes with an additional factor of $\alpha = e^2/4\pi \sim 1/137$.

The spin-dependent splitting between triplet and singlet spin configurations predicted by (6.5.37) also is relevant to Helium, but plays a role for excited states for which spin-triplet combinations are possible. For instance the first excited level for He puts one electron into the $(n, \ell, \ell_z) = (1, 0, 0)$ ground state but puts the other into one of the $n = 2$ states $(2, \ell, \ell_z)$ with $\ell = 0, 1$. For any state

[13] Using the Coulomb interaction does neglect nuclear recoil and finite-nuclear-size effects, but these are suppressed by powers of the electron to nuclear mass ratio: $\mu/M \sim 10^{-4}$ for He.

(n, ℓ, ℓ_z) eq. (6.5.37) predicts that it is the spin-1 combination (called *ortho-Helium*) that has a lower energy than the spin-0 combination (called *para-Helium*). Since the energy of a Hydrogen-like state is proportional to Z^2/n^2, where n is the principal quantum number, in the approximation used here their energies are given by

$$\mathcal{E}_n = -Z^2 R_\infty - \frac{Z^2}{n^2} R_\infty + (U_c \pm U_e) \tag{6.5.50}$$

where the upper (lower) sign is for $S = 0$ ($S = 1$) and (6.5.35) gives the following 'direct' and 'exchange' integrals

$$\begin{aligned} U_c &:= \frac{e^2}{4\pi} \int \mathrm{d}^3x \, \mathrm{d}^3y \, \frac{\psi^*_{100}(\mathbf{x},t)\psi_{100}(\mathbf{x},t)\; \psi^*_{n\ell\ell_z}(\mathbf{y},t)\psi_{n\ell\ell_z}(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|} \\ \text{and} \quad U_e &:= \frac{e^2}{4\pi} \int \mathrm{d}^3x \, \mathrm{d}^3y \, \frac{\psi^*_{100}(\mathbf{x},t)\psi_{n\ell\ell_z}(\mathbf{x},t)\; \psi^*_{n\ell\ell_z}(\mathbf{y},t)\psi_{100}(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|} \,. \end{aligned} \tag{6.5.51}$$

7 Semiclassical methods

This section describes some practical examples of the interactions described in the previous section, using the phenomenon of Bose-Einstein condensation to illustrate the use of semi-classical methods.

7.1 Bose-Einstein condensation

Earlier sections discussed coherent states as energy eigenstates that can arise for bosonic fields in the presence of source particles when an interaction allows these sources to create or destroy the bosons. This provided a simple model of how quantum bosonic fields can behave as classical fields, doing so in situations where bosons can carry very small energy and so be copiously produced by large static sources.

This section describes a second, related, example of this type – Bose-Einstein condensation – where even more massive bosons, such as atoms, can behave as classical fields. Bose-Einstein condensation happens in situations where a boson carries a conserved charge and so the total number of bosons can be fixed. When a boson does not carry a conserved charge the energy of a system can always be reduced simply by removing bosons from it. The ground state is then the state with no bosons (such as is the case for photons in Quantum Electrodynamics, for example).

But if a boson carries a conserved charge then the minimum energy for a (weakly interacting) system carrying nonzero charge puts all the bosons into the same minimum single-particle energy state. Minimizing the energy for a given charge can put macroscopic numbers of bosons into the lowest-energy single-particle state available. For example, for a system of non-interacting bosons described by the Hamiltonian

$$H = E_0 + \sum_p \left(\frac{\mathbf{p}^2}{2m} + \varepsilon_0 \right) a^\star_{\mathbf{p}} a_{\mathbf{p}} = E_0 + \int \mathrm{d}^3p \, \left(\frac{\mathbf{p}^2}{2m} + \varepsilon_0 \right) \mathfrak{a}^\star_{\mathbf{p}} \mathfrak{a}_{\mathbf{p}} \,, \tag{7.1.1}$$

the total number of particles, $\mathcal{N} = \sum_p a_p^\star a_p$, is conserved and the ground-state, $|\Phi\rangle$, for a collection of N particles satisfies

$$\mathcal{N}|\Phi\rangle = N|\Phi\rangle \quad \text{and} \quad H|\Phi\rangle = (E_0 + N\varepsilon_0)|\Phi\rangle\,, \tag{7.1.2}$$

corresponding to putting all particles into the minimum-energy state (which has $\mathbf{p} = 0$): $|\Phi\rangle \propto (a_0^\star)^N|0\rangle$. The same would be approximately true if weak interactions were included that also do not change N. By contrast, if weak interactions were to allow N to change the ground state would instead be found by reducing N (assuming $\varepsilon_0 > 0$) leading to a ground-state energy that is approximately simply E_0.

Worked example: Bose-Einstein condensation

This has physical implications, in particular for statistical distributions of particles for which N can fluctuate. To see how this works it is useful to reconsider the Grand Canonical ensemble considered in §1.6.1. To this end recall that the Grand Canonical ensemble assigns probabilities to any given state of the form

$$p_n = \frac{e^{-\beta(E_n - \mu N_n)}}{Z} \qquad \text{where} \qquad Z = \sum_n e^{-\beta(E_n-\mu N_n)} = \mathrm{Tr}\left[e^{-\beta(H-\mu\mathcal{N})}\right], \tag{7.1.3}$$

so that $\sum_n p_n = 1$. The parameter μ is to be chosen so that the average number of particles takes a specified value. That is, μ is determined as a function of $\langle\mathcal{N}\rangle$ by solving

$$\langle\mathcal{N}\rangle = \sum_n p_n N_n = \frac{1}{Z}\sum_n N_n\, e^{-\beta(E_n-\mu N_n)} = \frac{1}{\beta Z}\frac{\partial}{\partial\mu}\sum_n e^{-\beta(E_n-\mu N_n)} = \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z\,. \tag{7.1.4}$$

Because $\langle\mathcal{N}\rangle$ and β are positive this shows that Z is a monotonically increasing function of μ. Differentiating again shows that

$$\frac{1}{\beta}\frac{\partial^2}{\partial\mu^2}\ln Z = \frac{\partial}{\partial\mu}\langle\mathcal{N}\rangle = \frac{\partial}{\partial\mu}\left[\frac{1}{Z}\sum_n N_n\, e^{-\beta(E_n-\mu N_n)}\right] = \beta\langle\mathcal{N}^2 - \langle\mathcal{N}\rangle^2\rangle\,, \tag{7.1.5}$$

where the first term comes from differentiating the explicitly written μ-dependence and the second term comes from differentiating Z, using (7.1.4). Because $\langle\mathcal{N}^2 - \langle\mathcal{N}\rangle^2\rangle = \langle(\mathcal{N} - \langle\mathcal{N}\rangle)^2\rangle$, the right-hand side of (7.1.5) is also positive, showing that $\ln Z$ is concave up. When used in (7.1.4) this also shows that $\langle\mathcal{N}\rangle$ increases monotonically with μ.

As applied to free particles with the dispersion relation $\varepsilon(\mathbf{p}) = \varepsilon_0 + \mathbf{p}^2/(2m)$ expression (7.1.3) evaluates to

$$Z = \prod_p \sum_{N_p=0}^{\infty} e^{-\beta[\varepsilon(p)-\mu]N_p} = \prod_p \frac{1}{1-\exp\{-\beta[\varepsilon(p)-\mu]\}}\,, \tag{7.1.6}$$

and so (recalling that the grand thermodynamic potential, Ξ, is defined by $Z =: e^{-\beta\Xi}$) one finds

$$\Xi = -\frac{1}{\beta}\ln Z = \frac{1}{\beta}\sum_p \ln\left(1 - e^{-\beta[\varepsilon(p)-\mu]}\right), \tag{7.1.7}$$

and the average particle number (7.1.4) becomes

$$\langle\mathcal{N}\rangle = -\left(\frac{\partial\Xi}{\partial\mu}\right)_\beta = \sum_p \frac{1}{e^{\beta[\varepsilon(p)-\mu]} - 1}\,, \tag{7.1.8}$$

where $\varepsilon(\mathbf{p}) - \mu = (\varepsilon_0 - \mu) + \mathbf{p}^2/(2m)$.

The above manipulations show that the properties of these sums change dramatically once $\mu > \varepsilon_0$, since at this point the sign of the argument of the exponential changes for sufficiently small $|\mathbf{p}|$. When $\epsilon_0 - \mu$ is positive the probability of (7.1.3) is maximized when N_p is smallest (*i.e.* zero). How much of a penalty in probability is paid to occupy larger N_p then depends on the size of $\beta[\varepsilon(\mathbf{p}) - \mu]$. But once $\mu > \varepsilon_0$ this logic flips and the probability is maximized when N_p is as large as possible. In particular whenever $\varepsilon(p) - \mu < 0$ the exponential $e^{-\beta[\varepsilon(p)-\mu]N_p}$ is greater than unity and so the sum in (7.1.6) diverges.

So what happens if $\langle \mathcal{N} \rangle$ is ramped up to the point that μ first becomes equal to ε_0 for a real gas of bosons? As (7.1.6) shows, a problem develops, but at $\mu = \varepsilon_0$ this only happens for the specific mode $\mathbf{p} = 0$. The rest of the product over nonzero $\mathbf{p}$ satisfies $\varepsilon(\mathbf{p}) - \mu > 0$ and so remains convergent.

To understand what this implies in the large-$\mathcal{V}$ limit, separate out the $\mathbf{p} = 0$ state explicitly and combine the sum over nonzero momenta into an integral. In this case (7.1.7) and (7.1.8) become

$$\begin{aligned} \frac{\Xi}{\mathcal{V}} &= -\frac{1}{\beta\mathcal{V}} \ln Z = \frac{1}{\beta\mathcal{V}} \sum_p \ln\Bigl(1 - e^{-\beta[\varepsilon(p)-\mu]}\Bigr) \\ &= \frac{1}{\beta\mathcal{V}} \ln(1-z) + \frac{1}{\beta} \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \ln\Bigl(1 - z\, e^{-\beta p^2/(2m)}\Bigr) \\ &= \frac{1}{\beta\mathcal{V}} \ln(1-z) + \frac{4}{\sqrt{\pi}\beta\lambda^3} \int_0^\infty \mathrm{d}x\, x^2 \ln\Bigl(1 - z\, e^{-x^2}\Bigr), \end{aligned} \tag{7.1.9}$$

and

$$\frac{\langle \mathcal{N} \rangle}{\mathcal{V}} = -\frac{1}{\mathcal{V}} \frac{\partial \Xi}{\partial \mu} = \frac{1}{\mathcal{V}} \left(\frac{z}{1-z}\right) + \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \left[\frac{1}{z^{-1} e^{\beta p^2/(2m)} - 1}\right], \tag{7.1.10}$$

where the first term on the right-hand side of the last equality in each of these expressions is the contribution of the $\mathbf{p} = 0$ mode, while the *fugacity* z (a convenient proxy for μ) and the thermal length scale λ are defined by

$$z := e^{\beta(\mu - \varepsilon_0)} \quad \text{and} \quad \lambda := \sqrt{\frac{2\pi\beta}{m}} = \sqrt{\frac{2\pi}{mT}}. \tag{7.1.11}$$

In particular (7.1.10) shows that the total number of particles in the $\mathbf{p} = 0$ mode is

$$N_0 := \frac{z}{1-z}. \tag{7.1.12}$$

If z were finite then the *density* of such particles, $\langle N_0 \rangle / \mathcal{V}$, would vanish in the thermodynamic limit as $\mathcal{V} \to \infty$. What happens instead is that when $z \to 1$ the divergence in $z/(1-z)$ can become proportional to $\mathcal{V}$, allowing a finite macroscopic density to survive into the infinite-volume limit. The goal now is to identify the circumstances where this is what happens.

To this end it is useful to define the functions

$$g_n(z) := \sum_{k=1}^\infty \frac{z^k}{k^n} \tag{7.1.13}$$

because then term-by-term integration of the expansion of the integrand in powers of z shows that

$$\int_0^\infty \mathrm{d}x\, x^2 \ln\Bigl(1 - z e^{-x^2}\Bigr) = -\frac{\sqrt{\pi}}{4}\, g_{5/2}(z) \tag{7.1.14}$$

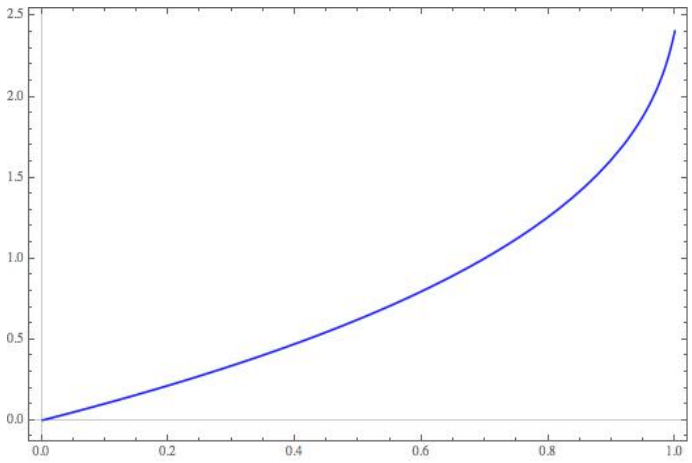


Figure 5. A plot of the function $g_{3/2}(z)$ relevant to Bose-Einstein condensation.

and so

$$\frac{\Xi}{\mathcal{V}} = \frac{1}{\beta\mathcal{V}} \ln(1-z) - \frac{1}{\beta\lambda^3}\, g_{5/2}(z)\,. \tag{7.1.15}$$

Similarly, using

$$g_{3/2} = z\frac{\partial g_{5/2}}{\partial z}\,, \tag{7.1.16}$$

then shows that

$$\frac{\langle\mathcal{N}\rangle}{\mathcal{V}} = \frac{1}{\mathcal{V}}\,\frac{z}{1-z} + \frac{1}{\lambda^3}\, g_{3/2}(z)\,. \tag{7.1.17}$$

What is important is that $g_{3/2}(z)$ is a monotonically increasing function of z that starts with $g_{3/2}(0) = 0$ and approaches a finite value as $z \to 1$

$$g_{3/2}(1) = \zeta_R(3/2) = 2.612\cdots \tag{7.1.18}$$

where $\zeta_R(s)$ is the Riemann zeta-function. Notice $g_{3/2}(z)$ approaches this value with infinite slope, since $\mathrm{d}g_{3/2}/\mathrm{d}z \to \infty$ as $z \to 1$ (see Fig. 5).

To see what this means in practice imagine solving (7.1.17) for z (and so also $\beta\mu$) starting from a given mean particle density, $\mathfrak{n} := \langle\mathcal{N}\rangle/\mathcal{V}$. As $\mathfrak{n}$ rises from zero so does z, and for any finite $z < 1$ the first term in (7.1.17) vanishes in the $\mathcal{V} \to \infty$ limit, leaving only the second term (from which the desired value of z can be found, for example, by solving graphically using Fig. 5). For large but finite $\mathcal{V}$ the first term does not vanish and so both terms must be used to determine z, and once z is found the total number of particles in the $\mathbf{p} = 0$ state is $\langle\mathcal{N}\rangle_0 = z/(1-z)$.

This all works until the density starts to approach the critical value

$$\mathfrak{n}_c = \frac{g_{3/2}(1)}{\lambda^3} \simeq \frac{2.612}{\lambda^3}\,. \tag{7.1.19}$$

But as $\mathfrak{n} \to \mathfrak{n}_c$ we know $z \to 1$ and so the first term in (7.1.17) starts to grow without bound. This shows that for $\mathfrak{n} > \mathfrak{n}_c$ the second term no longer increases beyond its value at $z = 1$ and so the only way to match the growth of the left-hand side is by growing $\langle\mathcal{N}\rangle_0$ in the first term; any additional

particles go into the ground state. Since $\langle\mathcal{N}\rangle$ is proportional to $\mathcal{V}$ the growth in $\langle\mathcal{N}\rangle_0$ this implies is proportional to $\mathcal{V}$, leaving the first term on the right-hand side of (7.1.17) finite in the limit $\mathcal{V}\to\infty$, with

$$\mathfrak{n} = \mathfrak{n}_0 + \frac{g_{3/2}(1)}{\lambda^3} \simeq \mathfrak{n}_0 + \frac{2.612}{\lambda^3}\,, \tag{7.1.20}$$

where $\mathfrak{n}_0 := \langle\mathcal{N}\rangle_0/\mathcal{V}$.

For densities $\mathfrak{n} > \mathfrak{n}_c$ this argument reveals there are two fluids: a Bose gas with $z = 1$ plus a macroscopically occupied ground state. In the limit $\mathcal{V}\to\infty$ this is a phase transition, with discontinuities in thermodynamic properties across the critical boundary, which occurs when $\mathfrak{n} = \mathfrak{n}_c$, or equivalently

$$\mathfrak{n}\lambda^3 = \mathfrak{n}\left(\frac{2\pi}{mT}\right)^{3/2} = g_{3/2}(1) \simeq 2.612\,. \tag{7.1.21}$$

This shows that the ground state becomes macroscopically occupied once the interparticle spacing is of order the thermal length scale λ.

If T is raised for fixed n then eq. (7.1.20) implies the fraction of particles in the ground state varies as

$$\frac{\mathfrak{n}_0}{\mathfrak{n}} = 1 - \frac{g_{3/2}(1)}{\mathfrak{n}}\left(\frac{mT}{2\pi}\right)^{3/2} = 1 - \left(\frac{T}{T_c}\right)^{3/2} \qquad (\text{for } T < T_c)\,, \tag{7.1.22}$$

and vanishes (for $\mathcal{V}\to\infty$) when $T > T_c$ where the critical temperature is defined by

$$T_c := \frac{2\pi}{m}\left[\frac{\mathfrak{n}}{g_{3/2}(1)}\right]^{2/3} \simeq 3.3\,\frac{\mathfrak{n}^{2/3}}{m}\,. \tag{7.1.23}$$

To get a feel for the numbers, if $m \simeq 4$ GeV (as for He atoms) and $\mathfrak{n} \simeq 10^9/\text{cm}^3 \simeq 10^{-30}/\text{fm}^3 \simeq 8\times10^{-33}$ GeV^3 then $T_c \simeq 3.3(8\times10^{-33})^{2/3}/4$ GeV$\simeq 3\times10^{-13}$ eV$\simeq 4$ nK.

7.1.1 Maximum density with repulsive interactions

In the absence of interactions there is no limit to the number $\mathfrak{n}_0$ of bosons that can be crammed in this way into the lowest-energy single-particle state. But this need no longer be true once the bosons interact, such as through the contact interaction of (6.4.1) (which is a repulsive interaction for $g > 0$). To see how this limit comes about adopt therefore the Hamiltonian

$$\begin{aligned} H &= \int \mathrm{d}^3x\, \left[\Phi^\star\left(-\frac{\nabla^2}{2m} + \varepsilon_0\right)\Phi + g(\Phi^\star\Phi)^2\right] \\ &= \sum_{\mathbf{p}}\left[\left(\frac{\mathbf{p}^2}{2m} + \varepsilon_0\right) a^\star_{\mathbf{p}} a_{\mathbf{p}}\right] + \frac{g}{\mathcal{V}}\sum_{\mathbf{pqkl}} \delta_{\mathbf{p}-\mathbf{q}+\mathbf{k}-\mathbf{l}}\, a^\star_{\mathbf{p}} a_{\mathbf{q}} a^\star_{\mathbf{k}} a_{\mathbf{l}}\,, \end{aligned} \tag{7.1.24}$$

and recall that the mode that is macroscopically occupied has $\mathbf{p} = 0$ and so contributes a position-independent amount to the position-space field:

$$\Phi(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{p}} a_{\mathbf{p}}\, e^{i\mathbf{p}\cdot\mathbf{x}} = \Phi_0 + \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\, \mathfrak{a}_{\mathbf{p}}\, e^{i\mathbf{p}\cdot\mathbf{x}} =: \Phi_0 + \hat\Phi(\mathbf{x})\,, \tag{7.1.25}$$

where Φ_0 is $\mathbf{x}$-independent and $\hat{\Phi}(\mathbf{x})$ contains all of the rest of the modes. In order not to double count the constant mode the field $\hat{\Phi}(\mathbf{x})$ must satisfy

$$\int \mathrm{d}^3x\ \hat{\Phi}(\mathbf{x}) = 0\,. \tag{7.1.26}$$

Using $\Phi(\mathbf{x}) = \Phi_0 + \hat{\Phi}(\mathbf{x})$ in the number operator gives

$$\mathcal{N} = \int \mathrm{d}^3x\ \Phi^\star(\mathbf{x})\Phi(\mathbf{x}) = \int \mathrm{d}^3x \Big[\Phi_0^\star\Phi_0 + \hat{\Phi}^\star(\mathbf{x})\hat{\Phi}(\mathbf{x})\Big]\,, \tag{7.1.27}$$

which uses (7.1.26) to eliminate the $\Phi_0\hat{\Phi}$ cross terms. The second term counts the particles in the Bose gas, as usual, revealing the quantity

$$\Phi_0^\star\Phi_0 = \mathfrak{n}_0 = \frac{\langle\mathcal{N}\rangle_0}{\mathcal{V}}\,, \tag{7.1.28}$$

to be the density of particles in the $\mathbf{p} = 0$ state.

Using $\Phi(\mathbf{x}) = \Phi_0 + \hat{\Phi}(\mathbf{x})$ in the Hamiltonian similarly gives

$$\begin{aligned} H &= \int \mathrm{d}^3x\ \left\{\varepsilon_0\ \Phi_0^\star\Phi_0 + \hat{\Phi}^\star\left(-\frac{\nabla^2}{2m} + \varepsilon_0\right)\hat{\Phi} + g\left[(\Phi_0 + \hat{\Phi})^\star(\Phi_0 + \hat{\Phi})\right]^2\right\} \\ &= \int \mathrm{d}^3x\ \left\{\varepsilon_0\ \Phi_0^\star\Phi_0 + \hat{\Phi}^\star\left(-\frac{\nabla^2}{2m} + \varepsilon_0\right)\hat{\Phi} + g(\Phi_0^\star\Phi_0)^2\right. \\ &\qquad\qquad +4g\,\Phi_0^\star\Phi_0\,\hat{\Phi}^\star\hat{\Phi} + g\Big[(\Phi_0^\star)^2\hat{\Phi}^2 + \Phi_0^2\,(\hat{\Phi}^\star)^2\Big] \\ &\qquad\qquad \left. + 2g\Big[\Phi_0^\star\,\hat{\Phi}^\star\hat{\Phi}^2 + \Phi_0\,\hat{\Phi}(\hat{\Phi}^\star)^2\Big] + g(\hat{\Phi}^\star\hat{\Phi})^2\right\}\,, \end{aligned} \tag{7.1.29}$$

which again uses (7.1.26) to eliminate the terms linear in $\hat{\Phi}$ and $\hat{\Phi}^\star$. When there are macroscopically many particles, most of which sit in the $\mathbf{p} = 0$ state (as the previous section shows happens for low enough temperatures), the matrix element of each factor of Φ_0 is of order $\sqrt{\mathfrak{n}_0} \gg 1$ and so the second and third lines of the last equality can be dropped relative to the first line, making $(\Phi_0^\star\Phi_0)^2$ dominate the other interactions terms.

To determine the energetically preferred value of $\mathfrak{n}_0$ consider now the contribution of this specific mode to the system's energy, including the repulsive contact interaction. The optimal value for $\mathfrak{n}_0$ is found by minimizing the energy $\langle H\rangle$, while holding fixed the total number $\langle\mathcal{N}\rangle$ of particles to equal whatever value is appropriate for the system of interest: $\langle\mathcal{N}\rangle = N_{\text{sys}}$. Such a minimization subject to a constraint can be performed using the method of Lagrange multipliers, summarized in Appendix A.2, which (denoting the Lagrange multiplier by $\lambda = -\mu$) asks us to freely extremize the following function

$$F := \langle H\rangle - \mu(\langle\mathcal{N}\rangle - N_{\text{sys}})\,, \tag{7.1.30}$$

against variations of all physical variables (such as $\mathfrak{n}_0$, but also including the new Lagrange multiplier, μ) *without* imposing any constraints. The constraint $\langle\mathcal{N}\rangle = N_{\text{sys}}$ is instead now

regardeded as a consequnce of extremizing with respect to μ (*i.e.* follows from the condition $\partial F/\partial\mu = 0$).

When there are macroscopically large numbers of particles sitting in the ground state the part of F involving $\mathfrak{n}_0$ is well-approximated by

$$F_0 = H_0 - \mu N_0 \simeq \int \mathrm{d}^3x \left[(\varepsilon_0 - \mu)\, \Phi_0^* \Phi_0 + g(\Phi_0^* \Phi_0)^2 \right] , \tag{7.1.31}$$

and so when the expectation value is evaluated in a state that diagonalizes $N_0 = a_0^\star a_0$ (and so also $\Phi_0^\star \Phi_0 = N_0/\mathcal{V} = \mathfrak{n}_0$) with a macroscopic number of $\mathbf{p} = 0$ particles this gives

$$\frac{\langle H - \mu \mathcal{N} \rangle}{\mathcal{V}} \simeq (\varepsilon_0 - \mu)\, \mathfrak{n}_0 + g\mathfrak{n}_0^2 \,. \tag{7.1.32}$$

This quantity vanishes when $\mathfrak{n}_0 = 0$ and this is also the minimizing configuration when $\varepsilon_0 > \mu$. But once $\mu > \varepsilon_0$ then $\langle H - \mu\mathcal{N} \rangle$ can be lowered by having $\mathfrak{n}_0 \neq 0$. When $g = 0$ there is no minimum because $\langle H - \mu\mathcal{N} \rangle$ can be made arbitrarily negative in this way, but for $g \neq 0$ there is an optimal value for $\mathfrak{n}_0$ above which further growth raises the energy because of the energy penalty required to overcome the repulsive interaction. This optimal value is found by minimizing $\langle H - \mu\mathcal{N} \rangle$ and so is given by

$$\mathfrak{n}_0^{\rm opt} = \frac{\mu - \varepsilon_0}{2g} \,. \tag{7.1.33}$$

This value lies within the regime of large occupation number provided g is small enough. When (7.1.33) is satisfied the free energy is lowered relative to the case $n_0 = 0$ by the amount

$$\frac{\langle H - \mu \mathcal{N} \rangle_{\rm min}}{\mathcal{V}} = - \frac{(\varepsilon_0 - \mu)^2}{4g} \,. \tag{7.1.34}$$

7.2 Bogoliubov transformation

This section explores how the above analysis can be developed more systematically as a perturbative expansion in powers of g in circumstances where $g \ll 1$, and how this expansion can also be regarded as a semiclassical expansion around a classical background field.

7.2.1 Classical Schrödinger field

The above argument shows that when $\varepsilon(\mathbf{p}) = \varepsilon_0 + \mathbf{p}^2/(2m)$ for bosonic fields the mode with minimum single-particle energy – *i.e.* the one with $\mathbf{p} = 0$ – can become macroscopically occupied.[14] This subsection explores this phenomenon in more detail, with the goal of better understanding the macroscopically occupied state and the relation between this state and a classical field, φ_0.

[14] The same can also happen to modes with nonzero momentum given the right combination of sources, such as found above for coherent states.

Later sections explore how such configurations transform under symmetries, and explores the implications of situations where φ_0 is *not* invariant under a symmetry transformation. Along the way we discuss why it is possible to have a non-invariant ground state at all, since although it is a common occurrence in quantum field theory it has no counterpart in single-particle quantum mechanics.

Both Φ_0 and $\hat{\Phi}(\mathbf{x})$ are quantum operators, but as we saw in §5.3 for coherent states, once a macroscopically large number of particles are placed into a Bose-Einstein condensate the quantum operator Φ_0 can be approximated by a classical number φ_0. In the present instance the failure of Φ_0 to commute follows from

$$[a_0, a_0^\star] = 1 \qquad \text{which implies} \qquad [\Phi_0, \Phi_0^\star] = \frac{1}{\mathcal{V}} \tag{7.2.1}$$

showing that quantum effects involving Φ_0 are suppressed by an inverse power of the volume. Approximating a quantum field by a classical field turns out to be useful, particularly when studying the symmetry properties of the ground state. The value to be chosen by this classical quantity φ_0 is determined by the particle density, $\mathfrak{n}_0 = \langle \mathcal{N} \rangle_0 / \mathcal{V}$ in the $\mathbf{p} = 0$ state.

To determine the value of φ_0 consider using $\Phi(\mathbf{x}) = \varphi_0 + \hat{\Phi}(\mathbf{x})$ in the number operator

$$N = \int \mathrm{d}^3x \; \Phi^\star(\mathbf{x})\Phi(\mathbf{x}) = \int \mathrm{d}^3x \Big[\varphi_0^* \varphi_0 + \hat{\Phi}^\star(\mathbf{x})\hat{\Phi}(\mathbf{x}) \Big] , \tag{7.2.2}$$

which uses (7.1.26) to eliminate the $\varphi_0 - \hat{\Phi}$ cross terms. The second term counts the particles in the Bose gas, as usual, revealing the combination

$$\varphi_0^* \varphi_0 = \mathfrak{n}_0 = \frac{\langle N_0 \rangle}{\mathcal{V}} , \tag{7.2.3}$$

to be the density of particles in the $\mathbf{p} = 0$ state.

This classical treatment of A_0 can be understood more formally as the use of a coherent state in the zero-momentum sector. That is, although (7.1.31) commutes with the number operator, $a_0^\star a_0$, the same is not true for the whole of (7.1.29). This means that the system's ground state need not be a Fock state that diagonalizes $a_0^\star a_0$ and instead could be closer to a coherent state, $|\alpha_0\rangle$, that satisfies $a_0|\alpha_0\rangle = \alpha_0|\alpha_0\rangle$. Diagonalizing a_0 automatically ensures Φ_0 is also diagonal, with

$$\Phi_0|\alpha_0\rangle = \frac{\alpha_0}{\sqrt{\mathcal{V}}} \, |\alpha_0\rangle =: \varphi_0|\varphi_0\rangle , \tag{7.2.4}$$

where the last equality just chooses to label the coherent state using φ_0 rather than α_0.

The state $|\varphi_0\rangle$ does not do a bad job of describing the expectation of (7.1.31) either, despite it not diagonalizing $a_0^\star a_0$. This is because (7.2.1) shows that the difference between $(\Phi_0^\star \Phi_0)^2$ and $(\Phi^\star)^2 \Phi_0^2$ is

$$\langle \varphi_0 | \Phi_0^\star \Phi_0 \Phi_0^\star \Phi_0 | \varphi_0 \rangle = \langle \varphi_0 | \left(\Phi_0^\star \Phi_0^\star \Phi_0 \Phi_0 + \frac{1}{\mathcal{V}} \, \Phi_0^\star \Phi_0 \right) | \varphi_0 \rangle = |\varphi_0|^4 + \frac{|\varphi_0|^2}{\mathcal{V}} , \tag{7.2.5}$$

and so

$$\frac{\langle\varphi_0|F_0|\varphi_0\rangle}{\mathcal{V}} = \left(\varepsilon_0 - \mu + \frac{g}{\mathcal{V}}\right)\varphi_0^*\varphi_0 + g(\varphi_0^\star\varphi_0)^2 \simeq (\varepsilon_0-\mu)\varphi_0^*\varphi_0 + g(\varphi_0^\star\varphi_0)^2\,. \tag{7.2.6}$$

As was the case for $\mathfrak{n}_0$, the value of φ_0 (and so also α_0) for the zero-mode state $|\varphi_0\rangle$ is chosen to minimize the expectation value of the free energy, (7.2.6). The same arguments as before therefore imply that

$$\varphi_0 = \sqrt{n_0^{\rm opt}}\; e^{i\Theta} = \sqrt{\frac{\mu-\varepsilon_0}{2g}}\; e^{i\Theta}\,, \tag{7.2.7}$$

where the phase Θ is arbitrary. Experience with coherent states tells us that treating the zero-mode in a classical approximation like this is best when the classical field is large (*i.e.* the state is highly occupied). Eq. (7.2.7) shows that a classical description therefore gets better and better the smaller g is (so long as g remains nonzero).

Finally, notice that minimization of $\langle F\rangle$ cannot determine the phase of φ_0 because H and N both are left invariant by the transformation

$$\Phi(\mathbf{x}) \to \Phi(\mathbf{x})\, e^{i\vartheta}\,, \tag{7.2.8}$$

where ϑ is an arbitrary real number. Because this symmetry takes $\varphi_0 \to \varphi_0\, e^{i\vartheta}$ it shifts the phase $\Theta \to \Theta + \vartheta$. Θ is not determined by minimizing F because F is invariant under the symmetry and this ensures it is minimized by *all* choices for Θ: the system's ground state is not unique and is instead parameterized by the continuous label Θ. Further implications of these symmetry properties are explored in §8.2.1 below.

7.2.2 Excitations

To understand the excitations around the Bose-Einstein condensate requires understanding the energy spectrum of the operator $\hat\Phi(\mathbf{x})$, defined by $\Phi(\mathbf{x}) = \Phi_0 + \hat\Phi(\mathbf{x})$, where Φ_0 can be replaced by the classical number φ_0 in the large-volume limit $\mathcal{V}\to\infty$. The dependence of the Hamiltonian on $\hat\Phi(\mathbf{x})$ is given in (7.1.29), and has the form

$$H = H_0 + H_2 + H_3 + H_4 \tag{7.2.9}$$

where H_s contains s powers of $\hat\Phi$, and $H_1 = 0$ once φ_0 is chosen to minimize the energy, as in (7.2.7). The nonzero terms are given by

$$\begin{aligned}
H_0 &= \int \mathrm{d}^3x\, \Big[\varepsilon_0\, \varphi_0^\star\varphi_0 + g(\varphi_0^\star\varphi_0)^2\Big] = \mathcal{V}\Big[\varepsilon_0\, \varphi_0^\star\varphi_0 + g(\varphi_0^\star\varphi_0)^2\Big] \\
H_2 &= \int \mathrm{d}^3x\, \left\{\hat\Phi^\star\left(-\frac{\nabla^2}{2m} + \varepsilon_0\right)\hat\Phi + 4g\,\varphi_0^\star\varphi_0\,\hat\Phi^\star\hat\Phi + g\Big[(\varphi_0^\star)^2\hat\Phi^2 + \varphi_0^2\,(\hat\Phi^\star)^2\Big]\right\} \\
H_3 &= 2g\int \mathrm{d}^3x\, \Big[\varphi_0^\star\,\hat\Phi^\star\hat\Phi^2 + \varphi_0\,\hat\Phi(\hat\Phi^\star)^2\Big] \\
\text{and}\quad H_4 &= g\int \mathrm{d}^3x\, (\hat\Phi^\star\hat\Phi)^2\,.
\end{aligned} \tag{7.2.10}$$

Eq. (7.2.7) shows that φ_0 can be regarded as order $g^{-1/2}$ in the limit when g is small, making this also the regime where a semiclassical expansion about a large classical background should be a good approximation. Since $H_0 \sim \mathcal{O}(g^{-1})$ in this limit while $H_2 \sim \mathcal{O}(g^0)$, $H_3 \sim \mathcal{O}(g^{1/2})$ and $H_4 \sim \mathcal{O}(g)$ the effects of H_2 through H_4 can be regarded as perturbations to the classical contribution H_0 when g is small, provided that matrix elements of $\hat{\Phi}$ are not also large for small g. In these circumstances it is worth working perturbatively in g, in which case it is H_2 (the part quadratic in $\hat{\Phi}$) that provides the leading $\mathcal{O}(g^0)$ description of quantum fluctuations of $\Phi(\mathbf{x})$ around φ_0, while H_3 contributes at order $g^{1/2}$ and H_4 at $\mathcal{O}(g)$.

Switching to momentum space by using (6.1.7) to trade $\hat{\Phi}(\mathbf{x})$ for the continuum-normalized $\mathfrak{a}_\mathbf{p}$ shows the quadratic piece H_2 has the form

$$H_2 = \int \mathrm{d}^3p \, \left[\varepsilon(\mathbf{p}) \, \mathfrak{a}^\star_\mathbf{p} \mathfrak{a}_\mathbf{p} + \frac{1}{2} W(\mathbf{p}) \, \mathfrak{a}_\mathbf{p} \mathfrak{a}_{-\mathbf{p}} + \frac{1}{2} W^*(\mathbf{p}) \, \mathfrak{a}^\star_\mathbf{p} \, \mathfrak{a}^\star_{-\mathbf{p}} \right] , \tag{7.2.11}$$

where the factors of $\frac{1}{2}$ prevent double counting in the sum over momenta, and the parameters ε and W are given in the above example by

$$\varepsilon(\mathbf{p}) = \left(\varepsilon_0 + 4g\varphi_0^*\varphi_0 \right) + \frac{\mathbf{p}^2}{2m} + \cdots \quad \text{and} \quad W(\mathbf{p}) = g\varphi_0^2 \, . \tag{7.2.12}$$

This does not yet have the form of a free-particle Hamiltonian because of the presence of the $W(\mathbf{p})$ terms, but it can be put into the standard free-particle form using an appropriate change of variables.

Bogoliubov transformation

The Hamiltonian H_2 can be diagonalized (*i.e.* put into free-particle form) by suitably redefining creation and annihilation operators, using the following *Bogoliubov* transformation

$$\mathfrak{a}_\mathbf{p} := X(p) \, \mathfrak{c}_\mathbf{p} + Y(p) \, \mathfrak{c}^\star_{-\mathbf{p}} \quad \text{and so} \quad \mathfrak{a}^\star_\mathbf{p} := X^*(p) \, \mathfrak{c}^\star_\mathbf{p} + Y^*(p) \, \mathfrak{c}_{-\mathbf{p}} \, , \tag{7.2.13}$$

with appropriately chosen coefficients $X(p)$ and $Y(p)$. Momentum conservation (or invariance under spatial translations) forbids similar terms mixing $\mathfrak{a}_\mathbf{p}$ with $\mathfrak{c}_{-\mathbf{p}}$ or $\mathfrak{c}^\star_\mathbf{p}$ (or mixing $\mathfrak{a}^\star_\mathbf{p}$ with $\mathfrak{c}_\mathbf{p}$ or $\mathfrak{c}^\star_{-\mathbf{p}}$), and rotation invariance allows the coefficients X and Y to depend only on $p = |\mathbf{p}|$.

The coefficients $X(p)$ and $Y(p)$ are determined by two conditions. First, we require $\mathfrak{c}_\mathbf{p}$ and $\mathfrak{c}^\star_\mathbf{q}$, to share the same commutation relations as do $\mathfrak{a}_\mathbf{p}$ and $\mathfrak{a}^\star_\mathbf{q}$ – *i.e.* $[\mathfrak{a}_\mathbf{p} \, , \mathfrak{a}^\star_\mathbf{q}] = [\mathfrak{c}_\mathbf{p} \, , \mathfrak{c}^\star_\mathbf{q}] = \delta^3(\mathbf{p} - \mathbf{q})$ – and this implies the coefficients X and Y must satisfy

$$XX^*(p) - YY^*(p) = 1 \, . \tag{7.2.14}$$

The second condition chooses X and Y by demanding the $\mathfrak{c}_\mathbf{p}\mathfrak{c}_{-\mathbf{p}}$ and $\mathfrak{c}^\star_\mathbf{p}\mathfrak{c}^\star_{-\mathbf{p}}$ terms to cancel in H_2, so that the remainder can be written

$$H_2 = E_0 + \int \mathrm{d}^3p \, \mathcal{E}(p) \, \mathfrak{c}^\star_\mathbf{p} \mathfrak{c}_\mathbf{p} \, , \tag{7.2.15}$$

for some calculable choices for E_0 and $\mathcal{E}(p)$. Once this is done $\mathcal{E}(p)$ is revealed as the approximate single quasi-particle energy for excitations above the ground state, with the ground state $|\Omega\rangle$ defined by $\mathfrak{c}_{\mathbf{p}}|\Omega\rangle = 0$.

To avoid notational clutter it is convenient in this section to suppress the label $\mathbf{p}$ completely, and keep track of the distinction between $\mathbf{p}$ and $-\mathbf{p}$ using only the sign $\pm$. With this notation the above transformations become

$$\begin{aligned} &\mathfrak{a}_+ := X\,\mathfrak{c}_+ + Y\,\mathfrak{c}_-^\star\,, \qquad \mathfrak{a}_- := X\,\mathfrak{c}_- + Y\,\mathfrak{c}_+^\star \\ \text{and so}\quad &\mathfrak{a}_+^\star \;=\; X^*\,\mathfrak{c}_+^\star + Y^*\,\mathfrak{c}_-\,, \qquad \mathfrak{a}_-^\star := X^*\,\mathfrak{c}_-^\star + Y^*\,\mathfrak{c}_+\,, \end{aligned} \tag{7.2.16}$$

and their inverse is

$$\begin{aligned} &\mathfrak{c}_+ := X\,\mathfrak{a}_+ - Y\,\mathfrak{a}_-^\star\,, \qquad \mathfrak{c}_- := X\,\mathfrak{a}_- - Y\,\mathfrak{a}_+^\star \\ \text{and so}\quad &\mathfrak{c}_+^\star \;=\; X^*\,\mathfrak{a}_+^\star - Y^*\,\mathfrak{a}_-\,, \qquad \mathfrak{c}_-^\star := X^*\,\mathfrak{a}_-^\star - Y^*\,\mathfrak{a}_+\,, \end{aligned} \tag{7.2.17}$$

which uses $X^*X - Y^*Y = 1$.

The constraint (7.2.14) removes one of the four real parameters contained within X and Y, and the remaining three can be written as

$$X = e^{i\xi}\cosh\mathcal{X} \quad \text{and} \quad Y = -e^{i\zeta}\sinh\mathcal{X}\,. \tag{7.2.18}$$

The phase $\xi(p)$ can be set to zero by appropriately rephasing $\mathfrak{c}_{\mathbf{p}}$ and $\mathfrak{a}_{\mathbf{p}}$ (since this is a symmetry of the problem) leaving two real parameters ζ and $\mathcal{X}$ (for each p), whose values are found by asking the $\mathfrak{c}_\pm\mathfrak{c}_\mp$ and $\mathfrak{c}_\pm^\star\mathfrak{c}_\mp^\star$ terms to cancel in H_2.

Inserting (7.2.13) into (7.2.11) gives (for each p)

$$\begin{aligned} H_2 &= \varepsilon\left(\mathfrak{a}_+^\star\mathfrak{a}_+ + \mathfrak{a}_-^\star\mathfrak{a}_-\right) + W\mathfrak{a}_+\mathfrak{a}_- + W^*\mathfrak{a}_+^\star\mathfrak{a}_-^\star \\ &= E_0 + 2\Big[\varepsilon\Big(X^*X + Y^*Y\Big) + WXY + W^*X^*Y^*\Big](\mathfrak{c}_+^\star\mathfrak{c}_+ + \mathfrak{c}_-^\star\mathfrak{c}_-) \\ &\qquad + \Big[\Big(2\varepsilon\,XY^* + WXX + W^*Y^*Y^*\Big)\mathfrak{c}_+\,\mathfrak{c}_- + \text{h.c.}\Big]\,, \end{aligned} \tag{7.2.19}$$

with — temporarily reinstating the integral over p and using $[\mathfrak{c}_\pm\,,\mathfrak{c}_\pm^\star] = \delta^3(\mathbf{p}=0)$ with $\delta^3(\mathbf{p}=0) = \mathcal{V}/(2\pi)^3$ — the parameter E_0 given by

$$E_0 = \mathcal{V}\int\frac{\mathrm{d}^3p}{(2\pi)^3}\,\left[\varepsilon(p)Y^*Y(p) + \frac{1}{2}\,WXY(p) + \frac{1}{2}\,W^*X^*Y^*(p)\right]. \tag{7.2.20}$$

The $c_+\,c_-$ and $c_+^\star\,c_-^\star$ terms in (7.2.19) therefore cancel if

$$\begin{aligned} 0 &= 2\varepsilon\,XY^* + WXX + W^*Y^*Y^* \\ &= -2\varepsilon\,e^{-i\zeta}\cosh\mathcal{X}\sinh\mathcal{X} + \mathfrak{w}\Big(e^{iw}\cosh^2\mathcal{X} + e^{-i(2\zeta+w)}\sinh^2\mathcal{X}\Big)\,, \end{aligned} \tag{7.2.21}$$

which uses (7.2.18) (with $\xi = 0$) and writes $W = \mathfrak{w}\, e^{iw}$ for real and positive $\mathfrak{w}$ and w. Each of these terms has the same phase if ζ is chosen equal to $-\omega$, after which $\mathcal{X}$ must satisfy

$$-2\varepsilon \tanh \mathcal{X} + \mathfrak{w}\Big(1 + \tanh^2 \mathcal{X}\Big) = 0\,. \tag{7.2.22}$$

This has as solution

$$\tanh \mathcal{X} = \frac{1}{\mathfrak{w}}\Big[\varepsilon - \sqrt{\varepsilon^2 - \mathfrak{w}^2}\Big] \tag{7.2.23}$$

where the root is chosen to ensure $\mathcal{X} \to 0$ (and so $Y \to 0$) in the limit $\mathfrak{w}/\varepsilon \to 0$. This root provides a real solution for $\mathcal{X}$ provided $\varepsilon > \mathfrak{w}$, which is the regime of interest in what follows.[15]

With these choices for ζ and $\mathcal{X}$ the Hamiltonian H_2 becomes

$$\begin{aligned} H_2 &= E_0 + \int \mathrm{d}^3p \,\Big[\varepsilon\Big(\cosh^2 \mathcal{X} + \sinh^2 \mathcal{X}\Big) - 2\mathfrak{w} \cosh \mathcal{X} \sinh \mathcal{X}\Big]\, \mathfrak{c}^\star_{\mathbf{p}} \mathfrak{c}_{\mathbf{p}} \\ &= E_0 + \int \mathrm{d}^3p\, \mathcal{E}(p)\, \mathfrak{c}^\star_{\mathbf{p}} \mathfrak{c}_{\mathbf{p}}\,, \end{aligned} \tag{7.2.24}$$

which has the standard free-particle form with single-particle, but with a modified dispersion relation $\mathcal{E}(p)$:

$$\mathcal{E}(p) = \sqrt{\varepsilon(p)^2 - \mathfrak{w}(p)^2}\,. \tag{7.2.25}$$

The quantity E_0, given by (7.2.20), similarly evaluates to

$$E_0 = -\mathcal{V} \int \frac{\mathrm{d}^3p}{(2\pi)^3}\Big[\varepsilon(p) - \sqrt{\varepsilon(p)^2 - \mathfrak{w}(p)^2}\Big]\,. \tag{7.2.26}$$

7.2.3 Quasi-particles and corrections to the ground-state energy

We now return to the application to Bose-Einstein condensation and so specialize to the special cases

$$\varepsilon(\mathbf{p}) = (\varepsilon_0 + 4g\mathfrak{n}_0) + \frac{\mathbf{p}^2}{2m} + \cdots \quad \text{and} \quad \mathfrak{w}(\mathbf{p}) = g\mathfrak{n}_0\,, \tag{7.2.27}$$

which uses $|\varphi_0|^2 = \mathfrak{n}_0$. Specializing to the optimal density from (7.2.7) shows that $\mathfrak{n}_0^{\text{opt}} = (\mu - \varepsilon_0)/(2g)$, and so $g\mathfrak{n}_0^{\text{opt}} \sim \mathcal{O}(1)$ for small g. In this limit the energy spectrum of H_2 provides the leading $\mathcal{O}(1)$ correction to the classical energy $H_0 \sim \mathcal{O}(g^{-1})$ found above.

Because H_2 has the standard oscillator form once written in terms of $c_{\mathbf{p}}$, its eigenstates and eigenvalues can be read off by inspection. In particular, its lowest-energy (ground) state $|\Omega\rangle$ has energy E_0. Because this ground-state energy, E_0, is negative, the state $|\Omega\rangle$ has a lower energy than the unperturbed ground state $|0\rangle$ (as would be expected for a better approximation to the system's ground state). For large p the square bracket in the integrand of (7.2.26) becomes $\mathfrak{w}^2/(2\varepsilon)$, which shows that the integral over $p = |\mathbf{p}|$ diverges as $p \to \infty$.

[15] Since $\mathfrak{w}$ is p-independent for the case of interest, the requirement that $\varepsilon(p) > \mathfrak{w}$ should hold for all $\mathbf{p}$ requires choosing $\varepsilon_0 > \mathfrak{w}$.

Just as was true in earlier sections, this divergence can be absorbed into the parameter in $\mathcal{H}$ that sets the zero of the classical energy density.

The state $|\Omega\rangle$ also does not contain a definite number of the original particles destroyed by $\mathfrak{a}_{\mathbf{p}}$ that are not in the macroscopic $\mathbf{p} = 0$ state. This happens when $\mathfrak{w} \neq 0$ because the quadratic Hamiltonian H_2 does not commute with $\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{p}}$. The mean number of 'normal' particles – *i.e.* those not in the Bose-Einstein state at $\mathbf{p} = 0$ – is found using

$$\begin{aligned} \langle\Omega|\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{q}}|\Omega\rangle &= \langle\Omega|\Big[X^*(p)\,\mathfrak{c}^\star_{\mathbf{p}} + Y^*(p)\,\mathfrak{c}_{-\mathbf{p}}\Big]\Big[X(q)\,\mathfrak{c}_{\mathbf{q}} + Y(q)\,\mathfrak{c}^\star_{-\mathbf{q}}\Big]|\Omega\rangle \\ &= Y(q)Y^*(p)\langle\Omega|\mathfrak{c}_{-\mathbf{p}}\,\mathfrak{c}^\star_{-\mathbf{q}}|\Omega\rangle = |Y(p)|^2\delta^3(\mathbf{p}-\mathbf{q})\,, \end{aligned} \tag{7.2.28}$$

and so

$$\begin{aligned} \mathfrak{n} := \frac{1}{\mathcal{V}}\int \mathrm{d}^3p\;\langle\Omega|\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{p}}|\Omega\rangle &= \frac{1}{\mathcal{V}}\int \mathrm{d}^3p\;|Y(p)|^2\langle\Omega|\mathfrak{c}_{\mathbf{p}}\mathfrak{c}^\star_{\mathbf{p}}|\Omega\rangle = \int\frac{\mathrm{d}^3p}{(2\pi)^3}|Y(p)|^2 \\ = \int\frac{\mathrm{d}^3p}{(2\pi)^3}\sinh^2\mathcal{X} &= \int\frac{\mathrm{d}^3p}{(2\pi)^3}\left[\frac{\varepsilon - \sqrt{\varepsilon^2-\mathfrak{w}^2}}{2\sqrt{\varepsilon^2-\mathfrak{w}^2}}\right]. \end{aligned} \tag{7.2.29}$$

The excited states are obtained from this ground state in the usual way by acting on it repeatedly with $\mathfrak{c}^\star_{\mathbf{p}}$. The states obtained in this way behave as independent non-interacting (at least so long as H_3 and H_4 are neglected) particles, called 'quasi-particles' to distinguish them from the underlying particles created by $\mathfrak{a}^\star_{\mathbf{p}}$. The energy cost for producing such a quasi-particle is $\mathcal{E}(p)$, which (because $\mathcal{E}(p) < \varepsilon(p)$) we see is smaller than the cost $\varepsilon(p)$ for producing an underlying particle in the absence of interactions with the background φ_0. It is smaller because a particle's interactions with the condensed $\mathbf{p} = 0$ mode allow it to lower its energy.

7.3 Graphical methods

yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada

8 Symmetries

This section switches focus to symmetries and how they are treated in quantum systems. A particuar focus is on how the physical implications of a symmetry can differ for a quantum field theory relative to what happens for garden variety quantum systems. A particularly important new feature that field theory introduces is the possibility that a symmetry does not leave invariant a system's ground state (such as is evidently the case above for Bose-Einstein condensation with a weak repulsive contact potential). To set up this discussion, first a digression on symmetries and their implications in quantum mechanics and in quantum field theory.

8.1 Symmetries in quantum mechanics

When repeated, the transformation (7.2.8) returns another transformation of the same type that also leaves H and N unchanged: $\Phi(\mathbf{x}) \to \left[\Phi(\mathbf{x})\, e^{i\vartheta_1}\right] e^{i\vartheta_2} = \Phi(\mathbf{x})\, e^{i(\vartheta_1+\vartheta_2)}$.

As is easy to verify, these properties (and the existence of the trivial transformation with $\vartheta = 0$) ensure the collection of transformations of the type (7.2.8) form what mathematicians call a 'group'. Because these particular transformations do not change the energy they are collectively called a *symmetry* group. Finally, because the group elements, $e^{i\vartheta}$, are labelled by a continuous parameter (in this case ϑ) with respect to which the elements are differentiable, the group is called a 'Lie group'. The symmetry is called a 'global' (or 'rigid') symmetry when the parameter ϑ is a spacetime-independent constant. Knowing these transformations can be regarded as a group (and in particular a Lie group) can be useful because the properties of groups in general (and Lie groups in particular) are well-studied.

In quantum mechanics the action of any such a transformation within the quantum-mechanical Hilbert space takes the form of a unitary transformation.[16] That is, there must be a family of unitary operators, $U(\vartheta)$ with $U(\vartheta)U^\star(\vartheta) = I$, that describe how symmetries act on states in the Hilbert space

$$|\psi(\vartheta)\rangle = U(\vartheta)|\psi\rangle \tag{8.1.1}$$

as well as on operators

$$U^\star(\vartheta)\Phi(\mathbf{x})U(\vartheta) = \Phi(\mathbf{x})\, e^{i\vartheta}\,. \tag{8.1.2}$$

that 'represent' the symmetry group in that they reproduce the multiplication rule:

$$U(\vartheta_1)U(\vartheta_2) = U(\vartheta_1+\vartheta_2) \tag{8.1.3}$$

as well as $U(0) = I$ and so

$$U(-\vartheta) = U^{-1}(\vartheta) = U^\star(\vartheta)\,. \tag{8.1.4}$$

How does one write these operators $U(\vartheta)$ in terms of the $\mathfrak{a}_{\mathbf{p}}$ and $\mathfrak{a}^\star_{\mathbf{p}}$ (or the fields $\Phi(\mathbf{x})$ and $\Phi^\star(\mathbf{x})$)? Eq. (8.1.3) is satisfied if we write

$$U(\vartheta) = \exp[i\vartheta Q] \tag{8.1.5}$$

for some operator Q and (8.1.4) is satisfied if Q is hermitian. To figure out how to choose Q to implement (8.1.2) Taylor expand this equation in powers of ϑ. It then says

$$\Phi(\mathbf{x}) - i\vartheta[Q,\Phi(\mathbf{x})] + \frac{(-i)^2\vartheta^2}{2}[Q,[Q,\Phi(\mathbf{x})]] + \cdots = \Phi(\mathbf{x})\left(1 + i\vartheta + \frac{i^2\vartheta^2}{2} + \cdots\right), \tag{8.1.6}$$

[16] The one exception to this statement is time-reversal, $t \to -t$, which when a symmetry is represented by an *anti-unitary* operator (for reasons explained more fully in §11.2.2).

which shows (to all orders in ϑ, as it turns out) that it suffices to find an operator Q for which

$$[Q, \Phi(\mathbf{x})] = -\Phi(\mathbf{x}) \quad \text{which then also implies} \quad [Q, \Phi^\star(\mathbf{x})] = \Phi^\star(\mathbf{x})\,. \tag{8.1.7}$$

Given the commutation relation $[\Phi(\mathbf{x}), \Phi^\star(\mathbf{y})] = \delta^3(\mathbf{x}-\mathbf{y})$ the solution to this condition is simply:

$$Q = \mathcal{N} = \int \mathrm{d}^3x\ \Phi^\star(\mathbf{x})\Phi(\mathbf{x})\,, \tag{8.1.8}$$

as can be seen because

$$[\mathcal{N}, \Phi(\mathbf{x})] = \int \mathrm{d}^3y\ [\Phi^\star(\mathbf{y})\Phi(\mathbf{y}), \Phi(\mathbf{x})] = \int \mathrm{d}^3y\ [\Phi^\star(\mathbf{y}), \Phi(\mathbf{x})]\Phi(\mathbf{y}) = -\Phi(\mathbf{x})\,, \tag{8.1.9}$$

as required. The quantity Q (or $\mathcal{N}$ in this instance) is called the generator of the symmetry transformation.

Transformation rules like (8.1.2) have been encountered earlier in these notes. For instance eq. (3.2.3) gives the time evolution of an operator in the Heisenberg picture as

$$\mathcal{O}_h(t) = e^{iH(t-t_0)}\mathcal{O}_h(t_0)\,e^{-iH(t-t_0)}\,. \tag{8.1.10}$$

One way to read (8.1.10) is that it states the unitary operator

$$U(\tau) := e^{-iH\,\tau} \quad \text{satisfies} \quad U(\tau_1)\,U(\tau_2) = U(\tau_1+\tau_2) \tag{8.1.11}$$

and

$$U^\star(\tau)\,\mathcal{O}_h(t_0)\,U(\tau) = \mathcal{O}_h(t_0+\tau)\,, \tag{8.1.12}$$

and so can be regarded as the operator that realizes the group of time translations in the quantum Hilbert space. Eq. (8.1.11) also reveals the Hamiltonian to be the generator of time translations.[17]

Spatial translations are similarly realized in the quantum space of states by $U(\mathbf{c}) := \exp(i\mathbf{P}\cdot\mathbf{c})$ where $\mathbf{P}$ is the total momentum operator. This is easiest to see in the interaction representation, where

$$\mathbf{P} := \sum_{\mathbf{p}} \mathbf{p}\,a^\star_{\mathbf{p}}a_{\mathbf{p}} = \int \mathrm{d}^3p\ \mathbf{p}\,\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{p}} = \int \mathrm{d}^3x\ \Phi^\star(\mathbf{x},t)(-i\nabla)\Phi(\mathbf{x},t)\,. \tag{8.1.13}$$

since $[\mathfrak{a}_{\mathbf{k}}\,, \mathfrak{a}^\star_{\mathbf{q}}] = \delta^3(\mathbf{k}-\mathbf{q})$ and $[\Phi(\mathbf{x},t)\,, \Phi^\star(\mathbf{y},t)] = \delta^3(\mathbf{x}-\mathbf{y})$ imply

$$\Big[\mathbf{P}\,, \mathfrak{a}_{\mathbf{k}}\Big] = -\mathbf{k}\,\mathfrak{a}_{\mathbf{k}} \quad \text{and} \quad \Big[\mathbf{P}\,, \Phi(\mathbf{x},t)\Big] = i\nabla\Phi(\mathbf{x},t)\,, \tag{8.1.14}$$

and so

$$U^\star(\mathbf{c})\,\mathfrak{a}_{\mathbf{k}}\,U(\mathbf{c}) = e^{-i\mathbf{P}\cdot\mathbf{c}}\mathfrak{a}_{\mathbf{k}}\,e^{i\mathbf{P}\cdot\mathbf{c}} = e^{i\mathbf{k}\cdot\mathbf{c}}\,\mathfrak{a}_{\mathbf{k}}\,, \tag{8.1.15}$$

[17] A similar thing is true in the interaction picture, but in this case it is the operator $\exp[-iH_{\text{free}}\tau]$ that satisfies (8.1.12) and so represents time translations on interaction-picture fields.

which in turn means

$$e^{-i\mathbf{P}\cdot\mathbf{c}}\,\Phi(\mathbf{x})\,e^{i\mathbf{P}\cdot\mathbf{c}} = \int \frac{\mathrm{d}^3k}{(2\pi)^{3/2}}\,e^{-i\mathbf{P}\cdot\mathbf{c}}\,\mathfrak{a}_{\mathbf{k}}\,e^{i\mathbf{P}\cdot\mathbf{c}}\,e^{i\mathbf{k}\cdot\mathbf{x}} = \Phi(\mathbf{x}+\mathbf{c})\,. \tag{8.1.16}$$

This representation of spatial translations then directly go over to the same expressions in Heisenberg and Schrödinger pictures provided $\mathbf{P}$ commutes with both H_{free} and H_{int}.

Relations like (8.1.10) and (8.1.16) are very useful in that they completely dictate the t- and $\mathbf{x}$-dependence of the matrix element of any operator taken using energy and momentum eigenstates. That is, if $\mathbf{P}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle$ and $H|\mathbf{p}\rangle = \varepsilon(\mathbf{p})|\mathbf{p}\rangle$ then

$$\begin{aligned}\langle\mathbf{q}|\mathcal{O}_h(\mathbf{x},t)|\mathbf{p}\rangle &= \langle\mathbf{q}|e^{iH(t-t_0)-i\mathbf{P}\cdot(\mathbf{x}-\mathbf{x}_0)}\mathcal{O}_h(\mathbf{x}_0,t_0)\,e^{-iH(t-t_0)+i\mathbf{P}\cdot(\mathbf{x}-\mathbf{x}_0)}|\mathbf{p}\rangle \\ &= \langle\mathbf{q}|\mathcal{O}_h(\mathbf{x}_0,t_0)|\mathbf{p}\rangle\,e^{i[\varepsilon(\mathbf{q})-\varepsilon(\mathbf{p})](t-t_0)-i(\mathbf{q}-\mathbf{p})\cdot(\mathbf{x}-\mathbf{x}_0)}\,.\end{aligned} \tag{8.1.17}$$

8.1.1 General implications of symmetries

Any operator, $\mathcal{O}(\Phi,\Phi^\star)$, that is invariant under the replacements $\Phi \to \Phi\,e^{i\vartheta}$ and $\Phi^\star \to \Phi^\star e^{-i\vartheta}$ automatically satisfies

$$U^\star(\vartheta)\mathcal{O}(\Phi,\Phi^\star)U(\vartheta) = \mathcal{O}(U^\star\Phi U, U^\star\Phi^\star U) = \mathcal{O}(\Phi\,e^{i\vartheta},\Phi^\star e^{-i\vartheta}) = \mathcal{O}(\Phi,\Phi^\star) \tag{8.1.18}$$

and so commutes with $U(\vartheta)$ (for all ϑ): $U(\vartheta)\,\mathcal{O} = \mathcal{O}\,U(\vartheta)$. (The first equality in this line of inference can be established, for example, by proving it term-by-term for the Taylor expansion of $\mathcal{O}$ in powers of Φ and $\Phi^\star$.) Inspection of (7.1.24) shows this is in particular true for the Hamiltonian itself, so

$$U(\vartheta)H = HU(\vartheta) \tag{8.1.19}$$

(which is indeed the defining feature[18] of a symmetry). This ensures in particular an important consequence of symmetries for quantum systems:

> **States linked by symmetries share the same energy:** Any two energy eigenstates related by a symmetry must share the same energy, since
>
> $$\text{if}\quad |\chi\rangle = U(\vartheta)|\psi\rangle \quad\text{and}\quad H|\psi\rangle = E_\psi|\psi\rangle \tag{8.1.20}$$
>
> then
>
> $$H|\chi\rangle = HU(\vartheta)|\psi\rangle = U(\vartheta)\,H|\psi\rangle = E_\psi U(\vartheta)|\psi\rangle = E_\psi|\chi\rangle\,. \tag{8.1.21}$$

Symmetry operators like $U(\vartheta)$ clearly must act *reducibly* inasmuch as energy eigenstates organize themselves into separate representations of any symmetries for each distinct eigenvalue.

[18] Strictly speaking, this slightly too restrictive a definition of a symmetry, since the Lorentz transformations of special relativity are practical examples of spacetime symmetries for which U does not commute with H. We return to this point when incorporating special relativity in §11 below.

If n_E states all share the same energy eigenvalue E, then a symmetry acts as an $n_E \times n_E$ matrix on these states.

Two other related consequences of (8.1.19) are

$$[H, Q\,] = 0 \qquad \text{and} \qquad U(t,t_0)\,Q = Q\,U(t,t_0)\,, \tag{8.1.22}$$

where (as usual) the time-evolution operator is $U(t,t_0) = \exp[-iH(t-t_0)]$. The first of these – the commutation relation $[H, Q\,] = 0$ – is also easy to verify for the case $Q = \mathcal{N}$ – with H given by (7.1.24) – by explicit calculation. This expresses a second general consequence of symmetries in quantum mechanics:

> **Existence of conserved charges:** A continuous symmetry implies the existence of an observable (*i.e.* hermitian operator, in the present case Q) that commutes with the system's Hamiltonian and time-evolution.

Because Q is hermitian it can be chosen to be a quantum observable, and because Q commutes with H both Q and H can be measured simultaneously. If at time t_0 a state $|\psi\rangle$ is measured to be an eigenstate of Q with eigenvalue q – *i.e.* $Q|\psi(t_0)\rangle = q|\psi(t_0)\rangle$ – then at a later time $|\psi(t)\rangle = U(t,t_0)|\psi(t)\rangle$ must also be an eigenstate with the same eigenvalue since

$$Q|\psi(t)\rangle = Q\,U(t,t_0)|\psi(t_0)\rangle = U(t,t_0)\,Q|\psi(t_0)\rangle = q\,U(t,t_0)|\psi(t_0)\rangle = q\,|\psi(t)\rangle\,. \tag{8.1.23}$$

Eq. (8.1.23) is the way charge conservation occurs within the Schrödinger picture, for which operators do not evolve but states do. The Heisenberg picture provides an alternative way to understand charge conservation, since it is the language in which it is the operators themselves – such as Q, for instance – that evolve in time, rather than the states. The conserved charge is given within the Heisenberg picture by

$$Q_h(t) := e^{iH(t-t_0)} Q\, e^{-iH(t-t_0)} = Q\,, \tag{8.1.24}$$

where the last equality uses that H and Q commute, and Q without a subscript means the Schrödinger-picture quantity. Equivalently, Heisenberg operators in general evolve in time according to the evolution equation (3.2.4), which for $Q_h(t)$ says:

$$\partial_t Q_h(t) = i\Big[H, Q_h(t)\Big] = 0\,. \tag{8.1.25}$$

8.2 Symmetries in field theory

Quantum field theory differs from single-particle quantum mechanics in several ways: (*i*) its states involve multiple particles of the form $|\psi\rangle \propto [a^\star_{p_1}]^{n_1} \cdots [a^\star_{p_k}]^{n_k}|0\rangle$, and (*ii*) conserved charges like H and Q arise as local integrals over position, of the form

$$H = \int \mathrm{d}^3x\; \mathcal{H}(\mathbf{x}) \qquad \text{and} \qquad Q = \int \mathrm{d}^3x\; \mathcal{Q}(\mathbf{x})\,, \tag{8.2.1}$$

for some Hamiltonian density $\mathcal{H}(\mathbf{x})$ and charge density $\mathcal{Q}(\mathbf{x})$ (*c.f.* for example eqs. (7.1.24) and (8.1.8) for the bosonic model considered above). Because of these differences the implications of symmetries in quantum field theory can also differ in detail from single-particle quantum mechanics.

8.2.1 Local conservation laws

Consider first conservation laws. In the example above it is actually the Hamiltonian *density* $\mathcal{H}(\mathbf{x})$, rather than just H, that is invariant under the replacement $A \to A\,e^{i\vartheta}$, and so eq. (8.1.18) actually leads to the local statement

$$U^\star(\vartheta)\mathcal{H}(\mathbf{x})\,U(\vartheta) = \mathcal{H}(\mathbf{x}) \quad \text{and so} \quad [Q, \mathcal{H}(\mathbf{x})] = 0\,, \tag{8.2.2}$$

which is a slightly stronger statement than (8.1.19) or (8.1.22). What is important is that although (8.1.19) and (8.1.22) remain true, these and (8.2.2) do *not* also imply the local version of (8.1.22). That is, $[H, \mathcal{Q}(\mathbf{x})] \neq 0$ in general. The most that can be concluded is

$$[H, \mathcal{Q}(\mathbf{x})] = i\,\nabla\cdot\mathbf{J}(\mathbf{x})\,, \tag{8.2.3}$$

for some vector field $\mathbf{J}(\mathbf{x})$. (The conventional factor of i is included since the left-hand side of (8.2.3) must be anti-hermitian because H and $\mathcal{Q}(\mathbf{x})$ are hermitian.)

The right-hand side of (8.2.3) is the most general form that is consistent with (8.1.22) (*i.e.* with $[H, Q\,] = 0$). To see why, integrate (8.2.3) over some region R of space, to get

$$\int_R \mathrm{d}^3x\;[H, \mathcal{Q}(\mathbf{x})] = i\int_R \mathrm{d}^3x\;\nabla\cdot\mathbf{J} = i\oint_{\partial R} \mathrm{d}^2x\;\mathbf{n}\cdot\mathbf{J}\,, \tag{8.2.4}$$

where the last equality uses Stoke's Law, with the final surface integral being over the boundary of R, denoted ∂R, for which $\mathbf{n}$ is the outward-pointing unit normal. If $Q_{\scriptscriptstyle R} := \int_{\scriptscriptstyle R} \mathrm{d}^3x\;\mathcal{Q}(\mathbf{x})$ denotes the amount of charge[19] within the region R, then (8.2.4) implies

$$[H, Q_{\scriptscriptstyle R}] = \int_R \mathrm{d}^3x\;[H, \mathcal{Q}(\mathbf{x})] = i\oint_{\partial R} \mathrm{d}^2x\;\mathbf{n}\cdot\mathbf{J}\,. \tag{8.2.5}$$

This says something very reasonable. In the Heisenberg picture (8.2.5) implies $Q_{\scriptscriptstyle Rh}(t)$ satisfies the evolution equation

$$\partial_t Q_{\scriptscriptstyle Rh}(t) = i\Big[H, Q_{\scriptscriptstyle Rh}(t)\Big] = -\oint_{\partial R} \mathrm{d}^2x\;\mathbf{n}\cdot\mathbf{J}\,, \tag{8.2.6}$$

which says the rate of change of Q within region R is equal to the rate with which Q gets moved out through the boundary of R. This shows that $\mathbf{J}(\mathbf{x})$ represents the local *flux* of Q (*i.e.* $\langle\psi|\mathbf{J}(\mathbf{x})|\psi\rangle$ is the flux of Q in any particular quantum state).

[19] Since $Q_{\scriptscriptstyle R}$ is an operator, more precisely $\langle\psi|Q_{\scriptscriptstyle R}|\psi\rangle$ is the amount of charge found in region R when the system is prepared in the state $|\psi\rangle$.

Eq. (8.2.6), or its local version

$$\partial_t \mathcal{Q}_h(\mathbf{x}, t) + \nabla \cdot \mathbf{J} = 0\,, \tag{8.2.7}$$

is the local expression of a conservation law. Eq. (8.2.7) and the existence of $\mathcal{Q}$ and $\mathbf{J}$ given a continuous symmetry is called *Noether's theorem*, and it carries more information than the statement $\partial_t Q_h(t) = 0$. The extra information arises because local conservation keeps track of how much charge moves into and out of any region R, rather than focussing exclusively on what happens to the total amount of charge everywhere. Eq. (8.2.6) is consistent with time-independence of Q_h because Q_h is obtained from Q_{Rh} by taking R to be all of space, pushing the boundary ∂R out to spatial infinity where there is no flux.

To make the above discussion more concrete, consider the example of Schrödinger field theory, for which the Hamiltonian is

$$H = \int \mathrm{d}^3x\; \Phi^\star \left[-\frac{\nabla^2}{2m} + V(\mathbf{x})\right] \Phi\,. \tag{8.2.8}$$

For this Hamiltonian the symmetry under the replacements $\Phi \to \Phi\, e^{i\zeta}$ and $\Phi^\star \to \Phi^\star\, e^{-i\zeta}$ implies the existence of the conserved charge

$$Q = \mathcal{N} = \int \mathrm{d}^3x\; \Phi^\star\Phi\,, \tag{8.2.9}$$

which counts the number of particles. The charge density in this example then is $\mathcal{Q}(\mathbf{x}) = \Phi^\star\Phi$. Recall also that for this system in the Heisenberg picture the field Φ satisfies the evolution equation (6.2.6), which reads:

$$i\partial_t \Phi = \left[-\frac{\nabla^2}{2m} + V(\mathbf{x})\right] \Phi\,, \tag{8.2.10}$$

and so

$$\partial_t \mathcal{Q} = (\partial_t \Phi^\star)\Phi + \Phi^\star(\partial_t \Phi) = \frac{i}{2m}\Big[\Phi^\star(\nabla^2\Phi) - (\nabla^2\Phi^\star)\Phi\Big] = -\nabla\cdot\mathbf{J} \tag{8.2.11}$$

where

$$\mathbf{J} = \frac{i}{2m}\Big[(\nabla\Phi^\star)\Phi - \Phi^\star(\nabla\Phi)\Big]\,. \tag{8.2.12}$$

This shows concretely how a specific form for the conserved current $\mathbf{J}$ and charge density $\mathcal{Q}$ arise for each symmetry, with local conservation in the form of (8.2.7) following as an automatic consequence of the equations of motion.

8.3 Spontaneous symmetry breaking

A major implication to be drawn from a symmetry in ordinary quantum mechanics is that energy eigenstates related by the symmetry automatically share the same energy eigenvalue

(as in eq. (8.1.20)). In quantum field theory it would therefore be tempting to conclude – and indeed once was believed – that if two different particle types are related by a symmetry then these particles must have the same single-particle dispersion relation $\varepsilon(\mathbf{p})$.

This conclusion is sometimes true, but also can break down under some circumstances. In quantum field theory the statement that particle type A is related to particle type B by the action of a symmetry means that their creation (and destruction) operators are related by[20]

$$U^\star a_{\mathbf{p}}\, U = b_{\mathbf{p}} \qquad \text{which also implies} \qquad U^\star a^\star_{\mathbf{p}}\, U = b^\star_{\mathbf{p}}\,. \tag{8.3.1}$$

Here U is a unitary symmetry-transformation operator, and the operators $a_{\mathbf{p}}$ and $b_{\mathbf{p}}$ satisfy

$$|A(\mathbf{p})\rangle = a^\star_{\mathbf{p}}|0\rangle \qquad \text{and} \qquad |B(\mathbf{p})\rangle = b^\star_{\mathbf{p}}|0\rangle\,, \tag{8.3.2}$$

for the two particle types, A and B. Clearly the fact that U commutes with H would immediately imply $\varepsilon_{\scriptscriptstyle A}(\mathbf{p}) = \varepsilon_{\scriptscriptstyle B}(\mathbf{p})$ if it could be shown that

$$|A(\mathbf{p})\rangle = U|B(\mathbf{p})\rangle\,. \tag{8.3.3}$$

The issue is whether or not this last equation actually follows from (8.3.1). To see when this follows (and when it does not) act on the no-particle state using (8.3.1) and (8.3.2). This leads to $U^\star a^\star_{\mathbf{p}} U|0\rangle = b^\star_{\mathbf{p}}|0\rangle = |B(\mathbf{p})\rangle$, which after multiplying through by U from the left gives

$$a^\star_{\mathbf{p}} U|0\rangle = U|B(\mathbf{p})\rangle\,. \tag{8.3.4}$$

Now comes the main point. Although eq. (8.3.4) follows from (8.3.1) it does *not* imply (8.3.3) unless the no-particle state is invariant under the symmetry:

$$U|0\rangle = |0\rangle\,. \tag{8.3.5}$$

When the no-particle state is invariant – *i.e.* when (8.3.5) holds, then (8.3.3) follows from (8.3.1) and so having the fields for A and B transform into one another under a symmetry automatically implies that the corresponding particles must share the same single-particle dispersion relation: $\varepsilon_{\scriptscriptstyle A}(\mathbf{p}) = \varepsilon_{\scriptscriptstyle B}(\mathbf{p})$. But (8.3.5) need not hold for a symmetry, and when $U|0\rangle \neq |0\rangle$ the symmetry is said to be *spontaneously broken*.

In single-particle quantum mechanics it happens to be a theorem that a system's ground state is unique, and so because $UH = HU$ this means that U acting on the ground state must return the ground state. So in single-particle quantum mechanics spontaneous symmetry breaking essentially never happens. But it *can* happen in quantum field theory, and the case of Bose-Einstein condensation (for nonrelativistic particles with a weak repulsive interaction) provides one of the simplest examples.

[20] This formula assumes the symmetry in question commutes with momentum, as turns out to be a very general requirement for internal symmetries in relativistic theories.

Recall that for this system in the presence of a large number of particles we found the scalar field $\Phi(\mathbf{x})$ has a ground state $|\varphi_0\rangle$ that satisfies $\langle\varphi_0|\Phi(\mathbf{x})|\varphi_0\rangle = \varphi_0$. Recall also that under the system's one-parameter symmetry transformations $U^\star(\vartheta)\Phi(\mathbf{x})U(\vartheta) = \Phi(\mathbf{x})\,e^{i\vartheta}$ and so taking the expectation of this equation using $|\varphi_0\rangle$ gives

$$\langle\varphi_0|U^\star(\vartheta)\Phi(\mathbf{x})U(\vartheta)|\varphi_0\rangle = \langle\varphi_0|\Phi(\mathbf{x})|\varphi_0\rangle\,e^{i\vartheta} = \varphi_0\,e^{i\vartheta}\,. \tag{8.3.6}$$

This equation shows that $U(\vartheta)|\varphi_0\rangle \neq |\varphi_0\rangle$ because if this were not so then the left-hand side of (8.3.6) would evaluate to φ_0 leading to a contradiction with the right-hand side for any $\vartheta \neq 0$. This is a general result: if any field that transforms nontrivially under a symmetry acquires a nonzero expectation value in a ground state then that ground state cannot be invariant under the symmetry. This makes any transforming field with a nonzero ground-state expectation of this type particularly interesting as a diagnostic for spontaneous symmetry breaking. Any such a diagnostic field is called an *order parameter* for the symmetry's spontaneous breaking.

Spontaneous symmetry breaking is observed to occur in many systems in nature, both for relativistic situations and for nonrelativistic ones. Examples of this are superfluids, for which Bose-Einstein condensation in a low-temperature fluid breaks the internal rephasing symmetry $\Phi(\mathbf{x}) \to \Phi(\mathbf{x})\,e^{i\vartheta}$ discussed above; solids for which the formation of a crystal lattice in the ground state spontaneously breaks the underlying translation invariance of the electromagnetic interactions between the atoms; or a ferromagnet where the macroscopic alignment of atomic spins spontaneously breaks the underlying rotation invariance of the interatomic interactions. It is also believed to happen at a more fundamental level, with the leading theory (the Standard Model) interpreting some of the patterns of elementary particle masses as being due to the non-invariance of the vacuum of elementary particles under a soecific class of symmetries.

8.3.1 Goldstone's theorem

Whenever a continuous internal symmetry of the type considered above is spontaneously broken there very generally always must exist a particle with a vanishing energy gap; a result known as *Goldstone's theorem*. The presence of this mode is often how one diagnoses the existence of spontaneously broken symmetries.

The reason such a particle must exist is because spontaneous symmetry breaking requires the system's ground state $|\Omega\rangle$ to satisfy $U(\vartheta)\,|\Omega\rangle \neq |\Omega\rangle$. But because $U(\vartheta) = \exp[i\vartheta Q]$ it must also be true that $Q|\Omega\rangle \neq 0$. Because $Q = \int \mathrm{d}^3x\ \mathcal{Q}(\mathbf{x})$ this in turn implies $\mathcal{Q}(\mathbf{x})|\Omega\rangle \neq 0$.

But if $\mathcal{Q}(\mathbf{x})|\Omega\rangle \neq 0$ then there must exist a state $|G\rangle$ for which $\langle G|\mathcal{Q}(\mathbf{x})|\Omega\rangle \neq 0$. Working in the Heisenberg picture (for which $\mathcal{Q}_h(\mathbf{x},t)$ depends on time as well as position) and assuming a system invariant under translations in space and time, this implies there exists an energy and momentum eigenstate, $|G(\mathbf{p})\rangle$, for which (see *e.g.* eq. (8.1.17))

$$\langle G(\mathbf{p})|\mathcal{Q}_h(\mathbf{x},t)|\Omega\rangle = F_Q\,e^{i(\varepsilon_G t - \mathbf{p}\cdot\mathbf{x})} \tag{8.3.7}$$

for some nonzero (and space- and time-independent) F_Q, where $\varepsilon_G(\mathbf{p})$ is the energy eigenvalue of the state $|G(\mathbf{p})\rangle$.

Next use charge conservation in its local form, (8.2.7). Taking the matrix element of this equation between $\langle G(\mathbf{p})|$ and $|\Omega\rangle$ gives

$$\partial_t \langle G(\mathbf{p})|\mathcal{Q}_h(\mathbf{x},t)|\Omega\rangle = -\nabla\cdot\langle G(\mathbf{p})|\mathbf{J}_h(\mathbf{x},t)|\Omega\rangle\,. \tag{8.3.8}$$

Writing – again using (8.1.17) – $\langle G(\mathbf{p})|\mathbf{J}_h(\mathbf{x},t)|\Omega\rangle = \mathbf{F}_J\, e^{i(\varepsilon_G t - \mathbf{p}\cdot\mathbf{x})}$, as well as (8.3.7) this implies

$$i\varepsilon_G(\mathbf{p}) F_Q\, e^{i(\varepsilon_G - \mathbf{p}\cdot\mathbf{x})} = i\mathbf{p}\cdot\mathbf{F}_J\, e^{i(\varepsilon_G - \mathbf{p}\cdot\mathbf{x})}\,. \tag{8.3.9}$$

If $\mathbf{p}\cdot\mathbf{F}_J = 0$ then because $F_Q \neq 0$ this implies $\varepsilon_G(\mathbf{p}) = 0$ for all $\mathbf{p}$. More commonly – such as for the concrete example (8.2.12) for instance – one finds $\mathbf{F}_J \propto \mathbf{p} \neq 0$ in which case (8.3.9) instead allows $\varepsilon_G(\mathbf{p})$ to be nonzero but gapless in the sense that the explicit factor of $\mathbf{p}$ on the right-hand side implies the zero-momentum limit of $\varepsilon_G(\mathbf{p})$ must satisfy[21]

$$\lim_{\mathbf{p}\to 0} \varepsilon_G(\mathbf{p}) = 0\,. \tag{8.3.10}$$

The presence of such a low-energy state is a robust symmetry prediction whenever a continuous global symmetry is spontaneously broken. More information about this state also follows from the symmetry, such as its general decoupling (to become very weakly interacting) for small $\mathbf{p}$. These additional conclusions can be derived by performing repeated symmetry transformations on other fields besides $\mathcal{Q}$, and asking what the symmetry transformations imply for matrix elements of other fields. Although it goes beyond the scope of these notes, one can show in this way that the low-energy interactions of Goldstone bosons are largely dictated by the group multiplication properties of the symmetry whose breaking ensures their existence.

9 Electromagnetic fields

So far the discussion of Hamiltonians and interactions has been quite general, and applies to a generic system involving non-relativistic particles. But in practice a particularly important role is played by nonrelativistic particles that interact with electromagnetic fields, since this is the interaction that is relevant in a vast number of ordinary systems encountered here on Earth.

This section explores how these electromagnetic interactions are set up in a quantum field theory context, partly because the interactions are interesting in their own right, and partly

[21] There is a loophole to this argument: if $\mathbf{F}_J \propto \mathbf{p}/|\mathbf{p}|^2$ (and so is singular as $|\mathbf{p}| \to 0$) then (8.3.9) need not imply $\varepsilon_G(\mathbf{p})$ vanish as $\mathbf{p} \to 0$. This is what happens in superconductors, for example, and more generally whenever the symmetry in question is a 'gauge' symmetry, for which the symmetry parameter, $\vartheta(\mathbf{x})$, varies with spacetime position. (More about gauge symmetries is encountered in §9 and an example that exploits this loophole is described in §14.4.)

because electromagnetic fields provide our first encounter with the relativistic quantum fields whose properties are examined in more detail in §11.

9.1 Classical electromagnetism

First, a brief reminder about some of the main features of electromagnetism that are relevant to what follows. Electromagnetism describes the properties and interactions of electric and magnetic fields,

$$\begin{aligned} \mathbf{E}(\mathbf{x},t) &= E_x(\mathbf{x},t)\,\mathbf{e}_x + E_y(\mathbf{x},t)\,\mathbf{e}_y + E_z(\mathbf{x},t)\,\mathbf{e}_z \\ \text{and}\quad \mathbf{B}(\mathbf{x},t) &= B_x(\mathbf{x},t)\,\mathbf{e}_x + B_y(\mathbf{x},t)\,\mathbf{e}_y + B_z(\mathbf{x},t)\,\mathbf{e}_z\,, \end{aligned} \tag{9.1.1}$$

both of which transform under proper rotations as vectors.

9.1.1 Maxwell's equations

Electric and magnetic fields arise due to the presence of charged particles, with centuries of experiments being summarized by four electromagnetic laws (which in their totality are called Maxwell's equations). The first of these equations express how electric fields are sourced by electric charges,

$$\nabla\cdot\mathbf{E} = \rho\,, \tag{9.1.2}$$

where $\rho(\mathbf{x},t)$ is the density of electric charge. The second equation expresses the equivalent for magnetic fields (together with the information that nature has not been observed to contain any magnetic 'monopole' charges):

$$\nabla\cdot\mathbf{B} = 0\,. \tag{9.1.3}$$

The remaining two Maxwell equations express how electric and magnetic fields respond to the presence of moving electric charges — *i.e.* electric current, $\mathbf{J}(\mathbf{x},t)$:

$$\nabla\times\mathbf{B} - \frac{\partial\mathbf{E}}{\partial t} = \mathbf{J}\,, \tag{9.1.4}$$

and

$$\nabla\times\mathbf{E} + \frac{\partial\mathbf{B}}{\partial t} = 0\,. \tag{9.1.5}$$

Notice that adding the time derivative of (9.1.2) to the divergence of (9.1.4) implies

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{J} = \frac{\partial}{\partial t}(\nabla\cdot\mathbf{E}) + \nabla\cdot\left[\nabla\times\mathbf{B} - \frac{\partial\mathbf{E}}{\partial t}\right] = 0\,. \tag{9.1.6}$$

This uses the identity $\nabla\cdot(\nabla\times\mathbf{B}) = 0$, which is true for any smooth vector field $\mathbf{B}$, and shows that Maxwell's equations *require* electric charge to be conserved (compare $\partial_t\rho + \nabla\cdot\mathbf{J} = 0$ to eq. (8.2.7) above (which expresses the local version of the conservation of any quantity). For any ρ and $\mathbf{j}$ satisfying the conservation equation (9.1.6), equations (9.1.2) through (9.1.5) determine the electric and magnetic fields that result.

9.1.2 Electromagnetic potentials

Although there are nominally six independent components (for every spacetime point) contained in the two vector fields $\mathbf{E}(\mathbf{x},t)$ and $\mathbf{B}(\mathbf{x},t)$, in practice the structure of Maxwell's equations is such that these six functions are not completely independent. (This can be seen from eqs. (9.1.3) and (9.1.5) which simply relate the components of $\mathbf{E}$ and $\mathbf{B}$ to one another in a way that does not involve ρ and $\mathbf{j}$.) It turns out that all six components of $\mathbf{E}$ and $\mathbf{B}$ can be completely specified in terms of three independent functions.[22]

It is therefore more efficient to express the field equations directly in terms of these independent functions. To see how to do this it is useful to define a new vector field $\mathbf{A}(\mathbf{x},t)$ from the condition

$$\mathbf{B} = \nabla \times \mathbf{A}\,, \tag{9.1.7}$$

since the identity $\nabla \cdot (\nabla \times \mathbf{A}) = 0$ for any $\mathbf{A}$ ensures that eq. (9.1.3) is solved. Notice that (9.1.7) does not uniquely specify $\mathbf{A}(\mathbf{x},t)$ because the identity $\nabla \times (\nabla\omega) = 0$ for any $\omega(\mathbf{x},t)$ shows that if $\mathbf{A}$ satisfies (9.1.7) then so does $\mathbf{A} + \nabla\omega$ for any scalar function ω.

Next, using (9.1.7) in (9.1.5) allows it to be written as

$$\nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = 0\,, \tag{9.1.8}$$

which locally means that the combination $\mathbf{E} + \partial\mathbf{A}/\partial t$ is the gradient of something. This suggests defining a scalar field ϕ so that

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi\,, \tag{9.1.9}$$

where the negative sign in front of $\nabla\phi$ is conventional.

Notice that although there are nominally four functions in total within the fields $\mathbf{A}(\mathbf{x},t)$ and $\phi(\mathbf{x},t)$, only three of these are independent because of the freedom to redefine

$$\mathbf{A} \to \mathbf{A} + \nabla\zeta \qquad \text{and} \qquad \phi \to \phi - \frac{\partial\zeta}{\partial t}\,, \tag{9.1.10}$$

which leaves both $\mathbf{B}$ and $\mathbf{E}$ – as given in terms of $\mathbf{A}$ and ϕ by (9.1.7) and (9.1.9) – unchanged. The transformation (9.1.10) is called a 'gauge transformation' and represents a redundancy of the description of electromagnetic fields when using the variables $\mathbf{A}$ and ϕ. This redundancy can be removed by imposing an additional arbitrary condition, called a 'gauge condition', such as $\nabla\cdot\mathbf{A} = 0$ (also called 'Coulomb gauge'). Other popular choices are 'temporal gauge', which sets $\phi = 0$; or axial gauge, which sets $A_z = 0$, or Lorentz gauge, which sets $\partial_t\phi + \nabla\cdot\mathbf{A} = 0$, and so on. Physical predictions do not care which of these conditions are used to remove the redundancy and so in practice one chooses the one that makes calculations most convenient.

[22] These three functions are not to be confused with the *two* degrees of freedom (or spin states) carried by the electromagnetic field, whose counting is made clearer below.

Finally, the remaining Maxwell equations, eqs. (9.1.2) and (9.1.4) can be used to determine $\mathbf{A}$ and ϕ given a specified charge distribution, ρ, and current distribution, $\mathbf{J}$. For instance, using (9.1.9) in (9.1.2) gives

$$\nabla \cdot \mathbf{E} = -\frac{\partial}{\partial t} \nabla \cdot \mathbf{A} - \nabla^2 \phi = \rho \,, \tag{9.1.11}$$

and similarly using (9.1.7) and (9.1.9) in (9.1.5) – see for example eq. (A.3.8) – gives

$$\nabla \times \mathbf{B} - \frac{\partial \mathbf{E}}{\partial t} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} + \frac{\partial^2 \mathbf{A}}{\partial t^2} + \frac{\partial}{\partial t} \nabla \phi = \mathbf{J} \,. \tag{9.1.12}$$

In Coulomb gauge (which sets $\nabla \cdot \mathbf{A} = 0$) these become the familiar equations:

$$-\nabla^2 \phi = \rho \qquad \text{and} \qquad -\nabla^2 \mathbf{A} + \frac{\partial^2 \mathbf{A}}{\partial t^2} + \frac{\partial}{\partial t} \nabla \phi = \mathbf{J} \,. \tag{9.1.13}$$

Because the equation $\nabla \cdot \mathbf{E} = -\nabla^2 \phi = \rho$ does not involve time derivatives in this gauge it is often called a 'constraint' equation; that is, it should not be regarded as an evolution equation for the field, but instead represents a limitation to the independent choices of initial conditions that are possible.[23]

Alternatively, in Lorentz gauge (which sets $\nabla \cdot \mathbf{A} + \partial_t \phi = 0$) eqs. (9.1.11) and (9.1.12) become inhomogeneous wave equations

$$\frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi = \rho \qquad \text{and} \qquad \frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla^2 \mathbf{A} = \mathbf{J} \,. \tag{9.1.14}$$

9.1.3 Electromagnetic waves

The general solution to equations (9.1.14) is given by any particular solution $(\phi_p, \mathbf{A}_p)$ of (9.1.14) plus the general solution, $(\phi_{\,\mathrm{hom}}, \mathbf{A}_{\mathrm{hom}})$, to the source-free homogeneous equations[24]

$$\frac{\partial^2 \phi_{\,\mathrm{hom}}}{\partial t^2} - \nabla^2 \phi_{\,\mathrm{hom}} = \frac{\partial^2 \mathbf{A}_{\mathrm{hom}}}{\partial t^2} - \nabla^2 \mathbf{A}_{\mathrm{hom}} = 0 \,. \tag{9.1.15}$$

Solutions to (9.1.15) describe electromagnetic waves, with for instance a plane-wave solution having the form

$$\mathbf{A}_{\mathrm{hom}} = \mathbf{A}_0 \, e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} + \text{c.c.} \qquad \text{and} \qquad \phi_{\mathrm{hom}} = \phi_0 \, e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} + \text{c.c.} \tag{9.1.16}$$

where (9.1.15) implies $\omega = |\mathbf{k}|$ and the Lorentz-gauge choice

$$\partial_t \, \phi + \nabla \cdot \mathbf{A} = 0 \tag{9.1.17}$$

[23] The number of degrees of freedom carried in the Electromagnetic field is then given by 4 (the components of $\mathbf{A}$ and ϕ), minus two (one each for the gauge freedom (9.1.10) and the constraint (9.1.2)), leaving two, as is shown below to be appropriate for the number of spin states available for a massless spin-one particle.

[24] This general result is a simple consequence of the linearity of the left-hand sides of (9.1.14), since (for example) if $L(\phi_1) = \rho$ and $L(\phi_2) = \rho$ is true for two solutions ϕ_1 and ϕ_2 then subtracting these equations implies $L(\phi_1 - \phi_2) = 0$ for any linear $L(a\phi_1 + b\phi_2) = aL(\phi_1) + bL(\phi_2)$. In the present instance $L = \partial_t^2 - \nabla^2$ is indeed linear.

implies $|\mathbf{k}|\phi_0 = \mathbf{k}\cdot\mathbf{A}_0$. The complex conjugate ('c.c.') is added in each case because physical electromagnetic fields are real.

Notice that (9.1.17) does not completely eliminate the gauge ambiguity in $\mathbf{A}$ and ϕ since it remains unchanged under the shift $\mathbf{A} \to \mathbf{A} + \nabla\zeta$ and $\phi \to \phi - \partial_t\,\zeta$ with $\zeta = \zeta_0\,\exp[-i|\mathbf{k}|t + i\mathbf{k}\cdot\mathbf{x}]$, since this shifts $|\mathbf{k}|\phi_0 \to |\mathbf{k}|\phi_0 + i\mathbf{k}^2\zeta_0$ and $\mathbf{k}\cdot\mathbf{A}_0 \to \mathbf{k}\cdot\mathbf{A}_0 + i\mathbf{k}^2\zeta_0$. As a consequence ζ_0 can be chosen to set $\phi_0 = \mathbf{k}\cdot\mathbf{A}_0 = 0$.

The upshot is that electromagnetic waves are transverse, being writable as

$$\phi_{\rm hom} = 0 \qquad \text{and} \qquad \mathbf{A}_{\rm hom} \propto \boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{-i|\mathbf{k}|t + i\mathbf{k}\cdot\mathbf{x}} + \text{c.c.}\,, \tag{9.1.18}$$

where the polarization vector $\boldsymbol{\epsilon}_\lambda(\mathbf{k})$ is perpendicular to the wave-vector: $\mathbf{k}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{k}) = 0$. For a wave travelling up the z-axis, for which $\mathbf{k} = k\,\mathbf{e}_z$, the polarization vectors can be chosen to be a linear combination of two basis vectors. Two convenient choices for this basis are

$$\boldsymbol{\epsilon}_x(\mathbf{k}) = \mathbf{e}_x \quad \text{and} \quad \boldsymbol{\epsilon}_y(\mathbf{k}) = \mathbf{e}_y \qquad \text{(linear polarization)} \tag{9.1.19}$$

or

$$\boldsymbol{\epsilon}_\pm(\mathbf{k}) = \frac{1}{\sqrt{2}}\Big(\mathbf{e}_x \pm i\mathbf{e}_y\Big) \qquad \text{(circular polarization)}\,. \tag{9.1.20}$$

For later purposes notice these polarization vectors satisfy the following normalization condition

$$\boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}_\zeta(\mathbf{k}) = \delta_{\lambda\zeta}\,, \tag{9.1.21}$$

as well as the completeness relation

$$\sum_{\lambda=\pm} \boldsymbol{\epsilon}^*_{\lambda i}(\mathbf{k})\cdot\boldsymbol{\epsilon}_{\lambda j}(\mathbf{k}) = \delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2}\,, \tag{9.1.22}$$

where $i, j = x, y, z$ here denote the vector components and the sum over λ in general goes over the two types of polarization.

With these choices the corresponding electric and magnetic fields for plane electromagnetic waves become

$$\mathbf{E}_{\rm hom} \propto i|\mathbf{k}|\,\boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{-i|\mathbf{k}|t + i\mathbf{k}\cdot\mathbf{x}} + \text{c.c.} \qquad \text{and} \qquad \mathbf{B}_{\rm hom} \propto i\mathbf{k}\times\boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{-i|\mathbf{k}|t + i\mathbf{k}\cdot\mathbf{x}} + \text{c.c.}\,. \tag{9.1.23}$$

9.1.4 Conservation of energy and momentum

Because Maxwell's equations are invariant under translations in space and time (in the absence of time- and position-dependent charge densities and currents), it is possible to define a conserved energy and momentum density.

The energy carried by a combination of electric and magnetic fields is given by

$$H = \frac{1}{2}\int \mathrm{d}^3x\,\Big(\mathbf{E}^2 + \mathbf{B}^2\Big)\,, \tag{9.1.24}$$

and this is locally conserved because Maxwell's equations imply

$$\partial_t \left[\frac{1}{2}\Big(\mathbf{E}^2 + \mathbf{B}^2\Big)\right] = \mathbf{E}\cdot\partial_t\mathbf{E} + \mathbf{B}\cdot\partial_t\mathbf{B} = \mathbf{E}\cdot\Big(\nabla\times\mathbf{B} - \mathbf{J}\Big) - \mathbf{B}\cdot\Big(\nabla\times\mathbf{E}\Big)$$
$$= -\nabla\cdot\Big(\mathbf{E}\times\mathbf{B}\Big) - \mathbf{E}\cdot\mathbf{J}\,. \tag{9.1.25}$$

This shows that this energy is locally conserved provided that $\mathbf{E}\cdot\mathbf{J} = 0$, and identifies the local density of energy flux carried by electromagnetic fields to be given by the 'Poynting vector':

$$\mathbf{S} := \mathbf{E}\times\mathbf{B}\,. \tag{9.1.26}$$

$\mathbf{S}$ gives the density of energy flux because the above arguments show it is related to the energy density $\mathcal{H} = \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2)$ by the local conservation equation $\partial_t\mathcal{H} + \nabla\cdot\mathbf{S} = 0$ whenever $\mathbf{E}\cdot\mathbf{J} = 0$.

It turns out that $\mathbf{S}$ plays a double role, also acting as the local momentum density of a collection of electromagnetic fields. This is perhaps most easily seen by evaluating $\mathcal{H}$ and $\mathbf{S}$ for the plane waves given in (9.1.18). Using $\phi = 0$ and $\mathbf{A} = C_{\mathbf{k}}\,\boldsymbol{\epsilon}_\lambda(\mathbf{k})\cos(-|\mathbf{k}|t + \mathbf{k}\cdot\mathbf{x} + \delta)$ implies $\mathbf{E}^2 = \mathbf{B}^2 = C_{\mathbf{k}}^2|\mathbf{k}|^2\cos^2(-|\mathbf{k}|t + \mathbf{k}\cdot\mathbf{x} + \delta)$ and $\mathbf{E}\times\mathbf{B} = C_{\mathbf{k}}^2|\mathbf{k}|\mathbf{k}\cos^2(-|\mathbf{k}|t + \mathbf{k}\cdot\mathbf{x} + \delta)$. It turns out that properly normalized modes have $C_{\mathbf{k}}^2 \propto /|\mathbf{k}|$. So if the normalization is chosen so that the energy obtained after integrating over a given volume commensurate with the wavelength is $E = \int \mathrm{d}^3x\ \mathcal{H} = N|\mathbf{k}|$, for some $\mathbf{k}$-independent constant N, then the same normalization gives $\mathbf{P} = \int \mathrm{d}^3x\ \mathbf{S} = N\mathbf{k}$. This is as would be expected if $\mathbf{S}$ were interpreted as the local momentum density in the same way that $\mathcal{H}$ is the local energy density. (This connection is also made more explicit in §9.2.)

9.2 Field quantization: photons

In the discussion to this point electromagnetic fields were implicitly regarded to be classical (though the point was left deliberately ambiguous). This section makes the transition to quantum fields starting from Einstein's interpretation of electromagnetic waves in terms of energy quanta (photons).

The starting points for defining the electromagnetic field operator are (as usual) the creation and annihilation operators for photons: $a^\star_{\mathbf{k}\lambda}$ and $a_{\mathbf{k}\lambda}$ which satisfy the usual commutation relations $[a_{\mathbf{k}\lambda}, a_{\mathbf{q}\xi}] = 0$ and

$$\Big[a_{\mathbf{k}\lambda}, a^\star_{\mathbf{q}\xi}\Big] = \delta_{\mathbf{kq}}\,\delta_{\lambda\xi}\,. \tag{9.2.1}$$

Here $\{\mathbf{k}, \lambda\}$ are the single-particle labels for photon states, with $\mathbf{k}$ being (as usual) momentum and λ being the polarization label. For linearly polarized states one might have $\lambda = 1, 2$ for the two perpendicular directions orthogonal to $\mathbf{k}$ and for circularly polarized photons it could instead be $\lambda = \pm$ (*c.f.* eqs. (9.1.19) and (9.1.20)).

A Fock space of multiple photon states are built up in the usual way by repeatedly acting with $a^\star_{\mathbf{k}\lambda}$:

$$|\{N_{\mathbf{k}\lambda}\}\rangle \propto \prod_{\mathbf{k}\lambda} (a^\star_{\mathbf{k}\lambda})^{N_{\mathbf{k}\lambda}} |0\rangle \,. \tag{9.2.2}$$

The energy of a collection of free photons is (as usual) given by

$$H_{\text{free}} = E_0 + \sum_{\mathbf{k}\lambda} \omega(\mathbf{k})\, a^\star_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} = E_0 + \sum_\lambda \int \mathrm{d}^3k\, \omega(\mathbf{k})\, \mathfrak{a}^\star_{\mathbf{k}\lambda} \mathfrak{a}_{\mathbf{k}\lambda} \tag{9.2.3}$$

where $\omega(\mathbf{k}) = |\mathbf{k}|$ is the single-particle energy of an individual photon with momentum $\mathbf{k}$, and (as usual) the continuum-normalized states satisfy

$$[\mathfrak{a}_{\mathbf{k}\lambda}, \mathfrak{a}^\star_{\mathbf{q}\zeta}] = \delta^3(\mathbf{k}-\mathbf{q})\delta_{\lambda\zeta} \,. \tag{9.2.4}$$

9.2.1 Electric and magnetic field operators

The connection between creation and annihilation operators and electromagnetic fields is made as in (6.1.7), by expanding the field operator in a basis of plane-wave states, keeping in mind that the electromagnetic field is real (or, as an operator, hermitian). In the Heisenberg picture (where operators are time-dependent) and working within Lorentz gauge as above, this suggests:

$$\begin{aligned}
\mathbf{A}_{\text{hom}}(\mathbf{x},t) &= \frac{1}{\sqrt{\mathcal{V}}} \sum_{\lambda=\pm1} \sum_{\mathbf{k}} \frac{1}{\sqrt{2\omega(\mathbf{k})}} \Big[a_{\mathbf{k}\lambda} \boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{-i\omega(\mathbf{k})t + i\mathbf{k}\cdot\mathbf{x}} + a^\star_{\mathbf{k}\lambda} \boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\, e^{i\omega(\mathbf{k})t - i\mathbf{k}\cdot\mathbf{x}} \Big] \\
&= \sum_{\lambda=\pm1} \int \frac{\mathrm{d}^3k}{\sqrt{(2\pi)^3 2\omega(\mathbf{k})}} \Big[\mathfrak{a}_{\mathbf{k}\lambda} \boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{-i\omega(\mathbf{k})t + i\mathbf{k}\cdot\mathbf{x}} + \mathfrak{a}^\star_{\mathbf{k}\lambda} \boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\, e^{i\omega(\mathbf{k})t - i\mathbf{k}\cdot\mathbf{x}} \Big]
\end{aligned} \tag{9.2.5}$$

and $\phi_{\text{hom}}(\mathbf{x},t) = 0$. Here the factor $[2\omega(\mathbf{k})]^{-1/2}$ – with $\omega(\mathbf{k}) = |\mathbf{k}|$ being (as above) the single-photon energy – is added for later convenience,[25] and the polarization vectors are as defined above in (9.1.19) or (9.1.20). In practical later applications circular polarizations are usually chosen as the polarization basis. Notice in particular that the property $\mathbf{k}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{k}) = 0$ implies that the field operator satisfies the Coulomb gauge condition

$$\nabla \cdot \mathbf{A}_{\text{hom}} = 0 \,. \tag{9.2.6}$$

The subscript 'hom' emphasizes that (so far) this description only applies to the wave part of the field (which in Heisenberg representation satisfies the homogeneous field equation (9.1.15)).

[25] The later convenience is to make transformation properties under special relativity more manifest, and this factor does the job because the combination $\mathrm{d}^3k/\omega(\mathbf{k})$ turns out to be Lorentz-invariant. The same factor also ensures that the commutation relation (9.2.4) implies the standard canonical commutation relations between $\partial_t \mathbf{A}$ and $\mathbf{A}$.

With this choice the Heisenberg picture electric field becomes (*c.f.* eq. (9.1.23))

$$\begin{aligned}\mathbf{E}_{\rm hom}(\mathbf{x},t) &= \frac{i}{\sqrt{\mathcal{V}}}\sum_{\lambda=\pm1}\sum_{\mathbf{k}}\sqrt{\frac{\omega(\mathbf{k})}{2}}\Big[a_{\mathbf{k}\lambda}\boldsymbol{\epsilon}_\lambda(\mathbf{k})\,e^{-i\omega(\mathbf{k})t+i\mathbf{k}\cdot\mathbf{x}} - a^\star_{\mathbf{k}\lambda}\boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\,e^{i\omega(\mathbf{k})t-i\mathbf{k}\cdot\mathbf{x}}\Big]\\ &= i\sum_{\lambda=\pm1}\int \mathrm{d}^3k\sqrt{\frac{\omega(\mathbf{k})}{2(2\pi)^3}}\Big[\mathfrak{a}_{\mathbf{k}\lambda}\boldsymbol{\epsilon}_\lambda(\mathbf{k})\,e^{-i\omega(\mathbf{k})t+i\mathbf{k}\cdot\mathbf{x}} - \mathfrak{a}^\star_{\mathbf{k}\lambda}\boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\,e^{i\omega(\mathbf{k})t-i\mathbf{k}\cdot\mathbf{x}}\Big]\end{aligned} \tag{9.2.7}$$

while the magnetic field in Heisenberg picture is

$$\begin{aligned}\mathbf{B}_{\rm hom}(\mathbf{x},t) &= \frac{i}{\sqrt{\mathcal{V}}}\sum_{\lambda=\pm1}\sum_{\mathbf{k}}\frac{1}{\sqrt{2\omega(\mathbf{k})}}\,\mathbf{k}\times\Big[a_{\mathbf{k}\lambda}\boldsymbol{\epsilon}_\lambda(\mathbf{k})\,e^{-i\omega(\mathbf{k})t+i\mathbf{k}\cdot\mathbf{x}} - a^\star_{\mathbf{k}\lambda}\boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\,e^{i\omega(\mathbf{k})t-i\mathbf{k}\cdot\mathbf{x}}\Big]\\ &= i\sum_{\lambda=\pm1}\int\frac{\mathrm{d}^3k}{\sqrt{(2\pi)^3 2\omega(\mathbf{k})}}\,\mathbf{k}\times\Big[\mathfrak{a}_{\mathbf{k}\lambda}\boldsymbol{\epsilon}_\lambda(\mathbf{k})\,e^{-i\omega(\mathbf{k})t+i\mathbf{k}\cdot\mathbf{x}} - \mathfrak{a}^\star_{\mathbf{k}\lambda}\boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\,e^{i\omega(\mathbf{k})t-i\mathbf{k}\cdot\mathbf{x}}\Big]\,.\end{aligned} \tag{9.2.8}$$

Notice that $\mathbf{A}_{\rm hom}(\mathbf{x},t)$ does not commute with $a_{\mathbf{k}\lambda}$ or $\mathfrak{a}_{\mathbf{k}\lambda}$ since, for instance

$$\begin{aligned}\Big[\mathfrak{a}_{\mathbf{p}\zeta},\mathbf{A}_{\rm hom}(\mathbf{x},t)\Big] &= \sum_{\lambda=\pm1}\int\frac{\mathrm{d}^3k}{\sqrt{(2\pi)^3 2\omega(\mathbf{k})}}\,\Big[\mathfrak{a}_{\mathbf{p}\zeta},\mathfrak{a}^\star_{\mathbf{k}\lambda}\Big]\,\boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\,e^{i\omega(\mathbf{k})t-i\mathbf{k}\cdot\mathbf{x}}\\ &= \frac{1}{\sqrt{(2\pi)^3 2\omega(\mathbf{p})}}\,\boldsymbol{\epsilon}^*_\zeta(\mathbf{p})\,e^{i\omega(\mathbf{p})t-i\mathbf{p}\cdot\mathbf{x}}\,,\end{aligned} \tag{9.2.9}$$

and so

$$\begin{aligned}\Big[\mathfrak{a}^\star_{\mathbf{p}\zeta}\mathfrak{a}_{\mathbf{p}\zeta},\mathbf{A}_{\rm hom}(\mathbf{x},t)\Big] &= \mathfrak{a}^\star_{\mathbf{p}\zeta}\Big[\mathfrak{a}_{\mathbf{p}\zeta}\,,\mathbf{A}_{\rm hom}(\mathbf{x},t)\Big] + \Big[\mathfrak{a}^\star_{\mathbf{p}\zeta}\,,\mathbf{A}_{\rm hom}(\mathbf{x},t)\Big]\mathfrak{a}_{\mathbf{p}\zeta}\\ &= \frac{1}{\sqrt{(2\pi)^3 2\omega(\mathbf{p})}}\Big[\boldsymbol{\epsilon}^*_\zeta(\mathbf{p})\,\mathfrak{a}^\star_{\mathbf{p}\zeta}\,e^{i\omega(\mathbf{p})t-i\mathbf{p}\cdot\mathbf{x}} - \boldsymbol{\epsilon}_\zeta(\mathbf{p})\,\mathfrak{a}_{\mathbf{p}\zeta}\,e^{-i\omega(\mathbf{p})t+i\mathbf{p}\cdot\mathbf{x}}\Big]\,.\end{aligned} \tag{9.2.10}$$

A similar relation also holds for the commutator of $\mathfrak{a}^\star_{\mathbf{p}\zeta}\mathfrak{a}_{\mathbf{p}\zeta}$ with $\mathbf{E}_{\rm hom}$ and $\mathbf{B}_{\rm hom}$. These show that the operators $\mathbf{A}_{\rm hom}(\mathbf{x},t)$, $\mathbf{E}_{\rm hom}(\mathbf{x},t)$ and $\mathbf{B}_{\rm hom}(\mathbf{x},t)$ cannot be diagonalized in the same basis that diagonalizes photon number (and so in particular the fields $\mathbf{A}_{\rm hom}(\mathbf{x},t)$, $\mathbf{E}_{\rm hom}(\mathbf{x},t)$ and $\mathbf{B}_{\rm hom}(\mathbf{x},t)$ must all fluctuate in any energy eigenstate built from the Fock basis of states, including in particular the ground state, or no-particle vacuum). That is, although the mean values of these fields vanish, $\langle 0|\mathbf{A}_{\rm hom}(\mathbf{x},t)|0\rangle = \langle 0|\mathbf{E}_{\rm hom}(\mathbf{x},t)|0\rangle = \langle 0|\mathbf{B}_{\rm hom}(\mathbf{x},t)|0\rangle = 0$, their variances $\langle 0|\mathbf{A}^2_{\rm hom}(\mathbf{x},t)|0\rangle$, $\langle 0|\mathbf{E}^2_{\rm hom}(\mathbf{x},t)|0\rangle$ and $\langle 0|\mathbf{B}^2_{\rm hom}(\mathbf{x},t)|0\rangle$ are all nonzero. It is the fluctuating values of these fields in the vacuum that are widely known as 'vacuum fluctuations'.

Notice also that with these expressions the photon commutation relations imply the following equal-time commutation relations in position space:

$$\begin{aligned}
\Big[A_{i\,\mathrm{hom}}(\mathbf{x},t), E_{j\,\mathrm{hom}}(\mathbf{y},t)\Big] &= -\Big[A_{i\,\mathrm{hom}}(\mathbf{x},t), \partial_t A_{j\,\mathrm{hom}}(\mathbf{y},t)\Big] \\
&= i\sum_{\lambda\zeta=\pm1}\int \frac{\mathrm{d}^3k\,\mathrm{d}^3q}{2(2\pi)^3}\sqrt{\frac{\omega(\mathbf{q})}{\omega(\mathbf{k})}}\Big\{-\Big[\mathfrak{a}_{\mathbf{k}\lambda},\mathfrak{a}^\star_{\mathbf{q}\zeta}\Big]\,\boldsymbol{\epsilon}_{\lambda i}(\mathbf{k})\boldsymbol{\epsilon}^*_{\zeta j}(\mathbf{q})\,e^{-i[\omega(\mathbf{k})-\omega(\mathbf{q})]t+i(\mathbf{k}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{y})} \\
&\qquad\qquad +\Big[\mathfrak{a}^\star_{\mathbf{k}\lambda},\mathfrak{a}_{\mathbf{q}\zeta}\Big]\,\boldsymbol{\epsilon}^*_{\lambda i}(\mathbf{k})\boldsymbol{\epsilon}_{\zeta j}(\mathbf{q})\,e^{i[\omega(\mathbf{k})-\omega(\mathbf{q})]t-i(\mathbf{k}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{y})}\Big\} \\
&= -i\sum_{\lambda=\pm1}\int\frac{\mathrm{d}^3k}{2(2\pi)^3}\Big\{\boldsymbol{\epsilon}_{\lambda i}(\mathbf{k})\boldsymbol{\epsilon}^*_{\lambda j}(\mathbf{k})\,e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}+\boldsymbol{\epsilon}^*_{\lambda i}(\mathbf{k})\boldsymbol{\epsilon}_{\lambda j}(\mathbf{k})\,e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\Big\} \qquad (9.2.11)\\
&= -i\int\frac{\mathrm{d}^3k}{(2\pi)^3}\left(\delta_{ij}-\frac{k_ik_j}{\mathbf{k}^2}\right)e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} = -i\left(\delta_{ij}-\frac{\partial_i\partial_j}{\nabla^2}\right)\delta^3(\mathbf{x}-\mathbf{y})\,.
\end{aligned}$$

The δ_{ij} term here has the same form as would the canonical quantization relations for position and momentum if $\partial_t A_i$ were the momentum conjugate to A_i (more about this in later sections). The $\partial_i\partial_j/\nabla^2$ term is that what is required to make the result consistent with the Coulomb gauge condition (9.2.6), and the homogeneous Maxwell equation $\nabla\cdot\mathbf{E}_{\mathrm{hom}}=0$.

9.2.2 Photon energy and momentum operators

It is a simple matter to substitute the above expressions for $\mathbf{E}_{\mathrm{hom}}$ and $\mathbf{B}_{\mathrm{hom}}$ as functions of $\mathfrak{a}_{\mathbf{k}\lambda}$ and $\mathfrak{a}^\star_{\mathbf{k}\lambda}$ to see what the Maxwell energy (9.1.24) and energy flux (9.1.26) become once expressed in terms of creation and annihilation operators.

Worked example: energy and momentum in terms of $a_{\mathbf{k}\lambda}$

For the energy operator this yields the result

$$\begin{aligned}
H &:= \frac{1}{2}\int \mathrm{d}^3x\,\Big(\mathbf{E}^2_{\mathrm{hom}}+\mathbf{B}^2_{\mathrm{hom}}\Big) \\
&= \frac{1}{4}\sum_{\lambda\zeta=\pm1}\int \mathrm{d}^3k\,\omega(\mathbf{k})\Big[\mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{k}\zeta}\;\boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}_\zeta(\mathbf{k})+\mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}^\star_{\mathbf{k}\zeta}\;\boldsymbol{\epsilon}_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}^*_\zeta(\mathbf{k}) \qquad (9.2.12)\\
&\qquad -\mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}_{-\mathbf{k}\zeta}\;\boldsymbol{\epsilon}_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}_\zeta(-\mathbf{k})\,e^{-2i\omega(\mathbf{k})t}-\mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}^\star_{-\mathbf{k}\zeta}\;\boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}^*_\zeta(-\mathbf{k})\,e^{2i\omega(\mathbf{k})t}\Big]+\mathbf{B}^2\text{ terms}\,, \\
&= \frac{1}{2}\sum_{\lambda=\pm1}\int \mathrm{d}^3k\,\omega(\mathbf{k})\Big[\mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{k}\lambda}+\mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}^\star_{\mathbf{k}\lambda}\Big]
\end{aligned}$$

which uses $\omega(-\mathbf{k})=\omega(\mathbf{k})$. Both the $\mathfrak{a}_{\mathbf{k}}\mathfrak{a}_{-\mathbf{k}}$ term and its adjoint vanish once the $\mathbf{E}^2_{\mathrm{hom}}$ and $\mathbf{B}^2_{\mathrm{hom}}$ terms are summed, while the $\mathbf{E}^2_{\mathrm{hom}}$ and $\mathbf{B}^2_{\mathrm{hom}}$ terms contribute equally for the $\mathfrak{a}^\star_{\mathbf{k}}\mathfrak{a}_{\mathbf{k}}$ and $\mathfrak{a}_{\mathbf{k}}\mathfrak{a}^\star_{\mathbf{k}}$ terms explicitly displayed. Notice the final result is precisely the same as H_{free}, as given in (9.2.3), with $\omega(\mathbf{k})=|\mathbf{k}|$ and

$$E_0=\frac{1}{2}\sum_{\lambda=\pm1}\int\mathrm{d}^3k\,\omega(\mathbf{k})=\int\mathrm{d}^3k\,|\mathbf{k}|\,, \qquad (9.2.13)$$

given by the sum of zero-point energies over all possible photon modes. This verifies that using the field expansion (9.2.5) in the Maxwell energy simply returns the energy of noninteracting photons.

The momentum operator is similarly obtained by inserting (9.2.5) into the energy flux (Poynting vector) and integrating over all space.[26] One finds in this way

$$\begin{aligned}\mathbf{P} &:= \int \mathrm{d}^3x\, \mathbf{E}_{\rm hom} \times \mathbf{B}_{\rm hom} \\ &= \frac{1}{2}\sum_{\lambda\zeta=\pm1} \int \mathrm{d}^3k\, \mathbf{k}\Big[\mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{k}\zeta}\, \boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}_\zeta(\mathbf{k}) + \mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}^\star_{\mathbf{k}\zeta}\, \boldsymbol{\epsilon}_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}^*_\zeta(\mathbf{k}) \\ &\qquad\qquad +\mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}_{-\mathbf{k}\zeta}\, \boldsymbol{\epsilon}_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}_\zeta(-\mathbf{k})\, e^{-2i\omega(\mathbf{k})t} + \mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}^\star_{-\mathbf{k}\zeta}\, \boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\cdot\boldsymbol{\epsilon}^*_\zeta(-\mathbf{k})\, e^{2i\omega(\mathbf{k})t}\Big], \\ &= \frac{1}{2}\sum_{\lambda=\pm1} \int \mathrm{d}^3k\, \mathbf{k}\Big[\mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{k}\lambda} + \mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}^\star_{\mathbf{k}\lambda}\Big] = \sum_{\lambda=\pm1} \int \mathrm{d}^3k\, \mathbf{k}\, \mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{k}\lambda}\end{aligned} \tag{9.2.14}$$

where the third equality uses the identity $\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = \mathbf{b}(\mathbf{a}\cdot\mathbf{c}) - \mathbf{c}(\mathbf{a}\cdot\mathbf{b})$ (true for any three vectors) and $\mathbf{k}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{k}) = 0$ (for both λ). In this case the $\mathfrak{a}_\mathbf{k}\mathfrak{a}_\mathbf{k}$ terms cancel between $\mathbf{k}$ and $-\mathbf{k}$ in the integral d^3k. There is no zero-point contribution to $\mathbf{P}$ because the divergent integral $\int \mathrm{d}^3k\, \mathbf{k}$ vanishes if it is regulated in a rotationally invariant way.

Again the Maxwell expression for field momentum reproduces the sum over photon momenta once the electromagnetic fields are expressed in terms of $\mathfrak{a}^\star_{\mathbf{k}\lambda}$ and $\mathfrak{a}_{\mathbf{k}\lambda}$ using (9.2.5). Treating the electromagnetic field like an operator is equivalent to treating multi-photon states in terms of creation and annihilation operators along the lines used for other particles in earlier sections.

9.3 Casimir energy and regularizations

As a simple application of a consequence of regarding electromagnetic fields as quantum operators, consider the zero-point energy, E_0, given by (9.2.13). Although this is not in itself measurable to the extent that experiments are only sensitive to energy differences,[27] what *can* be measured is any dependence of E_0 on external variables that can be varied in the lab.

An example of this is the change in zero-point energy associated with a change in boundary conditions, such as the zero-point energy of an electromagnetic field between the parallel conducting plates of a capacitor. This energy depends on the separation L between the plates and so can be measured by varying L: (the derivative of the zero-point energy with respect to L manifests itself as a force between the plates). This difference arises because the single-particle energies appearing in (9.2.13) themselves depend on L.

To see how this works in detail, consider parallel conducting plates, one situated at $z = 0$ and the other at $z = L$. Single-particle energies respond to the presence of these plates because any static electric field must be perpendicular to the surface of a conductor. (If it

[26] For aficionados: this works because the symmetry of the stress-energy tensor ensures that the energy flux density equals the momentum density.

[27] The gravitational consequences of the zero-point energy *are* measurable because gravity responds to the total energy density and not just to energy differences, but that is a subject for another chapter.

weren't then the part of the field tangent to the surface would drive currents in the conductor that would continue until the field became normal to the surface.)

Since $\mathbf{E} = -\partial_t \mathbf{A}$ (in a gauge for which $\phi = 0$) the conducting boundary condition is satisfied by the field expansion (9.4.5) if the vector potential satisfies

$$\mathbf{A}(x, y, z = 0) = \mathbf{A}(x, y, z = L) = 0\,. \tag{9.3.1}$$

This boundary condition is in turn satisfied if the normalized photon mode functions are modified from $\mathcal{V}^{-1/2} \exp[i\mathbf{p}\cdot\mathbf{x}]$ to

$$u_{\mathbf{q}n}(\mathbf{r}, z) = \mathcal{V}_{\parallel}^{-1/2} \sqrt{\frac{2}{L}}\, e^{i\mathbf{q}\cdot\mathbf{r}} \sin\left(\frac{\pi n z}{L}\right)\,, \tag{9.3.2}$$

where the momentum and position parallel to the plates are denoted $\mathbf{q} = \{q_x, q_y\}$ and $\mathbf{r} = \{x, y\}$ and are real numbers, while $n = 1, 2, \cdots$ is a positive integer. Here the system volume is written $\mathcal{V} = \mathcal{V}_{\parallel} L$ where $\mathcal{V}_{\parallel}$ is the volume in the two dimensions parallel to the plates.

Denoting the 3-momentum of the mode by $\mathbf{p}_n := \{\mathbf{q}, \pi n/L\}$ the single-particle energy of such a mode is then given by

$$\omega(\mathbf{q}, n) = |\mathbf{p}_n| = \sqrt{\mathbf{q}^2 + \left(\frac{\pi n}{L}\right)^2}\,. \tag{9.3.3}$$

With this mode energy the zero-point energy (9.2.13) per-unit-plate-area becomes

$$\frac{E_0(L)}{\mathcal{V}_{\parallel}} = \sum_{n=1}^{\infty} \int \frac{\mathrm{d}^2 q}{(2\pi)^2} \sqrt{\mathbf{q}^2 + \left(\frac{\pi n}{L}\right)^2}\,, \tag{9.3.4}$$

although in practice our interest is only in the difference

$$\sigma_c(L) := \frac{E_0(L) - E_0(\infty)}{\mathcal{V}_{\parallel}}\,. \tag{9.3.5}$$

Although the sum and integral in (9.3.4) diverge for large n and $\mathbf{q}$ this divergence cancels with a similar divergence in $E_0(\infty)$ leaving a finite result for the observable $\sigma_c(L)$.

9.3.1 Ultraviolet regulators

To evaluate $\sigma_c(L)$ the idea is to 'regulate' the divergent expression (9.3.4) to make intermediate steps well-defined, and remove the regularization once the well-behaved quantity σ_c is obtained. It does not matter precisely how this regularization is done provided that it satisfy the following two reasonableness criteria:

- The regularized version of a convergent integral (or sum) gives the convergent answer;
- The regularization is *linear* inasmuch as the regularization of the sum of two integrals is the same regardless of whether each integral is separately regularized, or only the sum over their combined integrands is regularized.

Any regularization schemes that obey these two conditions may differ on the values found for $E_0(L)$ and $E(\infty)$ separately, but must agree on their convergent difference.

Worked example: regulating the Casimiar energy

To simplify the calculation use a trick — consider the following integral:[28]

$$\int_0^\infty \mathrm{d}s\; s^p\, e^{-\lambda s} = \lambda^{-1-p}\,\Gamma(1+p)\,, \tag{9.3.6}$$

where $\Gamma(z)$ is the Euler gamma function satisfying $z\,\Gamma(z) = \Gamma(z+1)$. Although strictly speaking convergence of the integral assumes $p > -1$ and $\lambda > 0$ in (9.3.6), the right-hand side can also be taken to define the integral for general complex p and returns a finite value for any $p \neq -1, -2, -3, \cdots$. This extension defines the integral for more general complex values of p, and regarded as a regularization of this integral satisfies the two criteria listed above.

The idea is to imagine writing $\lambda = \omega^2$, so that ω can be formally rewritten as the limit

$$\omega = \sqrt{\lambda} = \lim_{p\to -3/2} \frac{1}{\Gamma(1+p)} \int_0^\infty \mathrm{d}s\; s^p\, e^{-\omega^2 s}\,. \tag{9.3.7}$$

Using this to represent the factor $\omega_{\mathbf{k}\lambda}$ in the expression (9.2.13) gives

$$\begin{aligned}
\frac{E_0(L)}{\mathcal{V}_\parallel} &= \sum_{n=1}^\infty \int \frac{\mathrm{d}^2 q}{(2\pi)^2}\, \omega(\mathbf{q}, n) \\
&= \lim_{p\to -3/2} \frac{1}{\Gamma(1+p)} \int_0^\infty \mathrm{d}s\; s^p \sum_{n=1}^\infty \int \frac{\mathrm{d}^2 q}{(2\pi)^2}\; \exp\left\{-\left[\mathbf{q}^2 + \left(\frac{\pi n}{L}\right)^2\right] s\right\} \\
&= \lim_{p\to -3/2} \frac{1}{4\pi\Gamma(1+p)} \int_0^\infty \mathrm{d}s\; s^{p-1} \sum_{n=1}^\infty \exp\left\{-\left(\frac{\pi n}{L}\right)^2 s\right\} \\
&= \lim_{p\to -3/2} \frac{1}{4\pi p} \left(\frac{L}{\pi}\right)^{2p} \sum_{n=1}^\infty \frac{1}{n^{2p}} \\
&= \lim_{p\to -3/2} \frac{1}{4\pi p} \left(\frac{L}{\pi}\right)^{2p} \zeta_R(2p) \\
&= -\frac{\pi^2}{6L^3}\, \zeta_R(-3) = -\frac{\pi^2}{720 L^3}\,,
\end{aligned} \tag{9.3.8}$$

where the second line uses

$$\int_{-\infty}^\infty \frac{\mathrm{d}q_x}{2\pi}\; e^{-q_x^2 s} = \frac{1}{2\pi}\sqrt{\frac{\pi}{s}}\,, \tag{9.3.9}$$

and similarly for the integral over q_y. The s integral is performed using (9.3.6) again and the final sum is recognized as the Riemann zeta-function, with the last equality using the result $\zeta_R(-3) = \frac{1}{120}$. All the intermediate steps (*e.g.* switching orders of integration and summation) are legitimate for the regularized quantities. The precise details of the regularizations, such as how the Riemann zeta function is evaluated for negative p, are not important for the final result for the reasons give above.

[28] Tricks like this are often more convenient than simply cutting off any integral at a large but finite upper limit, because cutting integrals off often breaks some of a problem's symmetries.

Since the final result in (9.3.8) vanishes as $L \to \infty$ there is no need to subtract $E_0(\infty)$ to obtain the energy difference, leading immediately to

$$\sigma_c(L) = -\frac{\pi^2}{720 L^3}\,. \tag{9.3.10}$$

Because this is negative, the system energy can be lowered by making L smaller. This amounts to there being an attractive force-per-unit-area (or pressure) between the plates, of size[29]

$$p_z = \frac{F_z}{\mathcal{V}_\parallel} = -\frac{\partial \sigma_c}{\partial L} = -\frac{\pi^2}{240 L^4}\,, \tag{9.3.11}$$

an effect that is both large enough to be measurable, and has actually been measured.

9.4 Atom-photon interactions

The next step is to combine the earlier treatment of nonrelativistic particles with the quantum formulation for the electromagnetic field to develop a description of non-relativistic particles interacting with photons.

For these purposes recall that the description of noninteracting nonrelativistic particles interacting with a potential $V(\mathbf{x})$ is described by Schrödinger field theory, with Hamiltonian

$$H_P = \int \mathrm{d}^3x\; \Phi^\star \left[-\frac{\nabla^2}{2m} + V(\mathbf{x})\right] \Phi \tag{9.4.1}$$

while photons are described by the Maxwell Hamiltonian

$$H_{EM} = \frac{1}{2}\int \mathrm{d}^3x\; \left(\mathbf{E}^2 + \mathbf{B}^2\right). \tag{9.4.2}$$

The fields in these cases are related to the creation and annihilation operators (in Schrödinger picture) by

$$\Phi(\mathbf{x}) = \sum_n c_n\, u_n(\mathbf{x})\,, \quad \Phi^\star(\mathbf{x}) = \sum_n c_n^\star\, u_n^*(\mathbf{x})\,, \tag{9.4.3}$$

where

$$\left[-\frac{\nabla^2}{2m} + V(\mathbf{x})\right] u_n = \varepsilon_n\, u_n \tag{9.4.4}$$

and

$$\mathbf{A}(\mathbf{x}) = \sum_\lambda \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2|\mathbf{k}|}} \left[\mathfrak{a}_{\mathbf{k}\lambda}\, \boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}} + \mathfrak{a}^\star_{\mathbf{k}\lambda}\, \boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\, e^{-i\mathbf{k}\cdot\mathbf{x}}\right]. \tag{9.4.5}$$

The question is how to couple these to one another. The idea is to do so in such a way that does not ruin the redundancy of description included in the freedom to make gauge

[29] For aficionados: an alternative derivation of (9.3.11) starts with the observaton that the problem's symmetries require the electromagnetic stress tensor to be $\langle 0|T_{\mu\nu}|0\rangle = \mathrm{diag}(\sigma_c, -\sigma_c, -\sigma_c, p_z)$, where p_z is the inter-plate pressure and σ_c is the energy density found above. But the electromagnetic stress-energy also satisfies $\langle 0|T^\mu{}_\mu|0\rangle = 0$ which implies $-3\,\sigma_c + p_z = 0$.

transformations $\mathbf{A} \to \mathbf{A} + \nabla\zeta$ for an arbitrary function $\zeta(\mathbf{x})$. After all, this redundancy is central to Maxwell's equations describing only the two spin states carried by a massless spin-one particle (more about this in §11 below).

The simplest way to do this is to couple only to the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$, rather than to $\mathbf{A}$ itself. For rotationally invariant particles the simplest such an interaction (*i.e.* the interaction involving the fewest powers of fields and derivatives) couples to the rotational scalars $\mathbf{E}^2$ and $\mathbf{B}^2$, such as in

$$H_{\rm pol} = \frac{1}{2}\int \mathrm{d}^3x\; \Phi^\star\Phi\Big[\kappa_E\,\mathbf{E}^2 + \kappa_B\,\mathbf{B}^2\Big]\,. \tag{9.4.6}$$

This type of interaction indeed turns out to describe well the low-energy interactions between photons and electrically neutral but polarizable particles (such as electrically neutral atoms that are built from charged consituents).

Written in terms of creation and annihilation operators $H_{\rm pol}$ involves four types of terms: $c_n^\star c_m \mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{q}\zeta}$, $c_n^\star c_m \mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}^\star_{\mathbf{q}\zeta}$, $c_n^\star c_m \mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{q}\zeta}$ and $c_n^\star c_m \mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}^\star_{\mathbf{q}\zeta}$. It is a general feature of electromagnetic interactions that whenever there is an interaction that preserves the number of photons (like $c_n^\star c_m \mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{q}\zeta}$ and $c_n^\star c_m \mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}^\star_{\mathbf{q}\zeta}$) there must also be interactions where the net number of photons changes (like $c_n^\star c_m \mathfrak{a}_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{q}\zeta}$ and $c_n^\star c_m \mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}^\star_{\mathbf{q}\zeta}$). These always come together because interactions are built in position space from fields like $\mathbf{A}$, $\mathbf{E}$ or $\mathbf{B}$, all of which involve a sum of terms of the schematic form $(c_1\mathfrak{a}_{\mathbf{k}\lambda} + c_2\mathfrak{a}^\star_{\mathbf{k}\lambda})$, such as in eq. (9.4.5) for example. This proves to be a general feature of *all* interactions once they are made consistent with special relativity, as it turns out, a point that is argued in more detail in §11.

As mentioned earlier, the complete Hamiltonian $H = H_P + H_{EM} + H_{\rm pol}$ turns out to describe the dominant low-energy interactions of photons and neutral, spherically symmetric objects.[30] The coupling constants κ_E and κ_B are called the nonrelativistic particle's 'polarizabilities', and arise when the object in question contains constituent electric charges and/or spins that allow the atom to acquire an induced dipole moment in the presence of an applied field: $\mathbf{d}_E = \kappa_E\mathbf{E}$ and/or $\mathbf{d}_B = \kappa_B\mathbf{B}$. Eq. (9.4.6) then expresses the energy this induced moment has due to its interaction with the applied field.

This picture of where polarizabilities come from also comes with an estimate of their expected size. Imagine perturbing the electrons in an atom or molecule with an interaction that is linear in the electric field: $H_{\rm pert} = -\mathbf{d}_E\cdot\mathbf{E}$ where $\mathbf{d}_E$ is some operator that acts on the electronic degrees of freedom. Provided that the electron state satisfies $\langle\mathbf{d}_E\rangle = 0$ (which turns out to be the condition that the atom or molecule does not have a static dipole moment in the absence of electric fields) the electron's energy shift arises at second order in perturbation theory, making the expression for the energy shift second order in the components E_i of the

[30] It happens also to capture the dominant low-energy interactions of photons with non-spherical objects provided these objects are polarizable and do not have permanent electric or magnetic dipole moments.

electric field – *c.f.* eq. (3.1.9)

$$\delta\mathcal{E}_N \simeq \sum_M \frac{|\langle M|H_{\rm pert}|N\rangle|^2}{\varepsilon_N - \varepsilon_M} = \frac{1}{2}\big(\kappa_E\big)_{ij} E_i E_j \,, \tag{9.4.7}$$

where ε_N denotes the unperturbed electronic energies. Because $\mathbf{d}_E$ has dimension (charge) $\times$ (length), and the denominator is an energy, this discussion shows that $\kappa_E \propto \mathbf{d}_E^2/\Delta\varepsilon$ should have dimension (charge)$^2\times$(length)^2/(energy). [Since magnetic fields require moving charges expressions for κ_B are often suppressed relative to κ_E by powers of $v \ll 1$, where v is the typical speed of the charged constituents internal to the polarizable object of interest.]

For instance, for an electron in a polarizable atom we'd expect $|\mathbf{d}_E| \sim e\, a_B$ where $-e$ is the electron charge and the Bohr radius, $a_B \sim (\alpha m_e)^{-1} \sim 0.1$ nm, is a typical atomic size, where $m_e \simeq 511$ keV is the electron mass and $\alpha := e^2/4\pi \simeq 1/137$ is the electromagnetic fine-structure constant. For atoms the energy denominator appearing in (9.4.7) similarly is of order a typical atomic energy level, and so $\Delta\varepsilon \sim e^2/a_B$ and a typical electronic speed is $v \sim \alpha$. These lead to the estimate (see also §9.5.4 for more details)

$$\kappa_E \sim \frac{(e\, a_B)^2}{e^2/a_B} \sim a_B^3 \,. \tag{9.4.8}$$

What is remarkable here is that the weak electromagnetic coupling cancels in κ_E. As we see in §10 this cancellation is the reason why the index of refraction for ordinary materials (like water or glass) can be significantly different from unity.

The Hamiltonian $H_{EM} + H_{\rm pol}$ dominate the low-energy electromagnetic interactions of small objects like spherically symmetric atoms. It also turns out more generally to dominate the low-energy electromagnetic interactions of most small and polarizable objects, even if they are not spherically symmetric, provided that they do not have permanent electric dipole moments (like water molecules do, for example). This Hamiltonian dominates essentially because its parameters κ_E and κ_B are the least suppressed by powers of a_B where a_B is the small size of the underlying polarizable objects. The rate of scattering of photons from matter to which it leads is a famous prediction (as we now see). This scattering is called 'Rayleigh' scattering, because it agrees with a similar 19th Century calculation performed for the scattering of electromagnetic waves from a simple model of an atom using classical electromagnetism.

Worked Example: Rayleigh scattering

Treating $H_{\rm pol}$ perturbatively allows its implications for photon/neutral-particle scattering to be computed using Fermi's Golden Rule. But what is the small parameter that justifies using perturbative methods in this case? Naively one wants the couplings κ_E and κ_B to be 'small', but because these are dimensionful parameters the question is: what other scale are they small in comparison to? The answer to this depends on what is being computed. For instance, if used to compute the scattering of

photons from atoms then the small dimensionless parameter is $\kappa_{_E} k^3$ or $\kappa_{_B} k^3$, where where k is a measure of the energy involved in the scattering. This should be much less than one to trust perturbation theory.

To see how this works in detail consider the reaction $\gamma(\mathbf{k},\lambda) + C(n) \to \gamma(\mathbf{k}',\lambda') + C(n')$ where C generically represents the non-relativistic polarizable particle. For example C might be an atom – with $V(\mathbf{x})$ perhaps describing a 'trap' that localizes it for experimental purposes, say – or any other small neutral symmetric object. The relevant matrix element for this reaction is given by

$$\begin{aligned}
&\langle \gamma(\mathbf{k}',\lambda')\, C(n') | H_{\rm pol} | \gamma(\mathbf{k},\lambda)\, C(n)\rangle \\
&\qquad = \frac{(-i)^2}{2(2\pi)^3\sqrt{|\mathbf{k}||\mathbf{k}'|}} \int \mathrm{d}^3x\; u^\star_{n'}(\mathbf{x}) u_n(\mathbf{x}) \\
&\qquad\qquad \times \Big[\kappa_{_E}\, |\mathbf{k}||\mathbf{k}'| (\boldsymbol{\epsilon}^*_{\lambda'}\cdot\boldsymbol{\epsilon}_\lambda)\; e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} + \kappa_{_B} (\mathbf{k}'\times\boldsymbol{\epsilon}^*_{\lambda'})\cdot(\mathbf{k}\times\boldsymbol{\epsilon}_\lambda)\; e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \Big] \\
&\qquad = \frac{(-i)^2}{2(2\pi)^3\sqrt{|\mathbf{k}||\mathbf{k}'|}}\; \varrho_{n'n}(\mathbf{k}-\mathbf{k}') \Big[\Big(\kappa_{_E}\, |\mathbf{k}||\mathbf{k}'| + \kappa_{_B}\, \mathbf{k}\cdot\mathbf{k}' \Big) (\boldsymbol{\epsilon}^*_{\lambda'}\cdot\boldsymbol{\epsilon}_\lambda) - \kappa_{_B} (\mathbf{k}'\cdot\boldsymbol{\epsilon}_\lambda)(\mathbf{k}\cdot\boldsymbol{\epsilon}^*_{\lambda'}) \Big]
\end{aligned} \tag{9.4.9}$$

where the last equality defines the (dimensionless) Fourier transform of the nonrelativistic particle density matrix element

$$\varrho_{n'n}(\mathbf{q}) := \int \mathrm{d}^3x\; u^*_{n'}(\mathbf{x}) u_n(\mathbf{x})\; e^{i\mathbf{q}\cdot\mathbf{x}}\,, \tag{9.4.10}$$

and uses the vector identity

$$(\mathbf{k}'\times\boldsymbol{\epsilon}^*_{\lambda'})\cdot(\mathbf{k}\times\boldsymbol{\epsilon}_\lambda) = (\mathbf{k}'\cdot\mathbf{k})(\boldsymbol{\epsilon}^*_{\lambda'}\cdot\boldsymbol{\epsilon}_\lambda) - (\mathbf{k}'\cdot\boldsymbol{\epsilon}_\lambda)(\mathbf{k}\cdot\boldsymbol{\epsilon}^*_{\lambda'})\,. \tag{9.4.11}$$

In the special case the C particle is free (*i.e.* if $V(\mathbf{x}) = V_0$ is constant) then $n, n' \to \mathbf{p}, \mathbf{p}'$ can be taken as momentum eigenstates, in which case

$$u_n(\mathbf{x}) \to \frac{1}{\sqrt{\mathcal{V}}}\, \exp[i\mathbf{p}\cdot\mathbf{x}] \quad \text{and so} \quad \varrho_{n'n}(\mathbf{k}-\mathbf{k}') \to \frac{(2\pi)^3}{\mathcal{V}}\; \delta^3(\mathbf{p}+\mathbf{k}-\mathbf{p}'-\mathbf{k}')\,. \tag{9.4.12}$$

In these expressions $\boldsymbol{\epsilon}_\lambda := \boldsymbol{\epsilon}_\lambda(\mathbf{k})$ and $\boldsymbol{\epsilon}_{\lambda'} := \boldsymbol{\epsilon}_{\lambda'}(\mathbf{k}')$ are polarization vectors that are referred to different momenta. It is convenient when evaluating this matrix element to choose the incoming photon momentum to define the z axis, and to choose the outgoing photon momentum to lie in the $z-x$ plane, in which case

$$\mathbf{k} = k\,\mathbf{e}_z \quad \text{and} \quad \boldsymbol{\epsilon}_\pm = \frac{1}{\sqrt{2}}(\mathbf{e}_x \pm i\,\mathbf{e}_y)\,, \tag{9.4.13}$$

for circularly polarized states, and so $\boldsymbol{\epsilon}^*_\pm\cdot\boldsymbol{\epsilon}_\pm = 1$ and $\boldsymbol{\epsilon}^*_\pm\cdot\boldsymbol{\epsilon}_\mp = \mathbf{k}\cdot\boldsymbol{\epsilon}_\pm = 0$ as required. Similarly

$$\mathbf{k}' = k'(\mathbf{e}_z\cos\theta + \mathbf{e}_x\sin\theta) \quad \text{and} \quad \boldsymbol{\epsilon}_{\pm'} = \frac{1}{\sqrt{2}}(\mathbf{e}_x\cos\theta - \mathbf{e}_z\sin\theta \pm i\,\mathbf{e}_y)\,, \tag{9.4.14}$$

and so $\mathbf{k}'\cdot\boldsymbol{\epsilon}_{\pm'} = 0$ and so on, as required. With these expressions the various dot products can be evaluated explicitly in terms of the photon scattering angle θ. Writing $|\mathbf{k}| = k$ and $|\mathbf{k}'| = k'$ one finds

$$\mathbf{k}\cdot\mathbf{k}' = kk'\,\cos\theta\,, \quad \mathbf{k}\cdot\boldsymbol{\epsilon}^*_{\pm'} = -\frac{k}{\sqrt{2}}\,\sin\theta\,, \quad \mathbf{k}'\cdot\boldsymbol{\epsilon}_\pm = \frac{k'}{\sqrt{2}}\,\sin\theta\,, \tag{9.4.15}$$

and

$$\boldsymbol{\epsilon}^*_{\pm'}\cdot\boldsymbol{\epsilon}_\pm = \frac{1}{2}(1+\cos\theta) = \cos^2\frac{\theta}{2} \quad \text{and} \quad \boldsymbol{\epsilon}^*_{\pm'}\cdot\boldsymbol{\epsilon}_\mp = -\frac{1}{2}(1-\cos\theta) = -\sin^2\frac{\theta}{2} \tag{9.4.16}$$

and so (for example)

$$\sum_{\lambda} |\boldsymbol{\epsilon}_{\lambda'} \cdot \boldsymbol{\epsilon}_{\lambda}|^2 = \cos^4 \frac{\theta}{2} + \sin^4 \frac{\theta}{2} = \frac{1}{2}\left(1 + \cos^2\theta\right) . \tag{9.4.17}$$

With these expressions in hand, the helicity-preserving amplitude (with $\lambda' = \lambda$) is

$$\begin{aligned} &\langle \gamma(\mathbf{k}'\pm') \, C(n') | H_{\rm pol} | \gamma(\mathbf{k}\pm) \, C(n) \rangle \\ &\qquad = \frac{(-i)^2}{2(2\pi)^3} \sqrt{|\mathbf{k}||\mathbf{k}'|} \; \varrho_{n'n}(\mathbf{k}-\mathbf{k}') \left[\Big(\kappa_{\scriptscriptstyle E} + \kappa_{\scriptscriptstyle B} \, \cos\theta \Big) \cos^2 \frac{\theta}{2} + \frac{\kappa_{\scriptscriptstyle B}}{2} \, \sin^2\theta \right] , \end{aligned} \tag{9.4.18}$$

while the helicity-flipping amplitude (with $\lambda' = -\lambda$) becomes

$$\begin{aligned} &\langle \gamma(\mathbf{k}'\mp') \, C(n') | H_{\rm pol} | \gamma(\mathbf{k}\pm) \, C(n) \rangle \\ &\qquad = \frac{(-i)^2}{2(2\pi)^3} \sqrt{|\mathbf{k}||\mathbf{k}'|} \; \varrho_{n'n}(\mathbf{k}-\mathbf{k}') \left[-\Big(\kappa_{\scriptscriptstyle E} + \kappa_{\scriptscriptstyle B} \, \cos\theta \Big) \sin^2 \frac{\theta}{2} + \frac{\kappa_{\scriptscriptstyle B}}{2} \, \sin^2\theta \right] . \end{aligned} \tag{9.4.19}$$

Fermi's Golden Rule then gives the total scattering rate for an initially polarized photon:

$$\begin{aligned} \mathrm{d}\Gamma[\gamma(\mathbf{k},\lambda) + C(n) \to \gamma' + X] \;&=\; 2\pi \sum_{\mathbf{k}' \in \Delta\mathbf{k}} \sum_{\lambda' n'} \Big| \big(\gamma(\mathbf{k}',\lambda') \, C(n') | H_{\rm pol} | \gamma(\mathbf{k},\lambda) \, C(n)\big) \Big|^2 \\ &\qquad\qquad \times \delta(k' + \varepsilon_{n'} - k + \varepsilon_n) \\ &=\; \frac{(2\pi)^4}{\mathcal{V}} \sum_{\lambda' n'} \Big| \langle \gamma(\mathbf{k}',\lambda') \, C(n') | H_{\rm pol} | \gamma(\mathbf{k},\lambda) \, C(n) \rangle \Big|^2 \\ &\qquad\qquad \times \delta(k' + \varepsilon_{n'} - k + \varepsilon_n) \; \mathrm{d}^3k' , \end{aligned} \tag{9.4.20}$$

where X in the final state indicates that it is assumed only the final-state photon is measured (what is called an 'inclusive' measurement) and the second equality passes to the continuum limit for photon momenta in the usual way.

Evaluating the matrix element in the special case where $\kappa_{\scriptscriptstyle B} \ll \kappa_{\scriptscriptstyle E}$ (which is the one of most practical interest for polarizable atoms, or other small systems in electro-static equilibrium) and assuming there are N_n initial C particles sitting in the state 'n' then gives

$$\begin{aligned} \mathrm{d}\Gamma[\gamma(\mathbf{k},\lambda) + C(n) \to \gamma' + X] \;=\; &\frac{\kappa_{\scriptscriptstyle E}^2 k k'}{8\pi} \, \frac{N_n}{\mathcal{V}} \left[\cos^4 \frac{\theta}{2} + \sin^4 \frac{\theta}{2} \right] \sin\theta \, \mathrm{d}\theta \\ &\times \sum_{n'} |\varrho_{n'n}(\mathbf{k}-\mathbf{k}')|^2 \delta(k' + \varepsilon_{n'} - k - \varepsilon_n) \, (k')^2 \mathrm{d}k' , \end{aligned} \tag{9.4.21}$$

where a factor of 2π comes from performing the integral over the azimuthal angle ϕ in d^3k.

Expression (9.4.21) has the nice property that details of the initial state $u_n(\mathbf{x})$ drop out in the limit that the spacing between energies $|\varepsilon_{n'} - \varepsilon_n|$ is negligible compared with the initial photon energy, since in this case $\delta(k' + \varepsilon_{n'} - k - \varepsilon_n) \simeq \delta(k' - k)$ and so the only dependence on n' is in $|\varrho_{n'n}(\mathbf{k}'-\mathbf{k})|^2$. This allows the sum over n' to be written

$$\sum_{n'} |\varrho_{n'n}(\mathbf{q})|^2 = \sum_{n'} \int \mathrm{d}^3x \, \mathrm{d}^3y \; u^*_{n'}(\mathbf{x}) u_n(\mathbf{x}) u^*_n(\mathbf{y}) u_{n'}(\mathbf{y}) \; e^{i\mathbf{q}(\mathbf{x}-\mathbf{y})} , \tag{9.4.22}$$

which simplifies once the completeness of the mode functions,

$$\sum_{n'} u^*_{n'}(\mathbf{x}) u_{n'}(\mathbf{y}) = \delta^3(\mathbf{x}-\mathbf{y}) , \tag{9.4.23}$$

is used to perform the d^3y integral, leaving the result

$$\sum_{n'} |\varrho_{n'n}(\mathbf{q})|^2 = \int \mathrm{d}^3x\; u_n(\mathbf{x}) u_n^*(\mathbf{x}) = 1\,, \tag{9.4.24}$$

with the final result following from mode-function normalization.

In this limit the photon scattering rate becomes $\mathrm{d}\Gamma = \mathrm{d}\sigma(N_n/\mathcal{V})$ with differential cross section for scattering into the element of solid angle $\mathrm{d}\Omega = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$ given by

$$\begin{aligned}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}[\gamma(\mathbf{k},\lambda) + C(n) \to \gamma' + X] &:= \frac{1}{2\pi\sin\theta}\frac{\mathrm{d}\sigma}{\mathrm{d}\theta}[\gamma(\mathbf{k},\lambda) + C(n) \to \gamma' + X] \\ &= \frac{\kappa_{\scriptscriptstyle E}^2 k^4}{16\pi^2}\left(\cos^4\frac{\theta}{2} + \sin^4\frac{\theta}{2}\right) = \frac{\kappa_{\scriptscriptstyle E}^2 k^4}{32\pi^2}\left(1+\cos^2\theta\right)\,,\end{aligned} \tag{9.4.25}$$

which is maximized in the forward and backward directions ($\theta = 0, \pi$) and minimized at $\theta = \frac{\pi}{2}$. This expression shows explicitly how the small dimensionless quantity in the perturbative expansion is, in this instance, $\kappa_{\scriptscriptstyle E} k^3$.

Recalling that the $\cos^4\frac{\theta}{2}$ in (9.4.25) comes from the helicity-preserving scattering while $\sin^4\frac{\theta}{2}$ comes from the helicity-flipping scattering, the direction that maximizes the net polarization of the scattered photon (from an initially unpolarized beam of incident photons) can be inferred from the asymmetry

$$\begin{aligned}A &:= \frac{(\mathrm{d}\sigma/\mathrm{d}\Omega)[\gamma(\pm) \to \gamma'(\pm')] - (\mathrm{d}\sigma/\mathrm{d}\Omega)[\gamma(\pm) \to \gamma'(\pm')]}{(\mathrm{d}\sigma/\mathrm{d}\Omega)[\gamma(\pm) \to \gamma'(\pm')] + (\mathrm{d}\sigma/\mathrm{d}\Omega)[\gamma(\pm) \to \gamma'(\pm')]} \\ &= \frac{\cos^4(\theta/2) - \sin^4(\theta/2)}{\cos^4(\theta/2) + \sin^4(\theta/2)} = \frac{2\cos\theta}{1+\cos^2\theta}\,,\end{aligned} \tag{9.4.26}$$

which monotonically falls from $A(\theta = 0) = +1$ to $A(\theta = \pi) = -1$.

Integrating over all angles gives the total cross section for Rayleigh scattering:

$$\sigma[\gamma(\mathbf{k},\lambda) + C(n) \to \gamma' + X] = \frac{\kappa_{\scriptscriptstyle E}^2 k^4}{6\pi}\,, \tag{9.4.27}$$

whose k^4 dependence famously explains why the sky is blue and why sunsets are red (since short-wavelength light scatters more effectively from dust in the air than does long-wavelength red light).

Table 1. Scattering lengths for $\lambda_{\mathrm{blue}} = 400$ nm and $\lambda_{\mathrm{red}} = 600$ nm.

	a in μm	n in cm^{-3}	D_{red} in m	D_{blue} in m
gas atoms	10^{-4}	10^{19}	2×10^8	3×10^7
liquid atoms	10^{-4}	10^{24}	2000	300
haze aerosol	1	10	200	30
fog droplets	1	100	20	3

To estimate how effective Rayleigh scattering is, suppose the mean separation between polarizable scattering particles is ℓ, so their density is $\mathcal{N}_n := N_n/\mathcal{V} =: 1/\ell^3$. Furthermore,

suppose the size of polarizable particles is denoted a, so $\kappa_E \sim a^3$. Finally, writing the light's wavelength as $\lambda = 2\pi/k$ then the mean distance a photon is likely to travel before scattering (the 'scattering length') is of order,

$$D = \frac{1}{\Gamma} = \frac{1}{\mathcal{N}_n \sigma} = 3\lambda \left(\frac{\lambda}{2\pi a}\right)^3 \left(\frac{\ell}{a}\right)^3 . \tag{9.4.28}$$

Defining 'blue' and 'red' light to have wavelength $\lambda_{\rm red} = 600$ nm and $\lambda_{\rm blue} = 400$ nm (putting them on opposite sides of the visible range), then (9.4.28) predicts the values given in Table 1 given a few representative numbers for the size and density of scatterers. Notice that the derivation given above strictly only applies in the low-energy, long-wavelength approximation, $\lambda \gg 2\pi a$, which is marginal for the last two rows of this table.

Calculations like these show that the simplest interactions built using $\mathbf{E}$ and $\mathbf{B}$, like (9.4.6), do a good job of describing how spherically symmetric, electrically neutral polarizable objects (like atoms or droplets) interact with photons. But suppose one wanted to compute a polarizability κ_E from a more microscopic understanding, starting from the interactions photons have with the underlying charged particles (electrons and nuclei, say) from which neutral things like atoms are made. This involves understanding how electromagnetic fields couple to charged particles.

9.5 Photons interacting with charged particles

How do charged particles interact with photons? The answer is *not* dominantly through an interaction like (9.4.6), since this does not reproduce (for example) the proper Coulomb attraction (or repulsion) felt by electrically charged particles (more about this in §9.6).

It turns out that interactions like (9.4.6) don't capture the physics of charged particles because they involve too many powers of momentum, and as a result vanish too quickly as momenta become small. But the powers of momentum that appear are those that originate from the derivatives that appear in the expression for $\mathbf{E}$ and $\mathbf{B}$ in terms of $\mathbf{A}$, so coupling to electric charge must be done using $\mathbf{A}$ alone and undifferentiated.

9.5.1 Gauge invariant interactions

The puzzle then is: the proper counting of photon polarization states relied on there being a gauge redundancy, under which $\mathbf{A} \to \mathbf{A} + \nabla\zeta$. That is, how can a Hamiltonian describing the coupling between Φ and $\Phi^\star$ and $\mathbf{A}$ be written down that is *not* built just from $\mathbf{E}$ or $\mathbf{B}$ and yet remains invariant under the replacement $\mathbf{A} \to \mathbf{A} + \nabla\zeta$ for an arbitrary function $\zeta(\mathbf{x})$?

The trick is to extend this transformation rule so that Φ and $\Phi^\star$ also transform. If such a transformation exists that leaves H unchanged, it should reduce to a symmetry involving Φ only in the limit that ζ becomes $\mathbf{x}$-independent, which suggests starting from a symmetry of H_P – such as of (9.4.1) – and promoting this symmetry so that its parameter can now depend

on local spacetime position. And the Hamiltonian H_P of (9.4.1) *does* have a symmetry, under the replacements $\Phi \to \Phi\, e^{i\zeta}$ and $\Phi^\star \to \Phi^\star\, e^{-i\zeta}$, provided ζ is constant.

The restriction to constant ζ comes because otherwise the combination $\Phi^\star\nabla^2\Phi$ is not invariant. But this can be promoted to being invariant for spacetime-dependent $\zeta(\mathbf{x})$ if $\nabla\Phi$ and $\nabla\Phi^\star$ are replaced everywhere by

$$\mathbf{D}\Phi := (\nabla - iq\mathbf{A})\Phi \quad \text{and} \quad \mathbf{D}\Phi^\star := (\nabla + iq\mathbf{A})\Phi^\star\,, \tag{9.5.1}$$

since these transform as $\mathbf{D}\Phi \to \mathbf{D}\Phi\, e^{iq\zeta(\mathbf{x})}$ and $\mathbf{D}\Phi^\star \to \mathbf{D}\Phi^\star\, e^{-iq\zeta(\mathbf{x})}$ under the *joint* replacements

$$\Phi \to \Phi\, e^{iq\zeta(\mathbf{x})}\,, \quad \Phi^\star \to \Phi^\star e^{-iq\zeta(\mathbf{x})} \quad \text{and} \quad \mathbf{A} \to \mathbf{A} + \nabla\zeta\,. \tag{9.5.2}$$

Here the real parameter q is arbitrary (and will turn out to be the particle's electric charge, so $q = e$ for protons and $q = -e$ for electrons *etc.*). This process of promoting a global symmetry – with constant parameter ζ – to a local (or 'gauge') symmetry – with position-dependent $\zeta(\mathbf{x})$ – is called 'gauging' the symmetry.

The resulting coupling between Φ, $\Phi^\star$ and $\mathbf{A}$ is then given by $H = H_{EM} + H_P$ with H_{EM} given in (9.4.2) and the replacement $\nabla \to \mathbf{D}$ in H_P of (9.4.1), so

$$H_P \to \widetilde{H}_P := \int \mathrm{d}^3x\; \Phi^\star \left[-\frac{1}{2m}\Big(\nabla - iq\mathbf{A}\Big)^2 + V(\mathbf{x})\right]\Phi = H_P + H_{PA} + H_{PAA}\,, \tag{9.5.3}$$

where $\mathbf{D}^2\Phi = (\nabla - iq\mathbf{A})^2\Phi = \delta^{ij}D_i(D_j\Phi)$ should be read as two covariant derivatives acting sequentially on Φ. After an integration by parts this gives

$$\begin{aligned} H_P &= \int \mathrm{d}^3x\; \Phi^\star \left[-\frac{\nabla^2}{2m} + V(\mathbf{x})\right]\Phi \\ H_{PA} &= \frac{iq}{2m}\int \mathrm{d}^3x\; \Big[\Phi^\star(\nabla\Phi) - (\nabla\Phi^\star)\Phi\Big]\cdot\mathbf{A} \\ \text{and} \quad H_{PAA} &= \frac{q^2}{2m}\int \mathrm{d}^3x\; \Phi^\star\Phi\; \mathbf{A}\cdot\mathbf{A}\,. \end{aligned} \tag{9.5.4}$$

Notice the term linear in $\mathbf{A}$ has the form

$$H_{PA} = -\int \mathrm{d}^3x\; \mathbf{j}\cdot\mathbf{A}\,, \tag{9.5.5}$$

where

$$\mathbf{j} = \frac{iq}{2m}\Big[(\nabla\Phi^\star)\Phi - \Phi^\star(\nabla\Phi)\Big] \tag{9.5.6}$$

is q times the conserved current (8.2.12) found earlier for the initial global symmetry of H_P. This is the current that corresponds to the charge density

$$\rho = q\Phi^\star\Phi\,, \tag{9.5.7}$$

which is itself q times the conserved number density, $\mathcal{Q}$, found earlier for H_P.

Furthermore, minimizing $\tilde{H} + H_{EM}$ with respect to time-independent variations of $\mathbf{A}(\mathbf{x})$ gives

$$\left[\nabla \times \mathbf{B} - \mathbf{j} + \frac{q^2}{m}\,\Phi^\star\Phi\,\mathbf{A}\right] \cdot \delta\mathbf{A} = 0 \tag{9.5.8}$$

which when compared to (9.1.4) (in the static limit where $\partial_t \mathbf{E} = 0$) shows that the electromagnetic current is given by

$$\mathbf{J} = \mathbf{j} - \frac{q^2}{m}\,\Phi^\star\Phi\,\mathbf{A} = \frac{iq}{2m}\,\Big[(\mathbf{D}\Phi^\star)\Phi - \Phi^\star(\mathbf{D}\Phi)\Big]\,. \tag{9.5.9}$$

9.5.2 Thomson scattering

A simple application of the Hamiltonian $\widetilde{H}$ is to photon scattering from electrically charged particles. This can be computed perturbatively, using Fermi's Golden Rule, provided the dimensionless combination $qk/m \ll 1$ is satisfied (to justify treating H_{PA} and H_{PAA} in perturbation theory).

Worked example: Thomson scattering

The leading contribution to the reaction $\gamma + C(n) \to \gamma' + C'(n)$ is in this case given by

$$\begin{aligned}\langle\gamma(\mathbf{k}',\lambda'), C(n')|H_{PAA}|\gamma(\mathbf{k},\lambda), C(n)\rangle \\ = \frac{2}{2(2\pi)^3\sqrt{|\mathbf{k}||\mathbf{k}'|}}\left(\frac{q^2}{2m}\right)\,(\boldsymbol{\epsilon}^*_{\lambda'}\cdot\boldsymbol{\epsilon}_\lambda)\,\varrho_{n'n}(\mathbf{k}-\mathbf{k}')\,,\end{aligned} \tag{9.5.10}$$

where $\varrho_{n'n}(\mathbf{q})$ is defined (as before) by (9.4.10) and the overall factor of 2 comes because each of the fields $\mathbf{A}$ can destroy the initial photon.

Repeating the steps leading to (9.4.20) leads in this case to

$$\begin{aligned}\mathrm{d}\Gamma[\gamma(\mathbf{k},\lambda) + C(n) \to \gamma' + X] &= \frac{(2\pi)^4}{\mathcal{V}}\sum_{\lambda' n'}\Big|\langle\gamma(\mathbf{k}',\lambda')\,C(n')|H_{\rm pol}|\gamma(\mathbf{k},\lambda)\,C(n)\rangle\Big|^2 \\ &\qquad\times\delta(k' + \varepsilon_{n'} - k + \varepsilon_n)\,\mathrm{d}^3k' \\ &= \frac{1}{(2\pi)^2|\mathbf{k}||\mathbf{k}'|}\left(\frac{q^2}{2m}\right)^2\frac{N_n}{\mathcal{V}}\sum_{\lambda'}|\boldsymbol{\epsilon}^*_{\lambda'}\cdot\boldsymbol{\epsilon}_\lambda|^2\sum_{n'}|\varrho_{n'n}(\mathbf{k}-\mathbf{k}')|^2 \\ &\qquad\times\delta(k' + \varepsilon_{n'} - k + \varepsilon_n)\,\mathrm{d}^3k'\,.\end{aligned} \tag{9.5.11}$$

In the case where $\varepsilon_{n'} - \varepsilon_n$ is negligible relative to $k - k'$ eq. (9.4.24) can be used, as can (9.4.17) for the helicity sum, leading to

$$\begin{aligned}\mathrm{d}\Gamma[\gamma(\mathbf{k},\lambda) + C(n) \to \gamma' + X] &\simeq \frac{1}{(2\pi)^2 kk'}\left(\frac{q^2}{2m}\right)^2\frac{N_n}{\mathcal{V}}\sum_{\lambda'}|\boldsymbol{\epsilon}^*_{\lambda'}\cdot\boldsymbol{\epsilon}_\lambda|^2\delta(k'-k)\,\mathrm{d}^3k' \\ &= \frac{1}{4\pi}\left(\frac{q^2}{2m}\right)^2\frac{N_n}{\mathcal{V}}\left(1+\cos^2\theta\right)\,\sin\theta\,\mathrm{d}\theta\,.\end{aligned} \tag{9.5.12}$$

Defining (as usual) the cross section from $\mathrm{d}\Gamma = \mathrm{d}\sigma(N_n/\mathcal{V})$ then gives the following expression for the differential cross section for low-energy scattering of polarized photons from nonrelativistic charged-particles:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{q^4}{32\pi^2m^2}(1+\cos^2\theta) = \frac{\alpha_q^2}{2m^2}(1+\cos^2\theta)\,, \tag{9.5.13}$$

where $\alpha_q := q^2/(4\pi)$. Integrating over solid angle then gives the total cross section

$$\sigma = \int \mathrm{d}\Omega \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) = \frac{q^4}{6\pi m^2} = \frac{8\pi\alpha_q^2}{3m^2}\,, \tag{9.5.14}$$

also called the Thomson cross section. Notice this cross section is independent of photon energy, unlike the Rayleigh cross section for photon scattering from neutral atoms, as computed earlier in (9.4.27).

The term H_{PA} linear in $\mathbf{A}$ also contributes to low-energy scattering of photons from charged particles, but only by an amount of order $\delta\sigma \sim (q^2k/m^2)^2$, and so is down relative to the leading contribution, (9.5.14), by a power of $(k/m)^2$, which must be much smaller than unity to justify using perturbation theory.

9.5.3 Absorption, emission and the dipole approximation

The term H_{PA} does provide the leading contribution to processes that emit and absorb a photon, however, such as $\gamma + C(n) \to C(n')$ or $C(n) \to C(n') + \gamma$. In this case the relevant matrix element for emission is

$$\langle \gamma(\mathbf{k}',\lambda'), C(n')|H_{PAA}|C(n)\rangle = \frac{1}{\sqrt{2(2\pi)^3|\mathbf{k}'|}}\,\boldsymbol{\epsilon}^*_{\lambda'}\cdot\mathbf{I}_{n'n}(-\mathbf{k}')\,, \tag{9.5.15}$$

where

$$\mathbf{I}_{n'n}(\mathbf{p}) := \left(\frac{iq}{2m}\right)\int \mathrm{d}^3x\,\Big[u^*_{n'}(\nabla u_n) - (\nabla u^*_{n'})u_n\Big]\,e^{i\mathbf{p}\cdot\mathbf{x}}\,. \tag{9.5.16}$$

Similarly, for absorption the matrix element is

$$\langle C(n')|H_{PAA}|\gamma(\mathbf{k},\lambda), C(n)\rangle = \frac{1}{\sqrt{2(2\pi)^3|\mathbf{k}|}}\,\boldsymbol{\epsilon}_{\lambda}\cdot\mathbf{I}_{n'n}(\mathbf{k})\,. \tag{9.5.17}$$

For applications to atoms the evaluation of $\mathbf{I}_{n'n}(\mathbf{k})$ simplifies, because typical mode-functions for atoms vary over distances of order the Bohr radius, $a_B = (\alpha\, m_e)^{-1}$, and so $\mathbf{I}_{n'n}(\mathbf{p})$ has most of its structure for momenta of order $|\mathbf{p}| \sim 1/a_B = \alpha\, m_e$. But because the photon's energy is $\omega(\mathbf{k}) = |\mathbf{k}|$ the value of $|\mathbf{k}|$ at which $\mathbf{I}_{n'n}(\mathbf{p})$ is evaluated in the above matrix elements is set by the energy change $\varepsilon_n - \varepsilon_{n'}$ released in the transition. But for atoms this energy difference is of order $|\mathbf{k}| \sim \alpha^2 m_e$ and because $\alpha \simeq 1/137$ this is much smaller than $1/a_B$. Physically this says that the photons emitted or absorbed by atomic transitions have wavelengths that are much larger than the sizes of the atoms themselves.

As a consequence, for the dominant part of the d^3x integral in $\mathbf{I}_{n'n}(\mathbf{k})$ the phase factor is unity: $e^{i\mathbf{k}\cdot\mathbf{x}} \simeq 1$, making it a good approximation to replace

$$\mathbf{I}_{n'n}(\mathbf{k}) \simeq \mathbf{I}_{n'n}(0) = \frac{iq}{2m}\int \mathrm{d}^3x\,\Big[u^*_{n'}(\nabla u_n) - (\nabla u^*_{n'})u_n\Big] = \frac{iq}{m}\int \mathrm{d}^3x\; u^*_{n'}\nabla u_n = -\frac{q}{m}\,\hat{\mathbf{p}}_{n'n}\,. \tag{9.5.18}$$

where the second-last equality integrates by parts and the final one identifies the single-particle quantum operator $\hat{\mathbf{p}} = -i\nabla$.

Recall that the mode functions $u_n(\mathbf{x})$ are eigenstates of the single-particle Schrödinger energy operator, $\mathfrak{h} u_n = \varepsilon_n u_n$ with

$$\mathfrak{h} = -\frac{\nabla^2}{2m} + V(\mathbf{x}) = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{x}) \,. \tag{9.5.19}$$

Furthermore, explicit calculation shows

$$i\Big[\mathfrak{h}, \mathbf{x}\Big] = \frac{i}{2m}\Big[\hat{\mathbf{p}}^2, \mathbf{x}\Big] = \frac{i\hat{\mathbf{p}}}{m}\Big[\hat{\mathbf{p}}, \mathbf{x}\Big] = \frac{\hat{\mathbf{p}}}{m} \,, \tag{9.5.20}$$

and so

$$\hat{\mathbf{p}}_{n'n} = \int \mathrm{d}^3x \; u^*_{n'} \, \hat{\mathbf{p}} \, u_n = im \int \mathrm{d}^3x \; u^*_{n'} \Big[\mathfrak{h}, \mathbf{x}\Big] u_n = im(\varepsilon_{n'} - \varepsilon_n) \int \mathrm{d}^3x \; \mathbf{x} \, u^*_{n'}(\mathbf{x}) \, u_n(\mathbf{x}) \,, \tag{9.5.21}$$

which when used in (9.5.18) allows the matrix element to be written

$$\mathbf{I}_{n'n}(\mathbf{k}) \simeq \mathbf{I}_{n'n}(0) = iq(\varepsilon_n - \varepsilon_{n'}) \int \mathrm{d}^3x \; \mathbf{x} \, u^*_{n'}(\mathbf{x}) \, u_n(\mathbf{x}) =: i(\varepsilon_n - \varepsilon_{n'}) \, \mathbf{d}_{n'n} \,. \tag{9.5.22}$$

Here the last equality defines the electric-dipole-moment matrix element $\mathbf{d}_{n'n}$:

$$\mathbf{d}_{n'n} := q \int \mathrm{d}^3x \; \mathbf{x} \, u^*_{n'}(\mathbf{x}) \, u_n(\mathbf{x}) \,. \tag{9.5.23}$$

This allows the matrix elements (9.5.15) and (9.5.17) to be written in their 'dipole' form:

$$\begin{aligned} \langle \gamma(\mathbf{k}', \lambda'), C(n') | H_{PAA} | C(n) \rangle \; &\simeq \; \frac{1}{\sqrt{2(2\pi)^3 |\mathbf{k}'|}} \, \boldsymbol{\epsilon}^*_{\lambda'} \cdot \mathbf{I}_{n'n}(0) \\ &= \; \frac{i(\varepsilon_n - \varepsilon_{n'})}{\sqrt{2(2\pi)^3 |\mathbf{k}'|}} \, \boldsymbol{\epsilon}^*_{\lambda'} \cdot \mathbf{d}_{n'n} = \frac{i\omega(\mathbf{k}')}{\sqrt{2(2\pi)^3 |\mathbf{k}'|}} \, \boldsymbol{\epsilon}^*_{\lambda'} \cdot \mathbf{d}_{n'n} \\ &= \; \langle \gamma(\mathbf{k}', \lambda') | \mathbf{E}(\mathbf{x} = 0) | 0 \rangle \cdot \mathbf{d}_{n'n} \,, \end{aligned} \tag{9.5.24}$$

where the second equality on the second line uses energy conservation to relate the photon energy to $\varepsilon_n - \varepsilon_{n'}$ and the final equality uses $\mathbf{E} = -\partial_t \mathbf{A}$, which holds for the radiation field, when evaluating the matrix element. Similarly, for absorption the matrix element becomes

$$\langle C(n') | H_{PAA} | \gamma(\mathbf{k}, \lambda), C(n) \rangle \simeq \frac{1}{\sqrt{2(2\pi)^3 |\mathbf{k}|}} \, \boldsymbol{\epsilon}_{\lambda} \cdot \mathbf{I}_{n'n}(0) = \langle 0 | \mathbf{E}(\mathbf{x} = 0) | \gamma(\mathbf{k}, \lambda) \rangle \cdot \mathbf{d}_{n'n} \,, \tag{9.5.25}$$

showing how the leading matrix element of H_{PA} can be interpreted as a matrix element of the dipole interaction $\mathbf{E} \cdot \mathbf{d}$.

9.5.4 Polarizability revisited

The above dipole form allows a more microscopic understanding of the origin of the polarizability energy, $H_{\rm pol}$, experienced by electrically neutral atoms in the presence of an applied electric field, given in (9.4.6).

This polarization energy arises once the energy levels of electrons in the atom are perturbed using the interaction H_{PA}, since the state $|C(n)\rangle$ has its energy perturbed by an amount given to second order by (3.1.8) and (3.1.9)

$$\begin{aligned}\delta E_n &\simeq \langle C(n)|H_{PA}|C(n)\rangle + \sum_N \frac{|\langle N|H_{PA}|C(n)\rangle|^2}{\varepsilon_n - E_N} + \cdots \\ &\simeq \sum_{n'\lambda'} \int \mathrm{d}^3k' \, \frac{|\langle \gamma(\mathbf{k}',\lambda'), C(n')|H_{PA}|C(n)\rangle|^2}{\varepsilon_n - \varepsilon_{n'} - \omega(\mathbf{k}')} + \cdots \\ &\simeq \sum_{n'\lambda'} \int \mathrm{d}^3k' \, \frac{|\langle \gamma(\mathbf{k}',\lambda')|\mathbf{E}(0)|0\rangle \cdot \mathbf{d}_{n'n}|^2}{\varepsilon_n - \varepsilon_{n'} - \omega(\mathbf{k}')} + \cdots .\end{aligned} \tag{9.5.26}$$

This shows how an energy quadratic in $\mathbf{E}$ arises because at first order in H_{PA} the electric field induces a transition dipole interaction in the initial atom and at second order this transition moment causes an energy shift in the original state.

Having a microscopic understanding of the origin of $H_{\rm pol}$ in this instance also allows an estimate of the size to be expected of the polarizability coefficient κ_E appearing in $H_{\rm pol}$. This should be of order

$$\kappa_E \sim \frac{4\pi}{(2\pi)^3} \frac{|\mathbf{d}_{n'n}|^2}{\Delta E} \sim \frac{4\pi}{(2\pi)^3} \frac{(e\, a_B)^2}{\alpha^2 m_e} \sim \frac{1}{2\pi^2} \left(\frac{e^2}{\alpha}\right) a_B^3 \sim a_B^3 \,, \tag{9.5.27}$$

where the Bohr radius, $a_B = 1/(\alpha\, m_e)$, is an estimate of a typical atomic orbital size and $\Delta E \sim \alpha^2 m_e$ is a typical energy spacing between atomic levels. The $(2\pi)^{-3}$ comes from the matrix elements of $\mathbf{E}$, as above, and the factor of 4π is meant as an estimate of the angular integrations made when integrating over d^3k'.

9.6 Electrostatic interactions

To this point only the photon contribution to the electromagnetic field has been considered, which is like keeping only the homogeneous 'wave' term in eqs. (9.1.14) and dropping the particular integral that satisfies the inhomogeneous equation and so knows about any charge density, ρ, and current density, $\mathbf{j}$, that might be present. The purpose of the present section is to complete the above story by including also the solutions to the inhomogeneous equation for a quantized electromagnetic field.

For the present purposes this is done in the interaction picture, with a more complete treatment given in §13. To that end write the total Hamiltonian as $H = H_0 + H_{\rm int}$ where

for concreteness' sake the 'free' Hamiltonian is given by $H_0 = H_P + H_{EM}$ with H_P and H_{EM} given as in (9.4.1) and (9.4.2), respectively (repeated here for convenience)

$$H_P = \int \mathrm{d}^3x\, \Phi^\star \left[-\frac{\nabla^2}{2\mu} + V(\mathbf{x})\right] \Phi = \sum_n \varepsilon_n\, c_n^\star c_n$$
$$H_{EM} = \frac{1}{2}\int \mathrm{d}^3x\, \left(\mathbf{E}_0^2 + \mathbf{B}_0^2\right) = \sum_{\lambda=\pm} \int \mathrm{d}^3k\, |\mathbf{k}|\, \mathfrak{a}_{\mathbf{k}\lambda}^\star \mathfrak{a}_{\mathbf{k}\lambda}\,. \tag{9.6.1}$$

The particle mass is denoted here by μ to distinguish it from state labels m and M that arise in what follows.

Because, in the interaction picture, the time evolution of the fields is controlled by H_0 their time-dependence and their expansion in terms of creation and annihilation operators is given precisely as they were above in the absence of interactions. For matter fields this implies (compare with (9.4.3))

$$\Phi(\mathbf{x},t) = \sum_n c_n\, u_n(\mathbf{x})\, e^{-i\varepsilon_n t}\,, \quad \Phi^\star(\mathbf{x},t) = \sum_n c_n^\star\, u_n^*(\mathbf{x})\, e^{+i\varepsilon_n t}\,, \tag{9.6.2}$$

where, given the form of H_P, the mode functions satisfy

$$\left[-\frac{\nabla^2}{2\mu} + V(\mathbf{x})\right] u_n = \varepsilon_n\, u_n\,. \tag{9.6.3}$$

The electromagnetic field is similarly given in interaction picture by (compare with (9.4.5))

$$\mathbf{A}(\mathbf{x},t) = \sum_{\lambda=\pm} \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2|\mathbf{k}|}} \left[\mathfrak{a}_{\mathbf{k}\lambda}\, \boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{-i|\mathbf{k}|t + i\mathbf{k}\cdot\mathbf{x}} + \mathfrak{a}_{\mathbf{k}\lambda}^\star\, \boldsymbol{\epsilon}_\lambda^*(\mathbf{k})\, e^{+i|\mathbf{k}|t - i\mathbf{k}\cdot\mathbf{x}}\right], \tag{9.6.4}$$

which continues to fix the gauge freedom using Coulomb gauge: $\nabla\cdot\mathbf{A} = 0$. Because interactions are not yet included the fields $\mathbf{E}_0$ and $\mathbf{B}_0$ should be read as being the radiation fields $\mathbf{E}_0 = -\partial_t\mathbf{A}$ and $\mathbf{B}_0 = \nabla\times\mathbf{A}$, with $\mathbf{A}$ as given in (9.6.4). They therefore satisfy $\nabla\cdot\mathbf{E}_0 = \nabla\cdot\mathbf{B}_0 = 0$ and the commutation relations given in (9.2.11).

The time dependence in (9.6.2) and (9.6.4) is obtained by using the free evolution of the creation and annihilation operators (*c.f.* eq. (3.2.8))

$$\partial_t c_n = i\Big[H_0, c_n\Big] = -i\varepsilon_n\, c_n \quad \text{and} \quad \partial_t \mathfrak{a}_{\mathbf{k}\lambda} = i\Big[H_0, \mathfrak{a}_{\mathbf{k}\lambda}\Big] = -i|\mathbf{k}|\, \mathfrak{a}_{\mathbf{k}\lambda}\,, \tag{9.6.5}$$

since these imply $c_n(t) = c_n\, e^{-i\varepsilon_n t}$ and $\mathfrak{a}_{\mathbf{k}\lambda}(t) = \mathfrak{a}_{\mathbf{k}\lambda}\, e^{-i|\mathbf{k}|t}$. It is this time dependence that is the main difference between the interaction-picture expressions (9.6.2) and (9.6.4) on one hand and the earlier Schrödinger-picture expressions given in (9.4.3) and (9.4.5).

The main ingredient that remains missing from the above is the interaction-picture interaction Hamiltonian, $H_{\rm int}$, since this is required in order to evolve the system's state forward

in time. This must be chosen in such a way as to ensure that it reproduces the full field equations – including in particular the Maxwell equations including the current and charge densities – once transformed to the Heisenberg picture. As can be checked relatively easily, the result that does so is (see §13 for a more constructive derivation)

$$H_{\rm int} = H_{\rm int}^{\rm mat} + H_{PA} + H_{PAA} + H_C\,, \tag{9.6.6}$$

where $H_{\rm int}^{\rm mat}$ contains any non-electromagnetic interactions of the Φ field that may be present, such as perhaps $H_{\rm int}^{\rm mat} = -g\int \mathrm{d}^3x\ (\Phi^\star\Phi)^2$ as considered in §7.1. Similarly H_{PA} and H_{PAA} are as given in (9.5.4) and so

$$H_{PA} + H_{PAA} = \int \mathrm{d}^3x\ \left[-\mathbf{j}\cdot\mathbf{A} + \frac{q^2}{2\mu}\Phi^\star\Phi\,\mathbf{A}\cdot\mathbf{A}\right] = \int \mathrm{d}^3x\ \left[-\mathbf{J}\cdot\mathbf{A} - \frac{q^2}{2\mu}\Phi^\star\Phi\,\mathbf{A}\cdot\mathbf{A}\right], \tag{9.6.7}$$

with $\mathbf{j}$ and $\mathbf{J}$ as defined in (9.5.6) and (9.5.9):

$$\mathbf{j} = \frac{iq}{2\mu}\Big[(\nabla\Phi^\star)\Phi - \Phi^\star(\nabla\Phi)\Big] \tag{9.6.8}$$

$$\text{and}\quad \mathbf{J} = \frac{iq}{2\mu}\Big[(\mathbf{D}\Phi^\star)\Phi - \Phi^\star(\mathbf{D}\Phi)\Big] = \mathbf{j} - \frac{q^2}{\mu}\,\Phi^\star\Phi\,\mathbf{A}\,.$$

Notice that using the commutation relations (9.2.11) in $[\mathbf{E}_0, H_{PA} + H_{PAA}]$ shows that it is the gauge-invariant quantity $\mathbf{J}$ rather than $\mathbf{j}$ that appears in the Heisenberg-picture Maxwell equation (9.1.4), as it should.

The new contribution to $H_{\rm int}$ not seen previously is the Coulomb interaction,[31]

$$H_C = \frac{1}{2}\int \mathrm{d}^3x\ \rho\,\phi = \frac{1}{8\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\ \frac{\rho(\mathbf{x},t)\,\rho(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\,, \tag{9.6.9}$$

where the charge density $\rho = q\Phi^\star\Phi$ is as defined in (9.5.7), and so inherits its time-dependence from the time dependence in $\Phi(\mathbf{x},t)$ in the interaction picture. What is important is that the electrostatic potential ϕ is not here regarded as an independent quantum field in its own right. Instead it is a field whose commutation properties are completely defined in terms of the other fields (in this case Φ and $\Phi^\star$) by solving the (Coulomb gauge) Maxwell equation $\nabla\cdot\mathbf{E} = -\nabla^2\phi = \rho$, since this gives

$$\phi(\mathbf{x},t) = \frac{1}{4\pi}\int \mathrm{d}^3y\ \frac{\rho(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\,. \tag{9.6.10}$$

The Coulomb interaction is strange in several ways. Firstly, it seems nonlocal when written in terms of the dynamical fields $\mathbf{A}$ and Φ. The physical predictions of electrodynamics

[31] The unusual factor of $\frac{1}{2}$ arises because of a partial cancellation between the usual electrostatic $\rho\,\phi$ interaction and the part of the electromagnetic Hamiltonian that is quadratic in ϕ, as is justified below using canonical methods once these are introduced in §13. Alternatively, the need for the factor of $\frac{1}{2}$ can be justified by ensuring that the energy is not double-counted when integrating the charge density twice over all of space, or by verifying $H_{\rm int}$ properly reproduces the equations of motion in Heisenberg picture.

remain local despite this, however, due to the fact that $H_{\rm Coul}$ can also be written in a local way once expressed also in terms of ϕ. Although ϕ does not independently propagate in the above formulation this is also an artifact of using Coulomb gauge, and so observables (which are gauge invariant) do not display this nonlocality. The Coulomb interaction also appears not to be Lorentz invariant inasmuch as it does not group with the current interaction into the form of the product of four-vectors, like $J^\mu A_\mu = \mathbf{J}\cdot\mathbf{A} - \rho\,\phi$. Again this turns out to be an artefact of the fact that Coulomb gauge is not Lorentz invariant, and Lorentz covariance can be made more manifest if quantized in other gauges (such as Lorentz gauge - see §16).[32]

But the Coulomb interaction is nonetheless very real and of great practical importance, as illustrated by its implications for atomic energy levels, such as those for the He atom computed in §6.5.

10 Collective Effects

Electromagnetic interactions provide our first window on how relativistic particles (photons) are discussed in quantum mechanical systems. Before turning to a more systematic discussion of how relativity combines with quantum mechanics, we first pause to describe applications to electromagnetic interactions to matter in bulk: systems involving more than just a few particles. We study various aspects of electromagnetic response, and in particular the propagation of different types of waves within matter.

One might think complicated systems must be complicated to understand, but there is an important regime that can be much simpler than what is naively expected: the regime where the predictions of interest involve length scales much longer than the scales intrinsic to the underlying complicated state. Examples of this regime include scattering of light whose wavelength is much longer than typical interatomic distances, or effects that take much longer times than typical microscopic scattering times.

In this long-distance regime things simplify because physical predictions can be expressed in terms of macroscopic averages of physical properties, rather than dealing with the state particle by particle. A special role is played in this regime by the local density of quantities that are conserved by the microscopic physics – things like energy, particle number, electric charge and so on. These are special because local conservation means that the only way their average values can change is by physically moving them out of the region of interest – as expressed for example by (8.2.6); typically a slow process for regions that are macroscopically large compared to microscopic time-scales (such as, for example, those associated with particle scattering). One reason to describe these systems here (besides their intrinsic interest) is to sketch how these argument proceed within a field-theoretic framework.

[32] This particular issue is a more pressing one when the sector describing charged particles is itself relativistic.

10.1 Dielectrics

For the first example we return to the interactions of electromagnetism with polarizable atoms, along the lines described above in §9.4. The Hamiltonian for this system is given explicitly in eqs. (9.4.1), (9.4.2) and (9.4.6), repeated here for convenience of reference: $H = H_0 + H_{\rm pol}$ which we group here into the 'free' Hamiltonian

$$H_0 = \int \mathrm{d}^3x \, \left\{ \Phi^\star \left[-\frac{\nabla^2}{2m} + V(\mathbf{x}) \right] \Phi + \frac{1}{2}\Big(\mathbf{E}^2 + \mathbf{B}^2 \Big) \right\} , \tag{10.1.1}$$

and the interaction term

$$H_{\rm pol} = \frac{1}{2} \int \mathrm{d}^3x \, \Phi^\star\Phi \Big[\kappa_{_E} \, \mathbf{E}^2 + \kappa_{_B} \, \mathbf{B}^2 \Big] . \tag{10.1.2}$$

The detailed form of the potential $V(\mathbf{x})$ experienced by the particles isn't important in what follows, but (unlike in following sections) we here assume that it localizes the atoms so that they do not move appreciably when hit by external electromagnetic waves.

The fields appearing here are related to the creation and annihilation operators for photons and for the underlying atoms in the usual way. For electromagnetism $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\partial_t \mathbf{A} - \nabla\phi$ with ϕ constrained by Gauss' law in terms of the local electric charge density (which we take to locally vanish for the long length scales of interest). The photon creation and annihilation operators appear within the vector potential, which in Schrödinger picture we write as

$$\mathbf{A}(\mathbf{x}) = \sum_\lambda \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2|\mathbf{k}|}} \left[\mathfrak{a}_{\mathbf{k}\lambda} \, \boldsymbol{\epsilon}_\lambda(\mathbf{k}) \, e^{i\mathbf{k}\cdot\mathbf{x}} + \mathfrak{a}^\star_{\mathbf{k}\lambda} \, \boldsymbol{\epsilon}^*_\lambda(\mathbf{k}) \, e^{-i\mathbf{k}\cdot\mathbf{x}} \right] . \tag{10.1.3}$$

with $[\mathfrak{a}_{\mathbf{k}\lambda}, \mathfrak{a}^\star_{\mathbf{q}\xi}] = \delta_{\lambda\xi}\delta^3(\mathbf{k}-\mathbf{q})$ as before. The atom destruction operators appear within $\Phi(\mathbf{x})$,

$$\Phi(\mathbf{x}) = \sum_n c_n \, u_n(\mathbf{x}) , \quad \Phi^\star(\mathbf{x}) = \sum_n c^\star_n \, u^*_n(\mathbf{x}) , \tag{10.1.4}$$

and we assume spinless bosonic atoms so $[c_m, c^\star_n] = \delta_{mn}$. The single-particle mode functions satisfy

$$\left[-\frac{\nabla^2}{2m} + V(\mathbf{x}) \right] u_n(\mathbf{x}) = \varepsilon_n \, u_n(\mathbf{x}) , \tag{10.1.5}$$

but because our interest is in complicated atomic states perhaps containing an enormous number of atoms – think: a slab of glass or a region of transparent fluid – we wish to avoid using the detailed form for $u_n(\mathbf{x})$ and ε_n.

Consider first the simplest case, for which all we know is that the medium is translation invariant on macroscopic scales, and so for which the atomic density

$$n_{_A} = \langle \Phi^\star\Phi \rangle , \tag{10.1.6}$$

is independent of spatial position and of time.[33] Notice that translation invariance is *not* assumed to be true microscopically – the potential $V(\mathbf{x})$ rarely vanishes. As a result the detailed state could have quite a complicated position dependence, such as by having atoms assemble into a crystal lattice with typical inter-atomic spacing a. What matters for (10.1.6) is that the state becomes translation invariance once averaged over scales much larger than a, since this is all that is seen by a photon whose wavelength satisfies $\lambda \gg a$.

For such an environment electromagnetic waves are approximately governed[34] by the average Hamiltonian obtained from (10.1.1) and (10.1.2) by replacing $\Phi^\star\Phi$ with $\langle\Phi^\star\Phi\rangle = n_A$, leading to:

$$H_{EM} + H_{\rm pol} = \frac{1}{2}\int \mathrm{d}^3x \Big[(1+n_A\kappa_E)\mathbf{E}^2 + (1+n_A\kappa_B)\mathbf{B}^2\Big] \,. \tag{10.1.7}$$

The idea is to see how the new terms from $H_{\rm pol}$ alter the evolution of the electromagnetic fields within matter. To this end we compute the operator field equations in the Heisenberg picture, since (*c.f.* the discussion of §3.2) it is in Heisenberg picture that the fields carry the entire burden of time evolution. We therefore use the Hamiltonian (10.1.7) to compute the equations of motion (3.2.4)

$$\partial_t \mathcal{O}_h = i\Big[H, \mathcal{O}_h\Big] \,, \tag{10.1.8}$$

using the commutation relations

$$\Big[A_i(\mathbf{x},t), \partial_t E_j(\mathbf{y},t)\Big] = -i\left(\delta_{ij} - \frac{\partial_i\partial_j}{\nabla^2}\right)\delta^3(\mathbf{x}-\mathbf{y}) \tag{10.1.9}$$

and $[A_i(\mathbf{x},t), B_j(\mathbf{y},t)] = 0$ that follow from (10.1.3) – see also eqs. (6.1.9) and (9.2.11) – (that are preserved when transforming to Heisenberg picture).

One finds in this way the modified Maxwell equations

$$\begin{aligned} \nabla\times\Big[(1+n_A\kappa_B)\mathbf{B}_h\Big] - \partial_t\Big[(1+n_A\kappa_E)\mathbf{E}_h\Big] = 0 \\ \text{and} \quad \nabla\cdot\Big[(1+n_A\kappa_E)\mathbf{E}_h\Big] = 0 \,, \end{aligned} \tag{10.1.10}$$

where the subscript 'h' is a reminder that these are Heisenberg-picture operators. No current $\mathbf{J}$ or charge density ρ appears on the right-hand side because these are assumed to average to zero $\langle\mathbf{J}\rangle = \langle\rho\rangle = 0$ in the atomic state of interest (more about this assumption below). The other two Maxwell equations – (9.1.2) and (9.1.3) – are unchanged since they follow from the relations that give $\mathbf{E}$ and $\mathbf{B}$ in terms of $\mathbf{A}$ and ϕ. So far these are operator equations, but for the practical applications discussed below the initial state of the field is so highly occupied that the field is well-approximated as classical, along the lines described in §5.

[33] The average $\langle\cdots\rangle$ here could denote a quantum average if the microscopic state is prepared in a pure state, but could equally well also include non-quantum probabilities (such as from a thermal distribution, as described in §1.6).

[34] This is called the 'mean-field' approximation, and there are systematic methods (beyond the scope of these notes) to quantify the size of corrections to it.

Now comes the main point. Eqs. (10.1.10) are precisely what would be appropriate for a dielectric medium with electric permittivity $\epsilon = 1 + n_A\kappa_E$ and magnetic permeability $\mu^{-1} = 1 + n_A\kappa_B$. For dielectrics Maxwell's equations are modified in this way because the effective electric field experienced on large scales when external fields are applied is given by the electric displacement $\mathbf{D} = \epsilon\,\mathbf{E}$ (and similarly for magnetic fields and the magnetic induction $\mathbf{H} = \mathbf{B}/\mu$). These macroscopic fields differ from the naive ones because any applied fields polarize the surrounding medium and this polarization generates a countering field that partially screens the effects of the applied field.

Ultimately the medium's ability to polarize in this way comes from the polarizability of the atoms/molecules from which it is built, since (for example) these can acquire dipole moments in the presence of applied electric fields. And these atoms/molecules polarize within an applied field because they are themselves built from electrically charged electrons and nuclei that have a limited ability to adjust their positions relative to one another in the presence of an applied field (as we saw when computing its size in §9.5.4).

It is no surprise then that using (10.1.10) to derive the wave equation for $\mathbf{A}_h$ along the lines used in §9.1 one finds – instead of (9.1.14) – the result one would have obtained for a dielectric medium.

$$\mathfrak{n}^2\,\frac{\partial^2\mathbf{A}}{\partial t^2} - \nabla^2\mathbf{A}_h = 0\,, \quad \text{where} \quad \mathfrak{n} := \sqrt{\frac{1+n_A\kappa_E}{1+n_A\kappa_B}} = \sqrt{\epsilon\mu}\,. \tag{10.1.11}$$

Solving this equation using plane waves of the form $\mathbf{A}_h(\mathbf{x},t) \propto \boldsymbol{\varepsilon}\,\exp[-i\omega t + i\mathbf{k}\cdot\mathbf{x}]$ shows that the dispersion relation for the wave predicted by (10.1.11) is $\omega = c_s|\mathbf{k}|$ where the wave 'speed' now is $c_s = 1/\mathfrak{n}$.

This identifies $\mathfrak{n}$ as the medium's index of refraction (see below) and (10.1.11) shows that it is given approximately by $\mathfrak{n} \simeq \sqrt{1+n_A\kappa_E}$ [because κ_B is usually negligible for the reasons described below eq. (9.4.7)]. The estimate (9.4.8) for the typical size of κ_E in particular shows why $\mathfrak{n}-1$ is small for dilute media (like air) but can be order unity for matter that is reasonably closely packed, with atomic density $n_A \sim 1/a_B^3$ (as is true for water and glass), independent of the size of the electromagnetic coupling e.

Worked Example: Refraction and reflection

To reinforce the interpreation of $\mathfrak{n}$ as an index of refraction we next derive Snells's Law for refraction using the above solution. Imagine a polarizable material with constant index of refraction $\mathfrak{n}$ fills the half of space satisfying $z > 0$ in rectangular coordinates. Imagine an electromagnetic plane wave starts in the vacuum at $z < 0$ and approaches the medium with a wave-vector

$$\mathbf{k}_0 = k(\mathbf{e}_x\,\sin\vartheta_0 + \mathbf{e}_z\,\cos\vartheta_0) \tag{10.1.12}$$

that lies within the $x-z$ plane and makes an angle ϑ_0 with the unit normal $\mathbf{n} = \mathbf{e}_z$ to the medium's surface. Assuming part of the wave is reflected and part is refracted, denote the angle of reflection by ϑ_s and the angle of refraction by ϑ_r (both measured relative to $\mathbf{n}$).

Energy and momentum conservation at the interface at $z = 0$ suffice to determine ϑ_s and ϑ_r as a function of ϑ_0. When doing so it is important to realize that momentum is *not* conserved in the z direction because the presence of the medium's boundary at $z = 0$ breaks translation invariance in the z direction. But translation invariance of the problem in x and y ensures momentum is conserved in these directions and time-translation invariance ensures energy is conserved.

To compute the reflection angle we use conservation to compute the wave-vector of the reflected wave, $\mathbf{k}_s$. Momentum conservation in the x direction ensures its x component remains unchanged and so is $k \sin\vartheta_0$, and conservation in the y direction ensures its y component remains zero. Energy conservation states that $\omega_s = \omega_0$ where $\omega_s = |\mathbf{k}_s|$ and $\omega_0 = |\mathbf{k}_0|$. This implies the z component of the outgoing reflected wave must be opposite to that of the incoming wave, so

$$\mathbf{k}_s = k\,(\mathbf{e}_x\,\sin\vartheta_0 - \mathbf{e}_z\,\cos\vartheta_0) \tag{10.1.13}$$

and so the reflected wave shares the same angle with the surface normal as the incoming wave: $\vartheta_s = \vartheta_0$.

The same argument gives the direction of the refracted wave, with the important difference that within the medium the dispersion relation is now $\omega_r = |\mathbf{k}_r|/\mathfrak{n}$. Conservation of momentum in the y direction again dictates that $k_y = 0$, but conservation of energy now becomes $|\mathbf{k}_r|/\mathfrak{n} = |\mathbf{k}_0|$. The refracted wave-vector can therefore be written

$$\mathbf{k}_r = \mathfrak{n}\,k\,(\mathbf{e}_x\,\sin\vartheta_r + \mathbf{e}_z\,\cos\vartheta_r) \tag{10.1.14}$$

where ϑ_r is to be determined by conservation of momentum in the x direction. This implies ϑ_r must satisfy $\mathfrak{n}\,k\,\sin\vartheta_r = k\,\sin\vartheta_0$ and so

$$\sin\vartheta_r = \frac{1}{\mathfrak{n}}\,\sin\vartheta_0\,, \tag{10.1.15}$$

in agreement with Snell's Law given that $\mathfrak{n}$ is the medium's index of refraction.

10.2 Conductors and plasmas

The next class of systems to explore are those for which the microscopic constituents contain charges (typically electrons) that are *mobile* in the sense that they are free to travel over macroscopic distances. In this case we must re-examine two related assumptions made above for dielectrics: (i) the absence of macroscopic electric charge and current densities, and (ii) the absence of microscopic motion that is buried in the assumption that densities like $\langle\Phi^\star\Phi\rangle$ can remain position- and time-independent.

In practice the main change relative to the previous section is to allow the field Φ to be charged, as appropriate if the underlying non-relativistic particles of interest have net electric charge. This means that the Hamiltonian of interest should be based on the one derived in §9.5 and §9.6 rather than §9.4. The first observation when doing so is that the Coulomb interaction makes it hard to get large dense systems of charged particles at all, since these particles mutually repel one another and prefer to remain widely spread out. Because of this most real examples arise in practice where there are two types of particles present with opposite charges – typically negatively charged electrons and positively charged nuclei. For

this reason in this section we consider coupling electromagnetism to *two* species of charged fields: nonrelativistic electrons represented by a Schrödinger field $\Phi(\mathbf{x},t)$ with charge $q_e=-e$ and nonrelativistic nuclei represented by a Schrödinger field Ψ with charge $+Ze$ where Z is a positive integer.

We also focus on those electrons that remain free to move relative to the nuclei, such as is true in practice for conduction electrons in conductors or for the freely moving charges in ionized plasmas. For these Z is usually the net charge of ionized atoms rather than bare nuclei since some electrons remain trapped by the nuclei and so screen their charge. In practice $Z=1$ or 2 is then not that large a positive integer. For simplicity we ignore the spin degree of freedom of both and use the following dispersion relations

$$E_e(\mathbf{p})=\varepsilon+\frac{\mathbf{p}^2}{2m}\quad\text{and}\quad E_n(\mathbf{p})=\mathcal{E}+\frac{\mathbf{p}^2}{2M}\,, \tag{10.2.1}$$

where the electron gap energy ε and mass m are both much smaller than the gap energy $\mathcal{E}$ and mass M for the ions.

Following the same steps outlined in §9.5 and §9.6, the Hamiltonian for this type of system coupled to electromagnetism is then given by $H=H_{eA}+H_{NA}+H_{EM}+H_C$ where

$$H_{eA}=\int \mathrm{d}^3x\,\left[\frac{1}{2m}(\mathbf{D}\Phi)^\star\cdot\mathbf{D}\Phi+\varepsilon\,\Phi^\star\Phi\right]\quad\text{with}\quad\mathbf{D}\Phi:=\nabla\Phi+ie\mathbf{A}\Phi \tag{10.2.2}$$

$$H_{NA}=\int \mathrm{d}^3x\,\left[\frac{1}{2M}(\mathbf{D}\Psi)^\star\cdot\mathbf{D}\Psi+\mathcal{E}\,\Psi^\star\Psi\right]\quad\text{and}\quad\mathbf{D}\Psi:=\nabla\Psi-iZe\mathbf{A}\Psi\,, \tag{10.2.3}$$

while the free electromagnetic action is as in (9.6.1) and the Coulomb interaction is

$$H_C=\frac{1}{8\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\frac{\rho(\mathbf{x},t)\,\rho(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|} \tag{10.2.4}$$

where ρ is the electric charge density

$$\rho=Ze\,\Psi^\star\Psi-e\,\Phi^\star\Phi\,. \tag{10.2.5}$$

Because the nuclei are much more massive, they typically respond much more slowly to a given applied electrostatic force. For instance, a momentum transfer $\mathbf{q}$ gives a nucleus an energy of order $\mathbf{q}^2/2M$ which is much smaller than the energy $\mathbf{q}^2/2m$ that would be given by the same momentum transfer to an electron. If we neglect terms in the energy suppressed by $1/M$ we can ignore the recoil of the heavier ions when they scatter, and so treat them as being approximately motionless. Dropping effects suppressed by $1/M$ also allows us to ignore the nuclear contribution to any electromagnetic currents in Maxwell's equations:

$$\frac{iZe}{2M}\Big\langle(\mathbf{D}\Psi)^\star\Psi-\Psi^\star(\mathbf{D}\Psi)\Big\rangle\simeq 0\,. \tag{10.2.6}$$

In practice the ions are often spaced by distances much smaller than the distances of practical interest and are sufficiently dense that fluctuations in their density can be neglected:

$$\langle \Psi^\star \Psi \rangle = n_N \quad \text{and} \quad \langle (\Psi^\star \Psi)^2 \rangle \simeq n_N^2 \quad \text{and so on}\,. \tag{10.2.7}$$

In this case we can regard n_N as a given number and ignore the nuclear motion, leaving electron motion described by the approximate Hamiltonian $H_{\rm el} := H_{eA} + H_{EM} + H_C$ with H_{eA} and H_{EM} given by (10.2.2) and (9.6.1), while

$$H_C \simeq \frac{e^2}{8\pi} \int \mathrm{d}^3x\, \mathrm{d}^3y\, \frac{[\Phi^\star\Phi(\mathbf{x},t) - \bar{n}_e][\Phi^\star\Phi(\mathbf{y},t) - \bar{n}_e]}{|\mathbf{x}-\mathbf{y}|} \tag{10.2.8}$$

where the parameter $\bar{n}_e$ is defined in terms of n_N by

$$\bar{n}_e = Z n_N\,. \tag{10.2.9}$$

$\bar{n}_e$ is the constant electron density that would be required to precisely cancel the charge of the assumed background density of nuclei, and (10.2.8) shows that the Coulomb interaction imposes an energy cost on any deviation of the electron density operator, $\Phi^\star\Phi$, away from this value.

10.2.1 Field evolution

Our goal is to predict time evolution in a complicated matter system and (like in the previous section) the tool used to that end is field equations derived from the above Hamiltonian. Whether it is more useful to do so in the interaction or Heisenberg picture depends on the application one has in mind.

Interaction picture:

For applications to perturbation theory it is the interaction picture that is most useful. For instance, suppose we write $H_{\rm el} = H_0 + H_{\rm int}$ where

$$\begin{aligned} H_0 &= \int \mathrm{d}^3x\, \left[\frac{1}{2m}\nabla\Phi^\star\cdot\nabla\Phi + \varepsilon\,\Phi^\star\Phi + \frac{1}{2}\Big(\mathbf{E}_0^2 + \mathbf{B}_0^2\Big)\right] \\ &= E_0 + \int \mathrm{d}^3p\, E_e(\mathbf{p})\, \mathfrak{c}^\star_{\mathbf{p}}\mathfrak{c}_{\mathbf{p}} + \sum_\lambda \int \mathrm{d}^3k\, \omega(\mathbf{k})\, \mathfrak{a}^\star_{\mathbf{k}\lambda}\mathfrak{a}_{\mathbf{k}\lambda}\,, \end{aligned} \tag{10.2.10}$$

while $E_e(\mathbf{p})$ is as given in (10.2.1) and $\omega(\mathbf{k}) = |\mathbf{k}|$. The interaction Hamiltonian would in this case then be

$$\begin{aligned} H_{\rm int} &= \int \mathrm{d}^3x \left\{ \frac{ie}{2m}\Big[(\nabla\Phi^\star)\Phi - \Phi^\star(\nabla\Phi)\Big]\cdot\mathbf{A} + \frac{e^2}{2m}\Phi^\star\Phi\,\mathbf{A}\cdot\mathbf{A}\right\} + H_C \\ &= \int \mathrm{d}^3x \left\{ \frac{ie}{2m}\Big[(\mathbf{D}\Phi)^\star\Phi - \Phi^\star(\mathbf{D}\Phi)\Big]\cdot\mathbf{A} - \frac{e^2}{2m}\Phi^\star\Phi\,\mathbf{A}\cdot\mathbf{A}\right\} + H_C \end{aligned} \tag{10.2.11}$$

with H_C as given in (10.2.8) and $\mathbf{D}\Phi = (\nabla + ie\mathbf{A})\Phi$, as defined in (10.2.2).

In the interaction picture fields evolve as they would in the absence of $H_{\rm int}$ and so the field equations can be explicitly solved. This is most usefully done using modes that diagonalize the unperturbed Hamiltonian in the usual way. For electromagnetic fields this leads as before to

$$\mathbf{A}(\mathbf{x},t) = \sum_\lambda \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\omega_k}} \left[\mathfrak{a}_{\mathbf{k}\lambda}\, \boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{-i\omega_k t + i\mathbf{k}\cdot\mathbf{x}} + \mathfrak{a}^\star_{\mathbf{k}\lambda}\, \boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\, e^{i\omega_k t - i\mathbf{k}\cdot\mathbf{x}} \right] , \qquad (10.2.12)$$

where single-particle states are labelled by momentum and photon helicity, with $\omega_k := |\mathbf{k}|$ and the time-dependence written explicitly so the operators satisfying $[\mathfrak{a}_{\mathbf{k}\lambda}, \mathfrak{a}^\star_{\mathbf{l}\xi}] = \delta_{\lambda\xi}\delta^3(\mathbf{k}-\mathbf{l})$ are time-independent.

A similar story applies to the electron operators as well, and unlike for dielectrics the assumption that electrons are mobile means that they experience an approximately translation-invariant environment on large length scales and so are usefully labelled by momentum (and spin, when not neglected). This means that the field operators are also usefully expanded in terms of operators satisfying $\{\mathfrak{c}_{\mathbf{p}}, \mathfrak{c}^\star_{\mathbf{q}}\} = \delta(\mathbf{q}-\mathbf{p})$, with the interaction-picture time dependence given by the usual expressions – *c.f.* (9.6.2) and (9.6.4) – repeated for completeness here:

$$\Phi(\mathbf{x},t) = \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\, \mathfrak{c}_{\mathbf{p}}\, e^{-iE_e(\mathbf{p})t + i\mathbf{p}\cdot\mathbf{x}} , \qquad (10.2.13)$$

together with the commutation relations this implies

$$\Big\{ \Phi(\mathbf{x},t)\,, \Phi^\star(\mathbf{y},t) \Big\} = \delta^3(\mathbf{x}-\mathbf{y})\,. \qquad (10.2.14)$$

As usual in the interaction picture the evolution of the quantum state is determined by $H_{\rm int}$ (as described in §3.2).

As usual in the interaction picture, the field evolution is completely solved and the focus is in the use of perturbative expressions like (3.2.22) to compute the time-evolution of initially prepared states.

Heisenberg picture:

For what follows it is also useful to record the operator evolution in the Heisenberg picture, in which it is the fields that carry the entire burden of time evolution. Because the presence of interactions usually means the evolution cannot be explicitly solved, it is more useful in this case to write down the differential field equations.

To this end we therefore construct the Heisenberg-picture fields $\Phi_h(\mathbf{x},t)$ and $\mathbf{A}_h(\mathbf{x},t)$ in the usual way and use the Hamiltonian $H = H_0 + H_{\rm int}$ given in (10.2.10) and (10.2.11) to compute the equations of motion (10.1.8) [*c.f.* eq. (3.2.4)], using the commutation relations (10.1.9) (10.2.14) (that are preserved when transforming to Heisenberg picture). One finds

in this way the usual Maxwell equations,[35] with

$$\nabla \times \mathbf{B}_h - \partial_t \mathbf{E}_h = \mathbf{J} = -\frac{ie}{2m}\Big[(\mathbf{D}\Phi_h^\star)\Phi_h - \Phi_h^\star(\mathbf{D}\Phi_h)\Big]\,, \tag{10.2.15}$$

and the Φ_h equation

$$iD_t\Phi_h = -\frac{1}{2m}\mathbf{D}^2\Phi_h + \varepsilon\,\Phi_h\,, \tag{10.2.16}$$

with $D_t\Phi := (\partial_t - ie\phi)\Phi$. Here ϕ denotes the electrostatic potential

$$\phi(\mathbf{x},t) := \frac{e^2}{4\pi}\int \mathrm{d}^3y\,\frac{[\bar{n}_e - \Phi_h^\star\Phi_h(\mathbf{y},t)]}{|\mathbf{x}-\mathbf{y}|}\,, \tag{10.2.17}$$

which carries within it the information of the Coulomb gauge Maxwell equation

$$\nabla\cdot\mathbf{E}_h = \rho = e(\bar{n}_e - \Phi_h^\star\Phi_h)\,. \tag{10.2.18}$$

Notice in particular that (10.2.16) implies conservation of electric charge in the form

$$\partial_t\rho + \nabla\cdot\mathbf{J} = -e\,\partial_t\Big(\Phi_h^\star\Phi_h\Big) - \frac{ie}{2m}\nabla\cdot\Big[(\mathbf{D}\Phi_h^\star)\Phi_h - \Phi_h^\star(\mathbf{D}\Phi_h)\Big] = 0\,, \tag{10.2.19}$$

a result often called the 'continuity' equation.

10.2.2 Fluid approximation

As the first applications of the above equations we assume the Φ system is well-approximated as a *fluid*, for which the density of electrons is also high enough that the microscopic fluctuations (*e.g.* thermal or quantum fluctuations) in macroscopic properties like density are too small to be important. This is often a reasonable approximation given that overall electrical neutrality makes the electron density similar to the density of nuclei, which has already been assumed to be in this regime.

Unlike for the nuclei we *do not* neglect the possibility of there being space or time dependence in the density, $n_e(\mathbf{x},t) = \langle\Phi^\star\Phi\rangle$, because the electrons are light enough that they can move on the time-scales of interest. The electron density *should* satisfy (10.2.9) once averaged over position, however,

$$\bar{n}_e := \frac{1}{\mathcal{V}}\int \mathrm{d}^3x\; n_e(\mathbf{x},t) = Zn_{\scriptscriptstyle N}\,, \tag{10.2.20}$$

because the total system is assumed to be electrically neutral. But because $n_e(\mathbf{x},t)$ can change in time it becomes crucial to know how its time evolution is constrained by microscopic field equations like (10.2.16).

Rather than using (10.2.16) directly it is more useful to use one of its consequences, eq. (10.2.19), since this expresses something robust against microscopic details: conservation

[35] This is no surprise, since getting the correct Maxwell equations in this way is how the electromagnetic coupling Hamiltonian is constructed. The other two Maxwell equations are unchanged since they follow from the relations that give $\mathbf{E}$ and $\mathbf{B}$ in terms of $\mathbf{A}$ and ϕ.

of the number of electrons. Using $n_e(\mathbf{x},t) = \langle \Phi^\star \Phi \rangle$ in the expectation value of (10.2.19) then leads to the evolution equation for n_e:

$$\partial_t n_e = -\frac{i}{2m} \nabla \cdot \Big\langle (\mathbf{D}\Phi_h^\star)\Phi_h - \Phi_h^\star (\mathbf{D}\Phi_h) \Big\rangle = -\nabla \cdot \Big(n_e \, \mathbf{u} \Big) \,, \tag{10.2.21}$$

where the last equality *defines* the quantity $\mathbf{u}(\mathbf{x},t)$ using

$$\mathbf{J} = -\frac{ie}{2m} \Big\langle (\mathbf{D}\Phi_h^\star)\Phi_h - \Phi_h^\star (\mathbf{D}\Phi_h) \Big\rangle =: -e \, n_e \, \mathbf{u} \,. \tag{10.2.22}$$

This definition is motivated by the physical picture of the microscopic system as a gas of charged particles with density n_e, since then if all of the particles shared the same velocity $\mathbf{v}(\mathbf{x},t)$ in a small region around a point $\mathbf{x}$ at time t then the local particle flux would be $n_e(\mathbf{x},t)\,\mathbf{v}(\mathbf{x},t)$. But even if the system were described by a bunch of teeny billiard-ball-like particles there is no reason why they should all share the same velocity, so even in this case $\mathbf{u}(\mathbf{x},t) = \langle \mathbf{v}(\mathbf{x},t) \rangle$ would be more like an local average of the particle velocities.

Further progress requires obtaining an expression for how $\mathbf{u}(\mathbf{x},t)$ evolves in time. In principle one simply differentiates the left-hand side of (10.2.22) and uses (10.2.16) to remove time derivatives of Φ. The problem is that the right-hand side of the result involves the average of yet another operator, whose evolution must also be determined and so on *ad infinitum*. Real progress requires finding an approximation – called a *constitutive relation* – that allows us to close the system of equations: *i.e.* to determine a collection of fields whose evolution only refers to these same fields.

In practice we'd like to be able to express $\partial_t \mathbf{u}$ in terms of the variables we already have (like $\mathbf{u}$, n_e, $\mathbf{E}$ and $\mathbf{B}$). It is the choices made to do this that differentiate different kinds of microscopic systems, such as plasmas or conductors. A particularly simple choice runs with the picture that the microscopic system is described by freely moving particles sharing a common local velocity, so $\mathbf{u}(\mathbf{x},t) = \langle \mathbf{v}(\mathbf{x},t) \rangle$. In this case the evolution of $\mathbf{v}$ should be governed by the equation of motions of these particles, $m\dot{\mathbf{v}} = \mathbf{F}$, and so

$$m \, \partial_t \mathbf{u} = \langle m \dot{\mathbf{v}} \rangle = \langle \mathbf{F} \rangle \,. \tag{10.2.23}$$

This becomes cleaner if inter-particle forces can be ignored since then the particle motion should be determined by the Lorentz force due to any local electromagnetic fields: $\mathbf{F} = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ (for particle charge $q = -e$). This suggests the choice

$$m \partial_t \mathbf{u} \simeq -e \langle \mathbf{E} + \mathbf{v} \times \mathbf{B} \rangle = -e \Big(\mathbf{E} + \mathbf{u} \times \mathbf{B} \Big) \quad \text{(cold plasma)} \,. \tag{10.2.24}$$

This is called a 'cold plasma' assumption because it assumes the electromagnetic forces dominate all others, and in particular neglects forces due to inter-particle collisions that for thermal systems are typically only negligible at low temperatures (more about these below).

It is constitutive equations like (10.2.24) that allow us to close the system of evolution equations. That is, eq. (10.2.21) gives $\partial_t n_e$ in terms of n_e and $\mathbf{u}$, (10.2.24) then gives $\partial_t \mathbf{u}$ in

terms of $\mathbf{u}$, $\mathbf{E}$ and $\mathbf{B}$. But the Maxwell equations (10.2.15) and (9.1.5) then give $\partial_t \mathbf{E}$ and $\partial_t \mathbf{B}$ in terms of themselves and n_e and $\mathbf{u}$, once we use (10.2.22).

Worked Example: Plasma oscillations

We explore the implications of the cold-plasma constitutive relation (10.2.24), in which we further assume electrostatic forces dominate magnetic ones (as is usually true for slowly moving charges). This, together with eqs. (10.2.21) and the expectation value of (10.2.15) – using (10.2.22) – leads to the following four equations for the four unknowns, n_e, $\mathbf{u}$, $\mathbf{E} = -\partial_t \mathbf{A} - \nabla\phi$ and $\mathbf{B} = \nabla \times \mathbf{A}$:

$$\partial_t n_e = -\nabla \cdot \Big(n_e \, \mathbf{u} \Big) \,, \tag{10.2.25}$$

$$m \partial_t \mathbf{u} \simeq -e\mathbf{E} \,, \tag{10.2.26}$$

$$\nabla \cdot \mathbf{E}_h = \langle \rho \rangle = e(\bar{n}_e - n_e) \,, \tag{10.2.27}$$

and

$$\nabla \times \mathbf{B} - \partial_t \mathbf{E} = \langle \mathbf{J} \rangle = -e \, n_e \, \mathbf{u} \,. \tag{10.2.28}$$

For everyday electromagnetic fields we can again treat $\mathbf{A}$ (and so also $\mathbf{E}$ and $\mathbf{B}$) as being prepared in such a sufficiently highly occupied state that the field is effectively classical. The trivial (ground-state) solution is given by a uniform fluid at rest: $\mathbf{u} = \mathbf{E} = \mathbf{B} = 0$ and $n_e = \bar{n}_e$, and we seek new solutions that are perturbatively close to this of the plane-wave form:

$$n_e - \bar{n}_e = \tilde{n}_{\mathbf{k}} \, e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} \,, \quad \phi = \tilde{\phi}_{\mathbf{k}} \, e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} \,, \quad \mathbf{u} = \tilde{\mathbf{u}}_{\mathbf{k}} \, e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} \text{ and } \mathbf{A} = \tilde{\mathbf{A}}_{\mathbf{k}} \, e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} \,, \tag{10.2.29}$$

where products of the small quantities $\tilde{n}_{\mathbf{k}}$, $\tilde{\phi}_{\mathbf{k}}$, $\tilde{\mathbf{u}}_{\mathbf{k}}$ and $\tilde{\mathbf{A}}_{\mathbf{k}}$ are dropped. Using these in eqs. (10.2.25) through (10.2.28) (as well as the gauge condition $\nabla \cdot \mathbf{A} = 0$) then gives the following two linearized scalar equations

$$\omega \tilde{n}_{\mathbf{k}} + \bar{n}_e \, \mathbf{k} \cdot \tilde{\mathbf{u}}_{\mathbf{k}} \quad \text{and} \quad k^2 \tilde{\phi}_{\mathbf{k}} = -e\tilde{n}_{\mathbf{k}} \tag{10.2.30}$$

(where $k = |\mathbf{k}|$), whose solutions are

$$\tilde{n}_{\mathbf{k}} = -\frac{\bar{n}_e}{\omega}(\mathbf{k} \cdot \tilde{\mathbf{u}}_{\mathbf{k}}) \quad \text{and} \quad \tilde{\phi}_{\mathbf{k}} = -\frac{e\tilde{n}_{\mathbf{k}}}{k^2} = \frac{e\bar{n}_e}{\omega k^2}(\mathbf{k} \cdot \tilde{\mathbf{u}}_{\mathbf{k}}) \,. \tag{10.2.31}$$

The two linearized vector equations similarly are

$$m\omega \tilde{\mathbf{u}}_{\mathbf{k}} = e\omega \tilde{\mathbf{A}}_{\mathbf{k}} + e\mathbf{k}\tilde{\phi}_{\mathbf{k}} \tag{10.2.32}$$

and

$$\omega^2 \tilde{\mathbf{A}}_{\mathbf{k}} + \omega \mathbf{k} \tilde{\phi}_{\mathbf{k}} - k^2 \tilde{\mathbf{A}}_{\mathbf{k}} - e\bar{n}_e \tilde{\mathbf{u}}_{\mathbf{k}} = 0 \,, \tag{10.2.33}$$

which can both be decomposed into directions transverse to and parallel to $\mathbf{k}$. For transverse waves these imply

$$\tilde{\mathbf{u}}^{\perp}_{\mathbf{k}} = \frac{e}{m} \tilde{\mathbf{A}}^{\perp}_{\mathbf{k}} \quad \text{and} \quad \Big(\omega^2 - k^2 - \omega_p^2 \Big) \tilde{\mathbf{A}}^{\perp}_{\mathbf{k}} = 0 \,, \tag{10.2.34}$$

which defines the *plasma frequency*

$$\omega_p^2 := \frac{e^2 \bar{n}_e}{m} \,. \tag{10.2.35}$$

We find that transverse electromagnetic waves within a plasma acquire an energy gap, since (10.2.34) reveals their dispersion relation to be

$$\omega^2(\mathbf{k}) = \omega_p^2 + k^2 \,. \tag{10.2.36}$$

Although this approaches the vacuum dispersion relation $\omega = k$ at large k it differs dramatically for longer wavelengths (smaller k). In particular energy conservation precludes an incident electromagnetic wave that in the vacuum has a frequency less than ω_p from entering a plasma, and this is the reason in practice that conductors strongly reflect visible light (and so tend to be shiny metals).

For longitudinal waves eq. (10.2.33) is consistent with the gauge condition $\tilde{A}^{\parallel} = \hat{\mathbf{k}} \cdot \tilde{\mathbf{A}} = 0$ because of the scalar relations (10.2.31). The remaining vector equation (10.2.32) then implies

$$m\omega \mathbf{k} \cdot \tilde{\mathbf{u}}_{\mathbf{k}} = e k^2 \tilde{\phi}_{\mathbf{k}} \,, \tag{10.2.37}$$

which is only consistent with (10.2.31) if $\omega = \omega_p$ for all k. The k-independence of the frequency of longitudinal modes proves to be an artefact of neglecting interparticle scattering.

Including scattering for a fluid that is locally in thermal equilibrium turns out to modify the linearized constitutive relation (10.2.26) to include a pressure-gradient term

$$m\partial_t \mathbf{u} \simeq -e\mathbf{E} - \frac{1}{\bar{n}_e} \nabla P \,, \tag{10.2.38}$$

where $P = P(n_e, T)$ is the pressure of the thermal fluid. The gradient of P can be re-expressed in terms of ∇n_e (and not also ∇T, for example) once the equation of state $P = P(n_e, T)$ is known, leading to $\nabla P = \gamma T \nabla n_e$ where the constant γ depends on whether or not the wave motion is isothermal or abiabatic. Including this and rederiving the solution for small longitudinal waves instead gives the dispersion relation

$$\omega^2 = \omega_p^2 + \left(\frac{\gamma T}{m}\right) k^2 \,, \tag{10.2.39}$$

which reduces to the previous k-independent result as $T \to 0$. Besides acquiring a gap, we see that electromagnetic waves within a plasma also acquire a third (longitudinal) polarization state.

10.2.3 Conductors

For later purposes it is worth exploring another type of common constitutive relation that is similar to (but different in detail) to the cold-plasma relation used in (10.2.26). To motivate the new choice consider writing (10.2.26) in Fourier space (assuming the space-time dependence $e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}}$) as $-im\omega \mathbf{u}_{\mathbf{k}} \simeq -e\mathbf{E}_{\mathbf{k}}$ and so

$$\mathbf{J}_{\mathbf{k}} \simeq -e\bar{n}_e \, \mathbf{u}_{\mathbf{k}} \simeq \frac{ie^2\bar{n}_e}{m\omega}\mathbf{E}_{\mathbf{k}} = \frac{i\omega_p^2}{\omega}\,\mathbf{E}_{\mathbf{k}} \,, \tag{10.2.40}$$

which shows that $\mathbf{J}_{\mathbf{k}}$ is proportional to $\mathbf{E}_{\mathbf{k}}$.

This proportionality motivates the *conducting* constitutive relation

$$\mathbf{J} = \sigma \, \mathbf{E} \tag{10.2.41}$$

where the coefficient is called the medium's *conductivity*. For oscillatory ('alternating current' or AC) fields eq. (10.2.41) can be written in Fourier space with each term regarded as being frequency dependent, in which case it is no different than (10.2.40) with AC conductivity $\sigma(\omega) = i\omega_p^2/\omega$.

A medium is called a electrical *conductor* if (10.2.41) is a good approximation *even as* $\omega \to 0$. In this case the nonzero limit $\sigma_0 = \lim_{\omega\to 0}\sigma(\omega)$ is called the medium's DC ('direct current') conductivity. The zero-frequency limit of (10.2.40) shows that cold plasmas are not conductors in this sense, because for cold plasmas it is $\partial_t \mathbf{J}$ that is proportional to $\mathbf{E}$ rather than $\mathbf{J}$ itself.

Real metals of common experience are DC conductors in this sense, and often very good ones. Nonzero DC conductivity arises when scattering allows charge carriers to dissipate their energy so that their speed is proportional to the applied force (much as a falling object in a gravitational field acquires a terminal velocity when falling through a frictional environment like the atmosphere). Simple models[36] of this dissipation predict DC conductivities to be of size $\sigma_0 \simeq e^2\bar{n}_e\tau_c/m$ where τ_c is a typical time between successive collisions of the charge carriers (assumed here to be electrons with mass m and charge $q = -e$).

The dissipation inherent in a DC conductor can also be seen by using (10.2.41) in Maxwell's equations. For instance, the conservation of electromagnetic energy (9.1.25) becomes

$$\partial_t\left[\frac{1}{2}\Big(\mathbf{E}^2 + \mathbf{B}^2\Big)\right] + \nabla\cdot\Big(\mathbf{E}\times\mathbf{B}\Big) = -\mathbf{J}\cdot\mathbf{E} = -\sigma_0\mathbf{E}^2 \leq 0\,, \tag{10.2.42}$$

showing that electromagnetic energy is drained into the charge carriers when an electric field is applied to a conductor. It is drained because it does work when accelerating the charge carriers and this charge-carrier energy is then dissipated by the collisions that give a nonzero DC conductivity.

Using (10.2.41) in the continuity equation for charge conservation – *c.f.* eq. (9.1.6) – similarly implies

$$\partial_t\rho = -\nabla\cdot\mathbf{J} = -\sigma_0\nabla\cdot\mathbf{E} = -\sigma_0\rho \tag{10.2.43}$$

whose solution $\rho(\mathbf{x},t) = \rho_0(\mathbf{x})\,e^{-\sigma_0 t}$ shows how an initial nonzero charge distribution $\rho_0(\mathbf{x})$ prepared at $t = 0$ dissipates away on a time-scale of order $1/\sigma_0$.

A third example comes from rederiving the wave equation for classical electromagnetic waves starting from Maxwell's equations. In particular taking the time derivative of the equation $\nabla\times\mathbf{B} - \partial_t\mathbf{E} = \mathbf{J}$ gives

$$\Big(\nabla\times\partial_t\mathbf{B}\Big) - \partial_t^2\mathbf{E} = \partial_t\mathbf{J} = \sigma_0\partial_t\mathbf{E} \tag{10.2.44}$$

which, after using $\partial_t\mathbf{B} + \nabla\times\mathbf{E} = 0$, implies

$$-\partial_t^2\mathbf{E} - \sigma_0\partial_t\mathbf{E} + \nabla^2\mathbf{E} = \nabla\rho\,. \tag{10.2.45}$$

[36] The formula quoted comes from the *Drude* model of conductivity, whose description goes beyond the scope of these notes.

As discussed at the beginning of this chapter, the general solution to this equation is obtained by adding any particular solution to a general solution, $\mathbf{E}_{\rm hom}(\mathbf{x},t)$, of the homogeneous equation obtained from (10.2.45) by setting $\rho = 0$. For plane wave the general solutions to the homogeneous equation are $\mathbf{E} \propto \tilde{\mathbf{E}}_{\mathbf{k}} \exp(-i\omega t + i\mathbf{k}\cdot\mathbf{x})$ where $\omega^2 + i\sigma_0\omega - \mathbf{k}^2 = 0$ and so

$$\omega = \sqrt{\mathbf{k}^2 - \frac{1}{4}\,\sigma_0^2} - \frac{i\sigma_0}{2}\,. \tag{10.2.46}$$

This shows how short-wavelength modes (those with $|\mathbf{k}| > \frac{1}{2}\,\sigma_0$) can propagate in a conductor, but are damped with an amplitude that falls with time like $|\mathbf{E}_{\rm hom}|^2 \propto e^{-\sigma_0 t}$. By contrast, long-wavelength modes are completely attenuated, since they are slow enough to be erased by the motion they induce in the charge carriers.

10.3 Superconductivity

This section examines the electromagnetic consequences of a different kind of state, one that would arise if the lighter mobile electrically charged field Φ were bosonic (rather than being fermions, as are electrons) and prepared in a classical coherent state, along the lines considered in §7. This in principle could occur if the effective gap energy ε in the dispersion relation (10.2.1) for the lighter charged state were for some reason to go to zero (or be cancelled by a chemical potential, μ) as described in more detail in §7.1. When this occurs the lowest-energy single-particle state for the field Φ can become macroscopically occupied when it undergoes Bose-Einstein condensation. We do not care so much about the details of *why* this should be energetically preferred, but instead ask how the electromagnetic response of such a system differs from the more mundane systems considered earlier. Suggestively, we find that the response resembles what is found experimentally for systems called *superconductors*.

To this end consider again the Hamiltonian given in (10.2.10) and (10.2.11), supplemented with the Coulomb interaction (10.2.8) and the repulsive contact interaction (6.4.1) (with the last of these introduced to ensure the stability of the Bose-Einstein condensate, as described in §7.1). This leads to

$$H = \int \mathrm{d}^3x\, \left\{ \frac{1}{2m}(\mathbf{D}\Phi)^\star \cdot \mathbf{D}\Phi + \varepsilon\,\Phi^\star\Phi + g(\Phi^*\Phi)^2 + \frac{1}{2}\Big(\mathbf{E}_0^2 + \mathbf{B}_0^2\Big) \right\} + H_C\,, \tag{10.3.1}$$

with $\mathbf{D}\Phi = \nabla\Phi - iq\mathbf{A}\,\Phi$ (assuming the boson has charge q) and the Coulomb interaction is

$$\begin{aligned} H_C &\simeq \frac{q^2}{8\pi} \int \mathrm{d}^3x\, \mathrm{d}^3y\, \frac{[\Phi^\star\Phi(\mathbf{x},t) - \bar{n}_e][\Phi^\star\Phi(\mathbf{y},t) - \bar{n}_e]}{|\mathbf{x}-\mathbf{y}|} \\ &= q \int \mathrm{d}^3x\, \phi(\mathbf{x},t) \Big[\Phi^\star\Phi(\mathbf{x},t) - \bar{n}_e\Big] \end{aligned} \tag{10.3.2}$$

where the electrostatic potential is

$$\phi(\mathbf{x},t) = \frac{q}{4\pi} \int \mathrm{d}^3y\, \frac{\Phi^\star\Phi(\mathbf{x},t) - \bar{n}_e}{|\mathbf{x}-\mathbf{y}|}\,. \tag{10.3.3}$$

The field equation for the Heisenberg-picture field Φ_h implied by this Hamiltonian is – *c.f.* eq. (10.2.16):

$$iD_t\Phi_h = -\frac{1}{2m}\mathbf{D}^2\Phi_h + \varepsilon\,\Phi_h + 2g(\Phi_h^\star\Phi_h)\,\Phi_h\,, \tag{10.3.4}$$

where $D_t\Phi = \partial_t\Phi + iq\phi\Phi$.

To describe the electromagnetic response we follow §7.2 and work in the semiclassical approximation, expanding Φ about a classical background φ_0 that captures the macroscopically occupied lowest-energy mode. The value of φ_0 is found by minimizing the (free) energy, as in §7.2. Restricted to $\Phi = \varphi_0$ the Coulomb energy (10.3.2) becomes

$$H_C \simeq \frac{q^2}{8\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\frac{(|\varphi_0|^2-\bar{n}_e)(|\varphi_0|^2-\bar{n}_e)}{|\mathbf{x}-\mathbf{y}|}\,, \tag{10.3.5}$$

and so Coulomb repulsion imposes a steep energy cost unless $\varphi_0^2 = \bar{n}_e$, which must be taken into account when deciding if nonzero φ_0 is energetically favourable. The details of this minimization are not needed for the present purposes, provided only that $\varphi_0 \neq 0$ once it is done.

An important conclusion of §7.2 was that the symmetry $\Phi \to e^{iq\omega}\Phi$ responsible for charge conservation ensures that the phase of φ_0 is never energetically determined, so rather than defining the complex fluctuation by $\hat{\Phi}(\mathbf{x},t) = \Phi - \varphi_0$ it is useful to explicitly isolate the phase and instead define two hermitian quantum fluctuation fields, χ and ψ, using

$$\Phi(\mathbf{x},t) = \Big[\varphi_0 + \psi(\mathbf{x},t)\Big]\exp[i\chi(\mathbf{x},t)] \simeq \varphi_0 + \psi(\mathbf{x},t) + i\varphi_0\,\chi(\mathbf{x},t) + \cdots\,, \tag{10.3.6}$$

where φ_0 is real. In terms of these variables the symmetry of $\Phi \to \Phi\, e^{iq\omega}$ becomes the shift symmetry $\chi \to \chi + q\omega$. In the semiclassical limit $\psi = 0$ in the ground state (by definition of φ_0), but the vacuum value of the field χ is not energetically fixed because this symmetry precludes it from having a potential energy.[37]

Our interest is in the form H takes once written in terms of $\mathbf{A}$, ϕ, χ and ψ, which is found by using

$$\Phi^\star\Phi = \Big(\varphi_0+\psi\Big)^2 \quad\text{and}\quad (\mathbf{D}\Phi)^\star\cdot\mathbf{D}\Phi = (\nabla\psi)^2 + (\varphi_0+\psi)^2\Big(\nabla\chi - q\mathbf{A}\Big)^2 \tag{10.3.7}$$

in (10.3.1). What is noteworthy here is that χ only appears in the specific combination $\nabla\chi - q\mathbf{A}$, and this is a consequence of the underlying gauge symmetry. Recall that §9.5 shows that physics must be invariant under the combined transformations[38] $\mathbf{A} \to \mathbf{A} + \nabla\omega$,

[37] This kind of transformation shows that χ is the Goldstone boson associated with the spontaneous breaking of this symmetry, an illustration of the general discussion given in §8.3 above.

[38] Invariance of the ϕ terms in H seems opaque here, but is made clearer in §13 since provides more systematic tools for thinking about field kinetic energies. But it is already evident in the invariance of the equation of motion (10.3.4).

$\phi \to \phi - \partial_t\omega$ and $\Phi \to \Phi\, e^{iq\omega}$ for any function $\omega(\mathbf{x}, t)$. In terms of the new variables this implies invariance under

$$\mathbf{A} \to \mathbf{A} + \nabla\omega\,, \quad \phi \to \phi - \partial_t\omega \quad \text{and} \quad \chi \to \chi - q\omega\,. \tag{10.3.8}$$

Invariance under this implies the total energy can only depend on ψ and the combinations

$$\Pi := \nabla\chi - q\mathbf{A} \quad \text{and} \quad \hat{\pi} := \partial_t\chi + q\phi\,, \tag{10.3.9}$$

rather than the four fields ψ, χ, ϕ and $\mathbf{A}$ separately. In particular the field χ can be *completely removed* by performing a gauge transformation (10.3.8) with transformation parameter chosen[39] to be $\omega = \chi/q$.

This dependence suffices to dictate much of the electromagnetic response. In particular, the same gradient and kinetic terms in the Hamiltonian that would normally imply that energy is minimized when $\nabla\Phi = 0$ and $\partial_t\Phi = 0$ in the absence of electromagnetic fields now imply that deep within a superconductor the energy is instead minimized by $\Pi = 0$ and $\hat{\pi} = 0$. This means that an applied classical electromagnetic field must satisfy $\mathbf{A} = \nabla\chi/q$ and $\phi = -\partial_t\chi/q$ and so $\mathbf{E} = \mathbf{B} = 0$. Electric and magnetic fields are excluded from deep within such a medium. Notice that this conclusion is drawn *without* assuming the fields are completely static.

Although we've seen that electric fields also tend to zero inside conductors (see the discussion surrounding eq. (10.2.46)), they can persist for times of order $1/\sigma_0$ and the same is not usually true for magnetic fields. Magnetic fields *are* excluded from materials called superconductors, however, a phenomenon called the *Meissner effect*. Superconductors are unusual materials obtained when some conductors are cooled to low temperatures until a critical temperature is reached. Below this temperature they behave as if they had infinite conductivity: electrical currents can persist in them indefinitely and in the absence of electric fields. Applied electric fields also never penetrate far into the sample; it is as if the time for electric fields to decay went to zero (as would be the case in a conductor if σ_0 were to become infinite).

The above picture of bose-condensed electric charge carriers provides a hint as to why this happens. Experiments reveal that superconducting charge carriers have charge $q = -2e$, so it is as if electrons pair up and bind together to become bosons that then condense. This is more or less what electrons actually do, though the picture is more subtle than the description here might lead one to think (for instance the bound electron pairs are not particularly small compared with underlying interatomic spacings).

[39] It is true that once this is done $\mathbf{A}$ will no longer satisfy $\nabla \cdot \mathbf{A} = 0$, but this need not be important since physical quantities do not care what gauge one chooses.

11 Special relativity in quantum mechanics

Electromagnetism provides the first example of a quantum field theory that is also consistent with special relativity. This turns out not to be an easy thing to do, and there are a number of requirements a quantum field theory must satisfy in order to consistently incorporate special relativity. The list of such requirements is respectably long, including the existence of antiparticles for all particle types, the spin-statistics connection, the requirement that all interactions be invariant under CPT (charge conjugation – more about which later – parity and time-reversal) transformations, something called 'crossing' symmetry and so on.

All of these consistency requirements for reconciling quantum mechanics and special relativity turn out actually to be realized in nature, and it is a great triumph of physics that they are so robustly predicted by relativistic quantum field theory. This chapter provides an introductory sketch of how and why these consistency requirements arise.

11.1 Review of special relativity

To start, a lightning review of special relativity. The goal here is not to teach it from scratch, but instead to provide a brief summary that emphasizes the role played by symmetries. Emphasizing the role of symmetries in special relativity is useful because it is through its symmetry predictions that its implications enter into quantum mechanics.

11.1.1 Inertial observers and the Minkowski metric

Special relativity traditionally proposes (similar to Newtonian mechanics) the existence of a class of preferred 'inertial' observers that can move relative to one another, but only with constant relative velocity. The laws of nature take precisely the same form for all such observers. For Newton these would be the non-accelerating observers for all of whom $\mathbf{F} = m\mathbf{a}$ is true.

The *Principle of Relativity* states that the laws of physics are invariant under the transformations that take us from any one inertial frame to any other, and this is as true in Newtonian mechanics as it is in Special Relativity. The difference between Special Relativity and Newtonian mechanics turns out to be the specific form of the transformations that relate the various inertial frames.

In Special Relativity the guiding principle for defining the transformation rules between inertial frames is the demand that all inertial observers must measure precisely the same numerical value, $c = 299,792,458$ m/s, for the speed of light in vacuum. This is a property of Maxwell's equations, which predict the speed of light in a way that seems not to depend on the reference frame. We now know it also turns out to be experimentally true, with many experiments verifying that the measured speed of light is independent of the observer's own speed.

Having everyone agree on the speed of light is certainly *not* true in Newtonian mechanics, due to the law of addition of velocities: if observer A moves with velocity $\mathbf{v}_{\rm rel}$ relative to observer B then the velocity $\mathbf{v}_A$ of a particle measured by observer A and its velocity $\mathbf{v}_B$ as measured by B are related by $\mathbf{v}_B = \mathbf{v}_A + \mathbf{v}_{\rm rel}$. If the object in question is moving along with the wave front of light then $v_A = |\mathbf{v}_A|$ defines the speed of light for observer A and $v_B = |\mathbf{v}_B|$ does the same for observer B. These cannot be the same for observers A and B when $\mathbf{v}_{\rm rel}$ is nonzero. Einstein's observation was that the error in this argument is that the two observers agree on their definition of t, and that once t_A and t_B become different there exists a relation between them that ensures that the speed of light is the same for all observers.

It is because all inertial observers measure the same value for c, that it is possible to define our units of distance so that $c = 1$, as was described in §1.1. (Such units would not be useful if all inertial observers did not agree on the speed of light.) These units are used throughout the rest of these notes, and (as discussed earlier) conversion of subsequent formulae to ordinary units is accomplished by inserting whatever factors of c are required to give the expression the correct dimensions. (*E.g.* for a result like $v = 0.2$ to have the dimensions of m/s, its right-hand-side must really be $0.2\,c$. Similarly, for E an energy, p a momentum and m a mass, $E = p$ becomes $E = p\,c$ and $E = m$ becomes $E = m\,c^2$.)

From a symmetry point of view, it is useful to cast the required transformation in terms of the motion of particles in a four-dimensional spacetime for which the rules for measuring distances (in space and time) are invariant under a class of transformations. Mathematically 'measuring distances' means that spacetime is endowed with a metric — that is, a position-dependent 4×4 matrix, $g_{\mu\nu}(x)$, in terms of which the distance $\mathrm{d}s$ corresponding to a given set of infinitesimal coordinate displacements, $\mathrm{d}x^\mu$, locally satisfies

$$\mathrm{d}s^2 = g_{\mu\nu}(x)\,\mathrm{d}x^\mu \mathrm{d}x^\nu\,. \tag{11.1.1}$$

Here the summation convention is in force, with any repeated Greek indices (like μ and ν in the above) being summed over the values $0, 1, 2, 3$, with $\{x^0, x^1, x^2, x^3\} = \{t, x, y, z\}$ where t denotes time and x, y and z are Cartesian position coordinates.

From this point of view Special Relativity can be summarized as the statement that for *all* inertial observers the metric that appears in (11.1.1) is independent of position and given everywhere by

$$\mathrm{d}s^2 = \eta_{\mu\nu}\,\mathrm{d}x^\mu\,\mathrm{d}x^\nu = -\mathrm{d}t^2 + \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2\,,$$

and so for rectangular coordinates $\{x^0, x^1, x^2, x^3\} = \{t, x, y, z\}$, we have

$$\eta_{\mu\nu} = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}\,, \tag{11.1.2}$$

where all non-written entries are zero. This particular metric is called the *Minkowski* metric.

Notice that this metric is *not* positive definite, unlike the metrics considered when thinking about the geometry of three-dimensional space. But $\mathrm{d}s^2$ *is* positive and agrees with our notion of distance in flat space if it is restricted to a purely spatial interval, along which $\mathrm{d}t = 0$. (The possibility that $\mathrm{d}s^2$ can be zero or negative is the main reason why the geometry of spacetime differs from that of the geometry of four-dimensional space.) If $\mathrm{d}s^2 > 0$ the interval is called *spacelike*, and will turn out represent the a spatial distance along the interval for the particular inertial observers who see $\mathrm{d}t = 0$ along the interval.

By contrast, the situation $\mathrm{d}s^2 = 0$ describes the trajectory of a light ray. That is, $\mathrm{d}s = 0$ implies $\mathrm{d}t^2 = \mathrm{d}\ell^2$, where $\mathrm{d}\ell^2 = \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2$ measures the spatial distance traversed. Clearly any such a trajectory satisfies $\mathrm{d}\ell/\mathrm{d}t = 1$, and so moves at the speed of light (since $c = 1$). The requirement that all inertial observers agree on the interval $\mathrm{d}s^2$ therefore includes as a special case the condition that all such observers agree on the speed of light *in vacuo*. An interval for which $\mathrm{d}s^2 = 0$ is called a *null* interval.

In the situation where $\mathrm{d}s^2 = -\mathrm{d}t^2 + \mathrm{d}\ell^2 < 0$, the interval corresponds to the world line of a trajectory of a particle moving at less than the speed of light, since $v^2 = (\mathrm{d}\ell/\mathrm{d}t)^2 = 1 + (\mathrm{d}s/\mathrm{d}t)^2 < 1$. In this case it is useful to define $\mathrm{d}\tau = \sqrt{-\mathrm{d}s^2}$, since this represents the proper time elapsed by the observer moving along this trajectory (for whom $\mathrm{d}\ell = 0$). For this reason intervals for which $\mathrm{d}s^2 < 0$ are called *timelike*.

11.1.2 Lorentz transformations

The transformations of special relativity may now be defined as those which do not change the Minkowski metric eq. (11.1.2), since all such observers will agree on physical distances and so also agree on physical laws that are expressed in terms of them. Special Relativity can then be regarded as the requirement that physics looks the same when expressed in terms of either coordinates, x^μ and x'^μ, when the transformation that relates them preserves the Minkowski metric of (11.1.2).

The resulting transformations are given by a combination of translations,

$$x^\mu \to x^\mu + a^\mu \,, \tag{11.1.3}$$

and linear transformations,

$$x^\mu \to \Lambda^\mu{}_\nu \, x^\nu \,, \tag{11.1.4}$$

where the constant matrices $\Lambda^\mu{}_\nu$ must satisfy

$$\eta_{\alpha\beta}\Lambda^\alpha{}_\mu\Lambda^\beta{}_\nu = \eta_{\mu\nu} \,. \tag{11.1.5}$$

The group of transformations defined by eqs. (11.1.3) through (11.1.5) is called the *Poincaré group*, while those defined by eqs. (11.1.4) and (11.1.5) alone are called the *Lorentz group*, or the group $O(3,1)$.

Poincaré transformations satisfy the defining properties of a group, and it is a Lie group because they are labelled by a continuous (rather than discrete) set of parameters. To get an idea of how many such parameters there are it is useful to examine transformations that are infinitesimally different from the identity transformation (*i.e.* the transformation that doesn't transform anything at all: $a^\mu = 0$ and $\Lambda^\mu{}_\nu = \delta^\mu_\nu$). Writing $\Lambda^\mu{}_\nu = \delta^\mu_\nu + \omega^\mu{}_\nu + ...$ and $a^\mu = \epsilon^\mu + ...$, the defining condition of invariance of the Minkowski metric them imposes no conditions on ϵ^μ, but implies $\omega^\mu{}_\nu$ must satisfy $\omega_{\mu\nu} = -\omega_{\nu\mu}$, where $\omega_{\mu\nu} := \eta_{\mu\lambda}\omega^\lambda{}_\nu$. This indicates there are 4 independent parameters in ϵ^μ, corresponding to the freedom to translate in all 3 spatial directions and in time. There are similarly $\frac{1}{2}\times 4\times 3 = 6$ independent parameters in the antisymmetric 4×4 matrix $\omega_{\mu\nu}$, and so the Poincaré group is a 10-parameter group, with its Lorentz subgroup containing 6 independent parameters.

Spatial rotations provide a special case of Lorentz transformations, for which

$$\Lambda^\mu{}_\nu = \begin{pmatrix} 1 & \\ & M^i{}_j \end{pmatrix} , \tag{11.1.6}$$

where $i, j = 1, 2, 3$ runs over purely spatial directions, and $M^i{}_j$ is an arbitrary 3×3 orthogonal matrix: $\delta_{ij}M^i{}_k M^j{}_l = \delta_{kl}$. The group of all such matrices is called $O(3)$. For instance, the matrices describing rotations about the x, y and z axes by an angle α_x, α_y and α_z are respectively given by

$$(M_x)^i{}_j = \begin{pmatrix} 1 & & \\ & c_x & s_x \\ & -s_x & c_x \end{pmatrix} , \; (M_y)^i{}_j = \begin{pmatrix} c_y & & s_y \\ & 1 & \\ -s_y & & c_y \end{pmatrix} , \; (M_z)^i{}_j = \begin{pmatrix} c_z & s_z & \\ -s_z & c_z & \\ & & 1 \end{pmatrix} , \tag{11.1.7}$$

where $s_i := \sin\alpha_i$ and $c_i := \cos\alpha_i$ for $i = x, y, z$. A general rotation is built from products of these basic three, and so rotations account for three of the six parameters of the Lorentz group.

A second class of Lorentz transformations involves both time and space directions. For instance, as is easy to verify, the matrix

$$(\Lambda_x)^\mu{}_\nu = \begin{pmatrix} \cosh\beta_x & \sinh\beta_x & & \\ \sinh\beta_x & \cosh\beta_x & & \\ & & 1 & \\ & & & 1 \end{pmatrix} , \tag{11.1.8}$$

that mixes the t and x directions satisfies the defining condition (11.1.5), for any value of the real parameter β_x. The same is true for the following matrices that similarly mix t with the y and z directions,

$$(\Lambda_y)^\mu{}_\nu = \begin{pmatrix} \cosh\beta_y & & \sinh\beta_y & \\ & 1 & & \\ \sinh\beta_y & & \cosh\beta_y & \\ & & & 1 \end{pmatrix} \quad \text{and} \quad (\Lambda_z)^\mu{}_\nu = \begin{pmatrix} \cosh\beta_z & & & \sinh\beta_z \\ & 1 & & \\ & & 1 & \\ \sinh\beta_z & & & \cosh\beta_z \end{pmatrix} , \tag{11.1.9}$$

for any real value of β_y and β_z. These provide the remaining three parameters of the Lorentz group, and are shown below to be related to *boosts* – *i.e.* to transformations that relate inertial observers that move relative to one another with nonzero velocity. This later discussion also provides an explicit relation between the three parameters β_i and the three components v_i that characterize the observer's relative velocity.

Exercise: Verify that the transformations (11.1.6) and (11.1.8) satisfy (11.1.5).

11.1.3 Improper Lorentz transformations

The group of Poincaré transformations as defined above turns out not to be a connected set, inasmuch as not all group elements can be continuously related to the identity transformation: $\Lambda^\mu{}_\nu = \delta^\mu_\nu$ and $a^\mu = 0$. Those transformations that can be continuously connected to the identity are called 'proper' Poincaré (or Lorentz) transformations.

The lack of connectedness arises within the Lorentz part of the group rather than from the translations. Improper Lorentz transformations are defined to be those that are not proper. To see that improper transformations exist notice that the defining condition (11.1.5) implies the determinant of the 4×4 matrix with components $\Lambda^\mu{}_\nu$ must satisfy $(\det \Lambda)^2 = 1$ and so $\det \Lambda = \pm 1$. Only transformations with $\det \Lambda = +1$ can be continuously connected to the identity transformation.

But having a negative determinant is not a necessary condition for a transformation to be improper. To see why, notice that evaluating (11.1.5) at $\mu = \nu = 0$ implies

$$-\Lambda^0{}_0\Lambda^0{}_0 + \delta_{ij}\Lambda^i{}_0\Lambda^j{}_0 = \eta_{00} = -1\,, \tag{11.1.10}$$

and so $(\Lambda^0{}_0)^2 = 1 + \delta_{ij}\Lambda^i{}_0\Lambda^j{}_0 \geq 1$. This means $\Lambda^0{}_0$ is either ≥ 1 or ≤ -1, and in particular cannot be continuously deformed from one of these categories into the other. Since the identity transformation satisfies $\Lambda^0{}_0 = 1$ it follows that one cannot continuously evolve from the identity transformation to any transformation with $\Lambda^0{}_0 < -1$.

All improper Lorentz transformations can be continuously related to two standard ones. One of these may be chosen to be parity, $\Lambda^\mu{}_\nu = P^\mu{}_\nu = \mathrm{diag}(+1, -1, -1, -1)$ corresponding to the inversion of all spatial coordinates. The other can be chosen to be time-reversal: $T^\mu{}_\nu = \mathrm{diag}(-1, +1, +1, +1)$. Both of these have negative determinant, but only $T^0{}_0$ is ≤ -1.

Connection to standard Lorentz transformations

To make contact between the above definition of Lorentz transformations and those that arise in introductory discussions of Special Relativity, consider the inertial motion of a free particle. Newton's first law states that a particle does not accelerate in the absence of external forces, and so in special relativity the spacetime trajectory (or world-line) of such an inertial particle (on which no forces act) is given by a straight line,

$$x^\mu(\lambda) = c^\mu + v^\mu\,\lambda\,, \tag{11.1.11}$$

where c^μ and v^μ are constant 4-vectors and λ is a parameter that labels the points along the line. For later purposes notice that any such a curve satisfies

$$\frac{\mathrm{d}x^\mu}{\mathrm{d}\lambda} = v^\mu \quad \text{and} \quad \frac{\mathrm{d}^2x^\mu}{\mathrm{d}\lambda^2} = 0\,, \tag{11.1.12}$$

and it is because the tangent vector $\mathrm{d}x^\mu/\mathrm{d}\lambda$ is constant that we know eq. (11.1.11) describes a straight world-line.

The invariant interval measured using the metric (11.1.2) along the trajectory is

$$\mathrm{d}s^2 = \eta_{\mu\nu}\,\frac{\mathrm{d}x^\mu}{\mathrm{d}\lambda}\,\frac{\mathrm{d}x^\nu}{\mathrm{d}\lambda}\,\mathrm{d}\lambda^2 = (v\cdot v)\,\mathrm{d}\lambda^2\,, \tag{11.1.13}$$

so it follows that v^μ must satisfy $v\cdot v = \eta_{\mu\nu}\,v^\mu v^\nu < 0$ for a timelike trajectory (*i.e.* motion with speed less than the speed of light), in which case the vector v^μ is also said to be timelike. (By contrast, for motion at the speed of light — such as for a photon — v^μ would instead be null: $v\cdot v = 0$.)

For motion slower than the speed of light define the proper time, τ, as the distance measured along the trajectory, and since this is negative for time-like trajectories define $\mathrm{d}s^2 = -\mathrm{d}\tau^2$. By definition of the metric this is the time as measured by an observer moving along this trajectory (*i.e.* the trajectory's proper time).

It is convenient to use τ rather than λ as the parameter labelling points along the curve. In this case $u^\mu := \mathrm{d}x^\mu/\mathrm{d}\tau$ is called the 4-velocity of the trajectory, and eq. (11.1.13) then implies $u\cdot u = -1$. Writing its components as

$$\begin{aligned}\frac{\mathrm{d}x^\mu}{\mathrm{d}\tau} = u^\mu &= \left(\frac{\mathrm{d}t}{\mathrm{d}\tau}, \frac{\mathrm{d}x}{\mathrm{d}\tau}, \frac{\mathrm{d}y}{\mathrm{d}\tau}, \frac{\mathrm{d}z}{\mathrm{d}\tau}\right) \\ &= \frac{\mathrm{d}t}{\mathrm{d}\tau}\left(1, \frac{\mathrm{d}x}{\mathrm{d}t}, \frac{\mathrm{d}y}{\mathrm{d}t}, \frac{\mathrm{d}z}{\mathrm{d}t}\right)\,,\end{aligned} \tag{11.1.14}$$

the condition $u\cdot u = -1$ implies $\mathrm{d}t/\mathrm{d}\tau$ satisfies $(\mathrm{d}t/\mathrm{d}\tau)^2(1-\mathbf{v}^2) = 1$, where the velocity 3-vector, $\mathbf{v}$, is defined to have components $v^i = \mathrm{d}x^i/\mathrm{d}t$. We read off from this the *time dilation* that relates the proper time τ to the time t of the observer with respect to which the trajectory has velocity $\mathbf{v}$:

$$\frac{\mathrm{d}t}{\mathrm{d}\tau} := \gamma = \frac{1}{\sqrt{1-\mathbf{v}^2}}\,. \tag{11.1.15}$$

where the condition $\mathrm{d}t/\mathrm{d}\tau > 0$ (*i.e.* both t and τ increase into the future) fixes the sign of the square root used in this expression.

We may now relate the parameter β appearing in a Lorentz boost to the speed, v, of the inertial observers involved, and thereby verify that eq. (11.1.8) describes a standard Lorentz transformation familiar from special relativity. To this end, suppose $\Lambda^\mu{}_\nu$ is the Lorentz boost which transforms from the frame of an observer at rest (and so whose 4-velocity is $u^\mu = (1,0,0,0)$) to the frame of an inertial observer moving with speed v along the x axis (and so whose 4-velocity from (11.1.14) is $u^\mu = (\gamma, \gamma v, 0, 0)$).

Requiring that the Lorentz transformation of eq. (11.1.8) be the one that relates these two 4-velocities gives the parameter β in terms of the speed, v. That is, if

$$\begin{pmatrix} \gamma \\ \gamma v \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \cosh\beta & \sinh\beta & & \\ \sinh\beta & \cosh\beta & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} , \tag{11.1.16}$$

then $\cosh\beta = \gamma$ and $\sinh\beta = \gamma v$, and so $\tanh\beta = v$. Notice that the definition $\gamma = (1-v^2)^{-1/2}$ is then equivalent to the identity $\cosh^2\beta - \sinh^2\beta = 1$. β is sometimes called the *rapidity* of the moving particle.

> **Exercise:** Prove the identity $\Lambda_x(\beta_1)\Lambda_x(\beta_2) = \Lambda_x(\beta_1 + \beta_2)$ for the composition of two boosts along the x axis, as in eq. (11.1.8), and use this to show that the inverse of the matrix $\Lambda_x(\beta)$ is $\Lambda_x^{-1}(\beta) = \Lambda_x(-\beta)$. Use your result with the relation $v/c = \tanh\beta$ to derive the relativistic law for adding velocities: if $\beta = \beta_1 + \beta_2$ then
>
> $$v = \frac{v_1 + v_2}{1 + v_1 v_2/c^2} . \tag{11.1.17}$$

Using this connection between β and v in the relation between the coordinates in these two frames, $x^{\mu'} = \Lambda^{\mu'}{}_{\nu} x^{\nu}$, or

$$\begin{pmatrix} t' \\ x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cosh\beta & \sinh\beta & & \\ \sinh\beta & \cosh\beta & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \begin{pmatrix} t \\ x \\ y \\ z \end{pmatrix} , \tag{11.1.18}$$

leads (temporarily replacing the factors of c) to the familiar expressions

$$t' = \frac{t + vx/c^2}{\sqrt{1 - v^2/c^2}} , \qquad x' = \frac{x + vt}{\sqrt{1 - v^2/c^2}} , \tag{11.1.19}$$

together with $y' = y$ and $z' = z$. The fact that these expressions imply that events sharing a common value for t are not the same as those sharing a common value for t' – *i.e.* the *relativity of simultaneity* — that makes it much more efficient to think in terms of spacetime, rather than space and time separately.

11.1.4 Tensors and covariant laws of motion

Consider two reference frames with coordinates $\{x^{\mu}\}$ and $\{x^{\mu'}\}$ that are related by a Lorentz transformation as in (11.1.4):

$$x^{\mu'} = \Lambda^{\mu'}{}_{\nu}\, x^{\nu} . \tag{11.1.20}$$

Any four quantities whose values in these two different inertial frames are related in the same way as are the coordinates x^μ themselves are called the components of a (contravariant) 4-vector. They are said in special relativity to transform as a 4-vector with respect to Lorentz transformations, which means their components in these two frames are related by

$$V^{\mu'} = \Lambda^{\mu'}{}_{\nu} V^\nu \,. \tag{11.1.21}$$

For example the components of the tangent, $u^\mu = \mathrm{d}x^\mu/\mathrm{d}\tau$, to the trajectory of any moving particle $x^\mu(\tau)$ are the components of a 4-vector provided τ is the proper time measured along the trajectory. The resulting 4-vector is called the particle's instantaneous 4-velocity. By contrast the components $\mathrm{d}x^\mu/\mathrm{d}t$, where t is the time coordinate, do not transform as a 4-vector when one transforms from one inertial frame to another (because, unlike τ, t is not invariant when one changes between inertial observers who move relative to one another).

More generally, physical quantities in different inertial frames in special relativity transform as tensors with respect to Lorentz transformations, which means their components in frames that are related by the transformation matrix $\Lambda^\mu{}_\nu$ are given by

$$T^{\mu'_1 .. \mu'_p}{}_{\lambda'_1 .. \lambda'_q} = T^{\nu_1 .. \nu_p}{}_{\rho_1 .. \rho_q} \left(\Lambda^{\mu'_1}{}_{\nu_1} \cdots \Lambda^{\mu'_p}{}_{\nu_p}\right) \left(\Lambda^{\rho_1}{}_{\lambda'_1} \cdots \Lambda^{\rho_q}{}_{\lambda'_q}\right) . \tag{11.1.22}$$

In particular, if all of the components of a tensor vanish in any particular inertial reference frame then they must also vanish in all other reference frames.

Vectors and tensors are important because if the laws of physics are expressed as a relationship with the schematic form of tensor = tensor, then the tensor transformation rule ensures that if the law is true for any one frame, the same law must be true for all inertial reference frames. In practice the Principle or Relativity is satisfied by demanding physical laws be expressed in terms of Lorentz vectors and Lorentz tensors in this way.

Example: particle kinematics

An example of such a law relates the instantaneous 4-momentum, p^μ, of a particle having rest-mass m to its 4-velocity u^μ, by

$$p^\mu = m \frac{\mathrm{d}x^\mu}{\mathrm{d}\tau} = m\, u^\mu \,. \tag{11.1.23}$$

The components of p^μ define the particle's instantaneous energy, $E = p^0$, and 3-momentum, p^i, and so (using the components for u^μ found in (11.1.14)):

$$p^0 = E = m\,\gamma = \frac{m}{\sqrt{1-v^2}} \qquad \text{and} \qquad p^i = m\,\gamma\, v^i = \frac{m v^i}{\sqrt{1-v^2}} \,. \tag{11.1.24}$$

Because (11.1.23) relates 4-vectors to 4-vectors it is true in any inertial frame, which implies the relations (11.1.24) also hold for the components of p^μ and u^μ in any inertial reference frame.

A second example of a physical relationship involving tensor quantities is the scalar condition $\eta_{\mu\nu}u^\mu u^\nu = -1$, which does not change at all when transforming between reference frames using (11.1.21). Together with (11.1.23) this also implies $\eta_{\mu\nu}p^\mu p^\nu = -m^2$, which is equivalent to the relativistic energy-momentum relation

$$E^2 = \mathbf{p}^2 + m^2 \,. \tag{11.1.25}$$

which must therefore also hold in all inertial frames.

The 4-momentum of a photon is described by the limit of the above as $m \to 0$ (with $\mathrm{d}\tau \to 0$ so that (11.1.23) doesn't imply $p^\mu \to 0$). The components of p^μ remain fixed and well-defined in this limit, and the $\mathrm{d}\tau \to 0$ limit implies that the 4-velocity $\mathrm{d}x^\mu/\mathrm{d}\lambda$ points in a null direction. Because u^μ is no longer time-like it is no longer possible to choose proper time, τ, as the parameter along the world line. The resulting 4-momentum satisfies $\eta_{\mu\nu}p^\mu p^\nu = p_\mu p^\mu = 0$, and so (11.1.25) reduces to $E = |\mathbf{p}|$.

Example: electric current

Conservation of electric charge provides another, more field-theoretic, instructive example of how physical laws can be expressed in terms of Lorentz tensors (if they are relativistic).

If there is an observer who sees a nonzero density of electric charge, $\sigma(x,t)$, then anyone else who moves relative to this observer must see a nonzero electric current density, $\mathbf{j}(x,t)$, in addition to seeing a charge density which is different due to the Lorentz contraction of space in the direction of motion, and due to the change in the relative motion of the moving charges. It follows that σ and $\mathbf{j}$ must transform into one another under Lorentz transformations, and it turns out that they transform as a 4-vector with components:

$$j^\mu = \begin{pmatrix} j^0 = \sigma \\ j^i \end{pmatrix} , \tag{11.1.26}$$

where j^i represent the 3 spatial components of the current density vector, $\mathbf{j}$. Being a 4-vector means that it transforms under a Lorentz transformation as

$$j^{\mu'} = \Lambda^\mu{}_\nu \, j^\nu \,, \tag{11.1.27}$$

and so in the specific case of a boost between inertial observers moving at relative speed $\mathbf{v}$, *c.f.* eqs. (11.1.8) and (11.1.19), this becomes

$$\sigma' = j^{0'} = \frac{\sigma + \mathbf{v}\cdot\mathbf{j}/c^2}{\sqrt{1 - v^2/c^2}} \,, \qquad \mathbf{j}' = \frac{\mathbf{j} + \mathbf{v}\sigma}{\sqrt{1 - v^2/c^2}} \,, \tag{11.1.28}$$

Conservation of electric charge may be expressed in terms of this 4-vector in a manifestly Lorentz-invariant way, as

$$\partial_\mu \, j^\mu = \frac{\partial j^0}{\partial t} + \nabla \cdot \mathbf{j} = 0 \,. \tag{11.1.29}$$

Since the left-hand side is a Lorentz scalar, if any observer finds the right-hand-side vanishes, then all inertial observers must find that it vanishes. That this equation expresses local charge conservation may be seen by integrating it over a volume V having boundary ∂V, and using Gauss' theorem

$$0 = \int_V \left[\frac{\partial j^0}{\partial t} + \nabla\cdot\mathbf{j}\right] \mathrm{d}^3x = \frac{\mathrm{d}}{\mathrm{d}t}\int_V \sigma\,\mathrm{d}^3x + \int_{\partial V} \mathbf{n}\cdot\mathbf{j}\,\mathrm{d}^2S\,, \tag{11.1.30}$$

where d^2S denotes an infinitesimal area element of the surface, whose outward-pointing normal vector is $\mathbf{n}$. Written this way it is clear that charge is conserved, inasmuch as the rate of change of the total charge in any volume V is equal to the net flux of charge carried by the current through the boundaries of V.

Example: electromagnetic fields

Since charges and currents are sources for electric, $\mathbf{E}$, and magnetic, $\mathbf{B}$, fields, these must similarly transform into one another under Lorentz transformations. It turns out that these six quantities transform as the components of an antisymmetric tensor, $F_{\mu\nu} = -F_{\nu\mu}$, according to

$$\begin{pmatrix} F_{00} & F_{01} & F_{02} & F_{03} \\ F_{10} & F_{11} & F_{12} & F_{13} \\ F_{20} & F_{21} & F_{22} & F_{23} \\ F_{30} & F_{31} & F_{32} & F_{33} \end{pmatrix} = \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & B_z & -B_y \\ E_y & -B_z & 0 & B_x \\ E_z & B_y & -B_x & 0 \end{pmatrix}, \tag{11.1.31}$$

which labels the inertial coordinates in the usual way, $x^\mu = \{x^0, x^1, x^2, x^3\} = \{t, x, y, z\}$.

> **Exercise:** Use the transformation properties under Lorentz transformations of a covariant tensor of rank 2 to compute how the components of electric and magnetic fields, $\mathbf{E}$ and $\mathbf{B}$, are related for observers who move relative to one another with constant speed v along the x-axis.

There are two types of fundamental laws in electromagnetism. One of these expresses the forces felt by charges in the presence of electric and magnetic fields, and states that a point charge of magnitude q moving with velocity $\mathbf{v}$ experiences a $U_{em}(1)$Lorentz force of magnitude

$$\mathbf{F} = q\Big(\mathbf{E} + \mathbf{v}\times\mathbf{B}\Big)\,. \tag{11.1.32}$$

The second type of law in electromagnetism relates the properties of the electric and magnetic fields to the distribution of charges and currents that source them, as summarized by Maxwell's equations:

$$\nabla\times\mathbf{E} + \frac{\partial\mathbf{B}}{\partial t} = 0\,, \qquad \nabla\cdot\mathbf{B} = 0 \tag{11.1.33}$$

and

$$\nabla\times\mathbf{B} - \frac{\partial\mathbf{E}}{\partial t} = \mathbf{j}\,, \qquad \nabla\cdot\mathbf{E} = \sigma\,. \tag{11.1.34}$$

Since all inertial observers must agree on the laws of electromagnetism, it should be possible to formulate these in terms of Lorentz tensors like $F_{\mu\nu}$ and j^μ. Indeed, the two source-free Maxwell equation, eqs. (11.1.33), can be written as the combined tensor equation

$$\partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} + \partial_\lambda F_{\mu\nu} = 0\,, \tag{11.1.35}$$

and the two Maxwell equations with sources, eqs. (11.1.34), similarly can be written

$$\partial_\nu F^{\mu\nu} = j^\mu\,. \tag{11.1.36}$$

Notice that the antisymmetry $F^{\mu\nu} = -F^{\nu\mu}$ implies $\partial_\mu\partial_\nu F^{\mu\nu}$ vanishes identically, showing that eq. (11.1.36) would be inconsistent if charge were not conserved, $\partial_\mu j^\mu \neq 0$.

The Lorentz force, eq. (11.1.32), can also be grouped into a force 4-vector,

$$F_\mu = qF_{\mu\nu}u^\nu\,, \tag{11.1.37}$$

where u^ν denotes the 4-velocity of the point charge.

Finally, the connection between $\mathbf{E}$ and $\mathbf{B}$ and the electromagnetic potentials, ϕ and $\mathbf{A}$,

$$\mathbf{B} = \nabla\times\mathbf{A} \qquad \text{and} \qquad \mathbf{E} = -\nabla\phi - \frac{\partial\mathbf{A}}{\partial t}\,, \tag{11.1.38}$$

can be grouped into the single tensor equation

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu\,, \tag{11.1.39}$$

with the *gauge potential 4-vector* defined by $A^\mu = \{A^0, A^i\} = \{\phi, A^i\}$.

> **Exercise:** Verify that eqs. (11.1.32), (11.1.33), (11.1.34) and (11.1.38) follow from eqs. (11.1.37), (11.1.35), (11.1.36) and (11.1.39), together with the definitions of $F_{\mu\nu}$, A_μ and j^μ.

11.2 The Poincaré group in quantum mechanics

So far so good, but how do we implement Special Relativity in quantum mechanics? The idea is to focus on its symmetry formulation since we know how symmetries are implemented in quantum systems. In particular, as described in §8 in quantum mechanics Lorentz transformations should be realized in terms of unitary operators.[40]

That is, suppose there are three inertial observers, O, O' and O'', who are related by Poincaré transformations (Λ, a) and $(\bar\Lambda, \bar a)$. Performing two Poincaré transformations in sequence, $y^\mu = \Lambda^\mu{}_\nu x^\nu + a^\mu$ and $z^\mu = \bar\Lambda^\mu{}_\nu y^\nu + \bar a^\mu$ shows that their net effect is

$$z^\mu = (\bar\Lambda\Lambda)^\mu{}_\nu\, x^\nu + (\bar\Lambda a)^\mu + \bar a^\mu\,. \tag{11.2.1}$$

[40] For aficionados: strictly speaking in quantum mechanics symmetries need only be described by 'ray representations' rather than unitary (or antiunitary) representations, but this distinction turns out not to matter for the Poincaré group.

This defines the Poincaré group's multiplication law.

Suppose now that these three observers characterize a particular physical state by the state vectors $|\psi\rangle$, $|\psi'\rangle$ and $|\psi''\rangle$, respectively. Then because physics is invariant under these transformations there should be unitary (probability preserving) operators $U(\Lambda, a)$ that express the Poincaré transformations in the space of quantum states:

$$|\psi'\rangle = U(\Lambda, a)\psi\rangle \quad \text{and} \quad |\psi''\rangle = U(\bar{\Lambda}, \bar{a})|\psi'\rangle = U(\bar{\Lambda}, \bar{a})U(\Lambda, a)|\psi\rangle\,. \tag{11.2.2}$$

This representation of the group should in particular express the above composition law for successive transformations, so $U(\Lambda, a)$ should satisfy:

$$U(\bar{\Lambda}, \bar{a})U(\Lambda, a) = U(\bar{\Lambda}\Lambda, \bar{\Lambda}a + \bar{a})\,. \tag{11.2.3}$$

We take, by convention, $U(1, 0) = I$ to be the unit operator.

It is convenient to first consider proper transformations, and in particular start with those that differ infinitesimally from the identity: $\Lambda^\mu{}_\mu = \delta^\mu_\nu + \omega^\mu{}_\nu + \cdots$ and $a^\mu = \epsilon^\mu + \cdots$. Expanding the corresponding operators $U(\Lambda, a)$ then defines the hermitian generators for Lorentz transformations, $J^{\mu\nu}$, and for translations, P^μ, by:

$$U(1 + \omega, \epsilon) = I + \frac{i}{2}\omega_{\mu\nu}J^{\mu\nu} + i\epsilon_\mu P^\mu + \cdots\,, \tag{11.2.4}$$

where the ellipsis denotes terms with higher powers of the parameters ω and ϵ. Because the infinitesimal version of the condition $\Lambda^\mu{}_\alpha\Lambda^\nu{}_\beta\eta^{\alpha\beta} = \eta^{\mu\nu}$ implies $\omega_{\mu\nu} = \eta_{\mu\lambda}\omega^\lambda{}_\nu = -\omega_{\nu\mu}$, this also implies the antisymmetry of the Lorentz generators: $J^{\mu\nu} = -J^{\nu\mu}$.

The group composition law (11.2.3) implies the generators P^μ and $J^{\mu\nu}$ satisfy a particular set of commutation relations. Sandwiching (11.2.4) between $U(\Lambda, a)$ on the left and $U^{-1}(\Lambda, a)$ on the right gives

$$\begin{aligned}
I + \frac{i}{2}\omega_{\mu\nu}\Big[U(\Lambda, a)J^{\mu\nu}U^{-1}(\Lambda, a)\Big] + i\epsilon_\mu\Big[U(\Lambda, a)P^\mu U^{-1}(\Lambda, a)\Big] + \cdots \\
&= U(\Lambda, a)\left[I + \frac{i}{2}\omega_{\mu\nu}J^{\mu\nu} + i\epsilon_\mu P^\mu + \cdots\right]U^{-1}(\Lambda, a) \\
&= U(\Lambda, a)U(1 + \omega, \epsilon)U^{-1}(\Lambda, a) \\
&= U(1 + \Lambda\omega\Lambda^{-1}, \Lambda\epsilon - \Lambda\omega\Lambda^{-1}a) \\
&= I + \frac{i}{2}\Lambda_\mu{}^\alpha\Lambda_\nu{}^\beta\omega_{\alpha\beta}J^{\mu\nu} + i(\Lambda_\mu{}^\nu\epsilon_\nu - \Lambda_\mu{}^\alpha\Lambda_\nu{}^\beta\omega_{\alpha\beta}a^\nu)P^\mu + \cdots
\end{aligned} \tag{11.2.5}$$

and so comparing the coefficients of $\omega_{\mu\nu}$ and ϵ_μ on both sides of this last equation gives

$$\begin{aligned}
U(\Lambda, a)J^{\mu\nu}U^{-1}(\Lambda, a) &= \Lambda_\alpha{}^\mu\Lambda_\beta{}^\nu(J^{\alpha\beta} - P^\alpha a^\beta + P^\beta a^\alpha) \\
\text{and} \quad U(\Lambda, a)P^\mu U^{-1}(\Lambda, a) &= \Lambda_\alpha{}^\mu P^\alpha\,.
\end{aligned} \tag{11.2.6}$$

Specializing to infinitesimal (Λ, a) finally gives the Poincaré algebra

$$\begin{aligned} \Big[J^{\mu\nu}, J^{\rho\lambda}\Big] &= -iJ^{\mu\lambda}\eta^{\rho\nu} + iJ^{\nu\lambda}\eta^{\rho\mu} - iJ^{\nu\rho}\eta^{\lambda\mu} + iJ^{\mu\rho}\eta^{\lambda\nu} \\ \Big[P^{\mu}, J^{\nu\lambda}\Big] &= -i\eta^{\mu\nu}P^{\lambda} + i\eta^{\mu\lambda}P^{\nu} \quad \text{and} \quad \Big[P^{\mu}, P^{\nu}\Big] = 0\,. \end{aligned} \tag{11.2.7}$$

These equations already say something important: even though the Poincaré group is a symmetry, its representation in terms unitary operators *cannot* commute with the system Hamiltonian. It cannot do so because the Hamiltonian is itself one of the symmetry generators: $P^0 = H$, because it generates time translations. Eqs. (11.2.7) then shows that the Poincaré group multiplication law forbids P^μ from commuting with the Lorentz generators $J^{\mu\nu}$. They cannot commute because the commutator of $J^{\mu\nu}$ with P^μ simply expresses that P^μ transforms under Lorentz transformations like a 4-vector. This also fits with what we know from introductory relativity: the energy measured by different inertial observers is observer-dependent because changing reference frames also changes a particle's energy.

But if $U(\Lambda)HU^{-1}(\Lambda) \neq H$ what do we mean by the statement that Lorentz transformations are a symmetry? We take this to mean that $U(\Lambda)$ must commute with the S matrix: $\mathcal{S} = \lim_{T\to\infty} e^{-iHT}$, as defined back in eq. (3.2.22). That is, if $|\psi\rangle_{\rm out} = \mathcal{S}|\psi\rangle_{\rm in}$ and $|\phi\rangle_{\rm out} = \mathcal{S}|\phi\rangle_{\rm in}$ and $|\psi\rangle_{\rm in} = U(\Lambda)|\phi\rangle_{\rm in}$ then it follows that $|\psi\rangle_{\rm out} = U(\Lambda)|\phi\rangle_{\rm out}$. Commuting with $\mathcal{S}$ is a weaker condition than is commuting with H. When push comes to shove, in later sections the quest to find a Lorentz invariant quantum theory is taken in practice to mean we seek a theory whose $\mathcal{S}$ matrix satisfies

$$U(\Lambda)\,\mathcal{S}\,U^{-1}(\Lambda) = \mathcal{S} \quad \text{and so} \quad \Big[U(\Lambda)\,, S\Big] = 0. \tag{11.2.8}$$

11.2.1 Particle States

As usual, the infinitesimal versions of the unitary operators that represent Poincaré symmetry in quantum mechanics provide a natural collection of hermitian operators that can be used as observables to label states. In particular, we know we can diagonalize all of the P^μ's simultaneously since they mutually commute among themselves. Since the corresponding symmetries are translations in time and space this corresponds to choosing states to be eigenstates of energy $H = P^0$ and momentum P^i. Choose, therefore states $|k, \sigma\rangle$, such that

$$P^\mu|k,\sigma\rangle = k^\mu|k,\sigma\rangle\,. \tag{11.2.9}$$

In general σ could label all of the other degrees of freedom required to pin down the state more precisely. A special role is played in many situations by 'point particles', which can be defined to be any states for which no internal structure is relevant for the questions being asked, allowing them to be characterized using only the centre-of mass and rigid-body motion (*i.e.* by their momentum and spin). The absence of extra labels beyond these for such states means they should be described in quantum mechanics by representations of the Poincaré

group that are irreducible. The goal now is to find what these irreducible representations look like for the Poincaré group.

Given any state $|k,\sigma\rangle$ one can always produce a state with eigenvalue $\Lambda^\mu{}_\nu k^\nu$ by applying $U(\Lambda) = U(\Lambda, 0)$, since, using (11.2.6):

$$\begin{aligned} P^\mu(U(\Lambda)|k,\sigma\rangle) &= U(\Lambda)\Big[U^{-1}(\Lambda)P^\mu U(\Lambda)\Big]|k,\sigma\rangle = U(\Lambda)(\Lambda^{-1})_\nu{}^\mu P^\nu|k,\sigma\rangle \\ &= \Lambda^\mu{}_\nu k^\nu (U(\Lambda)|k,\sigma\rangle). \end{aligned} \tag{11.2.10}$$

For physical states we require that the eigenvalue, k^μ, be one of three options:

1. $k^\mu = 0$,
2. k^μ timelike and future-directed, so that $k^2 = k^\mu k_\mu < 0$ and sign $k^0 > 0$, or
3. k^μ null and future-directed, so that $k^2 = 0$ and sign $k^0 > 0$.

Option (1) could be what happens for the no-particle state $|0\rangle$, and in this case the Poincaré group is represented trivially with $U = I$ for all group elements. Option (2) corresponds to a massive particle that moves more slowly than at light speed, while option (3) describes massless particles that move at the speed of light. We consider each of these last two in turn in what follows.

The action of Poincaré transformations on massive and massless particles is described in more detail in Appendix B, where the strategy used is to identify a standard form for k^μ and to first find representations of the subgroup of transformations (the so-called 'little' group) that preserve this standard form. Then all other momentum states are found by applying the remaining transformations that do not preserve the standard form, but these do not introduce any new representation labels beyond the momentum itself.

Massive particles

Massive particles are those whose four-momentum is timelike and future-directed, so $k \cdot k = -m^2 < 0$ and $k^0 > 0$. For any such a state it is always possible to perform a Lorentz transformation that brings k^μ into the standard form, conventionally chosen to be the rest frame, for which

$$k^0 = m > 0 \quad \text{and} \quad \mathbf{k} = 0\,. \tag{11.2.11}$$

The mass parameter m^2 can be used to label states since it is an eigenvalue of the operator $\eta_{\mu\nu}P^\mu P^\nu$, and this commutes with all of the Poincaré generators. Any other momentum, p^μ, is related to the standard momentum by a specific Lorentz transformation, $p^\mu = L^\mu{}_\nu(\mathbf{p}/m)k^\nu$, whose detailed form is given in Appendix B.

The 'little' group of proper Lorentz transformations that preserve this standard form for k^μ is simply the group of rotations in 3-dimensional space: $\Lambda^i{}_j = R^i{}_j$, $\Lambda^0{}_i = \Lambda^i{}_0 = 0$, and $\Lambda^0{}_0 = 1$, with $R^T R = 1$ and $\det R = 1$. States with $p^\mu = k^\mu$ must therefore fall into

unitary representations of this group, which are known from standard quantum mechanics courses to be labelled by an angular momentum quantum number j, where $2j$ is an integer. There are then $2j+1$ states at fixed k^μ that can be labelled by a quantum number $\sigma = -j, -j+1, \cdots, j-1, j$ and the action of any rotation in the little group is given by

$$U(R)|k,\sigma\rangle = \sum_{\sigma'} D^{(j)}_{\sigma',\sigma}(R)|k,\sigma'\rangle \tag{11.2.12}$$

where $D^{(j)}(R_1)$ are the explicit $(2j+1)\times(2j+1)$ matrices given in Appendix B. The angular momentum generators $J_i = \frac{1}{2}\epsilon_{ijk}J^{jk}$ that generate these rotations are represented on the states in the standard way for angular momentum in quantum mechanics:

$$\begin{aligned} [J_3]_{\sigma'\sigma} &= \sigma\delta_{\sigma'\sigma} \\ [J_1 \pm iJ_2]_{\sigma'\sigma} &= \sqrt{(j\mp\sigma)(j\pm\sigma+1)}\,\delta_{\sigma',\sigma\pm1} \\ \left[\mathbf{J}^2\right]_{\sigma'\sigma} &= j(j+1)\delta_{\sigma'\sigma}\,, \end{aligned} \tag{11.2.13}$$

which shows that the eigenvalue of total spin is $j(j+1)$ and σ is the eigenvalue of J_3.

The representations of massive particles are therefore labelled by the particle mass, m, and total spin, j, and there are $2j+1$ spin states for each p^μ that are conventionally chosen to diagonalize J_3 in the particle rest frame. The Appendix shows how to compute explicitly the action of an arbitrary Poincaré transformation in terms of these quantum numbers, leading to the general Lorentz transformation rule

$$U(\Lambda)|p,\sigma\rangle = \sqrt{\frac{\varepsilon(\Lambda\mathbf{p})}{\varepsilon(\mathbf{p})}}\sum_{\sigma'} D^{(j)}_{\sigma'\sigma}[W(\Lambda,\mathbf{p}/m)]|\Lambda p,\sigma'\rangle \tag{11.2.14}$$

where $W(\Lambda,p)$ is a specific type of 'little'-group rotation (called a Wigner rotation) that is constructed from $\Lambda^\mu{}_\nu$ and p^μ along the lines given in Appendix B. The factor $\sqrt{\varepsilon(\Lambda\mathbf{p})/\varepsilon(\mathbf{p})}$ appearing here might appear unusual, but arises because the momentum states are assumed to be normalized in the standard way: $\langle\mathbf{p}|\mathbf{q}\rangle = \delta^3(\mathbf{p}-\mathbf{q})$ (rather than normalizaing these states in an energy-dependent way to make the inner product more covariant).

Massless Particles

Massless particles correspond to states associated with future-directed null 4-vectors, $p\cdot p = 0$ and $p^0 > 0$. It is impossible to transform to a rest frame for such a momentum, but it is always possible to obtain such a 4-momentum by Lorentz-transforming a standard form

$$k^0 = k^3 = \kappa > 0 \quad \text{and} \quad k^1 = k^2 = 0\,. \tag{11.2.15}$$

The little group that preserves this form turns out to consist of a 3-parameter subset of Lorentz transformations consisting of a 2-parameter combination of boosts,[41] $S(a,b)$, com-

[41] See (C.2.15) for an explicit expression for $S(a,b)$.

bined with a rotation,

$$R(\theta) = \begin{pmatrix} 1 & & & \\ & \cos\theta & -\sin\theta & \\ & \sin\theta & \cos\theta & \\ & & & 1 \end{pmatrix} \tag{11.2.16}$$

about the 3-axis along which k^μ points.

It turns out that the only finite-dimesional representations of this little group represents $S(a,b)$ trivially (as the unit matrix) and represents the rotation $R(\theta)$ by a phase

$$U[R(\theta)]|k,\lambda\rangle = e^{i\lambda\theta}|k,\lambda\rangle\,, \tag{11.2.17}$$

where λ (with 2λ an integer) is the eigenvalue of the component of angular momentum in the 3-direction along which k^μ points. The eigenvalue, λ, of angular momentum in the direction of motion is called the massless particle's *helicity*, and (unlike for massive particles) only a single value of λ is required in an irreducible representation.

11.2.2 Parity and Time Reversal

The only Poincaré transformations whose action on particle states is not completely governed by the representations of the infinitesimal generators P^μ and $J^{\mu\nu}$ are those that are improper, because they cannot be obtained in a continuous way from the identity transformation. But because any improper Lorentz transformation can be written as a product of a proper Lorentz transformation with either parity or time-reversal or both, it suffices to specify how parity and time-reversal are represented in order to completely specify the action of any Poincaré transformation.

Recall that the parity and time-reversal Lorentz transformation matrices ${\Lambda^\mu}_\nu$ are given explicitly by

$${P^\mu}_\nu = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \quad \text{and} \quad {T^\mu}_\nu = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}. \tag{11.2.18}$$

Denote the representations of these two transformation in the quantum Hilbert space by $\mathcal{P} := U(P,0)$ and $\mathcal{T} := U(T,0)$. Not being continuously related to the identity, $\mathcal{P}$ or $\mathcal{T}$ may *a-priori* either be unitary or anti-unitary. We now show that $\mathcal{P}$ is represented by a unitary transformation while $\mathcal{T}$ must be represented by an anti-unitary one.

To determine which, go back to the group composition rule (11.2.6) for $U(\Lambda,a)$, which implies:

$$U(\Lambda,0) iP^\mu U^{-1}(\Lambda,0) = {\Lambda_\nu}^\mu iP^\nu \tag{11.2.19}$$

for any Lorentz transformation, Λ. It follows from this that

$$U(\Lambda,0) P^\mu U^{-1}(\Lambda,0) = \pm{\Lambda_\nu}^\mu P^\nu \tag{11.2.20}$$

where the upper (lower) sign applies if U is linear (antilinear). Consider, in particular, the energy, $P^0 = H$, for which the above becomes

$$\mathcal{P}H\mathcal{P}^{-1} = \pm P_0{}^0 H = \pm H \quad \text{and} \quad \mathcal{T}H\mathcal{T}^{-1} = \pm T_0{}^0 H = \mp H. \tag{11.2.21}$$

Now comes the main point. Since stability of the ground state require H must have a spectrum bounded from below, all symmetry operations must respect its sign. But this is only possible if $\mathcal{P}$ is unitary and $\mathcal{T}$ is anti-unitary. With these choices the transformation properties of the spatial components of P^μ are determined, and become

$$\mathcal{P}\mathbf{P}\mathcal{P}^{-1} = -\mathbf{P} \quad \text{and} \quad \mathcal{T}\mathbf{P}\mathcal{T}^{-1} = -\mathbf{P}\,. \tag{11.2.22}$$

An identical argument starting from the combination $U(\Lambda) i J^{\mu\nu} U^{-1}(\Lambda) = \Lambda_\alpha{}^\mu \Lambda_\beta{}^\nu i J^{\alpha\beta}$ similarly implies that the components of angular momentum, $J_i = \frac{1}{2}\epsilon_{ijk} J^{jk}$, satisfy

$$\mathcal{P}\mathbf{J}\mathcal{P}^{-1} = +\mathbf{J} \quad \text{and} \quad \mathcal{T}\mathbf{J}\mathcal{T}^{-1} = -\mathbf{J}. \tag{11.2.23}$$

These relations are needed to establish the effect of $\mathcal{P}$ and $\mathcal{T}$ on particle states, as is now done for massive and massless particles in turn.

Massive Multiplets

In the rest frame the momentum $k^\mu = (M, 0, 0, 0)$ is left unchanged by both $\mathcal{P}$ and $\mathcal{T}$. The action of the discrete symmetries on $\mathbf{J}$ then implies

$$\mathcal{P}|k,\sigma\rangle = \eta_{p,\sigma}|k,\sigma\rangle \quad \text{and} \quad \mathcal{T}|k,\sigma\rangle = \eta_{t,\sigma}|k,-\sigma\rangle \tag{11.2.24}$$

where η_p and η_t are phases that might depend on σ.

The σ-dependence is determined by demanding consistency with the action of the angular-momentum raising and lowering operators $J_\pm = J_1 \pm i J_2$. Acting on the relation

$$J_\pm|k,\sigma\rangle = \sqrt{(j \mp \sigma)(j \pm \sigma + 1)}\,|k,\sigma \pm 1\rangle \tag{11.2.25}$$

on both sides with $\mathcal{P}$ gives

$$\begin{aligned}
\sqrt{(j \mp \sigma)(j \pm \sigma + 1)}\,\eta_{p,\sigma\pm1}|k,\sigma\pm1\rangle &= \sqrt{(j \mp \sigma)(j \pm \sigma + 1)}\,\mathcal{P}|k,\sigma\pm1\rangle \\
&= \mathcal{P}J_\pm|k,\sigma\rangle = (\mathcal{P}J_\pm\mathcal{P}^{-1})\mathcal{P}|k,\sigma\rangle \\
&= J_\pm\mathcal{P}|k,\sigma\rangle = \sqrt{(j \mp \sigma)(j \pm \sigma + 1)}\,\eta_{p,\sigma}|k,\sigma\pm1\rangle
\end{aligned} \tag{11.2.26}$$

which implies[42] η_p must be independent of σ.

The identical argument for time-reversal uses

$$\mathcal{T}J_\pm\mathcal{T}^{-1} = \mathcal{T}(J_1 \pm i J_2)\mathcal{T}^{-1} = -(J_1 \pm (-i) J_2) = -J_\mp\,, \tag{11.2.27}$$

[42] This result is independent of the phase conventions assumed for the action of $J_\pm$ because $\mathcal{P}$ is unitary.

and so therefore

$$\begin{aligned}\sqrt{(j\mp\sigma)(j\pm\sigma+1)}\eta_{t,\sigma\pm1}|k,-(\sigma\pm1)\rangle &= \sqrt{(j\mp\sigma)(j\pm\sigma+1)}\mathcal{T}|k,\sigma\pm1\rangle \\ &= \mathcal{T}J_\pm|k,\sigma\rangle = (\mathcal{T}J_\pm\mathcal{T}^{-1})\mathcal{T}|k,\sigma\rangle \\ &= -J_\mp\mathcal{T}|k,\sigma\rangle = -\sqrt{(j\mp\sigma)(j\pm\sigma+1)}\eta_{t,\sigma}|k,-\sigma\mp1\rangle.\end{aligned} \tag{11.2.28}$$

This shows that the time-reversal phase satisfies: $\eta_{t,\sigma\pm1} = -\eta_{t,\sigma}$. This is a finite-difference equation whose solution is

$$\eta_{t,\sigma} = (-)^{j-\sigma}\eta_t\,, \tag{11.2.29}$$

where the conventional additional factor of $(-)^j$ is chosen to ensure that the exponent is an integer even for half-integer spins.

In summary, the action of $\mathcal{P}$ and $\mathcal{T}$ for states in the massive-particle rest-frame is

$$\mathcal{P}|k,\sigma\rangle = \eta_p|k,\sigma\rangle \quad \text{and} \quad \mathcal{T}|k,\sigma\rangle = \eta_t(-)^{j-\sigma}|k,-\sigma\rangle\,. \tag{11.2.30}$$

This can be extended to a state with general momentum by using the transformation properties (11.2.22) which imply

$$\mathcal{P}|\mathbf{p},\sigma\rangle = \eta_p|-\mathbf{p},\sigma\rangle \quad \text{and} \quad \mathcal{T}|\mathbf{p},\sigma\rangle = \eta_t(-)^{j-\sigma}|-\mathbf{p},-\sigma\rangle. \tag{11.2.31}$$

Many-particle states transform similarly, with the phase η being the product of the phases for each of its constituent single-particle states.

Because $\mathcal{P}$ is unitary, $\mathcal{P}H\mathcal{P}^{-1} = H$ and so $\mathcal{P}$ commutes with H. This ensures that parity-invariance implies a multiplicative conservation law — conservation of parity. There is no similarly conservation law for time-reversal because $\mathcal{T}$ is an anti-unitary operator. Because of this the phase η_t cannot be unambiguously defined for an entire ray within the quantum Hilbert space, and this keeps the existence of Time-Reversal Symmetry from leading to a conservation law. Time reversal invariance does, however, impose conditions on the S-matrix however since it requires it to be symmetric: $S = S^T$.

Some general constraints on parity quantum numbers also follow from the observation that the matrix $P^\mu{}_\nu$ satisfies $P^2 = 1$. This does *not* necessarily imply that the unitary operator, $\mathcal{P}$, must also square to one, however. All that must happen is $\mathcal{P}^2$ must be a (non-spacetime) symmetry of the system. In most cases of interest all multiplicative symmetries of the theory are subgroups of some continuous symmetry, of the generic form e^{iq}. In this case it is always possible to define their square root $e^{iq/2}$. Whenever this is true suppose that $\mathcal{P}^2 = Q$ and $\sqrt{Q}$ exists. We may then always redefine $\mathcal{P}$ to:

$$\mathcal{P}' \equiv Q^{-1/2}\mathcal{P} \text{ so } \mathcal{P}'^2 = 1\,, \tag{11.2.32}$$

and so whenever this is possible one can ensure $\eta_p^2 = 1$ so $\eta_p = \pm1$.

There are cases when such a choice is impossible, however. This occures, for instance, in theories with majorana fermions where it often is the case that $\mathcal{P}^2 = (-)^F$, where F is the fermion number. Since $e^{iF\theta}$ is not consistent with the majorana character of the fermions unless $\theta = 0$ or π, the square-root of $(-)^F = e^{i\pi F}$ cannot be defined. This precludes a redefinition of $\mathcal{P}$ to make it square to unity. In this case we have $\eta_p = \pm 1$ for bosons but $\eta_p = \pm i$ for fermions.

Massless Multiplets

For massless particles the standard frame is $k^\mu = (\kappa, 0, 0, \kappa)$, and neither parity or time-reversal preserve this standard four-vector. $T^\mu{}_\nu$ and $P^\mu{}_\nu$ do preserve this standard momentum however if combined with the following 180^o rotation about the 1-axis

$$R^\mu{}_\nu = \begin{pmatrix} +1 & & & \\ & +1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} . \tag{11.2.33}$$

As a result the combination $U(R)\mathcal{T}$ and $U(R)\mathcal{P}$ should be represented within the little group that preserves the form of k^μ. Since each Poincaré representation is characterized by a unique value for helicity λ, any dependence of η_t or η_p on λ is irrelevant. Using the relations

$$U(R)\mathcal{P}J_3\mathcal{P}^{-1}U^{-1}(R) = U(R)J_3U^{-1}(R) = -J_3 \tag{11.2.34}$$

and

$$U(R)\mathcal{T}J_3\mathcal{T}^{-1}U^{-1}(R) = -U(R)J_3U^{-1}(R) = +J_3\,, \tag{11.2.35}$$

it follows that for states in the standard frame

$$U(R)\mathcal{P}|k,\lambda\rangle = \eta_p|k,-\lambda\rangle \quad \text{and} \quad U(R)\mathcal{T}|k,\lambda\rangle = \eta_t|k,\lambda\rangle. \tag{11.2.36}$$

Because it flips the sign of the eigenvalue of J_3 (helicity), parity cannot be represented in the Hilbert space of a single massless particle. In a parity-invariant theory, therefore, massless particles must come in pairs with opposite helicities. Although time-reversal can be represented on state vectors representing massless particles, as for massive particles it cannot be unambiguously extended to a transformation among rays and so does not furnish a conserved quantum number.

11.3 Relativistic fields

The previous section shows that particle states within relativistic theories form representations of the Poincaré symmetry group that are labelled by their mass, m, and spin, j. Poincaré transformations $(\Lambda^\mu{}_\nu, a^\lambda)$ are represented in the quantum Hilbert space in terms of unitary operators $U(\Lambda, a)$ that act within these representations by changing the particle momentum

and spin labels $(\mathbf{p}, \sigma)$, in the way specified in detail in Appendix B. For massive particles the state label σ here represents the rest-frame z-component of angular momentum, while for massless particles it instead represents helicity.

But we would also like to be able to identify more constructively the circumstances under which these symmetries exist, such as by identifying what properties a system's Hamiltonian must have in order for Poincaré invariance to occur. To this end we have also seen, in §6, that the requirement of locality suggests that the Hamiltonian should be local (*i.e.* arise as the integral over space of a local Hamiltonian density), and that this observation requires creation and annihilation operators to appear within H only through local position-dependent fields of the general (interaction-picture) form

$$A_n(\mathbf{x}, t) = \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}} \; u_n(\mathbf{p}, \sigma) \, \mathfrak{a}_{\mathbf{p}\sigma} \; e^{-i\varepsilon(p)t + i\mathbf{p}\cdot\mathbf{x}} \,, \tag{11.3.1}$$

where $\varepsilon(p)$ denote the single-particle energies and the label n might run over a collection of fields (such as the components of electric or magnetic fields, $\mathbf{E}$ or $\mathbf{B}$, for example) for some coefficients functions $u_n(\mathbf{p}, \sigma)$.

The requirements of Poincaré invariance impose two conditions on such fields. The simplest condition is that Lorentz invariance implies the energy-momentum dispersion relation must satisfy (11.1.25), and so $\varepsilon(p) = \sqrt{\mathbf{p}^2 + m^2}$. It is also convenient to combine $\varepsilon(p)$ and $\mathbf{p}$ into a single 4-vector p^μ with $p^0 = \varepsilon(p)$, in which case the argument of the exponential is conveniently written $-i\varepsilon(p)t + \mathbf{p}\cdot\mathbf{x} = \eta_{\mu\nu} p^\mu x^\nu =: p \cdot x$.

There is also a second condition though, on the coefficient functions $u_n(\mathbf{p}, \sigma)$, which are most usefully chosen so that the field operator $A_n(\mathbf{x}, t)$ transforms *linearly* under Lorentz transformations so that $U(\Lambda) A_n(x) U^*(\Lambda)$ is a linear combination of the $A_n(\Lambda x)$'s evaluated at the transformed position $(\Lambda x)^\mu = \Lambda^\mu{}_\nu x^\nu$. When this is possible the result can be written more explicitly as

$$U(\Lambda) A_n(x) U^*(\Lambda) = \sum_m D_{nm}(\Lambda^{-1}) A_m(\Lambda x) \,, \tag{11.3.2}$$

for some choice of finite-dimensional matrices D_{mn}. This kind of transformation rule is useful because it makes the invariance properties of the theory more explicit and so easier to see. This section argues (with some of the details given in Appendix C.1) that condition (11.3.2) is actually very restrictive: once the particle spin and the matrices D_{mn} are chosen it completely determines the form of $u_n(\mathbf{p}, \sigma)$ up to normalization.

Performing a sequence of Lorentz transformations shows that the matrices, D_{mn}, must satisfy the same group multiplication law as do the unitary operators $U(\Lambda)$. That is to say, the D_{mn}'s furnish a finite-dimensional representation of the Lorentz group. To see why use the fact that $U(\Lambda_1) U(\Lambda_2) = U(\Lambda_1 \Lambda_2)$ two write two equivalent ways to express the operation

of two Lorentz transformations on $A_m(x)$:

$$\begin{aligned} U(\Lambda_1\Lambda_2)A_n(x)U^{-1}(\Lambda_1\Lambda_2) &= U(\Lambda_1)U(\Lambda_2)A_n(x)U^*(\Lambda_2)U^{-1}(\Lambda_1) \\ &= \sum_m D_{nm}(\Lambda_2^{-1})U(\Lambda_1)A_m(\Lambda_2 x)U^*(\Lambda_1) \\ &= \sum_{m\ell} D_{nm}(\Lambda_2^{-1})D_{m\ell}(\Lambda_1^{-1})A_\ell(\Lambda_1\Lambda_2 x). \\ &= \sum_\ell D_{n\ell}(\Lambda_2^{-1}\Lambda_1^{-1})A_\ell(\Lambda_1\Lambda_2 x). \end{aligned} \tag{11.3.3}$$

Since this must hold for any Lorentz matrices, consistency of these two expressions requires

$$\sum_\ell D_{n\ell}(\Lambda_1^{-1})D_{\ell m}(\Lambda_2^{-1}) = D_{nm}(\Lambda_1^{-1}\Lambda_2^{-1})\,, \tag{11.3.4}$$

and so the D_{nm}'s therefore furnish a representation of the Lorentz group, as claimed. This argument also shows why eq. (11.3.2) involves $D_{nm}(\Lambda^{-1})$ rather than $D_{nm}(\Lambda)$. It does so in order to ensure that the D's represent group multiplication in the conventional order: $D(\Lambda_1)D(\Lambda_2) = D(\Lambda_1\Lambda_2)$ as opposed to $D(\Lambda_2\Lambda_1)$.

If only a finite number of fields are used to represent each type of particle then the representation furnished by the D_{mn}'s must also be finite-dimensional. For the Lorentz group this means in particular that there is a theorem that states that they cannot be unitary, since faithful unitary representations of the Lorentz group cannot be finite-dimensional. Happily all of the finite-dimensional representations of the Lorentz group are known, with the general classification given in (B.2). This section works through a few special cases of the implications of (11.3.2), and then closes by quoting the main consistency results for the $u_n(\mathbf{p},\sigma)$ that apply in the general case.

11.3.1 Scalar fields

The simplest finite-dimensional Lorentz representation is the trivial one-dimensional one. In this case there is only a single real field and so the matrices $D_{mn}(\Lambda)$ degenerate into a number, that can be chosen to be 1 for all Λ. In this case the linear transformation rule (11.3.2) becomes

$$U(\Lambda)A(x)\,U^{-1}(\Lambda) = A(\Lambda x)\,. \tag{11.3.5}$$

A field that transforms in this way under Lorentz transformations is called a scalar field.

What does this transformation law say about the coefficient function $u(\mathbf{p},\sigma)$ that is allowed when $\mathbf{A}(x)$ is written as

$$A(x) = \sum_\sigma \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\; u(\mathbf{p},\sigma)\,\mathfrak{a}_{\mathbf{p}\sigma}\; e^{ip\cdot x}\,, \tag{11.3.6}$$

in terms of creation and annihilation operators? It turns out to say a lot because, on one hand $U(\Lambda)\,A(x)\,U^{-1}(\Lambda)$ acts according to the rule (11.3.7), and so

$$U(\Lambda)A(x)\,U^{-1}(\Lambda) = A(\Lambda x) = \sum_{\sigma}\int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\; u(\mathbf{p},\sigma)\,\mathfrak{a}_{\mathbf{p}\sigma}\;e^{ip\cdot\Lambda x}\,. \tag{11.3.7}$$

But on the other hand $U(\lambda)\,a_{\mathbf{p}\sigma}U^{-1}(\Lambda)$ can be independently evaluated given that the transformation rule (11.2.14) that specifies how the quantum states created by $\mathfrak{a}^\star_{\mathbf{p}\sigma}$ transform implies

$$U(\Lambda)\;\mathfrak{a}^\star_{\mathbf{p}\sigma}U^{-1}(\Lambda) = \sqrt{\frac{\varepsilon(\Lambda\mathbf{p})}{\varepsilon(\mathbf{p})}}\sum_{\sigma'} D^{(j)}_{\sigma'\sigma}[W(\Lambda,\mathbf{p}/m)]\;\mathfrak{a}^\star_{\Lambda\mathbf{p}\sigma'}\,, \tag{11.3.8}$$

and so

$$U(\Lambda)\;\mathfrak{a}_{\mathbf{p},\sigma}U^{-1}(\Lambda) = \sqrt{\frac{\varepsilon(\Lambda\mathbf{p})}{\varepsilon(\mathbf{p})}}\sum_{\sigma'} D^{(j)*}_{\sigma'\sigma}[W(\Lambda,\mathbf{p}/m)]\;\mathfrak{a}_{\Lambda\mathbf{p},\sigma'}\,, \tag{11.3.9}$$

and this means

$$\begin{aligned} U(\Lambda)A_n(x)U^{-1}(\Lambda) &= \sum_{\sigma}\int \mathrm{d}^3p\; u(\mathbf{p},\sigma)\Big[U(\Lambda)\;\mathfrak{a}_{\mathbf{p},\sigma}U^{-1}(\Lambda)\Big]\;e^{ip\cdot x} \\ &= \sum_{\sigma\sigma'}\int \mathrm{d}^3p\,\sqrt{\frac{\varepsilon(\Lambda\mathbf{p})}{\varepsilon(\mathbf{p})}}\;\mathfrak{a}_{\Lambda\mathbf{p},\sigma'}D^{(j)*}_{\sigma'\sigma}\,[W(\Lambda,\mathbf{p}/m)]\,u_n(\mathbf{p},\sigma)\;e^{ip\cdot x}\,. \end{aligned} \tag{11.3.10}$$

Comparing this with (11.3.7) then implies the desired condition on $u(\mathbf{k},\sigma)$:

$$\sum_{\sigma} D^{(j)*}_{\sigma'\sigma}\,[W(\Lambda,\mathbf{p}/m)]\,u(\mathbf{p},\sigma) = \sqrt{\frac{\varepsilon(\Lambda\mathbf{p})}{\varepsilon(\mathbf{p})}}\;u(\Lambda\mathbf{p},\sigma'). \tag{11.3.11}$$

This relation is the principal result that governs the form of $u(\mathbf{p},\sigma)$, and Appendix C.1.2 is devoted to solving it for the unknown functions $u(\mathbf{k},\sigma)$ for different choices for particle spin. The general solution obtained turns out to be quite simple to state:

- For any $j \neq 0$ the only solution is $u(\mathbf{p},\sigma) = 0$, which is to say that a scalar field can only be consistently chosen to represent spinless particles in a Poincaré invariant theory.
- For $j = 0$ the matrix $D^{(j)}$ becomes trivial and the solution $u(\mathbf{p}) \propto [\varepsilon(\mathbf{p})]^{-1/2}$ is then unique up to normalization.

Using the conventional normalization choice this implies the decomposition of a scalar field in terms of a spinless destruction operator takes the interaction-picture form

$$A(x) = \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\;\mathfrak{a}_{\mathbf{p}}\;e^{ip\cdot x}\,, \tag{11.3.12}$$

where $p \cdot x = \eta_{\mu\nu} p^\mu x^\nu = -\varepsilon(p)t + \mathbf{p} \cdot \mathbf{x}$.

Identical conclusions would also have been drawn for massless particles: a scalar field can only represent spinless massless particles, though it is not generically true that the types of fields that can represent a massless particle of helicity j need be the same as those that can represent a massive particle of spin j. (See §11.3.3 for a statement of the general case.)

11.3.2 4-vector fields

The previous section shows that consistency of the Lorentz transformation properties precludes some fields from being able to represent particles with some spins. In the above example a scalar field uniquely represents a spinless particle, but this is an extreme example and is not representative of what happens for other types of fields or particles with other spins. It is not generically true that there is a unique type of field that can represent a specific type of particle. Nor is it usually true that any particular type of field can only represent particles with a single value of spin. This section means to illustrate these points using the next most simple example: a 4-vector field $V^\mu(x)$.

A 4-vector field transforms in the same finite-dimensional representation as does x^μ, and so the representation matrices in this case are simply the Lorentz transformation matrices themselves: $D(\Lambda) = \Lambda$. In this case the linear transformation rule (11.3.2) becomes

$$U(\Lambda) V_\mu(x)\, U^{-1}(\Lambda) = \Lambda^\nu{}_\mu V_\nu(\Lambda x)\,. \tag{11.3.13}$$

The expansion of $V_\mu(x)$ in terms of creation and annihilation operators is given by

$$V_\mu(x) = \sum_\sigma \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}}\; u_\mu(\mathbf{p},\sigma)\, \mathfrak{a}_{\mathbf{p}\sigma}\; e^{ip\cdot x}\,, \tag{11.3.14}$$

and we seek to find the allowed coefficient functions $u_\mu(\mathbf{p},\sigma)$ as a function of the spin j of the particle that is destroyed by the operator $\mathfrak{a}_{\mathbf{p}\sigma}$. Repeating the same arguments as given above lead in this case to the consistency condition that must be satisfied by $u_\mu(\mathbf{p},\sigma)$:

$$\sum_\sigma D^{(j)*}_{\sigma'\sigma}\left[W(\Lambda,\mathbf{p}/m)\right] u_\mu(\mathbf{p},\sigma) = \sqrt{\frac{\varepsilon(\Lambda\mathbf{p})}{\varepsilon(\mathbf{p})}}\; \Lambda^\nu{}_\mu\, u_\nu(\Lambda\mathbf{p},\sigma')\,, \tag{11.3.15}$$

where the right-hand side contains an implied sum over the index ν (as usual for the Einstein summation convention). The explicit form on the left-hand side of this expression assumes the particle involved is massive.

As shown in general in Appendix C.1.2, the information content of this constraint is most transparently extracted by considering two special choices for Λ and for $\mathbf{p}$. In the first case choose $\Lambda = L(\mathbf{p}/m)$ to be the explicit Lorentz transformation that takes p^μ to the rest frame $k^\mu = (L\mathbf{p})^\mu$ for which $\mathbf{k} = 0$. In this case $\varepsilon(\Lambda p) = m$ and it happens that the Wigner rotation

$W(L, \mathbf{p}/m)$ becomes the identity transformation, and so the matrix $D^{(j)}_{\sigma\sigma'} = \delta_{\sigma\sigma'}$ for any j. In this case (11.3.15) reduces to the statement

$$u_\mu(\mathbf{p}, \sigma) = \sqrt{\frac{m}{\varepsilon(\mathbf{p})}}\, \Lambda^\nu{}_\mu\, u_\nu(\mathbf{0}, \sigma)\,, \tag{11.3.16}$$

which simply shows how to construct $u_\mu(\mathbf{p}, \sigma)$ in terms of the spin states in the rest frame. As such it does not in itself impose an obstruction to finding a solution to (11.3.15).

The constraint comes from the second special choice for Λ and $\mathbf{p}$: take $\mathbf{p} = 0$ (*i.e.* start in the rest frame), and choose $\Lambda = R$ to be one of the rotations within the little group that preserve the momentum in its rest frame. In this case (11.3.15) reduces to

$$\sum_\sigma D^{(j)*}_{\sigma'\sigma}(R) u_\mu(\mathbf{0}, \sigma) = R^\nu{}_\mu\, u_\nu(\mathbf{0}, \sigma')\,. \tag{11.3.17}$$

There are two choices for j that allow nontrivial solutions to this equation. One of these is to choose $j = 0$ in which case the matrix $D^{(j)}$ is one-dimensional and (11.3.17) says that $u_\mu(\mathbf{0})$ must satisfy $R^\nu{}_\mu u_\nu = u_\mu$ for all spatial rotations, which implies $u_\mu(\mathbf{0})$ must point purely in the time direction, and so be proportional to the 4-velocity of the rest frame. This, together with (11.3.16) then implies

$$u_\mu(\mathbf{p}) \propto \sqrt{\frac{m}{\varepsilon(p)}}\, p_\mu \quad \text{if } j = 0 \tag{11.3.18}$$

and so the field expansion (11.3.14) in this case can always be written

$$V_\mu(x) = i \int \frac{\mathrm{d}^3 p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\, p_\mu\, \mathfrak{a}_{\mathbf{p}\sigma}\, e^{ip\cdot x} = \partial_\mu A(x) \qquad (\text{spin } j = 0)\,, \tag{11.3.19}$$

where $A(x)$ is the scalar-field solution given in (11.3.12). Evidently a 4-vector field can represent a spinless particle, but it only does so by being the gradient of the scalar representation found earlier.

The second solution to (11.3.17) takes $j = 1$ and uses the 3-dimensional reprentation $D_{\sigma\sigma'}(R) = R_{\sigma\sigma'}$. For the three different eigenvalues $\sigma = -1, 0, 1$ of J_3 one can use circularly polarized polarization vectors, $\mathbf{u}(\mathbf{0}, \sigma) = \mathbf{e}_\sigma$, or for linearly polarized particles one can choose $u_i(\mathbf{0}, \sigma) = \delta_{i\sigma}$. Eq. (11.3.17) then simply expresses how these vector transform under spatial rotations. The field expansion (11.3.14) in this case then becomes

$$V_\mu(x) = \int \frac{\mathrm{d}^3 p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\, \epsilon_\mu(\mathbf{p}, \sigma)\, \mathfrak{a}_{\mathbf{p}\sigma}\, e^{ip\cdot x} \qquad (\text{spin } j = 1)\,, \tag{11.3.20}$$

where the polarization vectors $\epsilon_\mu(\mathbf{p}, \sigma) = u_\mu(\mathbf{p}, \sigma)$ for nonzero $\mathbf{p}$ are defined using (11.3.16).

The rules for combining angular momenta preclude nontrivial solutions to (11.3.17) for any other choices for j.

In this case the conclusions obtained would have been different if the particle had been assumed to be massless. Although the helicity zero solution (11.3.19) still exists for massless particles, the helicity one solution does not (more about which in §11.3.4).

11.3.3 Fields for general spin

One can press on in the same way for fields transforming in an arbitrary finite-dimensional representation of the Lorentz group, and for arbitrary spin j, for both the massive and massless particles, and for each representation consistent solutions for the functions $u_m(\mathbf{p}, \sigma)$ exist only for a restricted range of spins j, and when solutions do exist they are unique (for each j) up to normalization. This section summarizes the result for which spins can be represented for each choice for the field's Lorentz representation.

First, a brief summary of finite-dimensional Lorentz representations. As shown explicitly in Appendix B.2 a general finite-dimensional representation of the Lorentz group can be labelled by two spin-like quantum numbers (A, B), where $2A$ and $2B$ must be non-negative integers. [This labelling arises because the Lorentz algebra can be rewritten to look like a complexified version of the algebra for $SU(2) \times SU(2)$.] The Lorentz representation matrix is then built as a product of an ordinary rotation matrix for a particle having spin A and one with spin B, and so are $(2A+1)(2B+1)$-dimensional. The correspondence between this way of labelling Lorentz representations, and with some of the more commonly encountered representations (like scalars and 4-vectors) is given in Table 2.

(A, B)	Dim	Description	Example
$(0, 0)$	1	Scalar	ϕ
$(\frac{1}{2}, 0)$	2	Left-handed spinor	ψ_L
$(0, \frac{1}{2})$	2	Right-handed spinor	ψ_R
$(1, 0)$	3	Self-dual tensor	$\frac{1}{2}\epsilon_{\mu\nu\lambda\rho}F^{\lambda\rho} = iF_{\mu\nu}$
$(0, 1)$	3	Anti-self-dual tensor	$\frac{1}{2}\epsilon_{\mu\nu\lambda\rho}F^{\lambda\rho} = -iF_{\mu\nu}$
$(\frac{1}{2}, \frac{1}{2})$	4	4-vector	V^μ

Table 2. Common small-dimension representations of the Lorentz group.

Appendix C.1 repeats the above exercise of determining the form allowed for $u_m(\mathbf{p}, \sigma)$ for a general spin j (or helicity λ) and for a general Lorentz representation (A, B). For both massive and massless paricles are considered and in both cases it is the analog of the condition (11.3.17) that turns out to constrain which spins can be represented by fields transforming in any particular Lorentz representation.

For massive particles the general analog of condition (11.3.17) is given in (C.1.23), which reveals that the rules for determining if a field transforming in the (A, B) representation can represent a massive field of spin j are the same as the rules for whether an irreducible spin j object can be found from the product of a spin-A and a spin-B object using the usual rules of combining spins in single-particle quantum mechanics. That is, a massive paricle of spin j can be represented by a field transforming in the (A, B) Lorentz representation if and only if

$$j \in \Big\{ A+B, A+B-1, A+B-2, \cdots 1+|A-B|, |A-B| \Big\} . \tag{11.3.21}$$

This is consistent with the explicit examples considered above, since a scalar field corresponds to the $(0,0)$ representation, and so therefore only represents $j = 0$ particles. The 4-vector representation is similarly the $(\frac{1}{2}, \frac{1}{2})$ representation, which only allows $j = 0$ or $j = 1$.

For massless particles the analog of (11.3.17) turns out to be (C.1.26), which similarly restricts the helicities λ that are allowed for particles that can be represented by a field transforming in the (A, B) representation. The result there is that this is possible if and only if

$$\lambda = B - A\,. \tag{11.3.22}$$

This also agrees with the simplest example considered above, such as a scalar field in the $(0,0)$ representation, which the above says requires $\lambda = 0$ and so can represent only a spinless particle. For other fields the massless case particle result can be more surprising, however, such as is true in particular for the case of electromagnetism.

11.3.4 Electromagnetic fields

The photon is massless and was seen in earlier sections to contain two polarization states, which in the current language turn out to correspond to helicities $\lambda = \pm 1$. How does the result (11.3.22) work in the electromagnetic example?

Earlier sections provided explicit expansions of electromagnetic fields in terms of creation and annihilation operators, such as in (9.2.5) or (9.4.5), reproduced again here:

$$\mathbf{A}(\mathbf{x}) = \sum_\lambda \int \frac{\mathrm{d}^3 p}{\sqrt{(2\pi)^3 2|\mathbf{k}|}} \left[\mathfrak{a}_{\mathbf{k}\lambda}\, \boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}} + \mathfrak{a}^\star_{\mathbf{k}\lambda}\, \boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\, e^{-i\mathbf{k}\cdot\mathbf{x}} \right] . \tag{11.3.23}$$

This seems to say that a massless spin-one particle can be represented by a vector field, where $\mathbf{A}$ is regarded as the spatial part of a 4-vector potential A_μ, as described relativistically in (11.1.39). This seems to contradict (11.3.22) however, because a 4-vector field corresponds to the representation $(\frac{1}{2}, \frac{1}{2})$, and according to (11.3.22) this only allows $\lambda = \frac{1}{2} - \frac{1}{2} = 0$. What can be going on?

To find out, we sandwich (11.3.23) between $U(\Lambda)$ and $U^{-1}(\Lambda)$ and evaluate the result using the known transformation properties of $U(\Lambda)\, a_{\mathbf{k}\lambda}\, U^{-1}(\Lambda)$ that follow from the general representation for a massless state with helicity ± 1. When this is done one *almost* obtains the 4-velocity transformation rule, (11.3.13), for $U(\Lambda) A_\mu(x)\, U^{-1}(\Lambda)$, but not quite. What one finds instead (using $A_0 = 0$) is

$$U(\Lambda) A_\mu(x)\, U^{-1}(\Lambda) = \Lambda^\nu{}_\mu A_\nu(\Lambda x) + \Delta_\mu(x)\,, \tag{11.3.24}$$

where $\Delta_\mu = \partial_\mu \Omega$ is the gradient of some quantity Ω (whose detailed form is not important in what follows). This shows that A_μ as defined in (11.3.23) is *not* a 4-vector, and is instead only a 4-vector up to the addition of a gradient; it is only a 4-vector up to a gauge transformation.

This observation says that a field build from A_μ that is gauge invariant should therefore transform as a tensor if its transformation properties are computed using $U(\Lambda)\, a_{\mathbf{k}\lambda}\, U^{-1}(\Lambda)$

and (11.3.23) (with $A_0 = 0$). An example of a tensor with this property is $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ since the shift of A_μ by a gradient always cancels in this combination. Indeed computing $U(\Lambda)\, F_{\mu\nu}(x)\, U^{-1}(\Lambda)$ in this way leads to the covariant result

$$U(\Lambda) F_{\mu\nu}(x)\, U^{-1}(\Lambda) = \Lambda^\lambda{}_\mu \Lambda^\sigma{}_\nu F_{\lambda\sigma}(\Lambda x)\,. \tag{11.3.25}$$

This shows that the electromagnetic field strength, defined in terms of the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ as in (11.1.31), transforms covariantly under Lorentz transformations given that it is related to A_μ by (11.1.39).

Expression (11.3.25) is also consistent with (11.3.22), because (as summarized in Table 2) an antisymmetric tensor field transforms reducibly under Lorentz transformations; in the (A, B) notation transforming as the sum of a $(1, 0)$ and a $(0, 1)$ representation. These two fields are indeed precisely what are needed to represent particles with helicities $h = \pm 1$, as for a photon.

These observations say something important about the interactions of massless spin-one particles. They say that if you wish to describe the interactions of such a particle in terms of a field $A_\mu(x)$, such as in (11.3.23), then even if all interactions are constructed to be Lorentz invariant assuming that A_μ transforms like a 4-vector, the result can really only be Lorentz invariant if it is also assumed to be gauge-invariant (*i.e.* invariant under the shift $A_\mu \to A_\mu + \partial_\mu \Omega$). This is the simplest instance of a more general observation: the necessity of gauge invariance when describing massless particles with helicities $|h| \geq 1$ in Lorentz-invariant quantum theories.

11.4 Antiparticles and the spin-statistics connection

So far it has been taken for granted that for relativistic theories fields can always be expanded in terms of annihilation operators,

$$A_n(x) = \sum_\sigma \int \frac{\mathrm{d}^3 p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\, u_n(\mathbf{p}, \sigma)\, \mathfrak{a}_{\mathbf{p}\sigma}\, e^{ip\cdot x}\,, \tag{11.4.1}$$

along the lines of (11.3.12) and (11.3.14), just as they were for Schrödinger fields in (6.1.7). The purpose of this section is to show that this is wrong, and that it is no accident that for electromagnetism there are both creation and annihilation terms in field expansions like (11.3.23):

$$\mathbf{A}(\mathbf{x}) = \sum_\lambda \int \frac{\mathrm{d}^3 p}{\sqrt{(2\pi)^3 2|\mathbf{k}|}} \left[\mathfrak{a}_{\mathbf{k}\lambda}\, \boldsymbol{\epsilon}_\lambda(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}} + \mathfrak{a}^\star_{\mathbf{k}\lambda}\, \boldsymbol{\epsilon}^*_\lambda(\mathbf{k})\, e^{-i\mathbf{k}\cdot\mathbf{x}} \right]. \tag{11.4.2}$$

The argument that shows why this is necessary also provides the first step towards identifying the need for the existence of antiparticles.

11.4.1 The microcausality condition

To set up the issue recall that we seek conditions for when a theory is Lorentz invariant, and we ask the S matrix to commute with the $U(\Lambda)$, as in (11.2.8). Because the theory is specified by its Hamiltonian, in order to determine what it is required for Lorentz invariance, it is useful to express S in terms of the interaction Hamiltonian in order to see what is required of it.

Keeping in mind that the Hamiltonian is a local quantity, $H_{\rm int} = \int \mathrm{d}^3x\ \mathcal{H}(x)$, the perturbative expression for S is as given in (6.1.6),

$$S = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} d^4x_1 \cdots \mathrm{d}^4x_n\ T\left[\mathcal{H}(x_1)\cdots\mathcal{H}(x_n)\right]. \tag{11.4.3}$$

A sufficient condition for this expression to be Lorentz invariant is for $\mathcal{H}(x)$ to satisfy the following two conditions: (i) $\mathcal{H}(x)$ is a Lorentz scalar,

$$U(\Lambda)\ \mathcal{H}(x)\ U^{-1}(\Lambda) = \mathcal{H}(\Lambda x); \tag{11.4.4}$$

and (ii) $\mathcal{H}(x)$ and $\mathcal{H}(y)$ commute for spacelike separations,

$$\Big[\mathcal{H}(x), \mathcal{H}(y)\Big] = 0 \qquad \text{for} (x-y)^2 > 0\,. \tag{11.4.5}$$

The first of these conditions is really stronger than necessary. It is much stronger than just requiring $\mathcal{H}$ to transform as an energy density, which turns out to imply that $\mathcal{H}(x)$ should transform as the time-time component, $T^{00}(x)$, of a symmetric *stress tensor*: $T^{\mu\nu}$. It is nonetheless true that condition (11.4.4) is often satisfied in practice since it is just a condition on the interaction part of the Hamiltonian. For nonderivative interactions — like $\mathcal{H}_{\rm int} = gA^3(x)$, for example — it can indeed be true that the interaction contributes to the stress tensor an invariant form $T^{\mu\nu}_{\rm int} = \eta^{\mu\nu}\ \mathcal{H}(x)$, in which case $\mathcal{H}(x)$ is a scalar as in (11.4.4).

Condition (11.4.5) is necessary independent of Condition (11.4.4), even if $\mathcal{H}(x)$ should transform like a Lorentz scalar. This additional condition is required in order to ensure the invariance of the time ordering in eq. (11.4.3). Since different inertial observers can disagree on the ordering in time of spacelike separated events, if they are all to agree on what $T[\mathcal{H}(x)\,\mathcal{H}(y)]$ is we must demand that for spacelike separation the ordering of the $\mathcal{H}(x)$'s is irrelevant. This condition is required independent of the simplifying assumption that $\mathcal{H}(x)$ be a scalar, and is known as the condition of *microcausality*.

It is microcausality that gives relativistic quantum field theory most of its distinctive features. In particular, the remainder of this chapter argues that condition (11.4.5) is responsible for: (i) the existence of antiparticles and the rules that govern their properties; (ii) the Spin-Statistics connection; and (iii) the CPT Theorem.

The first step in making these connections is to see what the microcausality requirement implies for the fields $A_n(x)$. Since $\mathcal{H}(x)$ is constructed from multilinears of $A_n(x)$ and its Hermitian conjugate, the condition that it commute at spacelike separations would be

ensured if the fields themselves either commute or anticommute among themselves for spacelike separations. That is, writing $[A,B]_\pm \equiv AB \pm BA$ to denote either the commutator or anticommutator, a sufficient condition for (11.4.5) would be

$$\Big[A_m(x), A_n(y)\Big]_\mp = \Big[A_m(x), A_n^\star(y)\Big]_\mp = 0, \quad \text{for } (x-y)^2 > 0. \tag{11.4.6}$$

The first of these two conditions is actually easy to satisfy if the the sign $\pm$ in $[\cdot\,,\cdot]_\pm$ is chosen to correspond to the statistics of the particles involved. That is, local fields like (11.4.1) automatically commute at spacelike separations when $a_{\mathbf{p}\sigma}$ destroys bosons, or they automatically anticommute at spacelike separations if $a_{\mathbf{p}\sigma}$ destroys fermions. They do so because we know from earlier sections that the creation and annihilation operators for distinct particle types always commute or anticommute:

$$\Big[\mathfrak{a}_{\mathbf{p},\sigma}, \mathfrak{a}_{\mathbf{p}',\sigma'}\Big]_\pm = \Big[\mathfrak{a}^\star_{\mathbf{p},\sigma}, \mathfrak{a}^\star_{\mathbf{p}',\sigma'}\Big]_\pm = 0\,. \tag{11.4.7}$$

Notice though that if we demand that fermi fields anticommute for spacelike separation, then this only helps ensure that the commutator (and not anticommutator) $[\mathcal{H}(x), \mathcal{H}(y)]_- = 0$ if only even powers fermion fields can appear in $\mathcal{H}(x)$.

As a result the strongest consequences of microcausality should come from the condition that the commutator (or anticommutator) of $A_n(x)$ with its own conjugate, $A_n^\star(y)$, vanish for bosons (or fermions) at spacelike separations.

The Spinless Case

To explore the consequences of microscausality with a minimum of complications, consider first the case of a scalar field — *i.e.* the representation $(A,B) = (0,0)$ — representing a massive particle. From the considerations of §11.3.1 we know that such a field can represent only spinless particles: $j = 0$.

As mentioned in §11.3.1, it is conventional to normalize the fields such that

$$A(x) = \frac{1}{(2\pi)^{3/2}} \int \frac{\mathrm{d}^3p}{\sqrt{2\varepsilon(p)}}\, \mathfrak{a}_{\mathbf{p}}\, e^{ip\cdot x}. \tag{11.4.8}$$

With this choice the crucial commutator and anticommutator becomes:

$$\begin{aligned}
\Big[A(x), A^\star(y)\Big]_\mp &= \frac{1}{(2\pi)^3} \int \frac{\mathrm{d}^3p}{\sqrt{2\varepsilon(p)}} \frac{\mathrm{d}^3p'}{\sqrt{2\varepsilon(p)}} \Big[\mathfrak{a}_{\mathbf{p}}, \mathfrak{a}^\star_{\mathbf{p}'}\Big]_\mp e^{ip\cdot x - ip'\cdot y} \\
&= \frac{1}{(2\pi)^3} \int \frac{\mathrm{d}^3p}{2\varepsilon(p)}\, e^{ip\cdot(x-y)} \\
&=: \Delta_+(x-y),
\end{aligned} \tag{11.4.9}$$

in which the upper (lower) sign assumes the particles involved are bosons (fermions).

Exercise: Prove that the combination $\mathrm{d}^3p/\varepsilon(p)$ is Lorentz invariant.

We require the properties of $\Delta_+(x-y)$ in some detail, and so these are explored in the next few paragraphs. Since the combination $\mathrm{d}^3p/\varepsilon(p)$ is itself Lorentz invariant, the function $\Delta_+(z)$ is a manifestly Lorentz scalar function of the separation $z^\mu = x^\mu - y^\mu$. It can therefore only depend on the combinations $z^2 = \eta_{\mu\nu}z^\mu z^\nu$ and, if $z^2 \leq 0$, of $\mathrm{sign}(z^0)$. Consider, therefore, the cases of spacelike and timelike z^μ separately:

Timelike separations

Take first the case where $z^2 < 0$. Since $\Delta_+(z)$ is a scalar function it may be evaluated in the Lorentz frame for which the required algebra is the least tedious. Working in the frame for which $\mathbf{z} = 0$ and $z^0 = \pm\sqrt{-z^2}$ then gives:

$$\Delta_+(z) = \frac{1}{(2\pi)^3}\int \frac{\mathrm{d}^3p}{2\varepsilon(p)}\, e^{\mp i\varepsilon(p)\sqrt{-z^2}}. \tag{11.4.10}$$

Changing integration variables to the dimensionless combination $u \equiv |\mathbf{p}/m|$, and performing the integration over the direction of $\mathbf{p}$ then gives

$$\begin{aligned}\Delta_+(z) &= \frac{4\pi m^2}{2(2\pi)^3}\int_0^\infty \frac{u^2\,\mathrm{d}u}{\sqrt{u^2+1}}\, e^{\mp im\sqrt{u^2+1}\sqrt{-z^2}} \\ &= \frac{m}{8\pi\sqrt{-z^2}}\left[N_1\left(m\sqrt{-z^2}\right) \pm iJ_1\left(m\sqrt{-z^2}\right)\right],\end{aligned} \tag{11.4.11}$$

where the last equality uses the standard integral representations for Bessel functions:

$$\begin{aligned}N_1(z) &= \frac{2z}{\pi}\int_0^\infty \frac{u^2\,\mathrm{d}u}{\sqrt{u^2+1}}\,\cos\left(z\sqrt{u^2+1}\right) \\ J_1(z) &= -\frac{2z}{\pi}\int_0^\infty \frac{u^2\,\mathrm{d}u}{\sqrt{u^2+1}}\,\sin\left(z\sqrt{u^2+1}\right).\end{aligned} \tag{11.4.12}$$

Spacelike Arguments

Next choose a z^μ to be spacelike, so $z^2 > 0$. In this case it is convenient to work within the frame for which $z^0 = 0$ and so for which $|\mathbf{z}| = \sqrt{z^2}$. In this case

$$\begin{aligned}\Delta_+(z) &= \frac{1}{(2\pi)^3}\int \frac{\mathrm{d}^3p}{2\varepsilon(p)}\, e^{i\mathbf{p}\cdot\mathbf{z}} \\ &= \frac{4\pi m}{2(2\pi)^3}\int_0^\infty \frac{u^2\,\mathrm{d}u}{\sqrt{u^2+1}}\frac{\sin\left(mu\sqrt{z^2}\right)}{u\sqrt{z^2}} \\ &= \frac{m}{4\pi^2\sqrt{z^2}}\,K_1\left(m\sqrt{z^2}\right),\end{aligned} \tag{11.4.13}$$

where $K_1(z)$ is the modified Bessel function having integral representation:

$$K_1(z) = \int_0^\infty \frac{u\,\mathrm{d}u}{\sqrt{u^2+1}}\,\sin(uz). \tag{11.4.14}$$

This completes the evaluation of Δ_+ for spacelike and timelike arguments. Combining these results the commutator function for a massive scalar field turns out to be:

$$\begin{aligned}\Delta_+(x-y) &= \frac{m^2}{4\pi^2 z}\, K_1(z) \qquad\qquad \text{for} \quad (x-y)^2 > 0 \\ &= \frac{m^2}{8\pi z}\, \left[N_1(z) + \text{sign}\left(z^0\right)\; iJ_1(z)\right] \qquad \text{for} \quad (x-y)^2 < 0\,, \end{aligned} \tag{11.4.15}$$

in which the variables z and z^0 are defined by: $z^0 \equiv x^0 - y^0$ and $z = m\sqrt{|(x-y)^2|}$

Notice that $\Delta_+(z)$ is an even function of z^μ when z^μ is spacelike: *i.e.* $\Delta_+(z) = \Delta_+(-z)$ for $z^2 > 0$ (a property that proves useful in what follows). The same is not true for timelike z^μ due to the appearance in (11.4.15) of sign (z^0), which ensures $\Delta_+(z)$ has both odd and even parts under $z^\mu \to -z^\mu$ when $z^2 < 0$. The symmetry of $\Delta_+(x-y)$ for spacelike separations under the interchange of x and y can be simply understood as a consequence of Lorentz invariance because $x-y$ can be obtained from $y-x$ by a Lorentz transformation when x and y are spacelike separated.

Most importantly for the present purposes, notice that $\Delta_+(x-y)$ does *not* vanish for spacelike $x-y$. Consequently the fields $A_m(x)$ generically *do not* commute (or, for fermions, anticommute) with $A^\star(y)$ when $(x-y)^2 > 0$ and so a generic interaction Hamiltonian constructed from such fields will *not* satisfy the microcausality constraint (11.4.5). As a result the time-ordering appearing in expression (11.4.3) for the S matrix generically will differ for different inertial observers (and so therefore cannot be Lorentz invariant).

11.4.2 Antiparticles: the spinless case

Experience with electromagnetism suggests a way out of this problem, however. Continuing with the spinless example, suppose that the theory in question contains two particles which have the same mass and the same statistics[43] but not necessarily the same value for other quantum numbers. Denoting the destruction operator for this particle by $\overline{\mathfrak{a}}_{\mathbf{p}}$, the position-space field for this second particle — called the first particle's *antiparticle* — is denoted

$$B(x) = \frac{1}{(2\pi)^{3/2}} \int \frac{\mathrm{d}^3 p}{\sqrt{2\varepsilon(p)}}\; \overline{\mathfrak{a}}_{\mathbf{p}}\; e^{ip\cdot x}\,. \tag{11.4.16}$$

Define, then, the combination

$$\begin{aligned}\psi(x) &:= A(x) + \alpha B^\star(x) \\ &= \frac{1}{(2\pi)^{3/2}} \int \frac{\mathrm{d}^3 p}{\sqrt{2\varepsilon(p)}} \Big[\mathfrak{a}_{\mathbf{p}}\; e^{ip\cdot x} + \alpha\; \overline{\mathfrak{a}}^\star_{\mathbf{p}}\; e^{-ip\cdot x}\Big], \end{aligned} \tag{11.4.17}$$

[43] Once spinning particles are considered the antiparticle will also have the same total spin j.

with α some complex number. Then the commutator/anticommutator of $\psi(x)$ with its adjoint becomes

$$\begin{aligned}\Big[\psi(x),\psi^\star(y)\Big]_\mp &= \Big[A(x)+\alpha B^\star(x), A^\star(y)+\alpha^* B(y)\Big]_\mp \\ &= \Big[A(x),A^\star(y)\Big]_\mp \mp |\alpha|^2\Big[B(y),B^\star(x)\Big]_\mp \\ &= \Delta_+(x-y) \mp |\alpha|^2\Delta_+(y-x)\,,\end{aligned} \tag{11.4.18}$$

where the $[A(x),A(y)]_\mp$ and $[B(x),B(y)]_\mp$ terms vanish because it is the commutator that is used if the particles are bosons and it is the anticommutator that is used if they are fermions.

The basic observation at this point is that since $\Delta_+(x-y)$ is an even function for spacelike $x-y$ it is possible to make the commutator (and *not* the anticommutator) $[\psi(x),\psi^\star(y)]_-$ vanish for spacelike separations provided that we choose $|\alpha|^2=1$. Significantly, there is no choice for α that could similarly ensure that the anticommutator vanishes. Also notice that since $\Delta_+(x-y)$ is *not* even under interchange of x and y when $x-y$ is timelike, the commutator $[\psi(x),\psi^\star(y)]_-$ does not become trivial by vanishing everywhere.

For this choice for α the commutator becomes

$$\Big[\psi(x),\psi^\star(y)\Big]_- = \Delta_+(x-y)-\Delta_+(y-x) =: \Delta(x-y), \tag{11.4.19}$$

where (by construction) $\Delta(x-y)=0$ if $(x-y)^2>0$, while

$$\Delta(x-y) = \frac{im^2}{4\pi z}\,\mathrm{sign}\left(z^0\right)\; J_1(z) \qquad \text{for} \quad (x-y)^2<0\,, \tag{11.4.20}$$

where $z^0=x^0-y^0$ and $z=m\sqrt{-(x-y)^2}$.

At this point several things are worth emphasizing, because they also hold for higher spins and encapsulate the main consequences of combining special relativity with quantum mechanics.

- The interactions of spinless particles can be made consistent with causality provided that every particle has a partner – called its antiparticle – that is also spinless and has precisely the same mass.

- Microcausality forces the creation operator for the particle to systematically appear everywhere together with the destruction operator for the antiparticle (and vice versa). This ensures the impossibility of interactions that conserve the total particle number. As argued more explicitly below, should there be a symmetry in the problem for which $A(x)\to e^{i\theta}A(x)$ then it can only hope to remain a symmetry if $B(x)\to e^{-i\theta}B(x)$, and so the particle and antiparticle must have precisely opposite values for any additive quantum number (like electric charge).

- Causality forces the particle and its antiparticle to enter into all interactions with equal relative strength since $|\alpha|^2 = 1$. This relation between the couplings of particles and antiparticles is called *crossing symmetry*, and it implies that the amplitudes for destroying (creating) particles are precisely the same size as the amplitudes for creating (destroying) antiparticles.

- Since only the commutator, as opposed to the anticommutator, of $\phi(x)$ with its adjoint can be made to vanish for spacelike separations the spin-zero particle *must* be a boson—giving a connection between a particle's spin and it's statistics.

The new particle may, but need not, be the same particle type as the original. That is, it can be that $\overline{\mathfrak{a}}_{\mathbf{p}} = \mathfrak{a}_{\mathbf{p}}$, such as was found in (11.4.2) for the photon. In the event that a particle is its own antiparticle, it is called *self conjugate*. The requirement that particles and antiparticles have opposite vales of any conserved charge implies that a particle *cannot* be self-conjugate if it should carry nonzero charge for any additive conserved quantum number. It is only because photons carry no such charge that they can be their own antiparticles.

To make completely explicit the requirement that particles and antiparticles must carry opposite charges, notice that microcausality implies that it is ψ and its Hermitian conjugate that must enter the interaction Hamiltonian, $\mathcal{H}(x)$. It is therefore ψ which must transform linearly under any such a symmetry. Suppose then there is a charge, Q, for which $[Q, \mathfrak{a}_{\mathbf{p}}] = -iq\,\mathfrak{a}_{\mathbf{p}}$. (As discussed in §8.3, provided that the ground state satisfies $Q|0\rangle = 0$ this is equivalent to the condition that the corresponding particle states satisfy $Q|\mathbf{p}\rangle = q|\mathbf{p}\rangle$.) The field operator must therefore satisfy $[Q, A(x)] = -qA(x)$. The main point now is that if we therefore demand that $[Q, \psi(x)] = -q\psi(x)$ then consistency requires $[Q, B^*(x)] = -qB^*(x)$, or $[Q, \overline{\mathfrak{a}}_{\mathbf{p}}] = +q\,\overline{\mathfrak{a}}_{\mathbf{p}}$. Particle and antiparticle in this case therefore carry opposite charges and so cannot possibly be identical to one another.

11.4.3 Antiparticles: general spin

The above discussion goes through in a similar way for massless particles and for nonzero spins.

Massive spin one

For example, consider a massive spin-one particle represented by a 4-vector field — *i.e.* in the $(\frac{1}{2}, \frac{1}{2})$ representation. For this choice the relevant field expansion is

$$V_\mu(x) = \frac{1}{(2\pi)^{3/2}} \sum_\sigma \int \frac{\mathrm{d}^3 p}{\sqrt{2\varepsilon(p)}}\, u_\mu(\mathbf{p}, \sigma)\, \mathfrak{a}_{\mathbf{p}\sigma}\, e^{ip\cdot x}\,, \tag{11.4.21}$$

and so the crucial commutator/anticommutator (for bosons/fermions) becomes

$$\begin{aligned}\Big[V_\mu(x),V_\nu^\star(y)\Big]_\mp &= \frac{1}{(2\pi)^3}\sum_{\sigma\sigma'}\int\frac{\mathrm{d}^3p}{\sqrt{2\varepsilon(p)}}\frac{\mathrm{d}^3p'}{\sqrt{2\varepsilon(p)}}\,u_\mu(\mathbf{p},\sigma)u_\nu^*(\mathbf{p}',\sigma')\Big[\mathfrak{a}_{\mathbf{p}\sigma},\mathfrak{a}^*_{\mathbf{p}'\sigma'}\Big]_\mp\,e^{ip\cdot x-ip'\cdot y}\\ &= \frac{1}{(2\pi)^3}\sum_{\sigma}\int\frac{\mathrm{d}^3p}{2\varepsilon(p)}\,u_\mu(\mathbf{p},\sigma)u_\nu^*(\mathbf{p},\sigma)\,e^{ip\cdot(x-y)}\\ &= \frac{1}{(2\pi)^3}\int\frac{\mathrm{d}^3p}{2\varepsilon(p)}\,\left[\eta_{\mu\nu}+\frac{p_\mu p_\nu}{m^2}\right]\,e^{ip\cdot(x-y)}\\ &= \left[\eta_{\mu\nu}-\frac{\partial_\mu\partial_\nu}{m^2}\right]\Delta_+(x-y)=:\Delta_{\mu\nu}(x-y)\,,\end{aligned}\tag{11.4.22}$$

for which the upper (lower) sign again assumes the particles involved are bosons (fermions). The final result uses the completeness relation for a massive spin-one polarization vector,

$$\sum_\sigma u_\mu(\mathbf{p},\sigma)u_\nu^*(\mathbf{p},\sigma)=\eta_{\mu\nu}+\frac{p_\mu p_\nu}{m^2}\,,\tag{11.4.23}$$

where (as above) $p^\mu=\{\varepsilon(p)\,,\mathbf{p}\}$, and the right-hand side is the projection matrix onto the subpace of 4-vectors that satisfy $\eta_{\mu\nu}u^\mu p^\nu=0$ (as may be seen by contracting with p^μ and using $p\cdot p=\eta_{\mu\nu}p^\mu p^\nu=-m^2$).

Just as was true for spinless particles, this expression does not vanish for spacelike separations, but it can be cancelled if the theory contains another spin-one particle with the same mass and statistics. Denoting the destruction operator for this particle by $\overline{\mathfrak{a}}_{\mathbf{p}\sigma}$, and its position-space field as

$$W_\mu(x)=\frac{1}{(2\pi)^{3/2}}\sum_\sigma\int\frac{\mathrm{d}^3p}{\sqrt{2\varepsilon(p)}}\,u_\mu(\mathbf{p},\sigma)\,\overline{\mathfrak{a}}_{\mathbf{p}\sigma}\,e^{ip\cdot x}\,,\tag{11.4.24}$$

suggests writing the combination

$$\begin{aligned}\psi_\mu(x)&:=V_\mu(x)+\alpha W_\mu^\star(x)\\ &=\frac{1}{(2\pi)^{3/2}}\int\frac{\mathrm{d}^3p}{\sqrt{2\varepsilon(p)}}\Big[u_\mu(\mathbf{p},\sigma)\,\mathfrak{a}_{\mathbf{p}\sigma}\,e^{ip\cdot x}+\alpha\,u_\mu^*(\mathbf{p},\sigma)\,\overline{\mathfrak{a}}^\star_{\mathbf{p}\sigma}\,e^{-ip\cdot x}\Big],\end{aligned}\tag{11.4.25}$$

with α some complex number.

Then the commutator/anticommutator of $\psi(x)$ with its adjoint becomes

$$\begin{aligned}\Big[\psi_\mu(x),\psi_\nu^\star(y)\Big]_\mp &= \Big[V_\mu(x)+\alpha W_\mu^\star(x),V_\nu^\star(y)+\alpha^* W_\nu(y)\Big]_\mp\\ &= \Big[V_\mu(x),V_\nu^\star(y)\Big]_\mp\mp|\alpha|^2\Big[W_\nu(y),W_\mu^\star(x)\Big]_\mp\\ &= \Delta_{\mu\nu}(x-y)\mp|\alpha|^2\Delta_{\mu\nu}(y-x)\,,\end{aligned}\tag{11.4.26}$$

where (as before) the commutator is used if the particles are bosons and the anticommutator is used if they are fermions. This result also uses the same completeness relation (11.4.23) for $u_\mu(\mathbf{p},\sigma)$, a result expanded on in Appendix C.3.1.

It is again possible to make the commutator (but *not* the anticommutator) $[\psi_\mu(x), \psi^\star_\nu(y)]_-$ vanish for spacelike separations, provided we choose $|\alpha|^2 = 1$. For this choice for α the commutator becomes

$$\Big[\psi_\mu(x), \psi^\star_\nu(y)\Big]_- = \Delta_{\mu\nu}(x-y) - \Delta_{\mu\nu}(y-x) = \left[\eta_{\mu\nu} - \frac{\partial_\mu \partial_\nu}{m^2}\right] \Delta(x-y)\,, \tag{11.4.27}$$

which vanishes if $(x-y)^2 > 0$, with $\Delta(x-y)$ given by (11.4.20) for $(x-y)^2 < 0$.

The implications of microcausality are therefore much as they were for spinless particles. Most notably, every massive spin-one particle must be a boson, and has an antiparticle that is also a boson, also has $j = 1$ and has precisely the same mass. The antiparticle also has opposite values for any additive quantum numbers like electric charge.

11.4.4 The spin-statistics connection

The same logic as described in the previous section can be carried through for massive particles with arbitrary spin j represented by a generic field in the (A, B) representation. This section briefly summarizes the results that are found by doing so, with details given more explicitly in Appendix (C.3).

Suppose then that a massive spin-j particle and its antiparticle (with the same spin) are represented by a field $\psi_n(x)$ transforming in the (A, B) representation of the Lorentz group. Consistency of the Lorentz transformation properties then turns out to allow the following decomposition in terms of particle and antiparticle creation and annihilation operators (see eq. (C.3.1))

$$\psi_n(x) = \sum_\sigma \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}} \left[u_n(\mathbf{p}, \sigma)\; \mathfrak{a}_{\mathbf{p},\sigma}\; e^{ip\cdot x} + v_n(\mathbf{p}, \sigma)\; \overline{\mathfrak{a}}^\star_{\mathbf{p},\sigma}\; e^{-ip\cdot x}\right]. \tag{11.4.28}$$

Here the mode functions for general (A, B) are derived explicitly in Appendix C.2, and the antiparticle modes $v_n(\mathbf{p}, \sigma)$ are proportional to $u^*_n(\mathbf{p}, \sigma)$, or can equivalently be expressed in terms of $u_n(\mathbf{p}, \sigma)$ by (see eq. (C.3.2))

$$v_n(\mathbf{p}, \sigma) = \xi(-)^{j-\sigma} u_n(\mathbf{p}, -\sigma)\,, \tag{11.4.29}$$

and ξ is a complex number to be determined by requiring microcausality.

Microcausality requires fields and their adjoints to commute at spacelike separations, and for complete generality we ask what this implies for the commutator/anticommutator of two different types of fields, $\psi_n(x)$ and $\tilde{\psi}_n(x)$ — respectively transforming in the (A, B) and $(\tilde{A}, \tilde{B})$ representations — that both can represent a massive particle and antiparticle of spin j. Evaluating their commutator/commutator (whichever is appropriate for bose or fermi statistics) for spacelike separations is most easily done in the frame for which $x^0 = y^0 = t$, in which case the result becomes

$$\Big[\psi_n(x), \tilde{\psi}^\star_{\tilde{n}}(y)\Big]_\mp = m\Big[P_1(-i\nabla)\Big]_{n\tilde{n}} \int \frac{\mathrm{d}^3 p}{(2\pi)^3 \varepsilon(p)}\; e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \Big[1 \mp (-)^{2(A+\widetilde{B})} \xi\tilde{\xi}^*\Big]\,, \tag{11.4.30}$$

where the upper sign applies for bosons and the lower sign for fermions. The quantity $P_1(\mathbf{p})$ is a polynomial whose detailed form is calculated in (C.3) but does not matter in what follows.

Requiring (11.4.30) to vanish imposes the following condition on the complex constant ξ:

$$\pm(-)^{2(A+\widetilde{B})}\xi\tilde{\xi}^* = 1. \tag{11.4.31}$$

In the special case where both fields, $\psi(x)$ and $\tilde{\psi}(x)$, transform in the same Lorentz representation — so $\widetilde{A} = A$ and $\widetilde{B} = B$ — the modulus and phase of (11.4.31) gives the two conditions

$$|\xi| = 1 \qquad \text{and} \qquad \pm\,(-)^{2(A+B)} = 1. \tag{11.4.32}$$

The condition on $|\xi|$ provides the general foundations for 'crossing symmetry': particles and antiparticles always appear within any position-space field $\psi_n(x)$ with equal amplitudes, and as a result their interactions always have precisely the same strength.

The second condition contains within it the spin-statistics theorem. To see why, recall that a field transforming in the (A, B) Lorentz representation can only describe a massive particle of spin j if $j \in \{|A - B|, \cdots, A + B\}$. This implies that j differs from $A + B$ by an integer and so $(-)^{2(A+B)} = (-)^{2j}$. As a result the condition$\pm(-)^{2(A+B)} = 1$ can be rewritten

$$\pm(-)^{2j} = 1. \tag{11.4.33}$$

Keeping in mind that the upper sign applies for bosons and the lower sign applies for fermions, it follows that all integer-spin particles must satisfy Bose statistics while all half-odd-integer spin particles must be fermions.

Returning to the general case of eq. (11.4.31) with the fields $\psi(x)$ and $\tilde{\psi}(x)$ transforming differently, using the spin-statistics connection eq. (11.4.33) allows one to write $\pm(-)^{2A} = (-)^{2B}$, so that eq. (11.4.31) becomes $(-)^{2(B+\tilde{B})}\xi\tilde{\xi}^* = 1$. Since $\tilde{\xi}$ is a phase, its inverse is $\tilde{\xi}^{-1} = \tilde{\xi}^*$, which allows the microcausality condition to be written

$$\xi_0 := (-)^{2B}\xi = (-)^{2\tilde{B}}\tilde{\xi}. \tag{11.4.34}$$

This condition says that ξ_0 is a phase that is independent of the kind of field used to describe the particle of interest, and Appendix C.3 shows that it can therefore always be absorbed into the definition of the creation operator, $\overline{\mathfrak{a}}^*_{\mathbf{p}\sigma}$, for the particle and antiparticle. Once this is done we have $\xi = (-)^{2B}$ and so the general form for the relativistic field expansion finally becomes:

$$\psi_n(x) = \sum_\sigma \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\, u_n(\mathbf{p},\sigma)\left[\mathfrak{a}_{\mathbf{p}\sigma}\, e^{ip\cdot x} + (-)^{2B}(-)^{j-\sigma}\, \overline{\mathfrak{a}}^\star_{\mathbf{p}\sigma}\, e^{-ip\cdot x}\right]. \tag{11.4.35}$$

where B is the quantum number in the pair (A, B) defining the fields Lorentz-transformation properties.

11.5 C, P, T and CPT

A final class of general consequences of microcausality (and so of relativistic quantum field theory in general) concern three generic discrete symmetries that are associated with the disconnected parts of the Lorentz group — which §11.1.3 has shown are generated by two specific transformations: parity (P) and time-reversal (T) — as well as with *charge conjugation* (C), defined as the interchange of particles with antiparticles.

There are two types of general predictions to be made. First, although none of these transformations need separately be a symmetry, they often are for specific types of interactions of practical importance like the electromagnetic and strong interactions. When they are good symmetries they provide new multiplicative quantum numbers, and microscausality relates the values of these quantum numbers for antiparticles to those of their corresponding particles. This relation proves to be one of the very successful general predictions of relativistic quantum field theory.

The second general prediction – subject to very mild assumptions – is called the *CPT Theorem*, and states that the transformation CPT obtained by combining all three of C, P and T is on very general grounds always a symmetry even if each of them separately need not be.

11.5.1 Charge Conjugation

Since every particle type must come paired with an antiparticle that shares its mass, spin and statistics, it is possible to define an operation – *charge conjugation* – that interchanges all particles with their antiparticles. This is conventionally done without also changing their momentum. Its action on single-particle states is therefore defined as

$$\mathfrak{a}^\star_{\mathbf{p}\sigma}|0\rangle \to \eta_c\, \overline{\mathfrak{a}}^\star_{\mathbf{p}\sigma}|0\rangle, \tag{11.5.1}$$

in which η_c is a phase that might be different for each type of particle that is involved. The action on many-particle states is to similarly replace all particles in the state by the corresponding antiparticles. The no-particle state, $|0\rangle$, may be chosen to be invariant.

There is no guarantee that this replacement must be a symmetry of any given system. But when it is it may be represented in the Hilbert space by an operator, $\mathcal{C}$. The transformation rule (11.5.1) implies that this operator satisfies

$$\mathcal{C}\; \mathfrak{a}_{\mathbf{p}\sigma}\; \mathcal{C}^{-1} = \eta_c^*\; \overline{\mathfrak{a}}_{\mathbf{p}\sigma} \quad \text{and} \quad \mathcal{C}\; \overline{\mathfrak{a}}_{\mathbf{p}\sigma}\; \mathcal{C}^{-1} = \bar{\eta}_c^* \mathfrak{a}_{\mathbf{p}\sigma}. \tag{11.5.2}$$

When particle and antiparticle are different particles their charge-conjugation phases, η_c and $\bar{\eta}_c$, need not *a priori* be related to one another. However, they do turn out to be related by microcausality, as is demonstrated below.

When it exists, the charge conjugation operator defined in eq. (11.5.2) commutes with the Poincaré generators since it does not change any of the particle labels such as spin,

momentum, and mass. As a result it follows that for any Poincar'e transformation $U(\Lambda, a)$

$$\mathcal{C}\, U(\Lambda = 1, a)\, \mathcal{C}^{-1} = U(\Lambda = 1, a), \tag{11.5.3}$$

which in turn implies:

$$\mathcal{C}\, iP^0\, \mathcal{C}^{-1} = iP^0. \tag{11.5.4}$$

Consistency of this last equation with the positivity of the Hamiltonian, P^0, implies that $\mathcal{C}$ cannot be antilinear[44] and so must be represented a linear transformation.

Microcausality implies that the phases η_c and $\overline{\eta}_c$ appearing in (11.5.2) must be consistent with the existence of a transformation rule for the position-space field, $\psi_n(x)$, since it is only through this that $\mathfrak{a}_{\mathbf{p}\sigma}$ and $\overline{\mathfrak{a}}_{\mathbf{p}\sigma}$ actually appear in the interaction Hamiltonian. Appendix C.4.1 proves that this is only possible if the particle and antiparticle phases are related by:

$$\overline{\eta}_c = \eta_c^*. \tag{11.5.5}$$

Notice that in the particular case where particle and antiparticle (such as happens for photons) are the same particle then this implies $\overline{\eta}_c = \eta_c = \eta_c^*$ and so $\eta_c = \pm 1$.

The transformation rule for the field $\psi_n(x)$ in general becomes[45]

$$\mathcal{C}\, \psi_{ab}(x)\, \mathcal{C}^{-1} = \eta_c^*\, \tilde{\psi}_{ab}(x), \tag{11.5.6}$$

where $\tilde{\psi}_{ab}(x)$ is defined by the standard expansion, (11.4.35), but with $\mathfrak{a}_{\mathbf{p}\sigma}$ and $\overline{\mathfrak{a}}_{\mathbf{p}\sigma}$ interchanged. Appendix C.4.1 also shows that this transformation rule can also be written in terms of the Hermitian conjugate field, $\psi^\star_{ab}(x)$, rather than $\tilde{\psi}_{ab}(x)$, which implies that the representation (A, B) is mapped to the representation (B, A). Explicitly, (11.5.6) can also be rewritten

$$\mathcal{C}\, \psi_{\,ab}(x)\, \mathcal{C}^{-1} = \eta_c^*(-)^{2A-j-a-b}\, \psi^\star_{-b,-a}(x). \tag{11.5.7}$$

For example, these last two expressions are particularly simple in the special case of a scalar field $(A, B) = (0, 0)$ representing a spinless particle, $j = 0$, for which $u(\mathbf{p}) = [2\varepsilon(p)]^{-1/2}$ and so

$$\begin{aligned} \phi(x) &= \int \frac{\mathrm{d}^3 p}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \left[\mathfrak{a}_{\mathbf{p}}\, e^{ip\cdot x} + \overline{\mathfrak{a}}^\star_{\mathbf{p}}\, e^{-ip\cdot x}\right] \\ \text{and} \quad \tilde{\phi}(x) &= \int \frac{\mathrm{d}^3 p}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \left[\overline{\mathfrak{a}}_{\mathbf{p}}\, e^{ip\cdot x} + \mathfrak{a}^\star_{\mathbf{p}}\, e^{-ip\cdot x}\right], \end{aligned} \tag{11.5.8}$$

in terms of which (11.5.6) and (11.5.7) become

$$\mathcal{C}\, \phi(x)\, \mathcal{C}^{-1} = \eta_c^*\, \tilde{\phi}(x) = \eta_c^*\, \phi^\star(x). \tag{11.5.9}$$

[44] Recall that a transformation A is antilinear if $A(\alpha|\psi\rangle + \beta|\psi'\rangle) = \alpha^* A|\psi\rangle + \beta^* A|\psi'\rangle$.

[45] In order to be specific about the transformation properties of the fields, the generic index n for $\psi_n(x)$ is replaced in this section by the index pair (a, b) that is associated with the (A, B) Lorentz representation under which the field transforms – see Appendix C.2 for details.

11.5.2 Parity

The operator implementing the action of parity is a special case $\mathcal{P} = U(P, 0)$ of a Poincaré transformation, restricted to an improper Lorentz transformation, and this dictates how it acts on particle states. The result is worked out in §11.2.2, with the result for massive particle states being (*c.f.* eq. (11.2.31))

$$\mathcal{P}|\mathbf{p}, \sigma\rangle = \eta_p |-\mathbf{p}, \sigma\rangle \,, \tag{11.5.10}$$

for some (possibly species-dependent) phase η_p. This in turn implies

$$\mathcal{P}\; \mathfrak{a}_{\mathbf{p}\sigma}\; \mathcal{P}^{-1} = \eta_p^*\; \mathfrak{a}_{-\mathbf{p},\sigma} \quad \text{and} \quad \mathcal{P}\; \overline{\mathfrak{a}}_{\mathbf{p}\sigma}\; \mathcal{P}^{-1} = \bar{\eta}_p^*\; \overline{\mathfrak{a}}_{-\mathbf{p},\sigma}. \tag{11.5.11}$$

Microcausality again relates the parity phases, $\bar{\eta}_p$ and η_p, to one another because it demands these transformations be consistent with a single transformation law for the position-space fields $\psi_{ab}(x)$. This turns out to imply (see Appendix C.4.2 for details) that the particle and antiparticle parity phases are related by

$$\eta_p = (-)^{2B-2A}\; \bar{\eta}_p^* = (-)^{2(B+A)} \bar{\eta}_p^* = (-)^{2j} \bar{\eta}_p^*. \tag{11.5.12}$$

Notice that in the special case of self-conjugate particles, for which $a_{\mathbf{p}\sigma} = \overline{a}_{\mathbf{p}\sigma}$, this condition implies that $\eta_p = \overline{\eta}_p = (-)^{2j}$. In particular for self-conjugate bosons parity must take be real: $\eta_p = \pm 1$, while for self-conjugate (or *Majorana*) fermions we have instead: $\eta_p = \pm i$.

The field transformation property is also worked out in Appendix C.4.2, where it is shown to map the (A, B) representation onto the (B, A) representation, with the field components transforming as

$$\mathcal{P}\; \psi^{AB}_{ab}(x)\; \mathcal{P}^{-1} = (-)^{A+B-j} \eta_p^*\; \psi^{BA}_{ba}(x_p) \,, \tag{11.5.13}$$

where $x_p^\mu := P^\mu{}_\nu x^\nu$ with $P^\nu{}_\mu = \text{diag}(+1, -1, -1, -1)$ being the parity coordinate transformation, as defined in §11.1.3. Here the superscripts AB and BA indicate the representation for the corresponding field. Representations like $(0, 0)$ (scalars) and $(\frac{1}{2}, \frac{1}{2})$ (4-vectors) map to themselves under this law, and so for scalars the above transformation becomes $\mathcal{P}\, \phi(x)\, \mathcal{P}^{-1} = \eta_p^*\, \phi(x_p)$. For 4-vectors (keeping in mind the conversion dictionary given in eq. (B.2.13), and the observation that $\sigma^2 \sigma^\mu$ is antisymmetric for $\mu = 0$ and symmetric otherwise) it instead becomes

$$\mathcal{P}\, V_\mu(x)\, \mathcal{P}^{-1} = -\eta_p^*\, P^\nu{}_\mu\, V_\nu(x_p) \,, \tag{11.5.14}$$

consistent with the intuitive notion of parity for a 4-vector.

11.5.3 Time Reversal

The other independent improper Lorentz tranformation is time-reversal, whose operator representation within the quantum Hilbert space is denoted $\mathcal{T}$. The commutation relations of

$\mathcal{T}$ with the Poincaré generators is dicated by the Poincaré group multiplication law, as is the action of $\mathcal{T}$ on massive-particle states — see eq. (11.2.31):

$$\mathcal{T}|\mathbf{p},\sigma\rangle = \eta_t(-)^{j-\sigma}|-\mathbf{p},-\sigma\rangle\,, \tag{11.5.15}$$

where η_t is a phase. This implies the following transformation rule for particle annihilation operators,

$$\mathcal{T}\;\mathfrak{a}_{\mathbf{p}\sigma}\;\mathcal{T}^{-1} = \eta_t^*(-)^{j-\sigma}\;\mathfrak{a}_{-\mathbf{p},-\sigma} \quad \text{and} \quad \mathcal{T}\;\bar{\mathfrak{a}}_{\mathbf{p}\sigma}\;\mathcal{T}^{-1} = \bar{\eta}_t^*(-)^{j-\sigma}\;\bar{\mathfrak{a}}_{-\mathbf{p},-\sigma}. \tag{11.5.16}$$

Recall — *c.f.* the discussion below (11.2.21) — that $\mathcal{T}$ is an *anti*-unitary operator (as opposed to unitary), in the sense that $\mathcal{T}^\star\mathcal{T} = 1$ but $\mathcal{T}(\alpha|\psi\rangle) = \alpha^*\mathcal{T}|\psi\rangle$. As a result the phase η_t does not become a physical quantum number for labelling particle states, since it can be absorbed into the definition of the phase of these states, or equivalently into the phase of the creation operator, $\mathfrak{a}_{\mathbf{p}\sigma}$. A convenient choice for this arbitrary phase is given below.

The next step is to relate $\bar{\eta}_t$ to η_t as required by microcausality, as is done in detail in C.4.3. That is to say, even though η_t may be chosen conventionally by rephasing $\mathfrak{a}_{\mathbf{p}\sigma}$, the same cannot independently also be done with $\bar{\eta}_t$ because the phase of $\bar{\mathfrak{a}}_{\mathbf{p}\sigma}$ relative to $\mathfrak{a}_{\mathbf{p}\sigma}$ has already been chosen to eliminate the phase ξ_0, as described below eq. (11.4.34). Repeating the same arguments as before one finds

$$\bar{\eta}_t = \eta_t^*. \tag{11.5.17}$$

Appendix C.4.3 also shows that $\mathcal{T}$ maps fields transforming in the representation (A,B) onto itself, with the field components transforming as

$$\mathcal{T}\;\psi_{\,ab}(x)\;\mathcal{T}^{-1} = \eta_t^*(-)^{A+B-a-b}\;\psi_{-a,-b}(x_t)\,. \tag{11.5.18}$$

Here $x_t^\mu = T^\mu{}_\nu x^\nu$ is the time-reversal Lorentz matrix as defined in (11.2.18).

One final comment on these transformations, C, P, and T is worthwhile. If these are not symmetry transformations there need not in general exist a unitary representation for them in the Hilbert space. Furthermore, since C and P map fields from the (A,B) to the (B,A) Lorentz representations their action need not be represented on the fields if the symmetry group should have complex representations, involving differing numbers of (A,B) and (B,A) fields. In this case, even though neither C or P need be individually defined on the fields, the joint combination CP – that maps (A,B) representations to themselves – typically is.

11.5.4 C, P and CP for particle-antiparticle systems

It happens that all three of the transformations C, P and T are found experimentally to be symmetries of the electomagnetic and strong interactions. As a result the charge conjugation and parity phases, η_c and η_p, are conserved multiplicative quantum numbers for electromagnetic and strongly-interacting systems.

For these systems the relations just derived between these quantum numbers for particles and antiparticles can be tested, because it has several physical implications. One of these is that the charge-conjugation and parity quantum numbers for bound systems of particle-antiparticle pairs — such as the e^+e^- bound state *positronium* for instance — are completely determined because the *a priori* arbitrary phases, η_c and η_p, for the constituents necessarily cancel between particle and antiparticle.

To explore these implications in detail suppose that the bound system is represented by the state $|\Psi\rangle$ in the Hilbert space. $|\Psi\rangle$ may be expanded in terms of a basis of many-particle states according to

$$|\Psi\rangle = \sum_{\sigma\sigma'} \int \frac{\mathrm{d}^3p\ \mathrm{d}^3p'}{(2\pi)^6} \psi(\mathbf{p},\sigma;\mathbf{p}',\sigma')\ \mathfrak{a}^*_{\mathbf{p}\sigma}\ \overline{\mathfrak{a}}^*_{\mathbf{p}',\sigma'}|\Omega\rangle + \cdots . \tag{11.5.19}$$

This expansion is generally very complicated and it is a difficult problem both to determine the wavefunction, $\psi(\mathbf{p},\sigma;\mathbf{p}',\sigma')$, as well as all of the other basis states in the expansion—represented above by the ellipses. The main point is that knowledge of the detailed form of these extra states is irrelevant because they all must share the same charge-conjugation and parity qunatum numbers if the interactions involved have these as symmetries.

The no-electron state, $|\Omega\rangle$, is typically a complicated state of the electromagnetic (or, for the strong interactions, gluon) fields. Its only property for the present purposes is that its parity and charge-conjugation quantum numbers are the same as those of the no-particle state, $|0\rangle$. The phase of $\mathcal{C}$ is defined conventionally by requiring that the no-particle state be invariant: $\mathcal{C}|0\rangle = |0\rangle$.

The action of $\mathcal{C}$ on this state is:

$$\begin{aligned}\mathcal{C}\ |\Psi\rangle &= \sum_{\sigma\sigma'} \int \frac{\mathrm{d}^3p\ \mathrm{d}^3p'}{(2\pi)^6} \psi(\mathbf{p},\sigma;\mathbf{p}',\sigma')\ \left[\mathcal{C}\ \mathfrak{a}^*_{\mathbf{p}\sigma}\ \mathcal{C}^{-1}\right]\ \left[\mathcal{C}\ \overline{\mathfrak{a}}^*_{\mathbf{p}',\sigma'}\ \mathcal{C}^{-1}\right]|\Omega\rangle + \cdots \\ &= (-)^{2\sigma}\eta_c\bar{\eta}_c \sum_{\sigma\sigma'} \int \frac{\mathrm{d}^3p\ \mathrm{d}^3p'}{(2\pi)^6} \psi(\mathbf{p},\sigma;\mathbf{p}',\sigma')\ \mathfrak{a}^*_{\mathbf{p}',\sigma'}\ \overline{\mathfrak{a}}^*_{\mathbf{p}\sigma}|\Omega\rangle + \cdots .\end{aligned} \tag{11.5.20}$$

The overall sign, $(-)^{2\sigma}$, arises from the interchange of order of the creation operators that has been performed in arriving at the last line. It keeps track of the statistics of the particles involved, inasmuch as it is a minus sign (as appropriate for fermions) whenver σ is half-odd integer and it is a plus sign (as for bosons) whenver σ is an integer.

Eq. (11.5.20) may be written in the form of (11.5.19), if the summation and integration variables are redefined according to $\sigma \leftrightarrow \sigma'$ and $\mathbf{p} \leftrightarrow \mathbf{p}'$, and if the wavefunction has the symmetry property: $\psi(\mathbf{p},\sigma;\mathbf{p}',\sigma') = \pm\psi(\mathbf{p}',\sigma';\mathbf{p},\sigma)$. If so then:

$$\mathcal{C}\ |\Psi\rangle = \pm(-)^{2\sigma}\eta_c\bar{\eta}_c|\Psi\rangle. \tag{11.5.21}$$

The symmetry or antisymmetry of the wavefunction with respect to interchange of its arguments is usually determined in terms of its other quantum numbers, such as orbital angular momentum, total spin, and so on.

The main point is that the microcausality condition (11.5.5) – *i.e.* $\overline{\eta}_c = \eta_c^*$ – implies the dependence on the phases, η_c and $\overline{\eta}_c$ drops out of the relation (11.5.21), making the eigenvalue for $\mathcal{C}$ an absolute prediction.

Consider for definiteness a bound state consisting of spin-half fermion-antifermion pairs, $|f\overline{f}\rangle$, such as electrons and positrons or quarks and antiquarks. In this case the statistics sign is $(-)^{2\sigma} = -1$. Also, in this case the fermion spins can combine into a total spin singlet, $s = 0$, or a spin triplet, $s = 1$. The spin combines with the orbital angular momentum, ℓ, to give the total bound-state angular momentum $j \in \{|\ell - s|, ..., \ell + s\}$.

The total spin also fixes the symmetry of the wavefunction under spin interchange, $\sigma \leftrightarrow \sigma'$, with the singlet ($S = 0$) combination being antisymmetric under this interchange while the triplet ($S = 1$) is symmetric: $\psi(\mathbf{p}, \sigma; \mathbf{p}', \sigma') = (-)^{S+1}\psi(\mathbf{p}, \sigma'; \mathbf{p}', \sigma)$. Similarly the orbital angular momentum quantum number $\ell = 0, 1, \cdots$ is correlated with the symmetry under interchange of momenta by $\psi(\mathbf{p}, \sigma; \mathbf{p}', \sigma') = (-)^{\ell}\psi(\mathbf{p}', \sigma; \mathbf{p}, \sigma')$. The symmetry of the complete wavefunction therefore becomes: $\psi(\mathbf{p}, \sigma; \mathbf{p}', \sigma') = (-)^{\ell+S+1}\psi(\mathbf{p}', \sigma'; \mathbf{p}, \sigma)$, and so

$$\mathcal{C}|f\overline{f}\rangle = (-)^{\ell+S}|f\overline{f}\rangle. \tag{11.5.22}$$

This prediction is listed for low-j states in Table 3.

ℓ	S	j	$\mathcal{C}$	$\mathcal{P}$	$\mathcal{CP}$
0	0	0	+	−	−
0	1	1	−	−	+
1	0	1	−	+	−
1	1	0,1,2	+	+	+

Table 3. C and P quantum numbers for spin-half particle-antiparticle states

An identical argument goes through for the parity quantum number, implying

$$\mathcal{P}\,|\Psi\rangle = \eta_p\bar{\eta}_p \sum_{\sigma\sigma'} \int \frac{\mathrm{d}^3p\,\mathrm{d}^3p'}{(2\pi)^6}\, \psi(-\mathbf{p}, \sigma; -\mathbf{p}', \sigma')\, \mathfrak{a}^*_{\mathbf{p}\sigma}\, \overline{\mathfrak{a}}^*_{\mathbf{p}'\sigma'}|\Omega\rangle + \dots \tag{11.5.23}$$

and so using $\psi(\mathbf{p}, \sigma; \mathbf{p}', \sigma') = (-)^{\ell}\psi(-\mathbf{p}, \sigma; -\mathbf{p}', \sigma')$ the prediction for a spin-half fermion-antifermion pair is

$$\mathcal{P}|f\overline{f}\rangle = (-)^{\ell}|f\overline{f}\rangle. \tag{11.5.24}$$

This prediction is also summarized for low-j states in Table 3. The first two rows of this table may also be recognized as the parity and charge-conjugation quantum numbers for the light spinless and spin-one strong-interaction mesons observed in nature. From the above discussion this may be taken as support for the hypothesis that these are bound states of spin-half quarks and antiquarks.

A similar classification goes through for positronium states, that are Hydrogenlike 'atoms' consisting of a bound electron-positron pair. For positronium the $\mathcal{C}$ and $\mathcal{P}$ quantum numbers have significant implications for their mean decay lifetimes. They do so because the ground-states of positronium — which have $\ell = 0$ though can have spins either in the $S = 0$ or $S = 1$ combination — primarily decay electromagnetically through the annihilation of the electron-positron pair into photons. It turns out (see below) that these photons are necessarily charge-conjugation odd, so we see that the $S = 0$ singlet state can decay to two photons while the triplet $S = 1$ state can only decay into an odd number of photons. Since decay into a single photon is forbidden by energy-momentum conservation, triplet decays involve at least three photons in the final state. Since the probability to emit each photon involves a suppression by a factor of the fine-structure constant $\alpha \approx 1/137$ we expect that the $S = 0$ state should have a much longer lifetime. This expectation is indeed borne out quantitatively by experiment.

It is noteworthy that the intrinsic parity and charge-conjugation of all known bound fermion-antifermion pairs is correctly given by the above table—an experimental fact that goes unexplained in non-relativistic quantum mechanics and whose success is part of the evidence for microcausality.

11.5.5 CPT

The final topic of this section is known as the *CPT Theorem*. This theorem states that the combined transformation CPT is always a symmetry for any local Lorentz-invariant theory, regardless of whether or not the individual discrete symmetries, C, P or T, are themselves separately symmetries. Since CPT acting on a particle state gives its antiparticle, t is this symmetry that can be regarded as being responsible for keeping particle and antiparticle masses equal.

The line of reasoning used to prove the theorem shows that any Lorentz-invariant and local polynomials of the fields is automatically CPT invariant. To establish this reasoning it is therefore necessary to discuss the construction of Lorentz-invariant local interactions and then compute their CPT-transformation properties.

Lorentz-invariant combinations of fields

Building Lorentz scalars from fields that transform in finite-dimensional representations of the Lorentz group is an exercise in $SU(2)$ group theory. Since the Lorentz generators are given by $\mathbf{J} = \mathbf{A} + \mathbf{B}$ and $\mathbf{K} = -i(\mathbf{A} - \mathbf{B})$ it is clear that a Lorentz scalar must be a scalar separately for each of the $SU(2)$ generators, A's and the B. The problem is to combine multinomials of the fields into a singlet representation having labels $A_{\rm tot} = B_{\rm tot} = 0$.

The general solution to this problem is easily written down using Clebsch-Gordan coefficients. The simplest two cases — bilinars and trilinears of fields — are described here for simplicity. The rules for combining angular momenta — or alternatively Schur's lemma —

imply that invariant bilinears of fields can only be constructed if both of the fields transform in the same representation of the Lorentz group.

Taking this resprentation to be the (A, B) one, the invariant bilinear then is

$$\text{Invariant } = \sum_{aba'b'} \psi^{AB}_{ab}\ \psi^{AB}_{a'b'}\ C_{AA}(0,0;a,a')\ C_{BB}(0,0;b,b')\,, \tag{11.5.25}$$

while the invariant trilinear combination of fields is given by:

$$\begin{aligned}\text{Invariant } = \sum_{b''} \psi^{A_1B_1}_{a_1b_1}\ \psi^{A_2B_2}_{a_2b_2}\ \psi^{A_3B_3}_{a_3b_3}\ C_{A_1A_2}(A_3,a;a_1,a_2)\ C_{A_3A_3}(0,0;a,a_3)\\ \times C_{B_1B_2}(B_3,b;b_1,b_2)\ C_{B_3B_3}(0,0;b_1b_3)\,,\end{aligned} \tag{11.5.26}$$

where the particular combination,

$$\sum_a C_{A_1A_2}(A_3,a;a_1,a_2)\ C_{A_3A_3}(0,0;a_1a_3) =: \begin{pmatrix} A_1 & A_2 & A_3 \\ a_1 & a_2 & a_3 \end{pmatrix}, \tag{11.5.27}$$

that appears in (11.5.26) is Wigner $3-j$ symbol.

The CPT Theorem

We can now establish that any Lorentz-invariant quantity like these must also be invariant under the combined action of CPT.

The action of C, P and T for *any* field transforming in the (A, B) representation as found in the previous sections is

$$\begin{aligned}[\mathcal{CPT}]\ \psi^{AB}_{ab}(x)\ [\mathcal{CPT}]^{-1} &= \mathcal{CPT}\ \psi^{AB}_{ab}(x)\ \mathcal{T}^{-1}\mathcal{P}^{-1}\mathcal{C}^{-1}\\ &= \eta_t(-)^{A+B-a-b}\ \mathcal{CP}\ \psi^{AB}_{-a,-b}(x_t)\ \mathcal{P}^{-1}\mathcal{C}^{-1}\\ &= \eta_t\eta_p(-)^{2A+2B-a-b-j}\ \mathcal{C}\ \psi^{BA}_{-b,-a}(-x)\ \mathcal{C}^{-1}\\ &= \eta_t\eta_p\eta_c(-)^{2A-2j}\psi^{*AB}_{ab}(-x)\\ &= \eta_t\eta_p\eta_c(-)^{2B}\ \psi^{*AB}_{ab}(-x),\end{aligned} \tag{11.5.28}$$

in which the last equality uses the identity $(-)^{2(A+B)} = (-)^{2j}$.

We now use our freedom to choose the time-reversal phase, η_t, to ensure that the combination $\eta_t\eta_p\eta_c = 1$ for each particle type. The factor of $(-)^{2B}$ cannot be similarly absorbed into this phase since η_t is the same for all of the fields which describe a given particle, not all of which need share the same value for B. With this convention the final result for the CPT-transformation law becomes

$$(\mathcal{CPT})\ \psi^{AB}_{ab}(x)\ (\mathcal{CPT})^{-1} = (-)^{2B}\psi^{*AB}_{ab}(-x). \tag{11.5.29}$$

Now comes the key observation. The transformation law just derived, eq. (11.5.29), must also hold for a multilinear combination of basic fields provided only that it transform in the

$(A_{\rm tot}, B_{\rm tot})$ Lorentz representation. This is because the Clebsch-Gordan coefficients which pick out the $(A_{\rm tot}, B_{\rm tot})$ representation out of the reduction of the product $(A_1, B_1) \otimes \cdots \otimes (A_n, B_n)$ ensure that $B_{\rm tot}$ differs from the sum $B_1 + \cdots + B_n$ by an integer and so the sign which appears in (11.5.29) satisfies $(-)^{2B_{\rm tot}} = \prod_i (-)^{2B_i}$.

In particular any Lorentz-invariant combination, such as the interaction density itself, must have $B_{\rm tot} = 0$ and so satisfies

$$(\mathcal{CPT})\ \mathcal{H}(x)\ (\mathcal{CPT})^{-1} = \mathcal{H}^*(-x), \tag{11.5.30}$$

and it immediately follows that the integrated interaction Hamiltonian, $H_{\rm int} = \int d^3\mathbf{r}\ \mathcal{H}(\mathbf{r}, 0)$, satisfies:

$$(\mathcal{CPT})\ H_{\rm int} (\mathcal{CPT})^{-1} = H^\star_{\rm int} = H_{\rm int}. \tag{11.5.31}$$

The last equality uses the hermiticity of $H_{\rm int}$, which follows because conservation of probability requires that the time evolution, e^{-iHt}, must be unitary. It follows that Lorentz-invariance and locality for interactions imply their invariance under CPT.

Precisely the same arguments imply that a four-vector current built from powers of fields has $B_{\rm tot} = \frac{1}{2}$ and so must satisfy

$$(\mathcal{CPT})\ J_\mu(x)\ (\mathcal{CPT})^{-1} = -J^*_\mu(-x), \tag{11.5.32}$$

and so on. Once applied to the density of a conserved charge, this shows very robustly why particles and antiparticles must have precisely charge eigenvalues.

For the S-matrix, since CPT is antiunitary its conservation has the same effect as does that of time-reversal. That is to say,

$$S_{\beta\alpha} = S_{\tilde\alpha\tilde\beta}, \tag{11.5.33}$$

where $|\tilde\alpha\rangle$ is defined as the CPT-conjugate of the uninteracting states: $\mathcal{CPT}|\alpha\rangle$. Notice, however, that for the full scattering states $\mathcal{CPT}$ takes in-states to out-states, *etc.*

In the particular case that the initial state, $|\alpha\rangle$, is a single-particle state two other general consequence of $\mathcal{CPT}$ invariance may be obtained. Suppose first that the final state is the same particle as the initial state. For this case $\mathcal{CPT}$ invariance implies that the masses of particles and antiparticles must precisely agree. Alternatively, summing over all possible final states for a single-particle initial state shows that particles and antiparticles must also have precisely equal total decay lifetimes. Since the summation over all possible final states is crucial to this argument it does *not* also follow that their partial decay rates into particular final states must also agree.

12 Relativistic spinless particle

This section explores some simple implications of the simplest relativstic field theory, describing a relativistic spinless particle. To this end we first considering a Hamiltonian that

describes noninteracting relativistic spinless particles, after which – in §12.2 and §12.3 – the implications of a few simple interactions are included.

12.1 Klein-Gordon system

At one level the Hamiltonian for the non-interacting Hamiltonian is easy to write down:

$$H_0 = E_0 + \int \mathrm{d}^3p\, \varepsilon(p)\, \mathfrak{a}^\star_{\mathbf{p}}\, \mathfrak{a}_{\mathbf{p}}\,, \tag{12.1.1}$$

where as usual $[\mathfrak{a}_{\mathbf{p}}\,, \mathfrak{a}^\star_{\mathbf{q}}] = \delta^3(\mathbf{p}-\mathbf{q})$ (and the quantization chosen in terms of commutators rather than anticommutators because the spin-statistics theorem requires spinless particles to be bosons). E_0 is the energy of the zero-particle state $|0\rangle$ that is defined by $\mathfrak{a}_{\mathbf{p}}|0\rangle = 0$ for all $\mathbf{p}$ and the only specifically relativistic choice arises in the single-particle energy, which is

$$\varepsilon(p) = \sqrt{\mathbf{p}^2 + m^2}\,, \tag{12.1.2}$$

corresponding to the 4-momentum satisfying $\eta_{\mu\nu}p^\mu p^\nu = -m^2$. The parameter m has the usual interpretation of being the particle's rest mass.

12.1.1 Local Hamiltonian

But at another level we know from §6 that H_0 should come as a local integral $H_0 = \int \mathrm{d}^3x\, \mathcal{H}_0(x)$ where the energy density $\mathcal{H}_0(x)$ is expressed using a relativistic spin-zero field, which can always be chosen to be a scalar $\psi(x)$. As described in detail in §11.4.2 the consistency of Lorentz-transformation properties of $\psi(x)$ and $\mathfrak{a}_{\mathbf{p}}$ imply that the relation between them must be expressed as in (11.4.17), repeated here:[46]

$$\psi(x) = \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \Big[\mathfrak{a}_{\mathbf{p}}\, e^{ip\cdot x} + \overline{\mathfrak{a}}^\star_{\mathbf{p}}\, e^{-ip\cdot x}\Big], \tag{12.1.3}$$

where $\bar{\mathfrak{a}}_{\mathbf{p}}$ is the destruction operator for the particle's antiparticle, and p^μ has time component $p^0 = \varepsilon(p)$.

The antiparticle is chosen to be a distinct species from the particle, and this becomes compulsory if the spinless particle of interest has electric charge since the arguments of §11.4.2 show that the particle and antiparticle must have opposite values for any additive charge. In these circumstances $\psi(x)$ cannot be hermitian: $\psi^\star(x) \neq \psi(x)$, and the free Hamiltonian must really take the form

$$H_0 = E_0 + \int \mathrm{d}^3p\, \varepsilon(p) \left(\mathfrak{a}^\star_{\mathbf{p}}\, \mathfrak{a}_{\mathbf{p}} + \overline{\mathfrak{a}}^\star_{\mathbf{p}}\, \overline{\mathfrak{a}}_{\mathbf{p}}\right). \tag{12.1.4}$$

Several observations guide our guess for the form of $\mathcal{H}(x)$. First, since the result (12.1.4) is bilinear in creation and annihilation operators we seek $\mathcal{H}$ also to be bilinear in ψ and $\psi^\star$.

[46] The conventional phase appearing in (11.4.17) is set to unity by absorbing it into the definition of the particle and antiparticle states (or creation operators).

Furthermore, since (12.1.4) is invariant under

$$\mathfrak{a}_{\mathbf{p}} \to e^{-iq\theta}\,\mathfrak{a}_{\mathbf{p}} \quad \text{and} \quad \bar{\mathfrak{a}}_{\mathbf{p}} \to e^{iq\theta}\,\bar{\mathfrak{a}}_{\mathbf{p}}\,, \tag{12.1.5}$$

for all $\mathbf{p}$ — with precisely opposite transformation phases for $\mathfrak{a}_{\mathbf{p}}$ and $\bar{\mathfrak{a}}_{\mathbf{p}}$ being required by consistency with (12.1.3) — we demand that $\mathcal{H}$ be invariant under

$$\psi(x) \to e^{-iq\theta}\,\psi(x)\,, \tag{12.1.6}$$

for all x (where, for now, θ does not depend on x). Finally, we take (as usual) the Hamiltonian to be the sum of a kinetic energy and a potential energy, $\mathcal{H}_0 = \mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{pot}}$, where the kinetic energy is quadratic in time derivatives and so $\mathcal{H}_{\text{kin}} = \partial_t\psi^\star\,\partial_t\psi$. Since static properties like the potential energy should not care about the relativistic or nonrelativistic kinematics, which are associated with motion, we take for the potential energy the same expression as was used for nonrelativistic fields. Comparing with expression (6.3.1) — using its integrated-by-parts form (6.2.2) — for the nonrelativistic Hamiltonian for a spinless particle interacting with a constant static potential $V(\mathbf{x}) = \varepsilon_0$, this suggests writing $\mathcal{H}_0 = \mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{pot}}$

$$H_0 = \int \mathrm{d}^3x \Big(\mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{pot}}\Big) = \int \mathrm{d}^3x \Big[\rho_0 + \partial_t\psi^\star\,\partial_t\psi + Z\nabla\psi^\star\cdot\nabla\psi + \varepsilon_0\psi^\star\psi\Big]\,, \tag{12.1.7}$$

where the parameters Z, ε_0 and ρ_0 are chosen to reproduce (12.1.4).

Plugging (12.1.3) into (12.1.7) shows that agreement with (12.1.4) turns out to require $Z = 1$ and $\varepsilon_0 = m^2$, as may be seen using the intermediate steps

$$\begin{aligned}
\partial_t\psi(x) &= \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\Big[-i\varepsilon(p)\,\mathfrak{a}_{\mathbf{p}}\,e^{ip\cdot x} + i\varepsilon(p)\,\bar{\mathfrak{a}}^\star_{\mathbf{p}}\,e^{-ip\cdot x}\Big] \\
\nabla\psi(x) &= \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\Big[i\mathbf{p}\,\mathfrak{a}_{\mathbf{p}}\,e^{ip\cdot x} - i\mathbf{p}\,\bar{\mathfrak{a}}^\star_{\mathbf{p}}\,e^{-ip\cdot x}\Big]\,,
\end{aligned} \tag{12.1.8}$$

and

$$\begin{aligned}
\int \mathrm{d}^3x\;\psi^\star\psi &= \int \frac{\mathrm{d}^3p}{2\varepsilon(p)}\left[\bar{\mathfrak{a}}_{\mathbf{p}}\mathfrak{a}_{-\mathbf{p}}e^{-2i\varepsilon(p)t} + \mathfrak{a}^\star_{\mathbf{p}}\bar{\mathfrak{a}}^\star_{-\mathbf{p}}e^{+2i\varepsilon(p)t} + \frac{1}{2}\{\bar{\mathfrak{a}}_{\mathbf{p}},\bar{\mathfrak{a}}^\star_{\mathbf{p}}\} + \frac{1}{2}\{\mathfrak{a}_{\mathbf{p}},\mathfrak{a}^\star_{\mathbf{p}}\}\right] \\
\int \mathrm{d}^3x\;\partial_t\psi^\star\partial_t\psi &= \int \frac{\mathrm{d}^3p}{2\varepsilon(p)}\,[\varepsilon(p)]^2\left[-\bar{\mathfrak{a}}_{\mathbf{p}}\mathfrak{a}_{-\mathbf{p}}e^{-2i\varepsilon(p)t} - \mathfrak{a}^\star_{\mathbf{p}}\bar{\mathfrak{a}}^\star_{-\mathbf{p}}e^{+2i\varepsilon(p)t} + \frac{1}{2}\{\bar{\mathfrak{a}}_{\mathbf{p}},\bar{\mathfrak{a}}^\star_{\mathbf{p}}\} + \frac{1}{2}\{\mathfrak{a}_{\mathbf{p}},\mathfrak{a}^\star_{\mathbf{p}}\}\right] \\
\int \mathrm{d}^3x\;\nabla\psi^\star\cdot\nabla\psi &= \int \frac{\mathrm{d}^3p}{2\varepsilon(p)}\,\mathbf{p}^2\left[\bar{\mathfrak{a}}_{\mathbf{p}}\mathfrak{a}_{-\mathbf{p}}e^{-2i\varepsilon(p)t} + \mathfrak{a}^*_{\mathbf{p}}\bar{\mathfrak{a}}^\star_{-\mathbf{p}}e^{+2i\varepsilon(p)t} + \frac{1}{2}\{\bar{\mathfrak{a}}_{\mathbf{p}},\bar{\mathfrak{a}}^\star_{\mathbf{p}}\} + \frac{1}{2}\{\mathfrak{a}_{\mathbf{p}},\mathfrak{a}^\star_{\mathbf{p}}\}\right]
\end{aligned} \tag{12.1.9}$$

,

and so on. In these expressions the operator ordering $AB \to \frac{1}{2}\{A,B\} = \frac{1}{2}(AB + BA)$ is used when passing from classical to quantum variables, in order to preserve the hermiticity of the

result. When $Z = 1$ and $\varepsilon_0 = m^2$ we have

$$\begin{aligned}\int \mathrm{d}^3x\,\Big[\partial_t\psi^*\partial_t\psi + \nabla\psi^*\cdot\nabla\psi + m^2\psi^*\psi\Big] \\ &= \int\frac{\mathrm{d}^3p}{2\varepsilon(p)}\,\Big[(-[\varepsilon(p)]^2+\mathbf{p}^2+m^2)\Big(\mathfrak{a}_{\mathbf{p}}\mathfrak{a}_{-\mathbf{p}}e^{-2i\varepsilon(p)t}+\mathfrak{a}^\star_{\mathbf{p}}\bar{\mathfrak{a}}^\star_{-\mathbf{p}}e^{+2i\varepsilon(p)t}\Big) \\ &\qquad +([\varepsilon(p)]^2+\mathbf{p}^2+m^2)\left(\frac{1}{2}\{\bar{\mathfrak{a}}_{\mathbf{p}},\bar{\mathfrak{a}}^\star_{\mathbf{p}}\}+\frac{1}{2}\{\mathfrak{a}_{\mathbf{p}},\mathfrak{a}^\star_{\mathbf{p}}\}\right)\Big] \\ &= \frac{1}{2}\int\mathrm{d}^3p\Big[\varepsilon(p)\Big(\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{p}}+\mathfrak{a}_{\mathbf{p}}\mathfrak{a}^\star_{\mathbf{p}}\Big)+\varepsilon(p)\Big(\bar{\mathfrak{a}}^\star_{\mathbf{p}}\bar{\mathfrak{a}}_{\mathbf{p}}+\bar{\mathfrak{a}}_{\mathbf{p}}\bar{\mathfrak{a}}^\star_{\mathbf{p}}\Big)\Big]\,.\end{aligned} \tag{12.1.10}$$

We see that when $Z = 1$ and $\varepsilon_0 = m^2$ the Hamiltonian (12.1.7) becomes

$$H_0 = \int\mathrm{d}^3x\Big(\mathcal{H}_{\rm kin}+\mathcal{H}_{\rm pot}\Big) = \int\mathrm{d}^3x\Big[\rho_0+\partial_t\psi^\star\,\partial_t\psi+\nabla\psi^\star\cdot\nabla\psi+m^2\psi^\star\psi\Big]\,, \tag{12.1.11}$$

and produces precisely the form of (12.1.4) once we use (12.1.3) as well as $\mathfrak{a}_{\mathbf{p}}\,\mathfrak{a}^\star_{\mathbf{p}} = \mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{p}}+\delta^3(0)$ and similarly for $\bar{\mathfrak{a}}_{\mathbf{p}}\,\bar{\mathfrak{a}}^\star_{\mathbf{p}}$. The agreement works, provided we identify the ground state energy as

$$E_0 = \int\mathrm{d}^3x\;\rho_0+\delta^3(0)\int\mathrm{d}^3p\;\varepsilon(p) = \mathcal{V}\left[\rho_0+\int\frac{\mathrm{d}^3p}{(2\pi)^3}\;\varepsilon(p)\right]\,, \tag{12.1.12}$$

which uses $\delta^3(0) = \mathcal{V}/(2\pi)^3$. This shows the ground state energy is extensive — *i.e.* is proportional to the system volume $\mathcal{V}$ — and that the physical vacuum energy density, $E_0/\mathcal{V}$, is finite once the divergent integral over d^3p is absorbed into the unknown parameter ρ_0.

12.1.2 Commutation relations

Although the Hamiltonian (12.1.4) produces a relativistic single-particle energy (12.1.2), it does not look at face value all that relativistic. It is a useful exercise the check Lorentz covariance, such as by computing the field equation in the Heisenberg picture and verifying that it takes the same form in all intertial reference frames. That is, the field equations should be expressible in terms of Lorentz tensors, as defined in §11.1.4.

To this end first compute the equal-time commutation relations. The commutator of the field with its adjoint is computed in §11.4.2, with the result

$$\begin{aligned}\Big[\psi(x),\psi^\star(y)\Big] = \Delta(x-y) &= 0 && \text{if}\quad (x-y)^2>0\,, \\ &= \frac{im^2}{4\pi z}\,\mathrm{sign}\,\big(z^0\big)\;J_1(z) && \text{if}\;\;(x-y)^2<0\,,\end{aligned} \tag{12.1.13}$$

where $z^0 = x^0-y^0$ and $z = m\sqrt{-(x-y)^2}$. In particular $[\psi(\mathbf{x},t)\,,\psi^\star(\mathbf{y},t)] = [\psi(\mathbf{x},t)\,,\psi(\mathbf{y},t)] = 0$ at equal times. The equal-time commutator between ψ and $\partial_t\psi^\star$ can be computed from

scratch using (12.1.3) and (12.1.8) with $[\mathfrak{a}_{\mathbf{p}}\,,\mathfrak{a}^\star_{\mathbf{q}}]=\delta^3(\mathbf{p}-\mathbf{q})$, leading to $[\psi(\mathbf{x},t)\,,\partial_t\psi(\mathbf{y},t)]=0$ and

$$\begin{aligned}\Big[\psi(\mathbf{x},t)\,,\partial_t\psi^\star(\mathbf{y},t)\Big] &= \int \frac{\mathrm{d}^3q}{\sqrt{(2\pi)^3 2\varepsilon(q)}}\frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \\ &\qquad\times\Big[\Big(\mathfrak{a}_{\mathbf{q}}\,e^{iq\cdot x}+\bar{\mathfrak{a}}^\star_{\mathbf{q}}\,e^{-iq\cdot x}\Big)\,,i\varepsilon(p)\Big(\mathfrak{a}^\star_{\mathbf{p}}\,e^{-ip\cdot y}-\bar{\mathfrak{a}}_{\mathbf{p}}\,e^{ip\cdot y}\Big)\Big] \\ &= i\int\frac{\mathrm{d}^3p}{2(2\pi)^3}\Big[e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}+e^{i\mathbf{p}\cdot(\mathbf{y}-\mathbf{x})}\Big]=i\delta^3(\mathbf{x}-\mathbf{y})\,. \end{aligned} \tag{12.1.14}$$

Using these explicit expressions in the Heisenberg-picture field equation (3.2.4), $\partial_t\mathcal{O}_h = i\Big[H,\mathcal{O}_h\Big]$, gives (for ψ) a tautology

$$\partial_t\psi(\mathbf{x},t)=i\Big[H_0,\psi(\mathbf{x},t)\Big]=i\int\mathrm{d}^3y\,\Big[\partial_t\psi^\star\partial_t\psi(\mathbf{y},t)\,,\psi(\mathbf{x},t)\Big]=\partial_t\psi(\mathbf{x},t)\,. \tag{12.1.15}$$

as well as (for $\partial_t\psi$) the field equation

$$\begin{aligned}\partial_t^2\psi(\mathbf{x},t) &= i\Big[H_0,\partial_t\psi(\mathbf{x},t)\Big]=i\int\mathrm{d}^3y\,\Big[\nabla\psi^\star\cdot\nabla\psi(\mathbf{y},t)+m^2\psi^\star\psi(\mathbf{y},t)\,,\partial_t\psi(\mathbf{x},t)\Big] \\ &= \nabla^2\psi(\mathbf{x},t)-m^2\psi(\mathbf{x},t)\,. \end{aligned} \tag{12.1.16}$$

which uses

$$\Big[\nabla\psi(\mathbf{x},t)\,,\partial_t\psi^\star(\mathbf{x}',t)\Big]=\nabla\Big[\psi(\mathbf{x},t)\,,\partial_t\psi^\star(\mathbf{x}',t)\Big]=i\nabla\delta^3(\mathbf{x}-\mathbf{x}')\,, \tag{12.1.17}$$

where ∇ denotes differentiation with respect to $\mathbf{x}$ (and ∇' similarly represents differentiation with respect to $\mathbf{x}'$). The field equation (12.1.16) – called the Klein-Gordon equation – can indeed be written in a manifestly covariant tensor form by defining the 4-vector $\partial_\mu\psi(x)$ whose time component is $\partial_t\psi$ and whose space components are $\nabla\psi$. In terms of these (12.1.16) becomes

$$-\partial_t^2\psi+\nabla^2\psi-m^2\psi=\eta^{\mu\nu}\partial_\mu\partial_\nu\psi-m^2\psi=:(\Box-m^2)\psi\,, \tag{12.1.18}$$

where the last equality defines the d'Alembertian differential operator (the relativistic generalization of the Laplace operator $\nabla^2=\nabla\cdot\nabla$).

12.1.3 Conserved current

Notice that the following 4-vector quantity,

$$J_\mu=iq\Big(\psi\,\partial_\mu\psi^\star-\psi^\star\,\partial_\mu\psi\Big) \tag{12.1.19}$$

is conserved in the sense that it satisfies

$$\partial_\mu J^\mu=\partial_t J^0+\nabla\cdot\mathbf{J}=-\partial_t J_0+\nabla\cdot\mathbf{J}=0\,, \tag{12.1.20}$$

whenever ψ satisfies the Klein Gordon equation. This equation expresses conservation in the way described earlier for (8.2.7), where it was also stated that such currents arise whenever a system has a continuous symmetry. In the present instance the symmetry responsible for the conservation of J^μ is the symmetry $\psi \to e^{-i\theta}\psi$ enjoyed by H_0. (A constructive derivation of the conserved current given such a symmetry is given below in §13.3.)

Exercise: Using the hermitian replacement $AB \to \frac{1}{2}(AB + BA)$ to evaluate the charge operator

$$Q = \int \mathrm{d}^3x\; J^0 = iq \int \mathrm{d}^3x \Big[\psi^\star\, \partial_t\psi - \psi\, \partial_t\psi^\star\Big] \tag{12.1.21}$$

as a function of creation and annihilation operators, and thereby show that it can be written

$$Q = q \int \mathrm{d}^3p \left(\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{p}} - \bar{\mathfrak{a}}^\star_{\mathbf{p}}\bar{\mathfrak{a}}_{\mathbf{p}}\right). \tag{12.1.22}$$

Prove the commutation relations $[Q\,,\mathfrak{a}_{\mathbf{p}}] = -q\,\mathfrak{a}_{\mathbf{p}}$ while $[Q\,,\bar{\mathfrak{a}}_{\mathbf{p}}] = +q\,\bar{\mathfrak{a}}_{\mathbf{p}}$ and $[Q\,,\psi(\mathbf{x},t)] = -q\,\psi(\mathbf{x},t)$. These respectively show that $\mathfrak{a}_{\mathbf{p}}$ destroys a particle with charge q, $\bar{\mathfrak{a}}_{\mathbf{p}}$ destroys a particle of charge $-q$ and that Q is the generator of the symmetry $\delta\psi = -iq\psi$ that is the infinitesimal version of $U(\theta)\psi\,U^{-1}(\theta) = e^{-iq\theta}\psi$ where $U(\theta) = \exp(i\theta Q)$.

For later purposes it is useful to express the current operator $J_\mu(\mathbf{x},t)$ in terms of creation and annihilation operators

$$J_\mu(x) = q\int \frac{\mathrm{d}^3k\,\mathrm{d}^3p}{2(2\pi)^3\sqrt{\varepsilon(k)\varepsilon(p)}}\Big[\frac{1}{2}\{\mathfrak{a}^\star_{\mathbf{k}}\,,\mathfrak{a}_{\mathbf{p}}\}(p+k)_\mu e^{i(p-k)\cdot x} - \frac{1}{2}\{\bar{\mathfrak{a}}_{\mathbf{k}}\,,\bar{\mathfrak{a}}^\star_{\mathbf{p}}\}(p+k)_\mu e^{i(p-k)\cdot x} + \bar{\mathfrak{a}}_{\mathbf{k}}\mathfrak{a}_{\mathbf{p}}(p-k)_\mu e^{i(p+k)\cdot x} - \mathfrak{a}^\star_{\mathbf{k}}\bar{\mathfrak{a}}^\star_{\mathbf{p}}(p-k)_\mu e^{-i(p+k)\cdot x}\Big], \tag{12.1.23}$$

where care is taken to write all products of non-commuting operators in the hermitian combination $AB \to \frac{1}{2}(AB+BA)$. Notice that the 'zero-point' contributions proportional to $[\mathfrak{a}^\star_{\mathbf{k}},\mathfrak{a}_{\mathbf{p}}]$ and $[\bar{\mathfrak{a}}_{\mathbf{k}},\bar{\mathfrak{a}}^\star_{\mathbf{p}}]$ cancel here between particle and antiparticle (unlike for the energy), leaving

$$J_\mu(x) = q\int \frac{\mathrm{d}^3k\,\mathrm{d}^3p}{2(2\pi)^3\sqrt{\varepsilon(k)\varepsilon(p)}}\Big[\mathfrak{a}^\star_{\mathbf{k}}\mathfrak{a}_{\mathbf{p}}(p+k)_\mu e^{i(p-k)\cdot x} - \bar{\mathfrak{a}}^\star_{\mathbf{p}}\bar{\mathfrak{a}}_{\mathbf{k}}(p+k)_\mu e^{i(p-k)\cdot x} + \mathfrak{a}_{\mathbf{k}}\mathfrak{a}_{\mathbf{p}}(p-k)_\mu e^{i(p+k)\cdot x} - \bar{\mathfrak{a}}^\star_{\mathbf{k}}\bar{\mathfrak{a}}^\star_{\mathbf{p}}(p-k)_\mu e^{-i(p+k)\cdot x}\Big], \tag{12.1.24}$$

Eq. (12.1.24) shows in particular that the matrix element of $J_\mu(x)$ within the single-particle states $|\mathbf{p}\rangle := \mathfrak{a}^\star_{\mathbf{p}}|0\rangle$ and single-antiparticle states $|\overline{\mathbf{p}}\rangle := \bar{\mathfrak{a}}^\star_{\mathbf{p}}|0\rangle$ is given by

$$\langle\mathbf{k}|J_\mu(x)|\mathbf{p}\rangle = -\langle\overline{\mathbf{k}}|J_\mu(x)|\overline{\mathbf{p}}\rangle = \frac{q}{2(2\pi)^3\sqrt{\varepsilon(k)\varepsilon(p)}}\,(p+k)_\mu\; e^{i(p-k)\cdot x}\,. \tag{12.1.25}$$

The diagonal matrix elements of the charge density and the spatial current become

$$\begin{aligned} \langle \mathbf{p}|J^0(x)|\mathbf{p}\rangle \;&=\; -\langle \overline{\mathbf{p}}|J^0(x)|\overline{\mathbf{p}}\rangle \;=\; \frac{q}{(2\pi)^3} \\ \text{and}\quad \langle \mathbf{p}|\mathbf{J}(x)|\mathbf{p}\rangle \;&=\; -\langle \overline{\mathbf{p}}|\mathbf{J}(x)|\overline{\mathbf{p}}\rangle \;=\; \frac{q}{(2\pi)^3}\,\frac{\mathbf{p}}{\varepsilon(p)} \;=\; \frac{q\,\mathbf{v}}{(2\pi)^3}\,, \end{aligned} \tag{12.1.26}$$

which uses the relativistic relation between velocity, momentum and energy: $\mathbf{v} = \mathbf{p}/\varepsilon(p)$. In particular notice that the current carried by antiparticles (in units of q) is in the opposite direction from their momenta and velocities.

12.2 Local self-interactions

It is instructive to examine simple kinds of interactions for relativistic particles. This section explores the implications of two particularly simple kinds of such interactions: interactions of spinless charged particles with background potentials and their self-interactions. (Electromagnetic interactions are discussed in §14.1 below.) Both of these types of interactions lend themselves to analysis using tools similar to the ones already presented for non-relativistic particles (such as the perturbative methods introduced in §3 or the exploitation of redefinitions along the lines of the Bogoliubov transformations of §7.2).

As discussed in §11.4.1, a sufficient condition for an interaction to be Lorentz invariant is if the interaction-Hamiltonian density is a Lorentz scalar:

$$H_{\text{int}} = \int \mathrm{d}^3x\; \mathcal{H}(x) \quad \text{with} \quad U(\Lambda)\,\mathcal{H}(x)\,U^{-1}(\Lambda) = \mathcal{H}(\Lambda x)\,, \tag{12.2.1}$$

provided $\mathcal{H}$ is built from microcausal fields like (12.1.3). As later sections show, this condition is by no means necessary. A simple example of an interaction of this type for a scalar field might be given by a local function of ψ itself $\mathcal{H} = \mathcal{H}(\psi, \psi^\star)$, such as

$$H_{\text{int}} = \int \mathrm{d}^3x\; \left\{ \frac{\lambda}{4}\big[\psi^\star(x)\psi(x)\big]^2 + \Big[\frac{g}{4!}\;\psi^4 + \text{c.c.}\Big] \right\}, \tag{12.2.2}$$

for some real coupling λ and some complex coupling g. (Couplings like λ and g usually satisfy some positivity conditions to the extent that the total Hamiltonian, H, is to be bounded from below.) The two representative couplings shown in (12.2.2) are chosen to illustrate the point that some couplings (*e.g.* λ) might preserve the symmetry $\psi \to e^{i\theta}\psi$ that the Klein-Gordon Hamiltonian (12.1.11) has, while others (*e.g.* g) do not. In what follows only the coupling λ plays a role.

Worked example: $\psi - \psi$ scattering

As an illustration of how the implications of this type of interaction can be extracted, imagine using the interaction (12.2.1) to compute the leading contribution to 2-body scattering of our charged scalars — such as the reaction $\psi(p) + \psi(q) \to \psi(k) + \psi(l)$ where $p^\mu = \{\varepsilon(p), \mathbf{p}\}$ denotes the 4-momentum of

particle called $\psi(p)$ and so on. Imagine doing so perturbatively in $H_{\rm int}$, starting off with the Born-approximation prediction. The relevant matrix element (keeping in mind the continuum normalization used in (12.1.3)) is

$$\begin{aligned}\langle \mathbf{k}\,,\mathbf{l}|H_{\rm int}|\mathbf{p},\mathbf{q}\rangle &= \frac{\lambda}{4}\int \mathrm{d}^3x\ \langle \mathbf{k}\,,\mathbf{l}|[\psi^\star(x)\psi(x)]^2|\mathbf{p}\,,\mathbf{q}\rangle \\ &= 4\times\frac{\lambda}{4}\,\frac{1}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\frac{1}{\sqrt{(2\pi)^3 2\varepsilon(q)}}\frac{1}{\sqrt{(2\pi)^3 2\varepsilon(k)}}\frac{1}{\sqrt{(2\pi)^3 2\varepsilon(l)}}\int \mathrm{d}^3x\ e^{i(p+q-k-l)\cdot x} \\ &= \frac{\lambda}{(2\pi)^3}\,\frac{1}{\sqrt{2\varepsilon(p)2\varepsilon(q)2\varepsilon(k)2\varepsilon(l)}}\,\delta^3(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l})\end{aligned} \tag{12.2.3}$$

which uses the matrix elements (*c.f.* eq. (12.1.3))

$$\langle \mathbf{p}|\psi^\star(x)|0\rangle = \frac{e^{-ip\cdot x}}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \quad\text{and}\quad \langle 0|\psi(x)|\mathbf{p}\rangle = \frac{e^{ip\cdot x}}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\,, \tag{12.2.4}$$

and where the overall factor of $4 = 2\times 2$ comes from the two choices for the two initial particles that could be destroyed by any one field $\psi(x)$ and the two final particles that can be created by each $\psi^\star(x)$. The factor of $\frac{1}{4}\lambda\int \mathrm{d}^3x$ similarly comes from the definition of $H_{\rm int}$.

Using (12.2.3) in Fermi's Golden Rule then gives the reaction rate

$$\begin{aligned}\mathrm{d}\Gamma_{\rm tot} &= 2\pi\Big|(\mathbf{k}\,,\mathbf{l}|H_{\rm int}|\mathbf{p},\mathbf{q})\Big|^2\delta[\varepsilon(p)+\varepsilon(q)-\varepsilon(k)-\varepsilon(l)]\,\mathrm{d}n \\ &= \frac{(2\pi)^4}{\mathcal{V}}\,\frac{\lambda^2\delta^4(p+q-k-l)}{[(2\pi)^3 2\varepsilon(p)][(2\pi)^3 2\varepsilon(q)]}\left[\frac{\mathrm{d}^3k}{(2\pi)^3 2\varepsilon(k)}\right]\left[\frac{\mathrm{d}^3l}{(2\pi)^3 2\varepsilon(l)}\right],\end{aligned} \tag{12.2.5}$$

where $\delta^4(p-q) = \delta^3(\mathbf{p}-\mathbf{q})\,\delta(p^0-q^0)$ expresses conservation of 4-momentum. Although the $\mathcal{V}$-dependence here may look odd, it agrees with what would have been obtained if the scattering were to have taken place in the presence of an initial distribution of paticles with phase-space densities $f(\mathbf{p})$ – normalized so that $N/\mathcal{V} = \int \mathrm{d}^3p\, f(\mathbf{p})/(2\pi)^3$ – which gives

$$\begin{aligned}\mathrm{d}\Gamma_{\rm tot} &= 2\pi\Big|(N(\mathbf{k})\,,N(\mathbf{l})|H_{\rm int}|N(\mathbf{p})\,,N(\mathbf{q}))\Big|^2\delta[\varepsilon(p)+\varepsilon(q)-\varepsilon(k)-\varepsilon(l)]\,\mathrm{d}n \\ &= \frac{\lambda^2\mathcal{V}}{(2\pi)^2}\,\delta^4(p+q-k-l)\left[f(\mathbf{p})\frac{\mathrm{d}^3p}{(2\pi)^3 2\varepsilon(p)}\right]\left[f(\mathbf{q})\frac{\mathrm{d}^3q}{(2\pi)^3 2\varepsilon(q)}\right] \\ &\qquad\times\left[(1+f(\mathbf{k}))\frac{\mathrm{d}^3k}{(2\pi)^3 2\varepsilon(k)}\right]\left[(1+f(\mathbf{l}))\frac{\mathrm{d}^3l}{(2\pi)^3 2\varepsilon(l)}\right].\end{aligned} \tag{12.2.6}$$

The total rate is then proportional to the system volume, as it must be for a translation-invariant system, and the previous result is obtained assuming only two particles are initially present: $f(\mathbf{p}) = [(2\pi)^3/\mathcal{V}]\,\delta^3(\mathbf{p}-\mathbf{p}_0)$ and $f(\mathbf{q}) = [(2\pi)^3/\mathcal{V}]\,\delta^3(\mathbf{q}-\mathbf{q}_0)$ together with $f(\mathbf{k}) = f(\mathbf{l}) = 0$. The differential collision rate per particle with momentum $\mathbf{p}$ is then obtained by dividing $\mathrm{d}\Gamma_{\rm tot}$ by $\mathcal{V}f(\mathbf{p})\,\mathrm{d}^3p/(2\pi)^3$ and so is well-behaved as $\mathcal{V}\to\infty$:

$$\begin{aligned}\mathrm{d}\Gamma_{\rm pp} &= \frac{\lambda^2}{(2\pi)^2}\,\delta^4(p+q-k-l)\,\frac{1}{2\varepsilon(p)}\left[f(\mathbf{q})\frac{\mathrm{d}^3q}{(2\pi)^3 2\varepsilon(q)}\right] \\ &\qquad\times\left[(1+f(\mathbf{k}))\frac{\mathrm{d}^3k}{(2\pi)^3 2\varepsilon(k)}\right]\left[(1+f(\mathbf{l}))\frac{\mathrm{d}^3l}{(2\pi)^3 2\varepsilon(l)}\right].\end{aligned} \tag{12.2.7}$$

The factor of $1/\varepsilon(p)$ is precisely what is required to have the time-scale set by $\mathrm{d}\Gamma_{\rm pp}$ time-dilate properly due to the motion of the particle with momentum $\mathbf{p}$.

The cross section is then obtained by starting with (12.2.5) and defining $\mathrm{d}\sigma = \mathrm{d}\Gamma_{\rm tot}/F$ where F is chosen to agree with the particle flux in the rest-frame of one of the initial particles, and is also chosen to transform in such a way as to ensure that $\mathrm{d}\sigma$ is Lorentz invariant (and so is agreed on by all inertial observers). Because $\mathrm{d}^3k/\varepsilon(k)$ is Lorentz invariant, the second requirement says $F = \mathcal{F}/[\mathcal{V}\varepsilon(p)\varepsilon(q)]$ where $\mathcal{F}$ is a Lorentz scalar. Since the particle flux is its density ($n = 1/\mathcal{V}$) times their relative velocity, $v_{\rm rel}$, the first requirement then says $\mathcal{F} = v_{\rm rel}(-p\cdot q)$. This works because $-p\cdot q = -\eta_{\mu\nu}p^\mu q^\nu$ equals $\varepsilon(p)\varepsilon(q)$ in the rest frame of p^μ or q^μ and the relative speed between two particles of equal mass is Lorentz invariant and is given by

$$v_{\rm rel} = \sqrt{1 - \frac{m^4}{(p\cdot q)^2}}\,. \tag{12.2.8}$$

The result is the manifestly Lorentz-invariant expression

$$\mathrm{d}\sigma = \frac{\lambda^2}{4(2\pi)^2\mathcal{F}}\,\delta^4(p+q-k-l)\left[\frac{\mathrm{d}^3k}{(2\pi)^3 2\varepsilon(k)}\right]\left[\frac{\mathrm{d}^3l}{(2\pi)^3 2\varepsilon(l)}\right]. \tag{12.2.9}$$

12.2.1 Crossing symmetry

It is instructive to compute the rate for processes that are related to the one just computed by changing particle to antiparticle. For instance imagine computing the rate for $2 \to 2$ antiparticle scattering, $\overline{\psi}(p)+\overline{\psi}(q) \to \overline{\psi}(k)+\overline{\psi}(l)$, or for the process $\psi(p)+\overline{\psi}(q) \to \psi(l)+\overline{\psi}(k)$. These all turn out to have the same amplitude due to the fact that both $a_{\mathbf{p}}$ and $\bar{a}^\star_{\mathbf{p}}$ enter $\psi(x)$ with the same relative weight, as may be seen by comparing (12.2.4) to

$$\langle\overline{\mathbf{p}}|\psi(x)|0\rangle = \frac{e^{-ip\cdot x}}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \quad\text{and}\quad \langle 0|\psi^\star(x)|\overline{\mathbf{p}}\rangle = \frac{e^{ip\cdot x}}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\,, \tag{12.2.10}$$

where $|\overline{\mathbf{p}}\rangle := \bar{a}^\star_{\mathbf{p}}|0\rangle$ just as $|\mathbf{p}\rangle := a^\star_{\mathbf{p}}|0\rangle$.

For example, repeating the calculation that led to (12.2.3) for these other processes leads to the results

$$\begin{aligned}\langle\mathbf{k}\,,\mathbf{l}|H_{\rm int}|\mathbf{p},\mathbf{q}\rangle &= \frac{\lambda}{4}\int \mathrm{d}^3x\,\langle\mathbf{k}\,,\mathbf{l}|[\psi^\star(x)\psi(x)]^2|\mathbf{p}\,,\mathbf{q}\rangle = \frac{\lambda}{(2\pi)^3}\,\frac{\delta^3(\mathbf{p}+\mathbf{q}-\mathbf{k}-\mathbf{l})}{\sqrt{2\varepsilon(p)2\varepsilon(q)2\varepsilon(k)2\varepsilon(l)}}\\ &= \langle\overline{\mathbf{k}}\,,\overline{\mathbf{l}}|H_{\rm int}|\overline{\mathbf{p}},\overline{\mathbf{q}}\rangle = \langle\overline{\mathbf{k}}\,,\mathbf{l}|H_{\rm int}|\mathbf{p},\overline{\mathbf{q}}\rangle\,,\end{aligned} \tag{12.2.11}$$

implying immediately that the cross sections for these processes are all equal at this order and given by (12.2.9). This relation between the amplitudes for processes that differ by substituting particles and antiparticles is known as *crossing symmetry*.

12.3 Couplings to background fields

Another informative example considers a relativistic particle interacting with a fixed background potential, such as in

$$H_{\rm int} = \int \mathrm{d}^3x\,U(\mathbf{x})\,\psi^\star(x)\psi(x)\,, \tag{12.3.1}$$

where $U(\mathbf{x})$ is regarded to be a known explicit function of position. Although the implications of this kind of interaction can also be treated perturbatively in powers of U, because $H_{\rm int}$ is bilinear in ψ and $\psi^\star$ it is also possible do better than this. In this case it is often possible to explicitly diagonalize the entire Hamiltonian $H = H_0 + H_{\rm int}$, sometimes through use of a Bogoliubov transformation along the lines considered in §7.2.

12.3.1 Modified mode functions

The background field $U(\mathbf{x})$ breaks translation invariance — and so makes momentum no longer be conserved — and this makes momentum less useful as a label for single-particle setates. Experience with the Schrödinger field in §6.3 suggests that the full Hamiltonian

$$H = H_0 + H_{\rm int} = \int \mathrm{d}^3x \Big[\rho_0 + \partial_t\psi^\star\,\partial_t\psi + \nabla\psi^\star\cdot\nabla\psi + U(\mathbf{x})\psi^\star\psi\Big]\,, \tag{12.3.2}$$

might be put into the standard single-particle oscillator form by generalizing (12.1.3) to a more appropriate mode expansion of the form

$$\psi(x) = \sum_n \Big[a_n\, u_n(x) + \overline{a}^\star_n\, u^*_n(x)\Big], \tag{12.3.3}$$

for some choice of mode functions $u_n(x)$ whose properties are to be determined. In particular, since the a_n's and $\bar a_n$'s are intended to destroy single-particle energy eigenstates in the presence of the potential, we may assume $i\partial_t u_n(x) = \varepsilon_n\, u_n(x)$ for some choice of ε_n.

Plugging (12.3.3) into (12.3.2) helps determine the properties of $u_n(x)$, as follows. Writing

$$\begin{aligned}
\int \mathrm{d}^3x\ \psi^\star\psi &= \sum_{mn}\int \mathrm{d}^3x\left[\bar a_n a_m\, u_n u_m + a^\star_n\overline{a}^\star_m u^*_n u^*_m + \frac{1}{2}\{\bar a_m,\bar a^\star_n\}u^*_n u_m + \frac{1}{2}\{a_n,a^\star_m\}u_n u^*_m\right]\\
\int \mathrm{d}^3x\ \partial_t\psi^\star\partial_t\psi &= \sum_{mn}\varepsilon_n\varepsilon_m\left[-\bar a_n a_m\, u_n u_m - a^\star_n\overline{a}^\star_m u^*_n u^*_m + \frac{1}{2}\{\bar a_m,\bar a^\star_n\}u^*_n u_m + \frac{1}{2}\{a_n,a^\star_m\}u_n u^*_m\right]\\
\int \mathrm{d}^3x\ \nabla\psi^\star\cdot\nabla\psi &= \sum_{mn}\int \mathrm{d}^3x\,[\bar a_n a_m\,\nabla u_n\cdot\nabla u_m + a^\star_n\overline{a}^\star_m\nabla u^*_n\cdot\nabla u^*_m\\
&\qquad\qquad + \frac{1}{2}\{\bar a_m,\bar a^\star_n\}\nabla u^*_n\cdot\nabla u_m + \frac{1}{2}\{a_n,a^\star_m\}\nabla u_n\cdot\nabla u^*_m\Big]\\
&= -\sum_{mn}\int \mathrm{d}^3x\,\big[\bar a_n a_m\, u_n\nabla^2 u_m + a^\star_n\overline{a}^\star_m u^*_n\nabla^2 u^*_m\\
&\qquad\qquad + \frac{1}{2}\{\bar a_m,\bar a^\star_n\}u^*_n\nabla^2 u_m + \frac{1}{2}\{a_n,a^\star_m\}u_n\nabla^2 u^*_m\Big]\,,
\end{aligned} \tag{12.3.4}$$

where the last equality integrates by parts and the hermitian operator ordering $AB \to \frac{1}{2}\{A,B\} = \frac{1}{2}(AB+BA)$ is used. The goal is to choose $u_n(x)$ so that the $\bar a_n a_m$ terms cancel. Since the $\bar a_n a_m$ term in (12.3.2) is

$$\bar a_n a_m \int \mathrm{d}^3x\ u_n\Big[-\varepsilon_n\varepsilon_m - \nabla^2 + U(\mathbf{x})\Big]u_m\,, \tag{12.3.5}$$

this suggests asking u_n to satisfy

$$\nabla^2 u_m = \Big[-\varepsilon_m^2 + U(\mathbf{x})\Big] u_m \,, \tag{12.3.6}$$

because then (12.3.5) becomes

$$\bar{a}_n a_m \, \varepsilon_m(\varepsilon_m - \varepsilon_n) \int \mathrm{d}^3x \; u_n u_m \,. \tag{12.3.7}$$

This vanishes provided we also demand the orthogonality condition

$$\int \mathrm{d}^3x \; u_n u_m = 0 \quad \text{for any } n \neq m \,. \tag{12.3.8}$$

Notice that since $\partial_t u_n = -i\varepsilon_n \, u_n$ the equation (12.3.6) can also be written in the time domain, where it takes the Klein-Gordon form

$$\Big(-\partial_t^2 + \nabla^2 - U(\mathbf{x})\Big) u_n = \Big(\Box - U(\mathbf{x})\Big) u_n = 0 \,. \tag{12.3.9}$$

With these choices for u_n the remaining terms become

$$\begin{aligned} &\int \mathrm{d}^3x \, \Big[\partial_t\psi^*\partial_t\psi + \nabla\psi^* \cdot \nabla\psi + m^2\psi^*\psi\Big] \\ &\qquad = \sum_{mn} \frac{1}{2}\Big(\{a_n \,, a_m^\star\} + \{\bar{a}_n \,, \bar{a}_m^\star\}\Big)\varepsilon_m(\varepsilon_m + \varepsilon_n) \int \mathrm{d}^3x \; u_m^* u_n \,, \end{aligned} \tag{12.3.10}$$

which takes the single-particle harmonic oscillator form

$$\int \mathrm{d}^3x \, \Big[\partial_t\psi^*\partial_t\psi + \nabla\psi^* \cdot \nabla\psi + m^2\psi^*\psi\Big] = \sum_n \frac{1}{2}\Big(\{a_n \,, a_m^\star\} + \{\bar{a}_n \,, \bar{a}_m^\star\}\Big)\varepsilon_n \,, \tag{12.3.11}$$

if the mode-functions satisfy the normalization conditions

$$\delta_{mn} = (\varepsilon_m + \varepsilon_n) \int \mathrm{d}^3x \; u_m^* u_n = i \int \mathrm{d}^3x \, \Big(u_m^* \partial_t u_n - u_n \partial_t u_m^*\Big) \,. \tag{12.3.12}$$

Exercise: Prove that the inner product defined by the integral on the right-hand side of (12.3.12) is time independent (*i.e.* returns the same value regardless of the time where the spatial integral is evaluated) provided the functions u_n satisfy (12.3.9).

Exercise: Prove that the orthonormality and completeness of the mode functions $u_n(x)$ and $u_n^*(x)$ – defined using the inner product (12.3.12) – implies that if $\psi(x)$ satisfies the equal-time commutation relation $[\psi(\mathbf{x}, t) \,, \partial_t\psi^\star(\mathbf{y}, t)] = i\,\delta^3(\mathbf{x} - \mathbf{y})$ of (12.1.14) and if $\psi(x)$ is related to a_n and $\bar{a}_n^\star$ as in (12.3.3) then the operators a_n and $\bar{a}_n$ must satisfy the standard creation and annihilation operator relations

$$\Big[a_n \,, a_m^\star\Big] = \Big[\bar{a}_n \,, \bar{a}_m^\star\Big] = \delta_{mn} \,.$$

12.4 Feynman graphs and propagators

The entire formalism of perturbative methods described in §3 can be brought to bear on relativistic systems like the Klein Gordon field. This section describes this more explicitly in order to see in more detail how perturbation theory organizes itself in a manifestly Lorentz-covariant way.

To this end consider the Hamiltonian $H = H_0 + H_{\rm int}$ where the unperturbed (or 'free') Hamiltonian is as given in (12.1.11) (repeated here for convenience),

$$H_0 = \int \mathrm{d}^3x \Big[\rho_0 + \partial_t\psi^\star\,\partial_t\psi + \nabla\psi^\star\cdot\nabla\psi + m^2\psi^\star\psi\Big]\,, \tag{12.4.1}$$

and for illustrative purposes the interaction is taken from 12.2, with

$$H_{\rm int} = \frac{\lambda}{4}\int \mathrm{d}^3x\,\Big[\psi^\star(x)\psi(x)\Big]^2\,, \tag{12.4.2}$$

with real and positive coupling λ. As usual, the goal is first to quantize and solve the free theory, and then compute any observable of interest perturbatively in powers of λ, which is assumed to be small.

Quantizing the free theory is done as above by expanding the fields in terms of creation and annihiliation operators,

$$\psi(x) = \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\Big[\mathfrak{a}_{\mathbf{p}}\,e^{ip\cdot x} + \overline{\mathfrak{a}}_{\mathbf{p}}\,e^{-ip\cdot x}\Big] \tag{12.4.3}$$

where $p^\mu = \{\varepsilon(p), \mathbf{p}\}$ and $p\cdot x = p_\mu x^\mu = -\varepsilon(p)\,t + \mathbf{p}\cdot\mathbf{x}$ with $\varepsilon(p) = \sqrt{\mathbf{p}^2+m^2}$. The creation/annihilation operators for the particle and antiparticle satisfy the standard relations $[\mathfrak{a}_{\mathbf{p}}\,,\mathfrak{a}^\star_{\mathbf{k}}] = \delta^3(\mathbf{p}-\mathbf{k})$ and $[\overline{\mathfrak{a}}_{\mathbf{p}}\,,\overline{\mathfrak{a}}^\star_{\mathbf{k}}] = \delta^3(\mathbf{p}-\mathbf{k})$ with all other commutators vanishing. With these choices the free Hamiltonian is diagonal in the occupatoin number representation, since

$$H_0 = E_0 + \int \mathrm{d}^3p\;\varepsilon(p)\,\Big[\mathfrak{a}^\star_{\mathbf{p}}\mathfrak{a}_{\mathbf{p}} + \overline{\mathfrak{a}}^\star_{\mathbf{p}}\overline{\mathfrak{a}}_{\mathbf{p}}\Big] \tag{12.4.4}$$

with E_0 as given in §12.1.12.

Time-dependent perturbation theory then proceeds by evaluating the matrix elements

$$\langle\beta|\mathcal{S}|\alpha\rangle = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int \mathrm{d}^4x_1\cdots\mathrm{d}^4x_n\;\langle\beta|T\Big[\mathcal{H}_{\rm int}(x_1)\cdots\mathcal{H}_{\rm int}(x_n)\Big]|\alpha\rangle\,, \tag{12.4.5}$$

between the states

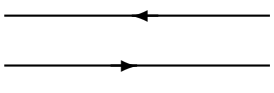
$$|\alpha\rangle = \mathfrak{a}^\star_{\mathbf{p}_1}\cdots\mathfrak{a}^\star_{\mathbf{p}_{N_\alpha}}\overline{\mathfrak{a}}^\star_{\mathbf{p}_{\overline{1}}}\cdots\overline{\mathfrak{a}}^\star_{\mathbf{p}_{\overline{N}_\alpha}}|0\rangle \quad\text{and}\quad \langle\beta| = \langle 0|\mathfrak{a}_{\mathbf{q}_1}\cdots\mathfrak{a}_{\mathbf{q}_{N_\beta}}\overline{\mathfrak{a}}_{\mathbf{q}_{\overline{1}}}\cdots\overline{\mathfrak{a}}_{\mathbf{q}_{\overline{N}_\beta}}\,, \tag{12.4.6}$$

with interaction-Hamiltonian density $\mathcal{H}_{\rm int}(x) = \frac{1}{4}\lambda\Big[\psi^\star(x)\psi(x)\Big]^2$ — *c.f.* eq. (12.4.2). Here $|\alpha\rangle$ is assumed to contain N_α particles and $\overline{N}_\alpha$ antiparticles (and similarly for $|\beta\rangle$ with N_β and $\overline{N}_\beta$).

In the end of the day, as always, the amplitude calculation boils down to evaluating the vacuum $\langle 0|\cdots|0\rangle$ matrix element of a string of creation and destruction operators. Because $\mathfrak{a}_{\mathbf{p}}|0\rangle = \langle 0|\mathfrak{a}^\star_{\mathbf{p}} = 0$ this matrix element is evaluated by moving all of the destruction operators to the right and all of the creation operators to the left, using the commutation relation $\mathfrak{a}_{\mathbf{p}}\,\mathfrak{a}^\star_{\mathbf{q}} = \mathfrak{a}^\star_{\mathbf{q}}\,\mathfrak{a}_{\mathbf{p}} + \delta^3(\mathbf{p}-\mathbf{q})$ (and similarly for the antiparticles). Nonzero contributions only come from the δ-functions arising from the failure of these operators to commute, and for any particular destruction operator one must sum over all of the possible 'pairings' with creation operators for which this can happen. These creation operators can arise either from within the initial state (12.4.6), or from creation operators that arise once the expansion (12.4.3) for ψ or $\psi^\star$ is inserted into[47] $\mathcal{H}_{\rm int}$.

12.4.1 Feynman graphs

The combinatorics of this sum is well captured by a graphical algorithm originally developed by Feynman. In this algorithm any 'contraction' coming from an $\mathfrak{a}$ failing to commute with an $\mathfrak{a}^\star$ is represented by a horizontal line, with an arrow on the line pointing to the left. A 'contraction' coming from an $\overline{\mathfrak{a}}$ failing to commute with an $\overline{\mathfrak{a}}^\star$ is similarly represented by a horizontal line, but with an arrow on the line pointing to the right, as in



(particle contraction)

(antiparticle contraction).

The arrow can heuristically be thought of as giving the flow of particle number through the graph (and so would not be present if the particle were the same as its antiparticle). The ends of the lines correspond to the two operators (*e.g.* $\mathfrak{a}$ or $\mathfrak{a}^\star$) that were paired.

Every interaction appearing in $\mathcal{H}_{\rm int}(x_i)$ is represented by a 'vertex' in the graph, at which lines end. The number of lines that can end at any vertex is given by the number of fields that appear in he interaction of interest. For instance an interaction involving $(\psi^\star\psi)^2$ involves 4 fields and so is represened by a vertex on which 4 lines can end. Since ψ destroys particles and creates antiparticles — see (12.4.3) — each ψ field in the interaction corresponds to a line entering the vertex with an incoming arrow. The field $\psi^\star$ similarly destroys an antiparticle and creates a particle so each $\psi^\star$ in a vertex corresponds to a line entering the vertex with an outgoing arrow, as in

$(\psi^\star\psi)^2$ vertex

[47] One other source of creation/annihilation operators arises if matrix elements of operators – like those considered in (3.3.9) – are considered instead of just S-matrix elements. In this case creation and annihilation operators also arise within the operators whose expectation values are being taken, but from the point of view of the Feynman rules they can treated in the same way as are terms in $\mathcal{H}_{\rm int}$.

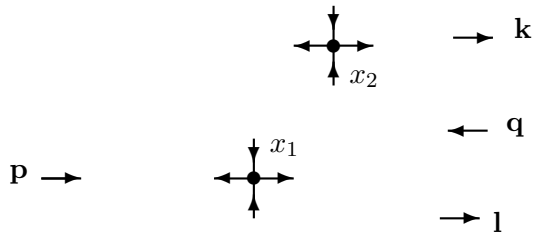


Figure 6. Ingredients of a Feynman graph, determined once the a set of interactions (vertices) and initial and final states (external lines) are chosen.

If one of the operators appearing in a contraction arises from within $\mathcal{H}_{\rm int}$ then the corresponding line is drawn to end on the corresponding vertex. If the operator instead comes from an initial state $|\alpha\rangle$ then that end of the line is left is not attached to any vertex and is drawn as if it enters the graph from the right-hand side of the page. If the operator arises in the final state $\langle\beta|$ then that end of the line also does not end at a vertex but is drawn as if it enters the graph from the left-hand side of the page (as if time flows from right to left).

The combinatorics of counting all ways that a creation operator can contract with a destruction operator, given a specific collection of operators $\mathcal{H}_{\rm int}(x_1)\cdots\mathcal{H}_{\rm int}(x_n)$ then is equivalent to drawing all possible graphs that connect the corresponding incoming lines from the right (for all particles in $|\alpha\rangle$), outgoing lines from the left (for all particles in $\langle\beta|$) and all of the vertices appearing in $\mathcal{H}_{\rm int}(x_1)\cdots\mathcal{H}_{\rm int}(x_n)$. Since $\mathfrak{a}^\star_{\mathbf{p}}$ commutes with $\overline{\mathfrak{a}}_{\mathbf{q}}$ the arrows on the lines must connect up in the same direction. (If particle and antiparticle were not distinct then no arrows would be drawn on the lines and any line could connect to any other.)

For example a graph contributing to the matrix element

$$\langle 0|\overline{\mathfrak{a}}_{\mathbf{p}}\, T\Big[\mathcal{H}_{\rm int}(x_1)\,\mathcal{H}_{\rm int}(x_2)\Big]\mathfrak{a}^\star_{\mathbf{q}}\overline{\mathfrak{a}}^\star_{\mathbf{k}}\overline{\mathfrak{a}}^\star_{\mathbf{l}}|0\rangle\,, \tag{12.4.7}$$

is built by connecting together the three incoming external lines, one outgoing external line and two vertices in all possible ways (see Fig. 6). An example of a graph (but not the only graph) that is obtained by connecting these initial ingredients is shown in Fig. 7. It perhaps goes without saying that the locations on the page of the vertices in the graph are arbitrary, and are usually chosen so that the final graph looks nice.

Feynman graphs drawn with a given initial and final state and interactions are in a one-to-one correspondence with the creation- and annihilation-operator pairings that contribute to any particular $\mathcal{S}$-matrix element. Drawing Feynman graphs represents a particularly efficient and visual way of finding all of the possible ways in which creation and annihilation operators can pair to give a nonzero result. The contributions to any particular scattering amplitude are found by drawing all possible Feynman graphs whose external lines correspond to the desired initial and final states, and whose vertices correspond to all of the possible interactions in the theory of interest. Furthermore, the explicit expression for the matrix element can also be

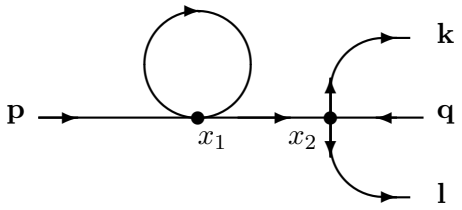


Figure 7. A particular Feynman graph constructed using the ingredients of Fig. 6.

read off from the graphs: one sums over all possible graphs where each graph contributes an expression that is determined by replacing each element (line and vertex) of the graph with an expression determined by the *Feynman rules* of the theory, as we now describe.

12.4.2 Feynman rules

The result for the matrix element is then obtained by associating the coefficent factors that are associated with the creation and annihilation operators in the matrix element in question. In the example considered here there are the following types of coefficients (each of which is associated with one of the constituent features of any graph):

Line touching no vertices: A line that directly connects an initial-state $\mathfrak{a}^\star_{\mathbf{p}}$ with a final-state $\mathfrak{a}_{\mathbf{q}}$ (or the same for an antiparticle) contributes the Feynman rule:[48]

$\mathbf{p}$ ·····◄····· $\mathbf{q}$ (particle) $\qquad$ $\mathbf{p}$ ·····►····· $\mathbf{q}$ (antiparticle)

$$\delta^3(\mathbf{p}-\mathbf{q}) \qquad \text{(disconnected line)}. \tag{12.4.8}$$

Line that touches only one vertex: Inspection of (12.4.3) line that connects an initial-state $\mathfrak{a}^\star_{\mathbf{q}}$ to an $\mathfrak{a}_{\mathbf{p}}$ appearing inside $\psi(x)$ contributes the Feynman rule:

x ●·····◄····· $\mathbf{q}$

$$\int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\, e^{ip\cdot x}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{iq\cdot x}}{\sqrt{(2\pi)^3 2\varepsilon(q)}} \qquad \text{(incoming particle)}. \tag{12.4.9}$$

An incoming antiparticle $\overline{\mathfrak{a}}^\star_{\mathbf{q}}$ pairing with an $\overline{\mathfrak{a}}_{\mathbf{p}}$ appearing in $\psi^\star(x)$ similarly gives

x ●·····►····· $\mathbf{q}$

[48] For later convenience from here on we conventionally use a dotted line in a Feynman graph to represent spinless particles, a solid line for spin-half particles and a dashed line for photons.

$$\int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\, e^{ip\cdot x}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{iq\cdot x}}{\sqrt{(2\pi)^3 2\varepsilon(q)}} \quad \text{(incoming antiparticle).} \tag{12.4.10}$$

By an identical argument, an outgoing particle $\mathfrak{a}_{\mathbf{q}}$ pairing with $\mathfrak{a}^\star_{\mathbf{p}}$ contained in $\psi^\star(x)$ gives

$$\int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\, e^{-ip\cdot x}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{-iq\cdot x}}{\sqrt{(2\pi)^3 2\varepsilon(q)}} \quad \text{(outgoing particle)}\,, \tag{12.4.11}$$

and an outgoing antiparticle $\overline{\mathfrak{a}}_{\mathbf{q}}$ pairing with $\overline{\mathfrak{a}}^\star_{\mathbf{p}}$ contained in $\psi(x)$ gives

$$\int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\, e^{-ip\cdot x}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{-iq\cdot x}}{\sqrt{(2\pi)^3 2\varepsilon(q)}} \quad \text{(outgoing antiparticle).} \tag{12.4.12}$$

Line that touches two vertices: The most interesting case arises when a contraction occurs between creation and annihilation operators appearing in two fields $\psi(x_1)$ and $\psi^\star(x_2)$ coming from two interaction Hamiltonians, $\mathcal{H}_{\rm int}(x_1)$ and $\mathcal{H}_{\rm int}(x_2)$.

This is called an *internal line* and contributes the result $\langle 0|T\big[\psi(x_1)\,\psi^\star(x_2)\big]|0\rangle$; often called the Feynman propagator:

$$\begin{aligned} G(x-y) &:= \langle 0|T\big[\psi(x)\,\psi^\star(y)\big]|0\rangle \\ &= \Theta(x^0-y^0)\langle 0|\psi(x)\,\psi^\star(y)|0\rangle + \Theta(y^0-x^0)\langle 0|\psi^\star(y)\,\psi(x)|0\rangle \\ &= \Theta(x^0-y^0)\int \frac{\mathrm{d}^3p}{(2\pi)^3 2\varepsilon(p)}\, e^{ip\cdot(x-y)} + \Theta(y^0-x^0)\int \frac{\mathrm{d}^3p}{(2\pi)^3 2\varepsilon(p)}\, e^{-ip\cdot(x-y)}\,, \end{aligned} \tag{12.4.13}$$

where the two terms arise because of the time-ordering. When $x^0 > y^0$ the field $\psi(x)$ stands to the left of $\psi^\star(y)$ and so the nonzero contribution comes from particles: $\langle 0|\mathfrak{a}_{\mathbf{p}}\mathfrak{a}^\star_{\mathbf{q}}|0\rangle$. When $y^0 > x^0$, on the other hand $\psi(x)$ stands to the right of $\psi^\star(y)$ and so the nonzero contribution comes from antiparticles: $\langle 0|\overline{\mathfrak{a}}_{\mathbf{p}}\overline{\mathfrak{a}}^\star_{\mathbf{q}}|0\rangle$. Although each of these terms is not itself separately Lorentz covariant (due to the step functions) *their sum is.* It is only because particles combine with antiparticles in this way that each step of the calculation can be kept manifestly Lorentz invariant.

To see why the result is covariant it is useful to re-express the integrals using the Fourier transform of a step function

$$\Theta(t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi i}\, \frac{e^{i\omega t}}{\omega - i\delta} = -\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi i}\, \frac{e^{-i\omega t}}{\omega + i\delta}\,, \tag{12.4.14}$$

where δ is an infinitesimal positive quantity that is taken to zero after performing the integral.[49] Using this one finds

$$\begin{aligned} G(x-y) &= i\int \frac{\mathrm{d}^3p\,\mathrm{d}\omega}{(2\pi)^4 2\varepsilon(p)}\left[\frac{e^{-i[\omega+\varepsilon(p)](x^0-y^0)+i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\omega+i\delta}+\frac{e^{i[\omega+\varepsilon(p)](x^0-y^0)-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\omega+i\delta}\right] \\ &= i\int \frac{\mathrm{d}^3p\,\mathrm{d}\omega}{(2\pi)^4 2\varepsilon(p)}\left[\frac{e^{-i\omega(x^0-y^0)+i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\omega-\varepsilon(p)+i\delta}+\frac{e^{i\omega(x^0-y^0)-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\omega-\varepsilon(p)+i\delta}\right] \\ &= i\int \frac{\mathrm{d}^3p\,\mathrm{d}\omega}{(2\pi)^4 2\varepsilon(p)}\left[\frac{e^{-i\omega(x^0-y^0)+i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\omega-\varepsilon(p)+i\delta}-\frac{e^{-i\omega(x^0-y^0)+i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\omega+\varepsilon(p)-i\delta}\right] \\ &= -i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{e^{i\bar{p}\cdot(x-y)}}{-(\bar{p}_0)^2+\mathbf{p}^2+m^2-i\bar{\delta}}\right]. \end{aligned} \tag{12.4.15}$$

The final line defines $\bar{\delta} := 2\varepsilon(p)\,\delta$ as a new positive infinitesimal, and writes the integration variable as $\bar{p}^\mu$ rather than p^μ because the time component $\bar{p}^0 = \omega$ is integrated independent of its spatial components, whereas the time component of the initial 4-momentum p^μ is a function of the components of 3-momentum through $p^0 = \varepsilon(p)$. Eq. (12.4.15) reveals $G(x-y)$ to be a Lorentz-invariant function, because both $\bar{p}\cdot(x-y) = \bar{p}_\mu(x-y)^\mu$ and $\bar{p}^2 = \bar{p}_\mu\bar{p}^\mu$ are Lorentz invariant, as is the measure $\mathrm{d}^4\bar{p}$.

This leads to the following Feynman rule for an internal line

$$-i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{e^{i\bar{p}\cdot(x-y)}}{\bar{p}^2+m^2-i\bar{\delta}}\right] \quad \text{(internal line)}. \tag{12.4.16}$$

Notice that this Feynman rule is the same if $x \leftrightarrow y$ and so is the same if the arrow were to point in the other direction.

Once the above factors are included, the result for the amplitude is obtained by performing several additional steps.

1. For each appearance of $\mathcal{H}_{\rm int}(x_i)$ a factor of all of the couplings must be included. For example for the interaction of (12.4.2) this requires including a factor

$$\frac{\lambda}{4}\int \mathrm{d}^4x_i \qquad \text{(vertex factor)}\,, \tag{12.4.17}$$

   and performing an integration over the spacetime position of the vertex: x_i^μ. For example the graph of Fig. 7 acquires two such factors — $(\lambda/4)^2$ — and must be integrated over both x_1 and x_2.

[49] The validity of this represntation of the step function can be seen by closing the contour in the complex ω-plane using a circular arc at infinity, and then evaluating the integral by residues using the pole at $\omega = i\delta$.

2. A graph involving n vertices arises at n'th order in perturbation theory, so expression (12.4.5) implies it must be accompanied by a factor $(-i)^n/n!$. For the graph of Fig. 7 this leads to a factor of $(-i)^2/2! = -\frac{1}{2}$.

3. There are usually a number of different ways that a given set of external lines and vertices can be combined to get a particular Feynman graph. Since all of these combinations give the same result (they have the same Feynman rules) it suffices to count the number of ways a particular graph can arise and multiply the result of the graph by this *symmetry factor*. For instance to obtain the graph of Fig. 7 from Fig. 6: the final **p** line can connect to either of the 2 vertices; and for each can connect to two of the lines on the vertex. Similarly the initial **q** line can connect to two of the lines of the other vertex, for another factor of 2. Once these are chosen there are two ways to tie off the loop, and the **k** initial line has two ways to connect to the remaining vertex, leading to an overall symmetry factor of $2 \times 2 \times 2 \times 2 \times 2 = 32$.

12.4.3 Momentum-space Feynman rules

A final simplification occurs because the integration over the positions x_i^μ mentioned above can be explicitly performed. This can be done because the only position dependence appearing in any of the rules comes through the exponential factors like $e^{ip\cdot x}$. Performing the integral over position then produces a factor of

$$\int \mathrm{d}^4x \; e^{i\sum_k p_k\cdot x} = (2\pi)^4\delta^4\left(\sum_k p_k\right) \tag{12.4.18}$$

for each vertex, which imposes 4-momentum conservation at each vertex. Once this is done we can drop the exponential factors in the above Feynman rules for the external lines and internal lines.

This leads to the following momentum-space Feynman rules:

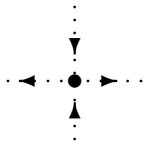
External lines: Each external line contributes the Feynman rule:

$$\frac{1}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \quad \text{(incoming or outgoing particle or antiparticle).} \tag{12.4.19}$$

Internal lines: Each internal line contributes the following momentum-space propagator

$$-i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{1}{\bar{p}^2+m^2-i\bar{\delta}}\right]. \tag{12.4.20}$$

Vertices: Each vertex contributes factors of coupling constants and an energy/momentum-conserving delta function. In the example considered here these were



$((\psi^\star\psi)^2$ interaction)

$$\frac{\lambda}{4}\,(2\pi)^4\,\delta\left(\sum_k p_k\right)\,, \tag{12.4.21}$$

where $\sum_k p_k^\mu$ is the sum over all 4-momenta entering the vertex.

To these must be added the symmetry factors and factors of $(-i)^n/n!$ described above. For instance, applying these rules to the graph of Fig. 7 gives the result

$$\begin{aligned}(\text{Fig. 7}) &= 32\left[\frac{(-i)^2}{2}\right]\left(\frac{\lambda}{4}\right)^2\int\frac{\mathrm{d}^4r}{(2\pi)^4}\frac{(-i)}{r^2+m^2-i\delta}\int\frac{\mathrm{d}^4s}{(2\pi)^4}\,\frac{(-i)}{s^2+m^2-i\delta}\\ &\qquad\times(2\pi)^4\delta(p-s)\;(2\pi)^4\delta(k+q+l-s)\left(\frac{1}{\sqrt{2(2\pi)^3}}\right)^4\frac{1}{\sqrt{\varepsilon(p)\,\varepsilon(k)\,\varepsilon(q)\,\varepsilon(l)}}\\ &=\frac{\lambda^2\Sigma}{4(2\pi)^6\sqrt{\varepsilon(p)\,\varepsilon(k)\,\varepsilon(q)\,\varepsilon(l)}}\;\frac{1}{p^2+m^2-i\delta}\;\delta^4(k+q+l-p)\,,\end{aligned} \tag{12.4.22}$$

where Σ is the momentum-independent (but UV-divergent — see §17.2 below for its evaluation) loop integral:

$$\Sigma := \int\frac{\mathrm{d}^4r}{r^2+m^2-i\delta}\,. \tag{12.4.23}$$

Once this amplitude is squared the factors of $\varepsilon^{-1/2}$ are precisely what is needed to combine with phase space integrals to give Lorentz-invariant integration measures of the form $\mathrm{d}^3k/\varepsilon(k)$. This ensures that physical rates that transform as they should under Lorentz transformations. Notice also the emergence of the overall delta function $\delta^4(k+q+l-p)$ that expresses conservation of overall 4-momentum for the entire process.

One can proceed very efficiently in this way for many problems, computing the effects of interactions in perturbation theory to any desired order.

12.4.4 Disconnected graphs

As argued above, any amplitude $\langle\beta|\mathcal{S}|\alpha\rangle$ can be expressed within perturbation theory as a sum over all possible Feynman graphs whose external lines correspond to the initial states α and β. Some simple physical observations are easiest to see within this kind of graphical representation.

One such is the distinction between *connected* and *disconnected* graphs. Connected graphs are defined to be those graphs for which it is possible to get from any vertex to any other in

the graph simply by following along the internal lines. A simple example of this distinction for the theory described here is given by:

Both of these graphs have the same external lines but only the left-hand graph is connected.

In the figure shown the right-hand disconnected graph also has no vertices and so describes a process where no interactions are involved. These contribute to the first (trivial) term in the expansion $\mathcal{S} = I + \cdots$ of the the S-matrix. But this is an artefact of the simplicity of the graph considered and disconnected graphs can also contain vertices in each of the disconnected parts. When this happens the Feynman rules ensure that 4-momentum is conserved separately for each of the disconnected pieces.

Physically the disconnected pieces of the graph describe independent processes where (say) the evolution of four particles involves two separate processes where different pairs of particles interact only with each other (such as if two of them scatter on Earth and the other two scatter on the star α-Centauri. Normally our interest is only in the amplitude for a specific scattering process, independent of other possible reactions that could be taking place elsewhere in the Universe, and for this reason one usually restricts the sum over Feynman graphs to include only the connected graphs.

The reasoning for keeping only connected graphs is slightly different if one computes the expectation values of operators, rather than S-matrix elements, such as if evaluating expressions like (3.3.9). In this case straightforward evaluation of (3.3.9) using the extended Feynman rules mentioned in footnote 47 does require including all graphs, connected and disconnected. Summing just the disconnected graphs instead computes the slightly different quantity. For example, if one computes

$$\frac{\langle\!\langle 0, \text{out}|T\Big[A_{h\,1}(t_1)\cdots A_{h\,2}(t_2)\Big]|0, \text{in}\rangle\!\rangle}{\langle\!\langle 0, \text{out}|0, \text{in}\rangle\!\rangle} - \left[\frac{\langle\!\langle 0, \text{out}|A_{h\,1}(t_1)|0, \text{in}\rangle\!\rangle}{\langle\!\langle 0, \text{out}|0, \text{in}\rangle\!\rangle}\right]\left[\frac{\langle\!\langle 0, \text{out}|A_{h\,2}(t_2)|0, \text{in}\rangle\!\rangle}{\langle\!\langle 0, \text{out}|0, \text{in}\rangle\!\rangle}\right], \tag{12.4.24}$$

instead of just $\langle\!\langle 0, \text{out}|T\Big[A_{h\,1}(t_1)\cdots A_{h\,2}(t_2)\Big]|0, \text{in}\rangle\!\rangle$ then the sum of disconnected graphs where the disconnected factor involves no external lines is cancelled by dividing by the vacuum amplitude $\langle\!\langle 0, \text{out}|0, \text{in}\rangle\!\rangle$. The disconnected graphs where each disconnected factor contains an extended Feynman rule for the $A_i(t_i)$ are similarly cancelled by subtracting the product $\langle\!\langle 0, \text{out}|A_{h\,1}(t_1)|0, \text{in}\rangle\!\rangle\, \langle\!\langle 0, \text{out}|A_{h\,2}(t_2)|0, \text{in}\rangle\!\rangle$.

12.5 Derivative interactions and the miracle of Lorentz invariance

Although beautiful, the discussion of microcausality in §11.4 is not quite the end of the story for reconciling quantum mechanics with special relativity, even in the special case where the interaction Hamiltonian is a Lorentz scalar. This is because there is a second way that time-ordering can ruin Lorentz covariance, that first arises for derivative interactions (as is explored in detail in this section).

It is because Lorentz invariance is so obscure using the Hamiltonian formulation that one is motivated to find the different, more efficient, formulation described below in §13 and then improved on even more in §21.

12.5.1 A simple derivative coupling

For the purpose of illustrating the issues, consider the system studied earlier involving a single spinless particle (that is distinct from its antiparticle), with non-interacting Hamiltonian

$$H_0 = \int \mathrm{d}^3x \, \Big[\partial_t\psi^\star \, \partial_t\psi + \nabla\psi^\star \cdot \nabla\psi + m^2 \, \psi^\star\psi\Big] \tag{12.5.1}$$

where — for $x^\mu = \{t\,, \mathbf{x}\}$ — the field $\psi(x)$ is related to the annihilation operators $\mathfrak{a}_{\mathbf{p}}$, $\bar{\mathfrak{a}}_{\mathbf{p}}$, $\mathfrak{a}^\star_{\mathbf{p}}$ and $\bar{\mathfrak{a}}^\star_{\mathbf{p}}$ by

$$\psi(x) = \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \Big[\mathfrak{a}_{\mathbf{p}} \, e^{ip\cdot x} + \bar{\mathfrak{a}}^\star_{\mathbf{p}} \, e^{-ip\cdot x}\Big] \,. \tag{12.5.2}$$

Suppose now that this system is supplemented by an interaction Hamiltonian of the form

$$H_{\rm int} = \int \mathrm{d}^3x \, \Big(W^\mu \, \partial_\mu\psi + \overline{W}^\mu \partial_\mu\psi^\star\Big) \,, \tag{12.5.3}$$

where $W^\mu(x)$ is some other 4-vector field from which the ψ particle can scatter and $\overline{W}^\mu$ is its complex conjugate. For the present purposes we imagine W^μ to be given by a classical profile, since this suffices to make the point towards which we are heading.

The S-matrix for ψ in the presence of the field W^μ is then (at second order)

$$\begin{aligned} \mathcal{S} \simeq \mathcal{I} - i \int_{-\infty}^{\infty} \mathrm{d}^4x \Big[W^\mu(x) \, \partial_\mu\psi(x) + \overline{W}^\mu(x) \, \partial_\mu\psi^\star(x)\Big] \qquad\qquad (12.5.4) \\ -\frac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}^4x \, \mathrm{d}^4y \, T\Big\{[W^\mu(x)\partial_\mu\psi(x) + \overline{W}^\mu\partial_\mu\psi^\star(x)][W^\nu(y)\partial_\nu\psi(y) + \overline{W}^\nu\partial_\nu\psi^\star(y)]\Big\} \end{aligned}$$

and so on, where T as usual denotes the time-ordered product

$$T\Big[A(x) \, B(y)\Big] = \Theta(x^0 - y^0) \, A(x) \, B(y) + \Theta(y^0 - x^0) \, B(y) \, A(x) \,. \tag{12.5.5}$$

For the sake of argument imagine computing the matrix element $\langle 0|\mathcal{S}|0\rangle$, just for the purpose of studying its Lorentz-transformation properties, leading at second order to

$$\langle 0|\mathcal{S}|0\rangle \simeq 1 - \int_{-\infty}^{\infty} \mathrm{d}^4x \, \mathrm{d}^4y \, W^\mu(x)\overline{W}^\nu(y) \, \langle 0|T\Big[\partial_\mu\psi(x) \, \partial_\nu\psi^\star(y)\Big]|0\rangle \,. \tag{12.5.6}$$

12.5.2 Non-covariant 'Schwinger terms'

Although (12.5.6) looks like it should be Lorentz invariant (provided W^μ transforms like a 4-vector), it turns out it is not because there is a subtlety to do with the derivatives acting on ψ.

At first sight this seems a surprise because (12.4.13) and (12.4.15) show that Feynman propagator $\langle 0|T[\psi(x)\,\psi^\star(y)]|0\rangle$ is a Lorentz-invariant function of the difference $(x-y)^\mu$, and so its derivative

$$\frac{\partial^2}{\partial x^\mu \partial y^\nu}\langle 0|T\Big[\psi(x)\,\psi^\star(y)\Big]|0\rangle = -i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{\bar{p}_\mu\,\bar{p}_\nu}{\bar{p}^2+m^2-i\bar{\delta}}\,e^{i\bar{p}\cdot(x-y)}\right] \tag{12.5.7}$$

also transforms covariantly. If this is so, then why is the same not true for the quantity

$$\begin{aligned}\langle 0|T\Big[\partial_\mu\psi(x)\,\partial_\nu\psi^\star(y)\Big]|0\rangle &= \int \frac{\mathrm{d}^3p}{(2\pi)^3 2\varepsilon(p)}\,p_\mu\,p_\nu\Big[\Theta(x^0-y^0)\,e^{ip\cdot(x-y)}+\Theta(y^0-x^0)\,e^{-ip\cdot(x-y)}\Big]\\ &= -i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{p_\mu\,p_\nu}{\bar{p}^2+m^2-i\bar{\delta}}\,e^{i\bar{p}\cdot(x-y)}\right]\end{aligned} \tag{12.5.8}$$

appearing in (12.5.6)?

The crucial difference is the replacement $p_\mu p_\nu \leftrightarrow \bar{p}_\mu\bar{p}_\nu$, since these differ in their time components: $p^0=\varepsilon(p)$ is a function of $\mathbf{p}$ while $\bar{p}^0$ is an independent integration variable. (That is $\bar{p}^2$ is arbitrary while $p^2=-m^2$; we say that p^μ is 'on shell' while $\bar{p}^\mu$ is not.) To see the problem more explicitly write the difference $p_\mu p_\nu - \bar{p}_\mu\bar{p}_\nu$ out explicitly:

$$p_\mu\,p_\nu - \bar{p}_\mu\,\bar{p}_\nu = \begin{pmatrix}\varepsilon^2(p)-\bar{p}_0^2 & [\varepsilon(p)-\bar{p}_0]p_j\\ p_i[\varepsilon(p)-\bar{p}_0] & 0\end{pmatrix}. \tag{12.5.9}$$

The off-diagonal term changes sign if $\mathbf{p}\to-\mathbf{p}$ and so vanishes when inserted into the integral, but the same is not true for the diagonal term. Using $\varepsilon^2(p)-\bar{p}_0^2 = -\bar{p}_0^2+\mathbf{p}^2+m^2 = \bar{p}^2+m^2$ and evaluating the remaining integrals then shows:

$$\begin{aligned}\langle 0|T\Big[\partial_\mu\psi(x)\,\partial_\nu\psi^\star(x')\Big]|0\rangle &= \partial_\mu\partial'_\nu\langle 0|T\Big[\psi(x)\,\psi^\star(x')\Big]|0\rangle - i\delta^0_\mu\,\delta^0_\nu\int\frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\,\frac{(\bar{p}^2+m^2)}{\bar{p}^2+m^2-i\bar{\delta}}\,e^{i\bar{p}\cdot(x-x')}\\ &= \partial_\mu\partial'_\nu\langle 0|T\Big[\psi(x)\,\psi^\star(x')\Big]|0\rangle - i\delta^0_\mu\,\delta^0_\nu\,\delta^4(x-x')\,.\end{aligned} \tag{12.5.10}$$

An alternative, more intuitive, way to see why this happens is to notice that time-ordering does not commute with differentiation. That is, imagine differentiating the definition (12.5.5) with respect to x^μ and y^ν. Differentiating once gives

$$\frac{\partial}{\partial x^\mu}\,T\Big[A(x)\,B(y)\Big] = T\Big[\partial_\mu A(x)\,B(y)\Big] + \delta^0_\mu\,\delta(x^0-y^0)\Big[A(x)\,,B(y)\Big]\,, \tag{12.5.11}$$

where the final term involving $\delta(x^0-y^0)$ comes from differentiating the step functions in the time-ordering. Differentiating again then gives

$$\begin{aligned}\frac{\partial^2}{\partial x^\mu\partial y^\nu}T\Big[A(x)\,B(y)\Big] &= T\Big[\partial_\mu A(x)\,\partial_\nu B(y)\Big] - \delta^0_\nu\,\delta(x^0-y^0)\Big[\partial_\mu A(x)\,,B(y)\Big]\\ &\quad +\delta^0_\mu\,\delta(x^0-y^0)\Big[A(x)\,,\partial_\nu B(y)\Big] - \delta^0_\mu\,\delta^0_\nu\,\delta'(x^0-y^0)\Big[A(x)\,,B(y)\Big]\,,\end{aligned} \tag{12.5.12}$$

which simplifies somewhat in the special case where A and B are either ψ or $\psi^\star$ because these fields have been designed to commute with each other at spacelike separations, and so $\delta'(x^0-y^0)[A(x)\,,B(y)]=0$. The remaining commutators are nonzero but local, such as

$$\begin{aligned}\Big[\partial_\mu\psi(x)\,,\psi^\star(y)\Big] &= \int \frac{\mathrm{d}^3p\,\mathrm{d}^3q}{(2\pi)^3 2\sqrt{\varepsilon(p)\varepsilon(q)}}\; ip_\mu\Big[\mathfrak{a}_{\mathbf{p}}\,e^{ip\cdot x}-\overline{\mathfrak{a}}^\star_{\mathbf{p}}\,e^{-ip\cdot x}\,,\mathfrak{a}^\star_{\mathbf{q}}\,e^{-iq\cdot y}+\overline{\mathfrak{a}}_{\mathbf{q}}\,e^{iq\cdot y}\Big]\\ &= \int \frac{\mathrm{d}^3p}{(2\pi)^3 2\varepsilon(p)}\; ip_\mu\Big[e^{ip\cdot(x-y)}+e^{-ip\cdot(x-y)}\Big]\,. \end{aligned} \tag{12.5.13}$$

and these are the source of the Lorentz-noninvariant contributions.

Now comes the main point. The first term on the right-hand side of (12.5.10) transforms covariantly, but the last term — sometimes called a 'Schwinger term' — does not because of the $\delta^0_\mu\,\delta^0_\nu$ factor. But this means that the left-hand side — which is the quantity appearing in the S-matrix — also cannot be covariant, and this causes invariance of the S-matrix to fail even if W^μ transforms as a 4-vector. Once again time ordering potentially poses a problem for special relativity. What to do?

12.5.3 Covariantizing interactions

All is not lost, because the terms that break Lorentz invariance are proportional to $\delta^4(x-y)$ and so are local. This means that the S-matrix for the theory can be made Lorentz-invariant by adding new noncovariant interactions to $H_{\rm int}$, in such a way as to cancel the contributions to the S-matrix from the non-covariant terms in (12.5.10).

For example, the Schwinger term in (12.5.10) contributes to (12.5.6) the non-covariant contribution

$$\begin{aligned}\langle 0|\mathcal{S}|0\rangle \ni -\int \mathrm{d}^4x\,\mathrm{d}^4x'\; W^\mu(x)\,\overline{W}^\nu(x')\,\langle 0|T\Big[\partial_\mu\psi(x)\,\partial_\nu\psi^\star(x')\Big]|0\rangle_{\rm non-cov}\\ = i\int \mathrm{d}^4x\; W^0(x)\,\overline{W}^0(x)\,,\end{aligned} \tag{12.5.14}$$

that would be cancelled if the Hamiltonian density were also to include a local but noncovariant interaction

$$\delta\mathcal{H}_{\rm int} = W^0(x)\overline{W}^0(x)\,, \tag{12.5.15}$$

since this contributes to the S-matrix (at first order) by an amount

$$\delta\mathcal{S} = -i\int \mathrm{d}^4x\;\delta\mathcal{H}_{\rm int}(x) = -i\int \mathrm{d}^4x\; W^0(x)\,\overline{W}^0(x)\,. \tag{12.5.16}$$

The ability to 'fix' non-covariant Schwinger terms by cancelling them with non-covariant interactions in $\mathcal{H}_{\rm int}(x)$ is possible because the non-covariance is local, and once this has been done the S-matrix is Lorentz invariant. The upshot is that the final result for physical processes is *as if* the noncovariant Schwinger terms in (12.5.10) were not present and $\mathcal{H}_{\rm int}$ were manifestly Lorentz invariant.

Given that such cancellations are possible, this suggests defining a modified covariant time ordering — denoted T^* and called '*T-star ordering*' — for which

$$T^*\Big[\partial_\mu\psi(x)\,\partial_\nu\psi^\star(x')\Big] = \partial_\mu\partial'_\nu\,T\Big[\psi(x)\,\psi^\star(x')\Big]\,. \tag{12.5.17}$$

In terms of this the S-matrix is built by using only manifestly invariant interactions and by T^* ordering in expressions like (12.5.4) for the S-matrix. This makes it sound as if there should be a simpler way to arrive directly at this simpler covariant expression without having to stray first through a complicated cancellation of non-covariant effects.

Such a formulation is indeed possible using a combination of canonical and path-integral methods. Canonical methods – described in §13 – do not remove the need for noncovariant terms in $\mathcal{H}_{\rm int}$, but removes the guesswork by providing an explicit way to generate them automatically. But the best progress comes once the path-integral techniques of §21 are used, since these completely dispense with the Hamiltonian and formulate predictions directly using the lagrangian density $\mathcal{L}$ (which must be covariant).

13 Canonical methods

Traditionally quantum mechanics is built around Hamiltonians, but the above examples show that this is not that convenient a framework for the purposes of discovering Lorentz-invariant quantum systems. This section sets out the alternative Lagrangian-based formulation of quantum mechanics that aims to make the criterion of Lorentz invariance more manifest at every step (though, as we shall see, does not completely succeed until §21).

13.1 Lagrangian methods

The further we go into the study of relativistic systems the more central a role gets played by the system's *action*, when formulating a theory. In earlier sections a system was specified by giving its Hamiltonian, and all predictions about its spectrum and time evolution followed from H. The action proves to be much more convenient in the long run, and contains the same information because the Hamiltonian can be derived from it using standard steps (that are now summarized). For those completely unfamiliar with Lagrangian methods, a brief summary is provided – both for field theories and for particle mechanics – in Appendix D.

13.1.1 Canonical quantization

Consider a collection[50] of fields $\psi^A(\mathbf{x},t)$. The action, $S[\psi]$, for this system of fields is a functional defined as a local integral over space and time of a function of the fields ψ^A and

[50]Here the index A runs over both any components within a Lorentz representation (such as the four components of a 4-vector field, V_μ) and over any label that distinguishes distinct fields that do not sit within the same representation of the Lorentz group. So for a collection of N 4-vector fields, $V^a_\mu(x)$ with $a = 1, \cdots, N$ and $\mu = 0, 1, 2, 3$, we have $\{A\} = \{a, \mu\}$.

its derivatives, all evaluated at the same spacetime point:

$$S[\psi] := \int_{-\infty}^{\infty} \mathrm{d}^4x \; \mathcal{L}(\psi^A, \partial_\mu \psi^A, \cdots) \,, \tag{13.1.1}$$

where the quantity $\mathcal{L}$ is called the system's *Lagrangian density*.[51] For slowly varying fields it suffices to restrict to functions $\mathcal{L}$ that depend only on undifferentiated and singly differentiated fields while neglecting any dependence on multiple derivatives like $\partial_\mu \partial_\nu \psi^A$.

Within the action formulation of quantum mechanics a system is specified through the choices made for $\mathcal{L}(\psi^A, \partial_\mu \psi^A)$ rather than for the Hamiltonian. As we shall see, $\mathcal{L}$ must be hermitian if the Hamiltonian that comes from it is also to be hermitian. In the lagrangian framework a symmetry is defined as a transformation that leaves the action S invariant, so we demand the action be unchanged under combined Lorentz transformations of the coordinates x^μ and the fields ψ^A. The presence of the measure d^4x in the action means that invariance of S requires $\mathcal{L}$ to transform as a Lorentz scalar, so $\mathcal{L}(x) \to \mathcal{L}(\Lambda x)$. This makes its form easier to guess than for the Hamiltonian.

Given a Lagrangian density $\mathcal{L}$ the Hamiltonian is constructed through the following algorithm (see Appendix D for the motivation for doing so). First one mentally separates the time and space derivatives from one another, denoting the time derivatives by $\dot{\psi}^A := \partial_t \psi^A = \partial_0 \psi^A$ and the spatial derivatives by $\partial_i \psi^A$. Canonical momenta are then defined by

$$\Pi_A(\mathbf{x}, t) := \frac{\partial \mathcal{L}}{\partial \dot{\psi}^A(\mathbf{x}, t)} \,, \tag{13.1.2}$$

making them functions of ψ^A, $\dot{\psi}^A$ and $\partial_i \psi^A$. Eq. (13.1.2) is regarded as an expression to be solved to eliminate the time derivatives $\dot{\psi}^A$ in favour of the Π_A, leading to an expression

$$\dot{\psi}^A = \dot{\psi}^A[\psi, \partial_i \psi, \Pi] \,. \tag{13.1.3}$$

It is assumed here that solutions of this type to (13.1.2) exist, though an extension of this formalism – called the theory of *constrained* Hamiltonian systems – has been developed (by Dirac, no less) to handle this case too.

With these definitions the system's Hamiltonian is a local quantity $H = \int \mathrm{d}^3x \; \mathcal{H}$, with Hamiltonian density given by[52]

$$\mathcal{H}[\psi, \partial_i \psi, \Pi] := \Pi_A \, \dot{\psi}^A - \mathcal{L}[\psi, \partial_i \psi, \dot{\psi}(\Pi)] \tag{13.1.4}$$

in which $\dot{\psi}^A$ is traded for Π_A using (13.1.3). Once this is done the Hamiltonian density is regarded as a function of ψ^A, $\partial_i \psi^A$ and Π_A (but not $\dot{\psi}^A$).

[51] This name arises because the quantity $L = \int \mathrm{d}^3x \; \mathcal{L}$ is the system's Lagrangian.

[52] As usual, the Einstein summation convention is in force throughout this section.

Given the Hamiltonian, quantization then proceeds by demanding the operators ψ^A and Π_A satisfy the canonical equal-time commutation relations

$$\Big[\psi^A(\mathbf{x},t)\,,\Pi_B(\mathbf{y},t)\Big] = i\,\delta^A{}_B\,\delta^3(\mathbf{x}-\mathbf{y})\,. \tag{13.1.5}$$

The next few subsections show how the above quantization algorithm captures the same physics as did the development in earlier sections where the algebra of creation and annihilation operators was the primitive concept.

13.1.2 Relevance to Lorentz covariance

But if canonical quantization simply reproduces what we already know then why bother with Lagrangian methods, given that the Hamiltonian-based methods already seem to work? There are several reasons for doing so, but the two that matter for the present purposes both involve Lorentz covariance.

Expressing $\mathcal{S}$ in terms of $\mathcal{L}_{\rm int}$:

The first reason is clearest in the simple case where the above algorithm is applied to perturbation theory, for which we write $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\rm int}$ and perturb in powers of $\mathcal{L}_{\rm int}$. This implies a similar split for the Hamiltonian density, $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\rm int}$, and it is often (but not always) the case that the interaction Hamiltonian obtained in this way is $\mathcal{H}_{\rm int} = -\mathcal{L}_{\rm int}$. This happens when the interactions in $\mathcal{L}_{\rm int}$ do not involve time derivatives of the fields and so do not enter into the definitions (13.1.2) of the canonical momenta, and so $\mathcal{L}_{\rm int}$ only enters the definition of $\mathcal{H}$ through the $-\mathcal{L}$ term of (13.1.4).

When this is true expressions like (6.1.6) for the S-matrix take a very suggestive form:

$$\mathcal{S} \simeq I + \sum_{n=1}^{\infty} \frac{i^n}{n!} \int_{-\infty}^{\infty} \mathrm{d}^4x_1 \cdots \int_{-\infty}^{\infty} \mathrm{d}^4x_n\; T\Big[\mathcal{L}_{\rm int}(x_1)\cdots\mathcal{L}_{\rm int}(x_n)\Big]\,. \tag{13.1.6}$$

As discussed below (11.4.3), this is suggestive because the integrals $\int \mathrm{d}^4x\,\mathcal{L}$ are *by construction* Lorentz invariant whenever the action is Lorentz invariant. Although the time-ordering could have been a problem, the microcausality condition (11.4.5) ensures this is not actually an issue. The successful derivation of manifest Lorentz invariance finally achieved in §21 ultimately does so by showing why (13.1.6) is *always* true, and not just when $\mathcal{H}_{\rm int} = -\mathcal{L}_{\rm int}$.

Generating required non-covariant terms in $\mathcal{H}_{\rm int}$:

In the general case where $\mathcal{H}_{\rm int} \neq -\mathcal{L}_{\rm int}$ we know from examples like that described in §12.5 that $\mathcal{H}_{\rm int}$ contains explicitly non-covariant interactions that then precisely cancel other non-covariant effects – such as the Schwinger terms of §12.5 (or the Coulomb interaction in electromagnetism). As we see later in this section, the second great merit of canonical methods is that they remove the guesswork when identifying these non-covariant interactions. Canonical methods provide a turn-the-crank method for finding them in a very explicit and systematic way.

13.2 The Klein-Gordon field

Consider first the Klein-Gordon system describing a single complex Lorentz-scalar field $\psi(x)$. We wish to determine the form for $\mathcal{L}$ that corresponds to the free Klein-Gordon Hamiltonian (12.1.11) or (12.3.2) and to interactions like those of (12.2.2) or (12.5.3).

13.2.1 Free theory

The first step is to guess the lagrangian density, $\mathcal{L}_0$, that reproduces the free Hamiltonian (12.1.11). Since this Hamiltonian is bilinear in ψ and $\psi^\star$ we demand the same of $\mathcal{L}_0$. We further require it to involve only the scalar field ψ, its space-time derivative $\partial_\mu\psi$ and their complex conjugates.

Because ψ is a Lorentz scalar its derivative transforms as a 4-vector and so the condition that $\mathcal{L}_0$ be a Lorentz scalar is simple: any derivatives must be contracted using the invariant metric $\eta^{\mu\nu}$. The most general option satisfying all of these conditions (and that is local) is

$$\mathcal{L}_0 = -\rho_0 - \mathfrak{c}_1\,\psi^\star\psi - \mathfrak{c}_2\,\eta^{\mu\nu}\partial_\mu\psi^\star\,\partial_\nu\psi = -\rho_0 - \mathfrak{c}_1\,\psi^\star\psi + \mathfrak{c}_2\left(\dot\psi^\star\,\dot\psi - \nabla\psi^\star\cdot\nabla\psi\right), \tag{13.2.1}$$

with constants ρ_0, $\mathfrak{c}_1$ and $\mathfrak{c}_2$ to be determined by agreement with (12.1.11). We here adopting the convenient notation where over-dots denote time derivatives: $\dot\psi := \partial_t\psi$ and similarly for other fields.

With this choice the canonical momenta become

$$\Pi := \frac{\partial\mathcal{L}_0}{\partial\dot\psi} = \mathfrak{c}_2\,\dot\psi^\star \quad\text{and}\quad \Pi^\star := \frac{\partial\mathcal{L}_0}{\partial\dot\psi^\star} = \mathfrak{c}_2\,\dot\psi\,, \tag{13.2.2}$$

and so the Hamiltonian density becomes

$$\mathcal{H}_0 = \Pi\,\dot\psi + \Pi^\star\,\dot\psi^\star - \mathcal{L}_0 = \frac{\Pi^\star\Pi}{\mathfrak{c}_2} + \mathfrak{c}_2\,\nabla\psi^\star\cdot\nabla\psi + \mathfrak{c}_1\,\psi^\star\psi + \rho_0\,. \tag{13.2.3}$$

This agrees with (12.1.11) when $\mathfrak{c}_1 = m^2$ and $\mathfrak{c}_2 = 1$, in which case

$$\mathcal{L}_0 = -\partial_\mu\psi^\star\partial^\mu\psi - m^2\psi^\star\psi - \rho_0 = \dot\psi^\star\dot\psi - \nabla\psi^\star\cdot\nabla\psi - m^2\psi^\star\psi - \rho_0 \tag{13.2.4}$$

while

$$\Pi = \dot\psi^\star \quad\text{and}\quad \mathcal{H}_0 = \Pi^\star\Pi + \nabla\psi^\star\cdot\nabla\psi + m^2\psi^\star\psi + \rho_0\,. \tag{13.2.5}$$

There is no loss of generality in making the choice $\mathfrak{c}_2 = 1$ because this can always be achieved (if not initially true) by rescaling the field ψ. The canonical equal-time commutation relations with this choice become

$$\Big[\psi(\mathbf{x},t)\,,\Pi(\mathbf{y},t)\Big] = \Big[\psi(\mathbf{x},t)\,,\dot\psi^\star(\mathbf{y},t)\Big] = i\delta^3(\mathbf{x}-\mathbf{y}) \tag{13.2.6}$$

in agreement with (12.1.14). This guarantees that if we expand the field as in (12.1.3)

$$\psi(x) = \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\Big[\mathfrak{a}_{\mathbf{p}}\;e^{ip\cdot x} + \overline{\mathfrak{a}}^\star_{\mathbf{p}}\;e^{-ip\cdot x}\Big], \tag{13.2.7}$$

the operators $\mathfrak{a}_{\mathbf{p}}$ and $\overline{\mathfrak{a}}_{\mathbf{p}}$ will inherit from (13.2.6) the usual creation and annihilation algebra $[\mathfrak{a}_{\mathbf{p}}\,,\mathfrak{a}^\star_{\mathbf{q}}] = \delta^3(\mathbf{p}-\mathbf{q}) = [\overline{\mathfrak{a}}_{\mathbf{p}}\,,\overline{\mathfrak{a}}^\star_{\mathbf{q}}]$. And this in turn ensures the Hamiltonian $H_0 = \int \mathrm{d}^3x\ \mathcal{H}_0$ can be written as (12.1.1) with the dispersion relation (12.1.2): $\varepsilon(p) = \sqrt{\mathbf{p}^2+m^2}$.

As described in Appendix D, the classical field equations for ψ are also determined by the action, by the requirement that the action is stationary with respect to arbitrary small changes of the fields, $\psi(\mathbf{x},t) \to \psi(\mathbf{x},t) + \delta\psi(\mathbf{x},t)$. The resulting field equation is given by (D.3.4), which for relativistic lagrangians built using ψ and $\partial_\mu\psi$ becomes

$$-\partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\psi^A)}\right] + \frac{\partial\mathcal{L}}{\partial\psi^A} = 0 \tag{13.2.8}$$

and its complex conjugate. For the lagrangian (13.2.4) this implies

$$\partial_\mu\partial^\mu\psi - m^2\psi = (\Box - m^2)\psi = \Big(-\partial_t^2 + \nabla^2 - m^2\Big)\psi = 0 \tag{13.2.9}$$

in agreement with (12.1.16).

We see in this way that we retrieve from canonical methods all of the standard results already encountered for noninteracting Klein-Gordon fields in §12.1.

13.2.2 Interactions

What about interactions? The simplest cases are interactions, like those of (12.2.2) or (12.3.1), that do not involve derivatives of ψ. Chasing through the definitions shows that these are simply incorporated by adding them (with an overall negative sign) to the Lagrangian density $\mathcal{L}$. For example, one might choose $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\text{int}}$ with

$$\mathcal{L}_{\text{int}} = -U(\mathbf{x})\,\psi^\star\psi - \frac{\lambda}{4}\big[\psi^\star(x)\psi(x)\big]^2 - \left[\frac{g}{4!}\,\psi^4 + \text{c.c.}\right]. \tag{13.2.10}$$

Because these types of interactions do not depend on $\dot\psi$ or $\dot\psi^\star$ they do not alter the relationship (13.2.5) giving Π in terms of $\dot\psi^\star$. Once the Hamiltonian is constructed using (13.1.4), the interaction part of the Hamiltonian density becomes

$$\mathcal{H}_{\text{int}} = -\mathcal{L}_{\text{int}} = U(\mathbf{x})\,\psi^\star\psi + \frac{\lambda}{4}\big[\psi^\star(x)\psi(x)\big]^2 + \left[\frac{g}{4!}\,\psi^4 + \text{c.c.}\right], \tag{13.2.11}$$

and because $\mathcal{L}_{\text{int}}$ is (by construction) a Lorentz scalar the same is then also true for $\mathcal{H}_{\text{int}}$.

Canonical methods are also useful in situations where the interaction Hamiltonian density is *not* a Lorentz scalar, because they efficiently identify the non-covariant interactions needed to cancel non-covariant contributions to correlation functions (like the Schwinger terms of §12.5). To see how this works consider again the simple derivative interaction considered in (12.5.3)

$$\mathcal{L}_{\text{int}} = -W^\mu\,\partial_\mu\psi - \overline{W}^\mu\partial_\mu\psi^\star = -W^0\,\dot\psi - \mathbf{W}\cdot\nabla\psi + \text{h.c.}\,, \tag{13.2.12}$$

where W^μ is a complex 4-vector field with complex conjugate $\overline{W}^\mu$.

In this case the interaction term modifies the relationship between the canonical momentum and the 'velocity' ($\dot\psi$). For $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\rm int}$, with $\mathcal{L}_0$ given in (13.2.4) and $\mathcal{L}_{\rm int}$ given in (13.2.12), the canonical momenta become

$$\Pi = \frac{\partial \mathcal{L}}{\partial \dot\psi} = \dot\psi^\star - W^0 \quad \text{and} \quad \Pi^\star = \frac{\partial \mathcal{L}}{\partial \dot\psi^\star} = \dot\psi - \overline{W}^0 \tag{13.2.13}$$

and so the Hamiltonian density becomes

$$\begin{aligned} \mathcal{H} &= \Pi\,\dot\psi + \Pi^\star\dot\psi^\star - \mathcal{L} = \Pi(\Pi^\star + \overline{W}^0) + \Pi^\star(\Pi + W^0) - \mathcal{L} \\ &= (\Pi^\star + \overline{W}^0)(\Pi + W^0) + \nabla\psi^\star\cdot\nabla\psi + m^2\psi^\star\psi + \rho_0 + \mathbf{W}\cdot\nabla\psi + \overline{\mathbf{W}}\cdot\nabla\psi^\star\,. \end{aligned} \tag{13.2.14}$$

It is instructive to treat this in perturbation theory and ask after the Lorentz-transformation properties expected for the S-matrix. In perturbation theory we write $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\rm int}$ with $\mathcal{H}_0$ given by (13.2.5) and the interaction Hamiltonian given by

$$\mathcal{H}_{\rm int} = \mathbf{W}\cdot\nabla\psi + \overline{\mathbf{W}}\cdot\nabla\psi^\star + \overline{W}^0\Pi + W^0\Pi^\star + W^0\overline{W}^0\,. \tag{13.2.15}$$

We also go to the interaction picture, for which the field equation defining the evolution of the fields uses only $\mathcal{H}_0$. Because of this the expression for the canonical momentum to be used in (13.2.15) is the non-interacting one of (13.2.5) rather than (13.2.13): $\Pi = \partial_t\psi^\star$ and $\Pi^\star = \partial_t\psi$.

Using this in $\mathcal{H}_{\rm int}$ shows that it can be written

$$\mathcal{H}_{\rm int} = W^\mu\partial_\mu + \overline{W}^\mu\partial_\mu\psi^\star + W^0\overline{W}^0\,, \tag{13.2.16}$$

showing that $\mathcal{H}_{\rm int} = -\mathcal{L}_{\rm int} + W^0\overline{W}^0$ consists of a covariant part plus a Lorentz non-covariant $W^0\overline{W}^0$ interaction. Notice that this non-covariant piece is precisely the interaction (12.5.15) required to cancel the non-covariance arising at second order in the S-matrix due to the appearance of non-covariant Schwinger terms in the propagator $\langle 0|T[\partial_\mu\psi^\star(x)\,\partial_\nu\psi(x')]|0\rangle$.

Perturbation theory gives a Lorentz-invariant S-matrix because the non-covariant parts of $\mathcal{H}_{\rm int}$ cancel the non-covariant Schwinger terms like those that appear in expressions like (12.5.10). It is *as if* we had simply used the covariant interaction Hamiltonian $\mathcal{H}_{\rm int} = -\mathcal{L}_{\rm int}$, and replaced everywhere naive time-ordering with the covariant T^* ordering, such as defined in (12.5.17). As mentioned earlier, a great virtue of the path-integral techniques described below in §21 is the more efficient derivation they provide of perturbation theory, by cutting directly to the manifestly covariant formulation in terms of $\mathcal{L}_{\rm int}$.

13.3 Symmetries and conservation laws

Formulating a theory in terms of an action using canonical methods has another benefit: it allows a direct derivation of the connection between continuous symmetries and local conservation laws. In particular it allows a more systematic construction of the conserved currents that such symmetries imply must exist.

Recall from §8.2.1 that the local version of a conservation law states that conserved charges arise as an integral $Q = \int \mathrm{d}^3x\ \rho$ over a charge density ρ, and local conservation of Q requires that ρ everywhere satisfies

$$\partial_t \rho + \nabla \cdot \mathbf{J} = 0\,, \tag{13.3.1}$$

for some current $\mathbf{J}$ that describes the local flux density of the conserved quantity, in the sense that the rate with which charge flows through a small surface area $\mathrm{d}A$ with unit normal $\mathbf{n}$ is given by $\mathbf{J}\cdot\mathbf{n}\,\mathrm{d}A$. Eq. (13.3.1) is consistent with special relativity because the charge and flux densities transform as the components of a current 4-vector $J^\mu = \{\rho\,, \mathbf{J}\}$, in terms of which (13.3.1) becomes the manifestly Lorentz-covariant expression

$$\partial_\mu J^\mu = 0\,. \tag{13.3.2}$$

This section asks: what does this have to do with symmetries, and how does one construct J^μ given a particular symmetry? The solution is a result called *Noether's theorem*, after its discoverer Emmy Noether.

13.3.1 Noether's theorem

For the purposes of answering these questions we define a symmetry to be a local transformation rule for the fields $\psi^A \to \tilde{\psi}^A$ for which the action is invariant

$$S[\tilde{\psi}] = S[\psi]\,. \tag{13.3.3}$$

This invariance is meant to hold for arbitrary field configurations (and not, for example, only for field configurations that satisfy the field equations).

For continuous symmetries the transformation can be made infinitesimal and so can differ from the original field by only a small amount: $\tilde{\psi}^A = \psi^A + \delta\psi^A$ where $\delta\psi^A = \eta^\alpha f^A_\alpha(\psi)$ for some functions $f^A_\alpha(\psi)$ and a collection of (x-independent) infinitesimal parameters η^α. For infinitesimal transformations eq. (13.3.3) implies $\mathcal{L}$ must satisfy $\int \mathrm{d}^4x\ \delta\mathcal{L} = 0$ and so

$$\delta\mathcal{L} = \frac{\partial\mathcal{L}}{\partial(\partial_\mu\psi^A)}\,\partial_\mu f^A_\alpha + \frac{\partial\mathcal{L}}{\partial\psi^A}\,f^A_\alpha = \partial_\mu V^\mu_\alpha\,, \tag{13.3.4}$$

for some 4-vector quantities V^μ_α. The special case where V^μ_α vanishes is called an 'internal' symmetry.

Now comes the main point. Eq. (13.3.4) can be rewritten

$$\delta\mathcal{L} = \partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\psi^A)}\,f^A_\alpha\right] + \left\{-\partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\psi^A)}\right] + \frac{\partial\mathcal{L}}{\partial\psi^A}\right\} f^A_\alpha = \partial_\mu V^\mu_\alpha\,, \tag{13.3.5}$$

and so when eq. (13.3.5) is evaluated at a solution to the field equation eq. (13.2.8), it simplifies to

$$\partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\psi^A)}\,f^A_\alpha - V^\mu_\alpha\right] = 0\,, \tag{13.3.6}$$

which takes the form of a conservation law $\partial_\mu J^\mu_\alpha = 0$ for each α, with the corresponding *Noether* current given by

$$J^\mu_\alpha = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi^A)}\, f^A_\alpha - V^\mu_\alpha \,. \tag{13.3.7}$$

This shows how to construct a current J^μ_α for each independent parameter η^a in the continuous symmetry group, that is conserved whenever ψ^A satisfies its field equation (13.2.8).

As an example consider the symmetry

$$\delta\psi = i\eta\,\psi \quad \text{and} \quad \delta\psi^\star = -i\eta\,\psi^\star \tag{13.3.8}$$

that is the infinitesimal version of a rephasing $\psi \to e^{i\eta}\psi$ and $\psi^\star \to e^{-i\eta}\psi^\star$. For this symmetry we therefore have a single parameter η for which $f(\psi) = i\psi$. The Klein-Gordon lagrangian density

$$\mathcal{L} = -\partial_\mu\psi^\star\partial^\mu\psi - m^2\psi^\star\psi \tag{13.3.9}$$

is invariant under (13.3.8), and so satisfies $\delta\mathcal{L} = \mathcal{L}(\psi + \delta\psi) - \mathcal{L}(\psi) = 0$, where we work to linear order in η. Comparing $\delta\mathcal{L} = 0$ to (13.3.5) shows that $V^\mu = 0$.

Using $V^\mu = 0$ in (13.3.7) and performing the required derivatives of $\mathcal{L}$ in (13.3.9) implies the conserved current for this symmetry is

$$J^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu\psi)}\, f(\psi) + \frac{\partial \mathcal{L}}{\partial(\partial_\mu\psi^\star)}\, f^\star(\psi) = i\Big(\psi^\star\partial^\mu\psi - \psi\,\partial^\mu\psi^\star\Big)\,. \tag{13.3.10}$$

Eq. (13.3.6) states that this current must satisfy the conservation condition $\partial_\mu J^\mu = 0$ when ψ satisfies its equation of motion — *i.e.* eq. (13.2.8) — which for the lagrangian density (13.3.9) are

$$\partial_\mu\partial^\mu\psi - m^2\psi = 0\,, \tag{13.3.11}$$

and its complex conjugate.

This conclusion is easily verified in the present instance by directly differentiating (13.3.10) and using (13.3.11), since this gives

$$\partial_\mu J^\mu = i\partial_\mu\Big(\psi^\star\partial^\mu\psi - \psi\,\partial^\mu\psi^\star\Big) = i\Big(\psi^\star\partial_\mu\partial^\mu\psi - \psi\,\partial_\mu\partial^\mu\psi^\star\Big) = 0\,, \tag{13.3.12}$$

as claimed. Although such currents can be constructed by trial and error for simple systems, the great power of Noether's theorem lies in its constructive nature since it provides a simple general algorithm for constructing the current once the symmetry transformations are known.

13.4 Canonical electromagnetism

The next relativistic system to examine in a Lagrangian light is electromagnetism itself. In this case the Lagrangian density turns out to be simple:

$$\mathcal{L}_{EM} = \frac{1}{2}\Big(\mathbf{E}^2 - \mathbf{B}^2\Big) = -\frac{1}{4}\,F_{\mu\nu}F^{\mu\nu}\,, \tag{13.4.1}$$

where the first way of writing things expresses the result directly in terms of the electric and magnetic fields while the second version shows that $\mathcal{L}_{EM}$ is manifestly a Lorentz scalar, since $F_{\mu\nu}$ is an antisymmetric Lorentz tensor. In this relativistic version the indices are raised and lowered as usual using the Minkowsky metric $\eta_{\mu\nu}$ and its matrix inverse $\eta^{\mu\nu}$, so that $F_{\mu\nu}F^{\mu\nu} = \eta^{\mu\lambda}\eta^{\nu\rho}F_{\mu\nu}F_{\lambda\rho} = 2F_{0i}F^{0i} + F_{ij}F^{ij}$.

Although neither $\mathbf{E}$ nor $\mathbf{B}$ are differentiated in $\mathcal{L}_{EM}$, we have seen that these are not all independent of one another in any case, and the basic variables in the problem are instead the vector potential $\mathbf{A}$ and the electrostatic scalar potential ϕ, related to $\mathbf{E}$ and $\mathbf{B}$ by $\mathbf{E} = -\partial_t\mathbf{A} - \nabla\phi$ and $\mathbf{B} = \nabla \times \mathbf{A}$, or $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ where the spatial parts of A_μ are given by the components of $\mathbf{A}$ and $A^0 = -A_0 = \phi$.

13.4.1 Constraints

Given the Lagrangian density the next step is to find the canonical momenta and for $\mathbf{A}$ the momentum turns out (up to a sign) to be the electric field itself, because

$$\mathbf{\Pi} = \frac{\partial \mathcal{L}_{EM}}{\partial(\partial_t \mathbf{A})} = -\mathbf{E}\,. \tag{13.4.2}$$

A complication arises once we seek the momentum for ϕ though because $\mathcal{L}_{EM}$ does not depend on $\partial_t\phi$ at all, and so its canonical momentum vanishes identically:

$$\Pi_0 = \frac{\partial \mathcal{L}_{EM}}{\partial(\partial_t A_0)} = 0\,. \tag{13.4.3}$$

Both (13.4.2) and (13.4.3) turn out to pose a problem for quantizing the electromagnetic field.

Eq. (13.4.3) is a problem because the vanishing of Π_0 means that the relationship between Π_0 and $\partial_t\phi$ is singular, since it is impossible to solve (13.4.3) for $\partial_t\phi$ as a function of Π_0. This is the hallmark of a 'constrained' system, which does not satisfy one of the assumptions that is usually made when discussing the Lagrangian and Hamiltonian formalisms. Constraints like (13.4.3) are a potential problem when quantizing the theory because they are generically inconsistent with the naive canonical equal-time quantization conditions that say that variables and their momenta do not commute. How can (13.4.3) be consistent with a relationship like

$$\Big[A_0(\mathbf{x},t)\,,\Pi_0(\mathbf{y},t)\Big] = i\delta^3(\mathbf{x}-\mathbf{y})\,? \tag{13.4.4}$$

There is a generalization of the standard quantization formalism that is designed to handle such cases, called the theory of contrained Hamiltonian systems. Much of this goes beyond the scope of these notes, so we here take an equivalent approach that reproduces the general results and suffices for the applications of interest here.

As applied to (13.4.3) this simpler procedure side-steps the problem of quantizing A_0 by recognizing that one of the equations of motion, namely the Maxwell equation

$$\nabla \cdot \mathbf{E} = \rho\,, \tag{13.4.5}$$

can be regarded as completely fixing A_0 as a function of the other fields that appear within the charge density ρ, and so it is not an independent degree of freedom. Rather than quantizing A_0 using (13.4.4) we instead think of A_0 as the operator found by expressing it in terms of other fields by explicitly solving (13.4.5). From then on we simply no longer think of it as an independent variable that needs quantizing.

The expression for A_0 can be made very explicit if we work within Coulomb gauge, for which $\nabla \cdot \mathbf{A} = 0$, since then (13.4.5) becomes $\nabla^2 A_0 = -\nabla^2 \phi = \rho$ and the general solution becomes

$$A^0(\mathbf{x}, t) = \phi(\mathbf{x}, t) = \frac{1}{4\pi} \int \mathrm{d}^3 y \, \frac{\rho(\mathbf{y}, t)}{|\mathbf{x} - \mathbf{y}|} \,. \tag{13.4.6}$$

In Coulomb gauge (13.4.6) effectively defines ϕ in terms of other fields, and so it inherits its operator character from these other fields. For example if the charged fields were described by a Schrödinger field $\Psi(\mathbf{x}, t)$ describing particles with charge q then we have seen that the charge density to be used in (13.4.6) is given by $\rho = q\, \Psi^\star \Psi$.

Eliminating ϕ in this way still leaves the problem posed by (13.4.2), however. The problem here arises because the twin conditions $\nabla \cdot \mathbf{A} = 0$ and $\nabla \cdot \mathbf{\Pi} = -\nabla \cdot \mathbf{E} = -\rho$ are not consistent with the naive quantization condition for a variable and its conjugate momentum, which in this case would be

$$\Big[A_i(\mathbf{x}, t) \,, \Pi_j(\mathbf{y}, t) \Big] = i \delta_{ij} \, \delta^3(\mathbf{x} - \mathbf{y}) \quad \text{(wrong)} \tag{13.4.7}$$

as can be seen by acting on both sides with $\partial/\partial x^i$ or $\partial/\partial y^j$. We handle this along the lines followed in §9.2 but because this involves working in the interaction picture its discussion we defer a discussion of commutation relations until first identifying the Hamiltonian.

13.4.2 Hamiltonian and interaction picture

To construct the Hamiltonian, suppose the coupling of charged matter to A_0 has a form that is linear in A_0, as in

$$\mathcal{L} = \mathcal{L}_{EM} + \mathcal{L}_{\text{matter}} + J^\mu A_\mu = \mathcal{L}_{EM} + \mathcal{L}_{\text{matter}} - \rho\, \phi + \mathbf{J} \cdot \mathbf{A} \,, \tag{13.4.8}$$

where $\mathcal{L}_{EM} = \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2)$ is as given in (13.4.1) while $\mathcal{L}_{\text{matter}}$ describes the rest of matter.

We assume for simplicity that neither $\mathcal{L}_{\text{matter}}$ nor J^μ depends on the electromagnetic fields A_μ. Not all systems can be written in this way, since (for example) the electromagnetic current $\mathbf{J}$ for Schrödinger fields found in (9.5.9) depends explicitly on $\mathbf{A}$. The current predicted in the next chapter – see eq. (14.1.4) – for relativistic charged spinless particles is

$$J_\mu = iq\Big(\psi\, \partial_\mu \psi^* - \psi^* \partial_\mu \psi \Big) + 2iq^2 A_\mu\, \psi^* \psi \,, \tag{13.4.9}$$

also depends on A_μ. But for some systems (13.4.8) is appropriate, such as for the Dirac field considered below in §16.2 relevant for Quantum Electrodynamics.

The field equation obtained using (13.4.8) by varying A_μ — see, for example, (D.3.4) and (D.3.5) — gives the usual two Maxwell equations involving currents and charges: $\partial_\nu F^{\mu\nu} = J^\mu$. This in particular includes the equation $\nabla \cdot \mathbf{E} = \rho$ that is used in (13.4.6) to determine ϕ in terms of other fields – *c.f.* (13.4.5).

Denoting the fields and momenta for the matter sector collectively as ψ^a and $\mathfrak{p}_a$, the Hamiltonian obtained from the Lagrangian (13.4.8) in the usual way is

$$\begin{aligned} H &= \int \mathrm{d}^3x \Big[\mathbf{\Pi} \cdot \partial_t \mathbf{A} + \mathfrak{p}_a \, \partial_t \psi^a - \mathcal{L}_{EM} - \mathcal{L}_{\text{matter}} - J^\mu A_\mu \Big] \\ &= \int \mathrm{d}^3x \left[\mathbf{E} \cdot \Big(\mathbf{E} + \nabla\phi \Big) - \frac{1}{2} \Big(\mathbf{E}^2 - \mathbf{B}^2 \Big) + \rho\,\phi - \mathbf{J} \cdot \mathbf{A} + \mathcal{H}_{\text{matter}} \right] \\ &= \int \mathrm{d}^3x \left[\frac{1}{2} \Big(\mathbf{E}^2 + \mathbf{B}^2 \Big) + \mathcal{H}_{\text{matter}} - \phi \, \nabla \cdot \mathbf{E} + \rho\,\phi - \mathbf{J} \cdot \mathbf{A} \right] , \end{aligned} \tag{13.4.10}$$

which uses $\mathcal{H}_{\text{matter}} = \mathfrak{p}_a \, \partial_t \psi^a - \mathcal{L}_{\text{matter}}$ and integrates by parts to rewrite $\mathbf{E} \cdot \nabla\phi$ as $-\phi \, \nabla \cdot \mathbf{E}$.

Interaction picture

Since our later aim is to use this in perturbative calculations, the next step is to divide H into a non-interacting and interaction part and go to the interaction picture. When doing so we follow the practice also followed in §9.2 of explicitly splitting the radiation part of the field from the constrained electrostatic part, writing

$$\mathbf{E} = \mathbf{E}_{\text{hom}} - \nabla\phi \quad \text{where} \quad \mathbf{E}_{\text{hom}} = -\partial_t \mathbf{A} \, . \tag{13.4.11}$$

Here ϕ carries the full burden of the constraint

$$\nabla \cdot \mathbf{E} = -\nabla^2 \phi = \rho \, , \tag{13.4.12}$$

whose explicit solution is (13.4.6). Because ϕ is regarded as a constrained function of other fields, the full interaction-picture electromagnetic field is $A^{\text{int}}_\mu = (0, \mathbf{A})$, satisfying the gauge choice used also for free fields in §9.2: $a^0 = \nabla \cdot \mathbf{A} = 0$. These imply $\nabla \cdot \mathbf{E}_{\text{hom}} = 0$.

With these choices the unperturbed Hamiltonian density becomes

$$\mathcal{H}_0 = \frac{1}{2} \Big(\mathbf{E}^2_{\text{hom}} + \mathbf{B}^2 \Big) + \mathcal{H}_{\text{mat}\,0} \, , \tag{13.4.13}$$

where we also split the matter Hamiltonian into an unperturbed and perturbed part: $\mathcal{H}_{\text{matter}} = \mathcal{H}_{\text{mat}\,0} + \mathcal{H}_{\text{mat}-\text{int}}$, where the matter interactions contain any non-electromagnetic interactions that might also be present. Subtracting this from (13.4.10) then gives the interaction Hamiltonian

$$\begin{aligned} H_{\text{int}} &= \int \mathrm{d}^3x \left[\frac{1}{2} \Big(\mathbf{E}^2 - \mathbf{E}^2_{\text{hom}} \Big) - \phi \, \nabla \cdot \mathbf{E} + \rho\,\phi - \mathbf{J} \cdot \mathbf{A} + \mathcal{H}_{\text{mat}-\text{int}} \right] \\ &= \int \mathrm{d}^3x \left[\frac{1}{2} (\nabla\phi)^2 + \phi \, \nabla^2 \phi + \rho\,\phi - \mathbf{J} \cdot \mathbf{A} + \mathcal{H}_{\text{mat}-\text{int}} \right] \\ &= \int \mathrm{d}^3x \left[\frac{1}{2} \, \rho\,\phi - \mathbf{J} \cdot \mathbf{A} + \mathcal{H}_{\text{mat}-\text{int}} \right] , \end{aligned} \tag{13.4.14}$$

where the second line uses (13.4.11) and the observation that $\nabla\cdot\mathbf{E}_{\rm hom} = 0$ implies $\mathbf{E}_{\rm hom}\cdot\nabla\phi = \nabla\cdot(\mathbf{E}_{\rm hom}\phi)$ is a total derivative that can be dropped. The third line similarly uses the constraint (13.4.12) to trade ϕ for ρ.

Notice that the first two terms of (13.4.14) give the same current and Coulomb interaction energy that was assumed in §9.5, in particular reproducing the correct Coulomb energy

$$H_C(t) = \frac{1}{2}\int \mathrm{d}^3x\;\rho\,\phi = \frac{1}{8\pi}\int \mathrm{d}^3x\,\mathrm{d}^3y\;\frac{\rho(\mathbf{x},t)\,\rho(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|}\,. \tag{13.4.15}$$

Notice also that because the interaction-picture field is $A^{\rm int}_\mu = (0,\mathbf{A})$, we have $\mathbf{J}\cdot\mathbf{A} = J^\mu A^{\rm int}_\mu$ and so the electromagnetic part of the interaction can be written as a covariant plus a non-covariant part, with

$$\mathcal{H}_{EM\,\rm int} = \frac{1}{2}\,\rho\,\phi - J^\mu A_\mu = \frac{1}{2}\,\rho\,\phi - \mathcal{L}_{EM\,\rm int}\,, \tag{13.4.16}$$

foreshadowing that the Coulomb interaction is also the noncovariant part of the Hamiltonian that will eventually be cancelling a noncovariant contribution to photon propagators (as we see explicitly in §16.1).

Commutation relations

We finally return to the the canonical commutation relation for $\mathbf{A}(\mathbf{x},t)$, within the interaction picture. Since fields satisfy the noninteracting field equations in the interaction picture, the appropriate canonical momentum for $\mathbf{A}(\mathbf{x},t)$ is $\mathbf{\Pi} = -\mathbf{E}_{\rm hom}$ rather than $\mathbf{E}$, and so both $\mathbf{A}$ and $\mathbf{\Pi}$ satisfy the constraint

$$\nabla\cdot\mathbf{A} = \nabla\cdot\mathbf{\Pi} = 0\,, \tag{13.4.17}$$

which is inconsistent with the naive canonical commutation relation (13.4.7).

This problem arises because all of the components of $\mathbf{A}$ are not independent. Because of this only the components of $\mathbf{A}$ that do not contribute to $\nabla\cdot\mathbf{A}$ should be regarded as being fully fledged quantum degrees of freedom for whom equal-time communtations can be imposed. The best one can ask is that the divergence-free part of $\mathbf{A}$ satisfy the standard commutation relations, which would instead lead to the quantization condition with $\nabla\cdot\mathbf{A}$ projected out, as in

$$\Big[A_i(\mathbf{x},t),\Pi_j(\mathbf{y},t)\Big] = i\left(\delta_{ij} - \frac{\partial_i\partial_j}{\nabla^2}\right)\delta^3(\mathbf{x}-\mathbf{y})\,. \tag{13.4.18}$$

Both sides of this condition vanish when operating with either $\partial/\partial x^i$ or $\partial/\partial y^j$, as is required by (13.4.17). Eq. (13.4.18) is indeed the commutation relation that was explicitly found in earlier chapters, such as in (9.2.11), and so is equivalent to the expansion of $\mathbf{A}$ in terms of photon creation and annihilation operators as in (9.2.5).

14 Scalar Electrodynamics

Electromagnetism is the best-known example of a relativistic field theory, but although the Maxwell equations are themselves relativistic, the descriptions so far — such as in §9 — only include slowly moving charged particles. This section uses the result of the previous chapters to formulate the dynamics of relativistic charged particles, which when coupled to electromagnetism gives what is called Quantum Electrodynamics (or QED for short). This chapter considers the simplest case: where the relativistic charged particles are spinless.

14.1 Charged Klein-Gordon Field

QED is usually formulated assuming that the relativistic charged particles have spin-half, since this covers many of the cases of most practical interest (electrons and protons and other spin-half 'elementary' particles). But it can also be formulated for charged particles with other spins, and this is our starting point here because it is relatively simple. Charged spinless particles also arise in Nature, such as for the spinless charged 'pions' $\pi^{\pm}$. The electromagnetic interactions of relativistic spinless charged particles are often called 'scalar electrodynamics' to distinguish from the coupling to spin-half charged particles.

This section starts with charged spinless particles, and so takes the relativistic spinless Klein-Gordon particle of the previous chapter and couples it to electromagnetism, thereby providing a first look at the electromagnetic behaviour of a completely relativistic system. The interactions we find involve derivative couplings, and so do not give rise to a Lorentz invariant Hamiltonian density, along the lines similar to the discussion in §12.5.2 and §13.2.2. This is why its discussion has been postponed to this point, so that canonical Lagrangian methods can be used to keep Lorentz invariance explicit.

To this end suppose we take the charged scalar to couple to electromagnetism in the same way as did the Schrödinger field, by promoting every derivative $\partial_\mu\psi$ to a covariant derivative,

$$D_\mu\psi = \partial_\mu\psi - iqA_\mu\psi \quad \text{and} \quad D_\mu\psi^\star = \partial_\mu\psi^\star + iqA_\mu\psi^\star\,, \tag{14.1.1}$$

where q is the electric charge of the particle destroyed by the (positive-frequency part of) ψ. Although $\partial_\mu\psi$ is a 4-vector when ψ is a Lorentz scalar, we saw in §11.3.4 that A_μ only transforms as a 4-vector *up to a gauge transformation* $A_\mu \to A_\mu + \partial_\mu\omega$, and so $A_\mu\psi$ is *not* a 4-vector. Consequently $\partial_\mu\psi$ is Lorentz covariant but not gauge covariant and $A_\mu\psi$ is neither Lorentz covariant nor gauge covariant. But the combination $D_\mu\psi$ *is* gauge covariant by construction and so is therefore also a 4-vector under Lorentz transformations, and this means a Lagrangian density built from it by contracting indices in the obvious way using $\eta^{\mu\nu}$ transforms as a Lorentz scalar, *provided* the lagrangian density is also gauge invariant.

Making the replacement (14.1.1) in the Klein-Gordon action therefore leads to an action that is both gauge-invariant and Lorentz-invariant

$$\begin{aligned} S &= -\int \mathrm{d}^4x \, \Big[D^\mu\psi^* D_\mu\psi + m^2\psi^*\psi \Big] \\ &= -\int \mathrm{d}^4x \, \Big[\partial^\mu\psi^*\partial_\mu\psi + m^2\psi^*\psi - A_\mu j^\mu + q^2 A_\mu A^\mu \psi^*\psi \Big] , \end{aligned} \tag{14.1.2}$$

where the zero-field EM current appearing here is (compare with (13.3.10))

$$j_\mu = iq\Big(\psi\,\partial_\mu\psi^* - \psi^*\partial_\mu\psi\Big) . \tag{14.1.3}$$

This is called the 'zero-field' current because it differs from the full conseved EM current that appears in Maxwell's equations, which is instead given by

$$J_\mu = iq\Big(\psi\, D_\mu\psi^* - \psi^* D_\mu\psi\Big) = j_\mu + 2iq^2 A_\mu\psi^*\psi . \tag{14.1.4}$$

To evaluate the Hamiltonian for this system write the lagrangian density for the charged spinless particle as

$$\mathcal{L} = \Big(\partial_t\psi - iqA_0\psi\Big)^*\Big(\partial_t\psi - iqA_0\psi\Big) - \mathbf{D}\psi^*\cdot\mathbf{D}\psi - m^2\psi^*\psi , \tag{14.1.5}$$

which shows that the canonical momenta are

$$\Pi := \frac{\partial\mathcal{L}}{\partial\dot\psi} = \partial_t\psi^\star + iqA_0\psi^* \quad \text{and} \quad \Pi^\star := \frac{\partial\mathcal{L}}{\partial\dot\psi^\star} = \partial_t\psi - iqA_0\psi . \tag{14.1.6}$$

Solving this for $\partial_t\psi$ as a function of ψ and Π then gives $\partial_t\psi = \Pi^* + iqA_0\psi$. The Hamiltonian density is then

$$\mathcal{H} := \Pi\,\partial_t\psi + \Pi^*\partial_t\psi^* - \mathcal{L} = \Pi^*\Pi + \mathbf{D}\psi^*\cdot\mathbf{D}\psi + m^2\psi^*\psi + iqA_0(\Pi\psi - \Pi^*\psi^*) . \tag{14.1.7}$$

It can sometimes also be useful to express $\mathcal{H}$ in terms of $\partial_t\psi$ rather than Π, and written in this way the above expression becomes

$$\mathcal{H} = \partial_t\psi^*\partial_t\psi + \nabla\psi^*\cdot\nabla\psi + (m^2 - q^2A_0^2)\psi^*\psi . \tag{14.1.8}$$

Notice that all terms linear in A_0 cancel out in this expression.

Although the Hamiltonian does not look very relativistic, the field equations for ψ obtained by commuting this Hamiltonian with $\partial_t\psi$ — or by using (13.2.8) — are (using a gauge $\partial_\mu A^\mu = 0$)

$$\begin{aligned} 0 &= (-D^\mu D_\mu + m^2)\psi = \Big(-\partial_\mu\partial^\mu + m^2 + 2iqA^\mu\partial_\mu + q^2A_\mu A^\mu\Big)\psi \\ &= \Big(\partial_t^2 - \nabla^2 + m^2 - q^2A_0^2 - 2iqA_0\partial_t + 2iq\mathbf{A}\cdot\nabla + q^2\mathbf{A}\cdot\mathbf{A}\Big)\psi , \end{aligned} \tag{14.1.9}$$

where $D_\mu D^\mu = \eta^{\mu\nu}D_\mu D_\nu$ is manifestly Lorentz covariant. For later purposes it is important to remember that the usual EM potential ϕ is related to A_0 by $\phi = A^0 = -A_0$, as may be seen because only then is $F_{0i} = \partial_0 A_i - \partial_i A_0$ consistent with $\mathbf{E} = -\partial_t\mathbf{A} - \nabla\phi$.

14.2 Background electrostatic fields

Before applying canonical methods to the electromagnetic field itself (for this see §13.4) we pause here to describe the above Klein-Gordon system in the presence of specified classical electrostatic background fields, in the spirit of §12.3, since this allows a discussion of scattering and pair production by an applied field.

14.2.1 Hamiltonian and field equations

For these purposes imagine specializing the above expressions to the case where $\mathbf{A} = 0$ and $A^0 = \phi$ is a specified function of space and time. In this case the lagrangian and Hamiltonian density for ψ become

$$\mathcal{L} = \Big(\partial_t\psi - iqA_0\psi\Big)^*\Big(\partial_t\psi - iqA_0\psi\Big) - \nabla\psi^*\cdot\nabla\psi - m^2\psi^*\psi\,, \tag{14.2.1}$$

and

$$\mathcal{H} = \Pi^*\Pi + \nabla\psi^*\cdot\nabla\psi + m^2\psi^*\psi + iqA_0(\Pi\psi - \Pi^*\psi^*)\,, \tag{14.2.2}$$

where the canonical momentum is given as before by (14.1.6).

Because this Hamiltonian is quadratic in ψ it can be diagonalized in principle by following the steps of §12.3 and expanding the fields as

$$\psi(x) = \sum_n \Big[\mathfrak{a}_n\, u_n(x) + \overline{\mathfrak{a}}_n^\star\, u_n^*(x)\Big], \tag{14.2.3}$$

for some choice of mode functions $u_n(x)$ chosen to be energy eigenstates — that is to satisfy $i\partial_t u_n(x) = \varepsilon_n\, u_n(x)$ — and to satisfy the field equations (14.1.9) specialized to this background:

$$\begin{aligned}(-D^\mu D_\mu + m^2)u_n &= \Big(\partial_t^2 - \nabla^2 + m^2 - q^2A_0^2 - 2iqA_0\partial_t\Big)u_n \\ &= \Big(-\varepsilon_n^2 - \nabla^2 + m^2 - q^2A_0^2 - 2iqA_0\partial_t\Big)u_n = 0\,.\end{aligned} \tag{14.2.4}$$

Notice that this is quadratic in ε_n and so admits solutions for ε_n that are both positive and negative. In general both of these solutions are required to form a complete basis of solutions, and with the convention $u_n(x) = v_n(\mathbf{x})\, e^{-i\varepsilon_n t}$ for $\varepsilon_n > 0$ it is $u_n^*(x)$ that contains the negative-frequency solutions.

The expansion (14.2.3) when substituted into the Hamiltonian $H = \int \mathrm{d}^3x\ \mathcal{H}$ – using (14.2.2) for $\mathcal{H}$ – leads to the harmonic oscillator form

$$H = E_0 + \sum_n \varepsilon_n\Big(\mathfrak{a}_n^\star\mathfrak{a}_n + \overline{\mathfrak{a}}_n^\star\overline{\mathfrak{a}}_n\Big)\,, \tag{14.2.5}$$

provided the mode functions are orthonormal $(u_n\,, u_m) = \delta_{nm}$ and $(u_n, u_m^*) = 0$ for an appropriate inner product.

14.2.2 Inner product

What is the appropriate inner product in this case? The required inner product can be inferred directly from the field equation and is defined for any two solutions, $f(x)$ and $g(x)$, of (14.2.4) by

$$(f,g) := i\int_{\Sigma_t} \mathrm{d}^3x\Big[f^* D_t g - (D_t f^*)g\Big] = i\int_{\Sigma_t} \mathrm{d}^3x\Big[f^*\partial_t g - (\partial_t f^*)g - 2iqA_0 f^* g\Big]\,, \qquad (14.2.6)$$

where Σ_t is a spatial surface of fixed time t. The inner product is defined in this way because this definition is independent of the time where the integration is performed, provided that f and g both satisfy $(-\Delta + m^2)f = (-\Delta + m^2)g = 0$ where $\Delta = D_\mu D^\mu$ and $D_\mu = \partial_\mu - iqA_\mu$ acts the same way on both f and g (*i.e.* both have the same charge).

The time-independence of the above definition can be seen by writing zero in the following suggestive way:

$$\begin{aligned}
0 &= \int_M \mathrm{d}^4x\Big[[(-\Delta+m^2)f]^* g - f^*(-\Delta+m^2)g\Big] = \int_M \mathrm{d}^4x\Big[(-\Delta f)^* g + f^*(\Delta g)\Big] \\
&= \int_M \mathrm{d}^4x\Big[-\partial_\mu[D^\mu f^* g] + D^\mu f^* D_\mu g + f^*(\Delta g)\Big] = \int_M \mathrm{d}^4x\,\partial_\mu\Big[-(D^\mu f)^* g + f^* D^\mu g\Big] \\
&= \int_{\partial M} \mathrm{d}^3x\, n_\mu\Big[-(D^\mu f)^* g + f^* D^\mu g\Big] \qquad (14.2.7) \\
&= \int_{\Sigma_{t'}} \mathrm{d}^3x\,\Big[-(D^0 f)^* g + f^* D^0 g\Big] - \int_{\Sigma_t} \mathrm{d}^3x\, n_\mu\Big[-(D^0 f)^* g + f^* D^0 g\Big]\,,
\end{aligned}$$

where M is the slab of spacetime lying between any two spatial slices, Σ_t and $\Sigma_{t'}$, of fixed time (with $t' > t$). In the above the second line performs two integrations by parts and the third line uses Stoke's theorem to write the result as a surface integral over ∂M: the oriented boundary of M. For functions that fall to zero quickly enough at spatial infinity the only boundary contributions come from Σ_t and $\Sigma_{t'}$ and these enter with opposite signs because n_μ is the outward-pointing normal to the boundary (and so n_μ points in the direction of increasing t for one of them and in the direction of decreasing t for the other, and so $n_\mu D^\mu = \pm D^0$). The conclusion that the final line vanishes shows that the inner product takes the same value for any Σ_t, as claimed.

Specialized to energy eigenmodes, which by definition satisfy $i\partial_t u_n(x) = \varepsilon_n\, u_n(x)$, the inner product becomes

$$(f,g) = \int_{\Sigma_t} \mathrm{d}^3x\Big[(\varepsilon_f + \varepsilon_g + 2qA_0) f^* g\Big]\,. \qquad (14.2.8)$$

14.2.3 Solutions for constant A_0

Suppose, for example, that A_0 is constant. Then the solutions to the field equation are plane waves, so the modes can be chosen to have the form $u_{\mathbf{p}}(t,\mathbf{x}) = C_{\mathbf{p}}\, e^{-i\varepsilon(p)\,t + i\mathbf{p}\cdot\mathbf{x}}$, for some

normalization $C_{\mathbf{p}}$, where (14.2.4) implies the mode energy $\varepsilon(p)$ satisfies

$$\Big[\varepsilon(p) + qA_0\Big]^2 = \mathbf{p}^2 + m^2\,. \tag{14.2.9}$$

The two branches of this solution are

$$\varepsilon_\pm(p) = -qA_0 \pm \sqrt{\mathbf{p}^2 + m^2}\,. \tag{14.2.10}$$

If we choose discrete momenta, such as by using periodic boundary conditions in a large box of finite volume $\mathcal{V}$, then (for constant A_0) the integral relevant for normalization is

$$(u_{\mathbf{p}}, u_{\mathbf{p}}) = 2\big[\varepsilon(p) + qA_0\big]\int_{\mathcal{V}} \mathrm{d}^3x\; u^*_{\mathbf{p}} u_{\mathbf{p}} = 2\mathcal{V}\big[\varepsilon(p) + qA_0\big]|C_{\mathbf{p}}|^2 \tag{14.2.11}$$

from which we learn $(u_{\mathbf{p}}\,, u_{\mathbf{p}}) = \mathrm{sign}[\varepsilon(p) + qA_0]$ where

$$|C_{\mathbf{p}}|^2 = \frac{1}{2|\varepsilon(p) + qA_0|\mathcal{V}}\,, \tag{14.2.12}$$

with absolute value required because some solutions can satisfy $\varepsilon(p) + qA_0 < 0$. The fact that some modes have negative norm is one of the reasons that the Klein-Gordon equation was abandoned as a relativistic version of the single-particle Schrödinger equation.

Modes energies and currents

The fact that $(u_{\mathbf{p}}, u_{\mathbf{p}})$ can be negative has implications when computing the contribution of any particular mode to the energy and conserved charge. For instance the contribution to the energy density of a mode $u_{\mathbf{p}} = C_{\mathbf{p}} e^{-i\varepsilon(p)\,t + i\mathbf{p}\cdot\mathbf{x}}$ is given by

$$\begin{aligned}
\mathcal{H}(u) &= \partial_t u^*_{\mathbf{p}} \partial_t u_{\mathbf{p}} + \nabla u^*_{\mathbf{p}} \nabla u_{\mathbf{p}} + (m^2 - q^2A_0^2) u^*_{\mathbf{p}} u_{\mathbf{p}} \\
&= \Big[\varepsilon^2(p) + \mathbf{p}^2 + m^2 - q^2A_0^2\Big]|C_{\mathbf{p}}|^2 \\
&= \Big[\varepsilon^2(p) + [\varepsilon(p) + qA_0]^2 - q^2A_0^2\Big]|C_{\mathbf{p}}|^2 \\
&= 2\varepsilon(p)\Big[\varepsilon(p) + qA_0\Big]|C_{\mathbf{p}}|^2 = \pm\frac{\varepsilon_\pm(p)}{\mathcal{V}}\,,
\end{aligned} \tag{14.2.13}$$

where the sign indicates which branch of frequency in (14.2.10) is under consideration, and arises because of the absolute value that appears when using (14.2.12) to eliminate $|C_{\mathbf{p}}|^2$. The total energy of the mode is therefore

$$E(u) = \mathcal{H}(u)\,\mathcal{V} = \pm\varepsilon_\pm(p) = \mp qA_0 + \sqrt{\mathbf{p}^2 + m^2}\,, \tag{14.2.14}$$

which is always positive for large $|\mathbf{p}|$. It is important that the mode energy be positive for large $|\mathbf{p}|$ because if this were not the case the Hamiltonian could not be bounded from below. Generically the system would then be be unstable, such as towards the spontaneous

production of arbitrarily many negative-energy modes from the vacuum. (As we see below, having $E(u)$ be negative in (14.2.14) for small $|\mathbf{p}|$, which can happen if $|qA_0| > m$, also implies a field-dependent type of instability – corresponding to the phenomenon of particle-antiparticle pair production by a sufficiently strong applied field.)

This expression for the energy shows that the positive (negative) frequency modes have their energy lowered (raised) with A_0, as they would if they had positive (negative) charge. To confirm the charge explicitly, evaluate the current density carried by a mode using

$$J^\mu(u) = iq\Big(u_{\mathbf{p}}\, D^\mu u^*_{\mathbf{p}} - u^*_{\mathbf{p}} D^\mu u_{\mathbf{p}}\Big) \tag{14.2.15}$$

and so its charge density is

$$\begin{aligned} J^0(u) &= -iq\Big(u_{\mathbf{p}}\, D_t u^*_{\mathbf{p}} - u^*_{\mathbf{p}} D_t u_{\mathbf{p}}\Big) = -iq\Big(u_{\mathbf{p}}\, \partial_t u^*_{\mathbf{p}} - u^*_{\mathbf{p}} \partial_t u_{\mathbf{p}}\Big) + 2q^2 A_0 u^*_{\mathbf{p}} u_{\mathbf{p}} \\ &= 2q\Big[\varepsilon_\pm(p) + qA_0\Big]|C_{\mathbf{p}}|^2 = \pm\frac{q}{\mathcal{V}}\,, \end{aligned} \tag{14.2.16}$$

where again the sign $\pm$ corresponds to the branches appearing in (14.2.10). This is proportional to $1/\mathcal{V}$ because it is the charge density, revealing the total integrated charge to be $\pm q$ for these modes (as expected).

The contribution of a mode to the current $\mathbf{J}$ is similarly

$$\mathbf{J}(u) = iq\Big(u_{\mathbf{p}}\, \nabla u^*_{\mathbf{p}} - u^*_{\mathbf{p}} \nabla u_{\mathbf{p}}\Big) = 2q|C_{\mathbf{p}}|^2\mathbf{p} = \frac{q\,\mathbf{p}}{|\varepsilon(p) + qA_0|\mathcal{V}} = \pm\frac{q\,\mathbf{v}}{\mathcal{V}}\,, \tag{14.2.17}$$

where

$$\mathbf{v} := \frac{\mathrm{d}\varepsilon_\pm(p)}{\mathrm{d}\mathbf{p}} = \frac{\mathbf{p}}{\varepsilon_\pm(p) + qA_0} = \pm\frac{\mathbf{p}}{\sqrt{\mathbf{p}^2 + m^2}}\,, \tag{14.2.18}$$

is the usual definition of group velocity associated with momentum $\mathbf{p}$. Notice that (14.2.17) shows how positive and negative frequency states carry charge in opposite directions — in the same way that (14.2.16) says they carry opposite charge densities — but *only* because (14.2.18) shows that the direction of particle motion, $\mathbf{v}$, is parallel to (antiparallel to) the direction of $\mathbf{p}$ for positive (negative) frequency states.

14.3 Scattering and pair production by background fields

It is useful to explore a few of the consequences of particles interacting with simple background potentials. This section does so by considering the scattering of Klein-Gordon charged particles from a simple (often piecewise constant) electrostatic potential. This is the same kind of toy potential that is often studied for introductory studies of the Schrödinger theory, which in that case lead to insights about the nature of scattering and tunneling. Both scattering and tunneling also occur in relativistic systems, but these are often also accompanied by the new phenomenon of pair production.

We consider in particular the case where the charged scalar's electric charge is $q = e$ and the classical background configuration is

$$A_0(x) = v \tanh\left(\frac{x}{\ell}\right) . \tag{14.3.1}$$

This potential (called a 'Sauter' potential) is one for which the Klein-Gordon equation is exactly solvable. We can always choose the direction of x to ensure that $ev > 0$. Because the electrostatic potential is $\phi = A^0 = -A_0$ for the choice $v > 0$ the electric field at the step points towards positive x and so accelerates positive charges in that direction and negative charges in the opposite direction. If pair production happens, in steady state we expect to see a current of positive charges flowing to the right and negative charges flowing to the left.

This potential approaches $A_0(\pm\infty) = \pm v$ like $e^{-|x|/\ell}$ and so is approximately constant apart from in a spatial interval of order ℓ around $x = 0$. For $|x| \gg \ell$ the potential is approximately a step-function, and the Klein-Gordon Lagrangian density becomes

$$\mathcal{L}_{KG} \simeq -\partial^\mu \psi^* \partial_\mu \psi - (m^2 - e^2 v^2)\psi^*\psi \pm iev\Big(\psi^*\dot{\psi} - \psi\,\dot{\psi}^*\Big) \tag{14.3.2}$$

where the upper and lower signs apply in the region $x = \pm|x|$.

14.3.1 First-quantized treatment

The first step is to find the mode functions for this potential, and we do so here and interpret these modes in a first-quantized way similar to what would have been done when solving the Schrödinger equation. This is followed by a full quantum-field description that justifies the interpretation used in the first-quantized description.

Thinking of the potential as a step simplifies the search for mode solutions since it allows the use of plane-wave solutions despite the step at $x = 0$ breaking translation invariance in the x direction. Plane waves are nonetheless useful because for step functions the breaking at $x = 0$ just mixes states with opposite x-components of momenta, just as happens in the Schrödinger case.

We seek mode solutions to (14.1.9) of the form $\varphi(x, y, z, t) \propto u(x)\, e^{i(k_y y + k_z z - \omega t)}$, where $u(x)$ satisfies

$$-u'' + \Big[-\omega^2 + k_T^2 + m^2 - e^2 A_0^2 - 2eA_0\,\omega\Big]u = 0 \tag{14.3.3}$$

where $k_T^2 = k_y^2 + k_z^2 = |\mathbf{k}_T|^2$ describes the conserved momentum parallel to the step. The solutions for $u(x)$ can be written $u_q(x) = C_R e^{iqx} + C_L e^{-iqx}$ where (14.3.3) implies $q \geq 0$ satisfies

$$q^2 = (\omega \pm ev)^2 - \mu_k^2 = (\omega - \mu_k \pm ev)(\omega + \mu_k \pm ev)\,, \tag{14.3.4}$$

where $\mu_k := \sqrt{k_T^2 + m^2} \geq m \geq 0$ provides a short form for the ubiquitous square root that contains the rest mass and the kinetic energy for motion parallel to the step.

The classically allowed regions correspond to those for which q is real (and positive, because we treat e^{iqx} and e^{-iqx} separately). Eq. (14.3.4) shows that solutions with real q

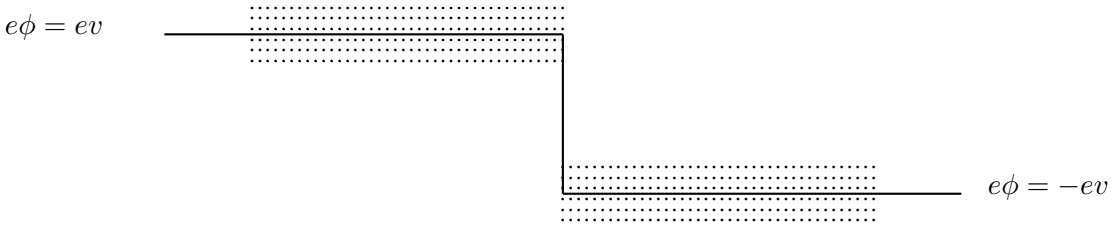


Figure 8. Sketch of the step potential $e\phi(x) = eA^0(x) = -eA_0(x)$ with the dotted area showing the forbidden energy bands in the region $e\phi + m > \omega > e\phi - m$.

exist only when the right-hand-side is positive. This condition is impossible to satisfy for any k_T when ω lies within a forbidden range of energies whose precise value depends on which side of the step one is:

$$\begin{aligned} -ev - m < \omega < -ev + m \qquad & \text{when } x \gg \ell \\ \text{and} \quad ev - m < \omega < ev + m \qquad & \text{when } x \ll -\ell \qquad \text{are forbidden}\,. \end{aligned} \tag{14.3.5}$$

This excludes there being single-particle states with energies in a band of width $2m$ centered on $-ev$ to the right of the step and centered on $+ev$ to its left, as sketched in Fig. 8. This gap separates the positive- and negative-frequency solutions from one another, just like in the absence of a background field, with the novelty being that the position of the gap differs on either side of the step.

The solutions for the energy, given a real q, have the same two branches as in (14.2.10):

$$\begin{aligned} \omega^R_{qk\pm} &= -ev \pm \sqrt{m^2 + k_T^2 + q^2} \quad \text{(right of step)} \\ \omega^L_{qk\pm} &= +ev \pm \sqrt{m^2 + k_T^2 + q^2} \quad \text{(left of step)}\,, \end{aligned} \tag{14.3.6}$$

and so simply differ in the sign of the square root in both cases. Notice in particular that $\omega^L_{qk\pm} = -\omega^R_{qk\mp}$. These also show that $\omega_{qk\pm} = \pm(\varepsilon_{qk} - \omega_0)$ where $\varepsilon_{qk} = \sqrt{k_T^2 + q^2 + m^2}$ and $\omega_{0R} = +ev$ and $\omega_{0L} = -ev$ when discussing positive-frequency states while $\omega_{0L} = +ev$ and $\omega_{0R} = -ev$ for negative energy states.

Because the band of classically forbidden states jumps at the step it can happen that the a classically allowed energy on one side of the step corresponds to a forbidden energy on the other side. In this case a tunneling solution allows an exponentially falling mode function in the forbidden region while there is an incoming and a reflected wave in the allowed region, much as in Schrödinger physics. If the step is large enough (*i.e.* when $ev > m$) it can also happen that the energy of a classically allowed positive-frequency state on one side of the step can correspond to a classically allowed negative-frequency state on the other side. When this is true it allows incident negative-frequency states on one side of the step to emerge as

positive frequency on the other side. As we shall see, this kind of transition lies at the root of the pair-production by the background electrostatic field.

Inspection of (14.3.5) shows that the energy window where classically allowed positive-frequency states on one side share the same energy as classically allowed negative frequency states on the other side corresponds to the interval

$$-ev + m < \omega < ev - m \tag{14.3.7}$$

(a regime whose existence clearly requires $ev > m$). The condition $ev > m$ has a natural interpretation for particle production because it is the condition for which it is possible to extract the rest energy of a particle-antiparticle pair ($E \geq 2m$) from the background-field part of the energy difference between the two sides of the step ($E_{\rm step} = 2ev$).

In the $\ell \to 0$ step-function limit the solutions to the left and right of the step are related to one another by demanding continuity of both the mode functions and their derivatives at $x = 0$ for all y, z and t. In the y, z and t directions this implies ω and $\mathbf{k}_T$ are the same on both sides of the step, with (14.3.6) then implying that q is obtained by solving $\omega^L_{q_L k} = \omega^R_{q_R k} = \omega$ on either side of the step. This means in particular that the value of q must differ on either side, with (from eq. (14.3.4))

$$q_L^2 = (\omega - ev)^2 - \mu_k^2 \quad \text{and} \quad q_R^2 = (\omega + ev)^2 - \mu_k^2 \,. \tag{14.3.8}$$

Notice the above results for q_L and q_R are the same regardless of whether the modes in question have positive frequency or negative frequency because the quantities $(\omega^L - ev)^2$ and $(\omega^R + ev)^2$ do not depend on which frequency branch we use.

For mode functions of the form $u_A = C_{A-} e^{-i(qx+\omega t)} + C_{A+} e^{i(qx-\omega t)}$, and $A = L, R$, continuity of $u_q(x)$ at $x = 0$ then implies

$$C_{L+} + C_{L-} = C_{R+} + C_{R-} \tag{14.3.9}$$

while continuity of $u_q'(x)$ implies

$$iq_R(C_{R+} - C_{R-}) - iq_L(C_{L+} - C_{L-}) = 0 \,. \tag{14.3.10}$$

These two conditions fix two of the four integration constants $C_{A\pm}$. One of the other two is always arbitrary and is fixed by normalizing the mode functions. The other is free parameter that can be fixed, for example, by a scattering boundary condition as described below.

Worked example: classically forbidden energy on left of step

Consider for example a case where a positive frequency mode has an energy that is allowed on the right of the step but where this energy is in the classically forbidden gap on the left of the step (so $\omega > -ev$ and $|\omega - ev| < m$). In this case $q_L = i\mathfrak{q}$ must be imaginary to the left of the step and we must choose the solution to be damped and so discard the term going like $e^{-|\mathfrak{q}|x}$. Using the convention

$\mathfrak{q} > 0$ (so that $iq_L = -\mathfrak{q} < 0$) we must take $C_{L+} = 0$. Then continuity ensures $C_{L-} = C_{R-} + C_{R+}$ while the jump condition gives (for $q = q_R$)

$$iq(C_{R+} - C_{R-}) - (-iq_L C_{L-}) = iq(C_{R+} - C_{R-}) - \mathfrak{q} C_{L-} = 0\,, \tag{14.3.11}$$

and so

$$\frac{C_{R+} - C_{R-}}{C_{R+} + C_{R-}} = \frac{1 - C_{R-}/C_{R+}}{1 + C_{R-}/C_{R+}} = \frac{\mathfrak{q}}{iq}\,. \tag{14.3.12}$$

This implies

$$\frac{C_{R-}}{C_{R+}} = \frac{q + i\mathfrak{q}}{q - i\mathfrak{q}}\,, \tag{14.3.13}$$

which is a pure phase because it implies $|C_{R-}/C_{R+}| = 1$. Once we connect these constants to physical transition amplitudes (see §14.3.2 below) the condition $|C_{R-}/C_{R+}| = 1$ will turn out to imply 100% reflection, just as it would have done in the Schrödinger case where u is more directly interpretable as a wave function.

These expressions for the $C_{A\pm}$ can be regarded as functions of ω (or q alone) by using (14.3.4), which in this case says

$$q^2 = (\omega - \mu_k + ev)(\omega + \mu_k + ev) \geq 0 \quad \text{and} \quad \mathfrak{q}^2 = (\mu_k + ev - \omega)(\omega + \mu_k - ev) \geq 0\,, \tag{14.3.14}$$

where the inequality uses the initial assumptions of positive frequency on the right ($\omega \geq -ev + \mu_k$) and overlap with the forbidden band on the left ($|\omega - ev| \leq \mu_k$).

Worked example: positive frequency on both sides of the step

Consider next the case where classically allowed states are present on both sides of the barrier, so $\omega > ev + m$ and so the momentum on each side of the step is

$$q_R^2 = (\omega - \mu_k + ev)(\omega + \mu_k + ev) \geq 0 \quad \text{and} \quad q_L^2 = (\omega - \mu_k - ev)(\omega + \mu_k - ev) \geq 0\,. \tag{14.3.15}$$

For a scattering state corresponding to a particle coming in from the right the appropriate boundary condition in a first quantized calculation chooses no right-movers to the left of the step. For positive-frequency states $\mathbf{v}$ is parallel to $\mathbf{p}$ and so this means that (as above) $C_{L+} = 0$. The implications of continuity of the wave-function and its derivative go through as before, leading this time to $C_{L-} = C_{R-} + C_{R+}$ and

$$iq_R(C_{R+} - C_{R-}) - iq_L(-C_{L-}) = 0\,, \tag{14.3.16}$$

and so

$$\frac{C_{R+} - C_{R-}}{C_{R+} + C_{R-}} = \frac{1 - C_{R-}/C_{R+}}{1 + C_{R-}/C_{R+}} = -\frac{q_L}{q_R}\,. \tag{14.3.17}$$

Solving these conditions implies

$$\frac{C_{R-}}{C_{R+}} = \frac{q_R + q_L}{q_R - q_L} \quad \text{and} \quad \frac{C_{L-}}{C_{R+}} = 1 + \frac{C_{R-}}{C_{R+}} = \frac{2q_R}{q_R - q_L} \quad \text{and so} \quad \frac{C_{L-}}{C_{R-}} = \frac{2q_R}{q_R + q_L}\,, \tag{14.3.18}$$

none of which is a pure phase.

If this were regarded as a first-quantized quantum scattering problem (as in an introductory quantum class) the reflection probability would be proportional to $|C_{R+}/C_{R-}|^2$ and the transmission

probability at the step would be proportional to $|C_{L-}/C_{R-}|^2$. But there is a subtlety in the precise definition because of the factors of energy appearing in the Klein-Gordon inner product – *c.f.* eq. (14.2.11). This energy dependence means that normalized states would be proportional to $q_L^{-1/2}$ on the left of the barrier and $q_R^{-1/2}$ to its right, and so because of this the transmission and reflection amplitudes are defined with a coefficient of $q_L^{-1/2}$ factored out. That is, one defines transmission and reflection amplitudes using

$$\tau := \frac{C_{L-}}{C_{R-}}\sqrt{\frac{q_L}{q_R}} \quad \text{and} \quad \rho := \frac{C_{R+}}{C_{R-}}\,, \tag{14.3.19}$$

where the above solutions imply

$$\rho = \frac{q_R - q_L}{q_R + q_L} \quad \text{and} \quad \tau = \frac{2\sqrt{q_R q_L}}{q_R + q_L}\,. \tag{14.3.20}$$

Notice that these satisfy $\left|\tau\right|^2 + \left|\rho\right|^2 = 1$, so the transmission and reflection probabilities sum to 1.

As a further check on the above solution we can verify that the boundary conditions ensure that the current J^μ remains conserved across the step. To this end notice that when $u = e^{-i\omega t}(C_+\, e^{iqx} + C_-\, e^{-iqx})$ then its contribution to the conserved charge density is

$$J^0(u) = 2e(\omega + eA_0)\, u^* u = 2e(\omega \pm ev)\Big[|C_+|^2 + |C_-|^2 + C_+^* C_- e^{-2iqx} + C_-^* C_+ e^{2iqx}\Big]\,, \tag{14.3.21}$$

where the upper (lower) sign applies to the right (left) of the step. In particular because this is time independent current conservation implies $\partial_x J^x = 0$.

To check this notice that the component of the current density in the x direction is

$$J^x(u) = ie\Big(u\,\partial_x u^* - u^*\partial_x u\Big) = 2eq\Big(|C_+|^2 - |C_-|^2\Big)\,, \tag{14.3.22}$$

with $q = q_L$ or q_R depending on which side of the step is of interest. Evaluating this using the solution for the C's found above in the case where $C_{L+} = 0$ (appropriate to a particle coming in from the right) then gives

$$J_L^x(u) = -2eq_L|C_{L-}|^2 = -\frac{8eq_L q_R^2}{(q_R + q_L)^2}\,|C_{R-}|^2\,, \tag{14.3.23}$$

where the first equality specializes to the left of the step. The same calculation to the right of the step one instead has

$$J_R^x(u) = 2eq_R\Big(|C_{R+}|^2 - |C_{R-}|^2\Big) = -\frac{8eq_L q_R^2}{(q_R + q_L)^2}\,|C_{R-}|^2\,, \tag{14.3.24}$$

Current conservation says these must be equal (as they are) because current conservation says J^x should be x-independent, even through the jump. The above verifies that the jump conditions properly encode this.

Worked example: negative frequency on left of the step

Finally consider the case where the energy corresponds to a positive frequency on the right of the step (so $\omega > m - ev$) but to a negative frequency to its left (so $\omega < ev - m$). These two limits are only consistent with one another if $ev > m$. In this case the momentum on each side of the step is given by

$$q_R^2 = (\omega - \mu_k + ev)(\omega + \mu_k + ev) \geq 0 \quad \text{and} \quad q_L^2 = (\mu_k + ev - \omega)(ev - \omega - \mu_k) \geq 0\,. \tag{14.3.25}$$

In this case the new wrinkle comes because of the observation – made above in (14.2.18) – that for negative frequency modes the group velocity $\mathbf{v}$ points in the *opposite* direction to the quantum number $\mathbf{p}$, and that this is required in order for antiparticles to carry currents of the opposite charge to their partner particles. (If thought of as a particle moving along a trajectory, this is one origin of observation that particles behave as in the same way as would their particle partners if these partners were to move backwards in time.) This provides a wrinkle because this means that a negative-frequency mode to the left of the step with $q < 0$ is *approaching* the step whilst a mode with $q > 0$ actually moves away from it.

With this in mind, the condition that expresses the absence of an incoming negative-frequency state on the left of the step in this case corresponds to choosing $C_{L-} = 0$ rather than $C_{L+} = 0$. Continuity of u and u' at $x = 0$ using the choice $C_{L-} = 0$ leads to the conditions $C_{L+} = C_{R-} + C_{R+}$ and

$$iq_R(C_{R+} - C_{R-}) - iq_L C_{L+} = 0\,, \tag{14.3.26}$$

and so

$$\frac{C_{R+} - C_{R-}}{C_{R+} + C_{R-}} = \frac{1 - C_{R-}/C_{R+}}{1 + C_{R-}/C_{R+}} = \frac{q_L}{q_R}\,. \tag{14.3.27}$$

This implies

$$\frac{C_{R-}}{C_{R+}} = \frac{q_R - q_L}{q_R + q_L} \quad \text{and} \quad \frac{C_{L+}}{C_{R+}} = 1 + \frac{C_{R-}}{C_{R+}} = \frac{2q_R}{q_R + q_L}\,, \tag{14.3.28}$$

which also means

$$\frac{C_{R+}}{C_{R-}} = \frac{q_R + q_L}{q_R - q_L} \quad \text{and} \quad \frac{C_{L+}}{C_{R-}} = \frac{2q_R}{q_R - q_L}\,. \tag{14.3.29}$$

The transition and reflection amplitudes in this case then are

$$\hat\rho = \frac{C_{R+}}{C_{R-}} = \frac{q_R + q_L}{q_R - q_L} \quad \text{and} \quad \hat\tau = \frac{C_{L+}}{C_{R-}}\sqrt{\frac{q_L}{q_R}} = \frac{2\sqrt{q_R q_L}}{q_R - q_L}\,. \tag{14.3.30}$$

which satisfy $|\hat\rho|^2 - |\hat\tau|^2 = 1$. Using the first-quantized interpretation (that is justified more fully in a second-quantized treatment below) the transmission probability of a negative-frequency antiparticle emerging on the left each time a particle is incident on the right is

$$|\hat\tau|^2 = \frac{4q_R q_L}{(q_R - q_L)^2}\,. \tag{14.3.31}$$

The likelihood of having a reflected particle emerge on the right is similarly

$$|\hat\rho|^2 = \frac{(q_R + q_L)^2}{(q_R - q_L)^2} = 1 + |\hat\tau|^2 \tag{14.3.32}$$

which is larger than unity. (Because of this surprise that the reflection probability could be larger than unity, this calculation was initially known as the 'Klein Paradox'.) The second-quantized treatment given below shows this is to be interpreted as 100% reflection of the incoming particle accompanied by the emission of a particle-antiparticle pair.

A check is again provided by evaluating $\mathcal{J}^x$ on either side of the step, to verify that it is x-independent. To the left of the step we have (by design) a current flowing to the right, as appropriate for left-moving antiparticles with charge $-e$:

$$\mathcal{J}^x_L = 2eq_L|C_{L+}|^2 = 2eq_L|C_{R-}|^2\left|\frac{2q_R}{q_R - q_L}\right|^2 = \frac{8eq_L q_R^2}{(q_R - q_L)^2}\,|C_{R-}|^2\,. \tag{14.3.33}$$

To the right of the step one instead has

$$\mathcal{J}_R^x = 2eq_R\Big(|C_{R+}|^2 - |C_{R-}|^2\Big) = 2eq_R|C_{R-}|^2\left(\left|\frac{q_R+q_L}{q_R-q_L}\right|^2 - 1\right) = \frac{8eq_Lq_R^2}{(q_R-q_L)^2}\,|C_{R-}|^2\,, \qquad (14.3.34)$$

in which the reflected current cancels out the incoming negative current (due to 100% reflection), leaving the residual pair produced current that agrees with the current on the left of the step.

The observation that negative-frequency states move in the opposite direction to $\mathbf{p}$ also allows an interpretation for the calculation leading to (14.3.20) that starts with $C_{L+} = 0$. Because the e^{-iqx} state describes an antiparticle coming *in* from infinity on the left rather than a particle escaping to infinity there, the 'transmission' amplitude, τ, found above should be interpreted as the annihilation amplitude between this incoming antiparticle on the left and the incident particle arriving from the right. By time reversal invariance this is also the amplitude for the pair production of precisely one particle-antiparticle pair starting from the vacuum.

If we denote by Λ_v the vacuum survival probability (*i.e.* the probability of producing zero pairs), then unitarity says that the sum of probabilities for producing any number of particles pairs should be unity, and so

$$1 = \Lambda_v + \Lambda_v|\tau|^2 + \Lambda_v|\tau|^4 + \cdots = \frac{\Lambda_v}{1-|\tau|^2}\,, \qquad (14.3.35)$$

which implies $\Lambda_v = 1 - |\tau|^2 = |\rho|^2$. The mean number of particle pairs produced is

$$\bar{n} = \Lambda_v|\tau|^2 + 2\Lambda_v|\tau|^4 + 3\Lambda_v|\tau|^6 + \cdots = \frac{\Lambda_v|\tau|^2}{(1-|\tau|^2)^2} = \frac{|\tau|^2}{1-|\tau|^2} = \frac{|\tau|^2}{|\rho|^2} = \frac{4q_Rq_L}{(q_R-q_L)^2}\,. \qquad (14.3.36)$$

Notice that comparing this last expression to (14.3.32) also shows that $\bar{n} = |\hat{\tau}|^2$, which is the transmission coefficient obtained above using the modes with only an outgoing antiparticle at infinity. This also has a simple physical interpretation, since it says that for each incoming particle on the right the probability of finding an antiparticle coming out at the left can be written

$$|\hat{\tau}|^2 = \frac{|\tau|^2}{1-|\tau|^2} = |\tau|^2(1+\bar{n})\,. \qquad (14.3.37)$$

This shows that this probability is larger than the probability $|\tau|^2$ for producing the pair in the vacuum, being enhanced by a stimulated-emission factor of $1+\bar{n}$ as expected for bosons.

14.3.2 Second-quantized calculation

This section now pins down more accurately the interpretation of ratios like $|C_{R+}/C_{R-}|^2$ and $|C_{L-}/C_{R-}|^2$ (or $|C_{L+}/C_{R-}|^2$) by computing time-evolution in a second-quantized framework within which we can ask explicitly for the amplitude for producing particle-antiparticle pairs. This connection to the mode functions described above made by expanding the field operator

$\psi(x)$ in two different bases of modes — a set that is simple to the left of the step and a another set that is simple on the right — and then performing a Bogoliubov transformation between these two bases, along the lines performed earlier in §7.2.

Some of the details of Bogoliubov transformations need updating — relative to the Schrödinger discussion of §7.2 — for the relativistic Klein-Gordon case. The main two changes involve (i) the presence of negative-frequency mode functions in any basis of solutions to the Klein-Gordon equation; and (ii) the different form for the inner product used for Klein-Gordon solutions, and its indefinite sign.

To make these issues explicit, consider two different bases of solutions to the Klein-Gordon equation: $u_i(x)$ and $v_a(x)$, both of which are taken to be energy eigenstates inasmuch as $i\partial_t u_j = \omega_j\, u_j$ and $i\partial_t v_a = \omega_a\, v_a$. We adopt the convention that ω_j and ω_a are bounded from below, in which case the negative frequency solutions are given by $u_i^*(x)$ and $v_a^*(x)$ (which, after all, automatically solve the Klein-Gordon equation provided that u_i and v_a do). Because both postive and negative frequency modes are required to form a complete basis of modes, the expansion of a generic solution $f(x)$ in terms of the either of these families of modes has the form

$$f(x) = \sum_j \Bigl[f_j\, u_j(x) + \bar{f}_j\, u_j^*(x) \Bigr] = \sum_a \Bigl[f_a\, v_a(x) + \bar{f}_a\, v_a^*(x) \Bigr] , \tag{14.3.38}$$

for some coefficients f_j, $\bar{f}_j$, f_a and $\bar{f}_a$. If the mode functions are orthonormal,[53] $(u_j, u_k) = \delta_{jk}$, $(v_a, v_b) = \delta_{ab}$ and $(u_j, u_k^*) = (v_a, v_b^*) = 0$, then the coefficients are given by $f_j = (u_j, f)$, $\bar{f}_j = (u_j^*, f)$, $f_a = (v_a, f)$ and $\bar{f}_a = (v_a^*, f)$.

Because both bases are complete they can be expanded in terms of one another

$$u_i(x) = \alpha_{ia}\, v_a(x) + \beta_{ia}\, v_a^*(x) \quad \text{and so} \quad u_i^*(x) = \alpha_{ia}^*\, v_a^*(x) + \beta_{ia}^*\, v_a(x) , \tag{14.3.39}$$

for some *Bogoliubov* coefficients α_{ia} and β_{ia}. For orthonormal states these coefficients are given explicitly in terms of inner products of the basis functions:

$$\alpha_{ia} = (v_a\,, u_i) = (u_i^*\,, v_a^*) \qquad \text{and} \qquad \beta_{ia} = (u_i^*\,, v_a) = (v_a^*\,, u_i) . \tag{14.3.40}$$

Written in matrix form the Bogoliubov transformation (14.3.39) becomes

$$\begin{pmatrix} u_i \\ u_j^* \end{pmatrix} = \begin{pmatrix} \alpha_{ia} & \beta_{ia} \\ \beta_{ia}^* & \alpha_{ia}^* \end{pmatrix} = \begin{pmatrix} v_a \\ v_a^* \end{pmatrix} \tag{14.3.41}$$

Orthonormality of both bases implies the above matrix must be unitary and so (in block form)

$$\text{if } \mathcal{B} := \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \quad \text{then} \quad \mathcal{B}^{-1} = \mathcal{B}^\dagger := \begin{pmatrix} \alpha^\dagger & \beta^T \\ \beta^\dagger & \alpha^T \end{pmatrix} \tag{14.3.42}$$

[53] We return below to the complications that arise when some of the states have $(u_i, u_i) < 0$.

which when written out implies the matrices α and β satisfy the relations

$$\alpha\alpha^\dagger + \beta\beta^\dagger = 1 \qquad \text{and} \qquad \alpha\beta^T + \beta\alpha^T = 0\,, \tag{14.3.43}$$

together with their complex conjugates

$$\alpha^*\alpha^T + \beta^*\beta^T = 1 \qquad \text{and} \qquad \alpha^*\beta^\dagger + \beta^*\alpha^\dagger = 0\,. \tag{14.3.44}$$

The above also show that the inverse relation giving the v_a in terms of the u_i is

$$v_a(x) = \alpha^*_{ia}\, u_i(x) + \beta_{ia}\, u^*_i(x) \quad \text{and so} \quad v^*_a(x) = \alpha_{ia}\, u^*_i(x) + \beta^*_{ia}\, u_i(x)\,, \tag{14.3.45}$$

Now comes the main point. Since $\{u_i, u^*_j\}$ and $\{v_a, v^*_b\}$ are both complete bases for solutions to the Klein Gordon equation we can expand the field operator in terms of either of them:

$$\psi(x) = \sum_i \Big[\mathfrak{a}_i\, u_i(x) + \overline{\mathfrak{a}}^\star_i\, u^*_i(x)\Big] = \sum_a \Big[\mathfrak{c}_a\, v_a(x) + \overline{\mathfrak{c}}^\star_a\, v^*_a(x)\Big] \tag{14.3.46}$$

and this implies a relationship between the operators $\mathfrak{a}_i$, $\overline{\mathfrak{a}}_j$ and $\mathfrak{c}_a$, $\overline{\mathfrak{c}}_b$:

$$\mathfrak{c}_a = \sum_i \Big(\alpha_{ia}\,\mathfrak{a}_i + \beta^*_{ia}\,\overline{\mathfrak{a}}^\star_i\Big) \quad \text{and} \quad \overline{\mathfrak{c}}^\star_a = \sum_i \Big(\beta_{ia}\,\mathfrak{a}_i + \alpha^*_{ia}\,\overline{\mathfrak{a}}^\star_i\Big)\,, \tag{14.3.47}$$

and

$$\mathfrak{a}_i = \sum_a \Big(\alpha^*_{ia}\,\mathfrak{c}_a + \beta^*_{ia}\,\overline{\mathfrak{c}}^\star_a\Big) \quad \text{and} \quad \overline{\mathfrak{a}}^\star_i = \sum_a \Big(\beta_{ia}\,\mathfrak{c}_a + \alpha_{ia}\,\overline{\mathfrak{c}}^\star_a\Big)\,, \tag{14.3.48}$$

and these relationships are consistent with the commutation relations $[\mathfrak{a}_i, \overline{\mathfrak{a}}^\star_j] = \delta_{ij}$ and $[\mathfrak{c}_a, \overline{\mathfrak{c}}^\star_b] = \delta_{ab}$ because of the conditions (14.3.43) and (14.3.44).

The above expressions imply the vacuum states, defined by $\mathfrak{a}_i|\Omega_A\rangle = \overline{\mathfrak{a}}_i|\Omega_A\rangle = 0$ and $\mathfrak{c}_a|\Omega_C\rangle = \overline{\mathfrak{c}}_a|\Omega_C\rangle = 0$, only coincide if $\beta_{ia} = 0$. Notice in particular that when these vacua differ there can be particles of one basis present in the vacuum of the other basis, since

$$\begin{aligned}
\langle\Omega_A|\mathfrak{c}^\star_b\,\mathfrak{c}_b|\Omega_A\rangle &= \sum_{ij}\langle\Omega_A|\Big(\alpha^*_{ib}\,\mathfrak{a}^\star_i + \beta_{ib}\,\overline{\mathfrak{a}}_i\Big)\Big(\alpha_{jb}\,\mathfrak{a}_j + \beta^*_{jb}\,\overline{\mathfrak{a}}^\star_j\Big)|\Omega_A\rangle = \sum_i \beta_{ib}\beta^*_{ib} = \Big(\beta^T\beta^*\Big)_{bb} \\
\langle\Omega_A|\overline{\mathfrak{c}}^\star_b\,\overline{\mathfrak{c}}_b|\Omega_A\rangle &= \sum_{ij}\langle\Omega_A|\Big(\beta_{ib}\,\mathfrak{a}_i + \alpha^*_{ib}\,\overline{\mathfrak{a}}^\star_i\Big)\Big(\beta^*_{jb}\,\mathfrak{a}^\star_j + \alpha_{jb}\,\overline{\mathfrak{a}}_j\Big)|\Omega_A\rangle = \sum_i \beta_{ib}\beta^*_{ib} = \Big(\beta^T\beta^*\Big)_{bb}\,.
\end{aligned} \tag{14.3.49}$$

and

$$\begin{aligned}
\langle\Omega_C|\mathfrak{a}^\star_i\,\mathfrak{a}_i|\Omega_C\rangle &= \sum_{ab}\langle\Omega_C|\Big(\alpha_{ia}\,\mathfrak{c}^\star_a + \beta_{ia}\,\overline{\mathfrak{c}}_a\Big)\Big(\alpha^*_{ib}\,\mathfrak{c}_b + \beta^*_{ib}\,\overline{\mathfrak{c}}^\star_b\Big)|\Omega_C\rangle = \sum_a \beta_{ia}\beta^*_{ia} = \Big(\beta\beta^\dagger\Big)_{ii} \\
\langle\Omega_C|\overline{\mathfrak{a}}^\star_i\,\overline{\mathfrak{a}}_i|\Omega_C\rangle &= \sum_{ab}\langle\Omega_C|\Big(\beta_{ia}\,\mathfrak{c}_a + \alpha_{ia}\,\overline{\mathfrak{c}}^\star_a\Big)\Big(\beta^*_{ia}\,\mathfrak{c}^*_a + \alpha^*_{ia}\,\overline{\mathfrak{c}}_a\Big)|\Omega_C\rangle = \sum_a \beta_{ia}\beta^*_{ia} = \Big(\beta\beta^\dagger\Big)_{ii}\,.
\end{aligned} \tag{14.3.50}$$

To apply this formalism to Klein-Gordon particles interacting with the step potential choose one of these bases to look like purely left-moving or purely right-moving states on the left of the step and choose the other to similarly look like left- and right-moving particles to the step's right. The Klein-Gordon equation and boundary conditions at $x = 0$ allow each of these to be extended to the other side of the step, where they necessarily include contributions with both signs of q.

From the point of view of an observer restricted to the right of the step a basis of modes describing left- and right-moving particles is

$$\mathfrak{r}_{qk\pm}(x,\mathbf{y},t) = \begin{cases} \sum_{a=\pm} \mathcal{C}^{\pm}_{La} \exp\Big[-i\omega t + i\mathbf{k}\cdot\mathbf{y} + iaq_L x\Big] & \text{if} \quad x < 0 \\ \mathcal{C}^{\pm}_{R} \exp\Big[-i\omega t + i\mathbf{k}\cdot\mathbf{y} \pm iq_R x\Big] & \text{if} \quad x > 0 \end{cases} \tag{14.3.51}$$

where $\mathcal{C}^{\pm}_R = \mathcal{C}^{\pm}_{R\pm}$ while q_L, q_R are positive and are related to ω using the dispersion relations (14.3.25) on either side of the step. Tracking through the boundary conditions as before gives the ratios of the coefficients to be

$$\frac{\mathcal{C}^{\pm}_{L-}}{\mathcal{C}^{\pm}_{R}} = \frac{q_L \mp q_R}{2q_L} \quad \text{and} \quad \frac{\mathcal{C}^{\pm}_{L+}}{\mathcal{C}^{\pm}_{R}} = \frac{q_L \pm q_R}{2q_L}\,. \tag{14.3.52}$$

The analogs of these (pure left- and right-movers) to the left of the step are

$$\mathfrak{l}_{qk\pm}(x,\mathbf{y},t) = \begin{cases} C^{\pm}_{L\pm} \exp\Big[-i\omega t + i\mathbf{k}\cdot\mathbf{y} \pm iq_L x\Big] & \text{if} \quad x < 0 \\ \sum_{a=\pm} C^{\pm}_{Ra} \exp\Big[-i\omega t + i\mathbf{k}\cdot\mathbf{y} + iaq_R x\Big] & \text{if} \quad x > 0 \end{cases} \tag{14.3.53}$$

where q_L and q_R again satisfy (14.3.25). Solving the boundary conditions at $x = 0$ in this case gives

$$\frac{C^{\pm}_{R-}}{C^{\pm}_{L}} = \frac{q_R \mp q_L}{2q_R} \quad \text{and} \quad \frac{C^{\pm}_{R+}}{C^{\pm}_{L}} = \frac{q_R \pm q_L}{2q_R}\,, \tag{14.3.54}$$

as was found earlier.

These are the two sets of basis functions, and the next step is to compute their overlap. It is useful when doing so to choose an unorthodox formulation of the inner product that takes advantage of the step geometry. Recall that (14.2.7) shows that the Klein-Gordon equation ensures that the integral of $n_\mu(f^*\partial^\mu g - g\,\partial^\mu f^*)$ over some 3-surface is independent of the particular 3-surface on which the integral is performed, and in earlier sections this 3-surface was chosen to be slices at fixed time t. Here the geometry of the step potential makes life easier if we instead choose the surfaces appearing in the inner product to be slices of fixed x rather than t, so that they are parallel to the step. With this in mind take the inner product to be

$$(f,g) = (g,f)^* = -i\int_\Sigma \mathrm{d}^2x\,\mathrm{d}t\,\Big(f^*\partial_x g - g\,\partial_x f^*\Big)\,, \tag{14.3.55}$$

where Σ denotes a 3-surface on which x does not vary and $\mathrm{d}^2x = \mathrm{d}y\,\mathrm{d}z$. Because this is proportional to J_x its value is guaranteed to be independent of Σ when evaluated for any pair of functions f and g that satisfy the Klein Gordon equation.

This inner product has the advantage that for any function of the form $f = e^{-i\omega t + i\mathbf{k}_T\cdot\mathbf{y}}u(x)$ the integrals over y, z and t evaluate to give $(2\pi)^3\,\delta(\omega-\tilde\omega)\,\delta^2(\mathbf{k}_T-\tilde{\mathbf{k}}_T)$. Evaluating this inner product for the modes (14.3.51) (which is simplest in the regime $x>0$, but which also gives the same result if evaluated at $x<0$) gives (with $a,\tilde a = \pm$)

$$(\mathfrak{r}_{qka},\mathfrak{r}_{\tilde q\tilde k\tilde a}) = (2\pi)^3\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}})(\tilde a\tilde q_R + aq_R)\,\mathcal{C}_R^{a*}\tilde{\mathcal{C}}_R^{\tilde a}\,. \tag{14.3.56}$$

Since $\omega=\tilde\omega$ implies $q_R=\tilde q_R$ it follows that the modes are orthogonal and they are also normalized to $(u_{qka},u_{qka}) = a\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}}) = \pm\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}})$ provided

$$|\mathcal{C}_R^{\pm}|^2 = \frac{1}{(2\pi)^3 2q_R}\,. \tag{14.3.57}$$

An identical discussion applied to the modes of (14.3.53) similarly implies

$$(\mathfrak{l}_{qka},\mathfrak{l}_{\tilde q\tilde k\tilde a}) = (2\pi)^3\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}})(\tilde a\tilde q_L + aq_L)\,C_{La}^{*}\tilde C_{L\tilde a}\,. \tag{14.3.58}$$

Again $\omega=\tilde\omega$ implies $q_L=\tilde q_L$ and so $(v_{qka},v_{qka}) = a\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}}) = \pm\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}})$ provided

$$|C_L^{\pm}|^2 = \frac{1}{(2\pi)^3 2q_L}\,. \tag{14.3.59}$$

The overlap of the $\mathfrak{r}$'s with the $\mathfrak{l}$'s similarly evaluates to

$$\begin{aligned}
(\mathfrak{r}_{qka},\mathfrak{l}_{\tilde q\tilde k\tilde a}) &= (2\pi)^3\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}})C_L^{\tilde a}\Big[(\tilde a\tilde q_L+q_L)\,\mathcal{C}_{L+}^{a*} + (\tilde a\tilde q_L - q_L)\,\mathcal{C}_{L-}^{a*}\Big] \qquad (14.3.60)\\
&= (2\pi)^3\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}})C_L^{\tilde a}\mathcal{C}_R^{a*}q_L\left[(\tilde a+1)\left(\frac{\mathcal{C}_{L+}^{a*}}{\mathcal{C}_R^{a*}}\right)+(\tilde a-1)\left(\frac{\mathcal{C}_{L-}^{a*}}{\mathcal{C}_R^{a*}}\right)\right]\\
&= (2\pi)^3\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}})C_L^{\tilde a}\mathcal{C}_R^{a*}q_L\left[(\tilde a+1)\left(\frac{q_L+aq_R}{2q_L}\right)+(\tilde a-1)\left(\frac{q_L-aq_R}{2q_L}\right)\right],
\end{aligned}$$

where the second line uses that $\tilde\omega=\omega$ implies $\tilde q_L = q_L$ while the last equality uses (14.3.52) to evaluate $\mathcal{C}_{L-}^{\pm}/\mathcal{C}_R^{\pm}$ and $\mathcal{C}_{L+}^{\pm}/\mathcal{C}_R^{\pm}$. The four cases found by using in this $a=\pm$ and $\tilde a=\pm$ are

$$(\mathfrak{r}_{qk\pm},\mathfrak{l}_{\tilde q\tilde k+}) = \delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}})\frac{q_L\pm q_R}{2\sqrt{q_Lq_R}} \quad\text{and}\quad (\mathfrak{r}_{qk\pm},\mathfrak{l}_{\tilde q\tilde k-}) = -\delta(\omega-\tilde\omega)\delta^2(\mathbf{k}-\tilde{\mathbf{k}})\frac{q_L\mp q_R}{2\sqrt{q_Lq_R}}\,, \tag{14.3.61}$$

once the normalization conditions (14.3.57) and (14.3.59) are used. An identical argument similarly shows

$$\begin{aligned}
(\mathfrak{r}_{qka},\mathfrak{l}^*_{\tilde q\tilde k\tilde a}) &= (2\pi)^3\delta(\omega+\tilde\omega)\delta^2(\mathbf{k}+\tilde{\mathbf{k}})C_L^{\tilde a*}\Big[(-\tilde a\tilde q_L+q_L)\,\mathcal{C}_{L+}^{a*} - (\tilde a\tilde q_L + q_L)\,\mathcal{C}_{L-}^{a*}\Big] \qquad (14.3.62)\\
&= (2\pi)^3\delta(\omega+\tilde\omega)\delta^2(\mathbf{k}+\tilde{\mathbf{k}})C_L^{\tilde a*}\mathcal{C}_R^{a*}q_L\left[(-\tilde a+1)\left(\frac{q_L+aq_R}{2q_L}\right)-(\tilde a+1)\left(\frac{q_L-aq_R}{2q_L}\right)\right]
\end{aligned}$$

leading to the four cases

$$(\mathfrak{r}_{qk\pm}, \mathfrak{l}^*_{\tilde{q}\tilde{k}+}) = -\delta(\omega+\tilde{\omega})\delta^2(\mathbf{k}+\tilde{\mathbf{k}})\frac{q_L \mp q_R}{2\sqrt{q_L q_R}} \quad \text{and} \quad (\mathfrak{r}_{qk\pm}, \mathfrak{l}^*_{\tilde{q}\tilde{k}-}) = \delta(\omega+\tilde{\omega})\delta^2(\mathbf{k}+\tilde{\mathbf{k}})\frac{q_L \pm q_R}{2\sqrt{q_L q_R}}\,. \tag{14.3.63}$$

Worked example: above barrier scattering

Returning now to the Bogoliubov transformation, the field can be expanded in terms of any complete basis of modes. For scattering problems we choose our two bases to be adapted to the initial and final states of a scattering process, so that the Bogoliubov transformation also corresponds to the time-evolution (or S-matrix) operation. To this end it is useful to redistribute the above modes into 'in' and 'out' modes, with solutions repsectively chosen to describe particles approaching and receding from the step. Consider for these purposes ordinary above-barrier scattering first, and then consider particle production by the step.

For above-barrier scattering we choose $\omega > m + ev$, so that mode functions both to the left and right of the step come from the positive-frequency branch. In this case define the 'in' basis to contain incoming particles and so

$$u^{\rm in}_{qk-} = u_{qk-} = \mathfrak{r}_{qk-} = \begin{cases} \mathcal{C}^-_{L+}e^{iq_L x} + \mathcal{C}^-_{L-}e^{-iq_L x} & \text{for } x<0 \\ \mathcal{C}^-_{R}e^{-iq_R x} & \text{for } x>0 \end{cases} \tag{14.3.64}$$

and

$$u^{\rm in}_{qk+} = u_{qk+} = \mathfrak{l}_{qk+} = \begin{cases} C^+_{L}e^{iq_L x} & \text{for } x<0 \\ C^+_{R+}e^{iq_R x} + C^+_{R-}e^{-iq_R x} & \text{for } x>0 \end{cases}, \tag{14.3.65}$$

since these look like a single plane wave moving to the right on the left of the step and moving to the left on the right of the step. According to the above calculations, these are linearly independent but not orthogonal.

At late times more convenient is the 'out' basis of outgoing particles, defined by

$$v^{\rm out}_{qk-} = v_{qk-} = \mathfrak{l}_{qk-} = \begin{cases} C^-_{L}e^{-iq_L x} & \text{for } x<0 \\ C^-_{R+}e^{iq_R x} + C^-_{R-}e^{-iq_R x} & \text{for } x>0 \end{cases} \tag{14.3.66}$$

and

$$v^{\rm out}_{qk+} = v_{qk+} = \mathfrak{r}_{qk+} = \begin{cases} \mathcal{C}^+_{L+}e^{iq_L x} + \mathcal{C}^+_{L-}e^{-iq_L x} & \text{for } x<0 \\ \mathcal{C}^+_{R}e^{iq_R x} & \text{for } x>0 \end{cases}, \tag{14.3.67}$$

which consists of left-moving particles on the left of the step and right-moving particles on its right.

Solving for the v's in terms of the u's gives

$$v_{qk+} = \frac{\mathcal{C}^+_R}{C^+_{R+}}\left[u_{qk+} - \frac{C^+_{R-}}{\mathcal{C}^-_R}\,u_{qk-}\right] = \frac{\mathcal{C}^+_R}{C^+_L}\frac{C^+_L}{C^+_{R+}}u_{qk+} - \frac{\mathcal{C}^+_R}{\mathcal{C}^-_R}\frac{C^+_{R-}}{C^+_{R+}}\,u_{qk-} = \alpha\,u_{qk+} - \beta\,u_{qk-}\,, \tag{14.3.68}$$

and so, using $\mathcal{C}^+_R/C^+_L = \sqrt{q_L/q_R}$ as well as $\mathcal{C}^+_R/\mathcal{C}^-_R = 1$ and expressions (14.3.52) and (14.3.54) for the other ratios, we find

$$\alpha := \frac{2\sqrt{q_L q_R}}{q_R+q_L} \quad \text{and} \quad \beta := \frac{q_R - q_L}{q_R+q_L}\,, \tag{14.3.69}$$

and so $|\alpha|^2 + |\beta|^2 = 1$. Similarly

$$v_{qk-} = \frac{C_L^-}{\mathcal{C}_{L-}^-}\left[u_{qk-} - \frac{\mathcal{C}_{L+}^-}{C_L^+}\,u_{qk+}\right] = \frac{C_L^-}{\mathcal{C}_R^-}\frac{\mathcal{C}_R^-}{\mathcal{C}_{L-}^-}\,u_{qk-} - \frac{C_L^-}{C_L^+}\frac{\mathcal{C}_{L+}^-}{\mathcal{C}_{L-}^-}\,u_{qk+} =: \alpha\,u_{qk-} - \beta\,u_{qk+}\,, \tag{14.3.70}$$

with the same expressions for α and β.

Expanding the field operator in both bases, as in (14.3.46), gives

$$\psi(x) = \int \mathrm{d}^2k\mathrm{d}q \sum_{i=\pm}\Big[\mathfrak{a}_{qki}\,u_{qki}(x) + \overline{\mathfrak{a}}^\star_{qki}\,u^*_{qki}(x)\Big] = \int \mathrm{d}^2k\mathrm{d}q \sum_{a=\pm}\Big[\mathfrak{c}_{qka}\,v_{qka}(x) + \overline{\mathfrak{c}}^\star_{qka}\,v^*_{qka}(x)\Big] \tag{14.3.71}$$

and so comparing these implies

$$\mathfrak{a}_{qk+} = \alpha\,\mathfrak{c}_{qk+} - \beta\,\mathfrak{c}_{qk-} \quad \text{and} \quad \mathfrak{a}_{qk-} = \alpha\,\mathfrak{c}_{qk-} - \beta\,\mathfrak{c}_{qk+}\,, \tag{14.3.72}$$

and similarly for the antiparticle destruction operators. The relation $|\alpha|^2 + |\beta|^2 = 1$ ensures that the canonical commutation relations are preserved under this transformation.

Defining the in and out vacua using $\mathfrak{a}_{qki}|\Omega_{\rm in}\rangle = 0$ and $\mathfrak{c}_{qka}|\Omega_{\rm out}\rangle = 0$ we have $|\Omega_{\rm out}\rangle = \mathcal{S}|\Omega_{\rm in}\rangle$ to define the S-matrix $\mathcal{S}$. The transmission and reflection amplitudes for an initial particle incoming from the right of the step then are given by the overlap between the initial state built by acting with a creation operator $\mathfrak{a}^\star$ on $|\Omega_{\rm in}\rangle$ and the final state built by acting on $|\Omega_{\rm out}\rangle$ with the appropriate creation operator $\mathfrak{c}^\star$. The reflection amplitude therefore is given by the overlap between the initial state $\mathfrak{a}^\star_{qk-}|\Omega_{\rm in}\rangle$ and the final state $\mathfrak{c}^\star_{qk+}|\Omega_{\rm out}\rangle$, and so

$$\langle\Omega_{\rm out}|\mathfrak{c}_{\tilde{q}\tilde{k}+}\mathfrak{a}^\star_{qk-}|\Omega_{\rm in}\rangle = \langle\Omega_{\rm out}|\mathfrak{c}_{\tilde{q}\tilde{k}+}\Big(\alpha^*\,\mathfrak{c}^\star_{qk-} - \beta^*\,\mathfrak{c}^\star_{qk+}\Big)|\Omega_{\rm in}\rangle =: \rho\,e^{iW}\,\delta(q-\tilde{q})\delta^2(\mathbf{k}-\tilde{\mathbf{k}}) \tag{14.3.73}$$

where $\rho = -\beta^*$ and $e^{iW} := \langle\Omega_{\rm out}|\Omega_{\rm in}\rangle$. Similarly, the transmission amplitude is given by the overlap between the initial state $\mathfrak{a}^\star_{qk-}|\Omega_{\rm in}\rangle$ and the final state $\mathfrak{c}^\star_{qk-}|\Omega_{\rm out}\rangle$, leading to

$$\langle\Omega_{\rm out}|\mathfrak{c}_{\tilde{q}\tilde{k}-}\mathfrak{a}^\star_{qk-}|\Omega_{\rm in}\rangle = \langle\Omega_{\rm out}|\mathfrak{c}_{\tilde{q}\tilde{k}-}\Big(\alpha^*\,\mathfrak{c}^\star_{qk-} - \beta^*\,\mathfrak{c}^\star_{qk+}\Big)|\Omega_{\rm in}\rangle =: \tau\,e^{iW}\,\delta(q-\tilde{q})\delta^2(\mathbf{k}-\tilde{\mathbf{k}})\,, \tag{14.3.74}$$

with $\tau = \alpha^*$. Evaluating α using (14.3.69), these expressions for ρ and τ agree with the naive results (14.3.20) found in a more hand-wavy way using first-quantized reasoning. Notice that unitarity is satisfied because the reflection and transmission probabilities sum to unity: $|\rho|^2 + |\tau|^2 = |\alpha|^2 + |\beta|^2 = 1$.

Worked example: pair production by the step

Now comes the main event. Consider now the situation where the incoming mode energy lies in the regime $ev - m > \omega > -em + m$, for which the solutions to the right of the step have positive frequency but those to its left must have negative frequency.

As discussed in the first-quantized discussion, having negative-frequency modes on the left has the important implication the group velocity, $\mathbf{v}$, is in the opposite direction from $\mathbf{p}$ and a mode like $\mathfrak{l}_{qk-} \propto e^{-iqx}$ (for $x < 0$) now describes antiparticles moving to the right rather than the left. This in particular reverses the notion of which modes are incoming and which are outgoing to the left of the step.

In this case we therefore choose as our 'in' basis for incoming particles the same as before to the step's right,

$$u^{\text{in}}_{qk-} = u_{qk-} = \mathfrak{r}_{qk-} = \begin{cases} \mathcal{C}^-_{L+} e^{iq_L x} + \mathcal{C}^-_{L-} e^{-iq_L x} & \text{for } x < 0 \\ \mathcal{C}^-_R e^{-iq_R x} & \text{for } x > 0 \end{cases} \tag{14.3.75}$$

but modify the ingoing choice on the left to

$$u^{\text{in}}_{qk+} = u_{qk+} = \mathfrak{l}_{qk-} = \begin{cases} C^-_L e^{-iq_L x} & \text{for } x < 0 \\ C^-_{R+} e^{iq_R x} + C^-_{R-} e^{-iq_R x} & \text{for } x > 0 \end{cases}, \tag{14.3.76}$$

because this describes a right-moving antiparticle due to the opposite direction of motion of the negative-frequency modes. The corresponding 'out' basis of outgoing antiparticles left of the step is now

$$v^{\text{out}}_{qk-} = v_{qk-} = \mathfrak{l}_{qk+} = \begin{cases} C^+_L e^{iq_L x} & \text{for } x < 0 \\ C^+_{R+} e^{iq_R x} + C^+_{R-} e^{-iq_R x} & \text{for } x > 0 \end{cases} \tag{14.3.77}$$

while the out-going particles to the right of the step remain as before:

$$v^{\text{out}}_{qk+} = v_{qk+} = \mathfrak{r}_{qk+} = \begin{cases} \mathcal{C}^+_{L+} e^{iq_L x} + \mathcal{C}^+_{L-} e^{-iq_L x} & \text{for } x < 0 \\ \mathcal{C}^+_R e^{iq_R x} & \text{for } x > 0 \end{cases}. \tag{14.3.78}$$

Solving for the v's in terms of the u's now gives

$$v_{qk+} = \frac{\mathcal{C}^+_R}{C^-_{R+}} \left[u_{qk+} - \frac{C^-_{R-}}{\mathcal{C}^-_R}\, u_{qk-} \right] = \frac{\mathcal{C}^+_R}{C^-_L} \frac{C^-_L}{C^-_{R+}}\, u_{qk+} - \frac{\mathcal{C}^+_R}{\mathcal{C}^-_R} \frac{C^-_{R-}}{C^-_{R+}}\, u_{qk-} = \hat{\alpha}\, u_{qk+} - \hat{\beta}\, u_{qk-}\,, \tag{14.3.79}$$

with the coefficients evaluating to

$$\hat{\alpha} := \frac{2\sqrt{q_L q_R}}{q_R - q_L} = \frac{\alpha^*}{\beta^*} \quad \text{and} \quad \hat{\beta} := \frac{q_R + q_L}{q_R - q_L} = \frac{1}{\beta^*} \tag{14.3.80}$$

with α and β as defined in (14.3.69). Clearly these new coefficients satisfy $|\hat{\beta}|^2 - |\hat{\alpha}|^2 = 1$. Similarly

$$v_{qk-} = \frac{C^+_L}{\mathcal{C}^-_{L+}} \left[u_{qk-} - \frac{\mathcal{C}^-_{L-}}{C^-_L}\, u_{qk+} \right] = \frac{C^+_L}{\mathcal{C}^-_R} \frac{\mathcal{C}^-_R}{\mathcal{C}^-_{L+}}\, u_{qk-} - \frac{C^+_L}{C^-_L} \frac{\mathcal{C}^-_{L-}}{\mathcal{C}^-_{L+}}\, u_{qk+} = -\hat{\alpha}\, u_{qk-} + \hat{\beta}\, u_{qk+}\,,$$

with $\hat{\alpha}$ and $\hat{\beta}$ as above. For later use notice the useful identities

$$|\beta|^2 = \frac{1}{|\hat{\beta}|^2} = \frac{|\alpha|^2}{|\hat{\alpha}|^2} = \frac{(q_R - q_L)^2}{(q_R + q_L)^2}\,. \tag{14.3.81}$$

Expanding the field operator in both bases (keeping in mind that the negative-frequency modes correspond to antiparticles on the left of the step) in this case gives

$$\begin{aligned} \psi(x) &= \int \mathrm{d}^2k\mathrm{d}q \Big[\mathfrak{a}_{qk-}\, u_{qk-}(x) + \overline{\mathfrak{a}}^\star_{qk+}\, u_{qk+}(x) + \overline{\mathfrak{a}}^\star_{qk-}\, u^*_{qk-}(x) + \mathfrak{a}_{qk+}\, u^*_{qk+}(x) \Big] \\ &= \int \mathrm{d}^2k\mathrm{d}q \Big[\mathfrak{c}_{qk+}\, v_{qk+}(x) + \overline{\mathfrak{c}}^\star_{qk-}\, v_{qk-}(x) + \overline{\mathfrak{c}}^\star_{qk+}\, v^*_{qk+}(x) + \mathfrak{c}_{qk-}\, v^*_{qk-}(x) \Big] \end{aligned} \tag{14.3.82}$$

and so this time comparing these implies

$$\overline{\mathfrak{a}}^{\star}_{qk+} = \hat{\alpha}\mathfrak{c}_{qk+} + \hat{\beta}\,\overline{\mathfrak{c}}^{\star}_{qk-} \quad \text{and} \quad \mathfrak{a}_{qk-} = -\hat{\beta}\,\mathfrak{c}_{qk+} - \hat{\alpha}\,\overline{\mathfrak{c}}^{\star}_{qk-}\,, \tag{14.3.83}$$

and its inverse

$$\overline{\mathfrak{c}}^{\star}_{qk-} = \hat{\alpha}\mathfrak{a}_{qk-} + \hat{\beta}\,\overline{\mathfrak{a}}^{\star}_{qk+} \quad \text{and} \quad \mathfrak{c}_{qk+} = -\hat{\beta}\,\mathfrak{a}_{qk-} - \hat{\alpha}\,\overline{\mathfrak{a}}^{\star}_{qk+}\,. \tag{14.3.84}$$

The relations $|\hat{\beta}|^2 - |\hat{\alpha}|^2 = 1$ again ensure that the standard commutation relations are preserved under this transformation.

Defining as before the in and out vacua using $\mathfrak{a}_{qki}|\Omega_{\rm in}\rangle = 0$ and $\mathfrak{c}_{qka}|\Omega_{\rm out}\rangle = 0$ we again have $|\Omega_{\rm out}\rangle = \mathcal{S}|\Omega_{\rm in}\rangle$. The quantity W in $e^{iW} := \langle\Omega_{\rm out}|\Omega_{\rm in}\rangle$ need not be real in this case because the vacuum is unstable to pair production, and so the vacuum survival probability is $|e^{iW}|^2 = \Lambda_v \neq 1$. Notice that the conditions $\mathfrak{a}_{qk-}|\Omega_{\rm in}\rangle = \overline{\mathfrak{a}}_{qk+}|\Omega_{\rm in}\rangle = 0$ imply

$$\hat{\beta}\,\mathfrak{c}_{qk+}|\Omega_{\rm in}\rangle = -\hat{\alpha}\,\overline{\mathfrak{c}}^{\star}_{qk-}|\Omega_{\rm in}\rangle \quad \text{and} \quad \hat{\beta}^*\,\overline{\mathfrak{c}}_{qk-}|\Omega_{\rm in}\rangle = -\hat{\alpha}^*\mathfrak{c}^{\star}_{qk+}|\Omega_{\rm in}\rangle\,. \tag{14.3.85}$$

The amplitude for spontaneously producing a single particle-antiparticle pair from the vacuum is therefore given by the overlap between $|\Omega_{\rm in}\rangle$ and $\mathfrak{c}^{\star}\mathfrak{c}^{\star}|\Omega_{\rm out}\rangle$, and so evaluates to

$$\langle\Omega_{\rm out}|\mathfrak{c}_{\tilde{q}\tilde{k}+}\overline{\mathfrak{c}}_{qk-}|\Omega_{\rm in}\rangle = -\frac{\hat{\alpha}^*}{\hat{\beta}^*}\langle\Omega_{\rm out}|\mathfrak{c}_{\tilde{q}\tilde{k}+}\mathfrak{c}^{\star}_{qk+}|\Omega_{\rm in}\rangle = -\frac{\hat{\alpha}^*}{\hat{\beta}^*}\,e^{iW}\,\delta(q-\tilde{q})\delta^2(\mathbf{k}-\tilde{\mathbf{k}})\,, \tag{14.3.86}$$

where

$$\left|\frac{\hat{\alpha}}{\hat{\beta}}\right|^2 = \frac{4q_{\scriptscriptstyle L}q_{\scriptscriptstyle R}}{(q_{\scriptscriptstyle R}+q_{\scriptscriptstyle L})^2} = |\alpha|^2\,. \tag{14.3.87}$$

The factor $|\hat{\alpha}/\hat{\beta}|^2 e^{iW}$ here agrees with the expression $\Lambda_v|\tau|^2 = e^{iW}|\alpha|^2$ as computed in the first-quantized discussion surrounding (14.3.35).

14.4 The Higgs mechanism

Previous sections in this chapter consider relativistic spinless particles that interact only through their electromagnetic interactions, but there is nothing that prevents these particles from having non-electromagnetic interactions as well. The competition amongst different interactions can cause interesting new effects when both electromagnetic and non-electromagnetic interactions are present. This section briefly explores one of these: the Higgs mechanism.

Consider therefore adding a scalar potential describing self-interactions for the spinless particles to the Klein-Gordon and electromagnetic lagrangians given in (13.4.1) and (14.1.2),

$$S = -\int \mathrm{d}^4x\,\left[\frac{1}{4}\,F_{\mu\nu}F^{\mu\nu} + D^\mu\psi^* D_\mu\psi + V(\psi^*\psi)\right]\,. \tag{14.4.1}$$

The scalar potential V is a function of $\psi^*\psi$ and so is invariant under the symmetry $\psi \to \psi\,e^{i\theta}$, and the case considered in (14.1.2) corresponds to the choice $V = m^2\psi^*\psi$. Self-interactions arise if V includes terms not just linear in $\psi^*\psi$, such as

$$V = m^2\psi^*\psi + \frac{\lambda}{4}(\psi^*\psi)^2\,. \tag{14.4.2}$$

Normally stability of the vacuum would imply that the coupling λ must be positive so that V is bounded from below.

Because V does not depend on derivatives of ψ or ψ^* its presence does not affect how the scalar field appears in the electromagnetic current or the canonical momenta, which remain given by (14.1.4) and (14.1.6) respectively. The Hamiltonian density for the scalar field therefore becomes

$$\mathcal{H} := \Pi\,\partial_t\psi + \Pi^*\partial_t\psi^* - \mathcal{L} = \Pi^*\Pi + \mathbf{D}\psi^*\cdot\mathbf{D}\psi + iqA_0(\Pi\psi - \Pi^*\psi^*) + V(\psi^*\psi)\,. \tag{14.4.3}$$

instead of (14.1.7). Observables can be computed perturbatively in the two dimensionless couplings, λ and the scalar electric charge q, provided these are both small.

We here focus on the special case where the scalar potential V is

$$V(\psi^*\psi) = V_0 - \mu^2\psi^*\psi + \frac{\lambda}{4}(\psi^*\psi)^2 = \frac{\lambda}{4}\Big(\psi^*\psi - v^2\Big)^2\,, \tag{14.4.4}$$

for real positive constants λ and v, where $\mu^2 = \frac{1}{2}\lambda v^2$ and $V_0 = \frac{1}{4}\lambda v^4$. This form for V is minimized when $\psi = \psi_0$ where $\psi_0^*\psi_0 = v^2 \neq 0$ – unlike (14.4.2) because of the opposite sign it implies for the quadratic term, for which $m^2 \to -\mu^2$. Furthermore, if λ is made small with μ^2 fixed then the value of ψ at the minimum, $\psi_0^*\psi_0 = v^2 = 2\mu^2/\lambda$, becomes large and so suggests using a semiclassical approximation for which the zero-momentum mode of ψ is regarded as classical, along the lines described for Schrödinger fields in §7.

To this end we therefore write $\psi = \psi_0 + \hat\psi$ where $\psi_0 = v = 2\mu/\sqrt{\lambda}$ and it is $\hat\psi$ that is expanded in terms of creation and annihilation operators. In terms of this expansion the derivatives become $\partial_\mu\psi = \partial_\mu\hat\psi$ and so

$$\begin{aligned} D_\mu\psi^* D^\mu\psi \;&=\; \Big[\partial_\mu\hat\psi^* + iqA_\mu(v+\hat\psi^*)\Big]\Big[\partial^\mu\hat\psi - iqA^\mu(v+\hat\psi)\Big] \\ &= \partial_\mu\hat\psi^*\partial^\mu\hat\psi + iqA_\mu\Big[v\,\partial^\mu(\hat\psi - \hat\psi^*) + (\hat\psi^*\partial^\mu\hat\psi - \hat\psi\partial^\mu\hat\psi^*)\Big] \\ &\qquad + \Big[v^2 + v(\hat\psi + \hat\psi^*) + \hat\psi^*\hat\psi\Big]q^2A_\mu A^\mu\,, \end{aligned} \tag{14.4.5}$$

while the scalar potential becomes

$$V = \frac{\lambda}{4}\Big[|v+\hat\psi|^2 - v^2\Big]^2 = \frac{\lambda v^2}{4}(\hat\psi + \hat\psi^*)^2 + \frac{\lambda v}{2}(\hat\psi + \hat\psi^*)\hat\psi^*\hat\psi + \frac{\lambda}{4}(\hat\psi^*\hat\psi)^2\,. \tag{14.4.6}$$

As usual in the semiclassical approximation we regard the quadratic part in the quantum fields as the unperturbed contribution and regard all terms involving three or more powers of quantum fields as interactions to be treated perturbatively. This leads to the Lagrangian

density $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\rm mix} + \mathcal{L}_{\rm int}$ where

$$\begin{aligned}
\mathcal{L}_0 &= -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - q^2v^2A_\mu A^\mu - \partial_\mu\hat\psi^*\partial^\mu\hat\psi - \frac{\lambda v^2}{4}(\hat\psi+\hat\psi^*)^2 \\
\mathcal{L}_{\rm mix} &= -iqv\,A_\mu\partial^\mu(\hat\psi-\hat\psi^*) \\
\mathcal{L}_{\rm int} &= -iqA_\mu(\hat\psi^*\partial^\mu\hat\psi - \hat\psi\partial^\mu\hat\psi^*) - \Big[v(\hat\psi+\hat\psi^*) + \hat\psi^*\hat\psi\Big]q^2A_\mu A^\mu \\
&\qquad -\frac{\lambda v}{2}(\hat\psi+\hat\psi^*)\hat\psi^*\hat\psi - \frac{\lambda}{4}(\hat\psi^*\hat\psi)^2\,.
\end{aligned} \tag{14.4.7}$$

Both $\mathcal{L}_0$ and $\mathcal{L}_{\rm mix}$ are quadratic in the fields, but only $\mathcal{L}_{\rm mix}$ is bilinear in A_μ and $\hat\psi - \hat\psi^*$.

Now comes the main point. The lagrangian $\mathcal{L}$ is *by construction* invariant under the simultaneous local transformation $A_\mu \to A_\mu + \partial_\mu\omega$ and $\psi \to \psi\, e^{iq\omega}$ for an arbitrary function $\omega(x)$, which represents a redundancy of description of the system. Since such transformations do not alter the physics (they are symmetries after all) we may as well use the freedom to perform them to simplify the problem as much as we can. It becomes irresitable to use this freedom to remove the phase of $\hat\psi$, after which $\hat\psi$ becomes real. With this choice $\mathcal{L}_{\rm mix}$ vanishes. It is conventional to denote the resulting real field as $\hat\psi := \chi/\sqrt{2}$, and once this is done the nonzero terms of the lagrangian are

$$\begin{aligned}
\mathcal{L}_0 &= -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - q^2v^2A_\mu A^\mu - \frac{1}{2}\,\partial_\mu\chi\partial^\mu\chi - \frac{\lambda v^2}{2}\chi^2 \\
\mathcal{L}_{\rm int} &= -\left(\sqrt{2}\;\chi + \frac{1}{2}\,\chi^2\right)q^2A_\mu A^\mu - \frac{\lambda v}{2\sqrt{2}}\,\chi^3 - \frac{\lambda}{16}\chi^4\,.
\end{aligned} \tag{14.4.8}$$

This unperturbed lagrangian is fairly simple to interpret. The χ-dependent terms in $\mathcal{L}_0$ is recognizable as the Klein Gordon lagrangian for a free massive field – *c.f.* eq. (13.2.4) – for a self-conjugate particle (that is its own antiparticle, and so carries no electric charge) with mass $m_\chi^2 = \lambda v^2$. The interpretation of the A_μ dependent terms can be obtained by examining the equation of motion that it implies:

$$\partial_\mu F^{\mu\nu} - 2q^2v^2A^\nu = \Box A^\nu - \partial^\nu\partial_\mu A^\mu - 2q^2v^2A^\nu = 0\,. \tag{14.4.9}$$

Taking the divergence of this equation once more by contracting with ∂_ν then gives the subsidiary condition $\partial_\nu A^\nu = 0$ (provided $qv \neq 0$), which allows (14.4.9) to be simplified to

$$\Big(\Box - 2q^2v^2\Big)A_\mu = 0\,. \tag{14.4.10}$$

This shows that each component of A_μ satisfies the Klein Gordon equation with mass $m_A^2 = 2q^2v^2$, and so that the spin-one photon has acquired a nonzero mass. This interpretation can also be verified by computing the hamiltonian for the electromagnetic field and verifying that it has the free-particle form for a massive spin-one particle with dispersion relation

$$\varepsilon_A(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m_A^2}\,. \tag{14.4.11}$$

There are several surprises buried in this interpretation. First, although a massless spin-one particle has only two helicity states a massive spin-one particle has three spin states. Where did the extra degree of freedom come from? The extra, longitudinal, degree of freedom turns out to come from the imaginary part of $\hat{\psi}$, which we used the gauge freedom to set to zero. But the gauge transformation required to do this acts as $A_\mu \to A_\mu + \partial_\mu \omega$ and so moves this scalar into the longitudinal part of the field A_μ, and so provides the required new spin state. It is said that the gauge field 'eats' the imaginary part of $\hat{\psi}$ (which would have been the Goldstone mode described in §8.3 for the broken symmetry if the symmetry had not been local). This process wherein a spin-one particle acquires a mass by eating a Goldstone boson when a local (gauge) symmetry is broken is called the *Higgs mechanism*. There are a number of fundamental spin-one particles known in nature and, so far as we know, this is the way all of the massive ones (the ones associated with the *weak interactions*) acquire their mass.

The second surprise is that the physical spectrum consists only of electrically neutral particles – a neutral but massive spin-one photon and a neutral and massive spin-zero scalar – despite our starting off with a charged spinless particle coupled to electromagnetism and adding only scalar self-interactions (whose crucial effect was to ensure $\langle\psi\rangle \neq 0$ in the ground state, so that the electromagnetic gauge symmetry is spontaneously broken in the sense given in §8.3. The neutrality of all particles is also confirmed by the final form for the interactions in $\mathcal{L}_{\rm int}$, which contains no derivative electromagnetic couplings of the type encountered earlier in this chapter for charged spinless particles. The only interactions are non-derivative couplings between χ and A_μ and self-couplings of χ, and the implications of these can be explored as in earlier sections using perturbative methods (provided λ and q are both small).

15 Relativistic spin-half particles

We next turn to the treatment of relativistic spin-half particles. This section works out their field representation, as a special case of the general results for fields of any spin described earlier in §11. Apart from the pedagogical interest of doing so, this is also a useful exercise for practical reasons since many fundamental particles, such as the electron and proton, do have spin one-half.

15.1 Spinors

The first step is to define the finite-dimensional representations of the Lorentz group to be used since these define how the fields transform. The general arguments of Appendix C.1 show that the smallest possible field content for spin-half particles are furnished by the $\left(\frac{1}{2},0\right)$ or $\left(0,\frac{1}{2}\right)$ representations. Since parity maps each of these representations onto the other both are required to describe a parity-invariant system. In such a case the smallest representation possible would instead be the direct sum: $\left(\frac{1}{2},0\right) \oplus \left(0,\frac{1}{2}\right)$. In what follows we work out all

three of these representations in detail starting with the $\left(\frac{1}{2},0\right)$ and $\left(0,\frac{1}{2}\right)$ examples, and then showing how these can be embedded into $\left(\frac{1}{2},0\right)\oplus\left(0,\frac{1}{2}\right)$.

15.1.1 Weyl spinors

Both the $\left(\frac{1}{2},0\right)$ and $\left(0,\frac{1}{2}\right)$ representations are two-dimensional, and so can be described using the standard Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \tag{15.1.1}$$

since these furnish an explicit two-by-two hermitian representation of the $SU(2)$ algebra. The hermitian matrices $S_k := \frac{1}{2}\sigma_k$, with $k = 1, 2, 3$ satisfy the $SU(2)$ commutation algebra: $[S_i, S_j] = i\epsilon_{ijk}S_k$, as can easily be proven by explicit matrix multiplication. Raising and lowering operators within the two-by-two representation may also be expressed in terms of these, through the linear combinations $S_\pm := S_1 \pm iS_2 = \frac{1}{2}(\sigma_1 \pm i\sigma_2)$:

$$S_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad S_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} . \tag{15.1.2}$$

The Lorentz generators in the $\left(\frac{1}{2},0\right)$ representation are defined by the matrix generators $\mathcal{A}_k = \frac{1}{2}\,\sigma_k$ and $\mathcal{B}_k = 0$, so the generators of rotations, $\mathcal{J}_k$, and boosts, $\mathcal{K}_k$, in this representation become:

$$\mathcal{J}_k = \mathcal{A}_k + \mathcal{B}_k = \frac{1}{2}\sigma_k \quad \text{and} \quad \mathcal{K}_k = -i(\mathcal{A}_k - \mathcal{B}_k) = -\frac{i}{2}\sigma_k \qquad \text{(left-handed)}\,. \tag{15.1.3}$$

In particular, the Pauli matrices give a representation for which both $\mathcal{J}_3$ and $\mathcal{K}_3$ are diagonal. The two-component spinors on which these matrices act are called 'left-handed' spinors and denoted χ_L.

The Lorentz generators in the $\left(0,\frac{1}{2}\right)$ representation are similarly written in terms of these Pauli matrices with $\mathcal{A}_k = 0$ and $\mathcal{B}_k = \frac{1}{2}\,\sigma_k$, implying that the generators of rotations and boosts become:

$$\mathcal{J}_k = \mathcal{A}_k + \mathcal{B}_k = \frac{1}{2}\,\sigma_k \quad \text{and} \quad \mathcal{K}_k = -i(\mathcal{A}_k - \mathcal{B}_k) = +\frac{i}{2}\,\sigma_k \qquad \text{(right-handed)}\,. \tag{15.1.4}$$

Again both $\mathcal{J}_3$ and $\mathcal{K}_3$ are diagonal. The two-component spinors on which these matrices act are called 'right-handed' spinors and denoted χ_R.

Although $\mathcal{J}_k$ is hermitian in both of these representations the $\mathcal{K}_k$ are not and so the representation is *not* unitary. Notice that the Pauli-matrix identity

$$\sigma_k^* = (i\sigma_2)\sigma_k(i\sigma_2) \tag{15.1.5}$$

implies these representations are complex conjugates of one another, up to a similarity transformation. This also implies that left-handed and right-handed spinors are related by complex conjugation, with

$$\chi_L = i\sigma_2\,\chi_R^\star = \mathfrak{e}\,\chi_R\,, \tag{15.1.6}$$

where

$$\mathfrak{e} := i\sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{15.1.7}$$

These two-component representations of the Lorentz group are called *Weyl spinors*.

15.1.2 Dirac spinors

For many applications a representation of parity is needed and in this case a reducible representation involving both left- and right-handed spinors is useful, corresponding to the Dirac representation $\left(\frac{1}{2},0\right)\oplus\left(0,\frac{1}{2}\right)$. This is a four-dimensional representation and so we may write the fields as a four-dimensional column vector – called a *Dirac spinor* – as follows:

$$\psi = \begin{pmatrix} \chi_L \\ \chi_R \end{pmatrix}, \tag{15.1.8}$$

in which the upper two elements correspond to the $\left(\frac{1}{2},0\right)$ representation and the lower two elements to the $\left(0,\frac{1}{2}\right)$.

The Lorentz generators in the $\left(\frac{1}{2},0\right)\oplus\left(0,\frac{1}{2}\right)$ representation may therefore be written as:

$$\mathcal{A}_k = \frac{1}{2}\begin{pmatrix} \sigma_k & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \mathcal{B}_k = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & \sigma_k \end{pmatrix}. \tag{15.1.9}$$

so the generators of rotations and boosts become

$$\mathcal{J}_k = (\mathcal{A}_k + \mathcal{B}_k) = \frac{1}{2}\begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}, \quad \mathcal{K}_k = -i(\mathcal{A}_k - \mathcal{B}_k) = -\frac{i}{2}\begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix}. \tag{15.1.10}$$

Weyl and Majorana reductions

The Dirac representation is written in a block-diagonal basis that emphasizes that all the generators act separately on the left- and right-handed spinors, and so the left- and right-handed components can be obtained simply by projecting out one or the other. The simplest way to do so defines a four-by-four matrix γ_5 whose eigenvalues distinguish left- and right-handed parts

$$\gamma_5 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{15.1.11}$$

where I is the two-by-two unit matrix. In terms of this left- and right-handed Weyl spinors are obtained by applying the projection matrices:

$$\gamma_L := \frac{1}{2}(1+\gamma_5) = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \gamma_R := \frac{1}{2}(1-\gamma_5) = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}. \tag{15.1.12}$$

If

$$\psi = \begin{pmatrix} \xi \\ \chi \end{pmatrix} \quad \text{then} \quad \psi_L := \gamma_L \psi = \begin{pmatrix} \xi \\ 0 \end{pmatrix} \quad \text{and} \quad \psi_R := \gamma_R \psi = \begin{pmatrix} 0 \\ \chi \end{pmatrix}. \tag{15.1.13}$$

An alternative way to reduce a Dirac spinor is to split it into its 'real' and 'imaginary' parts, rather than setting its left- and right-handed components to zero. This is achieved by imposing a reality condition, in a way that respect its Lorentz-transformation properties. Since left- and right-handed spinors are complex conjugates of one another, as in (15.1.6), it makes sense to reduce a Dirac spinor using the requirement that its lower two components transform as the complex conjugates of the upper two components. A *Majorana spinor* is therefore defined as one for which the left-handed component ξ is related to its right-handed component χ by $\chi = -\mathfrak{e}\xi^\star$ (and so $\chi = \mathfrak{e}\xi^\star$) with $\mathfrak{e}$ defined in (15.1.7):

$$\psi = \begin{pmatrix} \xi \\ -\mathfrak{e}\xi^\star \end{pmatrix} = C\,\psi^\star \quad \text{where} \quad C := \begin{pmatrix} 0 & \mathfrak{e} \\ -\mathfrak{e} & 0 \end{pmatrix}. \tag{15.1.14}$$

For reasons that become clearer below, C is known as the *charge-conjugation matrix*.

An arbitrary Dirac spinor can be decomposed as the sum of a left-handed and a right-handed spinor, $\psi = \psi_L + \psi_R$, or equivalently can be written as the sum of two Majorana spinors, $\psi = \psi_1 + i\psi_2$ where ψ_1 and ψ_2 are Majorana.

15.2 The Dirac field

Chapter §11 – and Appendix C – show that consistency of the field and particle transformation rules implies the relativistic field must be related to creation and annihilation operators by a relationship of the form

$$\psi_n(x) = \sum_\sigma \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}} \Big[u_n(\mathbf{p},\sigma)\; \mathfrak{c}_{\mathbf{p}\sigma}\; e^{ipx} + v_n(\mathbf{p},\sigma)\; \overline{\mathfrak{c}}^\star_{\mathbf{p}\sigma}\; e^{-ipx} \Big], \tag{15.2.1}$$

where the creation and destruction operators satisfy the fermionic commutation relations

$$\Big\{ \mathfrak{c}_{\mathbf{p}\sigma}, \mathfrak{c}^\star_{\mathbf{q}\xi} \Big\} = \Big\{ \bar{\mathfrak{c}}_{\mathbf{p}\sigma}, \mathfrak{c}^\star_{\mathbf{q}\xi} \Big\} = \delta_{\sigma\xi} \delta^3(\mathbf{p}-\mathbf{q}) \tag{15.2.2}$$

and with the mode functions, $u_n(\mathbf{p},\sigma)$ and $v_n(\mathbf{p},\sigma)$ determined up to normalization by the Lorentz-transformation properties of the field and the particle states.

For general spins the particle mode function in a general frame is related to its value in the rest frame by

$$u_n(\mathbf{p},\sigma) = \sqrt{\frac{m}{E_p}}\; D_{nm}\left[L(\mathbf{p}/m)\right] u_m(0,\sigma)\,, \tag{15.2.3}$$

where

$$D_{nm}\left[L(\mathbf{p}/m)\right] := \left[\exp\left(-i\phi \sum_k \hat{\mathbf{p}}_k \mathcal{K}_k \right) \right]_{nm}, \tag{15.2.4}$$

with $\hat{\mathbf{p}} := \mathbf{p}/|\mathbf{p}|$ the unit vector in the direction of $\mathbf{p}$ and $\mathcal{K}_k$ the representation's boost generators while

$$\sinh\phi := \frac{|\mathbf{p}|}{m} \quad \text{and} \quad \cosh\phi := \frac{E_p}{m} \tag{15.2.5}$$

where $E_p := \sqrt{\mathbf{p}^2 + m^2}$.

The antiparticle spinor is similarly given by

$$v_n(\mathbf{p},\sigma) = (-)^{2B}(-)^{j-\sigma}u_n(\mathbf{p},-\sigma) \tag{15.2.6}$$

where j is the particle spin while B is the spin label for the (A,B) representation of the Lorentz group described in §11.3.3 and Appendix B.2.

15.2.1 Particle and antiparticle spinors

We next write these spnors out explicitly for the special cases of the $\left(\frac{1}{2},0\right)$ and $\left(0,\frac{1}{2}\right)$ representations. The first step is to determine the mode function in the standard (rest) frame, $u_n(\sigma) \equiv u_n(0,\sigma)$. These functions are determined by demanding consistency between fields and particles for transformations restricted to the little group that preserves the rest frame. As reported in §11.3 and derived in Appendix C.2, the solutions are unique up to normalization and are given by Clebsch-Gordan coefficients as in eq. (C.2.2). The results for the $\left(\frac{1}{2},0\right)$ and $\left(0,\frac{1}{2}\right)$ representations are given explicitly by:

$$u_{a0}^{\left(\frac{1}{2},0\right)}(0,\sigma) = C_{\frac{1}{2}\,0}\left(\tfrac{1}{2},\sigma;a,0\right) = \delta_{\sigma a} \quad \text{and} \quad u_{0b}^{\left(0,\frac{1}{2}\right)}(0,\sigma) = C_{0\,\frac{1}{2}}\left(\tfrac{1}{2},\sigma;0,b\right) = \delta_{\sigma b}\,, \tag{15.2.7}$$

or, equivalently

$$\mathbf{u}_L\left(0,\sigma=+\tfrac{1}{2}\right) = \mathbf{u}_R\left(\sigma=+\tfrac{1}{2}\right) = \begin{pmatrix}1\\0\end{pmatrix}, \quad \mathbf{u}_L\left(0,\sigma=-\tfrac{1}{2}\right) = \mathbf{u}_R\left(\sigma=-\tfrac{1}{2}\right) = \begin{pmatrix}0\\1\end{pmatrix}, \tag{15.2.8}$$

which shows that the field and particle share the same eigenstate for J_3.

For the reducible $\left(\frac{1}{2},0\right)\oplus\left(0,\frac{1}{2}\right)$ representation we must take the direct sum of these two spinors. After including a conventional normalization factor, this leads to the following four-component rest-frame spinor in the $\left(\frac{1}{2},0\right)\oplus\left(0,\frac{1}{2}\right)$ representation:

$$\mathbf{u}\left(0,\sigma=+\tfrac{1}{2}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix} \quad \text{and} \quad \mathbf{u}\left(0,(\sigma=-\tfrac{1}{2}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\0\\1\end{pmatrix}. \tag{15.2.9}$$

Given these rest-frame spinors the result for arbitrary particle momenta, $\mathbf{u}(\mathbf{p},\sigma)$, is found using (15.2.3). The required matrix representation of the Lorentz boost, $D[L(\mathbf{p}/m)]$, is

$$D[L(\mathbf{p}/m)] = \exp\left(-i\phi\,\hat{\mathbf{p}}\cdot\vec{\mathcal{K}}\right) = \begin{bmatrix}\exp\left(-\frac{1}{2}\phi\,\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}\right) & 0\\ 0 & \exp\left(+\frac{1}{2}\phi\,\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}\right)\end{bmatrix}, \tag{15.2.10}$$

for which the exponentials can be evaluated explicitly using the Pauli-matrix identity $(\boldsymbol{\sigma}\cdot\hat{\mathbf{p}})^2 = \hat{\mathbf{p}}\cdot\hat{\mathbf{p}} = 1$, leading to

$$\exp\left(\pm\frac{1}{2}\phi\,\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}\right) = \cosh\left(\frac{\phi}{2}\right) \pm (\boldsymbol{\sigma}\cdot\hat{\mathbf{p}})\sinh\left(\frac{\phi}{2}\right), \tag{15.2.11}$$

where

$$\cosh\left(\frac{\phi}{2}\right) = \sqrt{\frac{\cosh\phi+1}{2}} = \sqrt{\frac{E_p+m}{2m}} \quad \text{and} \quad \sinh\left(\frac{\phi}{2}\right) = \sqrt{\frac{\cosh\phi-1}{2}} = \sqrt{\frac{E_p-m}{2m}}. \tag{15.2.12}$$

Combining everything, the final expression for the particle spinor $u_n(\mathbf{p},\sigma)$ then becomes

$$\mathbf{u}(\mathbf{p},\sigma) = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{\frac{E_p+m}{2E_p}} - \boldsymbol{\sigma}\cdot\hat{\mathbf{p}}\sqrt{\frac{E_p-m}{2E_p}} & 0 \\ 0 & \sqrt{\frac{E_p+m}{2E_p}} + \boldsymbol{\sigma}\cdot\hat{\mathbf{p}}\sqrt{\frac{E_p-m}{2E_p}} \end{pmatrix}\begin{pmatrix} \mathbf{w}(\sigma) \\ \mathbf{w}(\sigma) \end{pmatrix}. \tag{15.2.13}$$

in which $\mathbf{w}(\sigma)$ are the two-component spinors found earlier:

$$\mathbf{w}\left(\sigma=+\tfrac{1}{2}\right) = \begin{pmatrix}1\\0\end{pmatrix}; \qquad \mathbf{w}\left(\sigma=-\tfrac{1}{2}\right) = \begin{pmatrix}0\\1\end{pmatrix}. \tag{15.2.14}$$

Notice that these expressions also apply in the massless $m\to 0$ limit, in which case (15.2.13) approaches

$$\mathbf{u}(\mathbf{p},\sigma) \to \frac{1}{2}\begin{pmatrix} 1-\boldsymbol{\sigma}\cdot\hat{\mathbf{p}} & 0 \\ 0 & 1+\boldsymbol{\sigma}\cdot\hat{\mathbf{p}} \end{pmatrix}\begin{pmatrix} \mathbf{w}(\sigma) \\ \mathbf{w}(\sigma) \end{pmatrix}. \tag{15.2.15}$$

For massless states $\mathbf{w}$ is chosen to be an eigenstate of helicity, $\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}$, rather than spin, and so (15.2.15) shows that u_L and u_R each represent states of specific helicity (as required by the general results for the fields representing massless particles given in Appendix C.1).

The antiparticle spinors, $v_n(\mathbf{p},\sigma)$, are then found from eq. (15.2.6), which it is convenient to write in terms of the matrix γ_5 of (15.1.11) as

$$\mathbf{v}(\mathbf{p},\sigma) = (-)^{\frac{1}{2}-\sigma}\,\gamma_5\,\mathbf{u}(\mathbf{p},-\sigma). \tag{15.2.16}$$

In terms of these the expansion for the Dirac field in terms of creation and annihilation operators therefore becomes:

$$\psi(x) = \sum_{\sigma=\pm\frac{1}{2}}\int\frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\left[\mathbf{u}(\mathbf{p},\sigma)\;\mathfrak{c}_{\mathbf{p}\sigma}\;e^{ipx} + \mathbf{v}(\mathbf{p},\sigma)\;\overline{\mathfrak{c}}^{\star}_{\mathbf{p}\sigma}\;e^{-ipx}\right], \tag{15.2.17}$$

where (as usual) $px = p_\mu x^\mu = -E_p t + \mathbf{p}\cdot\mathbf{x}$ with $p^0 := E_p = \sqrt{\mathbf{p}^2+m^2}$.

15.2.2 The Dirac Equation

For scalar and vector fields the condition $p^0 = \sqrt{\mathbf{p}^2 + m^2}$ (or $\eta_{\mu\nu} p^\mu p^\nu = -m^2$) implies the field operator satisfies a field equation (the Klein-Gordon equation), and a similar statement is true for the spinor fields of interest in this section.

To see what this field equation is in the $\left(\frac{1}{2}, 0\right) \oplus \left(0, \frac{1}{2}\right)$ representation we start by noticing that the rest-frame spinors (15.2.9) satisfy a 'constraint' relation of the form

$$\beta\, \mathbf{u}(0,\sigma) = \mathbf{u}(0,\sigma) \quad \text{where} \quad \beta := \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \tag{15.2.18}$$

defines the matrix β, with 0 and I being two-by-two zero and unit submatrices.

The equation we seek is the expression of (15.2.18) in a general frame. It can therefore be found by explicitly performing the Lorentz boost $L(\mathbf{p}/m)$, since

$$\mathbf{u}(\mathbf{p},\sigma) = \sqrt{\frac{m}{E_p}}\, D[L(\mathbf{p}/m)]\, \mathbf{u}(0,\sigma). \tag{15.2.19}$$

It follows that constraint (15.2.18) becomes in a general frame

$$\Gamma(\mathbf{p})\, \mathbf{u}(\mathbf{p},\sigma) = \mathbf{u}(\mathbf{p},\sigma) \quad \text{where} \quad \Gamma(\mathbf{p}) := D[L(\mathbf{p}/m)]\, \beta\, D^{-1}[L(\mathbf{p}/m)]\,, \tag{15.2.20}$$

where using (15.2.10) the matrix $\Gamma(\mathbf{p})$ evaluates explicitly to

$$\begin{aligned} \Gamma(\mathbf{p}) &= \begin{pmatrix} B_- & 0 \\ 0 & B_+ \end{pmatrix} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \begin{pmatrix} B_+ & 0 \\ 0 & B_- \end{pmatrix} = \begin{pmatrix} 0 & B_-^2 \\ B_+^2 & 0 \end{pmatrix} \\ &= \frac{1}{m} \begin{pmatrix} 0 & E_p - \boldsymbol{\sigma}\cdot\mathbf{p} \\ E_p + \boldsymbol{\sigma}\cdot\mathbf{p} & 0 \end{pmatrix}, \end{aligned} \tag{15.2.21}$$

which defines the functions

$$B_\pm := \sqrt{\frac{E_p + m}{2m}} \pm \boldsymbol{\sigma}\cdot\hat{\mathbf{p}} \sqrt{\frac{E_p - m}{2m}}. \tag{15.2.22}$$

that appear in the matrix elements of $D[L(\mathbf{p}/m)]$.

Notice that (15.2.21) is linear and homogeneous in the components of the four-momentum $p^\mu = (E_p, \mathbf{p})$, and it is convenient to rewrite it in such a way as to make this explicit by writing

$$\Gamma(\mathbf{p}) = -\frac{i}{m}\, \gamma_\mu\, p^\mu = -i\frac{\not{p}}{m}\,. \tag{15.2.23}$$

The final equality introduces the 'slash' notation $\not{p} := \gamma_\mu\, p^\mu$ (and similarly for other 4-vectors besides p^μ) and defines the *Dirac matrices* γ_μ, and so reading off the coefficients shows that

$$\gamma_0 = -\gamma^0 := \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i\beta \quad \text{and} \quad \boldsymbol{\gamma} := \begin{pmatrix} 0 & -i\boldsymbol{\sigma} \\ i\boldsymbol{\sigma} & 0 \end{pmatrix}. \tag{15.2.24}$$

These satisfy the following anticommutation relation (or Clifford algebra)

$$\{\gamma_\mu, \gamma_\nu\} = 2\eta_{\mu\nu} \tag{15.2.25}$$

where $\eta_{\mu\nu}$ is the standard Minkowski metric. Eq. (15.2.25) can be established by matrix multiplication using the definitions (15.2.24), or by the arguments given in the next section.

In a general frame the constraint (15.2.18) therefore becomes (15.2.20) which in turn can be written more covariantly as

$$\Big(i\not{p} + m\Big)\mathbf{u}(\mathbf{p}, \sigma) = 0, \tag{15.2.26}$$

a result called the *Dirac equation*. As this derivation makes clear, the Dirac equation is merely a convention for normalizing the bottom two components of the Dirac field given the normalization of the top two.

Repeating this argument for the antiparticle spinors shows that for these the Dirac equation becomes

$$\Big(-i\not{p} + m\Big)\ \mathbf{v}(\mathbf{p}, \sigma) = 0, \tag{15.2.27}$$

as is easily seen once it is noticed that γ_5 anticommutes with all four of the Dirac matrices: $\{\gamma_5, \gamma_\mu\} = 0$.

Equations (15.2.26) and (15.2.27) satisfied by the spinors $\mathbf{u}(\mathbf{p}, \sigma)$ and $\mathbf{v}(\mathbf{p}, \sigma)$ together imply a differential condition on the field $\psi(x)$ of eq. (15.2.17):

$$\Big(\gamma^\mu \partial_\mu + m\Big)\psi(x) = \Big(\not{\partial} + m\Big)\psi(x) = 0. \tag{15.2.28}$$

This last equation also implies the further condition $(\Box - m^2)\psi = 0$, as can be seen by operating on both sides with the combination $(\not{\partial} - m)$. The result follows from the observation that $(\not{\partial} - m)(\not{\partial} + m)\psi = (\not{\partial}^2 - m^2)\psi$ and use of the identity

$$\not{\partial}^2 = \gamma^\mu\gamma^\nu\partial_\mu\partial_\nu = \frac{1}{2}\{\gamma^\mu, \gamma^\nu\}\partial_\mu\partial_\nu = \eta^{\mu\nu}\partial_\mu\partial_\nu = \Box \tag{15.2.29}$$

that follows from the anticommutation relation (15.2.25). The condition $(\Box - m^2)\psi = 0$ contains within it the momentum-space *mass-shell* condition $p^2 + m^2 = 0$, where $p^2 = \eta_{\mu\nu}p^\mu p^\nu$.

15.3 Gamma matrices

Because the Dirac matrices γ_μ appear in many applications it is useful to record here some of their properties. The most basic one is their anticommutation relation, (15.2.25), often also known as the *Dirac algebra*, that is repeated here for convenience:

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}. \tag{15.3.1}$$

One way to establish this property is to notice that the matrix $\Gamma(\mathbf{p}) = D(L)\ \beta\ D^{-1}(L)$ is the similarity transformation of a matrix that is idempotent: $\beta^2 = 1$. This implies the same is true of $\Gamma(\mathbf{p})$, so using the expression (15.2.23) then gives:

$$1 = \Gamma^2(\mathbf{p}) = -\frac{\not{p}^2}{m^2} = -\frac{1}{2m^2}\ \{\gamma^\mu, \gamma^\nu\}p_\mu p_\nu. \tag{15.3.2}$$

Using the relation $p^2 = p^\mu p_\mu = -m^2$ and recognizing that eq. (15.3.2) holds for all $\mathbf{p}$ then establishes identity (15.3.1).

It turns out that the matrix γ_5 enountered earlier can be written as a product of the γ_μ's, with

$$\gamma_5 = i\gamma_0\gamma_1\gamma_2\gamma_3 = \frac{i}{4!}\epsilon^{\mu\nu\lambda\rho}\gamma_\mu\gamma_\nu\gamma_\lambda\gamma_\rho\,, \tag{15.3.3}$$

where $\epsilon^{\mu\nu\lambda\rho}$ is the completely antisymmetric Levi-Civita tensor, with the convention that $\epsilon^{0123} = +1$. Eq. (15.3.3) is most easily proven by directly multiplying out the definitions, and has several immediate consequences. First, since (15.3.1) implies γ_μ and γ_ν anticommute when $\mu \neq \nu$, it follows that γ_5 must anticommute with all of the γ_μ's:

$$\{\gamma_5, \gamma_\mu\} = 0\,. \tag{15.3.4}$$

A second useful identity that follows from (15.3.3) is

$$\gamma_5\gamma^\mu\gamma^\nu = \gamma_5\,\eta^{\mu\nu} - \frac{i}{2}\,\epsilon^{\mu\nu\lambda\rho}\gamma_\lambda\gamma_\rho\,. \tag{15.3.5}$$

15.3.1 Lorentz Transformation Properties

The index 'μ' on the Dirac matrices γ^μ is suggestive of the index on a relativistic 4-vector, and this is not an accident as we now show. The point is that there is a sense that γ^μ does transform under Lorentz transformations as if it were a 4-vector, and it is because of this that it makes sense to raise and lower this index using the metric, as in

$$\gamma_\mu = \eta_{\mu\nu}\gamma^\nu \quad \text{and} \quad \gamma^\mu = \eta^{\mu\nu}\gamma_\nu\,. \tag{15.3.6}$$

To see why, evaluate the product $D(\Lambda)\,\gamma_\mu\,D^{-1}(\Lambda)$ where $D(\Lambda)$ is the matrix that represents Lorentz transformations in the $\left(\frac{1}{2},0\right)\oplus\left(0,\frac{1}{2}\right)$ representation, obtained by exponentiating the generators given in (15.1.10): $D(\Lambda) = \exp[i\theta_k\mathcal{J}_k + i\phi_k\mathcal{K}_k]$ for the parameters θ_k and ϕ_k labelling the transformation $\Lambda = \Lambda(\theta,\phi)$.

To evaluate $D(\Lambda)\,\gamma_\mu\,D^{-1}(\Lambda)$ we first notice the property that the matrix β defined in (15.2.18) commutes with all rotation matrices $D(R)$:

$$D(R)\,\beta\,D^{-1}(R) = \beta. \tag{15.3.7}$$

This follows from the observation that (15.1.10) implies that any rotation matrix always has the block-diagonal form:

$$D(R) = \begin{pmatrix} \exp(i\theta_k\mathcal{J}_k) & 0 \\ 0 & \exp(i\theta_k\mathcal{J}_k) \end{pmatrix}, \tag{15.3.8}$$

while β just swaps the lower-right two-by-two block with the upper-left one.

Since (15.3.7) is true for any rotation, it is in particular true for a Wigner rotation, $W(\Lambda, \mathbf{p}) = L^{-1}(\Lambda\mathbf{p}/m)\ \Lambda\ L(\mathbf{p}/m)$ — first encountered in (11.2.14) and defined in detail in (B.1.6) — and so $\beta = D(W)\,\beta\,D^{-1}(W)$, or

$$\beta = D^{-1}[L(\Lambda\mathbf{p}/m)]\,D(\Lambda)\,D[L(\mathbf{p}/m)]\,\beta\,D^{-1}[L(\mathbf{p}/m)]\,D^{-1}(\Lambda)\,D[L(\Lambda\mathbf{p}/m)]\,, \tag{15.3.9}$$

using the representation property $D(\Lambda_1\Lambda_2) = D(\Lambda_1)\,D(\Lambda_2)$. Moving the outermost two factors of D to the other side of this equation, and using the definition (15.2.20) to recognize that the result is $\Gamma(\Lambda\mathbf{p})$ then gives

$$\begin{aligned}\Gamma(\Lambda\mathbf{p}) &:= D[L(\Lambda\mathbf{p}/m)]\ \beta\ D^{-1}[L(\Lambda\mathbf{p}/m)] \\ &= D(\Lambda)\ D[L(\mathbf{p}/m)]\ \beta\ D^{-1}[L(\mathbf{p}/m)]\ D^{-1}(\Lambda) \\ &= D(\Lambda)\,\Gamma(\mathbf{p})\ D^{-1}(\Lambda).\end{aligned} \tag{15.3.10}$$

Finally, invoking the definition (15.2.23) for the gamma matrices and using $(\Lambda p)^\mu = \Lambda^\mu{}_\nu p^\nu$ then gives:

$$D(\Lambda)\,\gamma_\mu\,D^{-1}(\Lambda) = \Lambda^\nu{}_\mu\gamma_\nu\,, \tag{15.3.11}$$

which is the identity that we set out to derive. Notice that it gives a very precise sense in which the Dirac matrices 'transform' like a Lorentz four-vector.

Similarly, the definition (15.1.11) implies that because γ_5 is proportional to the unit matrix within each of the two-by-two subspaces, it must commute with all proper Lorentz transformations. Parity, on the other hand, should anticommute with γ_5 since it interchanges the $\left(\frac{1}{2}, 0\right)$ and $\left(0, \frac{1}{2}\right)$ subspaces. These properties are easily verified by combining (15.3.11) with (15.3.3) to obtain

$$\begin{aligned}D(\Lambda)\,\gamma_5\,D^{-1}(\Lambda) &= \frac{i}{4!}\epsilon^{\alpha\beta\gamma\delta}\Lambda^\mu{}_\alpha\gamma_\mu\Lambda^\nu{}_\beta\gamma_\nu\Lambda^\lambda{}_\gamma\gamma_\lambda\Lambda^\rho{}_\delta\gamma_\rho \\ &= \frac{i}{4!}(\det\Lambda)\epsilon^{\mu\nu\lambda\rho}\gamma_\mu\gamma_\nu\gamma_\lambda\gamma_\rho = (\det\,\Lambda)\ \gamma_5,\end{aligned} \tag{15.3.12}$$

indicating that the matrix γ_5 transforms as does a Lorentz *pseudo-scalar*. (Recall that $\det\Lambda = \pm 1$ for all Lorentz transformations.)

15.3.2 Tracing Dirac Matrices

As subsequent sections show, when calculating physical processes – such as cross section or energy level shifts – it is often necessary to take traces over products of gamma matrices. This subsection evaluates a useful selection of such traces for future purposes.

The generic trace of interest has the form $\mathrm{tr}\,[\gamma_{\mu_1}\ldots\gamma_{\mu_n}]$ or $\mathrm{tr}\,[\gamma_5\gamma_{\mu_1}\ldots\gamma_{\mu_n}]$. The simplest way to evaluate these traces is to take advantage of their transformation properties under the (improper) Lorentz group, since the property – *c.f.* (15.3.11)

$$D(\Lambda)\gamma_\mu D^{-1}(\Lambda) = \Lambda^\nu{}_\mu\gamma_\nu, \tag{15.3.13}$$

implies that a trace over n gamma matrices is an *invariant* tensor — as opposed to a *covariant* tensor — of the Lorentz group:

$$\Lambda^{\mu_1}{}_{\nu_1} \cdots \Lambda^{\mu_n}{}_{\nu_n} \mathrm{tr}\,[\gamma_{\mu_1} \ldots \gamma_{\mu_n}] = \mathrm{tr}\,[\gamma_{\nu_1} \ldots \gamma_{\nu_n}] \tag{15.3.14}$$

for all Lorentz transformations. A trace that includes a factor of the matrix γ_5 is similarly an invariant Lorentz *pseudotensor*:

$$\Lambda^{\mu_1}{}_{\nu_1} \cdots \Lambda^{\mu_n}{}_{\nu_n} \mathrm{tr}\,[\gamma_5 \gamma_{\mu_1} \ldots \gamma_{\mu_n}] = \det(\Lambda) \mathrm{tr}\,[\gamma_5 \gamma_{\nu_1} \ldots \gamma_{\nu_n}]. \tag{15.3.15}$$

Now comes the main point: *Any* such invariant tensor of the Lorentz group may be constructed from products of the invariant metric tensor, $\eta_{\mu\nu}$. Similarly, any invariant pseudotensor may be constructed from products of the metric tensor and an odd power of the completely antisymmetric *Levi-Civita symbol*, $\epsilon^{\mu\nu\lambda\rho}$, already encountered in (15.3.3). This last tensor is an invariant pseudotensor by virtue of the following identity that is true by *any* four-by-four matrix:

$$M^{\mu_1}{}_{\nu_1} M^{\mu_2}{}_{\nu_2} M^{\mu_3}{}_{\nu_3} M^{\mu_4}{}_{\nu_4} \epsilon^{\nu_1\nu_2\nu_3\nu_4} = \det(M)\, \epsilon^{\mu_1\mu_2\mu_3\mu_4}. \tag{15.3.16}$$

Traces are evaluated up to an overall multiplicative factor simply by writing down the most general combinations of metric and Levi-Civita tensors that has the same number and symmetry of indices. The multiplicative factor may then be chosen by evaluating the trace for a particularly simple choice of indices.

This procedure is illustrated by the following examples:

1. *Tensor with an odd number of indices:*

$$\mathrm{tr}\,[\gamma^{\mu_1} \ldots \gamma^{\mu_n}] = 0 \qquad \text{if } n \text{ is odd.} \tag{15.3.17}$$

   This follows from the impossibility of combining metrics and Levi-Civita symbols to produce an invariant tensor with an odd number of indices. This is impossible because the metric and Levi-Civita tensors themselves have an even number of indices and because their Lorentz-invariant contraction always removes two indices at a time.

2. *Pseudo-tensor with an odd number of indices:*

$$\mathrm{tr}\,[\gamma_5 \gamma^{\mu_1} \ldots \gamma^{\mu_n}] = 0 \qquad \text{if } n \text{ is odd.} \tag{15.3.18}$$

   This result is an immediate consequence of the previous one since $\gamma_5 = i\gamma_0\gamma_1\gamma_2\gamma_3$ involves an even number of gamma matrices. An alternative way to see the same result is to use the identity $\gamma_5 \gamma^{\mu_1} \ldots \gamma^{\mu_n} \gamma_5 = (-)^n \gamma^{\mu_1} \ldots \gamma^{\mu_n}$ together with the cyclic property of the trace.

3. *Tensor with two indices:*

$$\text{tr } [\gamma^\mu \gamma^\nu] = 4\eta^{\mu\nu}. \tag{15.3.19}$$

There is only one invariant second-rank symmetric tensor: the metric itself, $\eta^{\mu\nu}$. To fix the proportionality constant choose the special case where $\mu = \nu = 0$ for which $\text{tr } [(\gamma^0)^2] = \text{tr } [-1] = -4 = 4\eta^{00}$.

4. *Pseudo-tensor with two indices:*

$$\text{tr } [\gamma_5 \gamma^\mu \gamma^\nu] = 0. \tag{15.3.20}$$

This result follows from the cyclic property of the trace and the observation that $\{\gamma_5, \gamma_\mu\} = 0$ and as a result the trace must be antisymmetric under the interchange $\mu \leftrightarrow \nu$. Since the only second-rank invariant tensor is symmetric (and there is no invariant rank-two pseudo-tensor) the trace must be zero.

5. *Tensor with four indices:*

$$\text{tr } [\gamma^\mu \gamma^\nu \gamma^\lambda \gamma^\rho] = 4(\eta^{\mu\nu}\eta^{\lambda\rho} - \eta^{\mu\lambda}\eta^{\nu\rho} + \eta^{\mu\rho}\eta^{\nu\lambda}). \tag{15.3.21}$$

A fourth-rank invariant tensor (as opposed to pseudotensor) must be constructed from a sum of pairs of metric tensors. The three distinct pairs that are possible are those that appear on the right-hand-side of the above expression. The coefficient of each of these terms is most easily determined by evaluating both sides with a simple choice for the indices. For example, the coefficient of the first term is determined to be 4 by the choice $\mu = \nu = 0$ and $\lambda = \rho = 1$. With this choice only the first term on the right-hand side is nonzero since the metric is diagonal, and the left-hand side becomes: $\text{tr } [(\gamma^0)^2(\gamma^1)^2] = \text{tr } [-1] = -4 = 4\eta^{00}\eta^{11}$. Then repeat this exercise for two other similar choices that isolate the other two possible terms on the right-hand side.

6. *Pseudo-tensor with four indices:*

$$\text{tr } [\gamma_5 \gamma^\mu \gamma^\nu \gamma^\lambda \gamma^\rho] = 4i\epsilon^{\mu\nu\lambda\rho}. \tag{15.3.22}$$

The right-hand side of this equation is again the unique fourth-rank invariant pseudotensor. Its coefficient is easily determined by the evaluating the choice $\mu = 0$, $\nu = 1$, $\lambda = 2$ and $\rho = 3$ for which the right-hand-side is $4i\epsilon^{0123} = +4i$ and the left-hand-side is $\text{tr } [\gamma_5 \gamma^0 \gamma^1 \gamma^2 \gamma^3] = \text{tr } [i(\gamma_5)^2] = 4i$.

These results suffice for many purposes. Traces involving more than four gamma matrices may be evaluated in a similar fashion.

15.4 Bilinears

The next thing to be explored is how Dirac spinors may be combined into objects that transform as ordinary tensors with respect to Lorentz transformations.

15.4.1 The Dirac Adjoint

In order to construct tensors from multiples of an even number of spinors it is first necessary to determine how the adjoint field $\psi^\dagger$ transforms under Lorentz transformations. The formulae found here are special cases of the general results derived earlier in §11. Our notation throughout is to represent Hermitian conjugation in Hilbert space by an asterisk. A 'dagger' here is meant to indicate both conjugation in Hilbert space as well as taking the transpose in the four-by-four spinor space.

The starting point is the Lorentz-transformation rule for a Dirac spinor:

$$U(\Lambda)\,\psi(x)\,U^*(\Lambda) = D(\Lambda^{-1})\,\psi(\Lambda x), \tag{15.4.1}$$

in which $D(\Lambda) = \exp\left[i\theta_k \mathcal{J}_k + i\phi_k \mathcal{K}_k\right]$, with generators $\mathcal{J}_k$ and $\mathcal{K}_k$ defined in (15.1.10). The corresponding rule for the Hermitian conjugate spinor therefore is

$$U(\Lambda)\,\psi^\dagger(x)\,U^*(\Lambda) = \psi^\dagger(\Lambda x)\,D^\dagger(\Lambda^{-1}). \tag{15.4.2}$$

Unfortunately, since the representation matrices $D(\Lambda)$ are not unitary $\psi^\dagger$ does not transform in any particularly simple way.

Notice, however, that the definition of the generators imply that they satisfy the following reality properties:

$$\mathcal{J}_k^\dagger = \mathcal{J}_k = \beta\,\mathcal{J}_k\,\beta \quad \text{and} \quad \mathcal{K}_k^\dagger = -\mathcal{K}_k = \beta\,\mathcal{K}_k\,\beta. \tag{15.4.3}$$

These imply that a general Lorentz representation matrix must satisfy:

$$D^\dagger(\Lambda) = \exp\left[-i\theta_k(\beta\,\mathcal{J}_k\,\beta) - i\phi_k(\beta\,\mathcal{K}_k\,\beta)\right] = \beta\,D^{-1}(\Lambda)\,\beta\,. \tag{15.4.4}$$

Although the representation is not unitary, it is unitary up to a similarity transformation.

It follows that the *Dirac conjugate*, defined as:

$$\overline{\psi}(x) := \psi^\dagger(x)\,\beta = i\psi^\dagger(x)\,\gamma^0, \tag{15.4.5}$$

transforms *contragrediently* to ψ itself:

$$U(\Lambda)\,\overline{\psi}(x)\,U^*(\Lambda) = \overline{\psi}(\Lambda x)\,D^{-1}(\Lambda^{-1}) = \overline{\psi}(\Lambda x)\,D(\Lambda). \tag{15.4.6}$$

This is a special case of a result that is stated in §11.5 and argued on more general grounds in Appendix (C.4): the Hermitian conjugate of an (A, B) field transforms under Lorentz transformations in the (B, A) representation. The conjugate of a field in the $\left(\frac{1}{2}, 0\right) \oplus \left(0, \frac{1}{2}\right)$ representation must therefore necessarily transform in the same representation, or its contragredient, up to a similarity transformation. What the above shows is how to construct this similarity transformation explicitly.

In passing, notice that for majorana spinors the Dirac conjugate may be rewritten using the majorana reality condition (15.1.14),

$$\overline{\psi} = \psi^\dagger \, \beta = \psi^T \, C\beta = \psi^T \, \epsilon\gamma_5 \qquad \text{(Majorana spinors)} \tag{15.4.7}$$

where the superscript 'T' denotes the transpose and

$$\epsilon \equiv \begin{pmatrix} \mathfrak{e} & 0 \\ 0 & \mathfrak{e} \end{pmatrix} \quad \text{for} \quad \mathfrak{e} = i\sigma_2 \tag{15.4.8}$$

is used to rewrite the charge-conjugation matrix – *c.f.* eq. (15.1.14) – as $C = \gamma_5 \, \epsilon \, \beta = -\gamma_2$.

15.4.2 Covariant Bilinears

Using the transformation properties of ψ and $\overline{\psi}$ it is straightforward to compute the Lorentz-transformation properties of bilinears of Dirac spinors. If M is an arbitrary four-by-four matrix that acts in Dirac space then:

$$U(\Lambda) \, \overline{\psi}(x) M \psi(x) \, U^*(\Lambda) = \overline{\psi}(\Lambda x) \, D(\Lambda) \, M \, D^{-1}(\Lambda) \, \psi(\Lambda x). \tag{15.4.9}$$

The Lorentz-transformation properties of the bilinear is determined by the transformation properties of the matrix M under a similarity transformation by the matrix $D(\Lambda)$.

It is convenient to organize calculations by choosing a basis of sixteen independent four-by-four matrices that transform covariantly with respect to the Lorentz group. And this is easy to do because products of γ_μ and γ_5 will automatically be covariant because γ_μ and γ_5 themselves are separately. A convenient basis of 16 such matrices is listed in Table 4. Although it might not be obvious that these sixteen matrices are all linearly independent, this may be demonstrated by showing that they are all orthogonal with respect to the following inner product for the space of four-by-four matrices (prove this!):

$$(M, N) := \mathrm{tr}\,[M^\dagger N]\,. \tag{15.4.10}$$

As a consequence there always exist cofficients a, a_5, b^μ, b_5^μ and $c^{\mu\nu} = -c^{\nu\mu}$ for which an arbitrary matrix M can be expanded as

$$M = a\, I + a_5 \, \gamma_5 + b^\mu \gamma_\mu + b_5^\mu \gamma_5 \gamma_\mu + c^{\mu\nu} \gamma_{\mu\nu}\,. \tag{15.4.11}$$

The coefficients are given explicitly by

$$\begin{aligned} a = \tfrac{1}{4}\,\mathrm{tr}\,(M)\,, \quad a_5 = \tfrac{1}{4}\,\mathrm{tr}\,(\gamma_5 M)\,, \quad b^\mu = \tfrac{1}{4}\,\mathrm{tr}\,(\gamma^\mu M)\,, \\ b_5^\mu = \tfrac{1}{4}\,\mathrm{tr}\,(\gamma^\mu \gamma_5 M) \quad \text{and} \quad c^{\mu\nu} = \tfrac{1}{8}\,\mathrm{tr}\,(\gamma^{\mu\nu} M)\,. \end{aligned} \tag{15.4.12}$$

Some often-encountered examples of expansions of this form are

$$\begin{aligned} \gamma_\mu \gamma_\nu = \eta_{\mu\nu} + \gamma_{\mu\nu}\,, \quad \gamma_5 \gamma_{\mu\nu} = -\frac{i}{2}\,\epsilon_{\mu\nu\lambda\rho}\gamma^{\lambda\rho}\,, \\ \gamma_\mu \gamma_\nu \gamma_\lambda = \eta_{\mu\nu}\gamma_\lambda - \eta_{\mu\lambda}\gamma_\nu + \eta_{\nu\lambda}\gamma_\mu - i\epsilon_{\mu\nu\lambda\rho}\gamma^\rho\gamma_5 \end{aligned} \tag{15.4.13}$$

Matrix	Symbol	Transformation Property
I	S	Scalar
γ_5	P	Pseudo-scalar
γ_μ	V	Vector
$\gamma_5\,\gamma_\mu$	A	Axial-vector
$\gamma_{\mu\nu} := \frac{1}{2}[\gamma_\mu, \gamma_\nu]$	T	Skew-tensor.

Table 4. The Covariant Basis of Dirac Matrices

and so on.

An important special case of the general expansion (15.4.14) and (15.4.15) is the case where M is given by a dyadic of anticommuting fields: $M = \psi_1\,\overline{\psi}_2$. In this case the above formulae become

$$\psi_1\,\overline{\psi}_2 = a\,I + a_5\,\gamma_5 + b^\mu\gamma_\mu + b_5^\mu\gamma_5\gamma_\mu + c^{\mu\nu}\gamma_{\mu\nu}\,, \tag{15.4.14}$$

with coefficients

$$\begin{aligned} a = -\tfrac{1}{4}\,\overline{\psi_2}\psi_1\,, \quad a_5 = -\tfrac{1}{4}\,\overline{\psi_2}\gamma_5\psi_1\,, \quad b^\mu = -\tfrac{1}{4}\,\overline{\psi_2}\gamma^\mu\psi_1\,, \\ b_5^\mu = -\tfrac{1}{4}\,\overline{\psi_2}\gamma^\mu\gamma_5\psi_1 \quad \text{and} \quad c^{\mu\nu} = -\tfrac{1}{8}\,\overline{\psi_2}\gamma^{\mu\nu}\psi_1\,. \end{aligned} \tag{15.4.15}$$

These identities are called *Fiertz identities* when they are used to rearrange products of fermion fields. For instance (keeping in mind the easily-proven identities $\gamma_L\gamma_5 = \gamma_L$, $\gamma_L\gamma_R = \gamma_L\gamma^\mu\gamma^\nu\gamma_R = 0$ and $\gamma^\mu\gamma_\lambda\gamma_\mu = -2\gamma_\lambda$),

$$\begin{aligned} (\overline{\psi}_1\gamma^\mu\gamma_L\psi_2)\,(\overline{\psi}_3\gamma_\mu\gamma_L\psi_4) &= \overline{\psi}_1\gamma^\mu\gamma_L\Big[\psi_2\,\overline{\psi}_3\Big]\gamma_\mu\gamma_L\psi_4 \\ &= \overline{\psi}_1\gamma^\mu\gamma_L\Big[(b^\lambda + b_5^\lambda)\gamma_\lambda\Big]\gamma_\mu\gamma_L\psi_4 \\ &= -\frac{1}{2}(\overline{\psi}_3\gamma^\lambda\gamma_L\psi_2)\,(\overline{\psi}_1\gamma^\mu\gamma_\lambda\gamma_\mu\gamma_L\psi_4) \\ &= (\overline{\psi}_3\gamma^\lambda\gamma_L\psi_2)\,(\overline{\psi}_1\gamma_\lambda\gamma_L\psi_4)\,. \end{aligned} \tag{15.4.16}$$

It is worth noticing in passing that this covariant basis of Dirac matrices allows a translation between the labelling of Lorentz representations by the pair of spins, (A, B), and the conventional four-vector notation. The connection comes about because a bilinear of two Dirac fermions transform under Lorentz transformations in the $[(\frac{1}{2},0)\oplus(0,\frac{1}{2})]\otimes[(\frac{1}{2},0)\oplus(0,\frac{1}{2})]$ representation. This is a reducible representation and its reduction may be read off using the familiar rules for combining angular momenta:

$$\begin{aligned} \left[\left(\frac{1}{2},0\right)\oplus\left(0,\frac{1}{2}\right)\right]\otimes\left[\left(\frac{1}{2},0\right)\oplus\left(0,\frac{1}{2}\right)\right] = \\ (0,0)\oplus(0,0)\oplus\left(\frac{1}{2},\frac{1}{2}\right)\oplus\left(\frac{1}{2},\frac{1}{2}\right)\oplus(1,0)\oplus(0,1). \end{aligned} \tag{15.4.17}$$

It follows that the irreducible representations given on the right-hand-side can be identified with the types of tensors found in the table. Recalling that the dimension of an (A, B) representation is $(2A+1)(2B+1)$, the correspondence is

$$\begin{array}{lcccl} \text{Scalar} & \Longleftrightarrow & (0,0) & \Longleftrightarrow & \overline{\psi}\gamma_L\psi,\ \overline{\psi}\gamma_R\psi; \\ \text{Vector} & \Longleftrightarrow & \left(\frac{1}{2},\frac{1}{2}\right) & \Longleftrightarrow & \overline{\psi}\gamma^\mu\gamma_L\psi,;\ \overline{\psi}\gamma^\mu\gamma_R\psi \\ \text{Tensor} & \Longleftrightarrow & (1,0)\oplus(0,1) & \Longleftrightarrow & \overline{\psi}\gamma^{\mu\nu}\gamma_L\psi,\ \overline{\psi}\gamma^{\mu\nu}\gamma_R\psi. \end{array} \tag{15.4.18}$$

The one-dimensional $(0,0)$ representations correspond to the scalar and pseudo-scalar bilinears, the four-dimensional $\left(\frac{1}{2},\frac{1}{2}\right)$ representations are the vector and axial-vector bilinears and the two types of three-dimensional representations, $(0,1)$ and $(1,0)$, correspond to the six components of an antisymmetric tensor divided into its *self-dual* and *anti-self-dual* parts, according to the Lorentz-invariant conditions $\frac{1}{2}\epsilon^{\mu\nu\lambda\rho}F_{\lambda\rho} = \pm i\,F^{\mu\nu}$. Notice that the identities (15.4.13) imply that these respectively correspond to bilinears built from left- and right-handed spinors because

$$\tfrac{1}{2}\,\epsilon_{\mu\nu\lambda\rho}\,\gamma_L\gamma^{\lambda\rho} = +i\gamma_L\gamma_{\mu\nu} \quad \text{and} \quad \tfrac{1}{2}\,\epsilon_{\mu\nu\lambda\rho}\,\gamma_R\gamma^{\lambda\rho} = -i\gamma_R\gamma_{\mu\nu}\,. \tag{15.4.19}$$

15.4.3 Symmetry and Reality

Since majorana spinors satisfy a reality condition (15.1.14) bilinears that are built from majorana spinors have specific properties under complex conjugation or under interchange of the two spinors that are also worth enumerating.

The starting point is the following relations:

$$(\overline{\psi}_1\,M\,\psi_2)^* = \overline{\psi}_2\,\beta M^\dagger\beta\,\psi_1 \quad \text{and} \quad \overline{\psi}_1\,M\,\psi_2 = \overline{\psi}_2\,\epsilon\gamma_5 M^T\epsilon\gamma_5\,\psi_1\,, \tag{15.4.20}$$

that follow by explicitly taking the complex conjugate or pulling the anticommuting fields ψ_1 and ψ_2 past one another using (15.4.7) (prove them!). In the light of these transformation rules it is useful to know the effects on the basis matrices, M, of performing a similarity transformation with the matrices β, ϵ, and $C = \gamma_5\,\epsilon\,\beta$. Define, then, the signs $\eta, \zeta, \xi = \pm$ for each of the covariant basis matrices $M = S, P, V, A, T$ from the conditions:

$$M^T \equiv \xi\,\epsilon\,M\,\epsilon, \qquad M^\dagger \equiv \zeta\,\beta\,M\,\beta, \qquad M \equiv \eta\,\gamma_5\,M\,\gamma_5. \tag{15.4.21}$$

It is straightforward to check that the signs that correspond to each of the basis matrices of Table 4 are as listed in Table 5. This implies in particular the following symmetry and reality properties (for anticommuting spinors) for the bilinear $\overline{\psi}_1\,M\,\psi_2$:

$$\begin{array}{ll} M = S, P, A & \text{Symmetric under } 1 \leftrightarrow 2; \\ M = V, T & \text{Antisymmetric under } 1 \leftrightarrow 2; \\ M = S, V, T & \text{Real}; \\ M = P, A & \text{Imaginary}. \end{array} \tag{15.4.22}$$

Sign	S	P	V	A	T
ξ	$-$	$-$	$-$	$+$	$+$
ζ	$+$	$-$	$-$	$-$	$-$
η	$+$	$+$	$-$	$-$	$+$
$\xi\eta$	$-$	$-$	$+$	$-$	$+$
$\xi\zeta$	$-$	$+$	$+$	$-$	$-$
$\xi\zeta\eta$	$-$	$+$	$-$	$+$	$-$

Table 5. Some Symmetry Properties of Dirac Matrices

15.4.4 Mode completeness and normalization

Another useful calculational result is the *spinor density matrix* defined as the *dyadic* or *outer product* of the (commuting) mode function with its Dirac conjugate:

$$\mathbf{u}(\mathbf{p},\sigma)\,\overline{\mathbf{u}}(\mathbf{p},\sigma) =: \frac{m}{E_p}\Lambda(\mathbf{p},\sigma). \tag{15.4.23}$$

The explicit factor of m/E_p is reproduces the noncovariance of our definition for $\mathbf{u}(\mathbf{p},\sigma)$. We here evaluate the four-by-four matrix, $\Lambda(\mathbf{p},\sigma)$, by first computing it in the particle rest frame and then Lorentz transforming the result to a general frame. We work with massive particles and choose the direction of polarization to be measured in the z-direction. The result for massless particles may be obtained by taking the zero-mass limit in the result.

In the particle rest frame the product of the two possible polarization spinors may be simply computed and gives:

$$\mathbf{u}\left(\sigma=+\tfrac{1}{2}\right)\,\mathbf{u}^\dagger\left(\sigma=+\tfrac{1}{2}\right)=\frac{1}{2}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}\begin{pmatrix}1&0&1&0\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1&0&1&0\\0&0&0&0\\1&0&1&0\\0&0&0&0\end{pmatrix}, \tag{15.4.24}$$

and:

$$\mathbf{u}\left(\sigma=-\tfrac{1}{2}\right)\,\mathbf{u}^\dagger\left(\sigma=-\tfrac{1}{2}\right)=\frac{1}{2}\begin{pmatrix}0\\1\\0\\1\end{pmatrix}\begin{pmatrix}0&1&0&1\end{pmatrix}=\frac{1}{2}\begin{pmatrix}0&0&0&0\\0&1&0&1\\0&0&0&0\\0&1&0&1\end{pmatrix}. \tag{15.4.25}$$

These two results are succinctly summarized in terms of the Pauli matrices by:

$$\mathbf{u}\left(\sigma=\pm\tfrac{1}{2}\right)\,\mathbf{u}^\dagger\left(\sigma=\pm\tfrac{1}{2}\right)=\frac{1}{4}\begin{pmatrix}1\pm\sigma_3 & 1\pm\sigma_3\\ 1\pm\sigma_3 & 1\pm\sigma_3\end{pmatrix}. \tag{15.4.26}$$

The generalization to polarizations in an arbitrary direction is immediately obtained from rotation invariance. Defining the unit vector, $\mathbf{s}(\sigma)$, to point along the direction of polarization,

(15.4.26) becomes:

$$\mathbf{u}\,(\sigma)\;\mathbf{u}^{\dagger}\,(\sigma)=\frac{1}{4}\begin{pmatrix}1+\boldsymbol{\sigma}\cdot\mathbf{s} & 1+\boldsymbol{\sigma}\cdot\mathbf{s}\\ 1+\boldsymbol{\sigma}\cdot\mathbf{s} & 1+\boldsymbol{\sigma}\cdot\mathbf{s}\end{pmatrix}, \tag{15.4.27}$$

which reduces to the previous result when $\mathbf{s}\left(\sigma=\pm\frac{1}{2}\right)=\pm\mathbf{e}_z$.

The next step is to boost this last result to a general Lorentz frame. In order to do so it is convenient to re-express (15.4.27) in terms of Dirac matrices. Direct use of the definitions implies:

$$\begin{aligned}\mathbf{u}\,(\sigma)\;\mathbf{u}^{\dagger}\,(\sigma)&=\frac{1}{4}\left(1+\beta\right)\left(1+i\gamma_5\not{s}_0\beta\right)\\&=\frac{1}{4}\left(1+\beta\right)\left(1+i\gamma_5\not{s}_0\right)\beta.\end{aligned} \tag{15.4.28}$$

s_0^μ here is a four-vector that is defined by $s_0^\mu\equiv(0,\mathbf{s})$ in the particle rest frame. The corresponding vector in a general frame for which the particle momentum is $\mathbf{p}$ is obtained by boosting with the standard Lorentz boost given explicitly in (B.1.2): $s^\mu\equiv L^\mu{}_\nu(\mathbf{p}/m)\;s_0^\nu$. For example, in the frame for which $p^\mu=(E_p,0,0,p)$ this implies that $s^\mu=(s_zp/m,s_x,s_y,s_zE_p/m)$. Notice that the definition implies two Lorentz-invariant relations:

$$s\cdot s=+1\quad\text{and}\quad s\cdot p=0\,. \tag{15.4.29}$$

In a general frame the spinor mode function is related to the rest-frame result by:

$$\mathbf{u}(p,\sigma)=\sqrt{\frac{m}{E_p}}D(L)\;\mathbf{u}(\sigma), \tag{15.4.30}$$

in which $D(L)$ represents the standard Lorentz boost. Keeping in mind the definition of Dirac conjugation, the desired dyadic in a general frame therefore is:

$$\Lambda(\mathbf{p},\sigma)=D(L)\;\mathbf{u}(\sigma)\mathbf{u}^{\dagger}(\sigma)\;D^{\dagger}(L)\beta. \tag{15.4.31}$$

The final manipulations use some of the properties of $D\equiv D(L)$ that were derived in previous sections: $D^\dagger\beta=\beta D^{-1}$; $D\beta D^{-1}=-i\not{p}/m$; $D\gamma_5D^{-1}=\gamma_5$; and $D\not{s}_0D^{-1}=\not{s}$. These lead to the final result:

$$\mathbf{u}(\mathbf{p},\sigma)\;\overline{\mathbf{u}}(\mathbf{p},\sigma)=\frac{1}{4E_p}\;(m-i\not{p})\;(1+i\gamma_5\not{s}). \tag{15.4.32}$$

The corresponding relation for the antiparticle spinor may be read off using the relation $\mathbf{v}\left(\mathbf{p},\sigma=\pm\frac{1}{2}\right)=\mp\gamma_5\;\mathbf{u}\left(\mathbf{p},\sigma=\mp\frac{1}{2}\right)$. The result is:

$$\mathbf{v}(\mathbf{p},\sigma)\;\overline{\mathbf{v}}(\mathbf{p},\sigma)=-\frac{1}{4E_p}\;(m+i\not{p})\;(1+i\gamma_5\not{s}). \tag{15.4.33}$$

Notice that both of these last expressions are well behaved as $m\to0$ and give the correct result in this limit. Since s_μ changes sign when σ does it follows that summing over spins

gives

$$\sum_{\sigma=\pm 1/2} \mathbf{u}(\mathbf{p},\sigma)\,\overline{\mathbf{u}}(\mathbf{p},\sigma) = \frac{1}{2E_p}\,(m - i\not{p}) \quad \text{and} \quad \sum_{\sigma=\pm 1/2} \mathbf{v}(\mathbf{p},\sigma)\,\overline{\mathbf{v}}(\mathbf{p},\sigma) = -\frac{1}{2E_p}\,(m + i\not{p})\,. \tag{15.4.34}$$

There are two immediate corollaries to these expressions for $\mathbf{u}\overline{\mathbf{u}}$ and $\mathbf{v}\overline{\mathbf{v}}$. The first of these is the normalization convention which is satisfied by the Dirac spinors as they've been defined here. Together with the easily-proven orthogonality of the rest-frame spinors for different spins, the trace of eqs. (11.3.26) and (11.3.27) gives:

$$\overline{\mathbf{u}}(\mathbf{p},\sigma)\mathbf{u}(\mathbf{p},\sigma') = -\overline{\mathbf{v}}(\mathbf{p},\sigma)\mathbf{v}(\mathbf{p},\sigma') = \frac{m}{E_p}\,\delta_{\sigma\sigma'}. \tag{15.4.35}$$

More generally, tracing after multiplication on the right by one of the basis Dirac matrices gives:

$$\begin{aligned} \overline{\mathbf{u}}\gamma_5\mathbf{u} = \overline{\mathbf{v}}\gamma_5\mathbf{v} = -\frac{s\cdot p}{E_p} = 0\,, \quad \overline{\mathbf{u}}\gamma^\mu\mathbf{u} = \overline{\mathbf{v}}\gamma^\mu\mathbf{v} = -\frac{ip^\mu}{E_p}\,, \\ \overline{\mathbf{u}}\gamma_5\gamma^\mu\mathbf{u} = -\overline{\mathbf{v}}\gamma_5\gamma^\mu\mathbf{v} = -\frac{ims^\mu}{E_p}\,, \quad \overline{\mathbf{u}}\gamma_{\mu\nu}\mathbf{u} = \overline{\mathbf{v}}\gamma_{\mu\nu}\mathbf{v} = -\frac{i}{E_p}\,\epsilon_{\mu\nu\lambda\rho}p^\lambda s^\rho\,. \end{aligned} \tag{15.4.36}$$

Notice that unlike for (15.4.35) it is the *same* spinor that appears on both sides of the matrix elements in these last expressions.

15.4.5 Spin Sums

A further corollary of (15.4.32) and (15.4.33) we may evaluate the sum over the polarizations that often appears when computing scattering rates when initial or final spins are not measured,

$$\Pi_u(\mathbf{p}) \equiv \sum_{\sigma=\pm\frac{1}{2}} \mathbf{u}(\mathbf{p},\sigma)\,\overline{\mathbf{u}}(\mathbf{p},\sigma), \tag{15.4.37}$$

together with its analogue, $\Pi_v(\mathbf{p})$, for $\mathbf{v}(\mathbf{p},\sigma)$. The evaluation is trivially done given the identity $s^\mu(-\sigma) = -s^\mu(\sigma)$ that is satisfied in an arbitrary reference frame by the spin four-vector. This implies that the summed density matrix is:

$$\Pi_u(\mathbf{p}) = \frac{1}{2E_p}\,(m - i\not{p}) \quad \text{and} \quad \Pi_v(\mathbf{p}) = -\frac{1}{2E_p}\,(m + i\not{p})\,. \tag{15.4.38}$$

15.5 Discrete symmetries

The final useful calculational background result to be collected concerns how the spinor field transforms under the discrete symmetries of parity, time-reversal and charge-conjugation. After all, one of the principal motivations for using the Dirac representation (rather than a Weyl representation) is that parity and charge conjugation can be represented as matrices since, although they both interchange A with B when acting on a general (A,B) representation,

they map $(\frac{1}{2},0)\oplus(0,\frac{1}{2})$ onto itself. The purpose of this section is to specialize the general transformation properties of the fields given in Appendix C.4 explicitly to the special case of a Dirac spinor.

15.5.1 Parity

The general form for the parity transformation rule for a field in an arbitrary finite-dimensional Lorentz representation was found in C.4 to be given by:

$$\mathcal{P}\,\psi^{AB}_{ab}(x)\,\mathcal{P}^{-1}=(-)^{A+B-j}\eta^*_p\,\psi^{BA}_{ba}(x_p). \tag{15.5.1}$$

Applying this rule to each of the components of the $\left(\frac{1}{2},0\right)\oplus\left(0,\frac{1}{2}\right)$ representation then gives:

$$\mathcal{P}\,\psi(x)\,\mathcal{P}^{-1}=\mathcal{P}\begin{pmatrix}\psi_{a0}\ (x)\\ \psi_{0b}\ (x)\end{pmatrix}\mathcal{P}^{-1}=\eta^*_p\begin{pmatrix}\psi_{0a}(x_p)\\ \psi_{b0}(x_p)\end{pmatrix}=\eta^*_p\,\beta\psi(x_p)\,, \tag{15.5.2}$$

in which β is the matrix defined in (15.2.18) that interchanges the upper and lower two components of the four-component Dirac spinor. It is therefore here seen to carry the interpretation as the matrix which implements the action of parity on Dirac spinors: $D(P)=\beta$.

The action of parity on the Dirac conjugate, $\overline{\psi}$, is simply determined by taking the conjugate of its action on ψ itself. It is in this way found to be:

$$\mathcal{P}\,\overline{\psi}(x)\,\mathcal{P}^{-1}=\eta_p\,\overline{\psi}(x_p)\,\beta. \tag{15.5.3}$$

15.5.2 Charge Conjugation

The action of charge conjugation on a general irreducible field representation is similarly worked out in C.4, and is given by:

$$\mathcal{C}\,\psi^{AB}_{ab}(x)\,\mathcal{C}^{-1}=\eta^*_c(-)^{2A-j-a-b}\psi^{BA^*}_{-b,-a}(x). \tag{15.5.4}$$

When specialized to a Dirac spinor this implies the transformation law:

$$\mathcal{C}\,\psi(x)\,\mathcal{C}^{-1}=\mathcal{C}\begin{pmatrix}\psi_{\frac{1}{2},0}\\ \psi_{-\frac{1}{2},0}\\ \psi_{0,\frac{1}{2}}\\ \psi_{0,-\frac{1}{2}}\end{pmatrix}\mathcal{C}^{-1}=\eta^*_c\begin{pmatrix}+\psi^*_{0,-\frac{1}{2}}\\ -\psi^*_{0,\frac{1}{2}}\\ -\psi^*_{-\frac{1}{2},0}\\ +\psi^*_{\frac{1}{2},0}\end{pmatrix}=\eta^*_c\begin{pmatrix}\mathfrak{e}\,\psi^{(0,\frac{1}{2})*}\\ -\mathfrak{e}\,\psi^{(\frac{1}{2},0)*}\end{pmatrix}=\eta^*_c\,C\,\psi^*(x).$$

As usual the two-by-two matrix $\mathfrak{e}$ appearing in these equations is $\mathfrak{e}=i\sigma_2$. The four-by-four matrix C is the *charge-conjugation matrix* as defined in (15.1.14).

Acting on the Dirac conjugate, charge conjugation similarly becomes:

$$\mathcal{C}\,\overline{\psi}(x)\,\mathcal{C}^{-1}=-\eta_c\,\overline{\psi}^*(x)\,C=\eta_c\,\psi^T(x)\,\epsilon\,\gamma_5, \tag{15.5.5}$$

15.5.3 Time Reversal

These arguments may now be repeated for time-reversal transformations. The general transformation rule for a (A, B) field is given in Appendix C.4 as:

$$\mathcal{T}\ \psi^{AB}_{ab}(x)\ \mathcal{T}^{-1} = \eta_t^*(-)^{A+B-a-b}\,\psi^{AB}_{-a,-b}(x_t). \tag{15.5.6}$$

For Dirac spinors this specializes to:

$$\mathcal{T}\,\psi(x)\,\mathcal{T}^{-1} = \begin{pmatrix} \psi_{\frac{1}{2},0}(x) \\ \psi_{-\frac{1}{2},0}(x) \\ \psi_{0,\frac{1}{2}}(x) \\ \psi_{0,-\frac{1}{2}}(x) \end{pmatrix} \mathcal{T}^{-1} = \eta_t^* \begin{pmatrix} -\psi_{-\frac{1}{2},0}(x_t) \\ +\psi_{\frac{1}{2},0}(x_t) \\ -\psi_{0,-\frac{1}{2}}(x_t) \\ +\psi_{0,\frac{1}{2}}(x_t) \end{pmatrix} = -\eta_t^*\,\epsilon\,\psi(x_t)\,, \tag{15.5.7}$$

where ϵ is the four-by-four matrix defined in (15.4.8) above. The conjugate spinor therefore transforms as:

$$\mathcal{T}\ \overline{\psi}(x)\ \mathcal{T}^{-1} = \eta_t\ \overline{\psi}(x_t)\ \epsilon. \tag{15.5.8}$$

15.5.4 Transformation of the Bilinears

The C, P, and T transformation properties of the bilinears is also easily constructed using those of ψ and $\overline{\psi}$. The result for parity is:

$$\mathcal{P}\ \overline{\psi}_1(x)\,M\,\psi_2(x)\ \mathcal{P}^{-1} = (\eta_p)_1(\eta_p^*)_2\,\overline{\psi}_1(x_p)\,\beta\,M\,\beta\,\psi_2(x_p). \tag{15.5.9}$$

For charge conjugation the analogous result becomes:

$$\mathcal{C}\,\overline{\psi}_1(x)\,M\,\psi_2(x)\,\mathcal{C}^{-1} = -(\eta_c)_1(\eta_c^*)_2\,\overline{\psi}_2(x)\,C\,M^T\,C\,\psi_1(x). \tag{15.5.10}$$

Finally, keeping in mind the antiunitary character of the time-reversal operation:

$$\mathcal{T}\ \overline{\psi}_1(x)\,M\ \psi_2(x)\,\mathcal{T}^{-1} = (\eta_t)_1(\eta_t^*)_2\,\overline{\psi}_1(x_t)\,\epsilon\,M^*\,\epsilon\,\psi_2(x_t)\,. \tag{15.5.11}$$

15.6 Dirac action and interactions

In order to use the above field to describe physical processes we require its action (or, what is the same thing, its lagrangian density). This section constructs the lagrangian for the free Dirac field, and computes the implications of a simple interaction (one that describes radioactive β decays).

15.6.1 Dirac action

We start with the Dirac action, describing noninteracting spin-half particles. To this end we seek a lagrangian density $\mathcal{L}$ that depends on ψ and its derivatives. To keep things Lorentz invariant we require $\mathcal{L}$ to transform as a Lorentz scalar, and so the Lorentz transformation

properties of ψ imply it must involve at least one ψ and one $\overline{\psi}$. But if the lagrangian is to describe noninteracting particles it can be at most quadratic in the fields, so we require $\mathcal{L}$ to be bilinear in ψ and $\overline{\psi}$.

All possible bilinears are enumerated in §15.4 and we follow the practice of earlier sections by seeking only the terms involving the fewest nontrivial number of derivatives. We use the freedom to integrate by parts to move any derivatives from $\overline{\psi}$ and onto ψ. These conditions allow the following lagrangian density

$$\begin{aligned}\mathcal{L} &= -A\,\overline{\psi}\psi - iB\,\overline{\psi}\gamma_5\psi - C\,\overline{\psi}\gamma^\mu\partial_\mu\psi - iD\,\overline{\psi}\gamma^\mu\gamma_5\partial_\mu\psi \\ &= -\Big[(A+iB)\overline{\psi}\gamma_L\psi + (C+iD)\overline{\psi}\partial\!\!\!/\gamma_L\psi\Big] - \Big[(A-iB)\overline{\psi}\gamma_R\psi + (C-iD)\overline{\psi}\partial\!\!\!/\psi\gamma_R\Big]\,,\end{aligned} \tag{15.6.1}$$

where the second line uses the left- and right-handed projectors $\gamma_L = \frac{1}{2}(1+\gamma_5)$, $\gamma_R = \frac{1}{2}(1-\gamma_5)$ and the 'slash' notation $\partial\!\!\!/ = \gamma^\mu\partial_\mu$. Translation invariance in space and time implies the coefficients A, B, C and D appearing here are constants, and the reality conditions (15.4.22) imply they must all be real if $\mathcal{L}$ (and so also the Hamiltonian) is to be hermitian. The second line shows how it suffices to specify how the left-handed fields contribute to $\mathcal{L}$, with the right-handed parts then given automatically when adding the complex conjugate to make $\mathcal{L}$ hermitian.

Not all of these coefficients are physical because some can be removed simply by redefining the field ψ. To start it is conventional to put the kinetic terms into standard form by redefining[54]

$$\psi \to \frac{\gamma_L\psi}{C+iD} + \frac{\gamma_R\psi}{C-iD} = \frac{1}{C^2+D^2}(C - iD\gamma_5)\psi\,. \tag{15.6.2}$$

After this redefinition the lagrangian becomes

$$\mathcal{L} = -\left[\left(\frac{A+iB}{C+iD}\right)\overline{\psi}\gamma_L\psi + \overline{\psi}\partial\!\!\!/\gamma_L\psi\right] + \text{h.c.} = -\tilde{A}\,\overline{\psi}\psi - i\tilde{B}\,\overline{\psi}\gamma_5\psi - \overline{\psi}\partial\!\!\!/\psi\,, \tag{15.6.3}$$

where $\tilde{A}$ and $\tilde{B}$ are the real and imaginary parts of the complex number $(A+iB)/(C+iD)$.

This 'canonical' form for the kinetic (derivative) terms does not completely use up the freedom to redefine fields because $\overline{\psi}\partial\!\!\!/\psi$ remains unchanged under arbitrary and independent rephasings of the left- and right-handed parts:

$$\begin{aligned}\psi \to e^{i\alpha_L}\gamma_L\psi + e^{i\alpha_R}\gamma_R\psi &= e^{i\alpha_V}\Big[e^{i\alpha_A}\gamma_L + e^{-i\alpha_A}\gamma_R\Big]\psi \\ &= e^{i\alpha_V}\Big[\cos\alpha_A + i\gamma_5\sin\alpha_A\Big]\psi\,.\end{aligned} \tag{15.6.4}$$

After this transformation the lagrangian becomes

$$\mathcal{L} = -\left[\left(\tilde{A}+i\tilde{B}\right)e^{2i\alpha_A}\overline{\psi}\gamma_L\psi + \overline{\psi}\partial\!\!\!/\gamma_L\psi\right] + \text{h.c.}\,, \tag{15.6.5}$$

[54] Notice this redefinition would also be consistent even if the field ψ satisfied a reality condition like (15.1.14) because the left- and right-handed parts of ψ are rescaled by the complex conjugates of one another.

and so α_A can be chosen to ensure the vanishing of the imaginary part of $(\tilde{A} + i\tilde{B})\, e^{2i\alpha_A}$.

Once this is done the field is said to be canonically normalized and the lagrangian density takes its standard form

$$\mathcal{L} = -\overline{\psi}\Big(\partial\!\!\!/ + m\Big)\psi\,, \tag{15.6.6}$$

where $m = |\tilde{A} + i\tilde{B}| = \sqrt{\tilde{A}^2 + \tilde{B}^2}$. Notice that the field equation for ψ found from this by varying the action $S = \int \mathrm{d}^4x\, \mathcal{L}$ with respect to the fields is then the Dirac equation, already encountered in (15.2.28), which shows that the parameter m can be identified (for the noninteracting theory at least) with the particle's mass.

15.6.2 Sample interaction: β decay

As an application of the above formalism we consider β-decays of spin-half fermions through the weak interactions, such as for the decay of a neutron: $n \to p + e^- + \overline{\nu}_e$, or more generally the decay of a nucleon or nucleus, N, into a daughter, N' plus the two leptons. The half-life for this process is computed here as a demonstration of Dirac fields at work.

The starting point is the assumption that the interaction Hamiltonian responsible for β-decay has the form of a 'contact interaction' in which the decaying particle is destroyed and the three final-state particles are created. The hamiltonian density is then written as

$$\mathcal{H}_{\rm wk}(x) = \sum_m J_M(x)\; \overline{\psi}_e M \psi_\nu + \text{h.c.}\,. \tag{15.6.7}$$

This is known as a *four-fermion* interaction, or as the *Fermi* interaction Hamiltonian. ψ_e and ψ_ν here represent the fields that respectively destroy electrons and neutrinos, and the $J_M(x)$ are some unknown local operators that act exclusively on the strongly-interacting part of the Hilbert space which contains the initial and final nucleons or nuclei. The sum on M in principle runs over the complete set of Dirac covariants S, P, V, A, T.

The form permitted for the $J_M(x)$ is limited by some experimental facts, which may be summarized as the statement that the electrons that are emitted in β-decays are highly relativistic and have a definite helicity. Their helicity is found to be, on average $\langle h_{e^-}\rangle = -\frac{v}{2}$, where v is the electron's velocity (in units for which the speed of light is $c = 1$). The outgoing antineutrino likewise has helicity $h_{\overline{\nu}} = +\frac{1}{2}$. Similarly, for those reactions for which the outgoing lepton is a positron rather than an electron, *e.g.* $\overline{n} + p \to e^+ + \nu_e$, the positron helicity is $\langle h_{e^+}\rangle = +\frac{v}{2}$ and the neutrino helicity is $h_\nu = -\frac{1}{2}$.

Recalling that in the ultrarelativistic limit a field, $\psi^{AB}(x)$, transforming in the (A, B) representation of the Lorentz group can only destroy particles with helicity $\lambda = B - A$, we see that the electron and neutrino must both be created by a $\left(\frac{1}{2}, 0\right)$ field. That is, ψ_e and ψ_ν may only appear in the interaction hamiltonian, $\mathcal{H}_{\rm wk}$ through their left-handed combinations:

$$\gamma_L\, \psi_e = \frac{1}{2}(1 + \gamma_5)\, \psi_e \quad \text{and} \quad \gamma_L\, \psi_\nu = \frac{1}{2}(1 + \gamma_5)\, \psi_\nu\,. \tag{15.6.8}$$

This implies that a generic bilinear $\overline{\psi}_e M \psi_\nu$ may be replaced with no loss of generality in the interaction hamiltonian by $\overline{\psi}_e\, \gamma_R M \gamma_L\, \psi_\nu$. Since $\gamma_R \gamma_L = 0$ the only combination for which this replacement does not vanish is V or A: $M = \gamma^\mu$ or $M = \gamma_5 \gamma^\mu$.

For these two cases the interaction hamiltonian becomes:

$$\mathcal{H}_{\rm wk} = J^\mu_A\, \overline{\psi}_e\, \gamma_5 \gamma_\mu\, \gamma_L\, \psi_\nu + J^\mu_V\, \overline{\psi}_e\, \gamma_\mu\, \gamma_L\, \psi_\nu + \text{ h.c.} = \frac{1}{2}\, J^\mu\, \overline{\psi}_e\, \gamma_\mu (1+\gamma_5)\, \psi_\nu + \text{ h.c.} \tag{15.6.9}$$

where $J^\mu := J^\mu_V - J^\mu_A$. This is known as the '$V-A$' theory of the weak interactions, originally discovered by Feynman and Gell-Mann and Sudarshan and Marshak. The plan is to use this to perturbatively calculate the β–decay amplitude for the process $N \to N' + e^- + \overline{\nu}_e$.

Worked example: Beta decay rate

Referring back to Chapter 3, to lowest order in the interaction Hamiltonian the S-matrix for the reaction $N \to N' + e^- + \overline{\nu}_e$ is:

$$\langle N'; e^-; \overline{\nu}_e | S | N \rangle = -2\pi i\, \mathcal{A}\, \delta^4(p_N - p_{N'} - p_e - p_{\overline{\nu}}), \tag{15.6.10}$$

in which the reduced amplitude, $\mathcal{A}$, is:

$$\begin{aligned} \mathcal{A} &= \langle N'; e^-; \overline{\nu}_e | \mathcal{H}_{\rm wk}(0) | N \rangle \\ &= \langle N' | J^\mu(0) | N \rangle\, \langle e^-; \overline{\nu}_e | \overline{\psi}_e\, \gamma_\mu \gamma_L\, \psi_\nu | 0 \rangle \\ &= \langle N' | J^\mu(0) | N \rangle\, \left[\frac{\overline{\mathbf{u}}_e(\mathbf{p}_e, \sigma_e)}{(2\pi)^{3/2}} \right] \gamma_\mu \gamma_L \left[\frac{\mathbf{v}_\nu(\mathbf{p}_\nu, \sigma_\nu)}{(2\pi)^{3/2}} \right]. \end{aligned} \tag{15.6.11}$$

In terms of this matrix element, the decay rate is given by

$$\begin{aligned} \mathrm{d}\Gamma(N \to N' e^- \overline{\nu}) &= (2\pi)^7\, |\mathcal{A}|^2\, \delta^4(p_N - p_{N'} - p_e - p_{\overline{\nu}})\, \mathrm{d}^3 p_{N'}\, \mathrm{d}^3 p_e\, \mathrm{d}^3 p_{\overline{\nu}} \\ &= 2\pi\, W^{\alpha\beta}\, L_{\alpha\beta}\, \delta^4(p_N - p_{N'} - p_e - p_{\overline{\nu}})\, \mathrm{d}^3 p_{N'}\, \mathrm{d}^3 p_e\, \mathrm{d}^3 p_{\overline{\nu}}, \end{aligned} \tag{15.6.12}$$

in which

$$W^{\alpha\beta}(\mathbf{p}_N; \mathbf{p}_{N'}) := \langle N' | J^\alpha(0) | N \rangle\, \langle N | J^\beta(0) | N' \rangle, \tag{15.6.13}$$

and

$$\begin{aligned} L_{\alpha\beta} &:= \Big[\overline{\mathbf{u}}_e(\mathbf{p}_e, \sigma_e)\, \gamma_\alpha \gamma_L\, \mathbf{v}_\nu(\mathbf{p}_\nu, \sigma_\nu) \Big]\, \Big[\overline{\mathbf{u}}_e(\mathbf{p}_e, \sigma_e)\, \gamma_\beta \gamma_L\, \mathbf{v}_\nu(\mathbf{p}_\nu, \sigma_\nu) \Big]^* \\ &= -\Big[\overline{\mathbf{u}}_e(\mathbf{p}_e, \sigma_e)\, \gamma_\alpha \gamma_L\, \mathbf{v}_\nu(\mathbf{p}_\nu, \sigma_\nu) \Big]\, \Big[\overline{\mathbf{v}}_\nu(\mathbf{p}_\nu, \sigma_\nu)\, \gamma_\beta \gamma_L\, \mathbf{u}_e(\mathbf{p}_e, \sigma_e) \Big]. \end{aligned} \tag{15.6.14}$$

The definition $\overline{\mathbf{u}} = \mathbf{u}^\dagger \beta$ and the identity $\gamma_\mu^\dagger = -\beta \gamma_\mu \beta$ have been used to rewrite the complex conjugate in the last equality.

The next step is to use the trick of rewriting the spinor matrix elements that appear in $L_{\alpha\beta}$ in terms of a trace over Dirac matrices. This is done by rewriting (15.6.14) in terms of the dyadic spin density matrix of the previous section:

$$L_{\alpha\beta} = -\mathrm{Tr}\, \Big[\gamma_\alpha \gamma_L\, (\mathbf{v}_\nu \overline{\mathbf{v}}_\nu)\, \gamma_\beta \gamma_L (\mathbf{u}_e \overline{\mathbf{u}}_e) \Big]. \tag{15.6.15}$$

So far so good. Up until this point we have made no assumptions concerning the quantities that are to be measured during the decay. The calculation from here on may be greatly simplified if it is

recognized that experiments can usually detect only the outgoing electron momentum. Of the three components of electron momentum, only the magnitude—or, equivalently, the electron energy—is of real interest. This is because rotational invariance dictates that the decay rate is independent of the direction of the outgoing electron once all other momenta and spins are summed over. In order to determine the probability distribution for this variable only we may sum over all possible electron and antineutrino spins and integrate over all possible antineutrino and nuclear final momenta. In this case the unpolarized decay rate becomes:

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}^3 p_e} = (2\pi)^7 \int \mathrm{d}^3 p_{N'} \int \mathrm{d}^3 p_{\overline{\nu}}\, W^{\alpha\beta}\, \overline{L}_{\alpha\beta}\, \delta^4(p_N - p_{N'} - p_e - p_{\overline{\nu}}), \tag{15.6.16}$$

in which

$$\begin{aligned} \overline{L}_{\alpha\beta} &= -\sum_{\sigma_e,\sigma_\nu} \mathrm{Tr}\left[\gamma_\alpha\gamma_L\,(\mathbf{v}_\nu\overline{\mathbf{v}}_\nu)\,\gamma_\beta\gamma_L(\mathbf{u}_e\overline{\mathbf{u}}_e)\right] \\ &= +\frac{1}{4E_eE_{\overline{\nu}}}\,\mathrm{Tr}\left[\gamma_\alpha\gamma_L\,(m_\nu + i\not{p}_\nu)\,\gamma_\beta\gamma_L\,(m_e - i\not{p}_e)\right]. \end{aligned} \tag{15.6.17}$$

This evaluates the spin sum using (15.4.38) and the last expression assumes a nonzero neutrino mass, m_ν, in order to see how the result would depend on this parameter. In fact it is through precision measurements of the shape of this type of decay spectrum that the present upper bound on the electron-neutrino mass is derived.

This last form is the most useful for computing the decay rate since it may be evaluated using the trace theorems derived in section (11.5) above. The result is:

$$\begin{aligned} \overline{L}^{\alpha\beta} &= \frac{1}{4E_eE_{\overline{\nu}}}\,\mathrm{Tr}\left[\gamma^\alpha\gamma_L\,(m_\nu + i\not{p}_\nu)\,\gamma^\beta\gamma_L\,(m_e - i\not{p}_e)\right] \\ &= \frac{1}{4E_eE_{\overline{\nu}}}\,\mathrm{Tr}\left[\gamma^\alpha\gamma_L\not{p}_\nu\,\gamma^\beta\gamma_L\not{p}_e\right] \\ &= \frac{1}{8E_eE_{\overline{\nu}}}\,\mathrm{Tr}\left[(1+\gamma_5)\not{p}_e\gamma^\alpha\not{p}_\nu\gamma^\beta\right] \\ &= \frac{1}{2E_eE_{\overline{\nu}}}\left[(p_e^\alpha p_\nu^\beta + p_e^\beta p_\nu^\alpha - p_e\cdot p_\nu\,\eta^{\alpha\beta}) - i\epsilon^{\alpha\beta}{}_{\lambda\rho}\,p_e^\lambda p_\nu^\rho\right]. \end{aligned} \tag{15.6.18}$$

The next step is to perform the integrations over phase space, *i.e.* the unmeasured final-state momenta. Working in the rest frame of the decaying particle, $p_N^\mu = (M_N, 0, 0, 0)$, allows the phase space volume element to be written as:

$$\begin{aligned} &\delta^4(p_N - p_{N'} - p_e - p_{\overline{\nu}})\mathrm{d}^3p_{N'}\,\mathrm{d}^3p_{\overline{\nu}}\,\mathrm{d}^3p_e \\ &\quad= \delta(Q - E_e - E_{\overline{\nu}})\,\delta^3(\mathbf{p}_{N'} + \mathbf{p}_e + \mathbf{p}_{\overline{\nu}})\;\mathrm{d}^3p_{N'}\,\mathrm{d}^3p_{\overline{\nu}}\,\mathrm{d}^3p_e \\ &\quad= \delta(Q - E_e - E_{\overline{\nu}})|_{\mathbf{p}_{N'}=-\mathbf{p}_e-\mathbf{p}_{\overline{\nu}}}\;\mathrm{d}^3p_{\overline{\nu}}\,\mathrm{d}^3p_e. \end{aligned} \tag{15.6.19}$$

Here Q is defined as the net energy lost by the nucleons: $Q \equiv E_N - E_{N'}$, and the momentum-conserving δ-function has been used to perform the integral over $\mathbf{p}_{N'}$.

This is as much as can be done without some knowledge of the unknown matrix element $\langle N|J^\mu(0)|N'\rangle$ since this determines the dependence of $W^{\alpha\beta}$ on $\mathbf{p}_{N'} = -\mathbf{p}_e - \mathbf{p}_{\overline{\nu}}$. Things greatly simplify once it is recognized that in practice for all nuclear decays of the form we are considering the nucleons (or nuclei) are very heavy in comparison to the energy that is made available in the decay: $M_N, M_{N'} \gg Q$.

This is because dimensional analysis demands that the matrix element may be written as a function of the dimensionless combinations of the form $\mathbf{p}_{N'}/M$ where M denotes one of the nuclear masses, M_N or $M_{N'}$. Since these are at most of order $Q/M \ll 1$ in size it is a good approximation to simply neglect the nuclear recoil and take $W^{\alpha\beta}$ to be independent of the lepton momenta. In this same approximation the energy release becomes $Q \approx M_N - M_{N'}$.

The neglect of nuclear recoil then permits the evaluation of the integrals over the directions, $\hat{\mathbf{p}}_e$ and $\hat{\mathbf{p}}_{\overline{\nu}}$, of the outgoing leptons. The required integral is:

$$\begin{aligned} I_{\alpha\beta} &\equiv \int_0^{4\pi} \mathrm{d}^2\hat{\mathbf{p}}_e \int_0^{4\pi} \mathrm{d}^2\hat{\mathbf{p}}_{\overline{\nu}}\, L_{\alpha\beta}(\mathbf{p}_e, \mathbf{p}_{\overline{\nu}}) \\ &= (4\pi)^2\, L_{\alpha\beta}(\mathbf{p}_e = 0, \mathbf{p}_{\overline{\nu}} = 0). \end{aligned} \tag{15.6.20}$$

The integral is easy to perform because the integrand depends only linearly on $\hat{\mathbf{p}}_e$ and $\hat{\mathbf{p}}_{\overline{\nu}}$, as may be explicitly seen from (15.6.18).

Putting these results together and writing the phase space volume elements using $\mathrm{d}^3p = p^2\mathrm{d}p\,\mathrm{d}^2\hat{\mathbf{p}}$ and $p\mathrm{d}p = E\mathrm{d}E$ gives the final result for the differential energy spectrum:

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}E_e} = 16\pi^3\, E_e(Q - E_e)\sqrt{(E_e^2 - m_e^2)[(Q - E_e)^2 - m_\nu^2]}\,\Big(\mathcal{F} + \mathcal{G}\Big), \tag{15.6.21}$$

in which the nuclear matrix elements are for historical reasons written as:

$$\mathcal{F} := \Big|\langle N|J^0|N'\rangle\Big|^2, \qquad (\textit{Fermi}\text{ term}) \tag{15.6.22}$$

and

$$\mathcal{G} := \Big|\langle N|\mathbf{J}|N'\rangle\Big|^2, \qquad (\textit{Gamow-Teller}\text{ term}). \tag{15.6.23}$$

It has become conventional to display this spectrum using what is known as a *Kurie plot*. This is a plot of the combination

$$y := \left[\frac{\mathrm{d}\Gamma/\mathrm{d}E_e}{E_e\sqrt{E_e^2 - m_e^2}}\right]^{1/2} \tag{15.6.24}$$

against the energy of the electron, E_e. The motivation for plotting this particular combination of variables is that in early experiments Q, the energy released, was unknown. In the limit of vanishing neutrino mass the plot of y against E_e becomes a straight line of the form $y = C(Q - E_e)$, as in Fig. 9. Experimental determination of the slope and intercept of this line determine Q and C, and so also the strong matrix element $(\mathcal{F} + \mathcal{G})$. Searches for deviations in this curve from a straight line can be used to search for a nonzero neutrino mass.

A final historical note: we have taken the matrix elements of J^μ as being completely unknown. It turns out that for transitions between spinless nuclei the parity invariance of the strong interactions implies that only the vector (and not axial–vector) part, J^μ_V, contribute to the matrix element. In the standard model for particle interactions this matrix element is calculable in terms of the isospin quantum numbers of the nucleons and the *Fermi coupling constant*, G_F, that is measured in weak decays of muons, $\mu \to e + \overline{\nu}_e + \nu_\mu$.

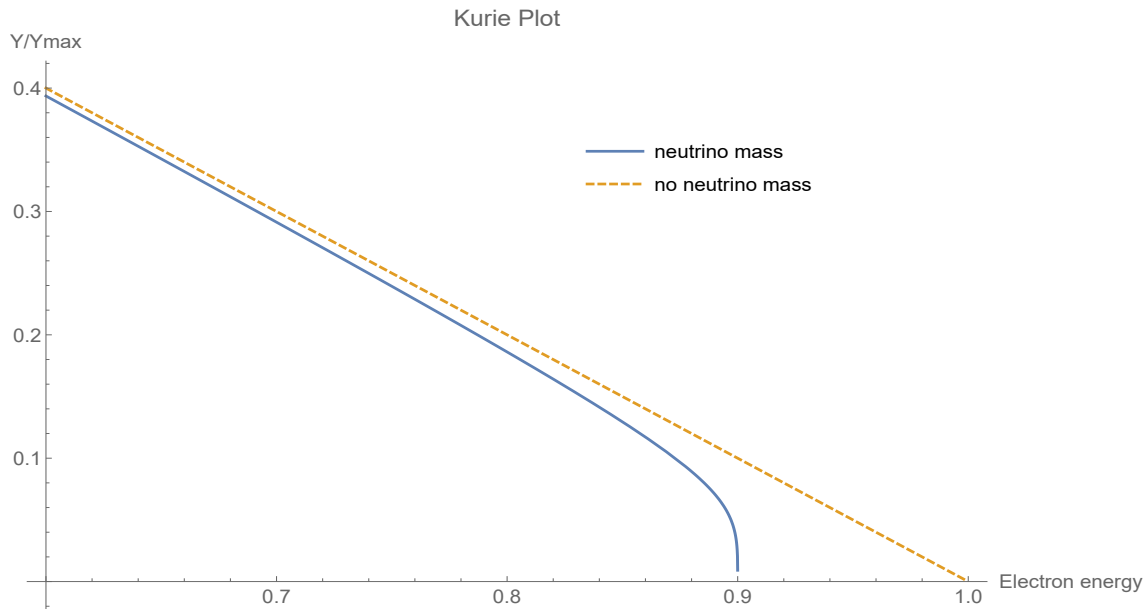


Figure 9. A Kurie Plot for both $m_\nu = 0$ and $m_\nu \neq 0$.

15.7 Propagator and Feynman rules

The final ingredient needed for applications is the spin-half Feynman propagator that appears once perturbative methods are used beyond leading order, as described for spinless particles in §12.4. The propagator appears in particular when contractions are sought between creation and annihilation operators that both arise from within the interaction Hamiltonian density $\mathcal{H}_{\rm int}(x)$ — or Lagrangian density $\mathcal{L}_{\rm int}(x)$.

For spin-half fields the quantity that arises in this way is the spinor propagator (or Dirac propagator) defined by

$$\begin{aligned} S_{mn}(x-y) &:= \langle 0|T\Big[\psi_m(x)\,\overline{\psi}_n(y)\Big]|0\rangle \\ &= \Theta(x^0-y^0)\langle 0|\psi_m(x)\,\overline{\psi}_n(y)|0\rangle - \Theta(y^0-x^0)\langle 0|\overline{\psi}_n(y)\,\psi_m(x)\,|0\rangle \\ &= \Theta(x^0-y^0)\Big\{\psi_m(x)\,,\overline{\psi}_n(y)\Big\} - \Theta(y^0-x^0)\Big\{\overline{\psi}_n(y)\,,\psi_m(x)\Big\}\,, \end{aligned} \tag{15.7.1}$$

where n and m are the 4-component Dirac indices. In what follows these indices are usually not written explicitly, instead writing S as a 4-by-4 dyadic matrix built from $\psi(x)$ and $\overline{\psi}(y)$.

The above also extends the previous definition of time-ordering — see (3.2.17) or (3.2.18) — to anticommuting fields:

$$T\Big[\mathcal{O}_{\scriptscriptstyle F}(x_1)\cdots\mathcal{O}_{\scriptscriptstyle F}(x_k)\Big] = \pm\mathcal{O}_{\scriptscriptstyle F}(x_{\rm latest})\cdots\mathcal{O}_{\scriptscriptstyle F}(x_{\rm earliest})\,, \tag{15.7.2}$$

where the $\pm$ counts the number of times pairs of fermionic fields interchange their order, with each interchange contributing a negative sign. This definition is chosen so that time

ordering does not matter for spacelike separations, given that bosonic fields commute there while fermionic fields anticommute.

Using the field expansion (15.2.1) (repeated here)

$$\psi(x) = \sum_\sigma \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}} \Big[\mathbf{u}(\mathbf{p},\sigma)\; \mathfrak{c}_{\mathbf{p}\sigma}\; e^{ipx} + \mathbf{v}(\mathbf{p},\sigma)\; \overline{\mathfrak{c}}^\star_{\mathbf{p}\sigma}\; e^{-ipx} \Big], \tag{15.7.3}$$

where $p^0 = E_p = \sqrt{\mathbf{p}^2 + m^2}$, and using the standard anticommutation rules $\{\mathfrak{c}_{\mathbf{p}\sigma}\,, \mathfrak{c}^\star_{\mathbf{q}\xi}\} = \delta_{\sigma\xi}\delta^3(\mathbf{p}-\mathbf{q}) = \{\overline{\mathfrak{c}}_{\mathbf{p}\sigma}\,, \overline{\mathfrak{c}}^\star_{\mathbf{q}\xi}\}$ — as well as $\{\mathfrak{c}_{\mathbf{p}\sigma}\,, \mathfrak{c}_{\mathbf{q}\xi}\} = \{\overline{\mathfrak{c}}_{\mathbf{p}\sigma}\,, \overline{\mathfrak{c}}_{\mathbf{q}\xi}\} = \{\mathfrak{c}_{\mathbf{p}\sigma}\,, \overline{\mathfrak{c}}_{\mathbf{q}\xi}\} = 0$ — one finds

$$\begin{aligned}
\langle 0|\psi_m(x)\,\overline{\psi}_n(y)|0\rangle \;&=\; \sum_{\sigma=\pm 1/2} \int \frac{\mathrm{d}^3p}{(2\pi)^3} e^{ip\cdot(x-y)}\; \mathbf{u}_m(\mathbf{p},\sigma)\,\overline{\mathbf{u}}_n(\mathbf{p},\sigma) \\
&= \int \frac{\mathrm{d}^3p}{(2\pi)^3}\; e^{ip\cdot(x-y)} \left(\frac{m - i\not{p}}{2E_p}\right)_{mn} \qquad (15.7.4) \\
&= \Big(m - \not{\partial}\Big)_{mn} \int \frac{\mathrm{d}^3p}{(2\pi)^3 2E_p}\; e^{ip\cdot(x-y)} \qquad (15.7.5)
\end{aligned}$$

where the derivative in $\not{\partial} = \gamma^\mu\partial_\mu$ acts on x (as opposed to y). Similarly,

$$\begin{aligned}
\langle 0|\overline{\psi}_n(y)\,\psi_m(x)|0\rangle \;&=\; \sum_{\sigma=\pm 1/2} \int \frac{\mathrm{d}^3p}{(2\pi)^3}\; e^{-ip\cdot(x-y)}\; \mathbf{v}_m(\mathbf{p},\sigma)\,\overline{\mathbf{v}}_n(\mathbf{p},\sigma) \\
&= -\int \frac{\mathrm{d}^3p}{(2\pi)^3}\; e^{-ip\cdot(x-y)} \left(\frac{m + i\not{p}}{2E_p}\right)_{mn} \qquad (15.7.6) \\
&= -\Big(m - \not{\partial}\Big)_{mn} \int \frac{\mathrm{d}^3p}{(2\pi)^3 2E_p}\; e^{-ip\cdot(x-y)}
\end{aligned}$$

which evaluates the spin sums using (15.4.34). Using these in (15.7.1) then gives

$$\begin{aligned}
S(x-y) \;&=\; \Theta(x^0-y^0)\Big(m - \not{\partial}\Big) \int \frac{\mathrm{d}^3p}{(2\pi)^3 2E_p}\; e^{ip\cdot(x-y)} \\
&\qquad\qquad + \Theta(y^0-x^0)\Big(m - \not{\partial}\Big) \int \frac{\mathrm{d}^3p}{(2\pi)^3 2E_p}\; e^{-ip\cdot(x-y)} \qquad (15.7.7) \\
&= \Big(m - \not{\partial}\Big) \int \frac{\mathrm{d}^3p}{(2\pi)^3 2E_p} \Big[\Theta(x^0-y^0)\, e^{ip\cdot(x-y)} + \Theta(y^0-x^0)\, e^{-ip\cdot(x-y)}\Big] \\
&= \Big(m - \not{\partial}\Big)\, G(x-y)\,, \qquad (15.7.8)
\end{aligned}$$

where $G(x-y)$ is the spinless Feynman propagator of (12.4.13). Notice that the second equality commutes $(m - \not{\partial})$ past the step functions because the difference is given by

$$-\gamma^0\delta(x^0-y^0) \int \frac{\mathrm{d}^3p}{(2\pi)^3 2E_p} \Big[e^{ip\cdot(x-y)} - e^{-ip\cdot(x-y)}\Big] = 0\,. \tag{15.7.9}$$

The manifestly covariant expression for $G(x-y)$ given in (12.4.15) then gives the covariant expression for $S(x-y)$ that we seek, since eq. (15.7.7) is then

$$\begin{aligned} S(x-y) &= \langle 0|T\Big[\psi(x)\,\overline{\psi}(y)\Big]|0\rangle = \Big(m-\not{\partial}\Big)G(x-y) \\ &= -i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{m-i\not{\bar{p}}}{\bar{p}^2+m^2-i\bar{\delta}}\right] e^{i\bar{p}\cdot(x-y)}\,, \end{aligned} \tag{15.7.10}$$

where (as before) the bar on $\bar{p}^\mu$ indicates that $\bar{p}^0$ is integrated independent of $\mathbf{p}$.

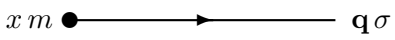
15.7.1 Feynman rules

With the propagator in hand, we can now proceed as in §12.4 and enunciate the new Feynman rules that arise when relativistic spin-half fermions are used at arbitrary order within a perturbative framework.

External spin-half lines: An external line that directly connects an initial-state $\mathfrak{c}^\star_{\mathbf{q}\sigma}$ to an $\mathfrak{c}_{\mathbf{p}\xi}$ appearing inside $\psi(x_1)$ contributes the Feynman rule:

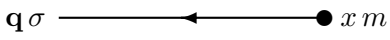
$$\sum_\xi \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\,\mathbf{u}_m(\mathbf{p},\xi)\,e^{ip\cdot x}\delta_{\sigma\xi}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{iq\cdot x}}{(2\pi)^{3/2}}\,\mathbf{u}_m(\mathbf{q},\sigma) \quad \text{(incoming particle).} \tag{15.7.11}$$

An incoming antiparticle $\bar{\mathfrak{c}}^\star_{\mathbf{q}\sigma}$ pairing with an $\bar{\mathfrak{c}}_{\mathbf{p}\xi}$ appearing in $\overline{\psi}(x_1)$ similarly gives



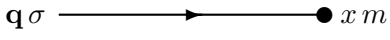
$$\sum_\xi \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\,\overline{\mathbf{v}}_m(\mathbf{p},\xi)\,e^{ip\cdot x}\delta_{\sigma\xi}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{iq\cdot x}}{(2\pi)^{3/2}}\,\overline{\mathbf{v}}_m(\mathbf{q},\sigma) \quad \text{(incoming antiparticle).} \tag{15.7.12}$$

By an identical argument, an $\mathfrak{c}_{\mathbf{q}\sigma}$ in the final state pairing with $\mathfrak{c}^\star_{\mathbf{p}\xi}$ contained in $\overline{\psi}(x_1)$ gives



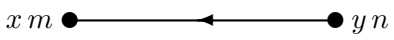
$$\sum_\xi \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\,\overline{\mathbf{u}}_m(\mathbf{p},\xi)\,e^{-ip\cdot x}\delta_{\sigma\xi}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{-iq\cdot x}}{(2\pi)^{3/2}}\,\overline{\mathbf{u}}_m(\mathbf{q},\sigma) \quad \text{(outgoing particle)}\,, \tag{15.7.13}$$

and an outgoing antiparticle $\bar{\mathfrak{c}}_{\mathbf{q}\sigma}$ pairing with $\bar{\mathfrak{c}}^\star_{\mathbf{p}\xi}$ contained in $\psi(x_1)$ gives



$$\sum_\xi \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\,\mathbf{v}_m(\mathbf{p},\xi)\,e^{-ip\cdot x}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{-iq\cdot x}}{(2\pi)^{3/2}}\,\mathbf{v}_m(\mathbf{q},\sigma) \quad \text{(outgoing antiparticle).} \tag{15.7.14}$$

Internal spin-half lines: When a contraction takes place between creation and annihilation operators that are both associated with a vertex one gets the propagator $S_{mn}(x-y)$ of (15.7.10), leading to the Feynman rule



$$-i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{m-i\bar{\not{p}}}{\bar{p}^2+m^2-i\bar{\delta}}\right]_{mn} e^{i\bar{p}\cdot(x-y)}\,. \tag{15.7.15}$$

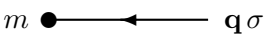
This expression assumes the momentum to be flowing in the same direction as the fermion-number flow.

The coupling and symmetry factors for a Feynman diagram are much the same as before but fermions do introduce a few new signs into the Feynman rules: each closed fermion loop comes with an additional factor of -1, as does the interchange of any two pairs of external lines.

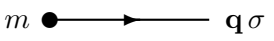
15.7.2 Momentum-space Feynman rules

Momentum-space Feynman rules are obtained by integrating over the positions x_i^μ for all the vertices, just as was done for the spinless case in §12.4, leading to the conservation of 4-momentum at each vertex. The resulting momentum-space Feynman rules for spin-half lines therefore are

External spin-half lines: contribute

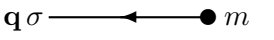


$\dfrac{\mathbf{u}_m(\mathbf{q},\sigma)}{(2\pi)^{3/2}}$ (incoming particle)

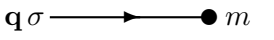


$\dfrac{\overline{\mathbf{v}}_m(\mathbf{q},\sigma)}{(2\pi)^{3/2}}$ (incoming antiparticle)\,, (15.7.16)

and



$\dfrac{\overline{\mathbf{u}}_m(\mathbf{q},\sigma)}{(2\pi)^{3/2}}$ (outgoing particle)



$\dfrac{\overline{\mathbf{v}}_m(\mathbf{q},\sigma)}{(2\pi)^{3/2}}$ (outgoing antiparticle)\,. (15.7.17)

Internal spin-half lines: The momentum space formulation for a spin-half internal line becomes

$$-i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{m-i\bar{\not{p}}}{\bar{p}^2+m^2-i\bar{\delta}}\right]_{mn}\,, \tag{15.7.18}$$

where m is the index associated with ψ_m (destroyer of particles and creator of antiparticles) and n is the index associated with $\overline{\psi}_n$ (destroyer of antiparticles and creator of particles). Notice that the integrand of (15.7.18) is not invariant under $\bar{p}^\mu \to -\bar{p}^\mu$ and so care should be

taken in the direction with which momentum flows through the fermion line. As written $\bar{p}$ is the 4-momentum that flows *into* the vertex corresponding to where ψ_m is, and so momentum flows in the same direction as fermion number.

With these rules the effects of fermion interactions can also (in principle) be pursued systematically to any perturbative order.

16 Quantum Electrodynamics

In this chapter we couple relativistic electrons to electromagnetic fields and by so doing arrive at the theory of Quantum Electrodynamics; in retrospect perhaps one of the most successful theories in the history of science. We do so by applying the general techniques of §11 to set up the relativistic quantum description of photons, and the resulting derivation provides yet another (so far, our third) perspective on quantizing the electromagnetic field.[55]

16.1 Photon field and propagator

The starting point for this iteration is to describe photons from first principles, using the general relativistic quantum treatment of massless spin-one particles. This allows us to establish the connection between fields and creation operators using only their transformation properties under Lorentz transformations (as opposed to finding them as operator solutions to Maxwell's equations).

16.1.1 First-principles field operator

Photons famously travel at the speed of light and so their particle states are labelled by their helicity λ. Since parity changes the sign of λ – see, for example, (11.2.36) – the parity invariance of electromagnetic interactions implies photons should come with two helicity states. The pattern of emission and absorption by atoms then argues that for photons $\lambda = \pm 1$.

We therefore seek the relativistic fields that can represent such a particle. As is argued in §11.3.4 – with explicit details given in §C.2.2 – fields transforming in the general finite-dimensional (A, B) Lorentz representation can only represent massless particles with helicity

$$\lambda = B - A\,. \tag{16.1.1}$$

The smallest field that can represent helicity ± 1 photons therefore is the $3+3 = 6$-dimensional representation $(1,0) \oplus (0,1)$. In more conventional tensor notation this is an antisymmetric tensor $F^{\mu\nu} = -F^{\nu\mu}$ (see Table 2), so

$$F^{\mu\nu}(x) = \sum_{\lambda=\pm} \int \frac{\mathrm{d}^3 p}{\sqrt{(2\pi)^3 2\omega_p}} \Big[u^{\mu\nu}(\mathbf{p},\lambda)\, \mathfrak{a}_{\mathbf{p}\lambda}\, e^{ip\cdot x} + v^{\mu\nu}(\mathbf{p},\lambda)\, \mathfrak{a}^\star_{\mathbf{p}\lambda}\, e^{-ip\cdot x} \Big]\,, \tag{16.1.2}$$

[55] For those counting, a fourth is yet to come – *c.f.* §21 below.

which uses that the photon is its own antiparticle.

The coefficient functions $u^{\mu\nu}(\mathbf{p},\lambda)$ and $v^{\mu\nu}(\mathbf{p},\lambda)$ are determined up to normalization by the consistency of the different Poincaré transformation rules for $F^{\mu\nu}(x)$ and $\mathfrak{a}_{\mathbf{p}\lambda}$. The form for $u^{\mu\nu}$ is a special case of the general result given in (C.2.24). For massive particles $v^{\mu\nu}$ is related to $u^{\mu\nu}$ by (C.3.2), but in the present instance this just amounts to choosing $v^{\mu\nu}$ to be the complex conjugate of $u^{\mu\nu}$. We must simply transcribe this general solution to more familiar Lorentz notation.

For a 4-vector field the finite-dimensional transformation matrix $D_{mn}(\Lambda)$ that represents the fields is given by the matrix $\Lambda^\mu{}_\nu$ itself and a tensor field inherits from this the transformation (11.1.22). The notation used when deriving the general rule assumed u_n transformed through matrix multiplication $u^n \to D^n{}_m(\Lambda)u^m$, and so comparing these transformation properties shows that for an antisymmetric tensor the index n becomes the antisymmetric pair $(\mu\nu)$ and

$$D^{\mu\nu}{}_{\lambda\rho}(\Lambda) = \frac{1}{2}\Big[\Lambda^\mu{}_\lambda\Lambda^\nu{}_\rho - \Lambda^\nu{}_\lambda\Lambda^\mu{}_\rho\Big]\,. \tag{16.1.3}$$

The generators in this representation are found by specializing to $\Lambda^\mu{}_\nu = \delta^\mu_\nu + \omega^\mu{}_\nu$ for an infinitesimal transformation and comparing the result to $D_{mn} = \delta_{mn} + \frac{i}{2}\,\omega_{\mu\nu}(\mathcal{J}^{\mu\nu})_{mn}$.

As usual $u^{\mu\nu}(\mathbf{p},\lambda)$ is first found in a special frame, which for massless states we choose to correspond to motion purely along the z-axis: $k^\mu = (k^0,k^1,k^2,k^3) = (\kappa,0,0,\kappa)$. The little group that preserves k^μ must act consistently on the field indices $(\mu\nu)$ as on the particle helicity label λ, as summarized in the general case by (C.1.25). The 3-parameter group of transformations $\Lambda^\mu{}_\nu$ forming the little group for k^μ is given explicitly by the 2-parameter boosts $S(a,b)$ given in (C.2.15) and the single rotation $R(\theta)$ given in (C.2.16).

Because we know $S(a,b)$ acts trivially on the particle labels it follows that it must also act trivially on the labels $(\mu\nu)$. This means that $u^{\mu\nu}(\mathbf{k},\lambda)$ must be a zero eigenvector of the generators found by linearizing S in a and b, leading to the conditions

$$\mathcal{T}^\mu{}_\lambda u^{\lambda\nu}(\mathbf{k},\lambda) + \mathcal{T}^\nu{}_\lambda u^{\mu\lambda}(\mathbf{k},\lambda) = 0 \tag{16.1.4}$$

for both $\mathcal{T}_a = (\partial S/\partial a)_{a=b=0}$ and $\mathcal{T}_b = (\partial S/\partial b)_{a=b=0}$, which evaluate explicitly to

$$(\mathcal{T}_a)^\mu{}_\lambda = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad \text{and} \quad (\mathcal{T}_b)^\mu{}_\lambda = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{16.1.5}$$

Particle states with helicity λ similarly rotate by a phase $e^{i\lambda\theta}$ when acted on by $R(\theta)$, and so for helicity $\lambda = \pm 1$ the generator $\mathcal{T}_\theta = (\partial R/\partial\theta)_{\theta=0}$ must satisfy

$$(\mathcal{T}_\theta)^\mu{}_\lambda u^{\lambda\nu}(\mathbf{k},\lambda) + (\mathcal{T}_\theta)^\nu{}_\lambda u^{\mu\lambda}(\mathbf{k},\lambda) = i\lambda u^{\mu\nu}(\mathbf{k},\lambda) \tag{16.1.6}$$

with

$$(\mathcal{T}_\theta)^\mu{}_\lambda = \begin{pmatrix} 0 & 0\,0\,0 \\ 0 & 0\,1\,0 \\ 0 & -1\,0\,0 \\ 0 & 0\,0\,0 \end{pmatrix} . \tag{16.1.7}$$

Because $\mathcal{T}_a$ and $\mathcal{T}_b$ act only in the two dimensions (t and z) spanned by k^μ and $\mathcal{T}_\theta$ only acts in the other two dimensions (x and y) the solution to these conditions (unique up to normalization) can be written

$$u^{\mu\nu}(\mathbf{k},\lambda) = i\Big[k^\mu\, e^\nu(\lambda) - k^\nu\, e^\mu(\lambda)\Big]$$

$$\text{where} \quad k^\mu = \begin{pmatrix} \kappa \\ 0 \\ 0 \\ \kappa \end{pmatrix} \quad \text{and} \quad e^\mu(\lambda=\pm1) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ \pm i \\ 0 \end{pmatrix} . \tag{16.1.8}$$

The result in a general frame with particle 4-momentum p^μ is then defined by transforming to this frame using the specific transformation — given explicitly in (B.1.2) — that satisfies $L^\mu{}_\nu k^\nu = p^\mu$. The action of $L^\mu{}_\nu$ on $e^\nu(\lambda)$ can be inferred by writing $L = R\,B$ where a boost B along the z axis (to get the correct frequency for a photon moving along the z axis) is followed by a rotation R that takes the z axis to $\hat{\mathbf{p}}$ (the direction of motion for photon momentum p^μ). The boost has no effect because $e^\mu(\lambda)$ is perpendicular to the z axis, leading to $\epsilon^\mu(\hat{\mathbf{p}},\lambda) = R^\mu{}_\nu e^\nu(\lambda)$, in agreement with the polarization vectors found in earlier sections. Notice that these definitions together with the fact $k_\mu\, e^\mu(\lambda) = 0$ imply that

$$p_\mu \epsilon^\mu(\hat{\mathbf{p}},\lambda) = 0 \qquad \text{for all } \mathbf{p} \text{ and } \lambda\,. \tag{16.1.9}$$

The final result for the massless spin-one mode function is

$$u^{\mu\nu}(\mathbf{p},\lambda) = i\Big[p^\mu\, \epsilon^\nu(\hat{\mathbf{p}},\lambda) - p^\nu\, \epsilon^\mu(\hat{\mathbf{p}},\lambda)\Big]\,, \tag{16.1.10}$$

and so the field expansion (16.1.2) implies $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ with

$$A_\mu = \sum_{\lambda=\pm1} \int \frac{\mathrm{d}^3 p}{\sqrt{(2\pi)^3 2\omega_p}} \Big[\mathfrak{a}_{\mathbf{p}\lambda}\, \epsilon_\mu(\hat{\mathbf{p}},\lambda)\, e^{ip\cdot x} + \mathfrak{a}^\star_{\mathbf{p}\lambda}\, \epsilon^*_\mu(\hat{\mathbf{p}},\lambda)\, e^{-ip\cdot x}\Big]\,. \tag{16.1.11}$$

This returns the same expression that we've been using throughout these notes up to this point, but justifies it on more general grounds than did earlier treatments. As mentioned earlier, eq. (16.1.11) is not inconsistent with (16.1.1), despite this implying that $\lambda = \pm1$ massless particles cannot be represented by a 4-vector field – *i.e.* a field in the $(\frac{1}{2},\frac{1}{2})$ representation. They are not inconsistent because the quantity A_μ defined by (16.1.11) is only a 4-vector up to a gauge transformation, as in (11.3.24).

16.1.2 Photon propagator

We have seen how the matrix elements that arise within time-dependent perturbation theory necessarily involve evaluating the field propagator, or time-ordered autocorrelation function — see for example (12.4.13) and (15.7.1) for the spin-zero and spin-half counterparts. For photons this is defined by

$$\begin{aligned}\Delta_{\mu\nu}(x-y) &:= \langle 0|T\Big[A_\mu(x)\,A_\nu(y)\Big]|0\rangle \qquad (16.1.12)\\ &= \sum_{\lambda=\pm1}\int\frac{\mathrm{d}^3p}{(2\pi)^3 2\omega_p}\Big[\Theta(x^0-y^0)\,\epsilon_\mu(\hat{\mathbf{p}},\lambda)\epsilon^*_\nu(\hat{\mathbf{p}},\lambda)\,e^{ip\cdot(x-y)}+(x,\mu\leftrightarrow y,\nu)\Big]\\ &= \int\frac{\mathrm{d}^3p}{(2\pi)^3 2\omega_p}\Big[\Theta(x^0-y^0)\,e^{ip\cdot(x-y)}+\Theta(y^0-x^0)\,e^{-ip\cdot(x-y)}\Big]\hat{\Pi}_{\mu\nu}(\hat{\mathbf{p}})\end{aligned}$$

where T denotes time ordering and the second line evaluates the matrix element using (16.1.11) together with the usual commutation relations $[\mathfrak{a}_{\mathbf{p}\lambda},\mathfrak{a}^\star_{\mathbf{q}\xi}]=\delta_{\lambda\xi}\delta^3(\mathbf{p}-\mathbf{q})$. The last line defines the quantity $\hat{\Pi}_{\mu\nu}(\hat{\mathbf{p}}):=\sum_{\lambda=\pm1}\epsilon_\mu(\hat{\mathbf{p}},\lambda)\,\epsilon^*_\nu(\hat{\mathbf{p}},\lambda)$, which must now be evaluated.

The starting point is to evaluate $\hat{\Pi}_{\mu\nu}(\hat{\mathbf{k}})$ in the special frame for which $p^\mu\to k^\mu$ and $\epsilon^\mu(\hat{\mathbf{p}},\lambda)\to e^\mu(\lambda)$. In this case explicit evaluation using (16.1.8) leads to

$$\hat{\Pi}_{\mu\nu}(\hat{\mathbf{k}})=\sum_{\lambda=\pm1}e_\mu(\lambda)\,e^*_\nu(\lambda)=\sum_{\lambda=\pm1}\frac{1}{2}\begin{pmatrix}0\\1\\i\lambda\\0\end{pmatrix}\begin{pmatrix}0&1&-i\lambda&0\end{pmatrix}=\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&0\end{pmatrix}. \qquad (16.1.13)$$

Since the general frame is constructed from this by the rotation that takes the positive z axis to the $\hat{\mathbf{p}}$ direction, the result for $\hat{\Pi}_{\mu\nu}(\hat{\mathbf{p}})$ must be a covariant tensor under rotations built using the components of $\hat{\mathbf{p}}$ that agrees with (16.1.13) when $\hat{\mathbf{p}}=\mathbf{e}_z$ points up the positive z axis. The most general matrix with these properties is

$$\hat{\Pi}_{ij}(\hat{\mathbf{p}})=\delta_{ij}-\hat{p}_i\,\hat{p}_j\,,\quad \hat{\Pi}_{i0}(\hat{\mathbf{p}})=\hat{\Pi}_{0i}(\hat{\mathbf{p}})=\hat{\Pi}_{00}(\hat{\mathbf{p}})=0\,. \qquad (16.1.14)$$

This can be written in a covariant notation by writing

$$\hat{\Pi}_{\mu\nu}(\hat{\mathbf{p}})=\eta_{\mu\nu}+\frac{(n_\mu p_\nu+n_\nu p_\mu)p_0-p_\mu p_\nu}{|\mathbf{p}|^2}+\frac{p_\sigma p^\sigma}{|\mathbf{p}|^2}\,n_\mu n_\nu\,, \qquad (16.1.15)$$

where we define $n_\mu:=\delta^0_\mu$ and $p_\mu:=(p_0,\mathbf{p})$ with p_0 arbitrary (because it completely cancels out of the right-hand side). As usual $p^2:=p_\sigma p^\sigma=-p_0^2+\mathbf{p}^2$.

The first two terms in (16.1.15) are the ones needed in what follows, since they provide the covariant part of the propagator. Fourier transforming the step functions along the same lines followed in (12.4.15), and using the result in (16.1.12) leads to the following expression for the covariant part of the propagator

$$\Delta_{\mu\nu}(x-y)=-i\int\frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\frac{\Pi_{\mu\nu}(\bar{p})}{\bar{p}^2-i\delta}\,e^{i\bar{p}\cdot(x-y)}\quad\text{with}\quad\Pi_{\mu\nu}(\bar{p})=\eta_{\mu\nu}+\alpha_\mu\bar{p}_\nu+\alpha_\nu\bar{p}_\mu\,, \qquad (16.1.16)$$

where δ is a small positive infinitesimal and the bar on $\bar{p}^\mu$ emphasizes that its time component is a separate integration variable from its spatial part – unlike in (16.1.12), say, where $p^0 = \omega_p = |\mathbf{p}|$.

The $\eta_{\mu\nu}$ term of (16.1.16) really is manifestly covariant, and is the important one for most purposes. The second term involves α_μ, where α_μ can be read off from (16.1.15) and although α_μ is not covariant this doesn't really matter. It doesn't matter because we prove a theorem below – in §16.3 – that shows that the underlying gauge invariance (and the associated conservation of charge) ensures that the $\alpha_\mu p_\nu + \alpha_\nu p_\mu$ term completely cancels out of all physical scattering amplitudes.

Because α_μ ultimately drops out of physical results, it can be convenient to choose it to be different than the definition that follows directly from (16.1.15). In particular, choosing $\alpha_\mu \propto \bar{p}_\mu$ allows Lorentz covariance to be made manifest in intermediate steps in calculations. Two common choices along these lines are $\alpha_\mu = 0$ or $\alpha_\mu = -\bar{p}_\mu/(2\bar{p}^2)$, for which

$$\begin{aligned} &\Pi_{\mu\nu}(\bar{p}) = \eta_{\mu\nu} && \text{(Feynman gauge)} \\ \text{or}\quad &\Pi_{\mu\nu}(\bar{p}) = \eta_{\mu\nu} - \frac{\bar{p}_\mu \bar{p}_\nu}{\bar{p}^2} && \text{(Landau gauge).} \end{aligned} \tag{16.1.17}$$

What about the not-at-all covariant $n_\mu n_\nu$ term in (16.1.15)? How does this contribute? Using this in (16.1.12) leads to the very non-covariant expression

$$\begin{aligned} \Delta^C_{\mu\nu}(x-y) &= -i\, n_\mu n_\nu \int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4} \frac{e^{i\bar{p}\cdot(x-y)}}{\bar{p}^2 - i\delta} \frac{\bar{p}^2}{|\mathbf{p}|^2} \\ &= -i\, n_\mu n_\nu\, \delta(x^0 - y^0) \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{|\mathbf{p}|^2} \\ &= -i\, n_\mu n_\nu \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\, \delta(x^0 - y^0)\,. \end{aligned} \tag{16.1.18}$$

Although this is not local it resembles the Coulomb potential inasmuch as it varies inversely with distance and acts instantaneously at a common time. In a story much like the cancellation between non-covariant interactions and Schwinger terms with derivative interactions, encountered earlier in §12.5, the non-covariance of $\Delta^C_{\mu\nu}$ goes through and systematically cancels out the noncovariant terms in the interaction Hamiltonian found using canonical methods.

To see how this cancellation works recall that canonical methods gave the interaction Hamiltonian (13.4.16) involving both a covariant $J^\mu A_\mu$ type interaction plus a noncovariant term, of the form

$$\begin{aligned} H_{\text{int}} &= \int \mathrm{d}^3 x \left(-J^\mu A_\mu + \frac{1}{2}\rho\,\phi \right) \\ &= -\int \mathrm{d}^3 x\, J^\mu A_\mu + \frac{1}{8\pi} \int \mathrm{d}^3 x \int \mathrm{d}^3 y\, \frac{J^0(\mathbf{x}, x^0)\, J^0(\mathbf{y}, x^0)}{|\mathbf{x}-\mathbf{y}|}\,. \end{aligned} \tag{16.1.19}$$

Suppose we consider J^μ to be a specified classical current (that consistency requires must be conserved $\partial_\mu J^\mu = 0$). Then the noncovariant terms quadratic in J^μ in the vacuum matrix element of the expansion (3.2.22),

$$\mathcal{S} = I - i\int \mathrm{d}^4x\; \mathcal{H}_{\rm int}(x) + \frac{1}{2}(-i)^2 \int \mathrm{d}^4x\, \mathrm{d}^4y\; T\Big[\mathcal{H}_{\rm int}(x)\,\mathcal{H}_{\rm int}(y)\Big] + \cdots\,, \tag{16.1.20}$$

receive a contribution at second order

$$\frac{1}{2}\,(-i)^2 \int \mathrm{d}^4x\, \mathrm{d}^4y\; J^\mu(x)\,\Delta^C_{\mu\nu}(x-y)\,J^\nu(y) = +\frac{i}{8\pi}\int \mathrm{d}^3x\, \mathrm{d}^3y\; \frac{J^0(\mathbf{x},x^0)\,J^0(\mathbf{y},x^0)}{|\mathbf{x}-\mathbf{y}|}\,, \tag{16.1.21}$$

from the noncovariant part of the propagator, where the last equality uses (16.1.18).

As advertised, eq. (16.1.21) precisely cancels the first-order contribution to (16.1.20) coming from the Coulomb interaction of (16.1.19). It is *as if* we could just use $\mathcal{H}_{\rm int} = -\mathcal{L}_{\rm int}$ inferred from (13.4.8) when computing scattering amplitudes, and at the same time simply drop the noncovariant piece $\Delta^C_{\mu\nu}$, keeping only the covariant propagator of (16.1.16).

The ugliness of this prescription cries out for a more manifestly covariant way to organize calculations. It drives home again that manifest covariance is subtle when perturbation theory is framed using Hamiltonians. Although canonical methods efficiently generate the noncovariant terms in $H_{\rm int}$ required to cancel noncovariant terms in time-ordered propagators, the very need for these cancellations is an abomination.

These observations are the core motivation for the path integral techniques described in §21, for which it is the Lorentz-invariant action $S = \int \mathrm{d}^4x\,\mathcal{L}$ that plays a starring role, rather than the intrinsically non-covariant Hamiltonian. Until then we compute using a covariant interaction and keeping only the covariant propagator (16.1.16).

16.2 Action and Feynman rules

The next step is to identify how relativistic spin-half particles, described by a 4-component Dirac spinor $\psi(x)$, can couple to the electromagnetic field $A_\mu(x)$. To keep things as covariant as possible we do so using the canonical framework, building an action $S = \int \mathrm{d}^4x\,\mathcal{L}$ with lagrangian density $\mathcal{L}(\psi, \overline{\psi}, \partial_\mu\psi, \partial_\mu\overline{\psi}, A_\mu, \partial_\nu A_\mu)$ that respects all of the symmetries we know experimentally hold for the electromagnetic interactions: Poincaré invariance, gauge invariance, parity invariance, charge conjugation invariance, and so on.

16.2.1 QED action

For the non-interacting lagrangian density for the spin-half particles we use the Dirac lagragian density (15.6.6), which is repeated here for convenience of reference:

$$\mathcal{L} = -\overline{\psi}\Big(\not{\partial} + m\Big)\psi\,. \tag{16.2.1}$$

This lagrangian has a symmetry $\psi \to e^{i\zeta}\psi$ where ζ is an arbitrary real parameter, and as a result the non-interacting field equation implies a conservation law (compare to (11.1.29)):

$$\Big(\not\partial + m\Big)\psi = 0 \quad \text{implies} \quad \partial_\mu\Big(\overline{\psi}\,\gamma^\mu\psi\Big) = 0\,. \tag{16.2.2}$$

Coupling to electromagnetism is now accomplished in the usual way, by promoting the ordinary derivative $\partial_\mu\psi$ to the covariant one

$$D_\mu\psi := \partial_\mu\psi + ieA_\mu\psi \qquad (\text{for charge } q = -e)\,, \tag{16.2.3}$$

and including the lagrangian (13.4.1) for free electromagnetic fields, written in terms of the manifestly Lorentz covariant fields $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. This leads to the defining lagrangian density for *Quantum Electrodynamics* (or QED for short):

$$\begin{aligned}\mathcal{L}_{QED} &= -\frac{1}{4}\,F_{\mu\nu}F^{\mu\nu} - \overline{\psi}\Big(\not D + m\Big)\psi \\ &= -\frac{1}{4}\,F_{\mu\nu}F^{\mu\nu} - \overline{\psi}\Big(\not\partial + m\Big)\psi - ie\,(\overline{\psi}\gamma^\mu\psi)\,A_\mu\,.\end{aligned} \tag{16.2.4}$$

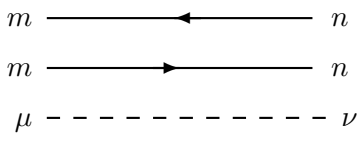
Notice that because the last, or interaction, term in (16.2.4) is linear in A_μ it falls into the class of theories given in (13.4.8) whose canonical quantization leads to (13.4.10). This includes in particular the Coulomb interaction whose Lorentz-non-covariant effects in scattering amplitudes cancel those of the non-covariant propagator $\Delta^C_{\mu\nu}$ (as described above). Because of this – and anticipating the results of the path-integral derivation of §21 – we now state the Feynman rules for QED assuming the propagator takes the covariant form (without the $\Delta^C_{\mu\nu}$ term) given in (16.1.16), and with the interaction Hamiltonian density taken to be

$$\mathcal{H}_{\text{int}} = -\mathcal{L}_{\text{int}} = ie\,(\overline{\psi}\gamma^\mu\psi)\,A_\mu\,. \tag{16.2.5}$$

16.2.2 Covariant Feynman rules

Perturbative predictions are made for QED by using (16.2.5) in standard perturbative expressions – like (6.1.6) for the S-matrix – and evaluating matrix elements of creation and annihilation operators in the usual way. This can be expressed as graphical Feynman rules along the lines initially explained for spinless particles (*c.f.* §12.4) and spin-half particles (*c.f.* §15.7), as is now briefly summarized.

For QED we draw a solid line to represent fermion flow (with an arrow denoting the direction of fermion-number flow) and draw a dashed line for photon propagation, with ends labelled by either Dirac matrix indices m, n or 4-vector indices μ, ν (see Fig. 16.2.6).



(fermion line)

(antifermion line).

(photon line).

External photon lines: An external line that directly connects an initial-state photon creation operator $\mathfrak{a}^\star_{\mathbf{q}\lambda}$ to an $\mathfrak{a}_{\mathbf{p}\xi}$ appearing inside an interaction-picture field $A_\mu(x_1)$ contributes the Feynman rule (using photon dispersion relation $\omega(k) = |\mathbf{k}|$):

$$x\,\mu \;\bullet\!\!-\!-\!-\!-\!-\!-\;\; \mathbf{q}\,\lambda \tag{16.2.6}$$

$$\sum_\xi \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\omega(p)}}\,\epsilon_\mu(\hat{\mathbf{p}},\xi)\,e^{ip\cdot x_1}\delta_{\lambda\xi}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{iq\cdot x_1}}{\sqrt{(2\pi)^3 2\omega(q)}}\,\epsilon_\mu(\hat{\mathbf{q}},\lambda) \quad \text{(incoming photon)}. \tag{16.2.7}$$

An $\mathfrak{a}_{\mathbf{q}\lambda}$ in the final state pairing with $\mathfrak{a}^\star_{\mathbf{p}\lambda}$ contained in $A_\mu(x_1)$ similarly gives

$$\mathbf{q}\,\lambda \;\;-\!-\!-\!-\!-\!-\!\bullet\; x\,\mu \tag{16.2.8}$$

$$\sum_\xi \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\omega(p)}}\,\epsilon^*_\mu(\hat{\mathbf{p}},\xi)\,e^{-ip\cdot x_1}\delta_{\lambda\xi}\delta^3(\mathbf{p}-\mathbf{q}) = \frac{e^{-iq\cdot x_1}}{\sqrt{(2\pi)^3 2\omega(q)}}\,\epsilon^*_\mu(\hat{\mathbf{q}},\lambda) \quad \text{(outgoing photon)}\,. \tag{16.2.9}$$

Internal photon lines: When a contraction takes place between creation and annihilation operators that are both associated with a vertex one gets the (covariant part of the) propagator $\Delta_{\mu\nu}(x-y)$ of (16.1.16), given explicitly by

$$x\,\mu \bullet\!\!-\!-\!-\!-\!-\!-\!-\!-\!-\!-\!\bullet\, y\,\nu$$

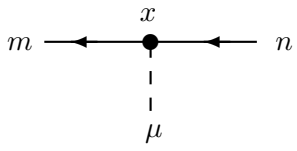
$$\langle 0|T\Big[A_\mu(x)\,A_\nu(y)\Big]|0\rangle = -i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{\Pi_{\mu\nu}(\bar{p})}{\bar{p}^2+m^2-i\bar{\delta}}\right]_{mn} e^{i\bar{p}\cdot(x-y)}\,, \tag{16.2.10}$$

with

$$\Pi_{\mu\nu}(p) = \eta_{\mu\nu} + \alpha_\mu\,p_\nu + \alpha_\nu\,p_\mu\,, \tag{16.2.11}$$

with α_μ arbitrary (since it drops out of physical amplitudes – see next section).

Interaction vertices: There is only one type of interaction vertex in QED, at which two fermion and one photon line meet. The Feynman rule associated with the vertex expresses all of the constants appearing in the interaction contained in $-i\mathcal{H}_{\rm int} = i\mathcal{L}_{\rm int}$ that the vertex represents. For the interaction (16.2.5) located at position x^μ the Feynman rule is



$$\Big(e\gamma^\mu\Big)_{mn}\int \mathrm{d}^4x\,, \tag{16.2.12}$$

where the index n is contracted with the incoming fermion line, the index m is contracted with the outgoing fermion line and the index μ is contracted with the photon line. Each

vertex comes associated with a position, corresponding to the position at which $\mathcal{H}_{\rm int}(x)$ is evaluated, and the positions of all vertices are integrated.

To these must be added the same coefficients described in previous discussions of Feynman rules:

- Divide by $N!$ where N is the number of vertices in the graph.
- Multiply any sign factors associated with permuting the position of two fermionic operators.
- Multiply by any symmetry factors, as described in §12.4.

16.2.3 Momentum-space Feynman rules

As in previous sections the momentum-space Feynman rules are obtained by performing the integration over the positions x_i^μ for all the vertices, which is possible because the only position dependence appears within exponentials. The result is a series of delta-functions that express the conservation of 4-momentum at each vertex. The resulting momentum-space Feynman rules for photon lines therefore are

External photon lines: contribute

μ ●- - - - - - $\mathbf{q}\,\lambda$

$$\frac{1}{\sqrt{(2\pi)^3 2\omega(q)}}\,\epsilon_\mu(\hat{\mathbf{q}},\lambda) \quad \text{(incoming photon).} \tag{16.2.13}$$

and

$\mathbf{q}\,\lambda$ - - - - - -● μ

$$\frac{1}{\sqrt{(2\pi)^3 2\omega(q)}}\,\epsilon^*_\mu(\hat{\mathbf{q}},\lambda) \quad \text{(outgoing photon).} \tag{16.2.14}$$

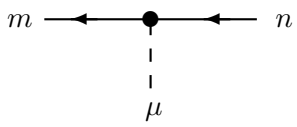
Internal photon lines: The momentum space formulation for an internal photon line becomes

μ ●- - - - - - - - - - -● ν

$$-i\int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4}\left[\frac{\eta_{\mu\nu}+\alpha_\mu\,p_\nu+\alpha_\nu\,p_\mu}{\bar{p}^2+m^2-i\bar{\delta}}\right], \tag{16.2.15}$$

where the indices μ and ν get contracted with the corresponding index for the vertex at which the line ends.

Vertices: The momentum space formulation for the QED vertex performs the integral over vertex position to get the delta function that expresses 4-momentum conservation:



$$\Big(e\gamma^\mu\Big)_{mn}(2\pi)^4\delta^4(p+q+k)\,, \tag{16.2.16}$$

where p^μ, q^μ and k^μ are the momenta flowing in through each of the three lines in the vertex, with the convention that all momentum point into the vertex.

With these rules the effects of electromagnetic photon-fermion interactions can (in principle) be pursued systematically to any perturbative order.

16.2.4 Validity of the expansion

As always when using perturbation theory, the first question is: What justifies its use? Naively, for QED the answer seems simple: the only interaction is proportional to the magnitude of the electron charge, e, and so the justification must be that $e \ll 1$. This is partially correct, but for the electron the physically relevant value of e turns out to be $e \simeq 0.303$, which is not actually that small. If this were the whole story we'd expect that neglecting the next term in an expansion in e could represent a 30% error in any prediction.

In reality the expansion is much better than this, because successive terms are proportional to

$$\Big(\frac{e}{4\pi}\Big)^2 = \frac{e^2}{16\pi^2} = \frac{\alpha}{4\pi} \simeq 5.81\times 10^{-4}\,, \tag{16.2.17}$$

where (as in earlier chapters) $\alpha := e^2/(4\pi) \simeq 1/137$ is the fine-structure constant (as measured from properties of low-energy systems, like those of atomic or condensed matter physics). The goal of this section is to justify the claim that this is the expansion parameter, and to identify which Feynman graphs contribute at any given order in it. The above claim shows that it will be important in practice to keep track of the powers of 2π when doing so.

To this end consider computing a scattering process that involves a total of E initial and final state particles. Any Feynman graph contributing to this process must have E external legs. There is no loss of generality in restricting to *connected* graphs (for which it is possible to get from any vertex to any other by walking along the lines in the graph), since the disconnected ones are just products of connected ones. Let us focus on a specific connected graph contributing to this process (it doesn't matter which one), and call the number of vertices in this graph V and the total number of internal lines I. Finally, denote the amplitude obtained by evaluating the graph as $\mathcal{A}_E$.

The goal is to count the powers of e and 2π appearing in $\mathcal{A}_E$ that are implied by the momentum-space Feynman rules, given that the graph is built using only the QED vertices and propagators described above. We do not count factors of 2π associated with the Feynman rules for external lines because these will be the same for all graphs that contribute to any particular scattering process. In every graph each of these factors come from one of three sources:

- Each vertex contributes a factor of $(2\pi)^4$ and a factor of e – see (16.2.16).
- Each internal line contributes a factor of $1/(2\pi)^4$ – see (15.7.18) and (16.2.15) – and an instruction to integrate over the 4-momentum p^μ flowing through the line.
- Some of the integrals over momenta are evaluated using the momentum-conserving delta functions at each vertex, but the angular part of each integral that is not evaluated this way contributes factors of 2π. This would be a factor of 4π solid angle if we were integrating only over three-dimensional vectors like $\mathbf{p}$, but for integrations over 4-vectors the corresponding estimate turns out to be half the surface area of a unit sphere embedded in four dimensions,[56] which turns out to be π^2.

To count the 2π's coming from angular integrations requires knowing how many of the integrals can instead be evaluated using the momentum-conserving delta functions. All told we know there is an integration over the 4-momentum for each internal line and we know that there is a delta function for each vertex, so the naive answer is that there are $I - V$ integrals with angular integrals contributing factors of π^2. But this is naive because we also know that one combination of delta functions expresses overall conservation of 4-momentum for the external momenta that flow into and out of the whole graph. Since this depends only on the *external* momenta it cannot be used to perform any integrals over the 4-momenta flowing through internal lines. Therefore only $V - 1$ delta functions can be used to perform internal momentum integrations, and so the total number of integrals contributing a factor π^2 is

$$L = I - V + 1\,. \tag{16.2.18}$$

The left-hand side of eq. (16.2.18) is labelled 'L' because this combination of I and V counts the number of 'loops' in a graph (draw some graphs and see).[57] The total number of factors of 2π and e appearing in our graph therefore is

$$\mathcal{A}_E \propto \left[\frac{1}{(2\pi)^4}\right]^I \left[e\,(2\pi)^4\right]^V \left(\pi^2\right)^L . \tag{16.2.19}$$

The estimate (16.2.19) can be simplified because the information that all graphs are drawn using the vertex (16.2.16) implies that E, V and I are not independent of one another. The relation between them can be expressed as the rule of 'conservation of ends', which states that the total number of ends of lines in a graph can be counted in two equivalent ways. Since all lines end on a vertex and three lines meet at the only vertex in our problem, the total

[56] Strictly speaking this is true for 4-vectors in Euclidian space, with metric $g_{\mu\nu} = \mathrm{diag}(+\,+\,+\,+)$, but as we see below the same result also applies for integrations over Minkowski-signature spaces, with metric $\eta_{\mu\nu} = \mathrm{diag}(-\,+\,+\,+)$, as well.

[57] For graphs that can be drawn on a piece of paper it happens that the number of loops, lines and vertices always satisfies $L - I + V = 1$ because this is a topological invariant. For graphs that cannot be drawn on a plane (16.2.18) is the *definition* of the number of loops.

number of ends must be $3V$. But it is also true that each internal line has two ends and each external line has one, so

$$3V = 2I + E \qquad \text{(conservation of ends)}. \tag{16.2.20}$$

Eqs. (16.2.18) and (16.2.20) can be used to eliminate I and V in terms of E and L,

$$I = E + 3L - 3 \quad \text{and} \quad V = E + 2L - 2\,, \tag{16.2.21}$$

and once this used (16.2.19) becomes

$$\mathcal{A}_E \propto (2\pi)^4\, e^E \left(\frac{e^2}{16\pi^2}\right)^L . \tag{16.2.22}$$

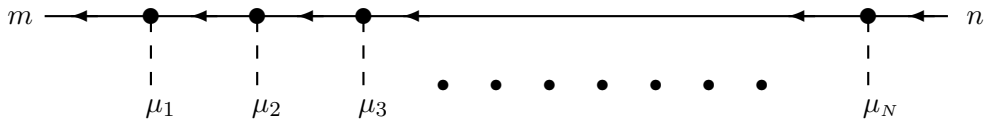
Besides justifying the statement that perturbation theory generates a series in powers of $(e/4\pi)^2$, (16.2.22) also tells us that processes with more external lines are suppressed by at least one power of e appearing in $\mathcal{A}_E$ for every external line. For fixed E it is the number of loops in a graph that controls how suppressed that graph's contribution is to $\mathcal{A}_E$. Furthermore *all* graphs with the same number of loops are equally important at any given order in this expansion. Because of this the perturbative expansion in QED is also often known as the *loop expansion*. The least suppressed (and so leading) contribution for any E has $L = 0$, and these graphs are called *tree* graphs.

16.3 Ward identities

Before using the above rules (or, equivalently, directly evaluating the expectaton of $\mathcal{S}$ between initial and final states) this section pauses to show why the term $\alpha_\mu\, p_\nu + \alpha_\nu\, p_\mu$ in the photon propagator (16.2.15) does not contribute to physical amplitudes. The physical reason for this is that the lagrangian (16.2.4) shows that photons couple to the conserved Dirac current (16.2.2): $\mathcal{L}_{\rm int} \propto J^\mu A_\mu$ with $\partial_\mu J^\mu = 0$. In momentum space conservation implies $p_\mu J^\mu(p) = 0$ and so it is the appearance of the p_μ's in $\alpha_\mu\, p_\nu + \alpha_\nu\, p_\mu$ that make it drop out of physical amplitudes.

This discussion appears in a section titled 'Ward identities' because for operators current conservation $\partial_\mu J^\mu = 0$ implies conditions on correlation functions, like $\langle 0|T[J^\mu(x)\, J^\nu(y)]|0\rangle$ or $\langle 0|T[\psi(x)\, J^\mu(y)\, \overline{\psi}(z)]|0\rangle$, and these conditions satisfied by correlation functions are called Ward identities. Just like current conservation itself, they ultimately have their roots in symmetries (in this case gauge invariance), as is explored in more detail in §18.2 below. The identity proven in this section is a special case of one of these more general symmetry relations.

To see in more detail how $p_\mu J^\mu(p) = 0$ shows up in explicit calculations consider a Feynman graph and focus on a particular fermion line that appears in this graph. Suppose this line has N photon lines attached to it, so the contribution to the graph associated with this line is labelled by the Dirac matrix labels m, n (one for each end of the fermion line) and vector indices μ_i with $i = 1, \ldots, N$ (one for each vertex).



Suppose the 4-momentum flowing in at each photon line is denoted k_i^μ and the momentum flowing out of the left-hand end of the fermion line is p^μ. Then the Feynman rule for the Dirac matrices along this fermion line contribute the following factor to the graph:

$$\mathcal{M}^{\mu_1\mu_2\cdots\mu_N}_{mn} = \Big[\gamma^{\mu_1} S(p-k_1)\gamma^{\mu_2} S(p-k_1-k_2)\gamma^{\mu_3}\cdots\gamma^{\mu_{N-1}} S(p-k_1-\cdots-k_{N-1})\gamma^{\mu_N}\Big]_{mn} \tag{16.3.1}$$

where

$$S(p) := \frac{-i\not{p}+m}{p^2+m^2-i\delta} = (i\not{p}+m)^{-1}\,. \tag{16.3.2}$$

It could be that this line goes right through the graph, in which case the final ends would be external lines and the initial and final Dirac spinor labels (n,m) would be contracted with the spinors describing the corresponding initial and final state fermions to give, say, $\overline{\mathbf{u}}\,\mathcal{M}^{\mu_1\mu_2\cdots\mu_N}\mathbf{u}$. But it could also be true that this line closes on itself to form a loop, in which case we would set $n=m$ and sum over n to give Tr $[\mathcal{M}^{\mu_1\mu_2\cdots\mu_N}]$. No other options are possible because there are no vertices in QED on which a fermion line ends.

We now imagine attaching an $N+1$th photon to this line where the new photon momentum is q^ν. The complete amplitude will contain a sum over all the possible places on the line to which this new photon could attach, so the new amplitude becomes

$$\begin{aligned}\mathcal{N}^{\nu\mu_1\mu_2\cdots\mu_N}_{mn} \;=\; &\Big[\gamma^\nu S(p-q)\gamma^{\mu_1}\cdots\gamma^{\mu_{N-1}} S(p-q-k_1-\cdots-k_{N-1})\gamma^{\mu_N}\Big]_{mn}\\ &+\Big[\gamma^{\mu_1} S(p-k_1)\gamma^\nu S(p-q-k_1)\cdots\gamma^{\mu_{N-1}} S(p-q-\cdots-k_{N-1})\gamma^{\mu_N}\Big]_{mn}\\ &\qquad\vdots\\ &+\Big[\gamma^{\mu_1} S(p-k_1)\cdots\gamma^{\mu_N} S(p-q-\cdots-k_N)\gamma^\nu\Big]_{mn}\,.\end{aligned} \tag{16.3.3}$$

The claim to be proven is that the sum of these amplitudes vanishes once contracted with q_ν, so it suffices to keep only the $\eta_{\mu\nu}$ term in the propagator of the photon being added. Showing this to be true for arbitrary N then allows an inductive proof to be developed for why the $\alpha_\mu\, p_\nu + \alpha_\nu\, p_\mu$ terms always drop out of physical amplitudes.

To this end contract (16.3.3) with q_ν, which introduces a factor of $\not{q}$ at various points along the fermion line, and use

$$\begin{aligned}\text{in the 1st line:}\quad i\not{q} &= \Big(i\not{p}+m\Big) - \Big[i(\not{p}-\not{q})+m\Big]\\ &= S^{-1}(p) - S^{-1}(p-q)\\ \text{in the 2nd line:}\quad i\not{q} &= \Big[i(\not{p}-\not{k}_1)+m\Big] - \Big[i(\not{p}-\not{q}-\not{k}_1)+m\Big)\\ &= S^{-1}(p-k_1) - S^{-1}(p-q-k_1)\,,\end{aligned} \tag{16.3.4}$$

and so on for each line in (16.3.3). With this substitute the first line of (16.3.3) contributes

$$iq_\nu \mathcal{N}^{\nu\mu_1\cdots\mu_N}\Big|_{\rm 1st} = \Big[(i\not{p}+m)S(p-q)\gamma^{\mu_1}S(p-q-k_1)\gamma^{\mu_2}\cdots\gamma^{\mu_N}\Big]_{mn} - \Big[\gamma^{\mu_1}S(p-q-k_1)\gamma^{\mu_2}S(p-q-k_1-k_2)\cdots\gamma^{\mu_N}\Big]_{mn}, \tag{16.3.5}$$

while the second line becomes

$$iq_\nu \mathcal{N}^{\nu\mu_1\cdots\mu_N}\Big|_{\rm 1st} = \Big[\gamma^{\mu_1}S(p-q-k_1)\gamma^{\mu_2}S(p-q-k_1-k_2)\cdots\gamma^{\mu_N}\Big]_{mn} - \Big[\gamma^{\mu_1}S(p-k_1)\gamma^{\mu_2}S(p-q-k_1-k_2)\cdots\gamma^{\mu_N}\Big]_{mn}, \tag{16.3.6}$$

and so on. Notice how the second line of (16.3.5) cancels the first line of (16.3.6). A similar cancellation also occurs between the second line and third lines of (16.3.3) and the third and the fourth and so on, leaving only two uncancelled contributions:

$$iq_\nu \mathcal{N}^{\nu\mu_1\mu_2\cdots\mu_N}_{mn} = \Big[(i\not{p}+m)S(p-q)\gamma^{\mu_1}S(p-q-k_1)\gamma^{\mu_2}\cdots\gamma^{\mu_N}\Big]_{mn} - \Big[\gamma^{\mu_1}S(p-k_1)\gamma^{\mu_2}\cdots\gamma^{\mu_N}(i\not{p}'+m)\Big]_{mn}, \tag{16.3.7}$$

where $p' := p - k_1 - k_2 \cdots - k_N$ is the 4-momentum that enters the fermion line from the far right.

Now comes the main point. If the initial fermion line is a closed loop, and so contributes Tr $[\mathcal{M}^{\mu_1\cdots\mu_N}]$ to the Feynman graph, then the momentum entering from the right is the same as the momentum that leaving from the left: $p' = p$. Because of this the two terms in (16.3.7) cancel one another because of the cyclic property of the trace:

$$iq_\nu \text{Tr}\ [\mathcal{N}^{\nu\mu_1\cdots\mu_N}] = 0\,. \tag{16.3.8}$$

Suppose, on the other hand, the two ends of the fermion line are external lines and so the line contributes $\overline{\mathbf{u}}(p)\mathcal{M}^{\mu_1\cdots\mu_N}\mathbf{u}(p')$ to the amplitude. The result again vanishes once contracted with q_ν because both terms in (16.3.7) separately give zero. They give zero because the external spinors satisfy (*c.f.* eq. (15.2.26))

$$\Big(i\not{p}' + m\Big)\mathbf{u}(\mathbf{p}') = \overline{\mathbf{u}}(\mathbf{p})\Big(i\not{p} + m\Big) = 0\,. \tag{16.3.9}$$

Imagine now introducing a new photon propagator to any Feynman graph. The two ends of this propagator must end at a fermion line (possibly the same one) through the vertex (16.2.16), and the complete amplitude is the sum over all of the possible ways this attachment can be done. The piece of the propagator involving $\alpha_\mu\, q_\nu + \alpha_\nu\, q_\mu$ necessarily has a contraction of the type found to vanish above for one of these fermion lines or the other. It therefore drops out once one sums over all of the ways of connecting to the fermion lines. We henceforth ignore these terms when computing physical amplitudes.

16.4 Compton scattering

With the above preliminaries in place we can use the Feynman rules (or take matrix elements of the interaction lagrangian) to compute physical processes. This section does so for two practical examples: electron-photon (Compton) scattering, and electron-positron pair production. Besides being of practical interest in their own right, these illustrate the use of the Feynman rules for both fermions and antifermions.

We start with the scattering of photons with relativistic electrons (Compton scattering):

$$e^-(\mathbf{p},\sigma) + \gamma(\mathbf{q},\lambda) \to e^-(\mathbf{p}',\sigma') + \gamma(\mathbf{q}',\lambda')\,. \tag{16.4.1}$$

The power-counting estimate (16.2.22) applies (with $E = 4$) and so the leading contribution to the amplitude arises proportional to e^4, and this comes from tree graphs with two external electron and two external photon legs.

There are two steps for computing the cross section for Compton scattering: calculating the S-matrix element $\langle\beta|\mathcal{S}|\alpha\rangle$, whose general form is

$$\langle e^-(\mathbf{p}'),\gamma(\mathbf{q}')|\mathcal{S}|e^-(\mathbf{p}),\gamma(\mathbf{q})\rangle = -2\pi i\,\mathcal{M}_C\,\delta^4(p+q-p'-q')\,, \tag{16.4.2}$$

where the reduced matrix element $\mathcal{M}_C$ is to be computed using the Feynman rules. Once $\mathcal{M}_C$ is known then we follow the steps of §4.3 or §9.4 to compute the cross section.

Kinematics and phase space

Recall that for two-body scattering of the form $A+B \to A'+B'$, the differential cross section implied by $\mathcal{M}_C$ is given by dividing the reaction rate by the initial flux as in (4.3.11). In the relativistic case it is useful to define the flux in such a way that it agrees with (4.3.11) in the rest frame of A or B, and that the cross section takes the same value in any Lorentz frame. Once this is done the relativistic differential cross section is given by

$$\mathrm{d}\sigma = \frac{(2\pi)^4|\mathcal{M}_C|^2}{u}\,\delta^4(p+q-p'-q')\,\mathrm{d}^3\mathbf{p}'\,\mathrm{d}^3\mathbf{q}'\,, \tag{16.4.3}$$

with

$$u := \frac{1}{q^0p^0}\,\sqrt{(p\cdot q)^2 - m_A^2m_B^2}\,, \tag{16.4.4}$$

where m_A and m_B are the masses of the initial-state particles, where the energies are $\varepsilon = p^0 = \sqrt{\mathbf{p}^2+m_A^2}$ and $\omega = q^0 = \sqrt{\mathbf{q}^2+m_B^2}$. For the electron-photon scattering of interest here, this implies we take $m_A = m$ to be the electron mass and $m_B = 0$.

The dependence on the final-state momenta (phase space factors) in (16.4.3) can be simplified if we use the delta function to perform all of the final state integrals except for the integration over the solid angle for the final-state photon: $\mathrm{d}\Omega$. Conservation of energy and momentum then imply the final-state phase space integrals simplify to

$$\delta^4(p+q-p'-q')\,\mathrm{d}^3p'\,\mathrm{d}^3q' = \frac{|\mathbf{q}'|^2}{\hat{\mathbf{q}}'\cdot[(\mathbf{q}'/\omega')-(\mathbf{p}'/\varepsilon')]}\,\mathrm{d}\Omega\,, \tag{16.4.5}$$

where $\hat{\mathbf{q}}'$ is the unit vector in the $\mathbf{q}'$ direction while $\varepsilon' = (p^0)' = \sqrt{|\mathbf{p}'|^2 + m^2}$ and $\omega' = (q^0)' = |\mathbf{q}'|$, and $\mathrm{d}\Omega = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$ if we use polar coordinates for which the initial photon momentum $\mathbf{q}$ is chosen to point in the positive z direction, so $\hat{\mathbf{q}} \cdot \hat{\mathbf{q}}' = \cos\theta$.

Specializing to the rest frame of the initial electron we have $\mathbf{p} = 0$ and $\varepsilon = m$ and so (16.4.4) implies $u = 1$. In this case energy and momentum conservation imply

$$\mathbf{p}' = \mathbf{q} - \mathbf{q}' \quad \text{and} \quad m + \omega = \omega' + \sqrt{(\mathbf{q} - \mathbf{q}')^2 + m^2}\,, \tag{16.4.6}$$

which once solved for ω' gives

$$\omega' = \frac{\omega}{1 + (\omega/m)(1 - \cos\theta)}\,. \tag{16.4.7}$$

Using this (16.4.5) further simplifies to

$$\delta^4(p + q - p' - q')\,\mathrm{d}^3p'\,\mathrm{d}^3q' = \frac{(\omega')^3(m + \omega - \omega')}{m\omega}\,\mathrm{d}\Omega\,, \tag{16.4.8}$$

and so the differential cross section for Compton scattering finally becomes

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = (2\pi)^4 \frac{(\omega')^3(m + \omega - \omega')}{m\omega}\,\Big|\mathcal{M}_C\Big|^2\,. \tag{16.4.9}$$

It remains to compute the required S-matrix element to obtain $\mathcal{M}_C$.

Worked example: Compton matrix element

Now comes the main event: evaluating the S-matrix element using the Feynman rules. The first step is to draw all possible relevant graphs. The Feynman rules for QED allow only two possible connected tree graphs that can contribute to the reaction (16.4.1):

The next step is to evaluate these graphs (and thereby also illustrate the use of the Feynman rules). Denoting $S_C := \langle e^-\gamma|\mathcal{S}|e^-\gamma\rangle$, direct application of the rules for external lines and fermion propagators gives, for the right-hand graph

$$\begin{aligned} S_C^{\text{right}} &= 2 \times \left[\frac{1}{2!}\right]\left[\frac{\epsilon_\mu(k)}{(2\pi)^{3/2}\sqrt{2\omega}}\right]\left[\frac{\epsilon^*_\nu(k')}{(2\pi)^{3/2}\sqrt{2\omega'}}\right]\int \frac{\mathrm{d}^4k}{(2\pi)^4 i}\Big[e\,(2\pi)^4\delta^4(k - p - q)\Big] \\ &\qquad \times \Big[e\,(2\pi)^4\delta^4(k - p' - q')\Big]\frac{\overline{\mathbf{u}}(p')}{(2\pi)^{3/2}}\gamma^\nu\left[\frac{-i\not{k} + m}{k^2 + m^2 - i\delta}\right]\gamma^\mu\left[\frac{\mathbf{u}(p)}{(2\pi)^{3/2}}\right] \\ &= -i(2\pi)^4\delta^4(p + q - p' - q')\left[\frac{e^2}{2(2\pi)^6\sqrt{\omega\omega'}}\,\frac{\overline{\mathbf{u}}(p')\gamma^\nu[-i(\not{p} + \not{q}) + m]\gamma^\mu\mathbf{u}(p)}{(p + q)^2 + m^2 - i\delta}\right]. \end{aligned} \tag{16.4.10}$$

Here the propagator and external-line factors are precisely those listed above. The initial factor of 2 is the symmetry factor: there are two ways vertices the first photon can connect to, after which

the graph is uniquely set. The factor of $1/2!$ comes from the $1/n!$ in the expression for the S-matrix (6.1.6). The vertex factor is as given in (16.2.12), which is the coefficient of $-i\mathcal{H}_{\rm int}(x)$, as read off from (16.2.5).

The same steps evaluate the left-hand graph to be

$$\begin{aligned} S_C^{\rm left} &= 2\times\left[\frac{1}{2!}\right]\left[\frac{\epsilon_\mu(k)}{(2\pi)^{3/2}\sqrt{2\omega}}\right]\left[\frac{\epsilon^*_\nu(k')}{(2\pi)^{3/2}\sqrt{2\omega'}}\right]\int\frac{{\rm d}^4k}{(2\pi)^4 i}\Big[e\,(2\pi)^4\delta^4(k-p+q')\Big] \\ &\qquad\times\Big[e\,(2\pi)^4\delta^4(k-p'+q)\Big]\frac{\overline{\mathbf{u}}(p')}{(2\pi)^{3/2}}\gamma^\mu\left[\frac{-i\not{k}+m}{k^2+m^2-i\delta}\right]\gamma^\nu\left[\frac{\mathbf{u}(p)}{(2\pi)^{3/2}}\right] \\ &= -i(2\pi)^4\delta^4(p+q-p'-q')\left[\frac{e^2}{2(2\pi)^6\sqrt{\omega\omega'}}\,\frac{\overline{\mathbf{u}}(p')\gamma^\mu[-i(\not{p}-\not{q}')+m]\gamma^\nu\mathbf{u}(p)}{(p-q')^2+m^2-i\delta}\right]. \end{aligned} \tag{16.4.11}$$

Summing these and comparing to (16.4.2) reveals the reduced amplitude $\mathcal{M}_C$ to be

$$\mathcal{M}_C = \frac{e^2}{(2\pi)^3 2\sqrt{\omega\omega'}}\,\epsilon_\mu\epsilon^{*\prime}_\nu\,\overline{\mathbf{u}}'\left\{\frac{\gamma^\nu[-i(\not{p}+\not{q})+m]\gamma^\mu}{-2m\omega}+\frac{\gamma^\mu[-i(\not{p}-\not{q})+m]\gamma^\nu}{2m\omega'}\right\}\mathbf{u}\,, \tag{16.4.12}$$

which uses $p^2+m^2=(p')^2+m^2=0$ and $q^2=(q')^2=0$ as well as the rest-frame results $(p+q)^2+m^2=2p\cdot q=-2m\omega$ and $(p-q')^2+m^2=-2p\cdot q'=2m\omega'$. It is convenient in what follows to give a name to the Dirac-matrix valued quantity appearing here in the curly braces (after factoring out the common $2m$ from the denominator:

$$\mathcal{T}^{\mu\nu} := \frac{\gamma^\nu[-i(\not{p}+\not{q})+m]\gamma^\mu}{-\omega}+\frac{\gamma^\mu[-i(\not{p}-\not{q})+m]\gamma^\nu}{\omega'}\,. \tag{16.4.13}$$

In terms of this the squared matrix element needed in (16.4.9) is

$$\Big|\mathcal{M}_C\Big|^2 = \frac{e^4}{16(2\pi)^6 m^2\omega\omega'}\epsilon_\mu(q)\,\epsilon^*_\nu(q')\,\epsilon^*_\rho(q)\,\epsilon_\lambda(q')\mathcal{A}^{\mu\nu\rho\lambda} \tag{16.4.14}$$

where

$$\mathcal{A}^{\mu\nu\rho\lambda} := \overline{\mathbf{u}}(p')\mathcal{T}^{\mu\nu}\mathbf{u}(p)\,\overline{\mathbf{u}}(p)\,\beta\Big(\mathcal{T}^{\rho\lambda}\Big)^\dagger\beta\,\mathbf{u}(p')\,, \tag{16.4.15}$$

which uses the definition (15.4.5): $\overline{\mathbf{u}}=\mathbf{u}^\dagger\beta$ where $\beta=\beta^\dagger$ and $\beta^2=1$. The hermitian conjugate of $\mathcal{T}^{\rho\lambda}$ can be evaluated using the general identities (15.4.21) with the second row of Table 5, in the form

$$\beta\Big[\gamma^\rho S(p)\gamma^\lambda\Big]^\dagger\beta=\beta(\gamma^\lambda)^\dagger\beta\,\beta[S(p)]^\dagger\beta\,\beta(\gamma^\rho)^\dagger\beta=(-\gamma^\lambda)S(p)(-\gamma^\rho) \tag{16.4.16}$$

and so $\beta(\mathcal{T}^{\rho\lambda})^\dagger\beta=\mathcal{T}^{\lambda\rho}$. This allows $\mathcal{A}^{\mu\nu\rho\lambda}$ to be written as a Dirac trace:

$$\mathcal{A}^{\mu\nu\rho\lambda}=\overline{\mathbf{u}}(p')\mathcal{T}^{\mu\nu}\mathbf{u}(p)\,\overline{\mathbf{u}}(p)\mathcal{T}^{\lambda\rho}\mathbf{u}(p')={\rm Tr}\Big\{\mathcal{T}^{\mu\nu}[\mathbf{u}(p)\,\overline{\mathbf{u}}(p)]\mathcal{T}^{\lambda\rho}[\mathbf{u}(p')\overline{\mathbf{u}}(p')]\Big\} \tag{16.4.17}$$

where the dyadic $\mathbf{u}(p,\sigma)\,\overline{\mathbf{u}}(\mathbf{p},\sigma)$ is evaluated in terms of p^μ and the spin in (15.4.32):

$$\mathbf{u}(\mathbf{p},\sigma)\,\overline{\mathbf{u}}(\mathbf{p},\sigma)=\frac{1}{4\varepsilon}\,(m-i\not{p})\,(1+i\gamma_5\not{s}),, \tag{16.4.18}$$

where $s^\mu p_\mu=0$ and in the rest frame $\mathbf{s}(\sigma=\pm\frac{1}{2})=\pm\mathbf{e}_s$ where $\mathbf{e}_s$ is the unit vector pointing in the direction along which σ is measured. In the rest frame we may also use $-i\not{p}+m=m(1+\beta)$.

At this point evaluating $\mathcal{A}^{\mu\nu\rho\lambda}$ is simply a fairly tedious exercise in taking Dirac traces. Things simplify somewhat if the initial and final spins are not measured, though, since in this case the rules

of quantum mechanics tell us we should sum over the final spins λ' and σ', but we should *average* over the initial spins λ and σ, so we replace $|\mathcal{M}_C|^2$ in the cross section with

$$|\mathcal{M}_C|^2 \to \overline{|\mathcal{M}_C|^2} := \frac{1}{4}\sum_{\sigma\lambda}\sum_{\sigma'\lambda'}|\mathcal{M}_C|^2\,. \tag{16.4.19}$$

The average over initial spins corresponds to being uncertain in what the initial spin configuration is, and assigning equal probabilities to all four possible combinations of allowed values for σ and λ.

Since the spins only appear in the mode functions $\mathbf{u}$ and ϵ_μ the sum over electron spins can be performed by replacing (16.4.18) with (*c.f.* (15.4.34))

$$\sum_\sigma \mathbf{u}(\mathbf{p},\sigma)\,\overline{\mathbf{u}}(\mathbf{p},\sigma) = \frac{1}{2\varepsilon}\,(m - i\not{p})\,, \tag{16.4.20}$$

and for photon helicities using (16.1.15)

$$\sum_\lambda \epsilon_\mu(\mathbf{q},\lambda)\,\epsilon^*_\nu(\mathbf{q},\lambda) = \hat{\Pi}_{\mu\nu}(q) = \eta_{\mu\nu} + \frac{(n_\mu q_\nu + n_\nu q_\mu)q_0 - q_\mu q_\nu}{|\mathbf{q}|^2} + \frac{q_\sigma q^\sigma}{|\mathbf{q}|^2}\,n_\mu n_\nu\,. \tag{16.4.21}$$

This last expression is not as bad as it looks, however, because the $n_\mu n_\nu$ term is proportional to $q_\sigma q^\sigma = -\omega^2 + \mathbf{q}^2$ which vanishes because of the photon dispersion relation. The $n_\mu q_\nu + n_\nu q_\mu$ and $q_\mu q_\nu$ terms also drop out of the calculation, as a special instance of the general result proven in §16.3. So in practice only the $\eta_{\mu\nu}$ term contributes, leading to

$$\overline{|\mathcal{M}_C|^2} = \frac{e^4}{16(2\pi)^6 m^2\omega\omega'}\,\mathcal{B}\,, \tag{16.4.22}$$

where

$$\mathcal{B} := \frac{1}{4}\,\eta_{\mu\rho}\eta_{\nu\lambda}\sum_{\sigma\sigma'}\mathcal{A}^{\mu\nu\rho\lambda} = \frac{1}{16\varepsilon\varepsilon'}\mathrm{Tr}\left\{\mathcal{T}^{\mu\nu}(-i\not{p}+m)\mathcal{T}_{\nu\mu}(-i\not{p}'+m)\right\} \tag{16.4.23}$$

Evaluating the Dirac trace – using identities such as (15.3.17) through (15.3.22) and their generalizations to larger numbers of Dirac matrices – then gives (in the initial electron rest frame):

$$\mathcal{B} = \frac{2m}{m+\omega-\omega'}\left[\frac{\omega}{\omega'} + \frac{\omega'}{\omega} + 2m\left(\frac{1}{\omega}-\frac{1}{\omega'}\right) + m^2\left(\frac{1}{\omega}-\frac{1}{\omega'}\right)^2\right]. \tag{16.4.24}$$

It might come as a surprise that $\mathcal{B}$ remains finite in the limit $\omega' = \omega$ and $\omega \to 0$, given the explicit factors of $1/\omega$ and $1/\omega'$ appearing in (16.4.13). This happens because in this limit $p' \to p$ and so $-i\not{p}' + m \to -i\not{p} + m = m(1+\beta)$ (where the last equality holds in the initial electron's rest frame). But because $1+\beta$ is a projection matrix and β anticommutes with the spatial components of γ^μ this means that the only nonzero trace involves $\mathcal{T}^{00}$ and so vanishes because $\mathcal{T}^{\mu\nu}$ is antisymmetric in this limit.[58]

[58] This same cancellation need not hold for arbitrary tree-level graphs, which actually can diverge in the limit of very low-energy photons. The reason predictions nonetheless make sense is the topic of §18.5 below.

Collecting results then gives (after some algebra) the following famous expression for the differential cross section for Compton scattering

$$\begin{aligned}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \frac{e^4}{8(2\pi)^2 m^2}\left(\frac{\omega'}{\omega}\right)^2\left[\frac{\omega}{\omega'}+\frac{\omega'}{\omega}+2m\left(\frac{1}{\omega}-\frac{1}{\omega'}\right)+m^2\left(\frac{1}{\omega}-\frac{1}{\omega'}\right)^2\right] \\ &= \frac{e^4}{32\pi^2 m^2}\,\frac{1}{[1+(\omega/m)(1-\cos\theta)]^2}\left[1+\cos^2\theta+\frac{(\omega/m)^2(1-\cos\theta)^2}{1+(\omega/m)(1-\cos\theta)}\right],\end{aligned} \tag{16.4.25}$$

where the second equality uses energy conservation – eq. (16.4.7) – to eliminate ω' in terms of ω and scattering angle θ. Notice that in the non-relativistic limit $\omega \ll m$ this expression precisely reproduces the expression (9.5.13) for the Thomson cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \simeq \frac{e^4}{32\pi^2 m^2}(1+\cos^2\theta) = \frac{\alpha^2}{2m^2}(1+\cos^2\theta)\,, \tag{16.4.26}$$

found earlier (using $\alpha = e^2/(4\pi)$).

Unlike in earlier sections the opposite limit, $\omega \gg m$, is allowed in the above result, and dropping subdominant powers of m/ω gives

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \simeq \frac{e^4}{32\pi^2 m\omega(1-\cos\theta)}\,, \tag{16.4.27}$$

showing how the scattering is sharply peaked in the forward direction ($\theta \to 0$) in this limit. The result does not actually diverge at $\theta = 0$ because once $\theta \lesssim \sqrt{m/\omega}$ the expansion in powers of $(\omega/m)(1-\cos\theta)$ breaks down. Taking instead $\theta \to 0$ for fixed ω/m in (16.4.25) shows that the full differential cross section actually approaches $e^4/(16\pi^2 m^2)$.

16.5 Pair production

At face value the basic interaction (16.2.5) of QED seems to allow the process $\gamma \to e^+e^-$, because the matrix element for particle-antiparticle production

$$\begin{aligned}\langle e^-(\mathbf{p},\sigma)\,, e^+(\mathbf{p}',\sigma')|\mathcal{H}_{\rm int}(x)|\gamma(\mathbf{k},\lambda)\rangle &= ie\,\langle e^-(\mathbf{p},\sigma)\,, e^+(\mathbf{p}',\sigma')|(\overline{\psi}\gamma^\mu\psi)\,A_\mu|\gamma(\mathbf{k},\lambda)\rangle \\ &= ie\left[\frac{\overline{\mathbf{u}}(p)}{(2\pi)^{3/2}}\right]\gamma^\mu\left[\frac{\mathbf{v}(p')}{(2\pi)^{3/2}}\right]\left[\frac{\epsilon_\mu(k)}{\sqrt{(2\pi)^3 2\omega}}\right]e^{i(k-p-p')\cdot x} \\ &= \frac{ie}{\sqrt{(2\pi)^9 2\omega}}\,\overline{\mathbf{u}}(p)\gamma^\mu\mathbf{v}(p')\,\epsilon_\mu(k)\,e^{i(k-p-p')\cdot x}\end{aligned} \tag{16.5.1}$$

is nonzero. Things are not quite this simple, however, because the S-matrix involves an integration d^4x of this, leading to the 4-momentum conserving delta function $\delta^4(k-p-p')$.

The problem is that there does not exist a choice of 4-vectors k, p and p' that can satisfy $k^\mu = (p+p')^\mu$ given that k is light-like ($k^2 = 0$) while p and p' are time-like ($p^2 < 0$ and $(p')^2 < 0$). The simplest way to see this is to recognize $p\cdot p' < 0$ since it is Lorentz invariant and evaluates to $-m\varepsilon' < 0$ in the rest frame of p. But this ensures that $(p+p')^2 = p^2+(p')^2+2p\cdot p'$

is also strictly negative and so cannot be light-like. Energy-momentum conservation is what keeps energetic photons from spontaneously turning into electron-positron pairs.

But electron-positron pairs can be (and are) produced by photons passing through matter, because the matter can then carry away some of the momentum, making the process kinematically allowed. This can be estimated with the tools available to this point by preparing the electromagnetic field be the sum of a classical background field (due, for instance, to the presence of a nearby atomic nucleus) plus the incident photon. Although we do not solve the Dirac equation in the presence of background fields until §19.1, the background field can instead be treated perturbatively by slightly modifying the Feynman rules.

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17 Radiative corrections and renormalization

We have seen that perturbation theory in QED is a series in $\alpha/(4\pi)$ and that for any fixed process – *i.e.* for a fixed number of external lines – each loop in a graph costs an additional factor of $\alpha/(4\pi)$. The tree graphs (no loops) of the previous section therefore provide the leading contribution to any specific process, and higher loops (historically called *radiative corrections*) provide potentially ever-more-precise predictions.[59]

This section calculates several of the leading such corrections, both because the examples examined provide good tests of the theory and because the calculations provide a vehicle for examining several conceptual issues that first arise at the one-loop level. Prominent among these is the phenomenon of ultraviolet (UV) divergences, and how these are handled by renormalization when making predictions. Although renormalization often is discussed purely in the context of handling divergences it is discussed here separately because it is logically distinct, with renormalization in principle required even in the absence of divergences.

The starting observation begins with the discussion above eq. (16.2.18), that identifies the number of integrations that remain to be done in a general (connected) Feynman graph after all of the 4-momentum conserving delta functions have been used up. There it was concluded that an integration over an internal 4-momentum remains for each loop in the graph (so no integrations arise at tree level, as found explicitly in the previous chapter). Unfortunately these integrals in general do not converge, often diverging in particular in the limit of infinite momentum (the 'far UV' limit).

[59]There is good evidence that the series in α is actually asymptotic rather than convergent so in practice successive terms only provide a better approximation for the first $N \sim 1/\alpha \sim 137$ terms. Although this could be a problem for theories with stronger coupling, it seems only an academic one in practice for QED.

Such divergences are not unique to relativistic theories since we already encountered them in previous section, like §5.1, §6.5 and §9.3. These divergences arise very commonly in quantum theories and indicate a sensitivity of the calculation to the shortest distance scales, usually in a regime beyond current theoretical reach. In past examples these divergences always arose together with one of the parameters of the theory, in such a way that only the sum of the parameter and the divergence is actually measurable. Because of this we could imagine absorbing the divergences into the definitions of the parameters, ending up with predictions that do not diverge when expressed in terms of the new parameters. This logic continues to work in the relativistic case, though with a few refinements.

Path-integral techniques provide a more systematic way to see why this is a reasonable way for theories to behave – see §21.7 – but the upshot of the message can be stated here. The fact that the effects of short wavelengths (divergent or not) can be absorbed into the parameters of a Hamiltonian reflects a deep property of Nature called *decoupling*. Decoupling says that most of the details of physics at very short distances is irrelevant to understanding what goes on at much longer distances. It is the reason why you can understand atomic physics, say, before you have fully understood nuclear physics.[60] It is also the reason science works at all: you don't have to understand all of the scales in the Universe at once.

The fact that divergences enter into physical predictions in the same way that parameters do in our theories tells us that you'd actually need to know the details at very small distances *if* you hoped to be able to predict the values of these parameters (such as the value of the electron mass or charge in QED). It is because we do not really know how Nature works at the smallest of distances that we have to parameterize our ignorance when making other predictions, and that is what the parameters in our theories are for.

This also provides a second insight into why theories are local: the uncertainty principle forces the influence of states with high energy and high momentum to act only over short distances and time intervals. If the theories we write down parameterize the unknown effects of states with much higher energies then we should expect them to come to us expressed as interactions at specific positions and times. In the end, decoupling expresses the remarkable fact that despite our ignorance of unknown small-distance physics, we can still make sensible predictions at the distances we do understand, *provided* we agree that the parameters within our local Hamiltonians are intrinsically unknown quantities whose values are likely to be sensitive to the details of UV physics. The key idea is that this sensitivity does not matter since we must in any case infer their values from experiments rather than from first principles.

17.1 Regularization of divergences

To see how this works requires having a way to describe very short-distance contributions, and this is what regularization schemes provide. To keep the discussion concrete it is useful

[60] You have to know *some* things about nuclear physics to understand atoms – notably the charge and mass of the nucleus – but (significantly) what needs knowing boils down to a few *parameters*.

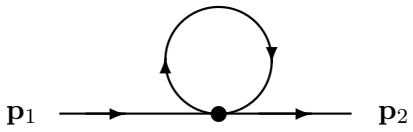


Figure 10. A representative one-loop 'tadpole' Feynman graph for a $(\chi^\star\chi)^2$ interaction.

to have a specific loop integral in mind, so consider a relativistic scalar field (with particle distinct from antiparticle) subject to a local self-interaction

$$\mathcal{L} = -\partial_\mu\chi^\star\,\partial^\mu\chi - m^2\chi^\star\chi - \frac{g}{4}(\chi^\star\chi)^2\,, \tag{17.1.1}$$

where g is a real and positive coupling constant (we return to QED shortly). For this theory we compute the 1-loop Feynman graph given in Fig. 10 that arises at first order in g.

Ignoring symmetry factors and the factors associated with the external lines, using the Feynman rules of §12.4 shows that this graph gives a result proportional to $g\,I_1(m^2)$ where I_1 denotes the integral

$$I_1(m^2) := \int_{-\infty}^{\infty} \frac{\mathrm{d}^4q}{(2\pi)^4}\,\frac{1}{q^2+m^2-i\delta}\,. \tag{17.1.2}$$

Because the momentum in the loop both flows in and out of the vertex, the delta function at the vertex ends up being $\delta^4(p_1-p_2)$ and so simply expresses overall 4-momentum conservation for the whole graph. As a result the integrand appearing in the loop integral is independent of external momentum. This integral has dimension $(\text{mass})^2$ and diverges as the upper limit of integration is taken to infinity since for large q it has the form $\int^\Lambda \mathrm{d}^4q/q^2$, which diverges like Λ^2 as $\Lambda\to\infty$ (as might have been guessed on dimensional grounds).

In order to sensibly discuss and manipulate divergent integrals like this one it is first necessary to define what they mean. This is done as in earlier sections by 'regularizing' them, which means replacing an ill-defined integral with a one-parameter family of integrals that converge for at least part of the parameter range. Then the integrals can be manipulated for values of the parameters that converge with the limit ultimately taken back to the value that gives the original integral at the end of the calculation (after the divergence has been dealt with – typically by renormalizing some parameter).

This regularization parameter might be as simple as the addition of an explicit UV cutoff, like Λ introduced below (17.1.2). But it could also be a more sophisticated deformation, along the lines followed when computing the Casimir energy starting with (9.3.6) (for which the new parameter was the variable p). Because the divergences are ultimately cancelled by being absorbed into a parameter in the theory (more about which below), the details of the regularization scheme do not matter so long as it satisfies the two key principles outlined in the discussion above (9.3.6). This leaves a lot of freedom of choice for regularization scheme,

and this freedom is most usefully exploited by ensuring the regularization makes calculations as easy as possible. In particular, the best regularization schemes preserve as many of the symmetries of the problem as possible.

17.1.1 Dimensional regularization

For most applications (particularly for relativistic theories with gauge symmetries) the regularization of choice is *dimensional regularization*, because this keeps both Lorentz-invariance and gauge invariance explicit at each step (which it turns out is fairly hard to do otherwise).

Dimensional regularization is based on a very simple idea: define the integration to be in n spacetime dimensions but treat n as an arbitrary non-integer variable in a way that allows the integral to converge. At the end of the day the limit $n \to 4$ is taken, after the divergences have been cancelled (usually by absorbing them into one of the theory's parameters).

To see how this works we apply it to the integral $I_1(m^2)$ defined in (17.1.2), which we deform to depend on the new parameter n

$$I_1(m^2) := \mu^{4-n} \int_{-\infty}^{\infty} \frac{\mathrm{d}^n q}{(2\pi)^n} \, \frac{1}{q^2 + m^2 - i\delta} = \mu^{4-n} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega \, \mathrm{d}^{n-1} q}{(2\pi)^n} \, \frac{1}{-\omega^2 + \mathbf{q}^2 + m^2 - i\delta} \,, \tag{17.1.3}$$

with $n \to 4$ to be taken at the end. The factor μ^{4-n} is present to ensure the answer still has dimension $(\text{mass})^2$, where μ is an arbitrary mass scale (that does not appear in any physical predictions). The next step is to perform the integrals, and the second equality separates the integration over $\omega = q^0$ from the remaining spatial integration, in order to perform this integral first. It is here that the infinitesimal δ plays a role, because it puts the poles of the integrand at $\omega = \pm\sqrt{\mathbf{q}^2 + m^2 - i\delta}$, which for nonzero δ lie slightly off the integration path along the real axis.

Wick rotation

Because these poles lie in the upper-left and lower-right quadrants of the complex ω plane it is useful to deform the contour of integration by rotating it 90 degrees counterclockwise – called a *Wick rotation* – to run up the imaginary axis: $\omega = i\omega_E$ with ω_E running from $-\infty$ to ∞. This rotation is possible because there are no poles encountered in the upper-right and lower-left quadrants.

Once this is done we have $\mathrm{d}\omega = i\mathrm{d}\omega_E$ and $-\omega^2 + \mathbf{q}^2 = +\omega_E^2 + \mathbf{q}^2 =: q_E^2$, where the subscript '$E$' stands for 'Euclidean' since q_E^2 is the length of a vector in a space with a positive-definite Euclidean signature metric (rather than the Minkowski one of special relativity). After this rotation the desired integral becomes

$$I_1(m^2) := i\mu^{4-n} \int_{-\infty}^{\infty} \frac{\mathrm{d}^n q_E}{(2\pi)^n} \, \frac{1}{q_E^2 + m^2} \,. \tag{17.1.4}$$

The infinitesimal δ can now be dropped because the denominator never vanishes anywhere near the integration contour and so there is no ambiguity in how to perform the integral.

Evaluation of the integral

The remaining integral can be done in polar coordinates because the integrand only depends on the magnitude q_E^2 of the vector. For later use we do so here for a slightly broader class of integrals than considered in (17.1.4); instead evaluating

$$\begin{aligned} J(A,B;a) &:= \int \mathrm{d}^n q_E \, \frac{(q_E^2)^A}{(q_E^2+a)^B} \\ &= \frac{\Omega_n}{2} \int_0^\infty \mathrm{d}x \, \frac{x^{A+\frac{1}{2}(n-2)}}{(x+a)^B} \\ &= \frac{\Omega_n}{2} \, a^{A-B+\frac{1}{2}n} \frac{\Gamma\left(A+\frac{1}{2}n\right)\,\Gamma\left(B-A-\frac{1}{2}n\right)}{\Gamma(B)} \\ &= \pi^{n/2} a^{A-B+\frac{1}{2}n} \frac{\Gamma\left(A+\frac{1}{2}n\right)\,\Gamma\left(B-A-\frac{1}{2}n\right)}{\Gamma(B)\Gamma\left(\frac{1}{2}n\right)} \,. \end{aligned} \tag{17.1.5}$$

Here $\Gamma(z)$ is Euler's generalized factorial function, and the second line evaluates the integral in polar coordinates. In n dimensions the angular integrations give a factor of the area, Ω_n of the unit $(n-1)$-sphere embedded within n-dimensions. This is given explicitly by:[61]

$$\Omega_n = \frac{2\pi^{n/2}}{\Gamma(n/2)} \,. \tag{17.1.6}$$

(The properties $\Gamma(\frac{1}{2}) = \sqrt{\pi}$, $\Gamma(1) = 1$ and $z\Gamma(z) = \Gamma(z+1)$ show that the first few terms agree with common sense: $\Omega_2 = 2\pi$; $\Omega_3 = 4\pi$, $\Omega_4 = 2\pi^2$ and so on.) The final line uses the integral

$$\int_0^\infty \mathrm{d}x \, \frac{x^M}{(x+y)^N} = y^{M-N+1} \frac{\Gamma(M+1)\,\Gamma(N-M-1)}{\Gamma(N)} \,. \tag{17.1.7}$$

Here comes the main point: although these manipulations were done as if n were a positive integer, we now *define* the integral $J(A,B;a)$ for all A, B, n and a by (17.1.5), even for complex n and for parameters A, B and n where the original integral does not converge. For instance the integral $I_1(m^2)$ corresponds to the choices $A = 0$ and $B = 1$ and so

$$I_1(m^2) = i\mu^{4-n} \frac{\Omega_n}{2(2\pi)^n} J(0,1;m^2) = \frac{im^2}{(4\pi)^{n/2}} \left(\frac{m}{\mu}\right)^{n-4} \Gamma\left(1-\tfrac{1}{2}n\right) \,, \tag{17.1.8}$$

with the original divergence reappearing here in the limit $n \to 4$ because $\Gamma(z)$ diverges when $z = -n$ is a nonpositive integer.

To isolate the divergent part of $I_1(m^2)$ write $n = 4 - 2\epsilon$ where $\epsilon \to 0$ is the limit of physical interest, and expand in powers of ϵ using the Laurent expansion of $\Gamma(z)$ about $z = 0$:

$$\Gamma(z) = \frac{1}{z} - \gamma + \mathcal{O}(z) \quad \text{with} \quad \gamma = 0.5772157... \quad \text{(the Euler-Mascheroni constant)}. \tag{17.1.9}$$

[61] This result is most easily derived by evaluating the integral over $e^{-\frac{1}{2}(x_1^2+x_2^2+\cdots+x_n^2)}$ over all of space. The result is the product of n identical factors if done in rectangular coordinates, but gives the desired expression for Ω_n if done in polar coordinates.

Combining this with the identity $(z-1)\Gamma(z-1)=\Gamma(z)$ then also shows

$$\Gamma(-1+z)=\frac{\Gamma(z)}{z-1}=-\frac{1}{z}+(\gamma-1)+\mathcal{O}(z)\,, \tag{17.1.10}$$

with a similar argument giving the expansion about any other negative integer. Keeping in mind $x^{n-4}=e^{(n-4)\log x}=1+(n-4)\log x+\mathcal{O}[(n-4)^2]$ one finds

$$I_1(m^2)=\frac{im^2}{(4\pi)^2}\left(\frac{m^2}{4\pi\mu^2}\right)^{-\epsilon}\Gamma\left(-1+\epsilon\right)=\frac{im^2}{(4\pi)^2}\left[-\frac{1}{\epsilon}+\log\left(\frac{m^2}{4\pi\mu^2}\right)+(\gamma-1)+\mathcal{O}(\epsilon)\right]. \tag{17.1.11}$$

The pole describes the divergent part and the goal when renormalizing is to see how these poles can be absorbed into the definitions of the parameters of the theory.

It is noteworthy that if $m=0$ the dimensionally regularized integral vanishes, for want of a dimensionful parameter to which it can be proportional for n near to but not equal to 4. Eq. (17.1.5) shows the same is true for $J(A,B;a)$ when $a\to 0$. This might come as a surprise in the case $B-A=2$ for which the integral is dimensionless in four dimensions. Why should dimensional regularization assign a value of zero to $J(A,A+2;0)$? To see why it is useful to examine the $a=0$ case with $A=0$ and $B=2$ more closely, rewriting it as the sum of two contributions

$$J(0,2;0)=\int\frac{\mathrm{d}^n q_E}{(2\pi)^n}\,\frac{1}{q_E^4}=\int\frac{\mathrm{d}^n q_E}{(2\pi)^n}\,\frac{1}{q_E^2(q_E^2+m^2)}+\int\frac{\mathrm{d}^n q_E}{(2\pi)^n}\,\frac{m^2}{q_E^4(q_E^2+m^2)}\,. \tag{17.1.12}$$

Both of the integrals on the right-hand side diverge as $n\to 4$, but while this is a UV divergence (from $q_E^2\to\infty$) for the first integral, the second integral actually converges in the ultraviolet. The divergence in the second integral instead comes from the $q_E^2\to 0$ limit, what is called an *infrared* (or IR) divergence. Both of these integrals can be dimensionally regularized using (17.1.5), leading to the result

$$J(0,2;0)=J(-1,1;m^2)+m^2J(-2,1;m^2)=\frac{1}{(4\pi)^2}\left(\frac{1}{\epsilon_{UV}}-\frac{1}{\epsilon_{IR}}\right), \tag{17.1.13}$$

where the regularization parameter for each integral is labelled with 'UV' and 'IR' to remind that a different type of divergence is involved in each case. This indeed vanishes once we use $\epsilon_{UV}=\epsilon_{IR}=\epsilon$, but this exercise shows that it does so because of a cancellation between an infrared and ultraviolet divergence, because dimensional regularization handles them in an identical way. Because UV and IR divergences have different interpretatons (IR divergences are *not* removed by renormalization), it is sometimes worth keeping them separate when calculating dimensionless integrals.

Feynman parameters

Before returning to QED it is worth adding one more trick to the bag. To see the reason for its necessity we must examine a more interesting divergent Feynman graph than the one in

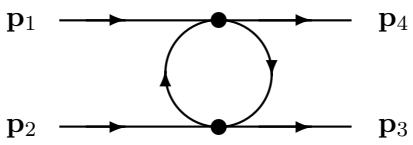


Figure 11. A more complicated divergent one-loop Feynman graph for a $(\chi^\star\chi)^2$ interaction.

Fig. 10. Consider therefore the second-order graph given in Fig. 11, whose Feynman rules reveal it to be proportional to $g^2 I_2$ where I_2 is the following dimensionally regularized loop integral:

$$I_2 := \mu^{4-n} \int \frac{\mathrm{d}^n q}{(2\pi)^n} \, \frac{1}{[q - \frac{1}{2}(p_2 - p_3)]^2 + m^2 - i\delta} \, \frac{1}{[q + \frac{1}{2}(p_2 - p_3)]^2 + m^2 - i\delta} \,. \tag{17.1.14}$$

For the present purposes, the main difference between this and the previous case is the presence of the external momenta in the denominators, which is allowed in this case by 4-momentum conservation at each vertex. This is a complication because it stops us from directly using (17.1.5) when using dimensional regularization. This problem can be fixed through the judicious use of a useful identity. The identity starts by evaluating the following integral:

$$\int_0^1 \frac{\mathrm{d}x}{[C_1 x + C_2(1-x)]^2} = \frac{1}{C_1 - C_2} \int_{C_2}^{C_1} \frac{\mathrm{d}u}{u^2} = \frac{1}{C_1 C_2} \,, \tag{17.1.15}$$

and applying it with C_1 and C_2 being the two factors in the denominator of (17.1.14). Temporarily suppressing the $i\delta$ factors and writing $k^\mu := \frac{1}{2}(p_2 - p_3)^\mu$, we take $C_1 = (q-k)^2 + m^2$ and $C_2 = (q+k)^2 + m^2$ so that

$$\frac{1}{(q-k)^2 + m^2} \, \frac{1}{(q+k)^2 + m^2} = \int_0^1 \frac{\mathrm{d}x}{D^2} \,. \tag{17.1.16}$$

where the denominator is

$$\begin{aligned} D &:= [(q-k)^2 + m^2]x + [(q+k)^2 + m^2](1-x) \\ &= q^2 + 2q \cdot k(1-2x) + k^2 + m^2 \\ &= [q + k(1-2x)]^2 + 4k^2 x(1-x) + m^2 \,. \end{aligned} \tag{17.1.17}$$

This final form can be further simplified by performing the change of integration variables from q^μ to $r^\mu := q^\mu + (1-2x)k^\mu$, after which I_2 becomes

$$I_2 = \mu^{4-n} \int \frac{\mathrm{d}^n r}{(2\pi)^n} \int_0^1 \mathrm{d}x \, \frac{1}{\{r^2 + 4k^2 x(1-x) + m^2 - i\delta\}^2} \,. \tag{17.1.18}$$

This disentangles the integration momentum from the external momenta and so allows the n-dimensional integral to be explicitly performed in the same way as was done for I_1.

Performing the Wick rotation as before then leads to a form to which (17.1.5) can be directly applied:

$$\begin{aligned} I_2 &= i\mu^{4-n} \int_0^1 \mathrm{d}x \int \frac{\mathrm{d}^n r_E}{(2\pi)^n} \, \frac{1}{\{r_E^2 + 4k^2x(1-x) + m^2\}^2} \\ &= i\mu^{4-n} \int_0^1 \mathrm{d}x \, J[0,2;4k^2x(1-x)+m^2] \,. \end{aligned} \tag{17.1.19}$$

From here on divergences can be isolated as before by expanding $n = 4 - 2\epsilon$ and dropping terms that are $\mathcal{O}(\epsilon)$.

Before returning to the main discussion we pause to record a useful generalization of (17.1.15) to involve products of more factors. The result can be proven by induction (do so!) and states

$$\begin{aligned} \frac{1}{C_1 C_2 \cdots C_s} = (s-1)! \int_0^1 \mathrm{d}x_1 \int_0^{x_1} \mathrm{d}x_2 \cdots \int_0^{x_{s-2}} \mathrm{d}x_{s-1} \\ \times \Big[C_s x_{s-1} + C_{s-1}(x_{s-2} - x_{s-1}) + \cdots + C_1(1 - x_1) \Big]^{-s} . \end{aligned} \tag{17.1.20}$$

17.2 Renormalization

There is one last rabbit hole to explore before turning to examples of explicit loop calculations: the role played by parameters in quantum field theory (and in theories more generally). Having this clear helps when turning to the nitty gritty of how divergences are absorbed by renormalization.

17.2.1 Parameterizing observables

To start recall a few facts about parameterizing curves. One way to describe a circle of radius a centered on the origin in the $x - y$ plane is as the set of all solutions (x, y) to the relation

$$x^2 + y^2 = a^2 \,. \tag{17.2.1}$$

But an alternative way of describing it uses parameterizations, such as

$$x(\theta) = a \, \cos\theta \quad \text{and} \quad y(\theta) = a \, \sin\theta \,, \tag{17.2.2}$$

for which the circle is swept out as the parameter θ runs through some range (in this case $0 \leq \theta \leq 2\pi$). Such parameterizations are not unique, with for example a different one for the circle being

$$x(\xi) = a \, \tanh\xi \quad \text{and} \quad y(\xi) = \frac{a}{\cosh\xi} \,. \tag{17.2.3}$$

The point of the parameterizations is that the functions in (17.2.2) and (17.2.3) satisfy (17.2.1) automatically for all values of the parameters.

A similar thing happens in physics when theories are used to make predictions. In this case the role of the variables x and y is played by observables O_i: things that can be measured,

like the energy required to produce a particle in the lab, or the frequency of a photon emitted by an atom as it transitions between electron states. The role of the parameters θ or ξ is played by the theory's coupling parameters g_a: numbers like m and e in QED whose values are free to be chosen to explain observables.

The predictions of a theory are then like (17.2.2) and (17.2.3); one finds formulae

$$O_i = O_i(g) \tag{17.2.4}$$

that express the values of observables in terms of the theory's parameters. The values of the parameters are used by solving a subset $\{\widehat{O}_i\}$ of these relations for the g_a's given measurements of some of the $\widehat{O}_i$'s:

$$g_a = g_a(\widehat{O})\,. \tag{17.2.5}$$

A precise statement of how couplings are defined in terms of observables – $g_a(O)$ – is for historical reasons called a *renormalization scheme* (more about which below). If there are N_o observables and N_p parameters then the theory is predictive if $N_o > N_p$, since once the first N_p observables are used to determine the values of the g_a's the remaining $N_o - N_p$ observables can be predicted with no further freedom.[62]

What is important is that the physical content of a theory's predictions lies in the relation it provides amongst the observables – like (17.2.1) above – rather than the dependence of these observables on any particular set of parameters. This is why there can be a variety of equivalent ways to parameterize a theory and they are all equally good in principle[63] so far as making predictions is concerned.

Though not controversial, the above observation plays a role in the discussion of divergences. To see why imagine computing the formulae $O_i(g)$ in perturbation theory. To simplify the discussion imagine further there is only a single parameter g and two observables and the small perturbative parameter is g. In this case the predictions (17.2.4) have the form

$$O_i = O_i^{(0)} + gO_i^{(1)} + g^2O_i^{(2)} + \cdots\,. \tag{17.2.6}$$

In principle we learn the value of g by measuring O_1 and solving for g. The better the precision of the measurement the more terms in the series are required (assuming the solution for g is small enough to allow perturbative methods). For instance if linear order in g suffices we might have

$$g = \frac{1}{O_1^{(1)}}\left[O_1^{\text{measured}} - O_1^{(0)}\right], \tag{17.2.7}$$

[62] In practice what really happens is the N_p parameters are fit to the N_o observables, but this doesn't really change the story here.

[63] Of course they may be very different in practice, since the mechanics of *deriving* the formulae $O_i(g)$ might not be equally easy in all parameterizations.

which when put into the expression for O_2 predicts

$$O_2 = O_2^{(0)} + gO_2^{(1)} = O_2^{(0)} + \frac{O_2^{(1)}}{O_1^{(1)}}\left[O_1^{\text{measured}} - O_1^{(0)}\right]. \tag{17.2.8}$$

What we are finding in quantum field theory is that the coefficients $O_i^{(k)}$ are UV divergent for $k \geq 1$, so once regularized we have

$$O_i^{(k)} = O_i^{(k)}(p) \quad \text{for some regularization parameter } p. \tag{17.2.9}$$

But because the quantities O_i are measurable (they are observable after all) the left-hand sides of eqs. (17.2.6) cannot diverge (they must evaluate to the value of the corresponding measurement). This means that the solutions (17.2.7) for g must also diverge, and the divergences in g must then cancel the divergences in the coefficient of g in the first equality of (17.2.8): the divergences in $O_1^{(1)}$ and $O_2^{(1)}$ must cancel in the second equality of (17.2.8).

It doesn't really matter that much if observables diverge when expressed in terms of couplings, or when couplings are expressed in terms of observables. What should be well-behaved in any sensible theory is the relation between observables and other observables. This is what we shall see is what happens in QED.

17.2.2 Effective Field Theories: Why local interactions suffice

The above discussion is all very nice, but why should it be true that UV divergences contribute to physical quantities in exactly the same way as do the parameters in any given theory? After all, we do not normally include all possible interactions and in particular – due to the arguments of Chapter 6 – we usually assume that the Hamiltonian (or Lagrangian) is local in space and time.

The key point is that UV divergences express a dependence on unknown very high-energy – and, for relativistic systems at least, short wavelength – degrees of freedom. Energy conservation ensures these can only appear as virtual intermediate states when computing low-energy observables, but because of this Heisenberg's uncertainty principle ensures they can only influence events over very short distances and times. As a result their influence can very generally be parameterized in terms of some local *effective interaction* once these distances and times are too short for a low-energy observer to resolve.

To see how this happens more concretely, consider a Feynman graph for a low energy process in which a massive spinless[64] particle appears somewhere as an internal line. (This is the only way high-energy states can contribute at low energies to the extent that the low-energy assumption itself implies they do not appear amongst the initial or final states of the

[64] The same argument applies for other spins as well.

reaction of interest.[65]) In this case the heavy propagator is given by (12.4.16), which when expanded in inverse powers of the heavy-particle mass becomes

$$G(x,y) = -i \int \frac{\mathrm{d}^4\bar{p}}{(2\pi)^4} \left[\frac{e^{i\bar{p}\cdot(x-y)}}{\bar{p}^2 + m^2 - i\delta} \right] \simeq -\frac{i}{m^2} \left[1 + \frac{\Box}{m^2} + \cdots \right] \delta^4(x-y)\,, \qquad (17.2.10)$$

showing that each term is manifestly local in space and time (but only *after* expanding order by order in $1/m$).

This is ultimately the reason why the effects of high-energy physics can always be captured at a low energy E by some choice of coupling for a local interaction, provided these effects are computed perturbatively in an expansion in powers of the small ratio E/m. This expansion should be a good approximation for particles that are so heavy that they have not yet been discovered, which is precisely the situation relevant for UV divergences: we cut off momentum integrals at a scale above which we do not know what the right high-energy physics really is.

Divergences are just the specific case where the leading dependence on the unknown heavy scale appears in the numerator (or within a logarithm) and not the denominator, and so these should only arise for couplings that have non-negative dimension (in fundamental units for which all dimensions are regarded as energy to a power), such as electron charge and mass in QED. The key observation is that there are usually not that many of couplings with non-negative dimension and so provided one includes all possible such interactions in the initial Hamiltonian they are guaranteed to capture any UV effects.

Notice that the above reasoning applies equally well if the high-energy physics under discussion is not yet understood, or if it is well-understood but just happens to be much heavier then the reaction of interest. An historically important example of this type is the W boson – whose mass $M_W = 80$ GeV is much higher than the energies released in weak decays that take place due to virtual W exchange. In this case we might be interested in studying effects (like radioactive decays) that involve inverse powers of M_W but only to a fixed order (say, M_W^{-2}). In this case it is often much simpler to work with the effective interactions that capture W-boson effects at this order rather than keeping the higher-energy theory in all its glorious detail. Historically it was this effective theory – the Fermi theory of the weak interactions – that was first discovered, before the full theory – the Standard Model of particle physics – involving the W boson was constructed.

The tools for finding and exploiting the effective interactions relevant to the low-energy limit of any particular kind of process are called *Effective Field Theories* and are encountered again in Chapter 21.7 below.

[65] There is a subtlety here because sometimes very massive high-energy states actually *can* appear in low-energy observables, such as atoms with masses well above 1 GeV involved in low-energy chemical reactions whose interaction energies involve only fractions of an eV. In this case the low-energy limit only makes sense to the extent to which the energy locked up in the rest mass cannot be liberated (as is the case for stable particles like protons and neutrons in nuclei).

17.2.3 Renormalization in QED

What does the above mean in practice for QED? The main message is that we should make a crystal clear distinction between parameters and observables that actually get measured.

Inspection of the QED lagrangian given in (16.2.4) (repeated here for ease of reference),

$$\mathcal{L}_{QED} = -\frac{1}{4} F_{\mu\nu}F^{\mu\nu} - \overline{\psi}\Big(\not{D} + m\Big)\psi \tag{17.2.11}$$

with $D_\mu\psi = \partial_\mu\psi + ieA_\mu\psi$, shows that at face value it has only two parameters: e and m. So we must distinguish between the parameters appearing in (17.2.11) and the observed electron mass and charge – perhaps measured by asking how much energy is required to produce an electron-positron pair together with the rate for this reaction. To keep the difference between these clear we henceforth denote by e_B and m_B the 'bare' parameters appearing in (17.2.11), and reserve e and m for the physically measured (or 'dressed') mass and charge. Explicit perturbative calculations in QED give predictions of the form

$$m = m_B + \Delta m(m_B, e_B) \quad \text{and} \quad e = e_B + \Delta e(m_B, e_B)\,, \tag{17.2.12}$$

where Δm and Δe are order $e_B^2/(16\pi^2) = \alpha_B/(4\pi)$ in size (but nonzero). It is the inversion of these expressions that in principle tells us the value of e_B and m_B once e and m are measured.

But this counting of parameters is also a bit misleading because (17.2.11) only has two parameters because we previously used the freedom to rescale fields to set the coefficients of $F_{\mu\nu}F^{\mu\nu}$ and $\overline{\psi}\not{\partial}\psi$ to specific values – *c.f.* the discussion that transformed eq. (15.6.1) to eq. (15.6.6) – a choice called *canonical normalization*. We must recognize that loop corrections in general modify the normalization of these fields; *i.e.* matrix elements of the full Heisenberg-picture fields ψ_h and A_μ might not be the same as those of the interaction-picture fields once loop corrections are performed. If so we would have to rescale the fields again to preserve canonical normalization. (It is indeed this 're-normalization' of the fields that gives this section its name.)

As a result, in the same way we distinguish the bare parameters e_B and m_B from the 'renormalized' couplings e and m, we should also distinguish the bare fields (ψ_B and A^B_μ) appearing in (17.2.11) from the 'renormalized' fields (ψ and A_μ) that are canonically normalized after including the effects of interactions, making (17.2.11) become

$$\mathcal{L}_{QED} = -\frac{1}{4} F^B_{\mu\nu}F_B^{\mu\nu} - \overline{\psi}_B\Big(\not{D} + m_B\Big)\psi_B \tag{17.2.13}$$

with $D_\mu\psi_B = \partial_\mu\psi_B + ie_BA^B_\mu\psi_B$.

Conventionally the bare and renormalized fields are related to one another by[66]

$$e_B = Z_1\, Z_2^{-1} Z_3^{-1/2} e\,, \quad m_B = Z_m Z_2^{-1}\, m\,, \quad \psi_B = \sqrt{Z_2}\;\psi \quad \text{and} \quad A^B_\mu = \sqrt{Z_3}\;A_\mu\,, \tag{17.2.14}$$

[66] The coupling redefinitions are all written in 'multiplicative' form because it turns out in QED (with dimensional regularization) that the changes to both e and m vanish if the bare quantity vanishes. This need not be true in general, in which case one might instead write (for instance) $m_B = m - \delta m$.

for some renormalization constants Z_i whose values are to be determined. The strange conventions relating $e_{\scriptscriptstyle B}$ and $m_{\scriptscriptstyle B}$ to e and m are chosen so that

$$e_{\scriptscriptstyle B}(\overline{\psi}_{\scriptscriptstyle B}\gamma^\mu\psi_{\scriptscriptstyle B})A^{\scriptscriptstyle B}_\mu = Z_1 e\,(\overline{\psi}\gamma^\mu\psi)A_\mu \quad \text{and} \quad m_{\scriptscriptstyle B}\overline{\psi}_{\scriptscriptstyle B}\psi_{\scriptscriptstyle B} = Z_m m\,\overline{\psi}\psi \tag{17.2.15}$$

involve fewer renormalization parameters. Because the bare and renormalized quantities are the same at lowest order, the four renormalization constants Z_i can be calculated order by order in the loop expansion, with

$$Z_i = 1 + \sum_{k=1}^{\infty} z_{ik}\,\left(\frac{\alpha_{\scriptscriptstyle B}}{4\pi}\right)^k =: 1 + \delta Z_i\,, \tag{17.2.16}$$

with the coefficients z_{ik} depending on the dimensional-regularization parameter n (and typically diverging as $n \to 4$).

These definitions also make clear that not all of the Z_i's should be independent of one another. In particular, we know that gauge invariance implies $\partial_\mu\psi_{\scriptscriptstyle B}$ must always appear together with $ie_{\scriptscriptstyle B}A^{\scriptscriptstyle B}_\mu\psi_{\scriptscriptstyle B}$, and the same is true for $\partial_\mu\psi$ and $ieA_\mu\psi$. This means that gauge invariance requires

$$eA_\mu = e_{\scriptscriptstyle B}A^{\scriptscriptstyle B}_\mu \quad \text{which, using (17.2.14), implies} \quad Z_1 = Z_2\,. \tag{17.2.17}$$

This is something that should be an automatic consequence once Z_1 and Z_2 are computed explicitly, and can be proven to be true order-by-order in perturbation theory using the Ward identity of §16.3.

Now comes the main point: because the contributions δZ are suppressed by powers of $\alpha_{\scriptscriptstyle B}$ we should be treating them as perturbations when dividing the full lagrangian $\mathcal{L}$ into an unperturbed and perturbed part: $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\rm int}$. Furthermore, we want to perturb around a system of free particles *with the correct physical mass and field normalization* and so should write

$$\mathcal{L}_0 = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \overline{\psi}(\partial\!\!\!/ + m)\psi \qquad \text{(correct choice)} \tag{17.2.18}$$

instead of

$$\mathcal{L}_0^{\rm wrong} = -\frac{1}{4}F^{\scriptscriptstyle B}_{\mu\nu}F_{\scriptscriptstyle B}^{\mu\nu} - \overline{\psi}_{\scriptscriptstyle B}(\partial\!\!\!/ + m_{\scriptscriptstyle B})\psi_{\scriptscriptstyle B} \qquad \text{(incorrect choice)}\,. \tag{17.2.19}$$

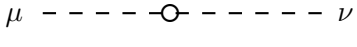
This distinction sounds trivial but is important because it means the naive (incorrect) choice misses an important set of interactions:

$$\begin{aligned}\mathcal{L}_{\rm int} &:= \mathcal{L} - \mathcal{L}_0 = -ie\,(1+\delta Z_1)\,(\overline{\psi}\gamma^\mu\psi)A_\mu - \frac{1}{4}\,\delta Z_3 F_{\mu\nu}F^{\mu\nu} - \delta Z_2\,\overline{\psi}\partial\!\!\!/\psi - \delta Z_m\, m\,\overline{\psi}\psi \\ &= -ie\,\overline{\psi}\gamma^\mu\psi A_\mu + \mathcal{L}_{\rm ct}\,,\end{aligned} \tag{17.2.20}$$

where the last line defines the *counter-term* lagrangian $\mathcal{L}_{\rm ct}$.

The momentum-space Feynman rules for the new counter-term interactions are identified in the same way as was used to obtain (16.2.16) and lead to the new vertices:

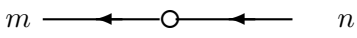
Photon counter-term: The momentum space formulation for the counter-term contribution to a photon line becomes



$$-\frac{i}{2}\,\delta Z_3\Big(p^2\eta_{\mu\nu}-p_\mu p_\nu\Big)(2\pi)^4\delta^4(p-q)\,, \tag{17.2.21}$$

where the indices μ and ν get contracted with the corresponding index for the line ending at the vertex and p^μ and q^μ are the 4-momenta flowing in one side and out of the other side of the vertex.

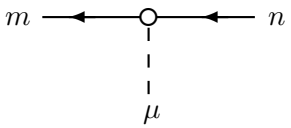
Fermion counter-term: The momentum space formulation for the counter-term contribution to a fermion line becomes



$$-i\Big(i\delta Z_2\not{p}+\delta Z_m m\Big)_{mn}(2\pi)^4\delta^4(p-q)\,, \tag{17.2.22}$$

where the Dirac indices m and n get contracted with the corresponding index for the lines ending at the vertex and p^μ is the 4-momentum entering from the right and q^μ is the 4-momenta flowing out on the left.

Vertex counter-term: The momentum space formulation for the QED vertex counter-term similarly is



$$\delta Z_1\left(e\gamma^\mu\right)_{mn}(2\pi)^4\delta^4(p+q+k)\,, \tag{17.2.23}$$

where p^μ, q^μ and k^μ are the momenta flowing in through each of the three lines in the vertex, with the convention that all momenta point into the vertex.

Renormalization conditions

Since the point of the counter-terms is to ensure we perturb around a free theory with canonically normalized fields and the physical mass, we have to demand that no corrections arise to these quantities in this reorganized perturbative expansion. It is this condition that determines the values taken by the renormalization constants δZ_i.

To see how this works we require a graphical criterion for identifying the physical mass and the canonical normalization of the fields. Although this is not justified in detail until §18.3 and §18.4 the criterion is simple to state: we demand the Fourier transform of the correlation functions of the Heisenberg-picture fields, such as

$$\widehat{S}(p) := \int \mathrm{d}^4x\, \frac{\langle\!\langle 0,\mathrm{out}|T[\psi_h(x)\,\overline{\psi}_h(0)]|0,\mathrm{in}\rangle\!\rangle}{\langle\!\langle 0,\mathrm{out}|0,\mathrm{in}\rangle\!\rangle}\, e^{ip\cdot x} \tag{17.2.24}$$

to preserve the lowest-order property that it have a pole at the physical particle mass, $p^2 = -m^2$, with unchanged residue at this pole. The corresponding photon correlation function similarly must have a pole at $p^2 = 0$ with residue unchanged relative to the unperturbed result.

To turn this into a calculation we require explicit Feynman rules for computing the corrections to correlation functions like these, as opposed to just having Feynman rules for computing S-matrix elements. These are easily obtained by applying the same steps as for the S-matrix to (3.3.9) of §3.3. As applied to propagators (3.3.9) states

$$\begin{aligned}&\langle\!\langle 0,\text{out}|T\Big[\psi_h(x)\overline{\psi}_h(y)\Big]|0,\text{in}\rangle\!\rangle \\ &\qquad = \sum_{N=0}^{\infty}\frac{(-i)^N}{N!}\int_{-\infty}^{\infty}\mathrm{d}^4x_1\cdots\mathrm{d}^4x_N\,\langle 0|T\Big[\psi(x)\overline{\psi}(y)\mathcal{H}_{\text{int}}(x_1)\cdots\mathcal{H}_{\text{int}}(x_N)\Big]|0\rangle\,,\end{aligned} \tag{17.2.25}$$

and this is computed by summing all Feynman graphs with one new Feynman rule relative to the ones constructed as usual from $\mathcal{H}_{\text{int}}$.

This new rule is taken from the fields $\psi(x)$ and $\overline{\psi}(y)$, along the lines discussed in footnote 47, and so can be drawn as:

where the small squares represent the fields $\overline{\psi}(x)$ and $\psi(y)$. The Feynman rules for these new vertices are given by the coefficients of $\mathfrak{c}_{\mathbf{p}\sigma}$ and $\mathfrak{c}^\star_{\mathbf{p}\sigma}$ appearing within the expansion (15.2.1) of the fields $\overline{\psi}(x)$ and $\psi(y)$). For these new Feynman rules external lines represent the same fermion propagator as appears in the internal fermion lines, with the difference that it simply ends at x or y.

Once Fourier transformed to momentum space this means that the external 4-momenta need not satisfy $p^2+m^2 = 0$ (*i.e.* they need not be 'on shell'). Often one doesn't use the special symbol on the external lines and takes these new Feynman rules as being implied. Dividing (17.2.24) by the vacuum amplitude $\langle\!\langle 0,\text{out}|0,\text{in}\rangle\!\rangle$ removes all of the diconnected graphs, as described at the end of §12.4, leaving $\widehat{S}(p)$ determined by the sum over all connected Feynman graphs with precisely these two external fermion lines.

Scalar propagator

As a warm-up consider first doing so for the scalar field χ described by the lagrangian (17.1.1). In this case denote the interacting momentum space propagator by $\widehat{G}(p)$, where the Heisenberg-picture correlation function is given by

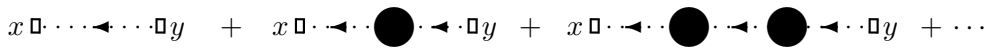
$$\frac{\langle\!\langle 0|T[\chi_h(x)\,\chi_h^\star(y)]|0\rangle\!\rangle}{\langle\!\langle 0,\text{out}|0,\text{in}\rangle\!\rangle} = -i\int\frac{\mathrm{d}^4p}{(2\pi)^4}\,\widehat{G}(p^2)\,e^{ip\cdot(x-y)}\,, \tag{17.2.26}$$

by analogy with the corresponding interaction-picture expression (12.4.20) for the free scalar propagator in the absence of interactions

$$\langle 0|T[\chi(x)\,\overline{\chi}(y)]|0\rangle = -i\int \frac{\mathrm{d}^4p}{(2\pi)^4}\,G(p^2)\,e^{ip\cdot(x-y)} \quad \text{where} \quad G(p^2) = \frac{1}{p^2+m^2-i\delta}\,. \tag{17.2.27}$$

Graphically, $\widehat{G}(p^2)$ is computed by summing all connected graphs with two external lines, which has the following general form:

Propagator Sum: The sum over all connected graphs with two external lines



(17.2.28)

where the large blobs represent the sum over all possible graphs from which the external legs are amputated (*i.e.* the Feynman rule for the external line is ignored) and that are *one-particle irreducible* (or 1PI). A graph is said to be 1PI if it cannot be cut into disconnected pieces by cutting only one internal line. The result for the sum of these 1PI graphs is denoted

$$i(2\pi)^4\Xi(p^2)\,\delta^4(p-q) \tag{17.2.29}$$

where $\Xi(p^2)$ is called the scalar's *self-energy*. Inserting this into the previous graph then implies

$$\begin{aligned}\widehat{G}(p^2) &= G(p^2) + G(p^2)\,\Xi(p^2)\,G(p^2) + G(p^2)\,\Xi(p^2)\,G(p^2)\,\Xi(p^2)\,G(p^2) + \cdots \\ &= G(p^2)\Big[1+\Xi(p^2)\widehat{G}(p^2)\Big]\end{aligned} \tag{17.2.30}$$

which can be solved to give

$$\frac{1}{\widehat{G}(p^2)} = \frac{1}{G(p^2)} - \Xi(p^2) \quad \text{and so} \quad \widehat{G}(p^2) = \frac{1}{p^2+m^2-\Xi(p^2)}\,. \tag{17.2.31}$$

We can now see what it means for the full propagator to have a pole at the same value $p^2=-m^2$ as the leading propagator. It means the self-energy must vanish at $p^2=-m^2$: $\Xi(-m^2)=0$. Writing $\Xi(p^2)=(p^2+m^2)\mathcal{Z}(p^2)$ then implies

$$\widehat{G}(p^2) = \frac{[1-\mathcal{Z}(p^2)]^{-1}}{p^2+m^2}\,. \tag{17.2.32}$$

Furthermore, requiring the residue of $\widehat{G}(p^2)$ for the pole at $p^2=-m^2$ to be unity implies $\mathcal{Z}(-m^2)=0$. In principle one would compute the self-energy and determine the renormalization constants $\chi_B=\sqrt{Z_\chi}\,\chi$ and $m_B^2=m^2-\delta m^2$ by imposing the conditions

$$\Xi(-m^2) = \left(\frac{\partial\Xi}{\partial p^2}\right)_{p^2=-m^2} = 0\,. \tag{17.2.33}$$

The graphs shown in (17.2.28) also provide some direct insight into why these are the right renormalization conditions for determining Z_χ and δm^2. Imagine that this particular collection of graphs were to arise as part of the calculation of a scattering amplitude, with one end attached to the rest of the graph and the other end representing an initial or final scattered particle. (This is called an 'external line correction'.) In this case the Feynman rule for the final external line representing the particle becomes the appropriate particle mode function associated with the particle's momentum $\mathbf{p}$.

But more importantly the particle energy $\varepsilon(p) = \sqrt{\mathbf{p}^2 + m^2}$ then implies the momentum flowing through this part of the graph is on-shell: $p^2 + m^2 = 0$. This is in principle a problem because each of the explicitly drawn internal lines in (17.2.28) is proportional to $(p^2 + m^2)^{-1}$ and so diverges when the momentum flowing through it is on shell. But no problem actually arises in practice *because* the self-energy graphs vanish like $\Xi \propto (p^2 + m^2)^2$ in this limit, as a consequence of the renormalization conditions (17.2.33).

Spin-half propagator

Identical reasoning goes through for the Dirac propagator, with the interacting Heisenberg-picture correlator defined by

$$\frac{\langle\langle 0|T[\psi_h(x)\,\overline{\psi}_h(y)]|0\rangle\rangle}{\langle\langle 0,\mathrm{out}|0,\mathrm{in}\rangle\rangle} = -i\int \frac{\mathrm{d}^4p}{(2\pi)^4}\,\widehat{S}(p)\,e^{ip\cdot(x-y)}\,, \tag{17.2.34}$$

in the same way that the interaction-picture (noninteracting) propagator is given by (15.7.18),

$$\begin{aligned}\langle 0|T[\psi(x)\,\overline{\psi}(y)]|0\rangle \;&=\; -i\int \frac{\mathrm{d}^4p}{(2\pi)^4}\,S(p)\,e^{ip\cdot(x-y)} \\ \text{where}\quad S(p) \;&=\; \frac{-i\not{p}+m}{p^2+m^2-i\delta} = \Big(i\not{p}+m\Big)^{-1}\,.\end{aligned} \tag{17.2.35}$$

In this case the fermion self-energy is the sum over amputated 1PI graphs with two fermion lines, denoted by

$$i(2\pi)^4\Sigma_{mn}(p)\,\delta^4(p-q)\,, \tag{17.2.36}$$

and the sum over all connected graphs implies $\widehat{S}(p)$ is given by (compare to (17.2.31)):

$$\Big[\widehat{S}(p)\Big]^{-1} = i\not{p} + m - \Sigma(p)\,. \tag{17.2.37}$$

Expanding the self-energy in powers of $(i\not{p} + m)$ then gives

$$\Sigma(p) = A + B(i\not{p} + m) + \mathcal{O}[(i\not{p} + m)^2] \tag{17.2.38}$$

so the requirement that the pole remain at $\not{p} = im$ sets $A = 0$ and the condition that the residue of the propagator at this pole be unity implies $B = 0$. These are the conditions that in principle fix the renormalization constants Z_2 and Z_m.

Photon propagator

The photon propagator tells much the same story, with gauge invariance imposing a minor complication. Defining the Heisenberg-picture correlator by

$$\frac{\langle\langle 0|T[A_h^\mu(x)\,A_h^\nu(y)]|0\rangle\rangle}{\langle\langle 0,\text{out}|0,\text{in}\rangle\rangle} = -i\int\frac{\mathrm{d}^4p}{(2\pi)^4}\,\widehat{\Delta}^{\mu\nu}(p)\,e^{ip\cdot(x-y)}\,, \tag{17.2.39}$$

ensures that $\widehat{\Delta}^{\mu\nu}(p)$ is defined in the same way as for the interaction-picture (noninteracting) propagator (16.2.10), for which we take the manifestly covariant form

$$\begin{aligned}\langle 0|T[A^\mu(x)\,A^\nu(y)]|0\rangle &= -i\int\frac{\mathrm{d}^4p}{(2\pi)^4}\,\Delta^{\mu\nu}(p)\,e^{ip\cdot(x-y)}\\ \text{where}\quad \Delta^{\mu\nu}(p) &= \frac{\eta^{\mu\nu}+\alpha\,p^\mu p^\nu}{p^2-i\delta}\,,\end{aligned} \tag{17.2.40}$$

where α is an arbitrary parameter.

The photon self-energy – traditionally called the *vacuum polarization* (for reasons made clearer below) – is the sum over 1PI graphs with two photon lines, denoted by

$$\mu \;\text{●}\; \nu \qquad\qquad i(2\pi)^4\Pi^{\mu\nu}(p)\,\delta^4(p-q)\,. \tag{17.2.41}$$

In this case gauge invariance implies $p_\mu\Pi^{\mu\nu}(p) = 0$, as follows by applying the argument of §16.3 to the graphs contributing to $\Pi^{\mu\nu}$. It follows that $\Pi^{\mu\nu}$ is determined by a single Lorentz-invariant function $\Pi(p^2)$:

$$\Pi^{\mu\nu}(p) = \Big(p^2\eta^{\mu\nu} - p^\mu p^\nu\Big)\,\Pi(p^2)\,. \tag{17.2.42}$$

Following the same steps as for the scalar and electron fields, the sum over all connected graphs with two external photon lines in this case implies

$$\widehat{\Delta}^{\mu\nu}(p) = \Delta^{\mu\nu}(p) + \Delta^{\mu\lambda}(p)\,\Pi_{\lambda\rho}(p)\,\widehat{\Delta}^{\rho\nu}(p)\,, \tag{17.2.43}$$

and once this – after using (17.2.42) – is solved for $\widehat{\Delta}^{\mu\nu}(p)$ one finds

$$\widehat{\Delta}^{\mu\nu}(p) = \frac{\eta^{\mu\nu}}{(p^2-i\delta)\,[1-\Pi(p^2)]} + \frac{p^\mu p^\nu}{p^2}\left\{\alpha - \frac{\Pi(p^2)}{p^2[1-\Pi(p^2)]}\right\}. \tag{17.2.44}$$

Notice that this automatically has a pole at $p^2 = 0$ so long as $\Pi(p^2)$ remains finite[67] as $p^2 \to 0$ (as explicit calculation – see below – shows that it does in QED). This is a consequence of gauge invariance, and in this case no special conditions are required to ensure the propagator has its pole at zero mass. The condition that the residue at this pole remain unity then implies $\Pi(p^2 = 0) = 0$, and this is the condition that fixes the renormalization constant Z_3.

[67] There can be physical situations where $\Pi(p^2)$ does acquire a pole at $p^2 = 0$, notably for superconductors where the pole comes from coupling to a Goldstone boson coming from an electrically charged field, as in §10.3. When this happens in a relativistic setting the pole in the photon propagator shifts away from $p^2 = 0$, indicating the photon has acquired a mass (such as was also found explicitly in §14.4).

Vertex correction

The final renormalization condition is the one that sets the physical value of the electric charge. The electron's electric charge is determined by the matrix element within a one-electron state of the electromagnetic current,

$$\frac{\langle\!\langle e^-(\mathbf{p}',\sigma'),\text{out}|J^\mu(x=0)|e^-(\mathbf{p},\sigma),\text{in}\rangle\!\rangle}{\langle\!\langle 0,\text{out}|0,\text{in}\rangle\!\rangle} = -\frac{ie}{(2\pi)^3}\,\overline{\mathbf{u}}(\mathbf{p}',\sigma')\,\Gamma^\mu(p',p)\,\mathbf{u}(\mathbf{p},\sigma)\,, \tag{17.2.45}$$

where (3.3.9) shows the numerator and denominator are given in interaction picture by

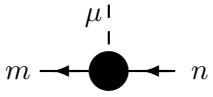
$$\begin{aligned}&\langle\!\langle e^-(\mathbf{p}',\sigma'),\text{out}|J^\mu(x=0)|e^-(\mathbf{p},\sigma),\text{in}\rangle\!\rangle \\ &\quad= \sum_{N=0}^{\infty}\frac{(-i)^N}{N!}\int_{-\infty}^{\infty}\mathrm{d}^4x_1\cdots\mathrm{d}^4x_N\;\langle e^-(\mathbf{p}',\sigma')|T\Big[J^\mu(0)\mathcal{H}_{\text{int}}(x_1)\cdots\mathcal{H}_{\text{int}}(x_N)\Big]|e^-(\mathbf{p},\sigma)\rangle\end{aligned} \tag{17.2.46}$$

and

$$\langle\!\langle 0,\text{out}|0,\text{in}\rangle\!\rangle = \sum_{N=0}^{\infty}\frac{(-i)^N}{N!}\int_{-\infty}^{\infty}\mathrm{d}^4x_1\cdots\mathrm{d}^4x_N\;\langle 0|T\Big[\mathcal{H}_{\text{int}}(x_1)\cdots\mathcal{H}_{\text{int}}(x_N)\Big]|0\rangle\,. \tag{17.2.47}$$

This shows that $\mathbf{u}(\mathbf{p},\sigma)$ is the single-particle mode function derived in (15.2.13) coming from the external line Feynman rules for the fermions, and whose properties are explored in detail in §15.2.

With these definitions $\Gamma^\mu(p',p)$ is the sum over all connected[68] Feynman graphs with two electron and one photon external line,



$$e\,(2\pi)^4\Gamma^\mu_{mn}(p',p)\,\delta^4(q+p'-p)\,. \tag{17.2.48}$$

where p^μ is the electron momentum flowing in from the right, $(p')^\mu$ is the electron momentum flowing out to the left and q^μ is the momentum flowing out along the photon line. Because the Feynman rule for the operator J^μ just differs from $\mathcal{H}_{\text{int}}$ by a factor of A_μ, no new Feynman rule need be associated with J^μ provided we regard the external photon line as being 'amputated' because there is no initial or final photon state associated with it. The factors out front of the definition of $\Gamma^\mu(p',p)$ are chosen to ensure that the leading order graph (which is simply the basic interaction vertex given in (16.2.16)) gives $\Gamma^\mu_{\text{lowest}-\text{order}} = \gamma^\mu$.

The expectation value of the electromagnetic current in a single-electron state is the $p'\to p$ limit of (17.2.45), and so the condition that $-e$ is the physical electron charge is that this limit should simply agree with the value $\Gamma^\mu_{\text{lowest}-\text{order}}$ obtained in the free theory. Writing the full result as

$$\Gamma^\mu_{mn}(p',p) = (\gamma^\mu)_{mn} + \Lambda^\mu_{mn}(p',p)\,, \tag{17.2.49}$$

[68] Disconnected graphs are cancelled here by the division by the vacuum matrix element, along the lines discussed around eq. (12.4.24).

this implies the renormalization condition becomes

$$\Lambda^\mu(p', p) \to 0 \quad \text{as} \quad p' \to p\,. \tag{17.2.50}$$

It is intuitive that Λ^μ should vanish as the electromagnetic 4-momentum tends to zero because the electron's electric charge can be measured by electromagnetic scattering at low energies and large distances, where the Coulomb interaction dominates and the charge can be read off using Gauss' law from the electromagnetic field at infinity. A more precise statement of this condition is given in (17.6.17) below.

17.2.4 Divergence counting

We now return to the issue of divergences and show that the above renormalization conditions automatically ensure that the divergences appearing in the renormalization constants δZ_i cancel all divergences in physical predictions. This verifies how predictions are UV finite once expressed in terms of physical couplings. As an intermediate step towards this end it is necessary to determine once and for all how badly any general Feynman graph diverges at short distances (or high momenta).

To make the argument as general as possible, consider a quantum field theory more general than QED containing a variety of particle types and a variety of interactions involving these particle types. Consider a specific (but arbitrary) Feynman graph in this theory. This contains:

- E_i external lines of particle type i, with a total of $E = \sum_i E_i$ external lines;
- I_i internal lines describing propagators of particle type i, for a total of $I = \sum_i I_i$ internal lines. We are interested in the large-momentum behaviour of the Feynman graph, so suppose that the propagator for particle i varies like

  $$G_i(p) \sim \frac{1}{(p^2)^{1-s_i}} \qquad \text{for large } p\,. \tag{17.2.51}$$

  Of the fields encountered so far we have seen $s_i = 0$ for spinless particles and photons while $s_i = \frac{1}{2}$ for spin-half particles.
- V_r vertices where r runs over all distinct monomials of fields in $\mathcal{L}_{\text{int}}$. Furthermore, we suppose the monomial involves precisely d_r derivatives and ℓ_{ri} fields of type i so that the corresponding vertex involves the meeting of ℓ_{ri} lines of type i and (in momentum space) a product of d_r factors of 4-momentum.

As described in §16.2 these variables are not all independent because relations are forced between them by the nuts and bolts of building graphs. In particular, the law of 'conservation

of ends' (counting the ends of lines using E_i and I_i must agree with the counting of ends that meet at all of the vertices) implies that for each i (compare with (16.2.20)):

$$E_i + 2I_i = \sum_r V_r \ell_{ri} \qquad \text{(conservation of ends, for each } i\text{)}. \tag{17.2.52}$$

For ultraviolet divergences it is the largest momenta in the problem that are of interest, so we ignore external momenta or masses in the Feynman rules. A diagnostic for whether the integrations in a graph diverge or not is then given by the total power of momentum in the numerator minus the total power of momentum in the denominator.[69]

The locality of the lagrangian implies the only momenta appearing in a denominator are those coming from the propagators, for which (17.2.51) shows that all of the internal lines combined contribute a factor $(1/p)^{N_{\text{denom}}}$ with

$$N_{\text{denom}} = \sum_i I_i(2 - 2s_i)\,. \tag{17.2.53}$$

There are two kinds of contribution to the numerator: explicit powers of momentum in the vertices $p^{N_{\text{vert}}}$ and a factor of d^4p for each independent integration. The power coming from vertices is simply d_r for each vertex and so

$$N_{\text{vert}} = \sum_r V_r d_r\,. \tag{17.2.54}$$

The same arguments as in §16.2 also show that the total number of integrations, N_{int}, is given by the number of internal lines minus the number of momentum-conserving delta functions plus one (because one delta function expresses conservation of external momentum and so does not depend the momentum being integrated):

$$N_{\text{int}} = \sum_i I_i - \sum_r V_r + 1\,. \tag{17.2.55}$$

This is again the number of loops L in the graph of interest.

Since each integral contributes four factors of $\mathrm{d}p$ the total net power of momentum carried by the graph is

$$\begin{aligned} D &= 4N_{\text{int}} + N_{\text{vert}} - N_{\text{denom}} \\ &= 4\left(\sum_i I_i - \sum_r V_r + 1\right) + \sum_r V_r d_r - \sum_i I_i(2 - 2s_i) \\ &= 4 - \sum_i E_i(1 + s_i) - \sum_r V_r \Delta_r\,, \end{aligned} \tag{17.2.56}$$

[69] It is in principle more complicated than this because we are really talking about multi-dimensional integrals for which the large momenta might only flow through a subset of the graph, potentially leaving residual dependence on external momenta. However a theorem due to Weinberg shows that these complications only contribute logarithmically and so the naive dimension counting given here actually works.

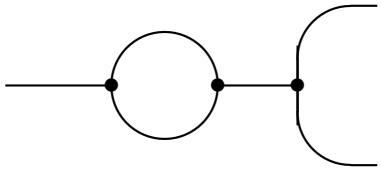


Figure 12. A representative Feynman graph for a scalar-field χ^3 interaction displaying a radiative correction to an external line for which the full graph has $D < 0$ while the self-energy subgraph has $D = 2$.

where the last line uses (17.2.52) to eliminate I_i and defines

$$\Delta_r := 4 - d_r - \sum_i \ell_{ri}(1 + s_i)\,. \tag{17.2.57}$$

The quantity Δ_r has a simple interpretation in terms of couplings in $\mathcal{H}_{\rm int}(x)$. A vertex with d_r derivatives and ℓ_{ri} external i-type lines must come from an interaction of schematic form

$$\mathcal{H}_{\rm int} \ni g_r\, \partial^{d_r} \prod_i \psi_i^{\ell_{ri}}\,, \tag{17.2.58}$$

where g_r is the coupling constant for this interaction. But the asymptotic condition (17.2.51) implies the field ψ_i has dimension $(\text{mass})^{1+s_i}$ because it states that there is a regime for which

$$\int \mathrm{d}^4x \langle 0|T\Big[\psi_i(x)\,\psi_i^\star(0)\Big]|0\rangle\; e^{ip\cdot x} \sim \frac{1}{p^{2-2s_i}}\,. \tag{17.2.59}$$

Because $\mathcal{H}_{\rm int}$ has dimension $(\text{mass})^4$ the dimension of the coupling g_r must be $(\text{mass})^{\Delta_r}$.

The quantity D is called the *superficial degree of divergence* and based on the above reasoning we expect a graph to diverge in the UV like

$$\int^\Lambda \mathrm{d}p\; p^{D-1} \sim \begin{cases} \Lambda^D & \text{when } D > 0 \\ \log\Lambda & \text{when } D = 0 \end{cases} \tag{17.2.60}$$

D is called the 'superficial' degree of divergence for several reasons besides the issues described in footnote 69. An important one is that graphs can also diverge even if $D < 0$ if they contain a subgraph for which $D \geq 0$ for the subgraph separately, such as is true in particular for the one-loop graph shown in Fig. 12. For this graph there is only one type of field (a scalar χ for which $s = 0$) and one type of cubic χ^3 vertex (which has $d = 0$ and $\ell = 3$ and so $\Delta = 1$). The graph satisfies $E = 3$, $V = 3$ and $L = 1$ and so for the entire graph $D = 4 - 3 - 3 = -2$. But the graph nonetheless diverges because of the self-energy loop subgraph, which if regarded as a graph on its own has $E = 2$, $V = 2$ and $L = 1$ and so $D = 4 - 2 - 2 = 0$.

Nonetheless, these expressions for D are useful because they give a way to think about which graphs should diverge and so might need absorbing into a parameter, particularly

when applied to *1-particle irreducible* (or 1PI) graphs. 1PI graphs are defined as those that cannot be broken into two disconnected graphs simply by cutting a single internal line, and are useful because *any* connected graph can be regarded as a tree graph (*i.e.* no loops) built using propagators and vertices constructed using only 1PI graphs. Since tree graphs do not diverge (because all internal momentum integrals can be performed using the 4-momentum conservation delta functions) this shows that any primitive divergences can be isolated by looking only at how 1PI graphs diverge.

17.2.5 Renormalizable theories

What is noteworthy about (17.2.56) is that all but the last sum is fixed purely by the graph's number of external lines. The last term also shows that only a limited number of graphs can diverge in theories for which all interactions have $\Delta_r \geq 0$. The kinds of divergences that arise is limited when this is true because $\Delta_r \geq 0$ for all r implies

$$D \leq D_{\max} = 4 - \sum_i E_i(1+s_i) \qquad (\text{if } \Delta_r \geq 0 \;\forall\; r)\,. \tag{17.2.61}$$

If only graphs with $D \geq 0$ are divergent then (17.2.61) shows that divergences only happen for graphs with a relatively small number of external lines. Theories are called *renormalizable* if $\Delta_r \geq 0$ for all of their interactions and if they include all possible such interactions consistent with their particle content and symmetries.

There is one final observation about divergences that plays an important role in what follows: any divergent part of a momentum-space Feynman graph can only involve a polynomial of the external momenta. This is because differentiating any amplitude with repect to external momenta takes D to $D-1$. This lowering of D through differentiation is clear on dimensional grounds because the more dimensions that are soaked up using external momenta, the fewer powers of loop momentum are possible in the above estimate of the graph's large-p behaviour. The reduction happens concretely because the external momenta appear in loop graphs in the denominator of a propagator, and differentiating these denominators introduces more powers of loop momenta into the denominator and so makes the graph more convergent. Sufficiently many derivatives eventially make D negative. In particular, the divergent contribution should be independent of external momenta for a $D=0$ graph; at most linear in momentum for a $D=1$ graph and so on. Schematically:

$$\begin{aligned} \mathcal{A}_{D=0}(p) &\sim C_1 \log\Lambda + \mathcal{A}_{\text{finite}}(p)\,, \qquad \mathcal{A}_{D=1}(p) \sim C_1\Lambda + C_2\, p\, \log\Lambda + \mathcal{A}_{\text{finite}}(p) \\ \mathcal{A}_{D=2}(p) &\sim C_1\Lambda^2 + C_2\, p\,\Lambda + C_3\, p^2 \log\Lambda + \mathcal{A}_{\text{finite}}(p)\,. \end{aligned} \tag{17.2.62}$$

Some of the C_i's in this expression may vanish if they are inconsistent with the symmetry-transformation properties of the amplitude of interest.[70]

[70] Unless the regularization procedure itself breaks the symmetries – which is why it is preferable to regulate in a way that respects the symmetries of the problem.

For QED there are two types of fields (corresponding to the photon and electron), so $i = p, e$ with $s_p = 0$ and $s_e = \frac{1}{2}$. There is only one interaction plus the counter-terms, and for all of these $\Delta_r \geq 0$. For instance, the photon-fermion vertex has $d = 0$, $\ell_p = 1$ and $\ell_e = 2$. Therefore $\Delta = 4 - 0 - 1 - 2(\frac{3}{2}) = 0$, consistent with its coupling e being dimensionless. Furthermore there are no other interactions that can be built from a spin-half fermion ψ and the electromagnetic field A_μ that are Lorentz invariant and have couplings with non-negative dimension, so QED turns out to be renormalizable.

Lorentz invariant divergent forms	E_e	E_p	D	gauge invariant form
$\mathcal{A}^{\mu\nu\lambda\rho} \propto \eta^{\mu\nu}\eta^{\lambda\rho} + \eta^{\mu\lambda}\eta^{\nu\rho} + \eta^{\mu\rho}\eta^{\lambda\nu}$	0	4	0	not allowed
$\mathcal{A}^{\mu\nu\lambda} \propto \eta^{\mu\nu}p^\lambda + \eta^{\mu\lambda}p^\nu + \eta^{\nu\lambda}p^\mu$	0	3	1	not allowed
$\mathcal{A}^{\mu\nu} \propto C_1\eta^{\mu\nu}p^2 + C_2 p^\mu p^\nu$	0	2	2	$\eta^{\mu\nu}p^2 - p^\mu p^\nu$
$\mathcal{A}^{\mu}_{mn} \propto (\gamma^\mu)_{mn}$	2	1	0	$(\gamma^\mu)_{mn}$
$\mathcal{A}_{mn} \propto C_3(\gamma^\mu)_{mn}p_\mu + C_4\delta_{mn}$	2	0	1	$C_3(\gamma^\mu)_{mn}p_\mu + C_4\delta_{mn}$

Table 6. Possible divergent amplitudes in QED with $D \geq 0$. Terms with γ_5 in the bottom two rows are not included on grounds of parity invariance.

In QED which graphs can have $D \geq 0$? The list consistent with Lorentz invariance is given in Table 6. As the table shows, not all of the options in the table actually diverge in QED, because gauge invariance implies that any amplitude with an external photon must vanish if the external photon polarization is replaced by the photon 4-momentum: $\epsilon_\mu(p) \to p_\mu$ (which follows from invariance under $A_\mu \to A_\mu + \partial_\mu\omega$), and this is inconsistent with the possible momentum dependence of divergent terms for graphs with three or four external photons. This implies amplitudes with three or four photons must also involve at least some additional factors of external momenta, which is enough to make them UV finite.

What is striking about the entries of Table 6 is that each entry has the same momentum dependence as the Feynman rules derived above for the counter-term interactions. So although the reorganization of perturbation theory around a free theory with the physical mass and field normalizations would have been important to do regardless of whether or not anything diverged, a side effect of this renormalization process is to precisely cancel the divergences that were encountered in calculations in the absence of the counter-terms.

17.3 Self-energies

To make the above discussion more concrete it is useful to explicitly evaluate several examples of one-loop effects. We start in this section with the one-loop self-energies for the electron and the photon (where the photon self-energy is usually called the vacuum polarization, for reasons that become clear in what follows).

17.3.1 Electron self-energy

The electron self-energy is given by the sum of all connected graphs that have precisely two electron external lines. We regard these graphs as arising from the evaluation of the matrix element of (17.2.24), though following the discussion below (17.2.35) we evaluate the self-energy by keeping only 1PI graphs and amputating the external legs. This leads to the following one-loop contribution, plus a counter-term graph:

(a) (b)

The vertex correction Feynman rule is as given in (17.2.22), repeated here:

$$-i\Big(i\delta Z_2 \not{p} + \delta Z_m m\Big)_{mn} (2\pi)^4 \delta^4(p-q)\,. \tag{17.3.1}$$

Worked example: Evaluating the electron self-energy

Denoting the result for the loop graph (after amputing the external lines) as $i(2\pi)^4\Sigma(p)\,\delta^4(p'-p)$, direct use of the Feynman rules evaluates it to give

$$\begin{aligned} i(2\pi)^4\Sigma(p) \;=\; 2\left[\frac{(-i)^2}{2!}\right]\int \frac{\mathrm{d}^4k}{(2\pi)^4 i}\,\frac{1}{k^2-i\delta}\,\Big[ie\gamma^\mu(2\pi)^4\Big] \\ \times\left[\frac{1}{(2\pi)^4 i}\,\frac{-i(\not{p}+\not{k})+m}{(p+k)^2+m^2-i\delta}\right]\Big[ie\gamma_\mu(2\pi)^4\Big]\,, \end{aligned} \tag{17.3.2}$$

where the initial factor of 2 arises from the two choices for the vertex that the incoming fermion can first connect to, the $(-i)^2/2!$ is the usual coefficient in the second order expansion of the S-matrix, and so on.

Combining terms and dimensionally regulating the integral (which diverges in the UV) gives

$$\Sigma(p) = ie^2\mu^{4-n}\int \frac{\mathrm{d}^n k}{(2\pi)^n}\,\frac{N}{D}\,, \tag{17.3.3}$$

where

$$N = \gamma^\mu\Big[-i(\not{p}+\not{k})+m\Big]\gamma_\mu = (n-2)i(\not{p}+\not{k})+nm\,. \tag{17.3.4}$$

Performing the Feynman trick using identity (17.1.15) allows the denominator to be written $D^{-1} = \int_0^1 \mathrm{d}x\;\mathcal{D}^{-2}$ with

$$\begin{aligned} \mathcal{D} \;&=\; (1-x)(k^2-i\delta) + x\Big[(p+k)^2+m^2-i\delta\Big] \\ &=\; \Big(k+xp\Big)^2 + p^2x(1-x) + xm^2 - i\delta\,. \end{aligned} \tag{17.3.5}$$

Changing integration variable to $\hat{k}^\mu := (k+xp)^\mu$ simplifies the denominator to $\mathcal{D} = \hat{k}^2 + a^2 - i\delta$ with $a^2 := p^2x(1-x) + xm^2$. Since the rest of the integral is symmetric under $\hat{k} \to -\hat{k}$ any term

linear in $\hat{k}$ in the numerator integrates to zero, and so can be dropped inside the integral. After Wick rotating to Euclidean signature using $\mathrm{d}^n k = i\mathrm{d}^n k_{\scriptscriptstyle E}$ this leads to the expression

$$\Sigma(p) = -e^2\mu^{4-n}\int_0^1 \mathrm{d}x \int \frac{\mathrm{d}^n\hat{k}_{\scriptscriptstyle E}}{(2\pi)^n}\,\frac{(n-2)(1-x)i\not{p}+nm}{(\hat{k}_{\scriptscriptstyle E}^2+a^2)^2}\,. \tag{17.3.6}$$

Evaluating the integral using (17.1.5) then gives

$$\begin{aligned}\mu^{4-n}\int \frac{\mathrm{d}^n\hat{k}_{\scriptscriptstyle E}}{(2\pi)^n}\frac{1}{(\hat{k}_{\scriptscriptstyle E}^2+a^2)^2} &= \frac{\mu^{4-n}}{(2\pi)^n}\,J(0,2;a^2) = \frac{1}{(4\pi)^2}\left(\frac{a^2}{4\pi\mu^2}\right)^{(n-4)/2}\Gamma\left(2-\tfrac{1}{2}n\right)\\ &= \frac{1}{(4\pi)^2}\left[\frac{1}{\epsilon}-\gamma-\log\left(\frac{a^2}{4\pi\mu^2}\right)+\mathcal{O}(\epsilon)\right],\end{aligned} \tag{17.3.7}$$

for $n = 4-2\epsilon$, and so the self-energy becomes

$$\Sigma(p) = C_1 m + iC_2\not{p} + \frac{e^2}{(4\pi)^2}\int_0^1 \mathrm{d}x\Big[2(1-x)i\not{p}+4m\Big]\log\left[\frac{x(1-x)p^2+xm^2}{4\pi\mu^2}\right], \tag{17.3.8}$$

where C_1 and C_2 are divergent constants.

With an explicit expression in hand we can see how the above combines with the counterterm to impose the renormalization conditions described earlier. These asked the self-energy not to change the position of the propagator's pole or its residue at that pole, which amounts to demanding

$$\Sigma + \Sigma_{\rm ct} = \Sigma_\star(p)\,, \tag{17.3.9}$$

where $\Sigma_\star$ vanishes at least quadratically in $(i\not{p}+m)$ as $\not{p}\to im$ so that

$$\lim_{\not{p}\to im}(i\not{p}+m)^{-1}(\Sigma+\Sigma_{\rm ct}) = \frac{1}{i\not{p}+m}\,\Sigma_\star(p) = 0\,. \tag{17.3.10}$$

Using this in (17.3.8) then gives the following expression for $\Sigma_\star(p)$:

$$\Sigma_\star(p) = \frac{e^2}{(4\pi)^2}\int_0^1 \mathrm{d}x\left\{\Big[2(1-x)i\not{p}+4m\Big]\log\left[\frac{1+(1-x)(p^2/m^2)}{x}\right]-\frac{4(1-x^2)}{x}(i\not{p}+m)\right\}. \tag{17.3.11}$$

Although this expression is UV finite, notice the divergence in the x integral near $x\to 0$. This arises because the denominator in (17.3.5) is singular in the limit that both x and k^2 are small, the sign of an *infrared* (or IR) divergence. More about the meaning of these IR divergences is explained in §17.5 and §18.5.6 below.

17.3.2 Photon self-energy

A similar calculation also applies for the photon self-energy, which shows why the physical renormalization conditions imply that self-energy graphs on external lines drop out in photon-scattering processes. For electromagnetic fields the off-shell value for the self-energy can have interesting physical consequences, as described in §17.4, since it shows how virtual particle-antiparticle pairs act to screen charges and so to cause the effective strength of electromagnetic

couplings to depend on the length scale on which they are measured. This contains the seeds of the idea of 'running' couplings.

The single one-loop photon self-energy graph, and its counter-term graph, are:

(c) (d) (17.3.12)

The Feynman rule for the counterterm is given by (17.2.21), reproduced here

$$-\frac{i}{2}\,\delta Z_3\Big(q^2\eta_{\mu\nu}-q_\mu q_\nu\Big)(2\pi)^4\delta^4(q'-q)\,, \tag{17.3.13}$$

where the 4-momentum flowing through this line is denoted q^μ.

Worked example: Evaluating the vacuum polarization

Denoting the result for the loop graph by $i(2\pi)^4\Pi^{\mu\nu}(q)\,\delta^4(q'-q)$, the Feynman rules for the loop graph show that it evaluates to the following expression:

$$\begin{aligned} i(2\pi)^4\Pi^{\mu\nu}(q) \;=\; -2\left[\frac{(-i)^2}{2!}\right]\int \mathrm{d}^4p\left[\frac{1}{(2\pi)^4 i}\;\frac{1}{p^2+m^2-i\delta}\right]\left[\frac{1}{(2\pi)^4 i}\;\frac{1}{(p-q)^2+m^2-i\delta}\right] \\ \times\mathrm{Tr}\left\{\Big[ie\gamma^\mu(2\pi)^4\Big]\Big[-i(\not{p}-\not{q})+m\Big]\Big[ie\gamma^\nu(2\pi)^4\Big]\Big(-i\not{p}+m\Big)\right\}, \end{aligned} \tag{17.3.14}$$

where the initial factor of 2 is the symmetry factor counting the number of ways the ingredients can assemble into this graph, the $(-i)^2/2!$ is the usual coefficient in the second order expansion of the S-matrix, and so on. The overall minus sign comes from the interchange of fermionic fields that is always present for a fermionic closed loop.

This simplifies down to the form

$$\Pi^{\mu\nu}(q) = -ie^2\int\frac{\mathrm{d}^4p}{(2\pi)^4}\;\frac{N^{\mu\nu}}{D}\,, \tag{17.3.15}$$

where

$$D := \Big[p^2+m^2-i\delta\Big]\Big[(p-q)^2+m^2-i\delta\Big] \tag{17.3.16}$$

and

$$N^{\mu\nu} = \mathrm{Tr}\left\{(-i\not{p}+m)\gamma^\mu[-i(\not{p}-\not{q})+m]\gamma^\nu\right\}. \tag{17.3.17}$$

The now-standard Feynman trick using identity (17.1.15) implies $D^{-1}=\int_0^1\mathrm{d}x\;\mathcal{D}^{-2}$ with

$$\begin{aligned}\mathcal{D} \;&=\; (1-x)(p^2+m^2-i\delta)+x\Big[(p-q)^2+m^2-i\delta\Big] \\ &=\; (p-xq)^2+q^2x(1-x)+m^2-i\delta\,,\end{aligned} \tag{17.3.18}$$

suggesting changing integration variable to $\hat{p}^\mu := (p+xq)^\mu$ so the denominator becomes $\mathcal{D}=\hat{p}^2+a^2-i\delta$ with $a^2 := q^2x(1-x)+m^2$. The symmetry of the rest of the integral under $\hat{p}\to-\hat{p}$ allows dropping

odd powers of $\hat{p}$ in the numerator as well as the replacement $\hat{p}_\mu\,\hat{p}_\nu \to (\hat{p}^2/n)\,\eta_{\mu\nu}$ (due to the Lorentz invariance of the rest of the integral). Dimensionally regularizing then leads to the expression

$$\begin{aligned} N^{\mu\nu} &= \mathrm{Tr}\left\{[-i\hat{\not{p}} - xi\not{q} + m]\gamma^\mu[-i\hat{\not{p}} + (1-x)i\not{q} + m]\gamma^\nu\right\} \\ &= \mathrm{Tr}\left\{-\frac{\hat{p}^2}{n}\gamma_\lambda\gamma^\mu\gamma^\lambda\gamma^\nu + x(1-x)\not{q}\gamma^\mu\not{q}\gamma^\nu + m^2\gamma^\mu\gamma^\nu\right\}, \end{aligned} \tag{17.3.19}$$

where the second line uses that Dirac traces vanish unless they involve an even number of gamma matrices. Evaluating the traces using (15.3.21) — but with $\mathrm{Tr}\, I = 2^\varpi$ in n dimensions, where $\varpi(n)$ interpolates between the values $\varpi(n) = \frac{1}{2}n$ when n is an even positive integer and $\varpi(n) = \frac{1}{2}(n-1)$ for n an odd positive integer — then gives

$$N^{\mu\nu} = 2^\varpi\left[\frac{n-2}{n}\hat{p}^2\eta^{\mu\nu} + x(1-x)\Big(2q^\mu q^\nu - q^2\eta^{\mu\nu}\Big) + m^2\eta^{\mu\nu}\right]. \tag{17.3.20}$$

Finally, Wick rotating and evaluating the $\mathrm{d}^4p_{\scriptscriptstyle E}$ integral using (17.1.5) gives

$$\begin{aligned} \mathcal{I} := \mu^{4-n}\int\frac{\mathrm{d}^np}{(2\pi)^n}\,\frac{1}{(p^2+a^2-i\delta)^2} &= \frac{i}{(4\pi)^{n/2}}\left(\frac{a}{\mu}\right)^{n-4}\Gamma\left(2-\tfrac{1}{2}n\right) \\ &= \frac{i}{(4\pi)^{n/2}}\left(\frac{a}{\mu}\right)^{n-4}\frac{n-2}{n}\,\Gamma\left(1-\tfrac{1}{2}n\right), \end{aligned} \tag{17.3.21}$$

where the second line uses $z\Gamma(z) = \Gamma(z+1)$. On the other hand the $\hat{p}^2$ terms involve the integral

$$\begin{aligned} \frac{n-2}{n}\,\mu^{4-n}\int\frac{\mathrm{d}^np}{(2\pi)^n}\,\frac{p^2}{(p^2+a^2-i\delta)^2} &= \frac{ia^2}{(4\pi)^{n/2}}\left(\frac{a}{\mu}\right)^{n-4}\frac{2-n}{2}\,\Gamma\left(1-\tfrac{1}{2}n\right) \\ &= -a^2\mathcal{I}\,. \end{aligned} \tag{17.3.22}$$

Using $n = 4-2\epsilon$ the required integral becomes

$$\mathcal{I} = \frac{i}{(4\pi)^{n/2}}\left(\frac{a}{\mu}\right)^{n-4}\Gamma\left(2-\tfrac{1}{2}n\right) = \frac{i}{(4\pi)^2}\left\{\frac{1}{\epsilon} - \gamma - \log\left[\frac{x(1-x)q^2+m^2}{4\pi\mu^2}\right]\right\}. \tag{17.3.23}$$

Combining these integrals then leaves

$$\begin{aligned} \Pi^{\mu\nu}(q) &= -2^\varpi ie^2\int_0^1\mathrm{d}x\,\mathcal{I}\Big\{-\Big[x(1-x)q^2+m^2\Big]\eta^{\mu\nu} + x(1-x)\Big(2q^\mu q^\nu - q^2\eta^{\mu\nu}\Big) + m^2\eta^{\mu\nu}\Big\} \\ &= 2^{\varpi+1}ie^2\Big(q^2\eta^{\mu\nu} - q^\mu q^\nu\Big)\int_0^1\mathrm{d}x\,\mathcal{I}\,x(1-x)\,, \end{aligned} \tag{17.3.24}$$

showing the expected gauge-invariant tensor structure[71] that satisfies $q_\mu\Pi^{\mu\nu}(q) = 0$. Writing

$$\Pi^{\mu\nu}(q) = (q^2\eta^{\mu\nu} - q^\mu q^\nu)\Pi(q^2) \tag{17.3.25}$$

shows that the self-energy is captured by the single Lorentz-invariant function

$$\Pi(q^2) = -\frac{2^{\varpi+1}e^2}{(4\pi)^2}\int_0^1\mathrm{d}x\,x(1-x)\left\{\frac{1}{\epsilon} - \gamma - \log\left[\frac{x(1-x)q^2+m^2}{4\pi\mu^2}\right]\right\}, \tag{17.3.26}$$

[71] It is noteworthy that this form relied in detail on doing the Dirac algebra in n dimensions as well as continuing momenta to n dimensions. This is because the Dirac lagrangian in n dimensions relies on there being n matrices $\gamma^{\mu_1},\cdots,\gamma^{\mu_n}$ satisfying $\{\gamma^\mu,\gamma^\nu\} = 2\eta^{\mu\nu}$ for all n indices μ and ν.

showing that all of the divergences and ambiguity contribute as an additive constant to $\Pi(q^2)$.

This last expression has precisely the form that allows the divergent part to be cancelled by the counter-term graph, in order to impose the renormalization condition discussed below (17.2.44) that states $\Pi(q^2) + \Pi_{\rm ct}(q^2) = \Pi_\star(q^2)$ vanishes at $q^2 = 0$, leaving the μ-independent result

$$\Pi_\star(q^2) = \frac{e^2}{2\pi^2}\int_0^1 \mathrm{d}x\; x(1-x)\log\left[\frac{x(1-x)q^2+m^2}{m^2}\right] . \tag{17.3.27}$$

For later reference – *c.f.* §17.4 – the renormalization constant that accomplishes this is

$$Z_3 = 1 + \Pi(q^2=0) = 1 - \frac{e^2}{12\pi^2}\left[\frac{1}{\epsilon} - \gamma - \log\left(\frac{m^2}{4\pi\mu^2}\right)\right] . \tag{17.3.28}$$

17.4 Vacuum polarization and running couplings

Before moving on to compute the one-loop correction to the photon-electron interaction – *i.e.* the *vertex correction* and its associated prediction for anomalous magnetic moments – this section pauses to explore the physical interpretation of the photon self-energy computed above, and the implications associated with renormalizing the photon field: $A^B_\mu = Z_3^{1/2} A_\mu$, with Z_3 given explicitly by (17.3.28).

17.4.1 Vacuum polarization

The main observation is the similarity between $A^B_\mu = Z_3^{1/2}A_\mu$ and relations like $\mathbf{D} = \epsilon\,\mathbf{E}$ between microscopic and macroscopic fields within a dielectric medium, such as the polarizable media discussed in §10.1. This similarity suggests that the photon self-energy $\Pi(q^2)$ can be interpreted as the polarization of the quantum vacuum itself due to the presence in it of fluctuating interaction energy density[72] $\mathcal{H}_{\rm int}(x)$ (which fluctuates in an energy eigenstate because it does not commute with the total Hamiltonian). It is for this reason that $\Pi(q^2)$ is often called the *vacuum polarization*.

To make this connection precise we compute in this section the local induced charge density that is implied by $\Pi_\star(q^2)$ and show how it acts to screen charges by an amount that precisely reproduces the size of Z_3 computed in (17.3.28). To this end it is more useful to have Z_3 expressed in terms of a microscopic length scale a (or a large energy scale Λ with $a = \Lambda^{-1}$) rather than the dimensional-regularization parameter $n-4$. Recall that the need for regularization arose because the integral in (17.3.14) diverges in the UV, and does so logarithmically if Λ were a UV cutoff, leading to $Z_3 = 1 + c\,\log(\Lambda^2/m^2) + (\text{finite})$ for some coefficient c.

The precise value for c can be found by comparing $m^2\,\partial Z_3/\partial m^2$ with the result found in (17.3.28) using dimensional regularization, since differentiating the original integral with respect to m^2 gives a UV finite integral on which all regularizations must agree (according to

[72] Because these fluctuations are described in perturbation theory using Feynman graphs like those in (17.3.12), they are often colloquiually called 'virtual electron-positron pairs'.

the rules on regularization laid out in §9.3.1). This (or direct calculation) shows that using a direct cutoff would imply $c = -e^2/(12\pi^2)$ and so

$$Z_3 = 1 - \frac{e^2}{12\pi^2} \log\left(\frac{\Lambda^2}{m^2}\right) . \tag{17.4.1}$$

Trusting perturbation theory requires the deviation from unity here to be small, but the small size of $e^2/(12\pi^2)$ ensures this is true even if Λ is enormous (such as beyond the Planck scale $\Lambda \gtrsim M_p \sim 10^{18}$ GeV).

What is significant in what follows is the sign of the logarithm in this expression, since it implies $0 < Z_3 < 1$. Because bare and renormalized charges are related by $e_B = Z_3^{-1/2} e$ – *c.f.* (17.2.14) and (17.2.17) – having $Z_3 < 1$ implies $e < e_B$ and so bare charges become screened by virtual electron-positron effects, leading to smaller physical charges. This resembles a dielectric for which a charge density ρ leads – *via* the Maxwell equation $\nabla \cdot \mathbf{D} = \rho$ – to an electric field $\mathbf{E}$ that is effectively sourced by a screened charge ρ/ϵ, where ϵ is the dielectric's permittivity.

The logarithmic divergence in Z_3 also has a physical interpretation in this picture. As we see below, the above calculation of $\Pi_\star(q^2)$ implies that when very small 'point' particles[73] with charge Q_B scatter electromagnetically, they do so in a way that looks as it would if each charge polarized the vacuum to induce a local charge density about itself with a specific profile $\varrho_{\rm pol}(r)$. The profile $\varrho_{\rm pol}(r)$ falls to zero exponentially for $r > m^{-1}$ but behaves as

$$\varrho_{\rm pol}(r) \simeq -\frac{e^2 Q_B}{48\pi^3 r^3} \quad \text{in the regime} \quad \Lambda^{-1} \ll r \ll m^{-1} . \tag{17.4.2}$$

Because of this the net charge seen at distances $r \gg m^{-1}$ is given by

$$Q = Q_B + 4\pi \int_{m^{-1}}^{\Lambda^{-1}} {\rm d}r\, r^2 \varrho_{\rm pol}(r) = Q_B \left\{1 - \frac{e^2}{6\pi^2}\left[\log\left(\frac{\Lambda^2}{m^2}\right) + (\text{finite})\right]\right\} , \tag{17.4.3}$$

in agreement with (17.4.1) once we define $Q = Z_3^{1/2} Q_B$.

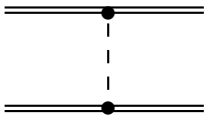
Of course the vacuum is electrically neutral and charge is conserved, so the above cannot be quite the full story. For instance, if we were to insert a charge Q_B into a small sphere of radius $a = \Lambda^{-1}$ excised out of a dielectric material, then besides inducing an extended charge density $\varrho_{\rm pol}(r)$ like the one described above, one would also induce a compensating surface charge density at the boundary of the sphere, with the surface charge cancelling the polarized 'bulk' charge. That is how the bulk charge builds up: opposite charges get attracted to the boundary, and then their accumulation there starts to distort the charge density in the rest of the bulk. In a real (electrically neutral) dielectric we know that the total charge seen at infinity agrees in the end with Q_B because of this cancellation. But in the vacuum we (by assumption) cannot resolve physics at distances as small as Λ^{-1} and so we have no way to separate the surface and interior charges. We instead lump them together into what we call Q_B, which then *can* differ from the charge seen at infinity.

[73] Here 'point' means the charged object is smaller in size than a sphere of radius $a = \Lambda^{-1}$.

Calculation of $\varrho_{\rm pol}(r)$

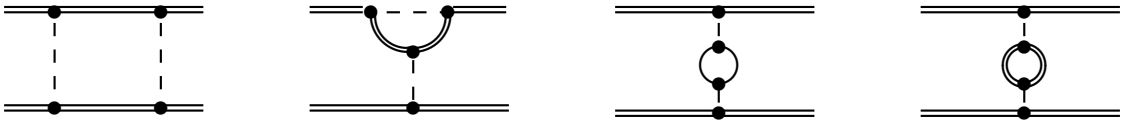
To calculate the charge distribution imagine computing the scattering of two particles with charges Q_1 and Q_2 and masses M_1 and M_2 that are both much larger than m. There are two reasons to take M_1 and M_2 to be large: it allows the electron-generated vacuum polarization graph to dominate the complete suite of one-loop contributions to the scattering; and it allows us to regard the scattered particles to be moving slowly enough that the scattering can be regarded as a form of non-relativistic potential scattering.

On one hand the amplitude for scattering of two (distinguishable) heavy particles can be computed from Feynman rules, and (representing the heavy particles by double solid lines) at tree level the relevant Feynman graphs are:



(a)

At one-loop order the required graphs are given by:



(b) (c) (d) (e)

and so on. In graph (d) it is the electron that circulates within the loop, while in graph (e) it is instead one of the heavy particles. For M_1, $M_2 \gg m$ it is only graph (d) that dominates, because it is proportional to $\Pi_\star(q^2)$ and so is proportional to q^2/m^2 while the others are suppressed by powers of the heavier masses.

Assuming the heavy particles have spin $\frac{1}{2}$ the amplitude for the scattering becomes approximately

$$\begin{aligned}\mathcal{A} &\simeq -\frac{iQ_1Q_2}{(2\pi)^2}\delta^4(p_1+p_2-p_1'-p_2')\,\overline{\mathbf{u}}(p_1')\gamma^\mu\mathbf{u}(p_1)\,\overline{\mathbf{u}}(p_2')\gamma^\nu\mathbf{u}(p_2)\left[\frac{\eta_{\mu\nu}}{q^2}+\frac{(q^2\eta_{\mu\nu}-q_\mu q_\nu)\Pi_\star(q^2)}{q^4}\right]\\ &= -\frac{iQ_1Q_2}{(2\pi)^2}\delta^4(p_1+p_2-p_1'-p_2')\,\overline{\mathbf{u}}(p_1')\gamma^\mu\mathbf{u}(p_1)\,\overline{\mathbf{u}}(p_2')\gamma_\mu\mathbf{u}(p_2)\left[\frac{1+\Pi_\star(q^2)}{q^2}\right], \qquad (17.4.4)\end{aligned}$$

where the first line directly applies the Feynman rules and the second line simplifies using $\overline{\mathbf{u}}(p')\not{q}\mathbf{u}(p)=0$, since the 4-momentum in the photon line is $q^\mu=(p_1'-p_1)^\mu=(p_2-p_2')^\mu$.

In the strict non-relativistic limit where all inverse powers of M_1 and M_2 are dropped we have $\overline{\mathbf{u}}(p')\gamma^\mu\mathbf{u}(p)\simeq -i\delta^\mu_0\,\delta_{\sigma\sigma'}$ and $q^2\simeq\mathbf{q}^2=(\mathbf{p}_1'-\mathbf{p}_1)^2$ so the amplitude becomes

$$\mathcal{A}\simeq -\frac{iQ_1Q_2}{(2\pi)^2}\delta^4(p_1+p_2-p_1'-p_2')\,\delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'}\left[\frac{1+\Pi_\star(\mathbf{q}^2)}{\mathbf{q}^2}\right]. \qquad (17.4.5)$$

This has the same form as does spin-independent scattering in ordinary quantum mechanics from a potential $V(\mathbf{x})$, which would have given (at leading order in V)

$$\mathcal{A}_{\rm pot} \simeq -\frac{i}{(2\pi)^2}\delta^4(p_1+p_2-p_1'-p_2')\,\delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'}\int \mathrm{d}^3x\; V(\mathbf{x})\,e^{-i\mathbf{q}\cdot\mathbf{x}}\,. \tag{17.4.6}$$

Comparing (17.4.5) and (17.4.6) implies

$$\frac{Q_1Q_2}{\mathbf{q}^2}\Big[1+\Pi_\star(\mathbf{q}^2)\Big] = \int \mathrm{d}^3x\; V(\mathbf{x})\,e^{-i\mathbf{q}\cdot\mathbf{x}}\,, \tag{17.4.7}$$

and so

$$V(\mathbf{x}) = \frac{Q_1Q_2}{(2\pi)^3}\int\frac{\mathrm{d}^3q}{\mathbf{q}^2}\,\Big[1+\Pi_\star(\mathbf{q}^2)\Big]\,e^{i\mathbf{q}\cdot\mathbf{x}}\,. \tag{17.4.8}$$

The first (tree-level) term is familiar since

$$V_c(\mathbf{x}) = \frac{Q_1Q_2}{(2\pi)^3}\int\frac{\mathrm{d}^3q}{\mathbf{q}^2}\,e^{i\mathbf{q}\cdot\mathbf{x}} = \frac{Q_1Q_2}{4\pi|\mathbf{x}|}\,, \tag{17.4.9}$$

just reproduces the Coulomb potential.

The final step is to show that the term in $V(\mathbf{x})$ coming from $\Pi_\star(\mathbf{q}^2)$ reproduces what would be expected for electrostatic scattering if each charge carried an associated charge distribution. To this end imagine that the charge distribution around each of the massive sources can be written

$$\rho_i(\mathbf{x}) = Q_i\Big[\delta^3(\mathbf{x}-\mathbf{x}_i)+\eta(\mathbf{x}-\mathbf{x}_i)\Big]\,, \tag{17.4.10}$$

where we write the polarization charge density as $\varrho_{{\rm pol},i}(\mathbf{x}) = Q_i\,\eta(\mathbf{x})$. In order for Q_i to be the physical charge measured from a distance we must demand

$$\int \mathrm{d}^3x\,\eta(\mathbf{x}) = 0\,. \tag{17.4.11}$$

The electrostatic potential generated by such a charge distribution is found from Coulomb's law to be

$$\phi_i(\mathbf{x}) = \frac{1}{4\pi}\int \mathrm{d}^3y\;\frac{\rho_i(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} = \frac{Q_i}{4\pi|\mathbf{x}-\mathbf{x}_i|} + \frac{Q_i}{4\pi}\int \mathrm{d}^3y\;\frac{\eta(\mathbf{y}-\mathbf{x}_i)}{|\mathbf{x}-\mathbf{y}|}\,. \tag{17.4.12}$$

The electrostatic interaction energy of these two charge distributions therefore is (dropping η^2 terms, in anticipation that $\eta\sim\mathcal{O}(\alpha)$)

$$\begin{aligned} V(\mathbf{x}_1,\mathbf{x}_2) &= \frac{1}{2}\int \mathrm{d}^3x\Big[\rho_1(\mathbf{x})\,\phi_2(\mathbf{x})+\rho_2(\mathbf{x})\,\phi_1(\mathbf{x})\Big] \\ &= \frac{Q_1Q_2}{4\pi|\mathbf{x}_1-\mathbf{x}_2|} + \frac{Q_1Q_2}{8\pi}\int \mathrm{d}^3x\left[\frac{\eta(\mathbf{x}-\mathbf{x}_2)}{|\mathbf{x}_1-\mathbf{x}|}+\frac{\eta(\mathbf{x}-\mathbf{x}_1)}{|\mathbf{x}_2-\mathbf{x}|}+(1\leftrightarrow 2)\right] \\ &= \frac{Q_1Q_2}{4\pi|\mathbf{x}_1-\mathbf{x}_2|} + \frac{Q_1Q_2}{4\pi}\int \mathrm{d}^3y\;\frac{\eta(\mathbf{y})+\eta(-\mathbf{y})}{|\mathbf{x}_1-\mathbf{y}-\mathbf{x}_2|}\,. \end{aligned} \tag{17.4.13}$$

Since $V(\mathbf{x}_1, \mathbf{x}_2)$ in this last expression is a function only of $|\mathbf{x}_1 - \mathbf{x}_2|$ we can ask what choice for $\eta(\mathbf{x})$ ensures this potential agrees with the one given in (17.4.8). The function $\eta(\mathbf{x})$ evidently must satisfy

$$\frac{1}{4\pi}\int \mathrm{d}^3y\,\frac{\eta(\mathbf{y})+\eta(-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} = \frac{1}{(2\pi)^3}\int \frac{\mathrm{d}^3q}{\mathbf{q}^2}\,\Pi_\star(\mathbf{q}^2)\,e^{i\mathbf{q}\cdot\mathbf{x}}\,. \tag{17.4.14}$$

The integral on the left-hand side can be removed by operating on this equation by ∇^2 (where the differentiation is with respect to $\mathbf{x}$), using the identity $\nabla^2(1/|\mathbf{x}-\mathbf{y}|) = -4\pi\,\delta^3(\mathbf{x}-\mathbf{y})$. This leads to

$$\eta(\mathbf{x})+\eta(-\mathbf{x}) = \frac{1}{(2\pi)^3}\int \mathrm{d}^3q\,\Pi_\star(\mathbf{q}^2)\,e^{i\mathbf{q}\cdot\mathbf{x}}\,. \tag{17.4.15}$$

Because the right-hand side is even under $\mathbf{x}\to-\mathbf{x}$ we can choose $\eta(\mathbf{x}) = \eta(-\mathbf{x})$ in which case the left-hand side of this last equation is simply $2\eta(\mathbf{x})$. Using the expression (17.3.27) for the photon self-energy then gives the inferred position-space charge density

$$\eta(\mathbf{x}) = \frac{e^2}{(2\pi)^5}\int_0^1 \mathrm{d}x\,x(1-x)\int \mathrm{d}^3q\,e^{i\mathbf{q}\cdot\mathbf{x}}\log\left[1+\frac{x(1-x)\mathbf{q}^2}{m^2}\right]. \tag{17.4.16}$$

It happens that the d^3q integration can be done in closed form – which would not have been possible if we'd solved instead directly for $V(\mathbf{x})$ – as follows. Evaluating the integral in polar coordinates leads to

$$\begin{aligned} I &:= \int \mathrm{d}^3q\,e^{i\mathbf{q}\cdot\mathbf{x}}\log\left[1+\frac{x(1-x)\mathbf{q}^2}{m^2}\right] \\ &= 4\pi\int_0^\infty \mathrm{d}q\,q^2\left(\frac{\sin qr}{qr}\right)\log\left[1+\frac{x(1-x)q^2}{m^2}\right] \\ &= \frac{2\pi}{ir}\int_{-\infty}^\infty \mathrm{d}q\,q\,e^{iqr}\log\left[1+\frac{x(1-x)q^2}{m^2}\right], \end{aligned} \tag{17.4.17}$$

where $r = |\mathbf{x}|$.

This last integral can be performed by deforming the integration contour in the complex q plane. Notice that the integrand has a branch point when $q^2 = -m^2/[x(1-x)]$, from which we choose the branch cut to run up the imaginary axis starting from $q = iq_\star$ with $q_\star = m/\sqrt{x(1-x)}$. Deforming the integration contour to wrap around this branch cut gives a contour integral that runs down just left of the cut from infinity to the branch point and then back up to infinity just to the right of the cut. Writing $q = iy$ the result then is

$$\begin{aligned} I &:= \frac{2\pi}{ir}\int_{q_\star}^\infty (i\mathrm{d}y)(iy)e^{-yr}\left\{\left[\log\left|1-\frac{x(1-x)y^2}{m^2}\right|+i\pi\right]-\left[\log\left|1-\frac{x(1-x)y^2}{m^2}\right|-i\pi\right]\right\} \\ &= -\frac{(2\pi)^2}{r}\int_{q_\star}^\infty \mathrm{d}y\,y\,e^{-yr} = -\frac{(2\pi)^2}{r^3}\left[1+\frac{mr}{\sqrt{x(1-x)}}\right]e^{-mr/\sqrt{x(1-x)}}\,. \end{aligned}$$

Using this in (17.4.16) leads to $\eta(\mathbf{x}) = \hat{\eta}(\mathbf{x})$, with

$$\hat{\eta}(\mathbf{x}) = -\frac{e^2}{(2\pi r)^3}\int_0^1 \mathrm{d}x\; x(1-x)\left[1+\frac{mr}{\sqrt{x(1-x)}}\right] e^{-mr/\sqrt{x(1-x)}}\,. \tag{17.4.18}$$

As advertised, this expression falls off exponentially once $mr \gg 1$ but takes the approximate form

$$\hat{\eta}(\mathbf{x}) \simeq -\frac{e^2}{48\pi^3 r^3} \quad \text{for } mr \ll 1. \tag{17.4.19}$$

This expression for $\hat{\eta}(\mathbf{x})$ cannot quite be final, since it is everywhere negative and so does not satisfy the neutrality condition (17.4.11). Based on the experience with the surface charge for a hole excised from a dielectric, we expect the neutralizing charge to be concentrated near the position of the massive charges themselves, and so write the full solution for the induced charge density as $\eta(\mathbf{x}) = N\,\delta^3(\mathbf{x}) + \hat{\eta}(\mathbf{x})$:

$$\eta(\mathbf{x}) = N\,\delta^3(\mathbf{x}) - \frac{e^2}{(2\pi r)^3}\int_0^1 \mathrm{d}x\; x(1-x)\left[1+\frac{mr}{\sqrt{x(1-x)}}\right] e^{-mr/\sqrt{x(1-x)}}\,, \tag{17.4.20}$$

where N is determined by the condition (17.4.11) and so satisfies

$$\begin{aligned} N = -\int \mathrm{d}^3x\,\hat{\eta}(\mathbf{x}) &= \frac{2e^2}{(2\pi)^2}\int_{\Lambda^{-1}}^{\infty}\frac{\mathrm{d}r}{r}\int_0^1 \mathrm{d}x\; x(1-x)\left[1+\frac{mr}{\sqrt{x(1-x)}}\right] e^{-mr/\sqrt{x(1-x)}} \\ &\simeq \frac{e^2}{12\pi^2}\int_{\Lambda^{-1}}^{m^{-1}}\frac{\mathrm{d}r}{r} = \frac{e^2}{24\pi^2}\log\left(\frac{\Lambda^2}{m^2}\right), \end{aligned} \tag{17.4.21}$$

where the last line focusses on the strongly Λ-dependent part.

Because $\eta(\mathbf{x})$ satisfies (17.4.11) the total charge of the source with charge density (17.4.10) is Q_i, while the bare charge is the charge contained within the region of size Λ^{-1}, and so is given by

$$Q_{B\,i} = Q_i\Big(1+N\Big) \simeq Q_i\left[1+\frac{e^2}{24\pi^2}\log\left(\frac{\Lambda^2}{m^2}\right)\right] \qquad (\text{for all } `i')\,. \tag{17.4.22}$$

Defining $Z_3^{1/2} = Q/Q_B$ then reproduces our starting expression (17.4.1) for the photon renormalization constant.

17.4.2 Running couplings

Notice that this polarization of the vacuum occurs for *all* charges, and since (unlike for dielectric materials) it is impossible to remove a charge from the vacuum it is better to write $Q_i = \mathcal{Z}_i\, e$ and $Q_{B\,i} = \mathcal{Z}_i\, e_B$ for $\mathcal{Z}_i$ some fixed number[74] (usually, in practice, an integer)

[74] Not to be confused with the renormalization constants Z_i!

and think of the Λ-dependence of the $Q_{B\,i}$ as a universal Λ-dependence to the measured electromagnetic coupling strength e_B,

$$e_B(\Lambda) = e\left[1 + \frac{e^2}{24\pi^2}\log\left(\frac{\Lambda^2}{m^2}\right)\right], \tag{17.4.23}$$

than to the charges of specific particles. Strictly speaking, this expression is only valid for $\Lambda \gg m$ because it neglects terms are suppressed by powers of m^2/Λ^2. The use of perturbative methods also assumes the combination $(e^2/24\pi^2)\log(\Lambda^2/m^2)$ is small. When both of these assumptions apply eq. (17.4.23) can be trusted and its derivative with respect to Λ can be computed, leading to a differential relation of the form

$$\Lambda\frac{\mathrm{d}e_B}{\mathrm{d}\Lambda} = \frac{e^3}{12\pi^2} + \mathcal{O}(e^5) = \frac{e_B^3}{12\pi^2} + \mathcal{O}(e^5)\,. \tag{17.4.24}$$

where we hold the physical charge e fixed as Λ varies and drop higher-order contributions.

What is interesting about (17.4.24) is that the right-hand side is independent of Λ (in the regime $\Lambda \gg m$) and so its domain of validity is broader than that of (17.4.23) because it only assumes $e^2/(16\pi^2)$ is small. Regarding (17.4.24) as a differential equation to be solved for $e_B(\Lambda)$ shows that it is equivalent to the expression

$$e_B^2 = \frac{e_{B\,0}^2}{1 - (e_{B\,0}^2/6\pi^2)\log(\Lambda/\Lambda_0)}\,, \tag{17.4.25}$$

where the initial condition $e_B(\Lambda_0) = e_{B\,0}$ is used. This expresses how $e_B^2(\Lambda)$ gets larger as Λ gets larger, as expected from the dielectric screening intuition described above.

Clearly (17.4.25) agrees with (17.4.23) if the denominator on the right-hand side is Taylor expanded out to linear order in the logarithm, and if we identify $e_{B\,0} = e$ when $\Lambda_0 = m$. But – unlike (17.4.23) – because (17.4.24) assumes only that $e^2/(16\pi^2)$ is small, this is also all that is needed to trust (17.4.25), and so in particular (17.4.25) remains valid even when $(e^2/16\pi^2)\log(\Lambda/\Lambda_0)$ is order unity. The prediction for $e_B(\Lambda)$ eventually breaks down, however because once the denominator starts to approach zero the value of e_B^2 starts to become large enough no longer to trust the perturbative evaluation.

The differential evolution (17.4.24) is called the *renormalization group* (RG) equation governing the way that the coupling $e_B(\Lambda)$ flows (or runs) with scale, so the extension of (17.4.23) to (17.4.25) is called a 'renormalization-group improvement' of the domain of validity of (17.4.23).

17.4.3 Shifts in Coulomb energy levels

The presence of an induced polarized charge distribution around a point charge has potentially measureable physical consequences. One of these is that the field of a point nucleus is no longer precisely Coulomb and this inevitably shifts the energy levels of atomic electrons. In

order to use the formulae derived above for the modified potential generated by vacuum polarization, we focus on bound states built using particles much heavier than electrons.[75]

At first order in perturbation theory (in ordinary single-particle quantum mechanics) a small potential $\delta V(\mathbf{x})$ added to the Coulomb potential shifts energy levels by an amount

$$\Delta E_N = \int \mathrm{d}^3x\, \delta V(\mathbf{x}) \left|\psi_N(\mathbf{x})\right|^2 , \tag{17.4.26}$$

where $\psi_N(\mathbf{x})$ is the unperturbed wave-function of the orbiting particle. If the orbiting particle moves within the Coulomb potential of a second heavy charge then $N = \{n, \ell, \ell_3\}$ denotes the usual quantum numbers for Hydrogen-like wave-functions. Assuming the orbiting particle has charge $Q_1 = -\mathcal{Z}_1 e$ and the 'nucleus' has charge $Q_2 = \mathcal{Z}_2 e$, using the potential (17.4.8) then gives

$$\Delta E_N = -\frac{\mathcal{Z}_1\mathcal{Z}_2 e^2}{(2\pi)^3} \int \mathrm{d}^3q\, \frac{\Pi_\star(\mathbf{q}^2)}{\mathbf{q}^2} \int \mathrm{d}^3x\, \left|\psi_N(\mathbf{x})\right|^2 e^{i\mathbf{q}\cdot\mathbf{x}} . \tag{17.4.27}$$

For example for the 1S and 2S Coulomb states the wave-functions are given by

$$\psi_{1S}(r) = \frac{1}{\sqrt{\pi}\, a_B^{3/2}}\, e^{-r/a_B} \quad \text{and} \quad \psi_{2S}(r) = \frac{1}{\sqrt{4\pi}\,(2a_B)^{3/2}} \left(2 - \frac{r}{a_B}\right) e^{-2r/a_B} , \tag{17.4.28}$$

and so on, where a_B is the characteristic orbit size

$$a_B := \frac{4\pi}{\mathcal{Z}_1\mathcal{Z}_2 e^2 M_{12}} = \frac{1}{\mathcal{Z}_1\mathcal{Z}_2 \alpha M_{12}} \quad \text{where} \quad M_{12} := \frac{M_1 M_2}{M_1 + M_2} . \tag{17.4.29}$$

The characteristic length scale associated with $\Pi_\star(q^2)$ is the electron Compton wavelength m^{-1}, while the characteristic size of the orbital wavefunction is a_B. Because the wavefunction with angular momentum ℓ behaves like $(r/a_B)^\ell$ as $r \to 0$, it is the $\ell = 0$ (S-wave) states that shift the most if $m^{-1} \ll a_B$. All S-wave states are functions only of the radial coordinate r, and so for them

$$\Delta E_{nS} = -\frac{2\mathcal{Z}_1\mathcal{Z}_2 e^2}{\pi} \int_0^\infty \mathrm{d}q\, \Pi_\star(q^2) \int_0^\infty \mathrm{d}r\, r \left|\psi_n(r)\right|^2 \frac{\sin(qr)}{q} . \tag{17.4.30}$$

where $n = 1, 2, \cdots$ is the principal quantum number. For the 1S state performing the radial integral then gives

$$\begin{aligned} \Delta E_{1S} &= -\frac{8\mathcal{Z}_1\mathcal{Z}_2 e^2}{\pi^2 a_B^4} \int_0^\infty \mathrm{d}q\, \frac{\Pi_\star(q^2)}{[q^2 + (4/a_B^2)]^2} \\ &= -\frac{\mathcal{Z}_1\mathcal{Z}_2 e^4}{2\pi^4 a_B} \int_0^1 \mathrm{d}x \int_0^\infty \mathrm{d}y\, \frac{x(1-x)}{(y^2+1)^2} \log\left[1 + \frac{4x(1-x)y^2}{a_B^2 m^2}\right] \\ &\simeq -\frac{\mathcal{Z}_1\mathcal{Z}_2 e^4}{60\pi^3 m^2 a_B^3} = -\frac{4(\mathcal{Z}_1\mathcal{Z}_2\alpha)^4 \alpha M_{12}^3}{15\pi m^2} \quad \text{when} \quad m a_B \gg 1 . \end{aligned} \tag{17.4.31}$$

[75] Practical examples of this type could include muonic atoms (a nucleus-muon bound state), pionic atoms (a nucleus-pion bound state), a muon-antimuon bound state, a proton-antiproton bound state and so on.

More generally, when $ma_B \gg 1$ then the wavefunction does not vary much within the region within a few electron Compton wavelengths of the nucleus for which the potential has its support, and so

$$\Delta E_N \simeq \left|\psi_N(0)\right|^2 \int \mathrm{d}^3x\; \delta V(\mathbf{x})\,, \tag{17.4.32}$$

where

$$\int \mathrm{d}^3x\; \delta V(\mathbf{x}) = -\mathcal{Z}_1\mathcal{Z}_2 e^2 \lim_{\mathbf{q}^2\to 0} \frac{\Pi_\star(\mathbf{q}^2)}{\mathbf{q}^2} = -\mathcal{Z}_1\mathcal{Z}_2 e^2 \Pi'_\star(0)\,, \tag{17.4.33}$$

with $\Pi'_\star(q^2) := \mathrm{d}\Pi_\star/\mathrm{d}q^2$. Differentiating (17.3.27) then gives

$$\Pi'_\star(0) = \frac{e^2}{60\pi^2 m^2} = \frac{\alpha}{15\pi m^2}\,, \tag{17.4.34}$$

and so

$$\Delta E_N \simeq -\mathcal{Z}_1\mathcal{Z}_2 e^2 \Pi'_\star(0) \left|\psi_N(0)\right|^2 = -\frac{\mathcal{Z}_1\mathcal{Z}_2 e^4}{60\pi^2 m^2} \left|\psi_N(0)\right|^2, \tag{17.4.35}$$

in agreement with (17.4.31) in the 1S special case.

This kind of energy shift is present and is measureable for muonic Hydrogen, in which a negative muon is captured by a nucleus before it decays. It happens, however, that the electron mass $m_e \simeq 0.51$ MeV is not that different from $a_B^{-1} = \alpha\, m_\mu \sim 0.77$ MeV, so for muonic atoms the approximation $ma_B \gg 1$ is not very good, and the integral must be performed more accurately using the muon wavefunction.

If applied to electrons responding to the polarization charge of the heavy nucleus in Hydrogen the above energy shift is also important because it contributes to the Lamb shift: a shift of the 2S state relative to the 2P state (which we see in §19.1 are predicted to be exactly degenerate when the Hydrogen atom is treated relativistically, but in the absence of radiative corrections). Since the 2S state for an electron orbiting a nucleus of charge $\mathcal{Z}e$ has $|\psi(0)|^2 = [\pi(2a_B)^3]^{-1} = \mathcal{Z}^2\alpha^3 m^3/(8\pi)$ eq. (17.4.35) predicts

$$\Delta E_{2S} \simeq -\frac{\mathcal{Z}e^4}{480\pi^3 m^2 a_B^3} = -\frac{\mathcal{Z}^4\alpha^5 m}{30\pi} \simeq -1.122\times 10^{-7}\,\mathrm{eV}\mathcal{Z}^4\,, \tag{17.4.36}$$

corresponding (when $\mathcal{Z}=1$) to a frequency $\Delta E/2\pi \simeq 37.13$ MHz.

Although a splitting between the 2S and 2P levels was famously found (by Lamb and Retherford) to be experimentally present, its observed value is 1057 MHz and so is not given purely by (17.4.36). This is because the vacuum polarization graph is not the only one that contributes to this energy shift at this order in powers of α. For electrons the vertex correction graph (see §17.6 and §19.3 below) in which the atomic electron emits and reabsorbs a photon also contributes at order $\mathcal{Z}^4\alpha^5$, but with a larger overall coefficient.[76] The same is not true for muonic Hydrogen because this vertex correction is proportional to $1/m_\mu^2$ rather than $1/m_e^2$ and so is suppressed relative to the vacuum polarization due to electrons.

[76] It also contains a factor of $\log\alpha \simeq -5$, which is numerically significant, for reasons elaborated in §19.3.

17.5 Renormalization group methods

Although the cutoff Λ makes explicit how UV divergences have their root in the short-distance part of the theory, calculations are much more conveniently performed in dimensional regularization because this preserves Lorentz and gauge symmetries in a way that cutoffs do not. It would be useful to be able to describe the running of the couplings and to use renormalization-group arguments starting directly from the dimension-regularization result (17.3.28) rather than (17.4.1).

To see how this is done recall that in dimensional regularization the bare coupling $e_B = e_B(n)$ is defined in n dimensions. Recall also that the couplings have different 'engineering' dimension in different numbers of spacetime dimensions. For example, for the QED lagrangian in n dimensions the action is

$$S = \int \mathrm{d}^n x \, \left[-\frac{1}{4} F^B_{\mu\nu} F_B^{\mu\nu} - \overline{\psi}_B \not{\partial} \psi_B - i e_B \overline{\psi}_B \gamma^\mu \psi_B A^B_\mu \right] , \tag{17.5.1}$$

and the action has the same units as $\hbar$ (and so is dimensionless in fundamental units, for which $\hbar = 1$). The lagrangian density must therefore have dimension $(\text{mass})^n$ to compensate for the dimensions of the integration measure $\mathrm{d}^n x$. This means that $F^B_{\mu\nu}$ must have dimension $(\text{mass})^{n/2}$ and because $F^B_{\mu\nu}$ is the derivative of the gauge potential it follows that A^B_μ has dimension $(\text{mass})^{(n-2)/2}$. The Dirac field ψ_B similarly has dimension $(\text{mass})^{(n-1)/2}$ and these in turn imply that e_B has dimension $(\text{mass})^{(4-n)/2}$.

17.5.1 Minimal subtraction

Consider the coupling $g_B := e_B^2$ that has dimension $(\text{mass})^{4-n}$. Because the physical coupling $g := e^2$ is dimensionless, the relation between g_B and g in dimensional regularization must involve the arbitrary scale μ with $g_B \propto \mu^{4-n} g$.

We also know that divergences arise in dimensional regularization as isolated singularities as $n \to 4$ (with more singular behaviour than a simple pole also possible once one goes beyond one loop), and these divergences are ultimately cancelled by allowing g_B to be n-dependent as well, in a way that cancels the singularities in observables. The expansion of g_B near $n = 4$ is a Laurent series, of the form

$$g_B(n) = \mu^{4-n} \left\{ g(\mu, n) + \sum_{k=1}^{\infty} \frac{b_k}{(n-4)^k} \right\} , \tag{17.5.2}$$

for some coefficients $g(\mu, n)$ and b_k. Because the curly bracket is dimensionless the coefficient functions b_k are independent of the electron mass m.

The coefficient $g(\mu, n)$ provides a very convenient definition for the renormalized coupling, since it is finite as $n \to 4$. This choice is called *minimal subtraction* (or MS for short) since it defines the renormalized coupling simply by subtracting the divergent part of the Laurent

expansion of g_B. The coefficients b_k should be regarded as functions of g, since they are generated through a perturbative expansion, so we write

$$b_k = b_k[g(\mu, n)]\,. \tag{17.5.3}$$

It must be emphasized that the renormalized coupling defined this way is not the same as the physical coupling defined above – for clarity now denoted $g_{\rm phys} = e^2_{\rm phys}$ – whose counter-term was determined by the condition that $\Pi(q^2 = 0) = 0$. This is an example of what is called a change of renormalization scheme.

Indeed even (17.5.2) leaves a great deal of freedom in precisely how to define g, since finiteness of the result at $n = 4$ leaves open considerable freedom to redefine couplings in a way that does not introduce a singularity at $n = 4$. For instance

$$\tilde{g}(\mu, n) := g(\mu, n) + \sum_{r=1}^{\infty} \mathfrak{e}_r\,(n-4)^r\,, \tag{17.5.4}$$

defines an equally consistent definition of the renormalized charge. Although these differ only by terms that vanish as $n \to 4$ this nonetheless allows the coefficients $\mathfrak{e}_r$ to appear in the finite part of correlation functions when the factor of $(n-4)^r$ combines with compensating powers of $1/(n-4)$ coming from a divergence.

The above notation also emphasizes how the renormalized coupling $g = g(\mu, n)$ defined this way must be an implicit function of μ if the bare coupling g_B is to be μ-independent, since the subdominant terms in the expansion of μ^{4-n} about $n = 4$ can survive when they multiply the inverse powers of $n - 4$ appearing in the sum. To see what this μ-dependence looks like, imagine changing $\mu \to \tilde{\mu} := \mu(1 + \delta)$ with n fixed. Because

$$\mu^{4-n} = \tilde{\mu}^{4-n}\Big[1 + (n-4)\ \log\delta + \cdots\Big]\,, \tag{17.5.5}$$

it is necessary also to do a redefinition of the type (17.5.4) in order to preserve the property that $g(\tilde{\mu}, n)$ remains defined by

$$g_B(n) = \tilde{\mu}^{4-n}\left\{g(\tilde{\mu}, n) + \sum_{k=1}^{\infty} \frac{b_k[g(\tilde{\mu}, n)]}{(n-4)^k}\right\}\,, \tag{17.5.6}$$

without additional nonsingular terms.

We can now determine how $g(\mu, n)$ varies with μ. To determine this, differentiate (17.5.2) with respect to μ holding n and g_B fixed:

$$0 = \mu^{n-4}\left(\mu\,\frac{{\rm d}g_B}{{\rm d}\mu}\right) = (4-n)\left[g + \sum_{k=1}^{\infty}\frac{b_k}{(n-4)^k}\right] + \left[1 + \sum_{k=1}^{\infty}\frac{b'_k}{(n-4)^k}\right]\beta(g, n)\,, \tag{17.5.7}$$

where $b'_k := {\rm d}b_k/{\rm d}g$ and

$$\beta(g, n) := \mu\,\frac{\partial g}{\partial \mu} = \beta(g) + \sum_{r=1}^{\infty}\kappa_r (n-4)^r \tag{17.5.8}$$

comes as a series in $(n-4)$ because of the redefinition (17.5.4) required to ensure (17.5.6) remains true as μ is varied. It is the first term, $\beta(g)$, that we seek since it determines how g depends on μ when $n=4$.

Eq. (17.5.7) is true for all n and so is equivalent to the conditions found by setting the coefficient of each power of $(n-4)$ to zero:

$$\begin{aligned}
(n-4)^r\ (r\geq 2):&\qquad \kappa_r = 0\,,\\
(n-4)^1:&\qquad -g+\kappa_1 = 0\,,\\
(n-4)^0:&\qquad \beta(g)+\kappa_1 b_1'(g) - b_1(g) = 0\,,\\
(n-4)^{-r}\ (r\geq 1):&\qquad -b_{r+1}(g)+\kappa_1 b_{r+1}'(g)+\beta(g)\,b_r'(g) = 0\,.
\end{aligned} \tag{17.5.9}$$

The first two of these imply

$$\beta(g,n) = \beta(g) + g\,(n-4)\,, \tag{17.5.10}$$

while the third gives $\beta(g)$ in terms of $b_1(g)$ as

$$\beta(g) = b_1(g) - g\,b_1'(g)\,. \tag{17.5.11}$$

The last provides a recursion relation that gives $b_{r+1}(g)$ as a function of $b_r(g)$ and $\beta(g)$. Clearly everything is determined once $b_1(g)$ is known.

To determine $g(\mu)$ at any order in g one simply asks what value of the bare coupling has the Laurent expansion that cancels all UV divergences, and then reads off from this the coefficient $b_1(g)$ of the $1/(n-4)$ term. For instance, at one-loop order in QED we know from (17.3.28) that

$$g_B = e_B^2 = Z_3^{-1} e_{\rm phys}^2 = e_{\rm phys}^2\left\{1+\frac{e_{\rm phys}^2}{12\pi^2}\left[\frac{2}{4-n}-\gamma-\log\left(\frac{m^2}{4\pi\mu^2}\right)\right]+\mathcal{O}(e_{\rm phys}^4)\right\}. \tag{17.5.12}$$

which, when compared to (17.5.2) (using $g=e^2$), relates the minimal-subtraction coupling to the physical one,

$$e^2 = e_{\rm phys}^2\left\{1-\frac{e_{\rm phys}^2}{12\pi^2}\left[\gamma+\log\left(\frac{m^2}{4\pi\mu^2}\right)\right]+\mathcal{O}(e_{\rm phys}^4)\right\}\qquad (\text{MS})\,, \tag{17.5.13}$$

while the pole term gives

$$b_1(g) = -\frac{g^2}{6\pi^2}\,. \tag{17.5.14}$$

Using (17.5.14) in (17.5.11) then implies

$$\beta(g) = b_1(g) - g\,b_1'(g) = +\frac{g^2}{6\pi^2} \tag{17.5.15}$$

and so

$$\mu\,\frac{\mathrm{d}e^2}{\mathrm{d}\mu} = \frac{e^4}{6\pi^2}\,, \tag{17.5.16}$$

consistent with directly differentiating (17.5.13) with e_{phys} held fixed. Integrating (17.5.16) then gives the RG-improved solution

$$e^2(\mu) = \frac{e_0^2}{1 - (e_0^2/6\pi^2)\log(\mu/\mu_0)}\,, \tag{17.5.17}$$

where $e(\mu_0) =: e_0$.

It is often convenient to have the scale μ_0 for the initial condition chosen so that $e(\mu_0) = e_{\text{phys}}$, and because of this it is often more convenient to define e^2 by also subtracting off the ubiquitous factor $\gamma - \log(4\pi)$ together with the pole, so that (17.5.13) instead becomes

$$e^2 = e_{\text{phys}}^2 \left[1 - \frac{e_{\text{phys}}^2}{12\pi^2}\log\left(\frac{m^2}{\mu^2}\right) + \mathcal{O}(e_{\text{phys}}^4)\right] \qquad (\overline{\text{MS}})\,, \tag{17.5.18}$$

a renormalization scheme called *modified minimal subtraction* (or $\overline{\text{MS}}$). In this scheme (17.5.17) becomes

$$e^2(\mu) = \frac{e_{\text{phys}}^2}{1 - (e_{\text{phys}}^2/6\pi^2)\log(\mu/m)}\,. \tag{17.5.19}$$

It is worth being clear at this point that – despite the notation e_{phys} – there is no one unique right answer for what the 'physical' charge is. This is because what we mean by e depends on how we measure it. The definition used above for e_{phys} is chosen to be what one would measure using Coulomb's law (such as by comparing scattering measurements to scattering from a Coulomb potential), which can be done at very large distances and arbitrarily small momentum transfers.[77] This gets converted to $\mu = m$ because the charge measured this way does not change at energies lower than m because the polarization cloud found above does not extend out beyond m^{-1}. But we could instead choose to measure e using a scattering experiment at a much higher energy E, and this is an equally good choice. In this case the resulting value found for $e(E)$ need not agree with the one found in low-energy scattering, and the above running calculation helps quantify how it differs.

Asymptotic freedom

Notice both (17.4.25) and (17.5.17) imply that the respective couplings become larger at higher energies (or lower distances), as the above arguments show is physically expected when the scale-dependence is due to screening. But this need not be generally true for couplings in other theories. An example where $\beta(g)$ has the opposite sign – implying the coupling *shrinks*

[77] In practice e is really measured using the Josephson effect in superconductors or the Quantum Hall effect, both of which involve electrons in condensed matter settings and are chosen because the observable in each case (Josephson frequency or quantized Hall resistivity) can both be computed and measured extremely accurately. Potato-potahto, since for the present purposes these can also be regarded as complicated scattering experiments at very low energies.

at higher energies – is provided by Quantum Chromodynamics (or QCD), the theory of the strong interactions.

QCD has a dimensionless coupling $g_s = e_s^2$ that controls the strength with which a collection of helicity-one photon-like particles (called gluons) couple to a new charge (called colour) that is carried by elementary spin-half particles called quarks. The theory is structured much like the electromagnetic interactions are, and successfully describes how quarks bind together into protons and neutrons (and ultimately also explains why protons and neutrons in turn bind into nuclei). For the present purposes what is important is that for QCD eq. (17.5.16) is replaced by

$$\mu \frac{\mathrm{d}e_s^2}{\mathrm{d}\mu} = -\frac{e_s^4}{8\pi^2}\left(11 - \frac{2n_q}{3}\right) , \tag{17.5.20}$$

where $n_q = 6$ is the number of species of quarks.

Quarks contribute a positive amount to the right-hand side of eq. (17.5.20) because virtual quarks and antiquarks act to screen the long-distance effects of any colour charge (just like electrons screen electric charge in QED). By contrast, the factor of 11 in (17.5.20) has the opposite sign. This term comes from virtual gluons – which themselves carry colour (unlike for photons in QED, which do not carry electric charge). For QCD the charge carried by the virtual gluons amplifies the strength of any colour charge, in much the same way that the energy in a gravitational field can itself gravitate and thereby amplify the gravitational effects of a test mass. In QCD the growth/reduction of couplings with scale is a competition between quark screening and gluon amplification, and in the end the gluons win because there are too few quarks for screening to prevail.

Theories (like QCD) for which couplings shrink at high energies (and, conversely, grow at low energies) are called *asymptotically free*. Indeed in QCD it is the growth of the coupling at low energies that is ultimately the reason why the strong interactions are in practice strong in everyday life.

Renormalization-scheme dependence

Although it is at first sight comforting that (17.5.16) and (17.5.17) agree with (17.4.24) and (17.4.25), this agreement is also puzzling because the couplings and scales being followed are defined differently in these two cases. And the minimal-subtraction coupling definition seems convenient but arbitrary; why should we care how it evolves with scale if it – unlike e_{phys} – is not the coupling strength of the physical electron?

This last question actually has two separate answers. The first one is that *all* renormalized couplings g agree on the first few terms in the expansion of $\beta(g)$ in powers of g. The second answer argues that there are situations where the running of the minimal-subtraction coupling can be shown to track more conveniently the physical dependence of observables on physical mass scales. We consider each of these in turn.

First, let us ask how two differently defined couplings run. To this end suppose that we have two ways to define a renormalized coupling, $g(\mu)$ and $\tilde{g}(\mu)$, with

$$\tilde{g} = F(g) = g + k_1 g^2 + k_2 g^3 + \cdots . \tag{17.5.21}$$

In writing the series form we imagine the differences in definition between the couplings only arise at subdominant order in perturbation theory (like the difference between minimal subtraction and the physical coupling examined above). If the coupling g satisfies $\mu(\mathrm{d}g/\mathrm{d}\mu) = \beta(g)$ then the evolution of the other coupling is given by

$$\tilde{\beta}(\tilde{g}) := \mu \frac{\mathrm{d}\tilde{g}}{\mathrm{d}\mu} = \frac{\mathrm{d}F}{\mathrm{d}g}\, \beta(g) = \Big(1 + 2k_1 g + 3k_2 g^2 + \cdots\Big)\beta(g)\,. \tag{17.5.22}$$

Suppose the perturbative expansion for $\beta(g)$ is known:

$$\beta(g) = b_1\, g^2 + b_2\, g^3 + b_3\, g^4 + \cdots . \tag{17.5.23}$$

Then the expansion for $\tilde{\beta}(\tilde{g})$ becomes

$$\begin{aligned} \tilde{\beta}(\tilde{g}) &= \Big(1 + 2k_1 g + 3k_2 g^2 + \cdots\Big)\Big(b_1\, g^2 + b_2\, g^3 + b_3\, g^4 + \cdots\Big) \\ &= b_1 g^2 + (b_2 + 2k_1 b_1) g^3 + (b_3 + 2k_1 b_2 + 3k_2 b_1) g^4 + \mathcal{O}(g^5) \\ &= b_1\, \tilde{g}^2 + b_2\, \tilde{g}^3 + (b_3 + b_2 k_1 + b_1 k_1^2 - b_1 k_2)\tilde{g}^4 + \mathcal{O}(\tilde{g}^5)\,. \end{aligned} \tag{17.5.24}$$

This shows that $\tilde{\beta}(\tilde{g})$ and $\beta(g)$ agree with one another quite generally both at leading and next-to-leading order. This is a boon because it means the subdominant term of the running for the physical coupling (at asymptotically large values for Λ/m) can be obtained much more simply by instead computing the running in minimal subtraction.

But differently defined couplings differ in general beyond the first two terms, and indeed the coefficients k_i could in principle be chosen to set all but the first two terms in $\tilde{\beta}(\tilde{g})$ to zero, should we want to do so.[78]

17.5.2 Resumming large logarithms

We close out the discussion of vacuum polarization and running couplings by making a more explicit connection between the running of the couplings and the dependence of physical observables on the logarithms of large physical mass ratios.

Suppose we are interested in an observable, O, (perhaps a cross section, energy threshold or reaction rate associated with some scattering process), which in QED depends in a calculable way on the parameters e and m as well as some observable-specific information like

[78] Although this would simplify the calculation of the running of $\tilde{g}$ at higher orders, the price would be that the connection between the value of $\tilde{g}$ and physical observables would become more obscure.

scattering energy E or dimensionless quantities (like scattering angles) collectively denoted by x:

$$O = O\Big(E\,, m\,, e_{\rm phys}\,, x\Big) = E^\Delta\, f\left(\frac{m}{E}\,, e_{\rm phys}\,, x\right)\,. \tag{17.5.25}$$

Here the last line uses dimensional analysis to scale out an overall factor of E, assuming O has engineering dimension (energy)$^\Delta$, so that the function f is dimensionless.

It is very tempting when writing things in this way to think that the energy dependence becomes simple in the limit $E \gg m$, because then

$$O \simeq E^\Delta\, \mathfrak{c}(e_{\rm phys}, x) \quad \text{where} \quad \mathfrak{c}(a,b) := f(0,a,b) \qquad \text{(naive)}\,. \tag{17.5.26}$$

It turns out that this expectation is wrong. When such quantities are computed explicitly in perturbation theory one instead finds

$$O \simeq E^\Delta \left[\mathfrak{c}_0(e_{\rm phys}, x) + \mathfrak{c}_1(e_{\rm phys}, x)\, \log\left(\frac{E}{m}\right) + \mathfrak{c}_2(e_{\rm phys}, x)\, \log^2\left(\frac{E}{m}\right) + \cdots\right]\,, \tag{17.5.27}$$

in the $E \gg m$ limit, for calculable functions $\mathfrak{c}_i$. The error in the naive reasoning was to assume that the function $f(m/E, a, b)$ is nonsingular in the limit $m/E \to 0$.

Where do these singularities come from? Because they only appear for small masses, they are dominated by long-wavelength modes and become infrared (IR) divergences in the limit $m \to 0$. One general source of this type of divergence in the presence of massless particles arises in scattering problems and is caused when massless states are emitted or absorbed by on-shell external lines. (This kind of IR problem is described in detail in §18.5 below.) As discussed in these later sections, when these kinds of honest-to-God IR divegences arise it is normally a sign that the putative observable being computed is actually not really observable, so the resolution is to identify an observable that is better behaved.

There is also a second source of mass singularities that arise for correlation functions and not just for scattering amplitudes, and these are the ones of interest here. A concrete example of a problem of this type can be seen in expressions like (17.3.11) for the renormalized electron self-energy $\Sigma_\star(p)$, or (17.3.27) for the photon vacuum polarization $\Pi_\star(p^2)$, both of which involve $\log(E/m)$ in the $E \gg m$ limit.

What is noteworthy about these examples is that the singularity as $m \to 0$ only really arises *after* imposing the physical renormalization condition that requires the relevant propagator to have unit residue at the physical particle mass. For instance, expression (17.3.26) for the vacuum polarization before imposing this condition has the following nonsingular limit when $m \to 0$:

$$\Pi(q^2) \simeq -\frac{2^{\varpi+1} e^2}{(4\pi)^2} \int_0^1 \mathrm{d}x\; x(1-x) \left\{\frac{1}{\epsilon} - \gamma - \log\left[\frac{x(1-x)q^2}{4\pi\mu^2}\right]\right\}\,. \tag{17.5.28}$$

The singularity in (17.3.27) as $m \to 0$ arises after the counter-term subtracts out the constant part; although this improves the UV convergence of the result it also makes its infrared behaviour worse.

Since it is the renormalization condition $\Pi(0) = 0$ that introduces the $m \to 0$ singularity, a simple way to avoid it in this case is to adopt another renormalization scheme besides the physical one (such as minimal subtraction or modified minimal subtraction). Then the dimensional estimate (17.5.25) instead becomes

$$O = O\Big[E\,, m\,, e(\mu)\,, \mu\,, x\Big] = E^\Delta\, f\left[\frac{m}{E}\,, e(\mu)\,, \frac{\mu}{E}\,, x\right]\,, \tag{17.5.29}$$

where μ is the arbitrary dimensional regularization scale. Because the coupling e does not use an on-shell renormalization scheme, the limit $m \to 0$ is now nonsingular, leading in the $E \gg m$ limit to

$$O \simeq E^\Delta\, f\left[0\,, e(\mu)\,, \frac{\mu}{E}\,, x\right]\,. \tag{17.5.30}$$

It is important for the rest of the story to realize (despite the notation) that the left-hand side of (17.5.29) is completely μ-independent:

$$\mu\,\frac{\mathrm{d}O}{\mathrm{d}\mu} = \frac{\partial O}{\partial \mu} + \frac{\partial O}{\partial e}\,\beta(e) = 0\,, \tag{17.5.31}$$

because any explicit dependence on μ is cancelled by the dependence on μ that is hidden within $e(\mu)$. This is just as well because (so far) μ is arbitrary. We can now exploit this arbitrariness to evaluate O at $\mu \sim E$,

$$O \simeq E^\Delta\, f\left[0\,, e(E)\,, 1\,, x\right]\,. \tag{17.5.32}$$

in which case there are no large scale ratios left on which large logarithms could depend, and the expression for f is relatively simple.

But we know that large logarithms must still be present if we were instead to use e_{phys}, and we can indeed see them emerge explicitly if we evaluate $e(E)$ as a function of e_{phys} using modified minimal subtraction (17.5.19), with initial condition $e(\mu = m) = e_{\text{phys}}$. Furthermore, because the large logarithms emerge through the functional form of $e(E, e_{\text{phys}})$, use of expressions like (17.5.19) rather than say (17.5.13) allows us to extend a perturbative result like (17.5.32) to all order in $e^2_{\text{phys}}\log(E/m)$, since (17.5.19) remains valid even if $e^2_{\text{phys}}\log(E/m)$ is order unity. The extension of a purely perturbative calculation to include all orders in $e^2_{\text{phys}}\log(E/m)$ is called a *renormalization-group resummation* of large logarithms.

17.6 Vertex Corrections

In this section we continue with explicit calculations, switching to the one-loop contribution to the vertex function and culminating with the famous QED prediction for the size of the electron's anomalous magnetic moment.

To this end we compute $\Gamma^\mu(p', p)$ appearing in the matrix element (17.2.45) of the electromagnetic current in a single-electron state, reproduced here:

$$\frac{\langle\!\langle e^-(\mathbf{p}', \sigma'), \text{out}|J^\mu(x=0)|e^-(\mathbf{p}, \sigma), \text{in}\rangle\!\rangle}{\langle\!\langle 0, \text{out}|0, \text{in}\rangle\!\rangle} = -\frac{ie}{(2\pi)^3}\,\overline{\mathbf{u}}(\mathbf{p}', \sigma')\,\Gamma^\mu(p', p)\,\mathbf{u}(\mathbf{p}, \sigma)\,. \tag{17.6.1}$$

As is argued below (17.2.45), $\Gamma^\mu_{mn}(p',p)$ in this expression is given by the sum of all connected graphs with two external electron lines and one external photon line, for which we are to ignore the Feynman rule associated with the external photon (but keep it for the external electron lines because of the appearance of explicit electron initial and final states in the matrix element).

17.6.1 Form factors

Before computing the one-loop contributions to $\Gamma^\mu_{mn}(p',p)$ it is worth seeing what constraints there are on its 4-momentum dependence on general symmetry grounds. In particular, we demand the matrix element be covariant under Lorentz, parity (because parity is conserved by the QED lagrangian) and gauge transformations.

Because $\Gamma^\mu(p',p)$ is a Dirac matrix (the m,n indices) it can be expanded in terms of the general covariant basis of Dirac matrices given in (15.4.14). The transformation properties of these matrices under Lorentz transformations and parity are listed in Table 4. Using these, the most general combination of the basis Dirac matrices and the two 4-momenta p and p' that have the same index structure as Γ^μ_{mn} and are parity invariant is given by

$$\begin{aligned}
S:&\quad p^\mu\, I\,,\quad p'^\mu\, I\\
V:&\quad \gamma^\mu\,,\quad \not{p}\, p^\mu\,,\quad \not{p}\, p'^\mu\,,\quad \not{p}'\, p^\mu\,,\quad \not{p}'\, p'^\mu\\
T:&\quad \gamma^{\mu\nu} p_\nu\,,\quad \gamma^{\mu\nu} p'_\nu\,,\quad \gamma^{\alpha\beta} p_\alpha p'_\beta p^\mu\,,\quad \gamma^{\alpha\beta} p_\alpha p'_\beta p'^\mu\\
A:&\quad \epsilon^{\mu\nu\lambda\rho}\gamma_5\gamma_\nu\, p_\lambda p'_\rho\\
P:&\quad \text{none}\,.
\end{aligned} \tag{17.6.2}$$

Parity invariance in particular implies that there must always be an even number of the two parity-odd quantities γ_5 and $\epsilon^{\mu\nu\lambda\rho}$. This then also implies that option P is not available because the only possible quantity – $\epsilon^{\mu\nu\lambda\rho}\gamma_5\gamma_\mu\gamma_\nu\gamma_\lambda\gamma_\rho$ – is proportional to the unit matrix, and so is not distinct from option S.

Each of these can in principle be multiplied by a Lorentz invariant function of momentum, which therefore must be a function of the external 4-momenta. But because 4-momentum conservation implies $q_\mu = p_\mu - p'_\mu$ it follows that any such an invariant can be built only using p and p'. The initial and final mode function $\overline{\mathbf{u}}'$ and $\mathbf{u}$ ensure the energy of the initial and final electrons have energies $\varepsilon^2 = \mathbf{p}^2 + m^2$ and so $p^2 = (p')^2 = -m^2$ are both constants. The only invariant bona-fide momentum variable is therefore $p\cdot p'$, or equivalently $q^2 = -2m^2 - 2p\cdot p'$. So any invariant coefficients can be regarded as being functions of q^2.

The number of independent tensors can also be reduced because the initial and final spinor mode functions satisfy

$$(i\not{p} + m)\mathbf{u} = \overline{\mathbf{u}}(i\not{p}' + m) = 0\,. \tag{17.6.3}$$

This allows the list given in (17.6.2) to be cut down to the following three independent structures:[79]

$$\overline{\mathbf{u}}(\mathbf{p}')\,\Gamma^\mu(p',p)\,\mathbf{u}(p) = \overline{\mathbf{u}}(p')\,\left[\gamma^\mu\,F(q^2) - \frac{i}{2m}(p+p')^\mu\,G(q^2) + \frac{i}{2m}\,q^\mu\,H(q^2)\right]\mathbf{u}(p)\,. \quad (17.6.4)$$

The factors of m are inserted to ensure the functions F, G and H are dimensionless and the factors of i ensure they are real. (The factors of 2 are purely conventional.)

The final piece of information implements gauge invariance by imposing the Ward identity proven in §16.3, which in this case implies

$$q_\mu\,\overline{\mathbf{u}}(p')\Gamma^\mu(p',p)\mathbf{u}(p) = 0\,. \quad (17.6.5)$$

Because (17.6.3) implies $\overline{\mathbf{u}}(p')\not{q}\,\mathbf{u}(p) = 0$ and because $q\cdot(p+p') = p^2 - (p')^2 = 0$ eq. (17.6.5) imposes no condition on $F(q^2)$ or $G(q^2)$ but does require $H(q^2) = 0$. The most general vertex function consistent with the symmetries of QED is therefore completely characterized by two Lorentz-invariant *form factors*, $F(q^2)$ and $G(q^2)$, through

$$\overline{\mathbf{u}}(\mathbf{p}')\,\Gamma^\mu(p',p)\,\mathbf{u}(p) = \overline{\mathbf{u}}(p')\,\left[\gamma^\mu\,F(q^2) - \frac{i}{2m}(p+p')^\mu\,G(q^2)\right]\mathbf{u}(p)\,. \quad (17.6.6)$$

Notice that in the absence of loop corrections we have $\Gamma^\mu(p',p) = \gamma^\mu$, which corresponds to the special case $F(q^2) = 1$ and $G(q^2) = 0$. Any q^2 dependence in $F(q^2)$ or any contributions to $G(q^2)$ at all is necessarily a sign of interactions of some sort. Notice also that Table 6 only allows UV divergences in the momentum-independent part of $\Gamma^\mu(p',p)$ and this implies that $G(q^2)$ is completely UV finite but $F(q^2)$ can involve an additive UV-divergent constant (but $\mathrm{d}F/\mathrm{d}q^2$ is UV finite).

Nonrelativistic limit

To interpret the meaning of these form factors it is worth specializing to a very slowly moving nonrelativistic electron, in which case the spinor mode function (15.2.13) reduces to

$$\mathbf{u}(\mathbf{p},\sigma) \simeq \frac{1}{\sqrt{2}}\begin{pmatrix} 1-\frac{1}{2m}\boldsymbol{\sigma}\cdot\mathbf{p} & 0 \\ 0 & 1+\frac{1}{2m}\boldsymbol{\sigma}\cdot\mathbf{p}\end{pmatrix}\begin{pmatrix}\mathbf{w}_\sigma \\ \mathbf{w}_\sigma\end{pmatrix}\,, \quad (17.6.7)$$

up to $1/m^2$ terms. Here $\mathbf{w}_\sigma$ are the two-component spinors

$$\mathbf{w}_{\sigma=+1/2} = \begin{pmatrix}1\\0\end{pmatrix}; \qquad \mathbf{w}_{\sigma=-1/2} = \begin{pmatrix}0\\1\end{pmatrix}. \quad (17.6.8)$$

Using this in the definitions then shows that

$$\overline{\mathbf{u}}(p')\,\gamma^0\,\mathbf{u}(p) \simeq \mathbf{w}^\dagger_{\sigma'}\left(1+\frac{\mathbf{p}'\cdot\boldsymbol{\sigma}}{2m}\right)\left(1+\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{2m}\right)\mathbf{w}_\sigma = -i\delta_{\sigma\sigma'} + \mathcal{O}(\mathbf{p}^2/m^2)\,, \quad (17.6.9)$$

[79] This is sometimes written with the second term proportional to $\gamma^{\mu\nu}q_\nu$, but this is not done here because having fewer Dirac matrices makes life computationally less complicated.

and

$$\begin{aligned}\overline{\mathbf{u}}(p')\,\boldsymbol{\gamma}\,\mathbf{u}(p) &\simeq \frac{i}{4m}\mathbf{w}^\dagger_{\sigma'}\left[-2(\mathbf{p}'\cdot\boldsymbol{\sigma})\boldsymbol{\sigma}-2\boldsymbol{\sigma}(\mathbf{p}\cdot\boldsymbol{\sigma})\right]\mathbf{w}_\sigma \\ &= -\frac{i}{2m}\mathbf{w}^\dagger_{\sigma'}\Big(\mathbf{p}+\mathbf{p}'-i\mathbf{q}\times\boldsymbol{\sigma}\Big)\mathbf{w}_\sigma+\mathcal{O}(\mathbf{p}^2/m^2) \\ &= -\frac{i}{2m}\Big[(\mathbf{p}+\mathbf{p}')\delta_{\sigma\sigma'}-i\mathbf{q}\times(\mathbf{w}^\dagger_{\sigma'}\boldsymbol{\sigma}\mathbf{w}_\sigma)\Big]+\mathcal{O}(\mathbf{p}^2/m^2)\,. \end{aligned} \tag{17.6.10}$$

Similarly

$$\overline{\mathbf{u}}(p')\,\mathbf{u}(p) \simeq \delta_{\sigma\sigma'}+\mathcal{O}(\mathbf{p}^2/m^2)\,, \tag{17.6.11}$$

and

$$q^2 \simeq \mathbf{q}^2+\mathcal{O}(\mathbf{p}^2/m^2)\,. \tag{17.6.12}$$

where $\mathbf{q}^2=(\mathbf{p}-\mathbf{p}')^2$. Combining these gives the nonrelativistic form for the vertex function:

$$\begin{aligned}\overline{\mathbf{u}}(p')\,\Gamma^0(p',p)\,\mathbf{u}(p) &\simeq -i\delta_{\sigma\sigma'}\Big[F(\mathbf{q}^2)+G(\mathbf{q}^2)\Big]+\mathcal{O}(\mathbf{p}^2/m^2) \\ \overline{\mathbf{u}}(p')\,\boldsymbol{\Gamma}(p',p)\,\mathbf{u}(p) &\simeq -\frac{i}{2m}\delta_{\sigma\sigma'}(\mathbf{p}+\mathbf{p}')\Big[F(\mathbf{q}^2)+G(\mathbf{q}^2)\Big] \\ &\qquad -\frac{1}{2m}\,\mathbf{q}\times\mathbf{M}_{\sigma\sigma'}\,F(\mathbf{q}^2)+\mathcal{O}(\mathbf{p}^2/m^2)\,,\end{aligned} \tag{17.6.13}$$

where $\mathbf{M}_{\sigma\sigma'}:=\mathbf{w}^\dagger_{\sigma'}\boldsymbol{\sigma}\,\mathbf{w}_\sigma$.

Electric charge

Having e be the magnitude of the electron charge means that the electric charge operator Q must satisfy

$$Q|e^-(\mathbf{p},\sigma)\rangle=-e|e^-(\mathbf{p},\sigma)\rangle \quad \text{where} \quad Q=\int \mathrm{d}^3x\; J^0\,, \tag{17.6.14}$$

since J^0 is the electric charge density operator. Therefore

$$\langle e^-(\mathbf{p}',\sigma')|Q|e^-(\mathbf{p},\sigma)\rangle=-e\,\delta_{\sigma\sigma'}\,\delta^3(\mathbf{p}-\mathbf{p}')\,. \tag{17.6.15}$$

But this is related to the vertex function form factors because

$$\begin{aligned}\frac{\langle\langle e^-(\mathbf{p}',\sigma')|Q|e^-(\mathbf{p},\sigma)\rangle\rangle}{\langle\langle 0,\mathrm{out}|0,\mathrm{in}\rangle\rangle} &= \int \mathrm{d}^3x\;\frac{\langle\langle e^-(\mathbf{p}',\sigma')|J^0(\mathbf{x})|e^-(\mathbf{p},\sigma)\rangle\rangle}{\langle\langle 0,\mathrm{out}|0,\mathrm{in}\rangle\rangle} \\ &= \int \mathrm{d}^3x\; e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}}\frac{\langle\langle e^-(\mathbf{p}',\sigma')|J^0(0)|e^-(\mathbf{p},\sigma)\rangle\rangle}{\langle\langle 0,\mathrm{out}|0,\mathrm{in}\rangle\rangle} \\ &= (2\pi)^3\delta(\mathbf{p}-\mathbf{p}')\;\left[-\frac{ie}{(2\pi)^3}\overline{\mathbf{u}}(p')\,\Gamma^0(p',p)\,\mathbf{u}(p)\right] \\ &= -e\,\delta_{\sigma\sigma'}\,\delta^3(\mathbf{p}-\mathbf{p}')\Big[F(0)+G(0)\Big]\,,\end{aligned} \tag{17.6.16}$$

which evaluates the position dependence of the matrix element using (8.1.16) and uses (17.6.1) to evaluate the matrix element itself. Comparing this last result with (17.6.15) shows that

the renormalization condition that the electron charge be $-e$ implies the form factors must satisfy the condition

$$F(0) + G(0) = 1\,. \tag{17.6.17}$$

This also automatically makes the spin-independent matrix element of the electric current in (17.6.13) also take the right form for a moving charge.

Magnetic moment

We next interpret the physical meaning of the spin-dependent contribution to (17.6.13) involving $\mathbf{M}_{\sigma\sigma'}$. To this end imagine turning on a weak classical magnetic field by allowing the electron to interact with a classical $\mathbf{A}_{\rm ext}$. We have seen that the Dirac Hamiltonian states that the Hamiltonian governing the electron spin evolution is

$$H_{\rm int} = -\int \mathrm{d}^3x\; \mathbf{J}\cdot\mathbf{A}_{\rm ext}\,, \tag{17.6.18}$$

whose matrix elements can be evaluated using (17.6.1) and (17.6.13), leading to

$$\begin{aligned}
\langle e^-(\mathbf{p}',\sigma')|H_{\rm int}|e^-(\mathbf{p},\sigma)\rangle &= -\int \mathrm{d}^3x\; e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}}\langle e^-(\mathbf{p}',\sigma')|\mathbf{J}(0)|e^-(\mathbf{p},\sigma)\rangle\cdot\mathbf{A}_{\rm ext}(\mathbf{x}) \\
&= \frac{ie}{(2\pi)^3}\int \mathrm{d}^3x\; \overline{\mathbf{u}}(p')\,\mathbf{\Gamma}(p',p)\,\mathbf{u}(p)\;\cdot\mathbf{A}_{\rm ext}(\mathbf{x})\,e^{-i\mathbf{q}\cdot\mathbf{x}} \\
&\simeq \frac{eF(0)}{2m(2\pi)^3}\int \mathrm{d}^3x\;\Big[-i\mathbf{q}\times\mathbf{M}_{\sigma\sigma'}\Big]\cdot\mathbf{A}_{\rm ext}\,e^{-i\mathbf{q}\cdot\mathbf{x}} \\
&= \frac{eF(0)}{2m(2\pi)^3}\int \mathrm{d}^3x\;\mathbf{M}_{\sigma\sigma'}\cdot\mathbf{B}_{\rm ext}\,e^{-i\mathbf{q}\cdot\mathbf{x}}\,.
\end{aligned} \tag{17.6.19}$$

For a constant magnetic field this becomes

$$\langle e^-(\mathbf{p}',\sigma')|H_{\rm int}|e^-(\mathbf{p},\sigma)\rangle \simeq \frac{eF(0)}{2m}\,\delta^3(\mathbf{p}-\mathbf{p}')\mathbf{M}_{\sigma\sigma'}\cdot\mathbf{B}_{\rm ext}\,, \tag{17.6.20}$$

which has the form of a magnetic moment interaction, $H_{\rm int} = -\boldsymbol{\mu}\cdot\mathbf{B}_{\rm ext}$, with magnetic moment operator in spin space given by

$$\boldsymbol{\mu} = -\frac{e}{2m}\,F(0)\,\mathbf{M}_{\sigma\sigma'} = -\frac{e}{2m}\,F(0)\,\mathbf{w}^\dagger_{\sigma'}\boldsymbol{\sigma}\mathbf{w}_\sigma\,. \tag{17.6.21}$$

The size of the magnetic moment components is therefore $-eF(0)/2m$.

Recall that for a non-interacting Dirac field we had $F(q^2) = 1$ for all q^2, so for a free Dirac particle one expects the conventional magnetic moment whose magnitude is

$$\mu = \frac{e}{2m}\,, \tag{17.6.22}$$

a quantity that (for the electron) has come to be known as a Bohr magneton: $\mu_B = e/2m_e$. Comparing this with the historical parameterization $\mu = g_L\mu_B S$, where S is the particle's

spin (in units of $\hbar$) and $g_{\scriptscriptstyle L}$ is called the Landé g-factor, this reproduces the famous result that $g_{\scriptscriptstyle L} = 2$ for a free relativistic electron (given that the electron spin is $S = \frac{1}{2}$).

In the presence of interactions we know very generally that $F(0) + G(0) = 1$ and so with interactions the full prediction (17.6.22) is replaced by

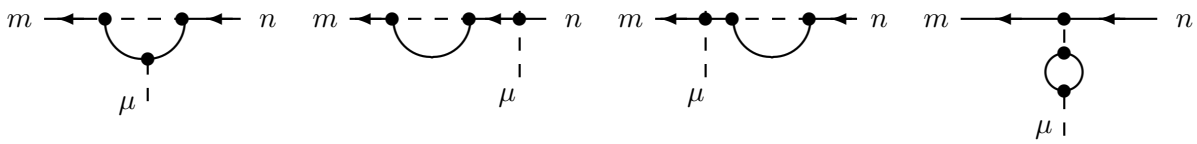
$$\mu = \frac{e}{2m}\Big[1 - G(0)\Big] \quad \text{or} \quad g_{\scriptscriptstyle L} = 2\Big[1 - G(0)\Big]\,. \tag{17.6.23}$$

Any deviation from $g_{\scriptscriptstyle L} = 2$ is called the anomalous magnetic moment and so the prediction for this from QED is found by evaluating the loop corrections to the function $G(q^2)$ (and so must also be UV finite).

17.6.2 Evaluation of the one-loop vertex correction

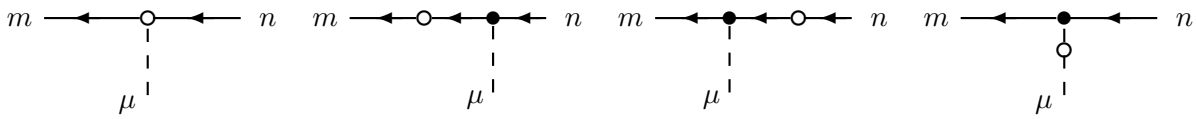
The next step is to compute $\Gamma^\mu(p', p)$ and thereby also compute $F(q^2)$ and $G(q^2)$. The explicit matrix element being computed in interaction picture is given in (17.6.1), and consists of the sum of all connected graphs with two external fermions and one external photon, though with the external photon line amputated (as described above).

At one loop there are several such graphs to be evaluated,



(a) (b) (c) (d)

as well as the counter-term graphs:



(e) (f) (g) (h)

The good news is that the discussion above shows that the contributions from graphs (b+f) vanishes one the electrons are put on shell as do also the graphs (c+g). They do so because they are proportional to $(i\not{p} + m)^{-1}\Sigma_\star$ which condition (17.3.10) implies vanishes as $\not{p} \to im$. The same is also true for the photon self-energy and counter-term contributions (d+h). All that needs doing is the evaluation of the vertex correction graph and counter-term (a+e). And because the vertex counter-term (e) only contributes to $F(0)$ all that is really needed to evaluate (17.6.23) is graph (a).

Worked example: Evaluating the one-loop vertex correction

The next step is to compute $\Gamma^\mu(p',p)$ and thereby also compute $F(q^2)$ and $G(q^2)$. The explicit matrix element being computed in interaction picture is given in (17.6.1), and consists of the sum of 1PI graphs with two external fermions and one external photon, though with the external photon line amputated (as described below (17.6.1)). At one loop there is one such graph that must be evaluated, plus the counter-term graph.

Denoting the result of the evaluation of the loop graph by $ie\,(2\pi)^4\Lambda^\mu_{mn}(p',p)\,\delta^4(q+p'-p)$ – so that $\Gamma^\mu(p',p)=\gamma^\mu+\Lambda^\mu(p',p)$ – we find

$$\begin{aligned} ie\,(2\pi)^4\Lambda^\mu(p',p) \;=\; 3!\left[\frac{(-i)^3}{3!}\right]\int\frac{\mathrm{d}^4k}{(2\pi)^4 i}\,\frac{1}{k^2-i\delta}\Big[ie\,(2\pi)^4\gamma^\rho\Big]\left[\frac{1}{(2\pi)^4 i}\;\frac{-i(\not p'-\not k)+m}{(p'-k)^2+m^2-i\delta}\right] \\ \times\Big[ie\,(2\pi)^4\gamma^\mu\Big]\left[\frac{1}{(2\pi)^4 i}\;\frac{-i(\not p-\not k)+m}{(p-k)^2+m^2-i\delta}\right]\Big[ie\,(2\pi)^4\gamma_\rho\Big]\,, \end{aligned} \tag{17.6.24}$$

where the initial 3! is the symmetry factor counting the number of ways the ingredients of the graph can be combined to produce this particular topology and $(-i)^3/3!$ is the factor $(-i)^N/N!$ appropriate for a graph with three vertices. Only the $\eta_{\mu\nu}$ piece of the photon polarization tensor is kept because the arguments of §16.3 show that the other terms do not contribute. Simplifying terms the result becomes

$$\Lambda^\mu(p',p)=\frac{ie^2}{(2\pi)^4}\int\mathrm{d}^4k\;\frac{N^\mu}{D}\,, \tag{17.6.25}$$

where

$$D:=\Big[(p'-k)^2+m^2-i\delta\Big]\Big[(p-k)^2+m^2-i\delta\Big]\Big(k^2-i\delta\Big)\,, \tag{17.6.26}$$

and

$$N^\mu:=\gamma^\rho\Big[-i(\not p'-\not k)+m\Big]\gamma^\mu\Big[-i(\not p-\not k)+m\Big]\gamma_\rho\,. \tag{17.6.27}$$

The numerator can be simplified because it appears sandwiched between $\overline{\mathbf{u}}(p')$ and $\mathbf{u}(p)$ and so we can use $\overline{\mathbf{u}}(p')\,(i\not p'+m)=(i\not p+m)\mathbf{u}(p)=0$. Using $\{\gamma^\alpha,\gamma^\beta\}=2\eta^{\alpha\beta}$ then implies

$$\overline{\mathbf{u}}'\gamma^\rho[-i(\not p'-\not k)+m]=\overline{\mathbf{u}}'\Big[-2i(p'-k)^\rho-i\not k\gamma^\rho\Big] \tag{17.6.28}$$

and similarly for $[-i(\not p-\not k)+m]\gamma^\rho\mathbf{u}$. This leaves

$$\begin{aligned} N^\mu \;&=\; \Big[-2i(p'-k)^\rho-i\not k\gamma^\rho\Big]\gamma^\mu\Big[-2i(p-k)_\rho-i\gamma^\rho\not k\Big] \\ &=\; -4(p'-k)\cdot(p-k)\gamma^\mu-2\gamma^\mu(\not p'-\not k)\not k-2\not k(\not p-\not k)\gamma^\mu-\not k\gamma^\rho\gamma^\mu\gamma_\rho\not k\,. \end{aligned} \tag{17.6.29}$$

Further simplifications come from repeated use of identities based on the Dirac algebra $\{\gamma^\mu,\gamma^\nu\}=2\eta^{\mu\nu}$, like

$$\not k\not p=k\cdot p+\gamma^{\mu\nu}k_\mu p_\nu \tag{17.6.30}$$

which implies in particular $\not k\not k=k^2$. Care must be used when doing so because some of these (though not the one shown above) differ when extended to $n\neq4$ dimensions. For instance one such is

$$\gamma^\rho\gamma^\mu\gamma_\rho=(-\gamma^\mu\gamma^\rho+2\eta^{\mu\rho})\gamma_\rho=(2-n)\gamma^\mu\,, \tag{17.6.31}$$

where the factor of n arises from $\gamma^\mu\gamma_\mu = \delta^\mu_\mu = \eta_{\mu\nu}\eta^{\mu\nu} = n$. Keeping this n-dependence is only important to the extent that the graph has a divergent contribution proportional to $1/(n-4)$ since then one can only take $n \to 4$ at the end of the calculation. One finds in this way the result

$$N^\mu = \Big[-4(p'-k)\cdot(p-k) + (6-n)k^2\Big]\gamma^\mu + 4imk^\mu + \Big[-4(p+p')^\mu + 2(n-2)k^\mu\Big]\not{k}\,. \qquad (17.6.32)$$

The denominator of (17.6.25) is simplified using the Feynman trick. Applying eq. (17.1.20) to the $s = 3$ factors in D gives

$$\frac{1}{D} = 2\int_0^1 \mathrm{d}x \int_0^x \mathrm{d}y\, \frac{1}{\mathcal{D}^3}\,, \qquad (17.6.33)$$

with denominator

$$\begin{aligned}\mathcal{D} &:= \Big[(p'-k)^2 + m^2 - i\delta\Big]y + \Big[(p-k)^2 + m^2 - i\delta\Big](x-y) + (k^2 - i\delta)(1-x) \\ &= \Big[k - p'y - p(x-y)\Big]^2 + \Big[y(p')^2 + (x-y)p^2 + m^2 x\Big] - a^2 - i\delta \\ &= \Big[k - p'y - p(x-y)\Big]^2 - a^2 - i\delta \qquad \text{when } p^2 = (p')^2 = -m^2\,,\end{aligned} \qquad (17.6.34)$$

where $a^\mu := [yp' + (x-y)p]^\mu$ and so

$$\begin{aligned}-a^2 &:= -\Big[yp' + (x-y)p\Big]^2 = m^2(x^2 - 2xy + 2y^2) - 2y(x-y)\, p\cdot p' \\ &= m^2x^2 + y(x-y)\, q^2\,.\end{aligned} \qquad (17.6.35)$$

In this expression the last equality on the first line uses $p^2 = (p')^2 = -m^2$ and the second line uses $q^\mu = (p-p')^\mu$ and so $q^2 = (p-p')^2 = -2m^2 - 2p\cdot p'$. We note in passing that the denominator and the measure and limits of the integration are invariant under the change of variables $y \to x - y$.

The next step is to shift the integration variable from k^μ to $\hat{k}^\mu := (k-a)^\mu = [k - yp' - (x-y)p]^\mu$, and re-express the numerator N^μ as a function of $\hat{k}^\mu$ rather than k^μ. Because the denominator and the integration region are both symmetric under $\hat{k}^\mu \to -\hat{k}^\mu$ we are free to drop any terms in N^μ that change sign under sign changes for $\hat{k}^\mu$, leaving the following symmetric terms as the only ones that survive the integration:

$$N^\mu_{\text{sym}} = \Big[-4(p'-a)\cdot(p-a) + (2-n)\hat{k}^2 + (6-n)a^2\Big]\gamma^\mu + 4ima^\mu - 4(p+p')^\mu\not{a} + 2(n-2)(\not{\hat{k}}\hat{k}^\mu + \not{a}a^\mu)\,. \qquad (17.6.36)$$

Because the rest of the integration is Lorentz invariant we can also replace $\hat{k}_\mu\hat{k}_\nu \to (\hat{k}^2/n)\,\eta_{\mu\nu}$ inside the integral, which further simplifies the numerator to

$$\begin{aligned}N^\mu_{\text{sym}} = \Big[-4p\cdot p' - 4(p+p')\cdot a - \frac{(n-2)^2}{n}\,\hat{k}^2 + (2-n)a^2\Big]\gamma^\mu \\ + 4ima^\mu + \Big[-4(p+p')^\mu + 2(n-2)a^\mu\Big]\not{a}\,.\end{aligned} \qquad (17.6.37)$$

Now use is the fact that the fermion lines are on-shell – *i.e.* that $\overline{\mathbf{u}}'(i\not{p}' + m) = (i\not{p} + m)\mathbf{u} = 0$ to set $\not{p}' = \not{p} = im$ and so $\not{a} = imx$ in (17.6.37). This allows its second line to be written

$$4ima^\mu + \Big[-4(p+p')^\mu + 2(n-2)a^\mu\Big]\not{a} = im\Big\{-4x(p+p')^\mu + \Big[4 + 2(n-2)x\Big]a^\mu\Big\}\,. \qquad (17.6.38)$$

The term linear in $a^\mu = y(p')^\mu + (x-y)p^\mu$ further simplifies if the change of variables $y \to x - y$ is performed in the p^μ term. This is a symmetry of the rest of the integral so has the effect of replacing

$a^\mu = [yp' + (x-y)p]^\mu$ with $y(p'+p)^\mu$. The same can be done for the term linear in a^μ in the first line of (17.6.37). Inside the integral the numerator therefore becomes

$$N^\mu_{\rm sym} = \left\{ \Big[2(1+2y) + (n-2)y(x-y)\Big] q^2 + \Big[4(1+4y) + (n-2)x^2\Big] m^2 - \frac{(n-2)^2}{n}\,\hat{k}^2 \right\} \gamma^\mu + \Big[4(y-x) + 2(n-2)xy\Big]\, im(p+p')^\mu \,. \tag{17.6.39}$$

Using this last expression and (17.6.33) in (17.6.25) finally gives

$$\Lambda^\mu(p',p) = 2ie^2\mu^{4-n} \int_0^1 \mathrm{d}x \int_0^x \mathrm{d}y \int \frac{\mathrm{d}^n k}{(2\pi)^n} \frac{1}{(k^2+M^2-i\delta)^3} \left\{ \left(\Big[2(1+2y) + (n-2)y(x-y)\Big] q^2 + \Big[4(1+4y) + (n-2)x^2\Big] m^2 - \frac{(n-2)^2}{n}\,k^2 \right) \gamma^\mu + \Big[4(y-x) + 2(n-2)xy\Big]\, im(p+p')^\mu \right\} , \tag{17.6.40}$$

where $M^2 = -a^2 = m^2x^2 + y(x-y)q^2$.

The $\mathrm{d}^n k$ integral can now be evaluated explicitly, by first Wick rotating – along the same lines used in passing from (17.1.3) to (17.1.4) – and then performing the resulting integral using the dimensionally regulated expressions (17.1.5). For the terms in the numerator that are independent of k^2 the integral converges and so we can directly take $n = 4$. The integral required in this case is

$$\int \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{1}{(k^2+M^2-i\delta)^3} = \frac{2i\pi^2}{(2\pi)^4} \int_0^\infty \frac{\mathrm{d}k_{\scriptscriptstyle E}\, k_{\scriptscriptstyle E}^3}{(k_{\scriptscriptstyle E}^2+M^2)^3} = \frac{i}{2(4\pi)^2 M^2} \,. \tag{17.6.41}$$

The k^2 term in the numerator gives a divergent integral:

$$I_{\rm div} := \mu^{4-n} \int \frac{\mathrm{d}^n k}{(2\pi)^n} \frac{k^2}{(k^2+M^2-i\delta)^3} = i\mu^{4-n} \int \frac{\mathrm{d}^n k_{\scriptscriptstyle E}}{(2\pi)^n} \frac{k_{\scriptscriptstyle E}^2}{(k_{\scriptscriptstyle E}^2+M^2)^3} = \frac{i\mu^{4-n}}{(2\pi)^n}\, J(1,3;M^2) = \frac{i}{(4\pi)^{n/2}} \left(\frac{M}{\mu}\right)^{n-4} \frac{n}{4}\, \Gamma\left(2 - \tfrac{1}{2}n\right) , \tag{17.6.42}$$

and so for $n = 4 - 2\epsilon$ this becomes (using (17.1.9)):

$$\frac{(n-2)^2}{n}\, I_{\rm div} = \frac{i(1-\epsilon)^2}{(4\pi)^2} \left(\frac{M^2}{4\pi\mu^2}\right)^{-\epsilon} \Gamma(\epsilon) = \frac{i}{(4\pi)^2} \left[\frac{1}{\epsilon} - \log\left(\frac{M^2}{4\pi\mu^2}\right) - \gamma - 2 + \mathcal{O}(\epsilon) \right] . \tag{17.6.43}$$

Combining results, the vertex correction becomes

$$\Lambda^\mu(p',p) = \frac{e^2}{(4\pi)^2} \int_0^1 \mathrm{d}x \int_0^x \mathrm{d}y \left\{ \left(2\left[\frac{1}{\epsilon} - \log\left(\frac{M^2}{4\pi\mu^2}\right) - \gamma - 2 \right] - \Big[2(1+2y) + 2y(x-y)\Big] \frac{q^2}{M^2} - \Big[4(1+4y) + 2x^2\Big] \frac{m^2}{M^2} \right) \gamma^\mu - \Big[4(y-x) + 4xy\Big]\, \frac{im}{M^2}(p+p')^\mu \right\} , \tag{17.6.44}$$

where (again) $M^2 = -a^2 = m^2x^2 + y(x-y)q^2$. As advertised, the divergent $1/\epsilon$ term only appears in the momentum-independent contribution proportional to γ^μ, and so can be cancelled by the right-hand counter-term graph shown in (17.6.24). The finite part of the remainder is chosen to ensure $F(0) + G(0) = 1$, as described above.

Explicit expressions for the form factors $F(q)^2$ and $G(q)^2$ can be read off from (17.6.44) by comparing the tensor structure of each term with (17.6.6). Recalling that $\Gamma^\mu(p',p) = (1+\delta Z_1)\gamma^\mu + \Lambda^\mu(p',p)$ – where δZ_1 comes from the counter-term graph – we can read off explicit expressions for the two form factors. One finds

$$\begin{aligned} F(q^2) = (\text{constant}) - \frac{2e^2}{(4\pi)^2}\int_0^1 \mathrm{d}x \int_0^x \mathrm{d}y \Bigg\{ \log\left(\frac{m^2x^2 + y(x-y)q^2}{4\pi\mu^2}\right) \\ + \Big[1 + 2y + y(x-y)\Big]\frac{q^2}{m^2x^2 + y(x-y)q^2} \\ + \Big[2(1+4y) + x^2\Big]\frac{m^2}{m^2x^2 + y(x-y)q^2}\Bigg\}\,. \end{aligned} \tag{17.6.45}$$

Notice that the value of the arbitrary scale μ contributes only as an additive constant in $F(q^2)$ and so is removed once the physical renormalization condition $F(0) + G(0) = 1$ is imposed. Notice the divergence in the Feynman parameter integration as $x, y \to 0$, reflecting a residual IR divergence as discussed in §17.3.

The other form factor is UV finite and is similarly given by

$$G(q^2) = \frac{8e^2m^2}{(4\pi)^2}\int_0^1 \mathrm{d}x \int_0^x \mathrm{d}y\, \frac{y - x + xy}{m^2x^2 + y(x-y)q^2}\,. \tag{17.6.46}$$

17.6.3 Anomalous magnetic moment

Knowledge of the form factor $G(q^2)$ allows a calculation of the anomalous magnetic moment, using (17.6.23). The result reproduces a famous result due to Schwinger:

$$G(0) = \frac{e^2}{2\pi^2}\int_0^1 \mathrm{d}x \int_0^x \mathrm{d}y\, \frac{y - x + xy}{x^2} = -\frac{e^2}{8\pi^2} = -\frac{\alpha}{2\pi}\,. \tag{17.6.47}$$

The corresponding Landé g-factor is

$$g - 2 = -2G(0) = \frac{\alpha}{\pi} + \mathcal{O}(\alpha^2)\,, \tag{17.6.48}$$

and the magnetic moment has magnitude

$$\mu = -\frac{e}{2m}\left(1 + \frac{\alpha}{2\pi} + \cdots\right) \simeq (-1.00116\cdots)\frac{e}{2m}\,. \tag{17.6.49}$$

Higher order corrections have been evaluated as well, and including also the next-order result leads to

$$\begin{aligned} F(0) = 1 - G(0) &= 1 + \frac{\alpha}{2\pi} + \frac{\alpha^2}{\pi^2}\underbrace{\left[\frac{197}{144} + \frac{\pi^2}{12} + \frac{3}{4}\,\zeta_R(3) - \frac{\pi^2}{2}\,\log 2\right]}_{-0.328} + \mathcal{O}(\alpha^3) \\ &= 1.001159639\,. \end{aligned} \tag{17.6.50}$$

The order α^3 is also known analytically as is the result numerically out to order α^5, leading to the state-of-the-art theoretical prediction

$$a_e(\text{th}) := \tfrac{1}{2}(g-2) = -G(0) = 0.001\,159\,652\,181\,643(764) \tag{17.6.51}$$

where the bracket is an estimate of the prediction's uncertainty in the last digits. This is to be compared with the experimentally measured value (which can also be inferred very precisely by measuring how electrons precess in magnetic fields)

$$a_e(\text{exp}) = 0.001\,159\,652\,180\,73(28)\,. \tag{17.6.52}$$

The concordance between these two numbers is among the most precise agreements in science.

The same calculation and measurement has also been done for the muon, which is another spin-half charged particle that is elementary (so far as we know) and shares identical properties to the electron apart from its mass (which is several hundred times heavier). For the muon the best measurements to date combine to give

$$a_\mu(\text{exp}) = 0.001\,165\,920\,61(41)\,. \tag{17.6.53}$$

The theoretical prediction for muons at $\mathcal{O}(\alpha)$ is precisely the same as found above for electrons, though higher orders differ for electrons and muons. At $\mathcal{O}(\alpha^2)$ the result is

$$\begin{aligned} 1 - G(0)_{\text{muon}} &= 1 + \frac{\alpha}{2\pi} + \frac{\alpha^2}{\pi^2}\left[-0.328 + \frac{1}{3}\,\log 2 - \frac{25}{36} + \frac{1}{6}\log\left(\frac{m_\mu^2}{m_e^2}\right)\right] + \mathcal{O}(\alpha^3) \\ &= 1.001\,165\,46\,, \end{aligned} \tag{17.6.54}$$

with the new explicitly written terms coming mostly from the graph obtained by inserting an electron-loop vacuum polarization into one of the internal photon lines.[80] The largest of the new contributions here comes from the logarithm of the mass ratio, whose origin can be traced because it arises by inserting a factor of the vacuum polarization (due to an electron loop) into the internal photon line, and so replaces $1/k^2 \to (1/k^2)[1 + \Pi_\star(k^2)]$, where we saw earlier that

$$\Pi_\star(k^2) = \frac{e^2}{2\pi^2}\int_0^1 \mathrm{d}x\; x(1-x)\log\left[1 + \frac{x(1-x)k^2}{m_e^2}\right] \simeq \frac{e^2}{12\pi^2}\ln\left(\frac{k^2}{m_e^2}\right) \quad \text{when } k^2 \gg m_e^2,. \tag{17.6.55}$$

This modifies the momentum integral (17.6.41) in the muon's vertex correction to become (for large momenta)

$$\mathcal{I} := \frac{e^2}{12\pi^2}\int \frac{\mathrm{d}^4k}{(k^2+a^2)^3}\;\log\left(\frac{k^2}{m^2}\right)\,, \tag{17.6.56}$$

[80] The corresponding graph where a muon circulates within a vacuum polarization graph within the electron's vertex correction also exists, but because the muon is much heavier than the typical momentum in the electron loop the result is in that case negligible because it is suppressed by a power of the mass ratio m_e/m_μ.

where for muons $a^2 = x^2 m_\mu^2 + \cdots$. Integrating this modifies the vertex correction to contribute

$$1 - G(0) = (\text{non-log contributions}) + \frac{\alpha}{2\pi}\left[\frac{e^2}{12\pi^2}\ln\left(\frac{m_\mu^2}{m_e^2}\right) + \cdots\right] \tag{17.6.57}$$

leading to logarithm whose coefficient is $(\alpha/2\pi)(\alpha/3\pi) = \frac{1}{6}(\alpha/\pi)^2$, as claimed in (17.6.54).

The best current theoretical predictions including even higher-order contributions give

$$a_\mu(\text{th}) = 0.001\,165\,918\,04(51) \tag{17.6.58}$$

and so (although in impressive overall agreement) is in modest tension with the measurement at about the 3-σ level. There is some controversy as to whether the theoretical errors – which depend on hard-to-calculate strongly interacting particles inside the loops – have been correctly assessed, however, and this remains an area of active research for both theory and experiment.

18 Beyond low-order perturbation theory

This section steps back from the immense satisfaction of computing physically measurable quantities in order to return and address several important broader questions of principle, some of which have already been encountered in previous sections. A common thread in this section is a focus on tools that can be used to derive consequences that apply beyond the leading order in perturbation theory.

A major tool for this is Low's theorem (3.3.9), relating the in-out matrix elements of time-ordered Heisenberg-picture operators to the interaction picture and repeated here for convenience of reference:

$$\begin{aligned}\langle\!\langle \beta, \text{out}|T\Big[A_{h\,1}(t_1)\cdots A_{h\,k}(t_k)\Big]|\alpha, \text{in}\rangle\!\rangle \qquad\qquad (18.0.1)\\ = \sum_{N=0}^{\infty}\frac{(-i)^N}{N!}\int_{-\infty}^{\infty} \mathrm{d}\tau_1\cdots\mathrm{d}\tau_N\ \langle\beta|T\Big[A_1(t_1)\cdots A_k(t_k)H_{\text{int},I}(\tau_1)\cdots H_{\text{int},I}(\tau_N)\Big]|\alpha\rangle\,,\end{aligned}$$

since this allows us to jump back and forth between Heisenberg picture (where some exact statements can be made) and interaction picture (which is more convenient for perturbative calculations).

18.1 Symmetry implications

Symmetries play a ubiquitous role in physics and one of the reasons this is so is the ability to use them to derive consequences that are exact predictions and not limited to various approximation schemes. That makes them a natural place to start a chapter aimed tools for going past leading order methods. We here make explicit some of these exact symmetry consequences for correlation functions, focussing on those associated with conserved charges and global symmetries, like Poincaré invariance and the global conservation of overall electric charge.

Poincaré transformations

We saw in §8 how in Heisenberg picture the Hamiltonian and momentum operators are the generators of translations in space and time, with (8.1.12) and (8.1.16) combinable into the more covariant form

$$U^\star(a)\,\mathcal{O}_h(x)\,U(a) = \mathcal{O}_h(x+a)\,, \tag{18.1.1}$$

where

$$U(a) = \exp\Bigl(ia_\mu P^\mu\Bigr) = \exp\Bigl(-iHa^0 + i\mathbf{a}\cdot\mathbf{P}\Bigr)\,. \tag{18.1.2}$$

and so

$$\Bigl[P^\mu\,,\mathcal{O}_h(x)\Bigr] = i\partial^\mu\mathcal{O}_h(x)\,. \tag{18.1.3}$$

Because our scattering states are eigenstates of P^μ these imply the exact relations

$$\begin{aligned}
&\langle\!\langle\beta,\text{out}|T\Bigl[\mathcal{O}_{h1}(x_1+y)\cdots\mathcal{O}_{hk}(x_k+y)\Bigr]|\alpha,\text{in}\rangle\!\rangle \\
&\qquad = \langle\!\langle\beta,\text{out}|T\Bigl[U^\star(y)\,\mathcal{O}_{h1}(x_1)\,U(y)\cdots U^\star(y)\,\mathcal{O}_{hk}(x_k)\,U(y)\Bigr]|\alpha,\text{in}\rangle\!\rangle \\
&\qquad = e^{i(p_\alpha-p_\beta)\cdot y}\langle\!\langle\beta,\text{out}|T\Bigl[\mathcal{O}_{h1}(x_1)\cdots\mathcal{O}_{hk}(x_k)\Bigr]|\alpha,\text{in}\rangle\!\rangle
\end{aligned} \tag{18.1.4}$$

where p^μ_α and p^μ_β are the 4-vector eigenvalues of P^μ on the in and out states. As applied to the two-point vacuum correlator this implies in particular

$$\langle\!\langle 0,\text{out}|T\Bigl[\mathcal{O}_{h1}(x)\,\mathcal{O}_{h2}(y)\Bigr]|0,\text{in}\rangle\!\rangle = \langle\!\langle 0,\text{out}|T\Bigl[\mathcal{O}_{h1}(x-y)\,\mathcal{O}_{h2}(0)\Bigr]|0,\text{in}\rangle\!\rangle\,. \tag{18.1.5}$$

A similar argument for Lorentz transformations shows how the Lorentz-transformation properties of correlation functions can be read off from the transformation properties of the operators and of the initial and final states in the matrix element.

Conservation of overall charge

Internal symmetries can be used in the same way, implying exact selection rules for correlation functions. For example suppose an internal conserved charge Q exists and is used to label the scattering states in addition to their energy and momentum:

$$Q|\alpha,\text{in}\rangle\!\rangle = q_\alpha|\alpha\,,\text{in}\rangle\!\rangle \quad\text{and}\quad Q|\beta,\text{out}\rangle\!\rangle = q_\beta|\beta\,,\text{out}\rangle\!\rangle\,. \tag{18.1.6}$$

Suppose also that the Heisenberg-picture field operators also have definite charge, so

$$\Bigl[Q\,,\mathcal{O}_{hi}(x)\Bigr] = -q_i\,\mathcal{O}_{hi}(x)\,, \tag{18.1.7}$$

as would be appropriate in particular (say) if $\mathcal{O}_{hi}(x)$ were to be a field that destroys a particle with charge q_i.

Now consider the operator

$$R(x_1,\cdots,x_N) := T\Bigl[\mathcal{O}_{h1}(x_1)\,,\cdots,\mathcal{O}_{hN}(x_N)\Bigr]\,. \tag{18.1.8}$$

On one hand (18.1.7) implies

$$\Big[Q\,,R(x_1,\cdots,x_N)\Big] = -q_R\,R(x_1,\cdots,x_N) \quad \text{with} \quad q_R := \sum_{k=1}^{N} q_k\,, \tag{18.1.9}$$

and so

$$\langle\!\langle\beta\,,\text{out}|\Big[Q\,,R(x_1,\cdots,x_N)\Big]|\alpha,\text{in}\rangle\!\rangle = -q_R\,\langle\!\langle\beta\,,\text{out}|R(x_1,\cdots,x_N)|\alpha,\text{in}\rangle\!\rangle\,. \tag{18.1.10}$$

On the other hand the left-hand side of this last equation can instead be evaluating by allowing Q to act on the in and out states, using (18.1.6), leading to

$$\langle\!\langle\beta\,,\text{out}|\Big[Q\,,R(x_1,\cdots,x_N)\Big]|\alpha,\text{in}\rangle\!\rangle = (q_\beta - q_\alpha)\,\langle\!\langle\beta\,,\text{out}|R(x_1,\cdots,x_N)|\alpha,\text{in}\rangle\!\rangle\,. \tag{18.1.11}$$

Equating (18.1.10) and (18.1.11) then implies

$$\Big(q_\beta - q_\alpha + q_R\Big)\,\langle\!\langle\beta\,,\text{out}|R(x_1,\cdots,x_N)|\alpha,\text{in}\rangle\!\rangle = 0\,, \tag{18.1.12}$$

and so $\langle\!\langle\beta\,,\text{out}|R(x_1,\cdots,x_N)|\alpha,\text{in}\rangle\!\rangle \neq 0$ necessarily implies $q_\beta = q_\alpha + q_R$. A special case of this that is used in what follows states that the matrix element

$$\langle\!\langle 0\,,\text{out}|A_h(x)|\alpha\,,\text{in}\rangle\!\rangle \tag{18.1.13}$$

can be nonzero for some Heisenberg-picture operator $A_h(x)$ only if $q_\alpha = q_A$ for all conserved charges, assuming that the ground state is invariant: $Q|0,\text{out}\rangle\!\rangle = 0$.

Charge conjugation

A special case of the above result applies it to discrete symmetries, like charge conjugation. Recall that charge conjugation is defined to swap particles with antiparticles and its action on a general relativistic field is given in (11.5.7). Specialized to the electron and photon fields of QED this becomes

$$\mathcal{C}\;A_\mu(x)\;\mathcal{C}^{-1} = -\;A_\mu(x)\,, \tag{18.1.14}$$

and

$$\mathcal{C}\;\psi(x)\;\mathcal{C}^{-1} = \eta_c^*\,C\,\psi^*(x)\,, \tag{18.1.15}$$

where η_c is a phase and C is the charge-conjugation matrix defined in (15.1.14). As is quick to check these transformations imply the QED Hamiltonian density satisfies

$$\mathcal{C}\,\mathcal{H}(x)\,\mathcal{C}^{-1} = \mathcal{H}(x), \tag{18.1.16}$$

and so is invariant.

Using this symmetry in the above general argument for the implications of symmetries for correlators to this particular case leads to a famous result. The transformation (18.1.14) in particular implies that correlators involving an odd number of electromagnetic fields must vanish when taken in a charge-conjugate invariant state, and applied to the vacuum this is called *Furry's theorem*:

$$\langle\!\langle 0,\text{out}|T\Big[A_{\mu_1}(x_1)\cdots A_{\mu_N}(x_N)\Big]|0,\text{in}\rangle\!\rangle = 0 \qquad \text{for } N \text{ odd}. \tag{18.1.17}$$

18.2 Ward identities (again)

We next turn to the implications of local conservation of electric charge, $\partial_\mu J^\mu = 0$, as opposed to only the overall conservation of the integrated charge $Q = \int \mathrm{d}^3x \; J^0$ considered above. Unlike global charge conservation local conservation also carries implications for correlations involving electromagnetic fields, since it is intimately tied to the underlying gauge invariance of the electromagnetic field.

In the examples considered so far local charge conservation and gauge invariance have already played important roles, such as by providing the underlying reason why the identity (16.3.7) proven in §16.3 was true, which in turn ensures that the $\alpha_\mu p_\nu + \alpha_\nu p_\mu$ terms in the photon propagator never play a role in physical processes. It has also been used in conclusions like $q_\mu \Pi^{\mu\nu}(q) = 0$ for the electromagnetic vacuum polarization discussed in §17.5.

This section derives a more general version of the identity $(p'-p)_\mu \, \overline{\mathbf{u}}(p') \Gamma^\mu(p',p) \, \mathbf{u}(p) = 0$ satisfied by the vertex correction discussed in §17.6 that also applies when the initial and final electrons are not on shell. To this end consider the correlation function

$$\int \mathrm{d}^4x \, \mathrm{d}^4y \, \frac{\langle\!\langle 0, \mathrm{out}| \, T\Big[\psi_n(x) \, J^\mu(0) \, \overline{\psi}_m(y)\Big] |0, \mathrm{in}\rangle\!\rangle}{\langle\!\langle 0, \mathrm{out}|0, \mathrm{in}\rangle\!\rangle} \, e^{-ip'\cdot x + ip\cdot y} \\ = -ie\Big[-i\widehat{S}(p')\Big]_{nk} \, \Gamma^\mu_{kl}(p',p) \, \Big[-i\widehat{S}(p)\Big]_{lm} , \tag{18.2.1}$$

where

$$J^\mu = -ie \, \overline{\psi} \, \gamma^\mu \psi \tag{18.2.2}$$

is the electromagnetic current appropriate for a spin-half fermion with charge $-e$ and

$$\Big[-i\widehat{S}(p)\Big]_{nm} := \int \mathrm{d}^4x \, \frac{\langle\!\langle 0, \mathrm{out}|T\Big[\psi_n(x) \, \overline{\psi}_m(0)\Big] |0, \mathrm{in}\rangle\!\rangle}{\langle\!\langle 0, \mathrm{out}|0, \mathrm{in}\rangle\!\rangle} \, e^{-ip\cdot x} \tag{18.2.3}$$

is that fermion's full momentum-space electron propagator encountered above.

The arguments of §18.4 below show that $\Gamma^\mu(p',p)$ is the same quantity encountered in §17.6, though here it does not appear between the spinors $\overline{\mathbf{u}}(p')$ and $\mathbf{u}(p)$ and so the momenta p and p' need not be on shell. From a graphical point of view (18.2.1) is true because the left-hand side is the sum of all connected graphs with an incoming and outgoing electron line and a photon line, but with the external electron lines describing propagators (rather than scattering mode functions) and the photon propagator amputated (see the discussions around (17.2.25) and (17.2.46)). But this is the same as inserting a single (amputated) external photon line in all possible ways to the connected graphs describing an electron propagator, which results in a 1PI vertex connected one each side to a propagator.

All operators here are Heisenberg-picture fields, for which the burden of time-evolution is carried by the fields, and so current conservation implies the operator $J^\mu(z)$ satisfies $\partial_\mu J^\mu(z) = 0$. To see what this implies for (18.2.1) we start by evaluating

$$\frac{\partial}{\partial z^\mu} \langle\!\langle 0, \mathrm{out}|T\Big[\psi_n(x) \, J^\mu(z) \, \overline{\psi}_m(y)\Big] |0, \mathrm{in}\rangle\!\rangle \, . \tag{18.2.4}$$

Although this derivative vanishes when it acts on $J^\mu(z)$ the above does not evaluate to zero because the derivative also acts on the z^0's appearing in the time ordering:

$$\begin{aligned} T\Big[\psi_n(x)\,J^\mu(z)\,\overline{\psi}_m(y)\Big] &:= \Theta(z^0-x^0)\,\Theta(x^0-y^0)\,J^\mu(z)\,\psi_n(x)\,\overline{\psi}_m(y) \\ &-\Theta(z^0-y^0)\,\Theta(y^0-x^0)\,J^\mu(z)\,\overline{\psi}_m(y)\,\psi_n(x) + \Theta(x^0-z^0)\,\Theta(z^0-y^0)\,\psi_n(x)\,J^\mu(z)\,\overline{\psi}_m(y) \\ &-\Theta(y^0-z^0)\,\Theta(z^0-x^0)\,\overline{\psi}_m(y)\,J^\mu(z)\,\psi_n(x) + \Theta(x^0-y^0)\,\Theta(y^0-z^0)\,\psi_n(x)\,\overline{\psi}_m(y)\,J^\mu(z) \\ &\quad -\Theta(y^0-x^0)\,\Theta(x^0-z^0)\,\overline{\psi}_m(y)\,\psi_n(x)\,J^\mu(z)\,, \end{aligned} \tag{18.2.5}$$

leading to

$$\begin{aligned} \frac{\partial}{\partial z^\mu}\langle\!\langle 0,\mathrm{out}|T\Big[\psi_n(x)\,J^\mu(z)\,\overline{\psi}_m(y)\Big]|0,\mathrm{in}\rangle\!\rangle &= \delta(z^0-x^0)\,\Theta(x^0-y^0)\Big[J^0(z),\psi_n(x)\Big]\overline{\psi}_m(y) \\ &+\delta(y^0-z^0)\,\Theta(x^0-y^0)\psi_n(x)\Big[J^0(z),\overline{\psi}_n(y)\Big] - \delta(z^0-y^0)\,\Theta(y^0-x^0)\Big[J^0(z),\overline{\psi}_n(y)\Big]\psi_n(x) \\ &-\delta(x^0-z^0)\,\Theta(y^0-z^0)\,\overline{\psi}_n(y)\Big[J^0(z),\psi_n(x)\Big]\,. \end{aligned} \tag{18.2.6}$$

The commutators with the current can be evaluated keeping in mind that the electron field's canonical momentum is

$$\Pi_\psi = \frac{\partial\mathcal{L}_{QED}}{\partial\dot{\psi}} = -\overline{\psi}\,\gamma^0\,, \tag{18.2.7}$$

and so the canonical commutation relations imply

$$\begin{aligned} &\Big[J^0(\mathbf{x},t)\,,\psi_n(\mathbf{y},t)\Big] = +e\,\delta^3(\mathbf{x}-\mathbf{y})\,\psi_n(\mathbf{y},t) \\ \text{and}\qquad &\Big[J^0(\mathbf{x},t)\,,\overline{\psi}_m(\mathbf{y},t)\Big] = -e\,\delta^3(\mathbf{x}-\mathbf{y})\,\overline{\psi}_m(\mathbf{y},t)\,. \end{aligned} \tag{18.2.8}$$

This gives

$$\begin{aligned} &\frac{\partial}{\partial z^\mu}\langle\!\langle 0,\mathrm{out}|T\Big[\psi_n(x)\,J^\mu(z)\,\overline{\psi}_m(y)\Big]|0,\mathrm{in}\rangle\!\rangle = \\ &\qquad -e\,\delta^4(y-z)\,T\Big[\psi_n(x)\,\overline{\psi}_m(y)\Big] + e\,\delta^4(x-z)\;T\Big[\psi_n(x)\,\overline{\psi}_m(y)\Big]\,. \end{aligned} \tag{18.2.9}$$

In order to use these to draw conclusions about (18.2.1) we next use the identity

$$\left(\frac{\partial}{\partial x^\mu}+\frac{\partial}{\partial y^\mu}+\frac{\partial}{\partial z^\mu}\right)\langle\!\langle 0,\mathrm{out}|T\Big[\psi_n(x)\,J^\mu(z)\,\overline{\psi}_m(y)\Big]|0,\mathrm{in}\rangle\!\rangle = 0\,, \tag{18.2.10}$$

which follows because translation invariance – *c.f.* eq. (18.1.4) – implies the correlation function is a function only of the coordinate differences, such as $(x-y)$ and $(z-y)$. Evaluating this at $z=0$ and Fourier transforming with respect to x and y then gives

$$\begin{aligned} &\int \mathrm{d}^4x\,\mathrm{d}^4y\;e^{-ip'\cdot x+ip\cdot y}\left[\left(-\frac{\partial}{\partial x^\mu}-\frac{\partial}{\partial y^\mu}\right)\langle\!\langle 0,\mathrm{out}|T\Big[\psi_n(x)\,J^\mu(0)\,\overline{\psi}_m(y)\Big]|0,\mathrm{in}\rangle\!\rangle\right] \\ &\qquad = -e\int \mathrm{d}^4x\;e^{-ip'\cdot x}\langle\!\langle 0,\mathrm{out}|T\Big[\psi_n(x)\,\overline{\psi}_m(0)\Big]|0,\mathrm{in}\rangle\!\rangle \\ &\qquad\qquad +e\int \mathrm{d}^4y\;e^{ip\cdot y}\langle\!\langle 0,\mathrm{out}|T\Big[\psi_n(0)\,\overline{\psi}_m(y)\Big]|0,\mathrm{in}\rangle\!\rangle\,, \end{aligned} \tag{18.2.11}$$

where the right-hand side uses (18.2.9) to evaluate the $\partial/\partial z^\mu$ term.

Dividing by the vacuum-to-vacuum amplitude and using (18.2.1) and (18.2.3) then gives (suppressing the Dirac spinor indices, using matrix notation):

$$(p'-p)_\mu \widehat{S}(p')\,\Gamma^\mu(p',p)\,\widehat{S}(p) = i\Big[\widehat{S}(p') - \widehat{S}(p)\Big]\,, \tag{18.2.12}$$

or, equivalently

$$i(p-p')_\mu \Gamma^\mu(p',p) = \widehat{S}^{-1}(p) - \widehat{S}^{-1}(p')\,. \tag{18.2.13}$$

This is called a Ward-Takahashi identity because it is a relation amongst correlation functions that follows as the consequence of a symmetry. Recall that at lowest order in perturbation theory we have $\Gamma^\mu(p',p) \to \gamma^\mu$ and $\widehat{S}^{-1}(p) \to S^{-1}(p) = i\not{p} + m$ and so (18.2.13) reduces to the trivially true statement

$$i(\not{p} - \not{p}') = (i\not{p} + m) - (i\not{p}' + m)\,. \tag{18.2.14}$$

The identity (18.2.13) can also be proven order-by-order in perturbation theory by recognizing that (18.2.1) corresponds to inserting an amputated photon line in all possible ways into an arbitrary electron propagator graph, and then using the argument of §16.3 to evaluate the result of contracting this graph with the external photon momentum.

18.3 Lehmann-Kählen representation

Earlier sections on renormalization used features of the full Heisenberg-picture propagator for various fields, so we next ask what can be said about these propagators on general grounds. For simplicity this is done here for a complex scalar field χ, such as first encountered in (17.2.26), though similar arguments can also be made for propagators for spinning particles.

18.3.1 Spectral density

Consider first the *Wightman function* for such a scalar field, defined by

$$\mathcal{W}(x,y) := \langle\!\langle 0,\mathrm{out}|\chi_h(x)\,\chi_h^\star(y)|0,\mathrm{in}\rangle\!\rangle\,. \tag{18.3.1}$$

Imagine inserting a partition of unity by summing over a complete basis of states between the two fields, with the basis chosen to be eigenstates of 4-momentum: $P^\mu|N\rangle\!\rangle = p_N^\mu|N\rangle\!\rangle$. This gives

$$\begin{aligned}\mathcal{W}(x,y) &= \sum_N \langle\!\langle 0,\mathrm{out}|\chi_h(x)|N\rangle\!\rangle\,\langle\!\langle N|\chi_h^\star(y)|0,\mathrm{in}\rangle\!\rangle \\ &= \sum_N e^{ip_N\cdot(x-y)}\Big|\langle\!\langle 0|\chi_h(0)|N\rangle\!\rangle\Big|^2\,,\end{aligned} \tag{18.3.2}$$

which extracts the position dependence of the fields using (18.1.1) and (18.1.2) and assumes the vacuum to be unique so that $|0,\mathrm{out}\rangle\!\rangle$ and $|0,\mathrm{in}\rangle\!\rangle$ are not distinct states. Similarly

$$\overline{\mathcal{W}}(x,y) := \langle\!\langle 0,\mathrm{out}|\chi_h^\star(y)\,\chi_h(x)|0,\mathrm{in}\rangle\!\rangle = \sum_N e^{ip_N\cdot(y-x)}\Big|\langle\!\langle 0|\chi_h^\star(0)|N\rangle\!\rangle\Big|^2 . \tag{18.3.3}$$

The idea is to use symmetries to simplify these expressions as much as possible, and do so *without* working in perturbation theory so the states $|N\rangle\!\rangle$ need not be simple single-particle states. To this end define the function

$$f(p) := \sum_N \Big|\langle\!\langle 0|\chi_h(0)|N\rangle\!\rangle\Big|^2 \,\delta^4(p-p_N)\,. \tag{18.3.4}$$

We know from the symmetry properties for correlations discussed above that $f(p)$ is a Lorentz-invariant function of momentum when $\chi_h(x)$ is a Lorentz scalar. We also know that $f(p)=0$ unless $p_\mu p^\mu \le 0$ and $p^0>0$ because when it is nonzero p^μ is the 4-momentum of some physical state $|N\rangle\!\rangle$.

This means we can always write

$$\sum_N \Big|\langle\!\langle 0|\chi_h(0)|N\rangle\!\rangle\Big|^2 \,\delta^4(p-p_N) = \frac{1}{(2\pi)^3}\,\Theta(p^0)\,\varrho(-p^2)\,, \tag{18.3.5}$$

where Θ is the Heaviside step function and $\varrho(\mu^2)$ is a real, positive function of a single argument that vanishes when this argument is negative. An identical argument also implies

$$\sum_N \Big|\langle\!\langle 0|\chi_h^\star(0)|N\rangle\!\rangle\Big|^2 \,\delta^4(p-p_N) = \frac{1}{(2\pi)^3}\,\Theta(p^0)\,\overline{\varrho}(-p^2)\,, \tag{18.3.6}$$

where the function $\overline{\varrho}$ is in principle independent (so far) of ϱ, but shares its properties of being real, positive and vanishing when its argument is negative.

Multiplying (18.3.5) by $e^{ip\cdot(x-y)}$, integrating over all p^μ and comparing the result to (18.3.2) shows that ϱ is related to $\mathcal{W}(x,y)$ by

$$\begin{aligned}\mathcal{W}(x,y) = \langle\!\langle 0|\chi_h(x)\,\chi_h^\star(y)|0\rangle\!\rangle &= \int \frac{\mathrm{d}^4p}{(2\pi)^3}\,\Theta(p^0)\,\varrho(-p^2)\,e^{ip\cdot(x-y)} \\ &= \int_0^\infty \mathrm{d}\mu^2\;\varrho(\mu^2)\,\Delta_+(x-y;\mu^2)\,,\end{aligned} \tag{18.3.7}$$

and

$$\begin{aligned}\overline{\mathcal{W}}(x,y) = \langle\!\langle 0|\chi_h^\star(y)\,\chi_h(x)|0\rangle\!\rangle &= \int \frac{\mathrm{d}^4p}{(2\pi)^3}\,\Theta(p^0)\,\overline{\varrho}(-p^2)\,e^{-ip\cdot(x-y)} \\ &= \int_0^\infty \mathrm{d}\mu^2\;\overline{\varrho}(\mu^2)\,\Delta_+(y-x;\mu^2)\,,\end{aligned} \tag{18.3.8}$$

where the final equalities use the function defined in (11.4.9), which we rewrite as

$$\begin{aligned}\Delta_+(x-y;m^2) &:= \frac{1}{(2\pi)^3}\int \frac{\mathrm{d}^3p}{2\varepsilon(p)}\, e^{ip\cdot(x-y)} \\ &= \frac{1}{(2\pi)^3}\int \mathrm{d}^4p\, \delta(p^2+m^2)\,\Theta(p^0)\, e^{ip\cdot(x-y)},\end{aligned} \tag{18.3.9}$$

where $\varepsilon(p) := \sqrt{\mathbf{p}^2+m^2}$ and the second line is proven by using the delta function to perform the p^0 integral.

We see that knowledge of $\varrho(\mu^2)$ completely determines the Wightman function $\mathcal{W}(x,y)$ and $\overline{\varrho}(\mu^2)$ similarly completely fixes $\overline{\mathcal{W}}(x,y)$, writing them as a superposition of free Wightman functions, summed over different masses weighted by a *spectral function* $\varrho(\mu^2)$ or $\overline{\varrho}(\mu^2)$. The noninteracting theory corresponds to the special case

$$\varrho(\mu^2) = \overline{\varrho}(\mu^2) = \delta(\mu^2-m^2) \qquad \text{(noninteracting theory)}. \tag{18.3.10}$$

General principles impose constraints on these functions, as we now describe. First, a connection between $\varrho(\mu^2)$ and $\overline{\varrho}(\mu^2)$ can be found either by imposing the canonical commutation relations on the fields (which implies in particular that $\chi_h(\mathbf{x},t)$ commutes with $\chi_h^\star(\mathbf{y},t)$ at equal times), or by imposing microcausality (which asks $\chi_h(x)$ to commute with $\chi^\star(y)$ when $x-y$ is spacelike. Either way, specializing (18.3.7) and (18.3.8) to equal times ($x^0=y^0$) and subtracting then gives

$$\langle\!\langle 0|\Big[\chi_h(\mathbf{x},t)\,,\chi_h^\star(\mathbf{y},t)\Big]|0\rangle\!\rangle = \int_0^\infty \mathrm{d}\mu^2\,\Big[\varrho(\mu^2)-\overline{\varrho}(\mu^2)\Big]\,\Delta_+(\mathbf{x}-\mathbf{y};\mu^2) = 0\,, \tag{18.3.11}$$

and because this must be true for all $\mathbf{x}-\mathbf{y}$ this further implies $\overline{\varrho}(\mu^2)=\varrho(\mu^2)$. The commutator at timelike or lightlike separations is not zero because

$$\langle\!\langle 0|\Big[\chi_h(x)\,,\chi_h^\star(y)\Big]|0\rangle\!\rangle = \int_0^\infty \mathrm{d}\mu^2\,\varrho(\mu^2)\,\Delta(x-y;\mu^2)\,, \tag{18.3.12}$$

where

$$\Delta(x-y;m^2) := \Delta_+(x-y;m^2)-\Delta_+(y-x;m^2)\,, \tag{18.3.13}$$

is given as an explicit function using (11.4.15).

A further constraint comes from the canonical commutation relation $[\dot\chi_h(\mathbf{x},t)\,,\chi_h^\star(\mathbf{y},t)] = -i\,\delta^3(\mathbf{x}-\mathbf{y})$. Using this with

$$\langle\!\langle 0|\Big[\dot\chi_h(x)\,,\chi_h^\star(y)\Big]|0\rangle\!\rangle = \int_0^\infty \mathrm{d}\mu^2\,\varrho(\mu^2)\,\frac{\partial}{\partial x^0}\Delta(x-y;\mu^2)\,, \tag{18.3.14}$$

leads to the conclusion

$$\int_0^\infty \mathrm{d}\mu^2\,\varrho(\mu^2) = 1\,. \tag{18.3.15}$$

The upshot is that the information in the Wightman function can be completely summarized by a single real, positive, Lorentz-invariant function and eqs. (18.3.5) and (18.3.6) ensure that this function only is nonzero when its argument coincides with the squared mass of a physical state in the theory for which the matrix elements $\langle\langle 0|\chi_h(0)|N\rangle\rangle$ or $\langle\langle 0|\chi_h^\star(0)|N\rangle\rangle$ are nonzero. For noninteracting theories this spectral weight is entirely concentrated at the squared-mass of the noninteracting particle, because only single-particle states can contribute to these matrix elements. Interactions allow multiparticle states also to do so and so spread out the support of $\varrho(\mu^2)$, but in a way that preserves the normalization (18.3.15).

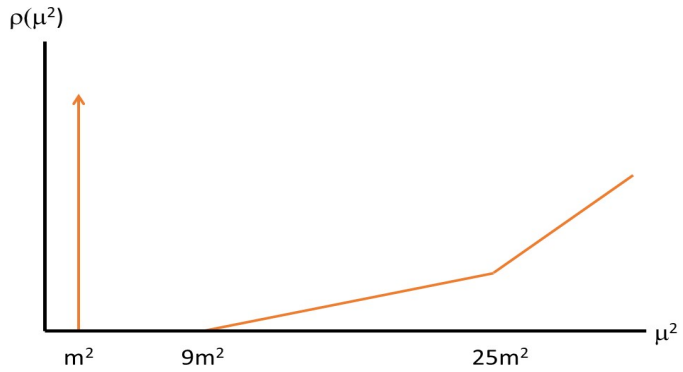


Figure 13. A sketch of the spectral function $\varrho(\mu^2)$ showing a single-particle pole, and the start of the 3-particle continuum and the 5-particle continuum and so on.

Because p^2 can run through continuous values when evaluated for multiparticle states, interactions end up giving spectral functions of the form sketched in Fig. 13, where the single-particle state remains as an isolated contribution at $\mu^2 = m^2$ but multiparticle states contributing continuous regions for which ϱ is nonzero. These regions are only available above a minimum energy threshold because expressions like (18.1.12) show that the multiparticle states must share the same charge assignments as the fields, and so the lowest energy multiple particle state contributing to $\varrho(\mu^2)$ is the energy $E_{\rm min} = 3m$ of two particles and an antiparticle. The next threshold above this occurs at $5m$, corresponding to a particle plus two particle-antiparticle pairs, and so on.

The contribution coming from the single-particle state, $|N\rangle\rangle = |\mathbf{k}\rangle\rangle$ of the interacting theory is strongly restricted since Lorentz-covariance determines the matrix element

$$\langle\langle 0|\chi_h(0)|\mathbf{k}\rangle\rangle = \frac{Z^{1/2}}{(2\pi)^{3/2}}\,\frac{1}{\sqrt{2\varepsilon(k)}}\,, \tag{18.3.16}$$

up to normalization (with numerical factors chosen here so that the non-interacting case

corresponds to $Z = 1$). Using this in the definition (18.3.5) then implies

$$\begin{aligned}\Theta(p^0)\,\varrho_{\rm sp}(-p^2) &= (2\pi)^3 \int \mathrm{d}^3k\, \left|\langle\!\langle 0|\chi_h(0)|\mathbf{k}\rangle\!\rangle\right|^2 \delta^4(p-k) \\ &= \frac{Z}{2\varepsilon(p)}\,\delta[p^0-\varepsilon(p)] = Z\,\Theta(p^0)\,\delta(p^2+m^2)\,,\end{aligned} \tag{18.3.17}$$

and so $\varrho(\mu^2)$ can be written

$$\varrho(\mu^2) = Z\,\delta(\mu^2-m^2) + \varrho_c(\mu^2)\,, \tag{18.3.18}$$

where the continuum contribution $\varrho_c(\mu^2)$ only has support for $\mu^2 \geq \mu^2_{\rm th} \simeq 9m^2$. The normalization condition (18.3.15) then implies

$$0 \leq Z = 1 - \int_{\mu^2_{\rm th}}^{\infty} \mathrm{d}\mu^2\; \varrho_c(\mu^2) \leq 1\,. \tag{18.3.19}$$

The parameter Z expresses the precise sense in which the normalization of the Heisenberg-picture field can differ in the interacting theory from the noninteracting theory about which perturbative methods expand.

18.3.2 Propagator singularities

Earlier sections on renormalization are phrased in terms of the singularities (positions of poles and their residues) in the time-ordered correlation function, so it is useful also to express this in terms of the spectral function $\varrho(\mu^2)$. To this end write

$$\begin{aligned}\mathcal{G}(x,y) &:= \langle\!\langle 0|T\Big[\chi_h(x)\,\chi_h^\star(y)\Big]|0\rangle\!\rangle = \Theta(x^0-y^0)\,\mathcal{W}(x,y) + \Theta(y^0-x^0)\,\overline{\mathcal{W}}(x,y) \\ &= \int_0^\infty \mathrm{d}\mu^2\; \varrho(\mu^2)\,G_{\scriptscriptstyle F}(x-y;\mu^2)\end{aligned} \tag{18.3.20}$$

where $G_{\scriptscriptstyle F}(x-y;m^2)$ is the free scalar propagator computed in (12.4.13):

$$G_{\scriptscriptstyle F}(x-y;m^2) := -i\int \frac{\mathrm{d}^4p}{(2\pi)^4}\,\frac{e^{ip\cdot(x-y)}}{p^2+m^2-i\delta}\,. \tag{18.3.21}$$

The spectral representation of the momentum-space Fourier transform for the exact propagator therefore is

$$\begin{aligned}i\widehat{G}(p^2) &= i\int \mathrm{d}^4x\; e^{-ip\cdot x}\,\langle\!\langle 0|T\Big[\chi_h(x)\chi_h^\star(0)\Big]|0\rangle\!\rangle \\ &= \int_0^\infty \mathrm{d}\mu^2\;\frac{\varrho(\mu^2)}{p^2+\mu^2-i\delta} \\ &= \frac{Z}{p^2+m^2-i\delta} + \int_{\mu^2_{\rm th}}^\infty \mathrm{d}\mu^2\;\frac{\varrho_c(\mu^2)}{p^2+\mu^2-i\delta}\,.\end{aligned} \tag{18.3.22}$$

The properties of $\varrho(\mu^2)$ show that the singularities of $\widehat{G}(p^2)$ only lie along the positive real axis in the complex $z = -p^2$ plane. Furthermore, eqs. (18.3.5) and (18.3.6) imply that $\varrho(\mu^2)$ is only nonzero if $\mu^2 = -p_N^2$ for some physical state $|N\rangle\!\rangle$ that has a nonzero matrix element $\langle\!\langle 0|\chi_h(0)|N\rangle\!\rangle$ or $\langle\!\langle 0|\chi_h^\star(0)|N\rangle\!\rangle$. As claimed in earlier sections, single-particle states (which have unique masses) correspond to isolated poles at $p^2 = -m^2$ where m is the mass of the single-particle state. The residue of this pole determines Z, and so measures the strength of matrix elements like $|\langle\!\langle 0|\chi_h(x)|\mathbf{k}\rangle\!\rangle|^2$. Multiparticle states (for which p^2 runs over a continuous range) correspond to branch cuts in $\widehat{G}(p^2)$, with a new branch point starting at each new particle threshold (see Fig. 13).

A similar discussion goes through for higher-spin fields as well, and for the electron and photon correlation functions, leading to expression like (18.3.22) for both the electron and photon fields.[81] Because the above arguments use canonical commutation relations and do not rely on perturbation theory the fields involved in them should be regarded as the 'bare' fields A_μ^B and ψ_B appearing in the lagrangian density (17.2.13). This means that the role played by Z above is taken by Z_2 and Z_3 for the electron and photon fields respectively. For these the value (given by expressions like (17.4.1)) do satisfy $0 \leq Z_3 < 1$ within the domain of validity of the perturbative calculation.

The general form (18.3.22), as applied to QED, justifies the renormalization condition that states that the full propagator must have its pole located at the physical particle mass, and also vindicates the introduction of the constants Z_2 and Z_3 based on the need to rescale fields. What is not explained yet is why the residue of the poles in the propagators should be chosen to be unity. The next section shows how the requirement to do this is more specific to calculations of S-matrix elements (as opposed to correlation functions).

18.4 LSZ reduction

To better understand renormalization conditions for the residue of the renormalized field at its single-particle pole it is worth digressing briefly to see what general non-perturbative arguments can say about how correlation functions are related to S-matrix elements (a connection called the Lehmann, Symanzik & Zimmermann – or LSZ – theorem).

At a purely perturbative level the connection between correlation functions and S-matrix elements is simple to state, based on the general relation (3.3.9) (or (18.0.1)). Comparing the Feynman rules for a correlation function of the fundamental fields (ψ and A_μ in QED, say, as opposed to composite operators like $J^\mu \propto \overline{\psi}\gamma^\mu\psi$), shows that there is a simple rule for obtaining the contribution of a graph to an S-matrix element from the contribution to the same graph to a correlation function. The rule is to strip off the propagator Feynman rule for each external line – *i.e.* 'amputate' the external lines – and then add in the mode-function

[81] The masslessness of the photon complicates things somewhat because it generically removes the threshold for producing multiparticle states.

factors describing the initial and final particles appearing in the scattering process. This process can also be understood more generally without direct use of perturbative rules.

To see how this works, consider a correlation function involving a collection of n local Heisenberg-picture operators

$$M(p; x_1, \cdots, x_n) := \int \mathrm{d}^4x \; e^{-ip\cdot x} \langle\!\langle 0, \mathrm{out}| T\Big[A_h(x)\, B_h(x_1)\, C_h(x_2) \cdots\Big] |0, \mathrm{in}\rangle\!\rangle \,, \tag{18.4.1}$$

and ask after the singularities that can arise when this is regarded as a function of p^μ. From the propagator example considered above we saw that singular features like $(p^2 + m^2)^{-1}$ ultimately arise from integrals over the time coordinate since these introduce the energy denominators in expressions like (12.4.15) that ultimately turn into the singular poles as a function of p^2.

Focussing on the time integrations, for those time orderings for which $A_h(x)$ appears between operators positioned at x_k^μ and x_r^μ we do not expect anything singular because the integration over x^0 is only over a finite range $x_k^0 < x^0 < x_r^0$. The potentially singular integrations occur only when $A_h(x)$ stands to the far left or to the far right of the correlation function, because only then is the integral over x^0 over an infinite range.

Consider first the case when $A_h(x)$ stands to the far left of the correlation function. Then

$$\begin{aligned} &M_{\mathrm{sing}}(p; x_1, \cdots, x_n) \\ &\quad = \int \mathrm{d}^4x \; e^{-ip\cdot x} \langle\!\langle 0, \mathrm{out}| A_h(x)\, T\Big[B_h(x_1)\, C_h(x_2) \cdots\Big] |0, \mathrm{in}\rangle\!\rangle \; \Theta(x^0 - \tau_{\max}) \\ &\qquad\qquad + (\text{non-pole terms}) \\ &\quad = \sum_N \int \mathrm{d}^4x \; e^{-ip\cdot x} \langle\!\langle 0, \mathrm{out}| A_h(x) |N\rangle\!\rangle \, \langle\!\langle N| T\Big[B_h(x_1)\, C_h(x_2) \cdots\Big] |0, \mathrm{in}\rangle\!\rangle \; \Theta(x^0 - \tau_{\max}) \\ &\qquad\qquad + (\text{non-pole terms}) \end{aligned} \tag{18.4.2}$$

where $\tau_{\max} := \max(x_1^0, \cdots, x_n^0)$ and the final equality inserts a complete set of states $|N\rangle\!\rangle$. The x-dependence of the matrix element can be identified using a special case of (18.1.4),

$$\langle\!\langle 0, \mathrm{out}| A_h(x) |N\rangle\!\rangle = e^{ip_N\cdot x} \, \langle\!\langle 0, \mathrm{out}| A_h(0) |N\rangle\!\rangle \,, \tag{18.4.3}$$

and so the d^4x integral can be performed explicitly, leading to

$$\begin{aligned} &\int \mathrm{d}^4x \; e^{-i(p-p_N)\cdot x} \, \Theta(x^0 - \tau_{\max}) \, F(x_1, \cdots, x_n) \\ &\qquad = (2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}_N) \int_{\tau_{\max}}^\infty \mathrm{d}x^0 \; e^{i(p^0 - p_N^0)x^0} F(x_1, \cdots, x_n) \\ &\qquad = -i(2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}_N) \frac{(p^0 + p_N^0)\, e^{i(p^0 - p_N^0)\tau_{\max}}}{-(p^0)^2 + (p_N^0)^2 - i(p^0 + p_N^0)\delta} \; F(x_1, \cdots, x_n) \,. \end{aligned} \tag{18.4.4}$$

The last line evaluates the x^0 integral by using the Fourier representation (12.4.14) of the step function so

$$\int_\tau^\infty \mathrm{d}x^0 e^{i(p^0-p_N^0)x^0} = \frac{i}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\frac{e^{i\omega\tau}}{\omega+i\delta}\int_{-\infty}^{\infty}\mathrm{d}x^0\;e^{i(p^0-p_N^0-\omega)x^0} = \frac{i\,e^{i(p^0-p_N^0)\tau}}{(p^0-p_N^0)+i\delta}\,, \quad (18.4.5)$$

and then multiplying numerator and denominator by a common factor $-(p^0+p_N^0)$.

The dependence on the 4-momentum p^μ when $A_h(x)$ stands to the far left of the correlator therefore has the general form

$$\begin{aligned}\int \mathrm{d}^4x\; e^{-i(p-p_N)\cdot x}\,\Theta(x^0-\tau_{\max})\,F(x_1,\cdots,x_n)&\\ = -i(2\pi)^3\delta^3(\mathbf{p}-\mathbf{p}_N)\frac{(p^0+p_N^0)\,e^{i(p^0-p_N^0)\tau_{\max}}}{p^2+m_N^2-i(p^0+p_N^0)\delta}\;F(x_1,\cdots,x_n)\,.&\end{aligned} \quad (18.4.6)$$

An identical argument gives the contribution from when $A_h(x)$ stands to the far right of the correlation function, and instead gives

$$\begin{aligned}\int \mathrm{d}^4x\; e^{-i(p-p_N)\cdot x}\,\Theta(\tau_{\min}-x^0)\,\widetilde{F}(x_1,\cdots,x_n)&\\ = i(2\pi)^3\delta^3(\mathbf{p}-\mathbf{p}_N)\frac{(p^0-p_N^0)\,e^{i(p^0+p_N^0)\tau_{\min}}}{p^2+m_N^2+i(p^0-p_N^0)\delta}\;\widetilde{F}(x_1,\cdots,x_n)\,.&\end{aligned} \quad (18.4.7)$$

Both therefore give a singularity as $p^2+m_N^2\to 0$ for the squared-mass of some physical state, but because

$$\frac{p^0+\varepsilon_N}{p^2+m_N^2-i(p^0+\varepsilon_N)\delta} = \frac{-1}{p^0-\varepsilon_N+i\delta} \quad\text{and}\quad \frac{p^0-\varepsilon_N}{p^2+m_N^2+i(p^0-\varepsilon_N)\delta} = \frac{-1}{p^0+\varepsilon_N-i\delta}\,, \quad (18.4.8)$$

the singularity when $A_h(x)$ stands to the far left only occurs when $p^0>0$ while the singularity when $A_h(x)$ stands to the far right only contributes when $p^0<0$.

From the discussion in the previous section we know that when the intermediate state $|N\rangle\!\rangle$ is a single particle state then the singularity found above is an isolated simple pole, because $m_N^2=m^2$ takes on a single value. But if the intermediate state is instead a multiparticle state the singularity is instead a branch cut because m_N^2 depends on continuous parameters (like the relative momentum of the particles within the multiparticle state).

Putting everything together, suppose we choose place p^2 at the position of a single-particle pole at $p^2=-m_N^2$ with $p^0>0$. Then the matrix element $M(p;x_1,\cdots,x_n)$ is dominated by the pole found above and becomes

$$M(p;x_1,\cdots) = -\frac{i(2\pi)^3 2\varepsilon_N}{p^2+m_N^2-i\epsilon}\,\langle\!\langle 0,\mathrm{out}|A_h(0)|\mathbf{p}\rangle\!\rangle\,\langle\!\langle \mathbf{p}|T\Big[B_h(x_1)\cdots\Big]|0\,\mathrm{in}\rangle\!\rangle + (\text{non-pole terms})\,, \quad (18.4.9)$$

where $\epsilon = (p^0 + \varepsilon_N)\delta$ is another positive infinitesimal. Sitting near the same pole but with $p^0 < 0$ instead gives the dominant term

$$M(p; x_1, \cdots) = -\frac{i(2\pi)^3 2\varepsilon_N}{p^2 + m_N^2 - i\epsilon} \langle\langle 0, \text{out}|T\Big[B_h(x_1)\cdots\Big]|\mathbf{p}\rangle\rangle \langle\langle \mathbf{p}|A_h(0)|0\,\text{in}\rangle\rangle + (\text{non-pole terms})\,, \tag{18.4.10}$$

Now comes the main point. This process can be repeated by Fourier transforming each of the remaining coordinates x_i^μ for all of the other operators in the correlation function. The same reasoning shows that if the new Fourier variable obtained by integrating over x_1^μ is put near a single-particle pole then the amplitude again factorizes as above, giving new factors involving matrix elements like $\langle\langle 0, \text{out}|B_h(0)|\mathbf{p}\rangle\rangle$ and $\langle\langle \mathbf{p}|T\Big[C_h(x_2)\cdots\Big]|0\,\text{in}\rangle\rangle$. Continuing on in this way eventually gives a final factor that is an S-matrix element, involving an initial-state particle for every pole that was chosen with $p^0 < 0$ and a final state particle every time a pole was chosen with $p^0 > 0$. Some of these singularities also can arise if (for example) the operator $B_h(0)$ annihilates the particle created by $A_h(0)$, and these singularities correspond to the disconnected graphs in a direct perturbative calculation.

To summarize, the prescription for obtaining an S-matrix element from a correlation function has two steps:

- Fourier transform the correlation function and seek the residue of the pole obtained by taking each Fourier variable near a single-particle pole, taking the pole with $p^0 > 0$ if the particle is to be in the final state and taking $p^0 < 0$ if it is in the initial state.
- Divide by the matrix element factors like $\langle\langle 0, \text{out}|A_h(0)|\mathbf{p}\rangle\rangle$ for the operator and particle involved, and divide by the factor $2\varepsilon_N(2\pi)^3$ for each particle in the initial and final state. This amounts to providing the correct Feynman rules for the external lines in a perturbative calculation.

Notice though that nothing in the above required the intermediate state $|N\rangle\rangle$ to be 'elementary' (like electrons or photons in QED), or that the operator $A_h(0)$ be the specific field for an elementary particle (like ψ and A_μ in QED). For instance, we could choose $|N\rangle\rangle$ to be positronium (a Hydrogen-like bound state of an electron and a positron) so long as we choose an operator for which there is a nonzero matrix element with the vacuum, like $A_h(0) = \overline{\psi}\Gamma\psi$ for some Dirac matrix Γ. The singularities of correlation functions occur at the mass of *any* physical state in the system, regardless of whether or not these states correspond to one of the system's elementary fields. This has physical consequences for scattering processes whose kinematics places them near such a singularity (for both bound states and elementary particles), which has the effect of increasing the observed scattering rate – what is called a 'resonant enhancement', as is seen in §18.6 below

A second noteworthy point is this: because we divide by the matrix element $\langle\langle 0|A_h(0)|N\rangle\rangle$ anyway it doesn't actually matter which field we use, so long as this matrix element is nonzero.

Any field with the required nonzero matrix element is called an *interpolating field* for the state $|N\rangle\!\rangle$, and they are all equally good for the purposes of reconstructing the S matrix from correlation functions. Taking $A_h = A_h(\chi)$ to be a function of the elementary fields then shows in detail (at least for scattering problems) that physical quantities are very generally insensitive to performing field redefinitions,[82] a result known as *Borcher's theorem*.

If we do choose to focus on elementary particles (like electrons and photons in QED) then the corresponding elementary fields provide natural interpolating fields. Then the above picture reproduces what we know must be done to obtain an S-matrix element from a correlation function. We amputate the external line for each operator (*i.e.* take the residue of the pole of the propagator describing the external line for the correlation function) and replace it with the correct factors describing external particle states.

There is an important caveat though: the previous section shows that the normalization of the Heisenberg-picture and interaction picture quantities need not be the same, even for elementary fields and particles, since

$$\langle\!\langle 0, \text{out}|A_h(0)|\mathbf{p}\rangle\!\rangle = Z^{1/2}\,\langle 0|A(0)|\mathbf{p}\rangle\,, \tag{18.4.11}$$

where Z is the residue of the full propagator. This means that if the residue of the full propagator is not unity, the above prescription for obtaining the S matrix instructs us to divide out by these factors of Z. It is this division that is enforced by renormalization conditions like $\Pi_\star(0) = 0$ that aim to ensure unit residue at the propagator's single-particle pole. Since *any* interpolating field is equally good, why not simplify life and work with a field like $\psi(x) = Z_2^{-1/2}\psi_B(x)$ or $A_\mu(x) = Z_3^{-1/2}A_\mu^B(x)$ that is designed to have unit residue at the pole? Such a choice conveniently dispenses with the requirement to divide by the residue for each external line.

18.5 IR divergences

Massless particles like photons can complicate some discussions because the energy cost for creating them can be arbitrarily small. For instance, as mentioned above, the absence of this energy gap complicates the clean association of single-particle states with isolated poles in correlation functions (rather than multiparticle branch cuts).

The present section argues that this is not just a mathematical inconvenience; it also has real physical implications. In particular, the negligible cost of emitting massless particles ensures that their emission often cannot be neglected even if the process of interest nominally doesn't directly involve photons. That is, even if your interest is only in understanding electron-electron scattering, processes in which one of the electrons accidentally throws off many low-energy (or 'soft') photons might be important.

[82] There are limits of course: in order to have no effect on the above S-matrix construction the redefinition $A_h(\chi)$ must be chosen such that its matrix element $\langle\!\langle 0|A_h|N\rangle\!\rangle$ does not introduce spurious new poles or singularities into the correlation functions (which makes nonlocal redefinitions generically dangerous).

In fact, at first glance it is worse that this because the summed rate for emitting soft photons is actually infinite: the amplitude for producing them is so large that the sum over final state photons diverges in the limit that their momenta goes to zero. This is true even for classical electromagnetism; what is sometimes called the *infrared catastrophe*. This section aims to isolate when this type of infrared (IR) divergence occurs and shows how it is the inclusion of virtual quantum processes that nevertheless allows sensible predictions to be made.

IR divergences, if they exist, are important to identify. Unlike UV divergences, IR divergences point to problems at very low energies and long distances; precisely the places where the theory was supposed to be true. As such, they cannot be swept into the meaning of effective local couplings, as part of the parameterization of our ignorance of short-distance physics. Instead, IR divergences are the theory's way of telling us that we are making a mistake. Physical processes should not diverge in the IR, so if you are finding one then you should be thinking again about how physical the process is that you are computing, or about whether your approximations are failing.

For QED the central message carried by IR divergences is that it is unphysical to try to specify the precise number of soft photons in a reaction, since this would require infinite precision to determine. They also provide a nice example of how quantizing electromagnetism actually cures a problem that remains unsolved if one remains purely within the classical theory.

18.5.1 Single soft-photon amplitude

Consider first the emission of soft photons. Suppose we have a scattering process that takes some initial state $|\alpha, \text{in}\rangle\rangle$ to a final state $|\beta, \text{out}\rangle\rangle$ where none of the initial or final states has particularly low energy. Suppose also the S-matrix element for this process is denoted

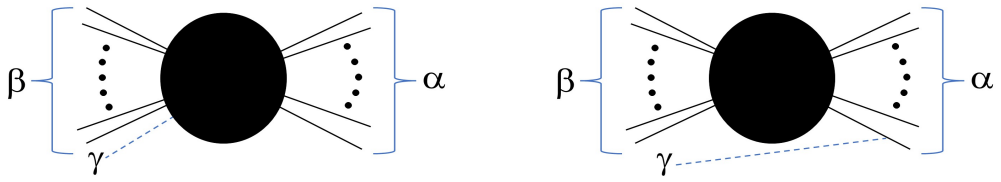
$$\mathcal{M}_{\beta\alpha} := \langle\langle \beta, \text{out} | \alpha, \text{in}\rangle\rangle = \langle \beta | \mathcal{S} | \alpha \rangle \,. \tag{18.5.1}$$

We ask what the dominant amplitude is for the same process to occur together with the emission of a soft photon, with a view to isolating the contributions that are dominant when the photon energy is very small.

The amplitude for emitting a single photon – *i.e.* for the process $\alpha \to \beta + \gamma(\mathbf{k}, \lambda)$ – can be written as

$$\mathcal{M}(\alpha \to \beta + \gamma) = \mathcal{M}^{\mu}_{\beta\alpha} \frac{\epsilon^*_\mu(\mathbf{k}, \lambda)}{\sqrt{(2\pi)^3 2\omega(k)}} \tag{18.5.2}$$

for some factor $\mathcal{M}^{\mu}_{\beta\alpha}$, with the rest (involving the photon's polarization vector $\epsilon_\mu(\mathbf{k}, \lambda)$ and energy $\omega(k) = |\mathbf{k}|$) coming from the standard Feynman rules given in (16.2.14) for an external photon state. Then the reaction rate (assuming the photon properties are not measured) is



(a) (b)

Figure 14. Two ways to attach an external photon to an existing scattering process where the black blob represents a connected Feynman graph. Graph (a) is infrared safe but graph (b) (and its counterpart with the photon attached to all of the other external lines) introduces an IR divergence into the rate for photon emission.

proportional to

$$\mathrm{d}\Gamma(\alpha \to \beta + \gamma) \propto \sum_{\lambda} \left| \mathcal{M}^{\mu}_{\beta\alpha}\, \epsilon^{*}_{\mu}(\mathbf{k}, \lambda) \right|^2 \frac{\mathrm{d}^3 k}{(2\pi)^3 2\omega(k)} \,. \tag{18.5.3}$$

Since $\mathrm{d}^3k = k^2 \mathrm{d}k\, \mathrm{d}^2\Omega$ and $\omega(k) = k = |\mathbf{k}|$ this shows that the integration over d^3k can only diverge in the $k \to 0$ limit if the amplitude $\mathcal{M}^{\mu}_{\beta\alpha}$ is proportional to $1/k$ (or worse) for small k. Why should this ever occur?

For a generic graph – such as panel (a) of Fig. 14 – it doesn't, because there is no particular reason why the propagator to which the external photon attaches in the amplitude $\mathcal{M}^{\mu}_{\beta\alpha}$ should be singular as $k \to 0$. The exception to this statement occurs when the photon attaches to one of the initial or final external lines in the initial amplitude $\mathcal{M}_{\beta\alpha}$, as in panel (b) of Fig. 14. To see why, suppose the photon is emitted from a final-state spin-half fermion line associated with the spinor $\overline{\mathbf{u}}(p)$ in the original amplitude $\mathcal{M}_{\beta\alpha}$. Then the amplitude $\mathcal{M}^{\mu}_{\beta\alpha}$ is obtained from the amplitude $\mathcal{M}_{\beta\alpha}$ by making the replacement

$$\overline{\mathbf{u}}(p) \to \overline{\mathbf{u}}(p) \Big[-(2\pi)^4 Q \gamma^{\mu} \Big] \left[\frac{1}{(2\pi)^4 i} \frac{-i(\not{p} + \not{k}) + m}{(p+k)^2 + m^2 - i\delta} \right] \simeq \frac{Q p^{\mu}}{p \cdot k - i\delta}\, \overline{\mathbf{u}}(p) \tag{18.5.4}$$

where Q denotes the fermion's charge and the final equality uses $\overline{\mathbf{u}}(p)(i\not{p} + m) = 0$ and $p^2 + m^2 = 0$ for external lines, and is only approximate because it drops the $\not{k}$ term in the numerator and k^2 term in the denominator (as appropriate for the small-k limit). Behold the advertised dangerous $1/k$ dependence.

A similar argument applies if the photon is emitted from an initial-state spin-half fermion line associated with the spinor $\mathbf{u}(p)$ in the original amplitude $\mathcal{M}_{\beta\alpha}$. In this case the amplitude $\mathcal{M}^{\mu}_{\beta\alpha}$ is obtained from $\mathcal{M}_{\beta\alpha}$ by making the replacement

$$\mathbf{u}(p) \to \left[\frac{1}{(2\pi)^4 i} \frac{-i(\not{p} - \not{k}) + m}{(p-k)^2 + m^2 - i\delta} \right] \Big[-(2\pi)^4 Q \gamma^{\mu} \Big] \mathbf{u}(p) \simeq \frac{-Q p^{\mu}}{p \cdot k + i\delta}\, \mathbf{u}(p) \tag{18.5.5}$$

again displaying the dangerous $1/k$ dependence. Summing over all external lines shows that the leading small-k limit of the emission amplitude factorizes, with

$$\mathcal{M}^{\mu}_{\beta\alpha} \simeq \sum_{n\in\alpha,\beta} \left(\frac{\eta_n Q_n p_n^{\mu}}{p_n \cdot k - i\eta_n \delta} \right) \mathcal{M}_{\beta\alpha} + (\text{nonsingular}) \,, \tag{18.5.6}$$

where we define

$$\eta_n = \begin{cases} +1 & \text{when } n \in \beta \\ -1 & \text{when } n \in \alpha \,. \end{cases} \tag{18.5.7}$$

The attentive reader will recognize these $1/\omega = 1/k$ factors from expressions like (16.4.12) encountered when computing the amplitude for Compton scattering. In the Compton-scattering case they did not cause a divergence because the amplitude $\mathcal{M}_{\beta\alpha}$ describing the process without emission vanishes because 4-momentum conservation forbids the absorption of a photon by an electron without the associated re-emission. Consequently the leading nonzero result for Compton scattering came from the nonsingular part, involving an additional power of k in the numerator.

Eq. (18.5.6) also contains a nice consistency check: recall that gauge invariance requires $k_\mu \mathcal{M}^{\mu}_{\beta\alpha} = 0$ and evaluating this with (18.5.6) gives

$$k_\mu \mathcal{M}^{\mu}_{\beta\alpha} \simeq \sum_{n\in\alpha,\beta} (\eta_n Q_n)\, \mathcal{M}_{\beta\alpha} + \mathcal{O}(k) = \left(\sum_{n\in\beta} Q_n - \sum_{n\in\alpha} Q_n \right) \mathcal{M}_{\beta\alpha} + \mathcal{O}(k) \,, \tag{18.5.8}$$

showing that the leading part vanishes because charge conservation implies $\sum_{n\in\alpha} Q_n = \sum_{n\in\beta} Q_n$, regardless of the details of $\mathcal{M}_{\beta\alpha}$. Again we see that low-energy photon interactions with charged particles would be inconsistent if charge were not conserved.

Before moving on to multiple emission of soft photons, we first pause to tidy up a loose end. The claim that IR dangerous graphs come when fermion lines are forced on shell is true, but it does not strictly mean that the soft photon must be emitted directly by an external line. The larger class of dangerous graphs is illustrated in Fig. 15, for which hard photons dress the soft-photon emission event while still leaving a fermion line free to go on-shell. One might worry that this class of graphs modifies the factorization shown in (18.5.6).

The short answer is that it does not. To see why not, notice that Fig. 15 changes the replacement (18.5.5) with

$$\mathbf{u}(p) \to iQ\widehat{S}_{\text{hard}}(p-k)\, \Gamma^{\mu}_{\text{hard}}(p, p-k)\mathbf{u}(p) \tag{18.5.9}$$

where $\widehat{S}(p)$ and $\Gamma^{\mu}(p', p)$ are the full propagators and vertex functions that include radiative corrections, but the label 'hard' emphasizes that these only include photons that are not soft. But we know from §18.3 that having the external momentum on-shell and the emitted photon

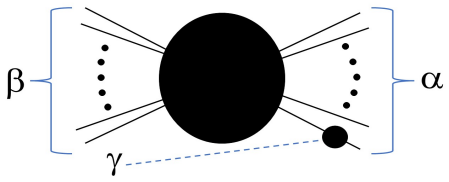


Figure 15. A dangerous graph for which a soft photon can be emitted without having the photon be directly emitted from an external line.

be soft forces the dressed propagator also to be very close to the pole that it very generally has at $p^2 = -m^2$, so the right-hand side of (18.5.9) becomes

$$iQ\widehat{S}_{\rm hard}(p-k)\,\Gamma^{\mu}_{\rm hard}(p,p-k)\mathbf{u}(p) = \frac{2iQ\,N^{\mu}}{(p-k)^2+m^2-i\delta}\,\mathbf{u}(p) \simeq \frac{-iQ\,N^{\mu}}{p\cdot k+i\delta}\,\mathbf{u}(p)\,, \quad (18.5.10)$$

for some function $N^{\mu}(p,k)$.

The function N^{μ} might be complicated, but it must be consistent with the Ward-Takahashi identity (18.2.13) (provided the split between 'hard' and 'soft' has been done in a gauge invariant way), so contracting the left-hand side of (18.5.10) with k_{μ} gives

$$Q\widehat{S}_{\rm hard}(p-k)\Big[\widehat{S}^{-1}_{\rm hard}(p) - \widehat{S}^{-1}_{\rm hard}(p-k)\Big]\mathbf{u}(p) \simeq -Q\,\mathbf{u}(p)\,, \quad (18.5.11)$$

which uses $\widehat{S}^{-1}_{\rm hard}(p)\,\mathbf{u}(p) = 0$ because of the proximity to the pole. Contracting the right-hand side of (18.5.10) therefore implies $ik\cdot N = k\cdot p$ and so $N^{\mu} = -ip^{\mu}$ up to subdominant k^{μ} terms, which ensures the dressed result again gives (18.5.5) in the soft limit. The upshot is that the Ward-Takahashi identity ensures that each external line contributes as in (18.5.6), even after summing over all self-energy and vertex corrections.

18.5.2 Multiple soft-photon amplitude

The above calculation contains both good news and bad news. On one hand, the fact that the amplitude for soft-photon emission diverges means that in principle the entire perturbative expansion is at risk. Perturbative methods are a good approximation if it is an expansion in powers of $\alpha/4\pi$, but not if the series really is in powers of $C\alpha/4\pi$ with C arbitrarily large. The divergence is telling us that contributions at low energies are so strong that they can overwhelm the suppression by α of nominally higher-order effects. This is bad news if true because it means we must explore these higher order effects to see what is going on.

The good news lies in the fact that the emission amplitude for a soft photon factorizes, since this makes it seem that the emission process and the underlying hard scattering process are statistically independent. If so, then it should be not much more difficult to compute the amplitude for multiple soft-photon emissions. This is important to compute, if so, because

the low energy cost and larger number of states available (called 'phase space' in the trade) will make multiple emissions likely if they are possible. In fact given the discussion in §5 we should not be surprised if multiple soft-photon emissions come to resemble radiation of a classical electromagnetic field.

For the emission of two soft photons the amplitude can be written

$$\mathrm{d}\Gamma(\alpha \to \beta + 2\gamma) \propto \sum_{\lambda_1 \lambda_2} \left| \mathcal{M}^{\mu_1\mu_2}_{\beta\alpha}\, \epsilon_{\mu_1}(\mathbf{k}_1, \lambda_1)\, \epsilon_{\mu_2}(\mathbf{k}_2, \lambda_2) \right|^2 \frac{\mathrm{d}^3 k_1}{(2\pi)^3 2\omega(k_1)} \frac{\mathrm{d}^3 k_2}{(2\pi)^3 2\omega(k_2)}\,, \quad (18.5.12)$$

and we seek an expression for $\mathcal{M}^{\mu_1\mu_2}_{\beta\alpha}$. There are two cases to consider – emission from different external lines and multiple emission from a single line – and we consider each in turn.

Emission from distinct lines

The simplest case is when each photon comes off a different external line because the argument for each line is identical to the argument given above, leading to

$$\mathcal{M}^{\mu_1\mu_2}_{\beta\alpha}(\text{lines } m, n) \simeq \left(\frac{\eta_m Q_m p_m^{\mu_1}}{p_m \cdot k_1 - i\eta_m \delta} \right) \left(\frac{\eta_n Q_n p_n^{\mu_2}}{p_n \cdot k_2 - i\eta_n \delta} \right) \mathcal{M}_{\beta\alpha} + (\text{nonsingular})\,. \quad (18.5.13)$$

This is to be summed over all possible pairs of lines from which the photons could come.

Emission from the same line

Next consider the emission of two photons in succession from a single line, with k_1^μ being emitted before k_2^μ. Repeating the above arguments gives the following result

$$\mathcal{M}^{\mu_1\mu_2}_{\beta\alpha}(1 \text{ then } 2) \simeq \left(\frac{\eta_n Q_n p_n^{\mu_1}}{p_n \cdot (k_1 + k_2) - i\eta_n \delta} \right) \left(\frac{\eta_n Q_n p_n^{\mu_2}}{p_n \cdot k_2 - i\eta_n \delta} \right) \mathcal{M}_{\beta\alpha} + (\text{nonsingular})\,. \quad (18.5.14)$$

To this must be added the amplitude for the photons to come out in the opposite order, leading to

$$\begin{aligned} \mathcal{M}^{\mu_1\mu_2}_{\beta\alpha}(2 \text{ then } 1) &\simeq Q_n^2\, p_n^{\mu_1} p_n^{\mu_2} \mathcal{M}_{\beta\alpha} \left[\frac{1}{p_n \cdot (k_1 + k_2)\, p_n \cdot k_2} + \frac{1}{p_n \cdot (k_1 + k_2)\, p_n \cdot k_1} \right] + \cdots \\ &= \frac{Q_n^2\, p_n^{\mu_1} p_n^{\mu_2}}{(p_n \cdot k_1)(p_n \cdot k_2)} \mathcal{M}_{\beta\alpha} + (\text{nonsingular})\,, \end{aligned} \quad (18.5.15)$$

where we suppress the dependence on the δ's to keep the notation manageable. This agrees with (18.5.13) specialized to $m = n$.

Emission of N soft photons

These arguments can be repeated for the emission of N soft photons. If all N photons are emitted by different external lines in the underlying process then the relevant part of the amplitude is

$$\mathcal{M}^{\mu_1 \cdots \mu_N}_{\beta\alpha}(\text{distinct}) = \mathcal{M}_{\beta\alpha} \prod_{r=1}^{N} \left(\frac{\eta_{n_r} Q_{n_r} p_{n_r}^{\mu_r}}{p_{n_r} \cdot k_r - i\eta_{n_r} \delta} \right) + (\text{nonsingular})\,. \quad (18.5.16)$$

It can be proven inductively that having all N photons come off the same external line gives

$$\mathcal{M}_{\beta\alpha}^{\mu_1\cdots\mu_N}(\text{same line}) = \mathcal{M}_{\beta\alpha}\prod_{r=1}^{N}\left(\frac{\eta_n Q_n p_n^{\mu_r}}{p_n\cdot k_r - i\eta_n\delta}\right) + (\text{nonsingular})\,. \tag{18.5.17}$$

using an argument like the one above that sums over the order of emission of the N'th photon, given the result is true for $N-1$ photons.

These show how – for any specific choice of external lines doing the radiating – the amplitude always factorizes into the same factors. The complete matrix element for the emission of N soft photons then sums the above expressions over all possible external lines that do the emitting:

$$\mathcal{M}_{\beta\alpha}^{\mu_1\cdots\mu_N}(\text{distinct}) = \mathcal{M}_{\beta\alpha}\sum_{n_1,\cdots n_N\in\alpha,\beta}\prod_{r=1}^{N}\left(\frac{\eta_{n_r} Q_{n_r} p_{n_r}^{\mu_r}}{p_{n_r}\cdot k_r - i\eta_{n_r}\delta}\right) + (\text{nonsingular})\,. \tag{18.5.18}$$

18.5.3 Emission rate

With the amplitude in hand we can compute the emission rate for multiple soft photons, with the goal of isolating the IR divergence in the phase space integrals. Rather than computing the rate to radiate a specific number of photons we instead ask a more physical question: what is the rate to emit soft photons whose total energy is less than some fixed energy E (which might be the energy resolution of the detector in an actual experiment), in association with a specific hard process $\alpha\to\beta$.

Worked example: Evaluating the soft-photon emission rate

The rate for this is given by

$$\begin{aligned}\Gamma_{\beta\alpha}(E) \;=\; \sum_{N=0}^{\infty}\frac{1}{N!}\sum_{\lambda_1\cdots\lambda_N}\int_{\mathfrak{E}}^{\infty}\frac{\mathrm{d}^3k_1}{(2\pi)^3 2k_1}\cdots\int_{\mathfrak{E}}^{\infty}\frac{\mathrm{d}^3k_N}{(2\pi)^3 2k_N} \\ \times\left|M_{\beta\alpha}^{\mu_1\cdots\mu_N}\epsilon_{\mu_1}(\mathbf{k}_1,\lambda_1)\cdots\epsilon_{\mu_N}(\mathbf{k}_N,\lambda_N)\right|^2\Theta\left(E-\sum_n k_n\right)\,\mathcal{P}_{\beta\alpha}\,,\end{aligned} \tag{18.5.19}$$

where $\mathcal{P}_{\beta\alpha}$ contains all of the phase-space factors for the reaction $\alpha\to\beta$, the $1/N!$ is required because the photons are all indistinguishable and $\mathfrak{E}$ is an infrared cutoff, introduced to display the divergence that is present when $\mathfrak{E}\to 0$. Using the standard photon polarization sum

$$\sum_{\lambda}\epsilon_\mu(\mathbf{k},\lambda)\,\epsilon_\nu^*(\mathbf{k},\lambda) = \eta_{\mu\nu} + \alpha_\mu k_\nu + \alpha_\nu k_\mu \tag{18.5.20}$$

and recognizing that $\mathcal{M}_{\beta\alpha}^{\mu_1\cdots\mu_N}$ vanishes when contracted on index μ_i with k_{μ_i} – *c.f.* eq. (18.5.8) – the rate becomes

$$\begin{aligned}\Gamma_{\beta\alpha}(E) \;=\; \Gamma_{\beta\alpha}\sum_{N=0}^{\infty}\frac{1}{N!}\int_{\mathfrak{E}}^{\infty}\frac{\mathrm{d}^3k_1}{(2\pi)^3 2k_1}\cdots\int_{\mathfrak{E}}^{\infty}\frac{\mathrm{d}^3k_N}{(2\pi)^3 2k_N}\,\Theta\left(E-\sum_n k_n\right) \\ \times\prod_{s=1}^{N}\left[\sum_{m,n\in\alpha,\beta}\frac{\eta_n\eta_m Q_n Q_m\, p_n\cdot p_m}{(p_n\cdot k_s)(p_m\cdot k_s)}\right]\,,\end{aligned} \tag{18.5.21}$$

where $\Gamma_{\beta\alpha}$ is the rate for the hard scattering in the absence of soft photon radiation.

To proceed further notice the following inspired representation of the step function:

$$\Theta(x-a) = \int_{-\infty}^{\infty} \mathrm{d}\sigma \, \frac{\sin(x\sigma)}{\pi\sigma} \, e^{ia\sigma} \,, \tag{18.5.22}$$

To prove this rewrite the right-hand side in the following way:

$$\mathrm{RHS} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\sigma}{\pi\sigma} \, \sin(x\sigma)\, \cos(a\sigma) = \frac{1}{2}\int_{-\infty}^{\infty} \frac{\mathrm{d}\sigma}{\pi\sigma} \Big\{ \sin[(x+a)\sigma] + \sin[(x-a)\sigma] \Big\} \,, \tag{18.5.23}$$

and use the integral

$$\int_{-\infty}^{\infty} \mathrm{d}\sigma \, \frac{\sin(\beta\sigma)}{\pi\sigma} = \mathrm{sign}\ \beta \,, \tag{18.5.24}$$

to see that the right-hand side is RHS is $\frac{1}{2}(1+1) = 1$ when $x > a$ but is $\frac{1}{2}(1-1) = 0$ when $x < a$.

The beauty of (18.5.22) is that by exponentiating a it allows a simpler organization of the momentum integrals, which all become independent of one another:

$$\begin{aligned} \frac{\Gamma_{\beta\alpha}(E)}{\Gamma_{\beta\alpha}} &= \int_{-\infty}^{\infty} \mathrm{d}\sigma \, \frac{\sin(E\sigma)}{\pi\sigma} \sum_{N=0}^{\infty} \frac{1}{N!} \left[\sum_{mn} \frac{\eta_n \eta_m Q_n Q_m p_n \cdot p_m}{2(2\pi)^3} \int_{\mathfrak{E}}^{\infty} \frac{\mathrm{d}^3 k}{k} \, \frac{e^{ik\sigma}}{(p_n\cdot k)(p_m \cdot k)} \right]^N \\ &= \int_{-\infty}^{\infty} \mathrm{d}\sigma \, \frac{\sin(E\sigma)}{\pi\sigma} \exp\left[\sum_{mn} \frac{\eta_n \eta_m Q_n Q_m p_n \cdot p_m}{2(2\pi)^3} \int_{\mathfrak{E}}^{\infty} \frac{\mathrm{d}^3 k}{k} \, \frac{e^{ik\sigma}}{(p_n\cdot k)(p_m \cdot k)} \right] . \end{aligned} \tag{18.5.25}$$

The momentum integrations can now be performed explicitly by going to polar coordinates – $\mathrm{d}^3 k = k^2 \mathrm{d}k \, \mathrm{d}^2\Omega$. Defining

$$I_{nm} := \int_{\mathfrak{E}}^{\infty} \frac{\mathrm{d}^3 k}{k} \, \frac{e^{ik\sigma}}{(p_n\cdot k)(p_m\cdot k)} = W_{nm} \int_{\mathfrak{E}}^{E} \frac{\mathrm{d}k}{k} \, e^{ik\sigma} = W_{nm} \left[\log\frac{E}{\mathfrak{E}} + \int_0^E \frac{\mathrm{d}k}{k} \left(e^{ik\sigma} - 1 \right) \right] , \tag{18.5.26}$$

the last bracket isolates the divergent part as $\mathfrak{E} \to 0$, since the last integral is IR finite (and so in it $\mathfrak{E}$ is set to zero). The angular integration appears in the factor

$$W_{rs} := \int_0^{4\pi} \frac{\mathrm{d}^2\Omega}{2\,\varepsilon_r\,\varepsilon_s} \, \frac{1}{(\mathbf{v}_r\cdot\hat{\mathbf{k}} - 1)(\mathbf{v}_s\cdot\hat{\mathbf{k}} - 1)} \,, \tag{18.5.27}$$

where $\mathbf{v}_r := \mathbf{p}_r/\varepsilon_r$, $\hat{\mathbf{k}} := \mathbf{k}/k$ where $k = |\mathbf{k}|$ and $\varepsilon_r := \sqrt{\mathbf{p}_r^2 + m_r^2}$ and the angular integration is over the direction of $\hat{\mathbf{k}}$.

The angular integral W_{rs} is simplest to perform in the rest frame of one of the particle lines, which we choose to be line 's'. (It is possible to choose a convenient frame because the definition W_{rs} is Lorentz-invariant.) In this frame we choose $\mathbf{v}_r$ to define the z-axis for polar coordinates, so defining $u := \cos\theta$ and $\mathrm{d}^2\Omega = \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$, the desired integral becomes

$$W_{rs} = -\frac{\pi}{\varepsilon_r m_s} \int_{-1}^{1} \frac{\mathrm{d}u}{v_r u - 1} = \frac{\pi}{\varepsilon_r m_s v_r} \, \log\left(\frac{1+v_r}{1-v_r} \right) . \tag{18.5.28}$$

The result in a general frame is then found by finding those invariants built from p_r^μ and p_s^μ that agree with the result in this frame. To this end notice that in the rest frame

$$p_r \cdot p_s = -m_s \varepsilon_r = -\frac{m_s m_r}{\sqrt{1-v_r^2}} \,. \tag{18.5.29}$$

This shows that the Lorentz invariant $-p_r \cdot p_s$ evaluates in the rest frame to $m_s \varepsilon_r$. The last equality also shows that the relative speed β_{rs} of any two particles is also a Lorentz invariant and agrees with v_r in the rest frame. β_{rs} is given explicitly in terms of $p_r \cdot p_s$ by solving (18.5.29) for $v_r = \beta_{rs}$, and so

$$\beta_{rs} = \sqrt{1 - \frac{m_r^2 m_s^2}{(p_r \cdot p_s)^2}} \,. \tag{18.5.30}$$

The upshot is that W_{rs} evaluates in a general frame to

$$W_{rs} = -\frac{\pi}{(p_r \cdot p_s)\beta_{rs}} \, \log\left(\frac{1+\beta_{rs}}{1-\beta_{rs}}\right) . \tag{18.5.31}$$

Putting everything together the soft-photon emission rate becomes

$$\Gamma_{\beta\alpha}(E) = \Gamma_{\beta\alpha} \left(\frac{E}{\mathfrak{E}}\right)^A B(A) \,, \tag{18.5.32}$$

where

$$A := -\frac{1}{8\pi^2} \sum_{n,m \in \alpha,\beta} \frac{\eta_n \eta_m Q_n Q_m}{\beta_{nm}} \, \log\left(\frac{1+\beta_{nm}}{1-\beta_{nm}}\right) , \tag{18.5.33}$$

and

$$\begin{aligned} B(A) \,&:=\, \int_{-\infty}^{\infty} \mathrm{d}\sigma \, \frac{\sin\sigma}{\pi\sigma} \, \exp\left[A \int_0^1 \frac{\mathrm{d}x}{x} \left(e^{ix\sigma} - 1\right)\right] \\ &\simeq\, 1 - \frac{\pi^2 A^2}{12} + \mathcal{O}(A^4) \qquad \text{when} \quad A \ll 1 \,, \end{aligned} \tag{18.5.34}$$

where the small-A limit is relevant because $A = \mathcal{O}(\alpha/4\pi) \ll 1$ if we choose $Q = \pm e$.

Several things are noteworthy about this calculation.

- The order-by-order expansion in powers of α (or A) gives a series involving all possible powers of $A \log(E/\mathfrak{E})$, showing how the emission rate diverges logarithmically at any fixed order in A as $\mathfrak{E} \to 0$. This means that just summing over the possibility to emit multiple soft photons does not in itself solve the IR divergence problem.

- Notice that $A \to 0$ in the strictly nonrelativistic limit for which all of the β_{nm} are negligible. The vanishing in this case is a consequence of charge conservation, which ensures $\sum_n \eta_n Q_n = 0$. This is partly why experience with nonrelativistic charged particles does not immediately raise flags that a potential problem exists.

- Whether the resummed rate (18.5.32) is amplified or suppressed for $E \gg \mathfrak{E}$ depends on the sign of A. It can be shown that A is always positive so the emission rate diverges as $\mathfrak{E} \to 0$. A simple example for which the sign is easy to compute is hard scattering for which all but one particle in the initial and final state is neutral. Then A evaluates to

$$A(\beta) = -\frac{Q^2}{4\pi^2} \left[2 - \frac{1}{\beta} \log\left(\frac{1+\beta}{1-\beta}\right)\right] , \tag{18.5.35}$$

where β is the speed of the final state charged particle relative to the initial one. The function of β in the second term starts at 2 when $\beta \to 0$ but then grows monotonically with β.

- This divergence is already present classically since the differential rate

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}E} = \frac{A\Gamma}{E} \tag{18.5.36}$$

is typical of bremstrahlung and is what one obtains within classical electromagnetism in response to charges that undergo instantaneous acceleration, so have step-function velocities $\mathbf{v}(t) = \mathbf{v}_0\Theta(-t) + \mathbf{v}_1\Theta(t)$ (the classical counterpart to hard scattering). This is what the discussion in §5 would lead us to expect on general grounds, given that classical fields emerge when the low cost of producing bosons ensures that very many quanta end up being produced.

- The quantity A diverges as $\beta_{nm} \to 1$ and so diverges if there were to exist a massless charged particle. The origin of this can be seen in the angular integration in (18.5.27), whose integrand shows the characteristic Bremstrahlung peaking in the forward direction where $\mathbf{v}_n$ and $\mathbf{k}$ are parallel. This peaking becomes singular for massless particles, leading to a new *collinear* divergence to be dealt with. No such particle exists in QED but such additional collinear divergences can happen in theories like QCD where massless gluons carry colour charge. In this case the story of infrared divergences becomes more complicated, and is the gateway to there being much richer strongly interacting physics at low energies.

As we see in the next section, the cure for these divergences for QED comes from summing over the photons that are exchanged between external legs of the hard process, because this also diverges in the IR in precisely the way required to cancel the IR divergence in (18.5.32). In this way it is the quantum fluctuations of QED that ride to the rescue of the would-be divergences of the classical limit.

Alternatively, another side of the same coin states that it is the requirement to sum over multiple soft-photon emission that cures the IR divergences associated with radiative corrections in QED. IR divergences are Quantum Field Theory's way of saying you are making a mistake. In this alternative phrasing the mistake was to think that it is observable to specify the precise number of particles in the final state; in reality there are always soft photons along for the ride and one is infinitely mistaken to ignore them.

18.5.4 Virtual soft photons

To see how radiative corrections diverge and how this compensates for the IR divergence in the photon emission rate, we next compute the effects of soft photon *exchange* between pairs of external lines.

Worked example: Evaluating the amplitude for soft photon exchange

To compute the amplitude for soft-photon exchange we can use the same factor $\mathcal{M}_{\beta\alpha}^{\mu_1\cdots\mu_N}$ as before and, once specialized to even $N = 2K$, we can connect pairs of indices together using a photon propagator in all possible ways of forming K soft-photon internal lines. This leads to the following amplitude for the process $\alpha \to \beta$:

$$\widetilde{\mathcal{M}}_{\beta\alpha} = \mathcal{M}_{\beta\alpha} \sum_{K=0}^{\infty} \frac{1}{2^K K!} \left[\int_{\mathfrak{E}}^{\Lambda} \frac{\mathrm{d}^4 k}{(2\pi)^4 i} \frac{1}{k^2 - i\delta} \sum_{mn \in \alpha,\beta} \left(\frac{\eta_n Q_n p_n^\mu}{p_n \cdot k - i\eta_n \delta} \right) \left(\frac{\eta_m Q_m p_m^\nu}{-p_m \cdot k - i\eta_m \delta} \right) \right]^K \tag{18.5.37}$$

where $\mathcal{M}_{\beta\alpha}$ is the rate including dressing by hard photons (with energy more than some scale Λ much less than the energy of the reaction, but much more than the IR cutoff $\mathfrak{E}$. Here the sign change in the $p_m \cdot k$ term in the second denominator comes because the momentum k^μ flows out of one of the vertices and into the other one. The factor of 2^K arises because the m, n sum is performed as if the results with m and n interchanged are distinct from one another. The $K!$ comes because the mn sum treats having photon 1 connect external lines a and b and photon 2 connecting lines c and d as distinct from having 1 connect c and d and 2 connect a and b, and so on.

Again the result factorizes, with the soft-photon contribution independent of the underlying hard process, and the soft photon factor again exponentiates. Writing the Λ-dependence implicit in the hard-soft split explicitly, the result becomes

$$\widetilde{\mathcal{M}}_{\beta\alpha} = \mathcal{F}(\Lambda)\, \mathcal{M}_{\beta\alpha}(\Lambda) \quad \text{where} \quad \mathcal{F} = \sum_{K=0}^{\infty} \frac{F^K}{2^K K!} = e^{F/2}\,, \tag{18.5.38}$$

and

$$F := \frac{1}{(2\pi)^4} \sum_{mn \in \alpha\beta} \eta_n \eta_m Q_n Q_m (p_n \cdot p_m) J_{mn}\,, \tag{18.5.39}$$

with

$$J_{mn} := -i \int_{\mathfrak{E}}^{\Lambda} \frac{\mathrm{d}^4 k}{k^2 - i\delta} \left(\frac{1}{p_n \cdot k - i\eta_n \delta} \right) \left(\frac{-1}{p_m \cdot k + i\eta_m \delta} \right). \tag{18.5.40}$$

The next step is to perform the integral in J_{mn}. The integral over k^0 can be done by residues, where the poles in the integrand arise in four ways:

$$\begin{aligned}
&(i) \quad k^0 = |\mathbf{k}| - i\delta && \text{from} \quad k^2 - i\delta = 0 \\
&(ii) \quad k^0 = -|\mathbf{k}| + i\delta && \text{from} \quad k^2 - i\delta = 0 \\
&(iii) \quad k^0 = \mathbf{v}_n \cdot \mathbf{k} - i\eta_n \delta && \text{from} \quad p_n \cdot k - i\eta_n \delta = p_n^0 (\mathbf{v}_n \cdot \mathbf{k} - k^0 - i\eta_n \hat{\delta}) = 0 \\
&(iv) \quad k^0 = \mathbf{v}_m \cdot \mathbf{k} + i\eta_n \delta && \text{from} \quad p_m \cdot k + i\eta_m \delta = p_m^0 (\mathbf{v}_m \cdot \mathbf{k} - k^0 + i\eta_m \hat{\delta}) = 0\,.
\end{aligned} \tag{18.5.41}$$

Here $p^0 \hat{\delta} = \delta$ defines $\hat{\delta}$ and so $p^0 > 0$ ensures $\hat{\delta}$ is another positive infinitesimal. Consider the following four choices for η_n and η_m:

Case 1: $\eta_n = +1$ and $\eta_m = -1$ ('n' in final state 'm' in initial state)

In this case only pole (ii) is in the upper-half k^0 plane and so it is simplest to close the contour to an arc at large positive Im k^0, since this picks off only the one pole. Writing

$$\frac{1}{k^2 - i\delta} = \frac{1}{2|\mathbf{k}|} \left[\frac{1}{|\mathbf{k}| - k^0 - i\delta} + \frac{1}{|\mathbf{k}| + k^0 - i\delta} \right] \tag{18.5.42}$$

shows that the residue at pole (ii) is $(2|\mathbf{k}|)^{-1}$ and so $J_{mn} = \mathcal{J}_{mn}$ where

$$\mathcal{J}_{mn} := (-i)(2\pi i)\int_{\mathfrak{E}}^{\Lambda}\frac{\mathrm{d}^3k}{2|\mathbf{k}|}\left(\frac{1}{p_n\cdot k - i\delta}\right)\left(\frac{-1}{p_m\cdot k - i\delta}\right). \tag{18.5.43}$$

Evaluating the remaining integrations in polar coordinates $\mathrm{d}^3k = k^2\mathrm{d}k\,\mathrm{d}^2\Omega$ then gives

$$\begin{aligned}\mathcal{J}_{mn} &= 2\pi\int_{\mathfrak{E}}^{\Lambda}\frac{\mathrm{d}k}{k}\int_0^{4\pi}\frac{\mathrm{d}^2\Omega}{2\varepsilon_n\varepsilon_m}\left(\frac{1}{\mathbf{v}_n\cdot\hat{\mathbf{k}}+1}\right)\left(\frac{-1}{\mathbf{v}_m\cdot\hat{\mathbf{k}}+1}\right)\\ &= 2\pi W_{mn}\,\log\left(\frac{\Lambda}{\mathfrak{E}}\right),\end{aligned} \tag{18.5.44}$$

where W_{mn} is as defined in (18.5.27) and the infinitesimal δ's are dropped because the integrand is no longer singular (provided the external fermion is not massless).

Case 2: $\eta_n = -1$ and $\eta_m = +1$ ('m' in final state 'n' in initial state)

In this case it is simplest to close the contour to an arc at large negative Im k^0, since this again picks off only the one pole: this time the pole (i). Taking the residue at pole (i) gives the result $J_{mn} = \mathcal{J}^{(2)}_{mn}$ where

$$\begin{aligned}\mathcal{J}^{(2)}_{mn} &= (-i)(-2\pi i)\int_{\mathfrak{E}}^{\Lambda}\frac{\mathrm{d}^3k}{(-2|\mathbf{k}|)}\left(\frac{1}{p_n\cdot k}\right)\left(\frac{-1}{p_m\cdot k}\right)\\ &= -2\pi\int_{\mathfrak{E}}^{\Lambda}\frac{\mathrm{d}k}{k}\int_0^{4\pi}\frac{\mathrm{d}^2\Omega}{2\varepsilon_n\varepsilon_m}\left(\frac{1}{\mathbf{v}_n\cdot\hat{\mathbf{k}}-1}\right)\left(\frac{-1}{\mathbf{v}_m\cdot\hat{\mathbf{k}}-1}\right)\\ &= 2\pi W_{mn}\,\log\left(\frac{\Lambda}{\mathfrak{E}}\right) = \mathcal{J}_{mn}\,,\end{aligned} \tag{18.5.45}$$

where the identification with W_{mn} in the final line is done after changing variables $\hat{\mathbf{k}}\to-\hat{\mathbf{k}}$ in the integrand.

Case 3: $\eta_n = \eta_m = +1$ (both 'n' and 'm' in final state)

In this case we close the contour in the upper-half complex k^0 plane, and so receive contributions from two poles: poles (ii) and (iv). The pole at (ii) gives the same contribution $\mathcal{J}_{mn}$ as found in (18.5.44). The pole at (iv) contributes the additional contribution

$$\begin{aligned}\Delta\mathcal{J}_{nm} &= (-i)(2\pi i)\int_{\mathfrak{E}}^{\Lambda}\frac{\mathrm{d}^3k}{\varepsilon_m}\left[\frac{1}{\mathbf{k}^2-(\mathbf{v}_m\cdot\mathbf{k})^2}\right]\left(\frac{1}{\mathbf{p}_n\cdot\mathbf{k}-\varepsilon_n\mathbf{v}_m\cdot\mathbf{k}-i\delta}\right)\\ &= \frac{2\pi}{\varepsilon_m\varepsilon_n}\,\log\left(\frac{\Lambda}{\mathfrak{E}}\right)\int_0^{4\pi}\mathrm{d}^2\Omega\,\left[\frac{1}{1-(\mathbf{v}_m\cdot\hat{\mathbf{k}})^2}\right]\frac{1}{(\mathbf{v}_n-\mathbf{v}_m)\cdot\hat{\mathbf{k}}}\,,\end{aligned} \tag{18.5.46}$$

whose evaluation is delayed until the final choice for the signs η_n and η_m is described. Notice that $\Delta\mathcal{J}_{nm}$ need not *a priori* be symmetric under the interchange $n\leftrightarrow m$ (although it turns out to be once evaluated).

Case 4: $\eta_n = \eta_m = -1$ (both 'n' and 'm' in initial state)

In this case we again close the contour in the upper-half complex k^0 plane, and so receive contributions from the poles (ii) and (iii). The pole at (ii) again gives the result for $\mathcal{J}_{mn}$ found in (18.5.44), and

the pole at (iii) contributes the additional contribution

$$\Delta\mathcal{J}'_{nm} = (-i)(2\pi i)\int_{\mathfrak{E}}^{\Lambda}\frac{\mathrm{d}^3k}{\varepsilon_n}\left[\frac{1}{\mathbf{k}^2-(\mathbf{v}_n\cdot\mathbf{k})^2}\right]\left(\frac{1}{\mathbf{p}_m\cdot\mathbf{k}-\varepsilon_m\mathbf{v}_n\cdot\mathbf{k}-i\delta}\right) = \Delta\mathcal{J}_{mn} \tag{18.5.47}$$

and so differs from Case 3 only by the interchange $n \leftrightarrow m$.

In all of these cases the IR divergence arising as $\mathfrak{E}\to 0$ in the k integration over the virtual photon 4-momentum is explicit, but it remains to evaluate $\Delta\mathcal{J}_{nm}$. Because the initial integral J_{mn} is Lorentz invariant and $\mathcal{J}_{nm}$ also is the same is true for $\Delta\mathcal{J}_{nm}$. This means it can be evaluated in the most convenient frame, which we take as the frame for which $\mathbf{v}_n = 0$, and we use the rotational symmetry to put the z-axis in the direction of $\mathbf{v}_m$. Then $\mathbf{v}_m\cdot\hat{\mathbf{k}} = v_m\cos\theta$ and so (writing $x := \cos\theta$) the angular integration over the direction of $\hat{\mathbf{k}}$ becomes

$$\begin{aligned}\Delta\mathcal{J}_{nm} &= \frac{2\pi}{\varepsilon_m\varepsilon_n}\log\left(\frac{\Lambda}{\mathfrak{E}}\right)\int_0^{2\pi}\mathrm{d}\phi\int_{-1}^{1}\mathrm{d}x\,\left(\frac{1}{1-v_m^2x^2}\right)\left(\frac{1}{-v_mx-i\delta}\right)\\ &= -\frac{4\pi^2}{\varepsilon_m\varepsilon_n v_m}\log\left(\frac{\Lambda}{\mathfrak{E}}\right)\int_{-v_m}^{v_m}\frac{\mathrm{d}u}{(1-u^2)(u+i\delta)}\,,\end{aligned} \tag{18.5.48}$$

where $u := v_mx$.

The integration over u can now be performed explicitly though care must be taken when navigating the pole at $u = 0$. To this end use the identity

$$\frac{1}{u\pm i\delta} = \frac{u}{u^2+\delta^2}\mp\frac{i\delta}{u^2+\delta^2}\to\mathcal{P}\left(\frac{1}{u}\right)\mp i\delta(u)\,, \tag{18.5.49}$$

where the limit corresponds to taking $\delta\to 0$ and $\mathcal{P}$ denotes the principle part of the singularity. Because (18.5.48) involves an integration region that is symmetric about $u = 0$ only the delta function contributes to the integral and we find

$$\Delta\mathcal{J}_{nm} = \frac{4i\pi^3}{\varepsilon_m\varepsilon_n v_m}\log\left(\frac{\Lambda}{\mathfrak{E}}\right)\qquad\text{(in the frame with } \mathbf{v}_n = 0)\,. \tag{18.5.50}$$

In a general frame we take $\varepsilon_m\varepsilon_n\to -p_m\cdot p_n$ since this is Lorentz invariant and the result is true in the frame with $\mathbf{v}_n = 0$. Similarly $v_m\to\beta_{nm}$ is the relative speed, given explicitly in terms of $p_m\cdot p_n$ by (18.5.30), leading to

$$\Delta\mathcal{J}_{nm} = \frac{4i\pi^3}{|p_n\cdot p_m|\beta_{nm}}\log\left(\frac{\Lambda}{\mathfrak{E}}\right) = \frac{4i\pi^3}{\sqrt{(p_m\cdot p_n)^2-m_m^2m_n^2}}\log\left(\frac{\Lambda}{\mathfrak{E}}\right) = \Delta\mathcal{J}_{mn}\,. \tag{18.5.51}$$

Notice in particular that $\Delta\mathcal{J}_{mn}$ is pure imaginary while the expression (18.5.44) for $\mathcal{J}_{mn}$ is real.

Returning to the expression (18.5.38) we had $\widetilde{\mathcal{M}}_{\beta\alpha} = e^{F/2}\,\mathcal{M}_{\beta\alpha}(\Lambda)$ with F given by (18.5.39) (repeated here)

$$F := \frac{1}{(2\pi)^4}\sum_{mn\in\alpha\beta}\eta_n\eta_mQ_nQ_m(p_n\cdot p_m)J_{mn}\,, \tag{18.5.52}$$

and

$$J_{mn} = \begin{cases}\mathcal{J}_{mn} & \text{when } \eta_n\neq\eta_m\\ \mathcal{J}_{mn}+\Delta\mathcal{J}_{mn} & \text{when } \eta_n=\eta_m\,.\end{cases} \tag{18.5.53}$$

Consequently the final result is

$$\widetilde{\mathcal{M}}_{\beta\alpha} = \mathcal{M}_{\beta\alpha}(\Lambda) \left(\frac{\mathfrak{E}}{\Lambda}\right)^{A/2} e^{i\mathcal{G}/2}\,, \tag{18.5.54}$$

with A given by (18.5.33) (repeated here)

$$A := -\frac{1}{8\pi^2} \sum_{n,m\in\alpha,\beta} \frac{\eta_n\eta_m Q_n Q_m}{\beta_{nm}} \log\left(\frac{1+\beta_{nm}}{1-\beta_{nm}}\right)\,, \tag{18.5.55}$$

and the phase $\mathcal{G} = \sum_{mn\in\alpha,\beta} \mathcal{G}_{mn}$ with $\mathcal{G}_{mn} := 0$ when $\eta_n \neq \eta_m$ but

$$\mathcal{G}_{mn} := \frac{Q_m Q_n}{4\pi\beta_{mn}} \log\left(\frac{\Lambda}{\mathfrak{E}}\right) \qquad \text{when } \eta_m = \eta_n\,. \tag{18.5.56}$$

There are again several noteworthy features in this expression.

- The infrared behaviour as $\mathfrak{E} \to 0$ is explicit in the final result. At any fixed order in α the result diverges logarithmically in this limit, indicating a breakdown of the perturbative expansion. But once resummed over all possible soft-photon exchanges the final result tends to zero as $\mathfrak{E} \to 0$ (keeping in mind that $A > 0$) *regardless* of the nature of the underlying hard-exchange process $\mathcal{M}_{\beta\alpha}(\Lambda)$.

- The phase $\mathcal{G}$ is only present when soft photons are exchanged between particles that are both in the initial or final state, and is a phase shift associated with the mutual Coulomb interactions of these pairs of charges, including the famous 'Sommerfeld enhancement' implied by the $1/\beta_{mn}$ dependence that amplifies Coulomb effects for charged particles with small relative speeds. The resulting singularity as $\beta_{mn} \to 0$ implies that perturbing in the Coulomb interaction eventually becomes a poor approximation for sufficiently slowly moving charges, as must be the case given that non-perturbative things like bound states can form when slow charged particles interact through the Coulomb interaction. Because $\mathcal{G}$ is a phase it does not affect the rate $|\widetilde{\mathcal{M}}_{\beta\alpha}|^2$ and so is ignored in what follows.

18.5.5 Bloch-Nordsieck cancellation of IR divergences

Now comes the main event: the calculation of the scattering rate $\Gamma_{\beta\alpha}(E)$ that includes *both* a summation over all possible numbers of exchanged virtual soft photons *and* a summation over the emission of an indefinite number of real soft photons by the initial and final charged particles. For the present purposes what is noteworthy about this calculation is that the infrared divergences as $\mathfrak{E} \to 0$ precisely cancel between these two types of soft sums.

To this end reconsider the calculation of the rate for soft-photon emission described in §18.5.3. In particular, the arguments of that section go through precisely as before when the underlying hard-scattering amplitude $\mathcal{M}_{\beta\alpha}(\Lambda)$ is replaced by the amplitude $\widetilde{\mathcal{M}}_{\beta\alpha}$ that includes also virtual soft-photon exchange, leading expressions like (18.5.21) and (18.5.32) to

be replaced with the also-factorized form

$$\Gamma_{\beta\alpha}(E) = \widetilde{\Gamma}_{\beta\alpha} \sum_{N=0}^{\infty} \frac{1}{N!} \int_{\mathfrak{E}}^{\infty} \frac{\mathrm{d}^3 k_1}{(2\pi)^3 2k_1} \cdots \int_{\mathfrak{E}}^{\infty} \frac{\mathrm{d}^3 k_N}{(2\pi)^3 2k_N} \, \Theta\left(E - \sum_n k_n\right) \times \prod_{s=1}^{N} \left[\sum_{m,n \in \alpha,\beta} \frac{\eta_n \eta_m Q_n Q_m \, p_n \cdot p_m}{(p_n \cdot k_s)(p_m \cdot k_s)} \right]$$
$$= \widetilde{\Gamma}_{\beta\alpha} \left(\frac{E}{\mathfrak{E}}\right)^A B(A) \,, \tag{18.5.57}$$

where (18.5.54) implies $|\widetilde{\mathcal{M}}_{\beta\alpha}|^2 \simeq |\mathcal{M}_{\beta\alpha}(\Lambda)|^2 (\mathfrak{E}/\Lambda)^A$ and so

$$\widetilde{\Gamma}_{\beta\alpha} = \Gamma_{\beta\alpha}(\Lambda) \left(\frac{\mathfrak{E}}{\Lambda}\right)^A \tag{18.5.58}$$

is the rate for the hard scattering in the absence of soft photon radiation but including the summation over all possible exchanges of virtual soft photons as computed above.

Combining these last two results leads to a final expression for $\Gamma_{\beta\alpha}(E)$

$$\Gamma_{\beta\alpha}(E) = \Gamma_{\beta\alpha}(\Lambda) \left(\frac{E}{\Lambda}\right)^A B(A) \,, \tag{18.5.59}$$

from which the singular $\mathfrak{E}$ dependence cancels (and so remains finite in the limit $\mathfrak{E} \to 0$). From this point of view the infrared divergence in each of the partial calculations is a sort of divine retribution for sin: in this case the sin of believing that amplitudes with a specific number of final photons is observable. Any physical measurement must involve a sum over an indefinite number of soft photons with energies smaller than the measurement's finite energy resolution, and the divergences in this sum cancel the divergent sum over virtual photons in precisely the way required to give a well-behaved answer for the physical question.

One might wonder about the dependence of expressions like (18.5.59) on Λ, the (arbitrary) dividing line between what is thought of as hard scattering and what counts as being soft. Since this is not a physical quantity the left-hand side of (18.5.59) cannot depend on it. In practice this occurs because in the limit $E \gg \Lambda$ the hard-scattering process satisfies $\Gamma_{\beta\alpha}(\Lambda) \propto (\Lambda/E_h)^A$, where E_h is an energy characteristic of the hard process. This type of simple inference of the leading Λ-dependence of $\Gamma_{\beta\alpha}(\Lambda)$ is a particularly simple version of the renormalization-group arguments already encountered in §17.5.

The fact that IR divergences ultimately cancel does not mean that they have no content, however. As the previous paragraph argues, the singular logarithmic dependence on made-up scales like Λ and $\mathfrak{E}$ ultimately turns into a dependence $\Gamma_{\beta\alpha}(E) \propto (E/E_h)^A = \exp[A \log(E/E_h)]$ on physically relevant scale ratios like $E \ll E_h$. The sensitivity to small energies that underlies the IR divergences implies that physical results typically invove large logarithms of physical energy ratios – like E/E_h – once expanded order-by-order in powers of

$\alpha/4\pi$ (or A). Although these logarithms enter in a different way than did the large logarithms encountered in §17.5, in practice they can be equally important numerically.

For instance suppose one has $E \simeq 1$ GeV energy resolution for a hard scattering process that involves $E_h \simeq 10$ TeV. In this case $E/E_h \simeq 10^{-4}$ and so $\log(E_h/E) \simeq 9$. Such factors can convert a nominally $\mathcal{O}(\alpha/4\pi) \sim 10^{-3}$ radiative correction into something that is ten times larger. This is even more important for interactions not as weak as electromagnetism; for an interaction with coupling $\tilde{\alpha}/4\pi \sim 10^{-2}$ such a logarithm could representing a 10% rather than 1% correction, or could be order unity if $\tilde{\alpha}/4\pi \sim 10^{-1}$.

It was argued earlier that the singular dependence of factors like A as $\beta_{mn} \to 1$ point to even stronger IR singularities if charged particles were ever to be massless, and the existence of massless coloured gluons in the theory of the strong interactions – Quantum Chromodynamics (QCD) – makes this not only a purely hypothetical problem. The fact that the $\beta_{mn} \to 1$ singularities survive in the above formulae shows that these additional divergences are *not* cured simply by summing over multiple final-state soft particles. It happens though that IR divergences nonetheless still drop out of physical quantities, but in this case the required cancellations only occur once amplitudes are summed over indefinite numbers of both initial *and* final soft particles – a theorem called the KLN theorem (for Kinoshita, Lee and Nauenberg). For QCD the need also to sum over initial soft and collinear states is related to the fact that strongly interacting states are necessarily bound composites of the fundamental gluons and quarks that carry QCD's charge.

18.5.6 Infrared divergent self-energies

We close out this section by making a connection between the above general description of IR divergences and the singularities encountered earlier for the electron self-energy in §17.3 (see for example eq. (17.3.11) and the discussion immediately thereafter). This section shows why these are the same divergences (and so ultimately why IR divergences in the self-energies cancel other divergences in physical processes).

The connection starts with the observation that the above discussion of soft photons is necessarily being done in a renormalization scheme (for UV divergences) that does not use physically normalized operators. If we'd been using physically renormalized fields we would not have needed to sum over corrections to external lines as external lines are put on shell, since these would all have been removed by the counterterms by virtue of on-shell renormalization conditions – such as (17.3.10) satisfied by $\Sigma_\star(p)$.

Instead the calculations described above can be regarded as using a mixed scheme where the effects of renormalizations by hard particles (with energies larger than Λ) are included but soft loops on external lines are explicitly not subtracted by the counterterms. Instead of using (17.2.14) the 'renormalized' field as used in this section would be written

$$\psi_\Lambda = Z_\Lambda^{-1/2}\psi_B = z_\Lambda^{1/2}\psi_{\rm ren} \tag{18.5.60}$$

where ψ_B and $\psi_{\rm ren}$ are the bare and renormalized fields discussed in §17.3, and the renormalization constant Z_2 of (17.2.14) is divided into hard and soft contributions:

$$Z_2 := Z_\Lambda \, z_\Lambda \,. \tag{18.5.61}$$

Imagine computing the scattering amplitude $\mathcal{M}_{\beta\alpha}(\Lambda)$ for the hard-scattering process by examining the poles of a correlation function of fields $\langle 0|T\psi_\Lambda(x_1)\cdots\psi_\Lambda(x_n)|0\rangle$, using the LSZ reduction procedure described in §18.4. Because $\mathcal{M}_{\beta\alpha}(\Lambda)$ omits the contributions of soft photons to external lines it is obtained in the standard way starting from the residue of correlation functions of the fields ψ_Λ near their on-shell poles:

$$\mathcal{M}_{\beta\alpha}(\Lambda) \sim \langle 0|T\psi_\Lambda\cdots\psi_\Lambda|0\rangle_{\rm res} \,, \tag{18.5.62}$$

in precisely the same way that the full amplitude $\widetilde{\mathcal{M}}_{\beta\alpha}$ is obtained from the residue of the fully renormalized fields

$$\widetilde{\mathcal{M}}_{\beta\alpha} \sim \langle 0|T\psi_{\rm ren}\cdots\psi_{\rm ren}|0\rangle_{\rm res} \sim \frac{\langle 0|T\psi_\Lambda\cdots\psi_\Lambda|0\rangle_{\rm res}}{\prod_n z_\Lambda^{1/2}} \,, \tag{18.5.63}$$

where the final equality uses (18.5.60). This last equality also makes sense from the point of view of the LSZ reduction formulae because ψ_Λ are interpolating fields for electrons, but satisfy $\langle \mathbf{p}\sigma|\psi_\Lambda(x)|0\rangle \propto z_\Lambda^{1/2}$ and so each on-shell electron line in a correlation of ψ_Λ operators has residue z_Λ at the pole, rather than unity. The procedure of §18.4 instructs us to divide out these residues to obtain the S-matrix, and so

$$\mathcal{M}_{\beta\alpha}(\Lambda) \sim \widetilde{\mathcal{M}}_{\beta\alpha} \prod_{n\in\alpha,\beta} z_\Lambda^{1/2} \,. \tag{18.5.64}$$

The point of this story is that there are now two equivalent ways to compute the soft-contribution z_Λ to the electron's renormalization constant, and this provides a check on the previous calculations. On one hand, the soft self-energy corrections described by z_Λ are simply a special case of eq. (18.5.54) specialized to the case where the soft photons are emitted and absorbed by the same external line. This corresponds to specializing formula (18.5.33) to the special case $\beta_{nm} \to 0$ and $\eta_n = \eta_m$, in which case

$$A \to A_{\rm self} = -\sum_{n\in\alpha,\beta} \frac{Q_n^2}{4\pi^2} \,. \tag{18.5.65}$$

This contributes to the soft dressing of the scattering amplitude by an amount

$$\widetilde{\mathcal{M}}_{\beta\alpha} \ni \mathcal{M}_{\beta\alpha}(\Lambda) \left(\frac{\mathfrak{E}}{\Lambda}\right)^{A_{\rm self}/2} = \mathcal{M}_{\beta\alpha}(\Lambda) \prod_{n\in\alpha,\beta} \left(\frac{\mathfrak{E}}{\Lambda}\right)^{-Q_n^2/8\pi^2} \,, \tag{18.5.66}$$

which, when compared with (18.5.64) implies

$$z_\Lambda \simeq \left(\frac{\mathfrak{E}}{\Lambda}\right)^{Q_n^2/4\pi^2} \simeq 1 - \frac{Q_n^2}{4\pi^2}\,\log\left(\frac{\Lambda}{\mathfrak{E}}\right) + \cdots\,. \tag{18.5.67}$$

This can be compared with the IR divergence found by directly evaluating the electron self-energy, along the lines performed in §17.3. Since we saw in that section that the IR nature of the divergence becomes obscured by the introduction of the Feynman parameter x, it is easier to make contact with the above by returning to the initial formula (17.3.2) for the self-energy, repeated here for convenience (for charge Q_n):

$$\Sigma(p) = iQ_n^2 \int \frac{\mathrm{d}^4k}{(2\pi)^4}\,\frac{1}{k^2 - i\delta}\,\left\{\frac{\gamma^\mu[-i(\not{p}+\not{k})+m]\gamma_\mu}{(p+k)^2+m^2-i\delta}\right\} + (\text{counterterms})\,. \tag{18.5.68}$$

Our interest is in the IR divergent part of the renormalization constant implied by this expression. Since the renormization constant is determined by the residue near the on-shell pole we can take $p = p_\star + p'$ where p' is also small and $p_\star^2 + m^2 = 0$ is on shell. Since we seek the IR divergent part it suffices to treat k as also being small. This leads to

$$\Sigma_{IR}(p_\star + p') \simeq iQ_n^2 \int_{\mathfrak{E}}^{\Lambda} \frac{\mathrm{d}^4k}{(2\pi)^4}\,\frac{1}{k^2-i\delta}\,\left[\frac{i\not{p}_m + 2m}{p_\star\cdot(p'+k) - i\delta}\right] + (\text{counterterms})\,, \tag{18.5.69}$$

for which the numerator can be further simplified by using $\not{p}_\star = im + \mathcal{O}(p')$ when at the far right or left. Mass renormalization is simply incorporated by subtracting the result with $p' = 0$, leading to

$$\Sigma_{IR}(p_\star + p') - \Sigma_{IR}(p_\star) \simeq -iQ_n^2 m \int_{\mathfrak{E}}^{\Lambda} \frac{\mathrm{d}^4k}{(2\pi)^4}\,\frac{1}{k^2-i\delta}\,\left[\frac{p_\star\cdot p'}{(p_m\cdot k - i\delta)^2}\right] + \mathcal{O}[(p')^2]\,. \tag{18.5.70}$$

To read off the IR part of the wave-function counterterm we must write the term linear in p' as being proportional to $i\not{p} + m$, which can be done using the identity $p^2 + m^2 = (i\not{p}+m)(-i\not{p}+m)$ which when evaluated with $p = p_\star + p'$ implies $p_\star\cdot p' \simeq im\not{p}'$. This means we can replace $p_\star\cdot p' \to m(i\not{p}+m) + \mathcal{O}[(p')^2]$ in the above and write

$$\Sigma_{IR}(p_\star + p') - \Sigma_{IR}(p_\star) \simeq -iQ_n^2 m^2 \left(i\not{p}+m\right) \int_{\mathfrak{E}}^{\Lambda} \frac{\mathrm{d}^4k}{(2\pi)^4}\,\frac{1}{k^2-i\delta}\,\frac{1}{(p_m\cdot k - i\delta)^2}\,, \tag{18.5.71}$$

dropping $(p')^2$ terms. From this we read off the IR divergent part of the residue (that would have been cancelled by the IR counterterm if we'd been using fully renormalized fields):

$$z_\Lambda \simeq 1 - iQ_n^2 m^2 \int_{\mathfrak{E}}^{\Lambda} \frac{\mathrm{d}^4k}{(2\pi)^4}\,\frac{1}{k^2-i\delta}\,\frac{1}{(p_m\cdot k - i\delta)^2} = 1 - \frac{Q_n^2 m^2}{(2\pi)^4}\,\mathcal{J}_{nn}\,, \tag{18.5.72}$$

where the final equality is obtained by comparing the integral to (18.5.40), and keeping in mind that we drop the phase $e^{i\mathcal{G}/2}$ when comparing to z_Λ and so can drop $\Delta\mathcal{J}_{mn}$ in (18.5.53), leading to

$$\mathcal{J}_{nn} = 2\pi W_{nn}\,\log\left(\frac{\Lambda}{\mathfrak{E}}\right) = \frac{4\pi^2}{m^2}\,\log\left(\frac{\Lambda}{\mathfrak{E}}\right)\,, \tag{18.5.73}$$

where the final equality uses the diagonal limit of (18.5.31): $W_{nn} = 2\pi/m^2$.

Combining (18.5.72) with (18.5.73) then agrees with the second equality of (18.5.67). The agreement also works beyond leading order in Q_n^2 because the sum of multiple soft-photon exchanges in the electron self-energy exponentiates in precisely the way found in the first equality of (18.5.67). In this way the IR divergence of the electron self-energy – which manifests itself as the divergence in the Feynman parameter integral in (17.3.11) – is seen to be a special case of the above general description for IR divergences in which the soft photons are emitted and absorbed by the same external line.

At first sight this might seem odd, because this section shows how IR divergences arise in scattering amplitudes because external lines are on shell while the self-energy is an off-shell quantity. It is because the physical (or on-shell) renormalization prescription enforces a condition on how quickly the self-energy must vanish as $p^2 + m^2 \to 0$ that this off-shell quantity acquires the IR divergence, but only does so *after* it is renormalized.

18.6 Resonance and unstable states

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18.6.1 Factorization on poles

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18.6.2 Resonances

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19 Bound states

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19.1 The Dirac-Coulomb problem

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19.2 NRQED

yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada yada

19.3 Precision bound-state energy levels

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Worked example: Lamb shift

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Worked example: positronium

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20 Path integrals

Earlier sections several times made the point – see the discussion below eqs. (12.5.17), (13.1.6) and (16.1.21), for example – that the operator/Hamiltonian formulation of quantum field theory could be inconvenient, particularly for making the Lorentz invariance of special relativity manifest at each step in a calculation. In these earlier discussions path-integral techniques were sometimes held out as providing a better way to proceed (because they are framed in terms of the system's *action* rather than its Hamiltonian). The remaining chapters aim to finally provide an introduction to these techniques, starting in this chapter with single-particle quantum mechanics and continuing to field theory in §21.

20.1 Path integrals in quantum mechanics

We start by deriving the basic path-integral representation of transition amplitudes and correlation functions in ordinary quantum mechanics. To this end consider[83] a collection of quantum variables Q^a with canonical momenta P_a whose dynamics is described by a Hamiltonian $H(Q, P)$.

[83]See Appendix D for a refresher on canonical methods.

We work in the Heisenberg picture for which the quantum operators are time-dependent – $Q = Q(t)$ and $P = P(t)$ – and satisfy the usual equal-time commutation relations

$$[Q^a(t)\,, P_b(t)] = i\,\delta^b_a\,. \tag{20.1.1}$$

Because the operators are time-dependent, the same is also true of their eigenvalues and eigenvectors:

$$Q^a(t) = e^{iHt}\,Q^a(0)\,e^{-iHt} \qquad \text{and} \qquad P_b(t) = e^{iHt}\,P_b(0)\,e^{-iHt}\,, \tag{20.1.2}$$

implies

$$Q^a(t)\,|q,t\rangle = q^a(t)\,|q,t\rangle \qquad \text{and} \qquad P_b(t)\,|p,t\rangle = p_b(t)\,|p,t\rangle\,, \tag{20.1.3}$$

where

$$|q,t\rangle = e^{iHt}\,|q,0\rangle \qquad \text{and} \qquad |p,t\rangle = e^{iHt}\,|p,0\rangle\,. \tag{20.1.4}$$

Standard arguments tell us that the commutation relations (20.1.1) imply the overlap beween these eigenstates is given at equal times by

$$\langle q,t|p,t\rangle = \frac{1}{(2\pi)^{N/2}}\;e^{ip_aq^a}\,, \tag{20.1.5}$$

with the usual implied sum over repeated indices (in this case over 'a', running from 1 to N).

We seek the expression for the analog of the overlap (20.1.5) between eigenstates at different times, using the fact that Heisenberg-picture eigenstates evolve in time according to (20.1.4). This is comparatively simple for infinitesimal time differences $t' = t + \mathrm{d}t$ because then

$$\begin{aligned}\langle q,t+\mathrm{d}t|p,t\rangle \;&=\; \langle q,t|\,e^{-iH(Q,P)\mathrm{d}t}\,|p,t\rangle \simeq \langle q,t|[1-iH(Q,P)\mathrm{d}t]|p,t\rangle = \langle q,t|[1-iH(q,p)\mathrm{d}t]|p,t\rangle \\ &\simeq e^{-iH(q,p)\mathrm{d}t}\langle q,t|p,t\rangle = \frac{1}{(2\pi)^{N/2}}e^{-iH(q,p)\mathrm{d}t+ip_aq^a}\,,\end{aligned} \tag{20.1.6}$$

where we assume $H(Q,P) = H[Q(t),P(t)]$ has the operator-ordering convention that all of the P's are written to the right of the Q's (as can always be ensured if not initially true by repeatedly using the commutation relation (20.1.1). A similar expression for the overlap between two position eigenstates at slightly different times can be derived by inserting a partition of unity expressed in terms of momentum eigenstates, as follows:

$$\langle q,t+\mathrm{d}t|\tilde{q},t\rangle = \int \mathrm{d}^Np\;\langle q,t|\,e^{-iH(Q,P)\mathrm{d}t}\,|p,t\rangle\,\langle p,t|\tilde{q},t\rangle = \int \frac{\mathrm{d}^Np}{(2\pi)^N}\;e^{-iH(q,p)\mathrm{d}t+ip_b(q-\tilde{q})^b}\,, \tag{20.1.7}$$

where $\mathrm{d}^Np := \prod_{a=1}^N \mathrm{d}p_a$.

Now comes the main point. An expression for the overlap between position eigenstates separated by a finite time difference $T := t_f - t_i > 0$ can be found by inserting a complete set of intermediate position eigenstates at slightly different times, each displaced relative to

the previous one by a time step $\mathrm{d}\tau$. That is, define $\mathcal{N}+2$ evenly spaced instants in time, t_k, chosen such that $t_0 = t_i$ and $t_{\mathcal{N}+1} = t_f$ and with $\Delta t := t_{k+1} - t_k = T/(\mathcal{N}+1)$ approaching $\mathrm{d}t$ as $\mathcal{N} \to \infty$. Then

$$\langle q_f, t_f | q_i, t_i \rangle = \int \mathrm{d}q_1 \cdots \mathrm{d}q_{\mathcal{N}} \, \langle q_f, t_f | q_{\mathcal{N}}, t_N \rangle \cdots \langle q_2, t_2 | q_1, t_1 \rangle \, \langle q_1, t_1 | q_i, t_i \rangle \,, \tag{20.1.8}$$

and so using (20.1.7) for each of these overlaps then gives

$$\langle q_f, t_f | q_i, t_i \rangle = \int \prod_{k=1}^{\mathcal{N}} \frac{\mathrm{d}^N q_j}{(2\pi)^{N/2}} \prod_{j=0}^{\mathcal{N}} \frac{\mathrm{d}^N p_j}{(2\pi)^{N/2}} \, \exp\left\{ i \sum_{l=1}^{\mathcal{N}+1} \Big[(p_{l-1})_a (q_l - q_{l-1})^a - H(q_l, p_{l-1}) \, \Delta t \Big] \right\} , \tag{20.1.9}$$

where $q_0 := q_i$ and $q_{\mathcal{N}+1} := q_f$ are not integrated.

This becomes a path integral in the limit $\mathcal{N} \to \infty$. To see why, write the sequence of values $\{q_0, t_0; q_1, t_1; \cdots ; q_{\mathcal{N}}, t_{\mathcal{N}}; q_{\mathcal{N}+1}, t_{\mathcal{N}+1}\}$ and $\{p_0, t_0; p_1, t_1; \cdots ; p_{\mathcal{N}}, t_{\mathcal{N}}; p_{\mathcal{N}+1}, t_{\mathcal{N}+1}\}$ as curves $q^a(t)$ and $p_a(t)$ sampled at each of the t_l's with the endpoints of $q^a(t)$ anchored at the initial and final positions:

$$q^a(t_i) = q_i^a \qquad \text{and} \qquad q^a(t_f) = q_f^a \,. \tag{20.1.10}$$

The sum in the exponent of (20.1.9) becomes an integral involving these curves as $\mathcal{N} \to \infty$, with $\Delta t \to \mathrm{d}t$ and $(q_l - q_{l-1})^a \to \dot{q}^a(t)\, \mathrm{d}t$ in this limit, leading to the key result

$$\langle q_f, t_f | q_i, t_i \rangle = \int_{q_i}^{q_f} \mathcal{D}q^a(t) \int \mathcal{D}p_b(t) \, \exp\left\{ i \int_{t_i}^{t_f} \mathrm{d}t \Big[p_a(t)\, \dot{q}^a(t) - H[q(t), p(t)] \Big] \right\} . \tag{20.1.11}$$

The notation $\int \mathcal{D}q^a(t)$ and $\int \mathcal{D}p_a(t)$ denotes *functional* integration, meaning an integration over *all* possible different choices for the entire curves $q^a(t)$ and $p_a(t)$ (that in practice could be defined by the discretization (20.1.9)). All curves $q^a(t)$ and $p_a(t)$ are included in this integral – not just $q^a(t)$ and $p_a(t)$ satisfying the classical equations of motion – and each curve contributes a phase to the overall amplitude given by the integrand of (20.1.11). The limits on the $\mathcal{D}q^a(t)$ integration mean that only curves satisfying (20.1.10) are to be summed over, while the absence of limits on the $\int \mathcal{D}p_a(t)$ integral means this includes an integration over the initial and final values for $p_a(t_i)$ and $p_a(t_f)$.

It is worth pausing to listen to our equations and consider what (20.1.11) is telling us. The above derivation provides a completely different perspective on what time evolution means in quantum mechanics. In classical mechanics moving from q_i at time t_i to q_f at time t_f takes place along a specific trajectory, $q_c(t)$– together with the related momentum evolution, $p_c(t)$ – that is found by integrating the classical equations of motion. The entire discussion is about finding the correct trajectory.

The path-integral point of view – initially developed by Richard Feynman – is that the quantum amplitude for moving from q_i at time t_i to q_f at time t_f is *not* associated with a

specific path. Instead there is a quantum amplitude for *every* single possible path, $q(t)$ – together with its related $p(t)$ – that connects the initial and final configurations. The amplitude for any particular path is given by a phase $e^{iS[q(t),p(t)]}$ where $S[q(t),p(t)]$ is given explicitly by the exponent seen in (20.1.11). The total amplitude is then obtained by interfering all of these amplitudes together by summing the contribution over all possible paths. This is a very profound (and, as we shall see, very useful) reframing of what quantum evolution really is.

20.1.1 Gaussian integrals

Expressing amplitudes as path integrals is only a useful thing to do if there are ways to evaluate them. We pause here to record a general class of integrals that can be evaluated explicitly: *gaussian* functional integrals, defined as those for which the integrand is the exponential of a quadratic function of the curves $q^a(t)$ and $p_a(t)$.

The starting point is the well-known basic single-variable gaussian integral

$$\int_{-\infty}^{\infty} \mathrm{d}x \;\exp\left[-\tfrac{1}{2}\lambda x^2\right] = \sqrt{\frac{2\pi}{\lambda}}\,, \tag{20.1.12}$$

which converges absolutely if $\lambda > 0$. The analogous single-variable integral with imaginary exponent also converges (though not absolutely), as can be seen by performing the change of variables $t = \frac{1}{2}\,x^2$ and rotating the integration contour by $\frac{\pi}{4}$ in the complex plane, leading to

$$\int_{-\infty}^{\infty} \mathrm{d}x \;\exp\left[\tfrac{1}{2}i\lambda x^2\right] = e^{i\pi/4}\sqrt{\frac{2\pi}{\lambda}}\,, \tag{20.1.13}$$

for nonzero real λ.

The better convergence of the real gaussian (as opposed to the imaginary one) makes a difference once integrations over more than one variable are considered. For real integrals absolute convergence allows the two-dimensional integral to be equally well regarded as an iterated single integral or as an area integral in two dimensions. That is,

$$\int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{d}y \;\exp\left[-\tfrac{1}{2}\lambda(x^2+y^2)\right] = \left[\int_{-\infty}^{\infty} \mathrm{d}x \;\exp\left[-\tfrac{1}{2}\lambda x^2\right]\right]^2 = \frac{2\pi}{\lambda}\,, \tag{20.1.14}$$

is equivalent to

$$\int_0^{\infty} \mathrm{d}r \int_0^{2\pi} \mathrm{d}\theta\; r\;\exp[-\tfrac{1}{2}\lambda r^2] = 2\pi\int_0^{\infty} \mathrm{d}u\, e^{-\lambda u} = \frac{2\pi}{\lambda}\,, \tag{20.1.15}$$

but although squaring (20.1.13) as in (20.1.14) can also be used to define the two-dimensional imaginary integral, the absence of absolute convergence means this is no longer equivalent to the polar-coordinate version (20.1.15) (which does not converge for imaginary gaussians). In practice imaginary multidimensional integrals are defined as powers of the one-dimensional integral or one imagines λ to have a small imaginary part that ensures convergence.

A generic real gaussian involving N integration variables has the form

$$I_N := \int_{-\infty}^{\infty} \frac{\mathrm{d}x_1 \cdots \mathrm{d}x_N}{(2\pi)^{N/2}} \, \exp\Big[-\tfrac{1}{2}A_{kl}x_k x_l + B_k x_k + C\Big] \tag{20.1.16}$$

where the normalization of the measure is suggested by the measure of (20.1.9). The integral is evaluated by completing the square by defining $y_k := x_k - (A^{-1})_{kl}B_l$ – where A^{-1} is the matrix inverse of A (which must exist for the integral to make sense) – and integrating over y_k after rotating to a basis for which A_{kl} is diagonal, leading to the result

$$I_N = (\det\, A)^{-1/2} \, \exp\Big[+\tfrac{1}{2}(A^{-1})_{kl}B_k B_l + C\Big]\,, \tag{20.1.17}$$

where

$$\det\, A = \prod_{l=1}^{N} \lambda_l \tag{20.1.18}$$

and λ_l are the eigenvalues of A (all of which are nonzero because A has an inverse, but are also assumed to be positive so the integrals converge). Notice that the exponent in (20.1.17) is equal to $-\frac{1}{2}A_{kl}\overline{x}_k\overline{x}_l + B_k\overline{x}_k + C$ where the saddle point configuration, $\overline{x}_k$, is defined as the solution to

$$\frac{\partial}{\partial x_k}\Big(-\tfrac{1}{2}A_{kl}x_k x_l + B_k x_k + C\Big)\Big|_{x=\overline{x}} = -A_{kl}\overline{x}_l + B_k = 0\,. \tag{20.1.19}$$

Gaussian functional integrals can be evaluated in much the same way. Consider therefore a functional integral of the form

$$I_{\mathrm{FI}} := \int \mathcal{D}x(t) \, \exp\left\{-\tfrac{1}{2}\int_{t_i}^{t_f}\mathrm{d}t\int_{t_i}^{t_f}\mathrm{d}t'\Big[x(t)a(t,t')x(t')\Big] + \int_{t_i}^{t_f}\mathrm{d}t\Big[b(t)\,x(t) + c(t)\Big]\right\} \tag{20.1.20}$$

where $a(t,t')$, $b(t)$ and $c(t)$ are specified functions on the interval $t_i < t < t_f$. In practice the kernels $a(t,t')$ of most interest have the form

$$a(t,t') = \mathfrak{D}\,\delta(t-t')\,, \tag{20.1.21}$$

where $\mathfrak{D}$ is a hermitian differential operator acting on the coordinate t.

We must quantify what it means to integrate this expression over all possible curves $x(t)$ and one way to do so is to expand $x(t)$ in terms of a basis of functions $u_r(t)$ by writing $x(t) = \sum_r x_r\, u_r(t)$ and performing ordinary integrations over all possible values for the coefficients x_r: $\mathcal{D}x(t) := \prod_r \mathrm{d}x_r/\sqrt{2\pi}$. A particularly useful basis of functions for these purposes is provided by the eigenfunctions of the integral transformation with kernel $a(t,t')$, that satisfy

$$\int_{t_i}^{t_f}\mathrm{d}t'\; a(t,t')\,u_r(t') = \lambda_r\, u_r(t) \qquad \text{and} \qquad \int_{t_i}^{t_f}\mathrm{d}t\, u_r(t)\,u_s(t) = \delta_{rs}\,, \tag{20.1.22}$$

for some eigenvalues λ_r. When (20.1.21) holds, these are simply eigenfunctions of the operator $\mathfrak{D}$ itself:[84]

$$\mathfrak{D}u_r(t) = \lambda_r u_r(t)\,. \tag{20.1.23}$$

In either case, expanding $x(t)$ in terms of such a basis gives

$$I_{\rm FI} = e^C \int \left(\prod_r \frac{\mathrm{d}x_r}{\sqrt{2\pi}}\right) \exp\left\{\sum_r \left[-\tfrac{1}{2}\lambda_r x_r^2 + B_r\, x_r\right]\right\}, \tag{20.1.24}$$

where $B_r = \int_{t_i}^{t_f} \mathrm{d}t\, b(t)\, u_r(t)$ and $C := \int_{t_i}^{t_f} \mathrm{d}t\, c(t)$. The integral in (20.1.20) can now be evaluated as a product of ordinary single-variable gaussians, much as was done in (20.1.14) and (20.1.17), leading to

$$\begin{aligned} I_{\rm FI} &= e^C \prod_r \int_{-\infty}^{\infty} \mathrm{d}x_r\, \exp\left[-\tfrac{1}{2}\lambda_r x_r^2 + B_r\, x_r\right] \\ &= e^C \prod_r \lambda_r^{-1/2} \exp\left[+\tfrac{1}{2}B_r^2/\lambda_r\right] \\ &= \left(\prod_r \lambda_r\right)^{-1/2} \exp\left\{\tfrac{1}{2}\int_{t_i}^{t_f} \mathrm{d}t\,\mathrm{d}t' \left[b(t)\, G(t,t')\, b(t')\right] + \int_{t_i}^{t_f} \mathrm{d}t\, c(t)\right\}. \end{aligned} \tag{20.1.25}$$

The product[85] of eigenvalues appearing here is called the determinant of the kernel $a(t,t')$ (or the operator $\mathfrak{D}$) and the function $G(t,t')$ is defined by

$$G(t,t') := \sum_r \frac{u_r(t)\, u_r(t')}{\lambda_r}\,. \tag{20.1.26}$$

$G(t,t')$ can be regarded as the inverse of the kernel $a(t,t')$ in the sense that it satisfies

$$\begin{aligned} \int_{t_i}^{t_f} \mathrm{d}t''\, a(t,t'')\, G(t'',t') &= \sum_r \frac{u_r(t')}{\lambda_r} \int_{t_i}^{t_f} \mathrm{d}t''\, a(t,t'')\, u_r(t'') \\ &= \sum_r u_r(t)\, u_r(t') = \delta(t-t')\,, \end{aligned} \tag{20.1.27}$$

where the second equality uses (20.1.22) and the last equality uses completeness of the mode functions $u_r(t)$. When (20.1.21) holds, the same argument shows that $G(t,t')$ is the *Green's function* of the operator $\mathfrak{D}$:

$$\mathfrak{D}G(t,t') = \sum_r \frac{[\mathfrak{D}u_r(t)]\, u_r(t')}{\lambda_r} = \sum_r u_r(t)\, u_r(t') = \delta(t-t')\,, \tag{20.1.28}$$

[84] For example if $\mathfrak{D} = -(\mathrm{d}/\mathrm{d}t)^2$ then $u_r(t) = A_r\cos(\omega_r t) + B_r \sin(\omega_r t)$ and $\lambda_r = +\omega_r^2$, where the precise form for A_r, B_r and ω_r depends on the boundary conditions satisfied by the $u_r(t)$'s at $t = t_i$ and $t = t_f$.

[85] This product usually diverges and this must be dealt with using renormalization techniques as described in more detail below.

where $\mathfrak{D}$ acts only on the t argument of $G(t,t')$. This observation allows (20.1.25) to be written in terms of $\mathfrak{D}^{-1}$ as

$$I_{\rm FI} = (\det \mathfrak{D})^{-1/2} \exp\left\{ \int_{t_i}^{t_f} \mathrm{d}t \left[\tfrac{1}{2}\, b(t)\, \mathfrak{D}^{-1}\, b(t) + c(t) \right] \right\}, \tag{20.1.29}$$

which should be compared with the very similar expression (20.1.17).

The above suggests a very simple mnemonic for constructing the argument of the exponential appearing in the last line of (20.1.25). This exponent can be written $E[\overline{x}(t)]$, inasmuch as it can be obtained from the exponent appearing in the integrand of (20.1.20),

$$E[x(t)] := -\tfrac{1}{2} \int_{t_i}^{t_f} \mathrm{d}t \int_{t_i}^{t_f} \mathrm{d}t' \Big[x(t) a(t,t') x(t') \Big] + \int_{t_i}^{t_f} \mathrm{d}t \Big[b(t)\, x(t) + c(t) \Big], \tag{20.1.30}$$

by evaluating it at a particular 'saddle-point' configuration, $\overline{x}(t)$, where $\overline{x}(t)$ is defined by

$$\left. \frac{\delta E}{\delta x(t)} \right|_{x(t)=\overline{x}(t)} = -\int_{t_i}^{t_f} \mathrm{d}t' \Big[a(t,t')\, \overline{x}(t') \Big] + b(t) = 0\,. \tag{20.1.31}$$

In the present instance this means

$$\overline{x}(t) = \int_{t_i}^{t_f} \mathrm{d}t'\; G(t,t')\, b(t')\,, \tag{20.1.32}$$

or $\overline{x}(t) = \mathfrak{D}^{-1} b(t)$ when (20.1.21) holds.

20.1.2 Integrating out the momenta

We next return to expression (20.1.11), which can sometimes be written in a more useful form. In particular, suppose the system's Hamiltonian is quadratic in momenta:

$$H(q,p) = \tfrac{1}{2} A^{ab} p_a\, p_b + B^a p_a + V\,, \tag{20.1.33}$$

for some known coefficients $A^{ab}(q)$, $B^a(q)$ and $V(q)$ that in principle can all depend on q. When this is true (as it often is for the practical cases of interest) then the momentum functional integration in (20.1.11) is gaussian and so can be performed explicitly.

The functional integral to be evaluated is

$$\begin{aligned} J :&= \int \mathcal{D}p_b(t)\; \exp\left\{ i \int \mathrm{d}t \Big[p_a(t)\, \dot{q}^a(t) - H[q(t),p(t)] \Big] \right\} \\ &= \exp\left[-i \int_{t_i}^{t_f} \mathrm{d}t\; V[q(t)] \right] \int \mathcal{D}p_b(t)\; \exp\left\{ i \int \mathrm{d}t \Big[p_a(t)[\dot{q}^a(t) - B^a(t)] - \tfrac{1}{2}\, A^{ab}(q) p_a(t) p_b(t) \Big] \right\}, \end{aligned} \tag{20.1.34}$$

which has the general form of (20.1.20) with $c(t) \to -iV[q(t)]$, $b(t) \to i[q^a(t) - B^a[q(t)]]$ and

$$a(t,t') \to i A^{ab}(q)\, \delta(t-t') \qquad \text{and so} \qquad G(t,t') = -i A_{ab}(q)\, \delta(t-t')\,, \tag{20.1.35}$$

where A_{ab} is the inverse matrix in the sense that $A^{ab}A_{bc} = \delta^a_c$. Performing the functional integral therefore gives (20.1.25), which in this case is

$$J = \mathcal{A}^{-1/2} \exp\left\{ i \int_{t_i}^{t_f} \mathrm{d}t \left[\tfrac{1}{2} A_{ab}(q)[\dot{q}^a - B^a(q)][\dot{q}^b - B^b(q)]b(t) - V(q) \right] \right\} . \tag{20.1.36}$$

$\mathcal{A}$ here denotes the determinant of $a(t,t')$ and so just provides an overall multiplicative constant K if A^{ab} is independent of q, and in this case can usually be ignored because it can be rescaled into the variables q^a, a choice called canonical normalization.[86] We assume this has been done in what follows, or (more practically) show how to identify any constant coefficient K in the path integral. $\mathcal{A}$ cannot be ignored if A^{ab} is q-dependent, and in this case the determinant can be formally rewritten as a contribution to the action by using the identity[87]

$$\det \mathcal{O} = \exp\Big[\mathrm{Tr}\,(\log \mathcal{O}) \Big] . \tag{20.1.37}$$

For the examples that follow A^{ab} is q-independent, so we henceforth restrict to this case.

The exponential appearing in (20.1.36) has the form e^{iS} with $S[q(t)]$ given by

$$\begin{aligned} S[q(t)] &:= \int_{t_i}^{t_f} \mathrm{d}t\, L(q,\dot{q}) \qquad \text{with} \\ L(q,\dot{q}) &= \tfrac{1}{2} A_{ab}(q)[\dot{q}^a - B^a(q)][\dot{q}^b - B^b(q)]b(t) - V(q) . \end{aligned} \tag{20.1.38}$$

The main point is that $L(q,\dot{q})$ is something we recognize: it is precisely the Lagrangian corresponding to the Hamiltonian (20.1.33) (see Appendix D for a review). To see why, use $L(q,\dot{q})$ to construct the canonical momentum

$$p_a := \frac{\partial L}{\partial \dot{q}^a} = A_{ab} \Big[\dot{q}^b - B^b(q) \Big] , \tag{20.1.39}$$

which when solved for the velocity gives $\dot{q}^a(q,p) = A^{ab}p_b + B^a(q)$. The Hamiltonian constructed from this then becomes

$$H[q,p] := \Big(p_a\, \dot{q}^a - L[q,\dot{q}] \Big)_{\dot{q}=\dot{q}(q,p)} = \tfrac{1}{2} A^{ab} p_a\, p_b + B^a p_a + V , \tag{20.1.40}$$

in agreement with (20.1.33).

The quantity S obtained by integrating the Lagrangian with respect to time – as in (20.1.38) – is called the system's *action*. It is no accident that the integration over $p_a(t)$ gives the action because the expression for L in (20.1.38) is precisely what is obtained by solving (20.1.40) for L after using Hamilton's equation of motion $\dot{q}^a = \partial H/\partial p_a$ to eliminate p_a in favour of $\dot{q}^a$. And the equation of motion for $\dot{q}^a$ is precisely the saddle-point obtained

[86] Moreover constant overall factors in the path integral often drop out of calculations and when this is so can be ignored even if present.

[87] This follows when both sides are evaluated using $\det \mathcal{O} = \prod_r \lambda_r$ and $\mathrm{Tr}\,(\log \mathcal{O}) = \sum_r \log \lambda_r$.

when $p_a\dot{q}^a - H[q,p]$ is varied with respect to $p_a(t)$. Using (20.1.34), (20.1.36) and (20.1.38) in (20.1.11) then leads to the expression

$$\langle q_f, t_f | q_i, t_i \rangle = \int_{q_i}^{q_f} \mathcal{D}q^a(t) \, \exp\left\{ i \int_{t_i}^{t_f} \mathrm{d}t \, L(q,\dot{q}) \right\} . \tag{20.1.41}$$

Knowledge of the amplitude $\langle q_f, t_f | q_i, t_i \rangle$ can be regarded as a solution to the time-evolution problem by converting to the Schrödinger picture, in which case $|q,t\rangle_h = e^{iHt}|q\rangle_s$ and so

$${}_h\langle q_f, t_f | q_i, t_i \rangle_h = {}_s\langle q_f | e^{-iH(t_f - t_i)} | q_i \rangle_s = {}_s\langle q_f | U(t_f, t_i) | q_i \rangle_s \, , \tag{20.1.42}$$

is the matrix element of the time-evolution operator between two position eigenstates. In Schrödinger picture the amplitude for preparing a state as $|\Phi\rangle$ at $t = t_i$ and finding the state $|\Psi\rangle$ at $t = t_f$ can be found by convolving with the appropriate initial and final wave function:

$$\langle \Psi | U(t_f, t_i) | \Phi \rangle = \langle \Psi, t_f | \Phi, t_i \rangle = \int \mathrm{d}^N q_f \, \mathrm{d}^N q_i \, \Psi^*(q_f) \langle q_f, t_f | q_i, t_i \rangle \Phi(q_i) \, , \tag{20.1.43}$$

where $\Psi(q) = \langle q | \Psi \rangle$ and $\Phi(q) = \langle q | \Phi \rangle$.

20.2 Simple examples

We pause here to build up intuition by explicitly evaluating the path integral in two simple (but very useful) examples: the free particle and the simple harmonic oscillator.

Worked example: the free particle

Consider first the free particle of mass m moving in N-dimensional flat space, for which $q^a = x^a$ is the particle position and the Lagrangian is

$$L(x, \dot{x}) = \frac{m}{2} \, \delta_{ab} \, \dot{x}^a \, \dot{x}^b \qquad \text{and so} \qquad p_a := \frac{\partial L}{\partial \dot{x}^a} = m \, \dot{x}_a \, , \tag{20.2.1}$$

and so

$$H(x,p) := p_a \dot{x}^a - L = \frac{1}{2m} \, \delta^{ab} p_a \, p_b \, . \tag{20.2.2}$$

The path-integral expression (20.1.11) for the kernel $\langle x_f, t_f | x_i, t_i \rangle$ in this case is

$$\begin{aligned} \langle x_f, t_f | x_i, t_i \rangle &= \int_{x_i}^{x_f} \mathcal{D}x^a(t) \int \mathcal{D}p_b(t) \, \exp\left\{ i \int_{t_i}^{t_f} \mathrm{d}t \left[p_a(t) \, \dot{x}^a(t) - \frac{1}{2m} \, \delta^{ab} p_a \, p_b \right] \right\} \\ &= \int_{x_i}^{x_f} \mathcal{D}x^a(t) \, \exp\left\{ i \int_{t_i}^{t_f} \mathrm{d}t \left[\frac{m}{2} \, \delta_{ab} \, \dot{x}^a \, \dot{x}^b \right] \right\} , \end{aligned} \tag{20.2.3}$$

where the sum is over all paths satisfying $x^a(t_i) = x_i^a$ and $x^a(t_f) = x_f^a$ and the second line uses the fact that H is quadratic in p to integrate out the momenta.

In this case the remaining $x^a(t)$ functional integral is also gaussian and so can be performed explicitly along the lines described in §20.1.1, by evaluating at a saddle-point configuration and computing a determinant. The required saddle-point configuration is obtained by asking the variation

of $S[x(t)]$ to vanish, so expanding $S[x(t)+\delta x(t)]-S[x(t)]$ to linear order in $\delta x(t)$ and setting the coefficient to zero gives (after integrating by parts)

$$\left(\frac{\delta S}{\delta x^a(t)}\right)_{x=\overline{x}} = -m\ddot{\overline{x}}^a(t) = 0\,. \tag{20.2.4}$$

The general solution $x^a = \overline{x}^a(t)$ to this must be at most linear in t and the one that satisfies the boundary conditions $\overline{x}^a(t_i) = x_i^a$ and $\overline{x}^a(t_f) = x_f^a$ is therefore

$$\overline{x}^a(t) = x_i^a + \frac{(x_f - x_i)^a}{t_f - t_i}\,(t - t_i)\,. \tag{20.2.5}$$

Notice that this is simply the classical trajectory that a free particle would take to get between the specified initial and final positions in the time allotted. The action evaluated at this solution is

$$S[\overline{x}(t)] = \frac{m}{2}\int_{t_i}^{t_f} \mathrm{d}t\;\delta_{ab}\,\dot{\overline{x}}^a(t)\,\dot{\overline{x}}^a(t) = \frac{m\delta_{ab}\,(x_f - x_i)^a\,(x_f - x_i)^b}{2(t_f - t_i)}\,. \tag{20.2.6}$$

The determinant in this case involves the differential operator $\mathfrak{D} = im(\mathrm{d}/\mathrm{d}t)^2$ and although this is independent of the quantum variables (and so its value is not required in what follows), it does depend on the parameters m and $t_f - t_i$ so for some purposes its evaluation can be instructive. The eigenvalue equation is

$$\mathfrak{D}\,u_r(t) = im\ddot{u}_r(t) = \lambda_r\,u_r(t) \qquad \text{with} \qquad u_r(t_f) = u_r(t_i) = 0\,, \tag{20.2.7}$$

where the boundary conditions follow from the requirement that $x^a(t_i) = \overline{x}^a(t_i) = x_i^a$ and $x^a(t_f) = \overline{x}^a(t_f) = x_f^a$ for *all* paths, which implies $\delta x^a = x^a - \overline{x}^a$ must vanishing at the endpoints. The solution for the eigenfunctions is therefore

$$u_r(t) = A\sin[\omega_r(t - t_i)] \qquad \text{where} \qquad \omega_r = \frac{\pi r}{t_f - t_i} \quad \text{with } r \text{ a positive integer}\,, \tag{20.2.8}$$

and A a nonzero constant that is fixed by normalization. The eigenvalues therefore are

$$\lambda_r = -im\omega_r^2 = \frac{m\pi^2 r^2}{i(t_f - t_i)^2}\,. \tag{20.2.9}$$

The determinant involves the infinite product of the λ_r over all values of r, which generically diverges for large r and so requires regularization and renormalization. As earlier chapters emphasize (see §5.1, §9.3 and §17.2) a great variety of regularizations can be used provided they satisfy the properties listed in §9.3.1. A useful trick for regularizing the functional determinant of interest here starts by defining the *zeta*-function for the operator $\mathfrak{D}$ by

$$\zeta_{\mathfrak{D}}(s) := \sum_r \lambda_r^{-s}\,, \tag{20.2.10}$$

where s is a complex parameter. This sum typically converges when the real part of s is sufficiently large, and its value can be defined by analytic continuation for other complex s. Once this continuation is known then the functional determinant is related to its derivative

$$\zeta'_{\mathfrak{D}}(s) = \frac{\mathrm{d}\zeta_{\mathfrak{D}}}{\mathrm{d}s} = -\sum_r \lambda_r^{-s}\log\lambda_r \tag{20.2.11}$$

because

$$\log\Bigl(\det \mathfrak{D}\Bigr) = \sum_r \log \lambda_r = -\zeta'_{\mathfrak{D}}(0)\,. \tag{20.2.12}$$

Notice that this definition satisfies the reasonableness requirements given in §9.3.1.

For the specific operator of interest here $\mathfrak{D} = im(\mathrm{d}/\mathrm{d}t)^2$ it is convenient to divide λ_r by the cube of an arbitrary mass scale, μ^3, to make each term in the sum (or product) dimensionless. In this case the zeta function becomes

$$\zeta_{\mathfrak{D}}(s) := \left[\frac{m\pi^2}{i\mu^3(t_f-t_i)^2}\right]^{-s} \sum_{r=1}^{\infty} r^{-2s} = \left[\frac{m\pi^2}{i\mu^3(t_f-t_i)^2}\right]^{-s} \zeta_{\scriptscriptstyle R}(2s)\,, \tag{20.2.13}$$

where $\zeta_{\scriptscriptstyle R}(s) := \sum_{r=1}^{\infty} r^{-s}$ is the Riemann zeta function – previously encountered in (9.3.8) – which satisfies

$$\zeta_{\scriptscriptstyle R}(0) = -\tfrac{1}{2} \quad \text{and} \quad \zeta'_{\scriptscriptstyle R}(0) = -\tfrac{1}{2}\,\log(2\pi)\,. \tag{20.2.14}$$

Using this in (20.2.13) and keeping in mind that we have N variables x^a then gives[88]

$$\begin{aligned}\Bigl(\det \mathfrak{D}\Bigr)^{-N/2} &= \exp\Bigl[\tfrac{1}{2}\,N\zeta'_{\mathfrak{D}}(0)\Bigr] = \exp\left\{-\tfrac{1}{2}N\zeta_{\scriptscriptstyle R}(0)\log\left[\frac{m\pi^2}{i\mu^3(t_f-t_i)^2}\right] + N\zeta'_{\scriptscriptstyle R}(0)\right\} \\ &= \left[\frac{m}{4i\mu^3(t_f-t_i)^2}\right]^{N/4}\,. \end{aligned} \tag{20.2.15}$$

Notice that changes to the arbitrary scale μ change the determinant by a numerical factor and so can be absorbed into an overall multiplicative constant K in (20.2.3), whose value depends on the precise scheme used to regularize the determinant. In this case we are led to

$$\begin{aligned}\langle x_f, t_f | x_i, t_i\rangle &= K\,\Bigl(\det \mathfrak{D}\Bigr)^{-N/2} \exp\Bigl\{iS[\overline{x}(t)]\Bigr\} \\ &= K\,\left[\frac{m}{4i\mu^3(t_f-t_i)^2}\right]^{N/4} \exp\left\{\frac{im\delta_{ab}\,(x_f-x_i)^a\,(x_f-x_i)^b}{2(t_f-t_i)}\right\}\,, \end{aligned} \tag{20.2.16}$$

for constant K.

We can check that this evolution kernel properly evolves states forward in time. For instance, a system prepared in a momentum eigenstate at $t_i = 0$ has wave-function $\langle x_i, 0|p\rangle = (2\pi)^{-N/2}\exp(ip_a x_i^a)$, and so at later times this becomes

$$\begin{aligned}\langle x, t|p\rangle &= \int \mathrm{d}^N x_i\ \langle x, t|x_i, 0\rangle\,\langle x_i, 0|p\rangle \\ &= K\,\left[\frac{m}{16\pi^2 i\mu^3 t^2}\right]^{N/4} \int \mathrm{d}^N x_i\ \exp\left\{\frac{im\delta_{ab}\,(x-x_i)^a\,(x-x_i)^b}{2t} + ip_a x_i^a\right\} \\ &= K\,\left[\frac{i}{4\mu^3 m}\right]^{N/4} \exp\left\{-\frac{i\delta^{ab}p_a p_b t}{2m} + ip_a x^a\right\}\,, \end{aligned} \tag{20.2.17}$$

where the last line evaluates the gaussian integral using the saddle point $\overline{x}_i^a = x^a - (p_a t/m)$ of the argument of the exponential. This has the correct dependence on x^a and t required of a momentum eigenstate (whose energy is $p^2/2m$).

[88] Although the determinant could have diverged in the $r \to \infty$ limit, a plus of zeta-function regularization is that it returns a finite answer. Although convenient, this obscures the renormalizations that are in principle required to absorb divergences. A more careful treatment shows that zeta function regularization is equivalent to use of dimensional regularization once the divergences are removed by minimal subtraction.

The value of K can be determined by requiring the normalization of the state not change, and gives $K = (m\mu^3/i\pi^2)^{N/4}$, in which case the kernel (20.2.16) becomes

$$\langle x_f, t_f | x_i, t_i \rangle = \left[\frac{m}{2\pi i (t_f - t_i)} \right]^{N/2} \exp\left\{ \frac{im\delta_{ab} \, (x_f - x_i)^a \, (x_f - x_i)^b}{2(t_f - t_i)} \right\} . \tag{20.2.18}$$

Notice that explicit differentiation of (20.2.18) shows that $\langle x_f, t_f | x_i, t_i \rangle$ satisfies the free-particle Schrödinger equation

$$\left(i \, \frac{\partial}{\partial t_f} + \frac{1}{2m} \delta^{ab} \frac{\partial}{\partial x_f^a} \frac{\partial}{\partial x_f^b} \right) \langle x_f, t_f | x_i, t_i \rangle = 0 \tag{20.2.19}$$

provided $t_f \neq t_i$ together with the initial condition that $\langle x_f, t_f | x_i, t_i \rangle \to \delta^N(x_f - x_i)$ as $t_f \to t_i$.

A second useful example can also be computed explicitly knowing only how to evaluate gaussian integrals: the simple harmonic oscillator (which we take for simplicity to be in one spatial dimension).

Worked example: the harmonic oscillator

For a harmonic oscillator of mass m and spring constant k with position $q = x$ the Lagrangian is

$$L(x, \dot{x}) = \frac{m}{2} \, \dot{x}^2 - \frac{k}{2} \, x^2 \qquad \text{and so} \qquad p := \frac{\partial L}{\partial \dot{x}} = m \, \dot{x} \, , \tag{20.2.20}$$

and

$$H(x, p) := p\dot{x} - L = \frac{p^2}{2m} + \frac{kx^2}{2} \, . \tag{20.2.21}$$

The path-integral expression (20.1.11) for the kernel $\langle x_f, t_f | x_i, t_i \rangle$ in this case is

$$\begin{aligned} \langle x_f, t_f | x_i, t_i \rangle &= \int_{x_i}^{x_f} \mathcal{D}x(t) \int \mathcal{D}p(t) \, \exp\left\{ i \int_{t_i}^{t_f} \mathrm{d}t \left[p \, \dot{x} - \frac{p^2}{2m} - \frac{kx^2}{2} \right] \right\} \\ &= \int_{x_i}^{x_f} \mathcal{D}x(t) \, \exp\left\{ \frac{i}{2} \int_{t_i}^{t_f} \mathrm{d}t \left[m \, \dot{x}^2 - kx^2 \right] \right\} , \end{aligned} \tag{20.2.22}$$

where the sum is over all paths satisfying $x^a(t_i) = x_i^a$ and $x^a(t_f) = x_f^a$ and the second line again uses the fact that H is quadratic in p to integrate out the momenta.

Since the remaining $x(t)$ functional integral is also gaussian it can also be performed explicitly. The variation of $S[x(t)]$ vanishes at the saddle point, and so (after integrating by parts) the saddle-point condition is

$$\left(\frac{\delta S}{\delta x(t)} \right)_{x = \overline{x}} = -m\ddot{\overline{x}}(t) - k\overline{x}(t) = 0 \, . \tag{20.2.23}$$

The general solution to this is $\overline{x}^a(t) = A \cos(\omega t) + B \sin(\omega t)$ where A and B are integration constants and $\omega^2 = k/m$. The choice for A and B that satisfies the boundary conditions $\overline{x}^a(t_i) = x_i^a$ and $\overline{x}^a(t_f) = x_f^a$ then gives

$$\overline{x}(t) = x_i \cos[\omega(t - t_i)] + \left[\frac{x_f - x_i \cos[\omega(t_f - t_i)]}{\sin[\omega(t_f - t_i)]} \right] \sin[\omega(t - t_i)] \, , \tag{20.2.24}$$

from which we also learn

$$\dot{\overline{x}}(t) = -\omega x_i \sin[\omega(t - t_i)] + \omega \left[\frac{x_f - x_i \cos[\omega(t_f - t_i)]}{\sin[\omega(t_f - t_i)]} \right] \cos[\omega(t - t_i)] \, . \tag{20.2.25}$$

The action evaluated at this solution is simplest to write by integrating by parts to rewrite it as a surface term plus a term that vanishes when condition (20.2.23) is used. This leads to

$$\begin{aligned} S[\overline{x}(t)] &= \frac{1}{2}\int_{t_i}^{t_f} \mathrm{d}t\, \Big[m\dot{\overline{x}}^2(t) - k\,\overline{x}^2(t)\Big] = \Big[\frac{1}{2}m\overline{x}\,\dot{\overline{x}}\Big]_{t=t_i}^{t=t_f} - \frac{1}{2}\int_{t_i}^{t_f} \mathrm{d}t\; \overline{x}(t)\Big[m\ddot{\overline{x}} + k\,\overline{x}\Big] \\ &= \frac{m\omega}{2\sin[\omega(t_f-t_i)]}\Big[(x_f^2+x_i^2)\cos[\omega(t_f-t_i)] - 2x_ix_f\Big]\,. \end{aligned} \tag{20.2.26}$$

The differential operator relevant to the determinant in this case is

$$\mathfrak{D} = im\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + ik = im\left[\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + \omega^2\right] \tag{20.2.27}$$

where $\omega^2 := k/m$ is the harmonic oscillator's angular frequency. So the eigenvalue equation is

$$\mathfrak{D}\,u_r(t) = im\Big[\ddot{u}_r(t) + \omega^2 u_r(t)\Big] = \lambda_r\,u_r(t) \qquad \text{with} \qquad u_r(t_f) = u_r(t_i) = 0\,. \tag{20.2.28}$$

The required eigenfunctions are

$$u_r(t) = C\sin[\omega_r(t-t_i)] \qquad \text{where} \qquad \omega_r = \frac{\pi r}{t_f - t_i} \quad \text{with } r \text{ a positive integer}\,, \tag{20.2.29}$$

and C a nonzero normalization constant. The eigenvalues therefore are

$$\lambda_r = im\Big(-\omega_r^2 + \omega^2\Big) = \frac{m\pi^2}{i\mu^3(t_f-t_i)^2}\left(r + \frac{\omega(t_f-t_i)}{\pi}\right)\left(r - \frac{\omega(t_f-t_i)}{\pi}\right)\,. \tag{20.2.30}$$

To evaluate the determinant we start by defining the following zeta function,

$$\hat{\zeta}(s,a,z) := \sum_{r=1}^{\infty}\Big[\sqrt{z}(r+a)\Big]^{-s}\,, \tag{20.2.31}$$

for real a and complex s and z. This zeta function has the formal property that

$$\hat{\zeta}'(0,a,z) + \hat{\zeta}'(0,-a,z) = -\sum_{r=1}^{\infty}\Big\{\log[\sqrt{z}(r+a)] + \log[\sqrt{z}(r-a)]\Big\} = -\sum_{r=1}^{\infty}\log\Big[z(r^2-a^2)\Big]\,, \tag{20.2.32}$$

where the prime denotes differentiation with respect to s. The right-hand side agrees with $-\log(\det\mathfrak{D})$ with eigenvalues (20.2.30) provided we choose

$$z = \frac{m\pi^2}{i\mu^3(t_f-t_i)^2} \qquad \text{and} \qquad a = \frac{\omega(t_f-t_i)}{\pi}\,. \tag{20.2.33}$$

To compute the behaviour of $\hat{\zeta}(s,a,z)$ near $s=0$ we use the definition $\zeta_{\scriptscriptstyle H}(s,u) := \sum_{r=0}^{\infty}(r+u)^{-s}$ of the Hurwitz zeta-function, in terms of which (20.2.31) becomes

$$\hat{\zeta}(s,a,z) = z^{-s/2}\sum_{r=1}^{\infty}(r+a)^{-s} = z^{-s/2}\Big[\zeta_{\scriptscriptstyle H}(s,a) - a^{-s}\Big]\,. \tag{20.2.34}$$

In terms of this the functional determinant is

$$\begin{aligned} \Big(\det\mathfrak{D}\Big)^{-1/2} &= \exp\Big\{\tfrac{1}{2}\Big[\hat{\zeta}'(0,a,z) + \hat{\zeta}'(0,-a,z)\Big]\Big\} \\ &= \exp\Big\{-\tfrac{1}{4}\log z\Big[\zeta_{\scriptscriptstyle H}(0,a) + \zeta_{\scriptscriptstyle H}(0,-a) - 2\Big] + \tfrac{1}{2}\Big[\zeta_{\scriptscriptstyle H}'(0,a) + \zeta_{\scriptscriptstyle H}'(0,-a)\Big] + \log a\Big\}\,, \end{aligned} \tag{20.2.35}$$

with z and a as given in (20.2.33). Using the limits

$$\zeta_{\scriptscriptstyle H}(0,x) = -x + \tfrac{1}{2} \qquad \text{and} \qquad \zeta'_{\scriptscriptstyle H}(0,x) = \log\Big[\Gamma(x)\Big] - \tfrac{1}{2}\log(2\pi)\,, \tag{20.2.36}$$

the determinant evaluates to

$$\Big(\det \mathfrak{D}\Big)^{-1/2} = \left[\frac{m\omega^2}{4i\mu^3 \sin^2[\omega(t_f - t_i)]}\right]^{1/4} . \tag{20.2.37}$$

which uses the identities $\Gamma(1-a)\Gamma(a) = -a\Gamma(-a)\Gamma(a) = \pi/\sin(\pi a)$. Again changes to the arbitrary scale μ can be absorbed into an overall constant K, in which case the result becomes

$$\begin{aligned}\langle x_f, t_f | x_i, t_i\rangle \;=\; K\,&\left[\frac{m\omega^2}{4i\mu^3 \sin^2[\omega(t_f - t_i)]}\right]^{1/4} \\ &\times \exp\left\{\frac{im\omega}{2\sin[\omega(t_f - t_i)]}\Big[(x_f^2 + x_i^2)\cos[\omega(t_f - t_i)] - 2x_i x_f\Big]\right\} .\end{aligned} \tag{20.2.38}$$

To fix the constant K imagine preparing the system in the ground state $|g\rangle$ at $t_i = 0$, for which (see (2.1.3))

$$\langle x_i, 0 | g\rangle = \sqrt{\frac{m\,\omega}{\pi}}\, e^{-m\omega x_i^2/2}\,, \tag{20.2.39}$$

in which case the state at a later time is

$$\begin{aligned}\langle x_f, t_f | g\rangle \;&=\; \int_{-\infty}^{\infty} \mathrm{d}x_i\; \langle x_f, t_f | x_i, 0\rangle\, \langle x_i, 0 | g\rangle \\ &=\; K\,\left[\frac{m^3\omega^4}{4i\pi^2\mu^3 \sin^2(\omega t_f)}\right]^{1/4} \\ &\qquad\qquad \times \int_{-\infty}^{\infty} \mathrm{d}x_i\; \exp\left\{\frac{im\omega}{2\sin(\omega t_f)}\Big[(x_f^2 + x_i^2)\cos(\omega t_f) - 2x_i x_f\Big] - \frac{m\omega x_i^2}{2}\right\} \\ &=\; K\,\left[\frac{im\omega^2}{\mu^3}\right]^{1/4} \exp\left\{-\frac{i\omega t_f}{2} - \frac{m\omega x_f^2}{2}\right\} .\end{aligned} \tag{20.2.40}$$

Notice that the gaussian x_i integration uses the *complex* saddle point

$$\overline{x}_i = \frac{x_f}{\cos(\omega t_f) + i\sin(\omega t_f)} = x_f\, e^{-i\omega t_f} \tag{20.2.41}$$

even though the integration range is over real x_i.

Eq. (20.2.40) for $\langle x_f, t_f | g\rangle$ has the correct dependence on x_f and t_f required of the ground state (whose energy is $\omega/2$). This is no accident because, as is easily verified by direct differentiation, $\langle x_f, t_f | g\rangle$ satisfies the harmonic oscillator Schrödinger equation

$$\left[i\,\frac{\partial}{\partial t_f} + \frac{1}{2m}\left(\frac{\partial}{\partial x_f}\right)^2 - \frac{k x_f^2}{2}\right] \langle x_f, t_f | x_i, t_i\rangle = 0\,, \tag{20.2.42}$$

for any $t_f \neq t_i$. Normalization is preserved if we choose $K = (m\mu^3/i\pi^2)^{1/4}$, in which case (20.2.38) becomes

$$\langle x_f, t_f | x_i, t_i\rangle = \left[\frac{m\omega}{2\pi i \sin[\omega(t_f - t_i)]}\right]^{1/2} \exp\left\{\frac{im\omega}{2\sin[\omega(t_f - t_i)]}\Big[(x_f^2 + x_i^2)\cos[\omega(t_f - t_i)] - 2x_i x_f\Big]\right\} . \tag{20.2.43}$$

20.3 Semiclassical (WKB) methods

We next turn to non-gaussian examples that cannot be so easily solved and so for which approximate methods are required. Of particular interest are saddle-point approximations when evaluating path integrals, whose counterpart in traditional quantum mechanics is the WKB (Wentzel, Kramers, Brillouin) approximation[89] to solving the Schrödinger equation. Once we transition to field theory in §21 the same path-integral methods will parallel the semiclassical approximation described in §7.

We start with a brief review of WKB methods in single-particle quantum mechanics.

20.3.1 WKB methods

The WKB approximation is also sometimes called the semiclassical or quasiclassical approximation because it describes quantum systems that are close to what can be called a classical limit. To set up the approximation consider a single particle of mass m moving in the presence of a potential $V(x)$, where x is the particle's position. The time-independent Schrödinger equation for such a particle is

$$-\frac{1}{2m}\,\frac{\partial^2\psi}{\partial x^2} + V(x)\,\psi = E\,\psi\,, \tag{20.3.1}$$

which in the simplest case where $V(x) = V_0$ is constant has plane-wave solutions

$$\psi(x) = A_\pm e^{\pm ipx} \qquad \text{with} \qquad p = \sqrt{2m(E-V_0)}\,, \tag{20.3.2}$$

where $A_\pm$ are integration constants.

The solution (20.3.2) must remain approximately valid if $V(x)$ is not exactly constant, provided that V varies sufficiently slowly as a function of x, suggesting that solutions should have the approximate form

$$\psi(x) \simeq A(x)\,\exp\left[\pm i\int \mathrm{d}x\; p(x)\right] \qquad \text{where} \qquad p(x) = \sqrt{2m[E-V(x)]}\,. \tag{20.3.3}$$

Intuitively, the validity of the approximation requires both $V(x)$ and $A(x)$ to vary negligibly over a de Broglie wavelength $\lambda = 2\pi/p$ (as can often be the case, as seen in Figure 16). This approximate solution becomes exact – with $A(x) \to A_0$ becoming constant – in the limit that $V(x) \to V_0$ is also constant.

To systematize this approximation, and to show the sense in which it describes a semiclassical limit, it is convenient to temporarily use units for which the factors of $\hbar$ are explicit and rewrite the wavefunction in terms of its amplitude and phase,

$$\psi(x) = A(x)\,e^{iP(x)}\,, \tag{20.3.4}$$

[89] This is sometimes called the WKBJ approximation, where the J stands for Jeffreys, who developed similar methods within the mathematics community slightly earlier than W, K or B did so independently for quantum physics.

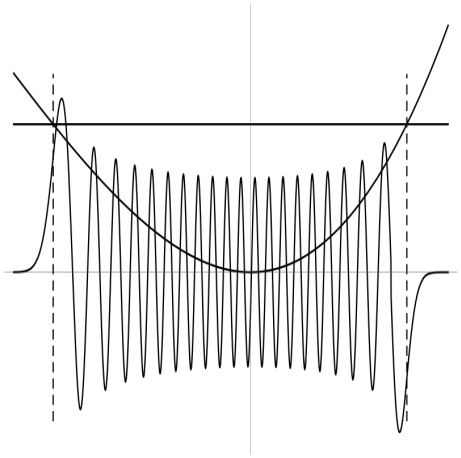

Figure 16. A sketch of the harmonic oscillator potential $V(x) = \frac{1}{2}kx^2$ together with the wavefunction of one of its excited eigenstates. Figure: Mathphysman - https://en.wikipedia.org/wiki/File:WKB_approximation_example.svg, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=97059556

where A and P are real functions. In terms of A and P the real and imaginary parts of (20.3.1) imply (with factors of $\hbar$ reintroduced)

$$\hbar^2\left[-\frac{A''}{A}+(P')^2\right]=2m[E-V(x)] \qquad \text{and} \qquad \hbar^2\Big[2A'P'+AP''\Big]=0\,, \tag{20.3.5}$$

where primes denote differentiation with respect to x. Notice that the second of these equations states $(A^2P')'=0$ and so integrates to give A as a function of P,

$$A=\frac{C}{\sqrt{P'}}\,, \tag{20.3.6}$$

where C is an integration constant.

Guided by the plane-wave example described above we seek solutions to (20.3.1) with the semiclassical series form

$$P=\frac{P_c}{\hbar}+P_1+\hbar P_2+\cdots\,, \tag{20.3.7}$$

once A is eliminated using (20.3.6). Substituting (20.3.7) into the first of eqs. (20.3.5) and setting to zero the coefficients of each power of $\hbar$ then leads to the following set of equations:

$$\begin{aligned}
&\mathcal{O}(\hbar^0): && \Big(P_c'\Big)^2=2m\Big[E-V(x)\Big]\,,\\
&\mathcal{O}(\hbar^1): && P_c'P_1'=0\\
&\mathcal{O}(\hbar^2): && -\frac{A_c''}{A_c}+\Big(P_1'\Big)^2+2P_c'P_2'=0\,,
\end{aligned} \tag{20.3.8}$$

and so on. The first of these has solution

$$P_c = \pm \int \mathrm{d}x\, p(x) \qquad \text{with } p(x) := \sqrt{2m[E - V(x)]}\,, \tag{20.3.9}$$

which when used in (20.3.6) gives the leading result

$$\psi_\pm(x) = \frac{C_\pm}{\sqrt{p(x)}} \exp\left[\pm i \int \mathrm{d}x\, p(x)\right], \tag{20.3.10}$$

extending (20.3.3) by also computing the amplitude.

The first subleading equation implies P_1 is a constant (which can be set to zero by absorbing P_1 into the phase of the constant $C_\pm$ appearing in (20.3.10)). The next equation can be integrated to give P_2, keeping in mind that (20.3.6) implies $A_c = C\sqrt{\hbar/|P_c'|} = C\sqrt{\hbar/p(x)}$ and so $A_c''/A_c = -(p''/2p) + 3(p'/2p)^2 = \mathcal{O}(\hbar^0)$, and

$$P_2' = \frac{A_c''}{P_c' A_c} = \pm\frac{1}{p}\left[-\frac{p''}{2p} + 3\left(\frac{p'}{2p}\right)^2\right]. \tag{20.3.11}$$

Although formally derived here as a series in $\hbar$, since $\hbar$ has dimensions (in ordinary units) this leaves open the thing relative to which $\hbar$ is small. The more precise statement is that the approximation relies on $\int_0^L p(x)\,\mathrm{d}x \gg \hbar$, where L is a characteristic length scale over which quantities like $V(x)$ and $p(x)$ vary appreciably. (In sensible units where $\hbar = 1$ the approximation relies on the condition $\int_0^L p(x)\,\mathrm{d}x \gg 1$.) That is, if $L \sim V(x)/V'(x) \sim p(x)/p'(x)$ then the approximation is controlled by the condition $L \gg \lambda = 2\pi/p$. Indeed, if $p' \sim p/L$ and $p'' \sim p/L^2$ then (20.3.11) implies $P_2'/P_c' \sim 1/(pL)^2 \sim \lambda^2/L^2$. In particular these corrections are *not* small when $p(x) \to 0$, such as occurs at any classical turning point for which $V(x) = E$. §20.4 has more to say about what one does instead near such turning points.

The WKB limit is a semiclassical approximation in the following practical sense. Any wavefunction of the form $\psi(x) = A(x)\, e^{i[P_c(x)/\epsilon] + \mathcal{O}(\epsilon^0)}$ has derivatives that for small ϵ are dominated by the derivatives of P_c, and consequently

$$-i\frac{\partial\psi}{\partial x} \simeq \frac{1}{\epsilon}\frac{\partial P_c}{\partial x}\,\psi\Big[1 + \mathcal{O}(\epsilon)\Big]. \tag{20.3.12}$$

But this means that to leading order in ϵ the function $\psi(x)$ is effectively an eigenstate of momentum whose eigenvalue is given by $\epsilon^{-1}\partial P_c/\partial x$ (and so is a function of position). Momentum and position can be simultaneously specified like this because the commutator of position and momentum acting on $\psi(x)$ is

$$\Big[\hat{X}, \hat{P}\Big]\psi(x) = \frac{1}{\epsilon}\left(x\,\frac{\partial P_c}{\partial x} - \frac{\partial P_c}{\partial x}\,x\right)\psi(x) + \mathcal{O}(\epsilon^0) = \mathcal{O}(\epsilon^0)\,, \tag{20.3.13}$$

and so when $\epsilon \ll 1$ the order-unity failure of $\hat{X}$ and $\hat{P}$ to commute is much smaller than the large eigenvalue of $\hat{P}$ itself.

20.3.2 Saddle-point approximation

With the semiclassical WKB approximation in mind we now return to the question of how to approximately evaluate functional integrals that are not strictly gaussian. The key idea to be used when doing so is the *saddle-point approximation*.

For ordinary integrals the saddle-point approximation states that when $\kappa \gg 1$ a convergent integral of the form

$$I(\kappa) := \int_{-\infty}^{\infty} \mathrm{d}x \ \exp\Big[-\kappa\, F(x)\Big] \tag{20.3.14}$$

can be well-approximated by expanding $F(x)$ about its minimum $x = x_c$ – found by solving[90] $F'(x_c) = 0$ and demanding $F''(x_c) > 0$ – and so writing

$$\begin{aligned} F(x, x_c) \ &= \ F(x_c) + \frac{1}{2}\, F''(x_c)(x - x_c)^2 + F_{\rm int}(x, x_c) \\ \text{with} \qquad F_{\rm int}(x, x_c) \ &:= \sum_{n=3}^{\infty} \frac{1}{n!}\, F^{(n)}(x_c)(x - x_c)^n \,, \end{aligned} \tag{20.3.15}$$

where $F^{(n)}(x_c) = (\partial^n F/\partial x^n)_{x=x_c}$ and no terms linear in $x - x_c$ appear because of the condition $F'(x_c) = 0$. The exponential involving all nongaussian terms is then Taylor expanded and the result is then integrated term by term, so

$$I(\kappa) \simeq \int_{-\infty}^{\infty} \mathrm{d}x \ \exp\Big[-\kappa\, F(x_c) - \tfrac{1}{2}\kappa\, F''(x_c)(x - x_c)^2\Big] \left\{1 + \sum_{n=1}^{\infty} \frac{1}{n!}\Big[-\kappa F_{\rm int}(x, x_c)\Big]^n\right\} . \tag{20.3.16}$$

The leading approximation is therefore given by

$$\begin{aligned} I(\kappa) \ &\simeq \ \exp\Big[-\kappa\, F(x_c)\Big] \int_{-\infty}^{\infty} \mathrm{d}x \ \exp\Big[-\tfrac{1}{2}\kappa\, F''(x_c)(x - x_c)^2\Big] \Big\{1 - \kappa F_{\rm int} + \cdots\Big\} \\ &= \ \sqrt{\frac{2\pi}{\kappa F''(x_c)}}\, \exp\Big[-\kappa\, F(x_c)\Big] \Big\{1 + \mathcal{O}(\kappa^{-1})\Big\} , \end{aligned} \tag{20.3.17}$$

and the corrections involving powers of $F_{\rm int}(x, x_c)$ form an asymptotic series in *inverse* powers[91] of κ starting at $\mathcal{O}(\kappa^{-1})$. The beauty of this expansion is that it involves only evaluating gaussian integrals weighted by powers of $(x - x_c)$, which can be performed explicitly. Indeed for gaussian integrals (for which $F_{\rm int} = 0$) the expansion around the saddle point provides the exact answer, as was explored in some detail in §20.1.1 and §20.2, with (20.2.41) providing an explicit example where the saddle point is complex and so does not lie on the original (real) contour of integration.

[90] Here primes denote derivatives with respect to x. If more than one local minimum exists then x_c is chosen so that $F(x_c)$ takes the smallest value. Notice that there is no requirement that x_c must lie on the original contour of integration.

[91] As we shall see, the series is in inverse powers (as opposed to positive powers) of κ because the integration over x brings enough powers of κ^{-1} to overwhelm the explicit κ's that premultiply each factor of $F_{\rm int}$.

We apply this technique to evaluating path integrals, such as to (20.1.41) which states

$$\langle q_f, t_f | q_i, t_i \rangle = \int_{q_i}^{q_f} \mathcal{D}q^a(t) \, \exp\left\{ i \int_{t_i}^{t_f} \mathrm{d}t \, L(q, \dot{q}) \right\} . \tag{20.3.18}$$

In this the integrand is $e^{iS[q(t)]/\hbar}$ – where $S[q(t)]$ is the action and powers of $\hbar$ are briefly reinstated – so the role of κF in (20.3.14) is here played by the action in Planck units: $iS/\hbar$. A saddle-point evaluation of (20.3.18) expands the integrand about the path $\overline{q}(t)$ that satisfies $\delta S/\delta q = 0$ – that is to say about the trajectory satisfying the classical equations of motion subject to the boundary conditions $\overline{q}(t_i) = q_i$ and $\overline{q}(t_f) = q_f$. The counterpart to the result (20.3.17) is then given by

$$\langle q_f, t_f | q_i, t_i \rangle \simeq \left(\det \overline{\mathfrak{D}} \right)^{-1/2} \exp\left\{ i \int_{t_i}^{t_f} \mathrm{d}t \, L(\overline{q}, \dot{\overline{q}}) \right\} \left[1 + \mathcal{O}(\hbar) \right] , \tag{20.3.19}$$

where $\overline{\mathfrak{D}} := \mathfrak{D}[\overline{q}(t)]$ with $-i\delta^2 S/\delta q(t)\delta q(t') = \mathfrak{D}\delta(t-t')$ being the operator that appears in the quadratic part of the fluctuations (found by taking the second functional derivative of the action).

For instance for

$$S = \int_{t_i}^{t_f} \mathrm{d}t \Big[\frac{m}{2} \, \dot{q}^2 - V(q) \Big] \qquad \text{we have} \qquad \frac{\delta S}{\delta q(t)} \bigg|_{q=\overline{q}} = -m\ddot{\overline{q}} - V'(\overline{q}) = 0 \, , \tag{20.3.20}$$

and the operator $\overline{\mathfrak{D}}$ then becomes

$$\overline{\mathfrak{D}} = i \left[\left(\frac{\mathrm{d}}{\mathrm{d}t} \right)^2 + V''(\overline{q}) \right] . \tag{20.3.21}$$

We have seen in §20.2 that in the special case of a quadratic or constant potential $V(q)$ this gives the exact result (without the $\mathcal{O}(\hbar)$ corrections) for what is then a gaussian functional integral, but the saddle-point approximation shows how gaussian integration can also give approximate results more generally even for a nongaussian path integral, at least within the semiclassical regime.

The semiclassical limit is justified for situations where $S \gg \hbar$ and so for which the exponential generically oscillates very rapidly, with nearby paths very efficiently destructively interfering with one another. The exception to this is in the vicinity of paths $\overline{q}(t)$ that are stationary points of the action $S[q(t)]$ because for these the stationarity condition $\delta S[\overline{q}(t)] = 0$ itself ensures that the action does not strongly vary. It is because of this that the saddle-point approximation works, with the role of κ played by $S/\hbar \gg 1$ and the corrections to the gaussian limit coming as powers of $1/\kappa \propto \hbar$. As discussed in §21, for field theories this expansion often corresponds to the perturbative expansion performed directly within the operator approach to quantum field theory described in earlier sections. From the perspective of quantum mechanics the saddle-point approximation is *why* solutions to the classical equations of motion $\delta S/\delta q(t) = 0$ are sometimes important.

20.3.3 State-dependence of saddle-point boundary conditions

The saddlepoint approximation dovetails very nicely with the WKB approximation as can be seen by using (20.3.21) to evolve a WKB energy eigenstate like the one given in (20.3.10) forward in time. In particular, the leading powers of $\hbar$ allow a very simple connection to be derived between the state that is evolved in a path integral and the boundary conditions that must be required of the classical path that semiclassically provides the dominant saddle point.

For example, for the lagrangian (20.3.20) there are two WKB energy eigenstates for each eigenvalue E, given by

$$\langle q, t_i | E, \pm \rangle = \psi_\pm(q, t_i) = C_\pm(q_0) \, \exp\left\{ \frac{i}{\hbar} \left[-E t_i \pm \int_{q_0}^{q} \mathrm{d}q \, \sqrt{2m[E - V(q)]} \right] \right\} + \mathcal{O}(\hbar^0) \,, \tag{20.3.22}$$

where we now work with full solutions to the time-dependent Schrödinger equation. The lower limit q_0 on the q integration is arbitary since changes to it can be absorbed into an appropriate change to $C_\pm$. $\hbar$ is once more reinstated in order to make explicit that we track here only the leading part of the semiclassical expansion.

At later times the wavefunction for these WKB energy eigenstates becomes

$$\begin{aligned} \langle q_f, t_f | E, \pm \rangle &= \int_{-\infty}^{\infty} \mathrm{d}q_i \, \langle q_f, t_f | q_i, t_i \rangle \langle q_i, t_i | E, \pm \rangle \\ &\simeq C_\pm(q_0) \int_{-\infty}^{\infty} \mathrm{d}q_i \, \exp\left\{ \frac{i}{\hbar} \left[W(q_f, q_i) - E t_i \pm \frac{i}{\hbar} \int_{q_0}^{q_i} \mathrm{d}q \, \sqrt{2m[E - V(q)]} \right] \right\} \\ &\qquad + \mathcal{O}(\hbar^0) \,, \end{aligned} \tag{20.3.23}$$

which works to the same order in the $\hbar$ expansion as does the WKB state (20.3.22) and so uses the saddle-point approximation (20.3.19) for $\langle q_f, t_f | q_i, t_i \rangle$ and drops $\mathcal{O}(\hbar^0)$ corrections. The function $W(q_f, q_i)$ is defined as the action (20.3.20) evaluated at the classical path satisfying $m\ddot{\overline{q}} + V'(\overline{q}) = 0$ that connects q_i to q_f in time $t_f - t_i$:

$$W(q_f, q_i) = \int_{t_i}^{t_f} \mathrm{d}t \Big[\frac{m}{2} \dot{\overline{q}}^2 - V(\overline{q}) \Big] \qquad \text{with} \qquad \overline{q}(t_i) = q_i \;\; \text{and} \;\; \overline{q}(t_f) = q_f \,, \tag{20.3.24}$$

regarded as a function of these endpoints.

To leading order in $\hbar$ the ordinary integral over q_i can also be performed using the saddle-point approximation, by expanding about the stationary point $\overline{q}_i$ of the exponent, which satisfies

$$\left(\frac{\partial W}{\partial q_i} \right)_{q_i = \overline{q}_i} \pm \sqrt{2m[E - V(\overline{q}_i)]} = 0 \,. \tag{20.3.25}$$

To evaluate $\partial W / \partial q_i$ compare the action for a trajectory $q(t)$ that differs from the classical solution $\overline{q}(t)$ by δq_i only very close to $t = t_i$. Writing $q(t) = \overline{q}(t) + \delta q(t)$ the variation of the

action is (see Appendix D)

$$\delta S[q(t)] = \Big[m\dot{\overline{q}}(t)\,\delta q(t)\Big]_{t_i}^{t_f} - \int_{t_i}^{t_f} \mathrm{d}t\,\Big[m\ddot{\overline{q}} + V'(\overline{q})\Big]\delta q(t) = -m\dot{\overline{q}}(t_i)\delta q_i\,, \tag{20.3.26}$$

where the last equality uses that $\overline{q}(t)$ satisfies the classical equation of motion $m\ddot{\overline{q}}+V'(\overline{q})=0$. We conclude $-\partial W/\partial q_i = m\dot{\overline{q}}_i$ is given by the saddle-point trajectory's classical momentum evaluated at $t=t_i$.

The saddle-point condition (20.3.25) then replaces the previous condition $\overline{q}(t_i)=q_i$ with

$$m\dot{\overline{q}}(t_i) = \pm\sqrt{2m[E-V(\overline{q}_i)]} \qquad \text{or, equivalently} \qquad \tfrac{1}{2}m\dot{\overline{q}}_i^{\,2} + V(\overline{q}_i) = E\,. \tag{20.3.27}$$

But the classical equations imply $\frac{1}{2}m\dot{\overline{q}}^{\,2}(t)+V[\overline{q}(t)]$ is a constant (equal to the energy) along any classical trajectory and so $\overline{q}(t)$ satisfies $\frac{1}{2}m\dot{\overline{q}}^{\,2}+V(\overline{q})=E$ for all t between t_i and t_f. The upshot is that semiclassical evaluation of the integral over the endpoint q_i when computing $\langle q_f,t_f|E,\pm\rangle$ converts the classical saddle point of the path integral from one that satisfies $\overline{q}(t_f)=q_f$ and $\overline{q}(t_i)=q_i$ (as was required for $\langle q_f,t_f|q_i,t_i\rangle$) into one that satisfies $\overline{q}(t_f)=q_f$ and has energy E, where E is the energy of the chosen WKB state.[92]

The value of the integral at this saddle point is given by

$$\langle q_f,t_f|E,\pm\rangle \simeq C_\pm(q_0)\,\exp\left\{\frac{i}{\hbar}\left[W(q_f,\overline{q}_i) - Et_i \pm \frac{i}{\hbar}\int_{q_0}^{\overline{q}_i}\mathrm{d}q\,\sqrt{2m[E-V(q)]}\right]\right\} + \mathcal{O}(\hbar^0)\,, \tag{20.3.28}$$

where evaluating $W(q_f,q_i)$ at $q_i=\overline{q}_i$ and using (20.3.27) and $\mathrm{d}t\,\dot{\overline{q}} = \mathrm{d}\overline{q}$ gives

$$\begin{aligned} W(q_f,\overline{q}_i) &= \int_{t_i}^{t_f}\mathrm{d}t\Big[\tfrac{1}{2}m\dot{\overline{q}}^{\,2} - V(\overline{q})\Big] = \int_{t_i}^{t_f}\mathrm{d}t\Big(m\dot{\overline{q}}^{\,2}\Big) - \int_{t_i}^{t_f}\mathrm{d}t\Big[\tfrac{1}{2}m\dot{\overline{q}}^{\,2}+V(\overline{q})\Big] \\ &= -E(t_f-t_i) \pm \int_{\overline{q}_i}^{q_f}\mathrm{d}q\sqrt{2m[E-V(q)]}\,. \end{aligned} \tag{20.3.29}$$

Using this allows (20.3.28) to be written

$$\langle q_f,t_f|E,\pm\rangle \simeq C_\pm(q_0)\,\exp\left[-\frac{i}{\hbar}E\,t_f \pm \frac{i}{\hbar}\int_{q_0}^{q_f}\mathrm{d}q\,\sqrt{2m[E-V(q)]}\right] + \mathcal{O}(\hbar^0)\,, \tag{20.3.30}$$

which at order $\hbar^{-1}$ has the correct time dependence and dependence on q_f for a WKB energy eigenstate (compare with (20.3.22)).

20.4 Turning points and reflection

The consistency of saddle-point and WKB methods seen above is gratifying and beautiful but also gives the false impression that not much happens: once one starts in a WKB energy

[92] Notice that if the state at $t=t_i$ were a momentum eigenstate with eigenvalue p_i then (20.3.27) instead becomes $m\dot{\overline{q}}(t_i)=p_i$, so the classical trajectory that semiclassically dominates $\langle q_f,t_f|p_i,t_i\rangle$ satisfies the boundary conditions $\overline{q}(t_f)=q_f$ and $m\dot{\overline{q}}(t_i)=p_i$.

eigenstate heading in one direction or the other – a choice made by choosing one of the '±' alternatives in (20.3.30) – this direction of motion never changes. Something must go wrong with the semiclassical approximation if phenomena like scattering from a barrier are to be described.

Something indeed does go wrong when semiclassical methods[93] are applied to scattering from a barrier: for motion in one spatial dimension classical scattering always involves changing the sign of the velocity (and momentum), which must therefore somewhere pass through zero. Expressions like (20.3.9) show that this zero happens at the classical turning points – *i.e.* positions, $x = a$, for which $V(a) = E$ – and the discussion below (20.3.11) shows that for precisely these points the semiclassical approximation *always* breaks down. The WKB approximation can only be trusted for $|x - a| > d$, for some positive d whose precise value depends on the desired accuracy of one's calculations.

20.4.1 Matching by analytic continuation

The calculation of reflection (and transmission) rates for scattering from a barrier therefore hinges on understanding how to evolve past the turning points. This is usually achieved by using a different approximation in the immediate vicinity of a turning point and matching this to the WKB solutions on either side of the turning point, thereby allowing the integration constants of the two WKB solutions to be related to one another.

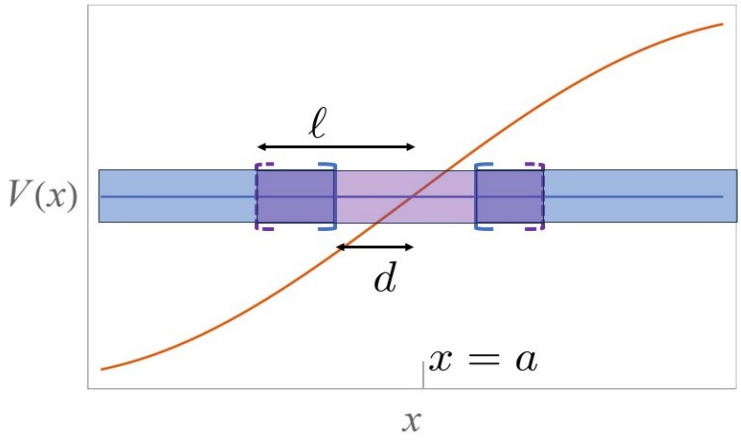

Figure 17. A sketch of $V(x)$ in the region near a turning point located at $x = a$. The purple region shows the domain of validity $|x - a| < \ell$ of the linear approximation $V \propto (x - a)$ and the blue region shows the domain of validity $|x - a| > d$ of the WKB approximation (assuming $d < \ell$).

[93] In quantum mechanics some reflection from a barrier occurs even if $E > V_{\max}$, even though in this regime the barrier only slows the speed of a classical particle without changing its direction of motion. This type of scattering is not in the semiclassical regime.

For instance, suppose a turning point occurs when $x = a$ with the classically allowed region being $x < a$ and the forbidden region being $x > a$ (see Fig. 17). Near $x = a$ we have

$$V(x) \simeq E + \frac{b^2}{2m}(x-a) + \mathcal{O}[(x-a)^2] \qquad \text{where} \qquad b^2 := 2mV'(a) > 0\,, \tag{20.4.1}$$

and the factor of particle mass m is included for later convenience. Suppose this is a good approximation for $|x-a| < \ell$ for some ℓ. In the usual telling of the story the WKB approximation can be propagated through the turning point if $\ell > d$ (where the WKB approximation holds only for $|x-a| > d$). One first solves the Schrödinger equation for a linear potential (not in the WKB approximation) in the domain $|x-a| < \ell$. If $\ell > d$ then the domains of validity of the linear-potential approximation and the WKB approximation overlap and so continuity allows the solution for the linear potential to be matched to the WKB solutions on both sides of the fixed points, thereby relating the integration constants for the WKB solutions on either side of the turning point.

If the WKB solution to the time-independent Schrödinger equation to the right of the turning point is assumed to be the solution (20.3.10) that is damped for large $x > a + d$,

$$\psi_{\scriptscriptstyle R}(x) \simeq \frac{C}{\sqrt{\mathfrak{p}(x)}} \exp\left[-\frac{1}{\hbar}\int_a^x \mathrm{d}u\, \mathfrak{p}(u)\right], \tag{20.4.2}$$

with $\mathfrak{p}(x) := \sqrt{2m[V(x)-E]}$ in the forbidden region, then this matching process implies the solution to the left of the turning point ($x < a - d$) is given by

$$\psi_{\scriptscriptstyle L}(x) \simeq \frac{C}{\sqrt{p(x)}} \cos\left[\frac{\pi}{4} + \frac{1}{\hbar}\int_a^x \mathrm{d}u\, p(u)\right], \tag{20.4.3}$$

where (as usual) $p(x) := \sqrt{2m[E-V(x)]}$.

We now rederive this standard result[94] without ever having to leave the semiclassical approximation, since this is more useful when making contact with saddle-points methods within the path-integral formulation. The idea is (again) to approximate the potential as being linear – as in (20.4.1) – but this time only use the WKB form of the solution with this potential rather than the exact result. In order for this to be done without WKB methods breaking down we adopt the trick of continuing the particle position x into the complex plane in order to avoid the breakdown at $x = a$.

For the linear potential (20.4.1) the momentum appearing in the WKB wavefunction in the forbidden region is $\mathfrak{p} = b\sqrt{x-a}$ and so the WKB wave-function (20.4.2) in the forbidden zone $x > a$ is

$$\psi(x) \simeq \frac{C}{\sqrt{\mathfrak{p}(x)}} \exp\left[-\frac{1}{\hbar}\int_a^x \mathrm{d}u\, \mathfrak{p}(u)\right] \simeq \frac{C}{\sqrt{b}|x-a|^{1/4}} \exp\left[-\frac{2b}{3\hbar}\,(x-a)^{3/2}\right]. \tag{20.4.4}$$

[94] This argument appears *e.g.* in *Quantum Mechanics (Non-relativistic Theory)* by Landau and Lifshitz.

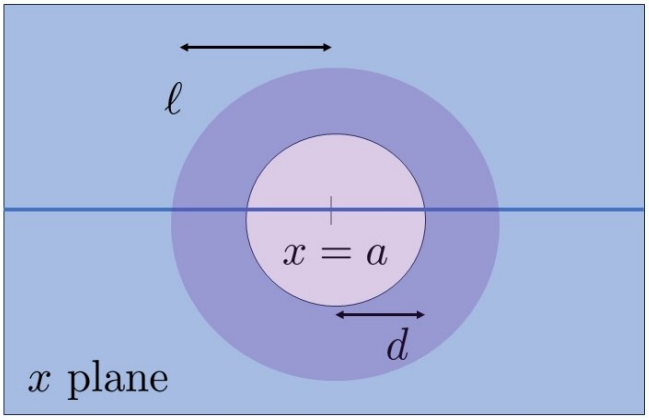

Figure 18. A sketch of the complex x plane near a turning point located at $x = a$. The purple circle shows the domain of validity $|x - a| < \ell$ of the linear approximation $V \simeq -b^2(x - a)$ and the blue region shows the domain of validity $|x - a| > d$ of the WKB approximation (assuming $d < \ell$).

We cannot get from $x > a + d$ to $x < a - d$ by simply using this expression for real x because doing so takes us outside the domain of validity for the WKB approximation, but we *can* use (20.4.4) to connect these regions if we evaluate it along a semicircle $x - a = R\, e^{i\theta}$ that lies in the annulus with radius $d < R < \ell$ in the complex x plane (see Fig. 18) for which the potential is approximately linear and the WKB approximation still holds. Along this curve the exponent of (20.4.4) becomes

$$\begin{aligned} -\frac{1}{\hbar}\int_a^x \mathrm{d}u\, \mathfrak{p}(u) \;&\simeq\; -\frac{2b}{3\hbar}|x-a|^{3/2}\Big[\cos\left(\tfrac{3}{2}\theta\right) + i\sin\left(\tfrac{3}{2}\theta\right)\Big] \\ &\to \pm\frac{2ib}{3\hbar}|x-a|^{3/2} \qquad \text{as } \theta \to \pm\pi\,, \end{aligned} \tag{20.4.5}$$

showing that different results are obtained for real $x < a$ depending on whether the contour moves along the semicircle in the upper or lower half plane. These are different because of the branch point at $x = a$, for which the branch cut can be taken to run for $x < a$ along the real axis, with the two results lying on different sheets.

Comparing to the WKB solutions for a linear potential in the classically allowed region, where $p(x) = \sqrt{2m[E - V(x)]} = b\sqrt{a - x}$,

$$\begin{aligned} \psi(x) \;&=\; \frac{C_+}{\sqrt{p(x)}}\exp\left[+\frac{i}{\hbar}\int_a^x \mathrm{d}u\, p(u)\right] + \frac{C_-}{\sqrt{p(x)}}\exp\left[-\frac{i}{\hbar}\int_a^x \mathrm{d}u\, p(u)\right] \\ &\simeq\; \frac{C_+}{\sqrt{p(x)}}\exp\left[-\frac{2ib}{3\hbar}\,(a-x)^{3/2}\right] + \frac{C_-}{\sqrt{p(x)}}\exp\left[+\frac{2ib}{3\hbar}\,(a-x)^{3/2}\right], \end{aligned} \tag{20.4.6}$$

shows that continuity along the contour in the upper half plane fixes C_- while continuity along the contour in the lower half plane fixes C_+. Keeping in mind that $\sqrt{\mathfrak{p}(x)} = \sqrt{b}|x-a|^{1/4}e^{\pm i\theta/4}$

along the two semicircles shows that continuity implies

$$C_\pm = C\, e^{\pm i\pi/4}\,, \tag{20.4.7}$$

in agreement with the classic result (20.4.3).

20.4.2 Saddle-point paths near turning points

With the above procedure in hand for navigating past the turning points purely within the WKB framework, we return to the question of how to handle the presence of classical turning points within the saddle-point approximation to the path integral.

The main thing needed for a saddle-point evaluation of the path integral is the classical path $\overline{x}(t)$ satisfying the boundary conditions appropriate for the amplitude of interest. To see why the presence of classical turning points complicates this consider the WKB energy eigenstate using (20.3.22) (reproduced here)

$$\langle x_i, t_i | E, \pm\rangle = C_\pm(x_0)\, \exp\left\{\frac{i}{\hbar}\left[-E\,t_i \pm \int_{x_0}^{x_i} \mathrm{d}x\, \sqrt{2m[E-V(x)]}\right]\right\} + \mathcal{O}(\hbar^0)\,, \tag{20.4.8}$$

which we wish to evolve to another position at a later time by convolving it with $\langle x_f, t_f | x_i, t_i\rangle$, doing so to leading order in $\hbar$ using saddle-point methods. Suppose for definiteness that the positions x_i and x_f are both to the left of the barrier and the energy is low enough that the barrier has classical turning points. Since x_0 is arbitrary we can always choose it also to be to the left of the barrier so that the integral in (20.4.8) is real.

We saw in §20.3.3 that the saddle point required to evolve (20.4.8) semiclassically to obtain $\langle x_f, t_f | E, \pm\rangle$ must satisfy

$$m\dot{x} = p(x) = \pm\sqrt{2m[E-V(x)]} \qquad \text{and} \qquad x(t_f) = x_f\,. \tag{20.4.9}$$

Real solutions to these conditions exist, one for each of the signs chosen in (20.4.9). What is new in the presence of turning points is that the classical trajectory is not unique: because p can change sign along a classical trajectory solutions with both signs of p can satisfy the boundary condition and so both must be included as saddle points within the path integral.

For x_f to the left of the barrier the trajectory with $p > 0$ goes through as described in earlier sections. For instance if we start to the left of the barrier with a right-moving wave so

$$\langle x, t | E, +\rangle = \frac{C_+}{\sqrt{p(x)}} \exp\left\{\frac{i}{\hbar}\left[-E\,t + \int_{x_0}^{x} \mathrm{d}u\, p(u)\right]\right\} \tag{20.4.10}$$

then convolving with the kernel $\langle y, t' | x, t\rangle$ using the saddle point solution to (20.4.9) with $p > 0$ everywhere propagates the state forward to another point y (assumed also to be to the left of the barrier) at a later time t' to give[95]

$$\frac{C_+}{\sqrt{p(y)}} \exp\left\{\frac{i}{\hbar}\left[-E\,t' + \int_{x_0}^{y} \mathrm{d}u\, p(u)\right]\right\} \tag{20.4.11}$$

[95] We use here the fact that the subdominant contributions of the path integral also convert $\sqrt{p(x)}$ to $\sqrt{p(y)}$ in the denominator of the amplitude (exercise: prove this!).

as before.

To this must be added the contribution of the other saddle point, which again solves (20.4.9) but with p changing sign at the classical turning point. The question is how to evaluate this contribution without leaving the domain of saddle-point methods which we know break down at this turning point. The answer is suggested by the discussion of WKB matching in the previous section: we should entertain the possibility of classical saddle points that venture out to complex values for x.

To see how this might work notice that for complex x (20.4.9) can be written

$$\frac{\mathrm{d}t}{\mathrm{d}x} = \sqrt{\frac{m}{2[E-V(x)]}} \qquad \text{with solution} \qquad t(x) = \sqrt{m}\int_{\mathcal{C}} \frac{\mathrm{d}x}{\sqrt{2[E-V(x)]}}\,, \tag{20.4.12}$$

where $\mathcal{C}$ is a trajectory in the complex plane that satisfies $t(y) = t'$. There is a lot of freedom in choosing this trajectory because the integrand depends only on x and not also on x^*, and $V(x)$ is an analytic function of x. The only singularities in the integrand therefore come from the square root and occur at the positions of the classical turning points like $x = a$, all of which lie on the real axis. These properties allow the contour of integration to be deformed arbitrarily provided only that it continues to satisfy $t(y) = t'$ and that it does not cross any of the singular turning points.

To start with we imagine choosing $\mathcal{C}$ to lie along the real x axis, and motivated by the discussion of the previous section we take the branch point of the integrand at $x = a$ to be associated with a branch cut that runs along the real axis for $x < a$. We regard x to have an infinitesimal imaginary part that puts $\mathcal{C}$ parallel to the real axis just above this branch cut.

Once the trajectory is close enough to the turning point we can approximate $V(x)$ with the linear potential (20.4.1). In this regime we know the momentum then satisfies $p(x) = b\sqrt{x-a}$ and the action can be evaluated explicitly as in the previous section. Rather than continuing too close to the singular turning point, once we get close enough to use the linear approximation for the potential we choose $\mathcal{C}$ to turn off the real axis and follow the circle $x = a + R\,e^{-i\theta}$ that skirts around the turning point as θ runs from $-\pi$ to π. Once back on the real axis just below the branch cut we can continue back just below the real axis towards smaller x along the classically reflected trajectory until we reach the point y (see the leftmost panel of Fig. 19).

Following the same steps as in the previous section the contribution of the path integral evaluated at this curve is

$$e^{-i\pi/2}\frac{C_+}{\sqrt{p(z)}}\exp\left\{\frac{i}{\hbar}\left[-E\,t' - \int_{x_0}^{z}\mathrm{d}u\,p(u)\right]\right\}\,, \tag{20.4.13}$$

where the phase prefactor comes from evaluating $[p(x)]^{-1/4}$ on the circular trajectory. Com-

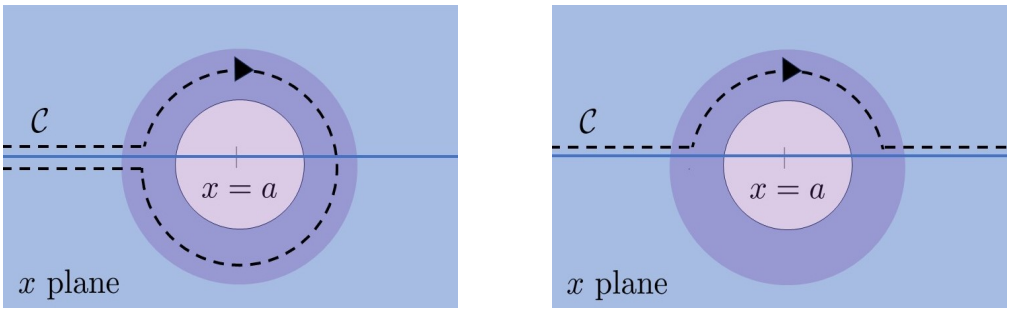

Figure 19. A sketch of two curves $\mathcal{C}$ in the complex x plane that are used to navigate about a classical turning point (located at $x = a$ with classically allowed region to the left) in the complex x plane. The purple circle shows the domain of validity $|x-a| < \ell$ of the linear approximation $V \simeq -b^2(x-a)$ and the blue region shows the domain of validity $|x-a| > d$ of the WKB approximation (assuming $d < \ell$). The left panel shows the contour used when computing the reflected-wave contribution to the saddle-point path integral while the right panel shows the contour used when computing the value of the wave function in the forbidden region.

bining this with (20.4.11) leads to the sum

$$\langle y, t'|E\rangle \simeq \frac{C_+}{\sqrt{p(y)}} \left\{ \exp\left[+\frac{i}{\hbar} \int_{x_0}^{y} \mathrm{d}u\, p(u) \right] + e^{-i\pi/2} \exp\left[-\frac{i}{\hbar} \int_{x_0}^{z} \mathrm{d}u\, p(u) \right] \right\} e^{-iE\,t'/\hbar} \tag{20.4.14}$$

in agreement with (20.4.3) once we use $C_+ = Ce^{i\pi/4}$. In this way the two types of classical trajectories to the left of the barrier respectively contribute to the incoming and reflected waves within the saddle-point approximation. Control of the saddle-point approximation is maintained despite the role played by a classical turning point by deforming the trajectory away from the real axis in the complex x plane.

Notice also that a similar story goes through if the point y is chosen to lie in the classically forbidden region. In this case only one trajectory contributes that circumnavigates the classical turning point, but this time the trajectory continues to the right on the real axis after having only gone halfway around the circle (see the right-hand panel of Fig. 19). The calculation of the previous section shows that this reproduces the correct damping solution but only because the incoming wave was chosen to lie just above the branch cut (and the outgoing wave just below) in the classically allowed region to the left of the barrier. A similar continuation can also be performed about any other turning points (if these exist) such as would arise in the computation of the transmission rate through a barrier, as we explore further in the next section.

20.5 Tunneling

It is instructive to use the above WKB/semiclassical path-integral approximations to compute a tunneling amplitude, both for it's own sake and because this has lessons for similar path-

integral calculations performed using fields in Chapter 21.

We focus again on one-dimensional, single-particle systems, for which particle position is denoted by x and the action is given by (20.3.20) (repeated here)

$$S[x(t)] = \int_{t_i}^{t_f} \mathrm{d}t \Big[\tfrac{1}{2}\, m\, \dot{x}^2 - V(x) \Big] \,. \tag{20.5.1}$$

To make things concrete consider the specific potential

$$V(x) = \frac{U}{2} \Big\{ \tanh\Big[\lambda(x+a)\Big] - \tanh\Big[\lambda(x-a)\Big] \Big\} \,, \tag{20.5.2}$$

which has the shape of a localized barrier of height U that extends from $x \simeq -a$ to $x \simeq +a$ (see Fig. 20). The parameter λ controls the steepness of the potential, and in the limit $\lambda \to \infty$ the potential $V(x)$ becomes a step potential

$$V_{\text{step}}(x) = \begin{cases} 0 & \text{for } |x| > a \\ U & \text{for } |x| < a \,. \end{cases} \tag{20.5.3}$$

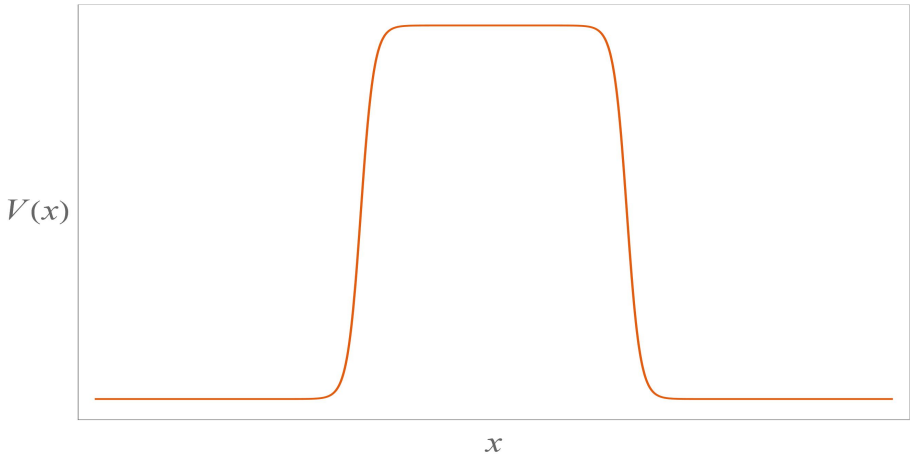

Figure 20. A sketch of the potential barrier described in (20.5.2) of the main text, with $\lambda = 10/a$.

20.5.1 A false start

It is tempting[96] to expect that tunneling amplitudes should be captured by computing $\langle x_f, t_f | x_i, t_i \rangle$ with x_f chosen on one side of the barrier and x_i chosen on the other, but this turns out not to be true. There are two ways to see why not.

The first way simply evaluates $\langle x_f, t_f | x_i, t_i \rangle$ semiclassically, which involves finding the classical trajectory that satisfies $m\ddot{\overline{x}} + V'(\overline{x}) = 0$ with boundary conditions $\overline{x}(t_i) = x_i$ and

[96] The temptation is largest if one first learns tunneling from some popular field theory accounts.

$\overline{x}(t_f) = x_f$. Tunneling might be expected to manifest itself by requiring this trajectory to pass through the classically forbidden region and so by finding that no real solutions exist. The problem with this approach is that a classical solution always does exist that satisfies the required boundary conditions and which is everywhere real, and so the amplitude $\langle x_f, t_f | x_i, t_i \rangle$ never is actually damped in the way expected for tunneling.

The existence of real solutions can be proven for potentials like (20.5.2) using a limiting procedure. We seek classical trajectories that go between two specified positions, $x_i < -a$ to $x_f > +a$, in a time interval $t_f - t_i$. Suppose first that $t_f - t_i$ is very small. In order to get from x_i to x_f in a very small time requires starting off at $t = t_i$ with a very large velocity, v_i, and we are not surprised to find classical real solutions in this case because for small enough $t_f - t_i$ the energy

$$E = \tfrac{1}{2}\, m\, v_i^2 + V(x_i) \tag{20.5.4}$$

associated with this large velocity ensures the trajectory's energy is high enough to go over top of the barrier: $E > U$. In this case we can construct the desired solution by starting off with the given initial position x_i and choose an initial large velocity v_i and use these to compute the E using (20.5.4). Given E the time taken to get to x_f is given by integrating $m\dot{x} = \sqrt{2m[E - V(x)]}$ to find

$$t_f - t_i = \int_{x_i}^{x_f} \frac{\mathrm{d}x}{\dot{x}} = \int_{x_i}^{x_f} \mathrm{d}x \sqrt{\frac{m}{2[E - V(x)]}}\,. \tag{20.5.5}$$

If this is not the correct value then we adjust v_i until the right value is obtained.

The only worry in this case would be that solutions might not exist if $t_f - t_i$ is taken to be extremely large, since then the required initial velocity might produce an energy that is not above the barrier. What actually happens in the large $t_f - t_i$ limit though is that the initial velocity must be chosen to make E very close to the top of the barrier: as $t_f - t_i \to \infty$ the energy approaches $E \to V_{\max}$ (where, for example, $V_{\max} = V(x = 0) = U \tanh(\lambda a)$ for the specific potential (20.5.2)).

To see why $t_f - t_i \to \infty$ when $E \to V_{\max}$ consider the time taken to go from $x = -\epsilon$ to $x = +\epsilon$ where ϵ is chosen small enough that we can approximate $E - V(x) \simeq \frac{1}{2}(\Delta + kx^2)$ with $\Delta = 2(E - V_{\max}) > 0$ and $k = -V''(0) > 0$. In this case (20.5.5) predicts

$$t(\epsilon) - t(-\epsilon) = \int_{-\epsilon}^{\epsilon} \mathrm{d}x \sqrt{\frac{m}{\Delta + kx^2}} = 2\sqrt{\frac{m}{k}}\ \tanh^{-1}\left[\sqrt{\frac{k\epsilon^2}{\Delta + k\epsilon^2}}\right], \tag{20.5.6}$$

which goes to infinity as $\Delta \to 0$ (and so $E \to V_{\max}$).

The absence of tunneling in the amplitude $\langle x_f, t_f | x_i, t_i \rangle = \langle x_f | U(t_f, t_i) | x_i \rangle$ can also be understood without resorting to path-integral methods. This is the amplitude for a process that starts with a state prepared at a position x_i on one side of the barrier and then is measured to have position x_f on the other side of the barrier at a time $t_f - t_i$ after starting.

But if the initial state really is a *position* eigenstate then the uncertainty principle means that the initial velocity can be anything, and in particular has an overlap with many states with enough energy to classically get over the barrier. Again no tunneling suppression is expected for this type of process.

20.5.2 Navigating the turning points

Both of these arguments also point to the problem in these calculations: tunneling occurs when it is the energy rather than position that is specified in the state. The boundary conditions that should be used are the ones like those in (20.4.9) that are appropriate for amplitudes of energy eigenstates like $\langle x, t|E\rangle$ studied in the previous section, since the boundary conditions required for this amplitude select saddle-point paths with a specified energy E that can be chosen to be below the top of the potential barrier.

A tunneling calculation therefore starts off as in the previous section, with an initial energy eigenstate like $\langle x_i, t_i|E, +\rangle$ such as shown in the semiclassical expression (20.4.10):

$$\langle x_i, t_i|E, +\rangle = \frac{C_+}{\sqrt{p(x_i)}} \exp\left\{\frac{i}{\hbar}\left[-E\,t_i + \int_{x_0}^{x_i} \mathrm{d}u\, p(u)\right]\right\} \tag{20.5.7}$$

with $p(x) = \sqrt{2m[E - V(x)]}$. We imagine that t_i is taken in the remote past, that x_i and x_0 are chosen well to the left of the barrier and that the energy eigenstate is chosen to be moving to the right. We then convolve this with the kernel $\langle x_f, t_f|x_i, t_i\rangle$ to find the form of the wavefunction elsewhere at later times. The previous section did so for positions x_f also to the left of the barrier in order to show how the presence of the classical turning point leads to both incoming and reflected waves.

Tunneling only differs from this by choosing x_f to the right of the barrier, and otherwise the problem is the same: we seek classical saddle points that start off to the left of the barrier moving to the right and ultimately end up to the right of the barrier still moving to the right. As always, the main problem is how to navigate around the classical turning points without leaving the domain of validity of saddle-point methods, and (like in the previous section) the resolution is to reframe the problem with x complex, with the solutions to the equation of motion given by expressions like (20.4.12) (repeated here)

$$t(x) = \sqrt{m} \int_{\mathcal{C}} \frac{\mathrm{d}x}{\sqrt{2[E - V(x)]}}\,. \tag{20.5.8}$$

This allows considerable freedom in the choice of the integration path $\mathcal{C}$, which must only satisfy $x(t_f) = x_f$ and must avoid singular points of the integrand (*i.e.* the classical turning points, which all lie on the real axis).

Imagine doing this in two steps. First convolve with $\langle y, t'|x_i, t_i\rangle$ with y chosen to be real and deep within the classically forbidden region. As discussed above, this is accomplished

using the contour that navigates around the turning point at $x = -a$ as in the right-hand panel of Fig. 19, leading to an expression that is the analog of (20.4.2),

$$\langle y, t'|E, +\rangle \simeq \frac{C}{\sqrt{\mathfrak{p}(y)}} \exp\left[-\frac{1}{\hbar}\int_{-a}^{y} \mathrm{d}u\, \mathfrak{p}(u)\right] e^{-iE\,t'/\hbar}\,, \tag{20.5.9}$$

with $\mathfrak{p}(x) = \sqrt{2m[V(x) - E]}$ and $C_+ = Ce^{i\pi/4}$. It remains to propagate past the right-hand turning point into the classically allowed region to the right of the barrier, and identify which semiclassical contour properly matches onto an outgoing (as opposed to an incoming) solution. As above, the incoming and outgoing solutions in the classically allowed zone can be regarded as lying on opposite sides of a branch cut that runs along the real axis.

We now argue that the required contour again is as in the right-hand panel of Fig. 19, doing so by repeating the steps of the previous section, but keeping track of the fact that for the second turning point the classically allowed region lies to the right rather than the left. To this end the potential is approximated as linear near the turning point at $x = a$, with

$$V(x) \simeq E - \frac{\tilde{b}^2}{2m}(x - a) \qquad \text{with} \qquad \tilde{b}^2 = -2mV'(a) > 0\,. \tag{20.5.10}$$

The exponent of (20.5.9) with this choice becomes

$$-\frac{1}{\hbar}\int_{-a}^{y} \mathrm{d}u\, \mathfrak{p}(u) = -\frac{1}{\hbar}\int_{-a}^{a} \mathrm{d}u\, \mathfrak{p}(u) - \frac{1}{\hbar}\int_{a}^{y} \mathrm{d}u\, \mathfrak{p}(u) = -\frac{1}{\hbar}\int_{-a}^{a} \mathrm{d}u\, \mathfrak{p}(u) + \frac{2\tilde{b}}{3\hbar}(a-y)^{3/2}\,, \tag{20.5.11}$$

and so transitioning to the allowed zone along the contour $y = a - |y - a|\, e^{-i\theta}$ with θ running from 0 to π (as appropriate for the contour in the right-hand panel of Fig. 19) gives the following exponent for $y > a$

$$-\frac{1}{\hbar}\int_{-a}^{a} \mathrm{d}u\, \mathfrak{p}(u) + \frac{2i\tilde{b}}{3\hbar}|y - a|^{3/2} = -\frac{1}{\hbar}\int_{-a}^{a} \mathrm{d}u\, \mathfrak{p}(u) + \frac{i}{\hbar}\int_{a}^{y} \mathrm{d}u\, p(u)\,, \tag{20.5.12}$$

as required to describe the outgoing wave.

The wave-function for $z > a$ at $t = t_f$ found by convolving with $\langle z, t_f|y, t'\rangle$ evaluated with this saddle point therefore becomes (keeping track of the θ-dependence of $\mathfrak{p}^{-1/2}$)

$$\langle z, t_f|E, +\rangle \simeq \frac{C_R}{\sqrt{p(z)}} \exp\left\{\frac{i}{\hbar}\left[-E\,t_f + \int_{a}^{z} \mathrm{d}u\, p(u)\right]\right\}\,, \tag{20.5.13}$$

with

$$C_R = C\, e^{+i\pi/4} \exp\left[-\frac{1}{\hbar}\int_{-a}^{a} \mathrm{d}u\, \mathfrak{p}(u)\right] = C_+ \exp\left[-\frac{1}{\hbar}\int_{-a}^{a} \mathrm{d}u\, \mathfrak{p}(u)\right]\,, \tag{20.5.14}$$

which implies the transmission amplitude

$$T := \frac{C_R}{C_+} = \exp\left[-\frac{1}{\hbar}\int_{-a}^{a} \mathrm{d}u\, \sqrt{2m[V(u) - E]}\right]\,, \tag{20.5.15}$$

in agreement with standard results.

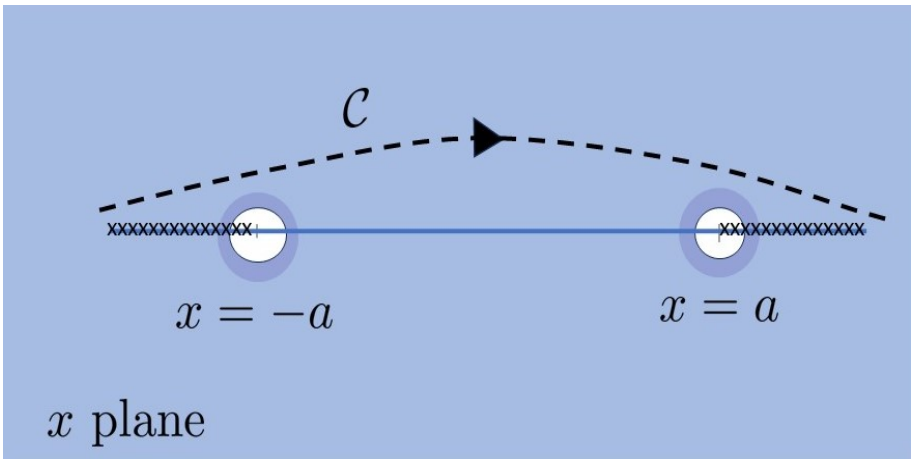

Figure 21. A sketch of an integration contour $\mathcal{C}$ that is deformed in the complex x plane away from the one used to compute the tunneling amplitude (20.5.13). The classical turning points are located at $x = \pm a$ and a branch cut is marked with 'xxx' along the real axis into the classically allowed zones. Trajectories moving to the right lie just above this cut and those moving to the left are just below the cut. The purple circle shows the domain of validity $|x - a| < \ell$ of the linear expansion of V about a turning point and the blue region shows the domain of validity $|x - a| > d$ of the WKB approximation (assuming $d < \ell$).

20.5.3 Imaginary time paths

Although the above is derived using a specific contour $\mathcal{C}$ that hugs the real axis apart from small semicircles near each turning point, it is important to recognize that $\mathcal{C}$ can be deformed away from this so long as the contour doesn't cross the singular points (such as to the contour illustrated in Fig. 21). And once x is complex the time inferred from the classical evolution through equations like (20.5.17)

$$t(x) = \int_{x_i}^{x} \mathrm{d}\overline{x} \sqrt{\frac{m}{2[E - V(\overline{x})]}} \tag{20.5.16}$$

is in general also complex (though becomes real once evaluated at $x = x_f$). Having x and t be complex like this does not cause a problem with physical amplitudes provided that the quantities specified by the amplitude (such as x_f, $t_f - t_i$ and E in $\langle x_f, t_f | E, \pm \rangle$, say) are real. The complex quantities drop out because they ultimately arise only as saddle points within an integral.

Although in general many variables can be extended into the complex plane for saddle-point calculations, for tunneling calculations in field theory there is a very specific type of continuation that is commonly encountered: continuation to imaginary time: $t = i\tau$ (usually with all other quantities kept real).[97] From the present point of view the focus on imaginary

[97] Because $-\mathrm{d}t^2 = +\mathrm{d}\tau^2$ this converts the Minkowski metric with signature $(-,+,+,+)$ to a Euclidean

time comes from expressions like (20.5.15) for tunneling amplitudes that depend only on integrations evaluated through the classically forbidden regime between the classical turning points, evaluated along a contour for which x is real. However, as (20.5.17) shows, the time evaluated along any such a profile

$$t(x) = \int_{-a}^{x} \mathrm{d}u \sqrt{\frac{m}{2[E - V(u)]}} \tag{20.5.17}$$

is then purely imaginary for real $x \in (-a, a)$ because $E < V(u)$.

20.6 Expectation values

Quantum mechanics involves more than the propagation forward of states; it also involves the evaluation of expectation values of operators. This section shows how some classes of expectations also have fairly simple expressions as path integrals.

To start off, consider the following matrix element of a Heisenberg-picture operator $\mathcal{O}[P(t), Q(t)]$, where we choose the ordering convention that all the P's are to the left of all the Q's.[98] In this case the path integral form for the matrix element $\langle q_f, t_f | \mathcal{O}[P(t), Q(t)] \, | q_i, t_i \rangle$ can be constructed exactly as before by integrating over a collection of time slices t_i, with the only difference that we choose one of these time slices to be located at the time t where the operator is evaluated. This choice requires us to replace (20.1.7) with

$$\begin{aligned} \langle q, t + \mathrm{d}t | \mathcal{O}[P(t), Q(t)] \, | \tilde{q}, t \rangle &= \int \mathrm{d}^N p \, \langle q, t | \, e^{-iH(Q,P)\mathrm{d}t} \, | p, t \rangle \, \langle p, t | \mathcal{O}[P(t), Q(t)] \, | \tilde{q}, t \rangle \\ &= \int \frac{\mathrm{d}^N p}{(2\pi)^N} \, e^{-iH(q,p)\mathrm{d}t + ip_b (q - \tilde{q})^b} \mathcal{O}(p, \tilde{q}) \,, \end{aligned} \tag{20.6.1}$$

but otherwise the path-integral derivation goes through exactly as before.

We are led in this way (in the limit of an infinite number of time slices) to the formula

$$\begin{aligned} \langle q_f, t_f | \mathcal{O}[P(t), Q(t)] \, | q_i, t_i \rangle = \int_{q_i}^{q_f} \mathcal{D}q^a(t) \int \mathcal{D}p_b(t) \;\; \mathcal{O}[p(t), q(t)] \\ \times \exp\left\{ i \int_{t_i}^{t_f} \mathrm{d}t \Big[p_a(t) \, \dot{q}^a(t) - H[q(t), p(t)] \Big] \right\} , \end{aligned} \tag{20.6.2}$$

where again $\int \mathcal{D}q^a(t)$ and $\int \mathcal{D}p_a(t)$ denotes *functional* integration over the curves $q^a(t)$ and $p_a(t)$ (that need *not* be related to one another through the classical equations of motion), with the curve $q^a(t)$ again satisfying the boundary condition (20.1.10):

$$q^a(t_i) = q_i^a \qquad \text{and} \qquad q^a(t_f) = q_f^a \,. \tag{20.6.3}$$

metric with signature $(+,+,+,+)$ so the resulting solutions are sometimes called Euclidean solutions. (God help you though if you mistakenly use the $(+,-,-,-)$ metric.)

[98] Notice this is precisely the opposite ordering as was used below eq. (20.1.6) for ordering within the Hamiltonian itself.

The same construction also works for expectation values of the product of many operators $\mathcal{O}_n[P(t_n),Q(t_n)]\cdots\mathcal{O}_1[P(t_1),Q(t_1)]$ *provided that* $t_n > t_{n-1} > \cdots > t_2 > t_1$. When this is true we may choose n of the time-slice points to be situated at t_1, $t_2\cdots,t_n$ and in this way generalize (20.6.2) to

$$\begin{aligned}\langle q_f,t_f|T\Big\{\mathcal{O}_n[P(t_n),Q(t_n)]\cdots\mathcal{O}_1[P(t_1),Q(t_1)]\Big\}|q_i,t_i\rangle \\ = \int_{q_i}^{q_f}\mathcal{D}q^a(t)\int\mathcal{D}p_b(t)\;\mathcal{O}_n[p(t_n),q(t_n)]\cdots\mathcal{O}_1[p(t_1),q(t_1)] \\ \times\exp\left\{i\int_{t_i}^{t_f}\mathrm{d}t\Big[p_a(t)\,\dot{q}^a(t)-H[q(t),p(t)]\Big]\right\},\end{aligned}\tag{20.6.4}$$

where (as in earlier chapters) T denotes the time-ordering operation defined[99] in (3.2.17).

Useful as these expressions are, more often than not expectation values for operators are required in other states (such as energy eigenstates) rather than position eigenstates. We consider next the specific case where the expectation value is taken within a harmonic oscillator ground state, $|\Omega\rangle$, as given in (20.2.39) (repeated here)

$$\langle q,t|\Omega\rangle=\sqrt{\frac{m\,\omega}{\pi}}\;\exp\Big[-\tfrac{1}{2}(m\omega q^2+i\omega t)\Big]\,,\tag{20.6.5}$$

because the result is useful in the field theory discussion of the next section. Multiplying (20.6.4) by $\langle\Omega|q_f,t_f\rangle\,\langle q_i,t_i|\Omega\rangle$ and integrating over $\mathrm{d}q_i$ and $\mathrm{d}q_f$ then gives the path-integral representation

$$\begin{aligned}\langle\Omega|T\Big\{\mathcal{O}_n[P(t_n),Q(t_n)]\cdots\mathcal{O}_1[P(t_1),Q(t_1)]\Big\}|\Omega\rangle \\ = \frac{m\omega}{\pi}\int_{-\infty}^{\infty}\mathrm{d}q_f\,\mathrm{d}q_i\;\exp\Big[-\tfrac{1}{2}m\omega(q_f^2+q_i^2)+\tfrac{i}{2}\omega(t_f-t_i)\Big] \\ \times\int_{q_i}^{q_f}\mathcal{D}q^a(t)\int\mathcal{D}p_b(t)\;\mathcal{O}_n[p(t_n),q(t_n)]\cdots\mathcal{O}_1[p(t_1),q(t_1)] \\ \times\exp\left\{i\int_{t_i}^{t_f}\mathrm{d}t\Big[p_a(t)\,\dot{q}^a(t)-H[q(t),p(t)]\Big]\right\}.\end{aligned}\tag{20.6.6}$$

Now comes the main point: this is more usefully written if the functional integral $\mathcal{D}q^a(t)$ with specified initial and final positions can be combined with the integral over initial and final position to obtain a functional $\mathcal{D}q^a(t)$ integral with unconstrained endpoints. When doing so we also use the identity (exercise: prove it!)

$$f(t_f)+f(t_i)=\lim_{\epsilon\to0^+}\epsilon\int_{t_i}^{t_f}\mathrm{d}t\;f(t)\,e^{-\epsilon|t|}\tag{20.6.7}$$

[99] As discussed in more detail in §21 below, the time-ordering appearing here is really the T^* ordering described in (12.5.17), rather than the naive time ordering (which is a good thing for relativistic applications in quantum field theory).

so that the terms $q_f^2 + q_i^2 = q^2(t_f) + q^2(t_i)$ can be written inside the time integration, leading to the expression

$$\begin{aligned}\langle\Omega|T\Big\{\mathcal{O}_n[P(t_n),Q(t_n)]\cdots\mathcal{O}_1[P(t_1),Q(t_1)]\Big\}|\Omega\rangle \\ = \int \mathcal{D}q^a(t)\int \mathcal{D}p_b(t)\;\mathcal{O}_n[p(t_n),q(t_n)]\cdots\mathcal{O}_1[p(t_1),q(t_1)] \\ \times\exp\left\{i\int_{t_i}^{t_f}\mathrm{d}t\Big[p_a(t)\,\dot{q}^a(t) - (H[q(t),p(t)] - \tfrac{1}{2}\omega) + \tfrac{1}{2}im\omega q^2(t)\,\epsilon e^{-\epsilon|t|}\Big]\right\},\end{aligned} \tag{20.6.8}$$

where the constant factor $m\omega/\pi$ is absorbed into the integration measure and the limit $\epsilon \to 0^+$ is taken at the end of the calculation.

Notice that the last two terms in the exponent of (20.6.8) can be absorbed into the Hamiltonian. For instance, if $H[q,p] = (p^2/2m) + \frac{1}{2}m\omega^2q^2 + V_0$ is the harmonic oscillator Hamiltonian[100] then the new Hamiltonian including the new terms becomes

$$\widetilde{H}(q,p) := \frac{p^2}{2m} + \frac{1}{2}m(\omega - i\delta)^2q^2 + (V_0 - \tfrac{1}{2}\omega)\,, \tag{20.6.9}$$

where $\delta(t) := 2\epsilon\, e^{-\epsilon|t|}$ is an infinitesimal positive quantity for all t that is taken to zero at the end of the calculation.

The final result (20.6.8) is quite simple: the vacuum-to-vacuum matrix element of a collection of time-ordered operators is obtained by performing a functional integral for which initial and final values of p and q are both unconstrained, provided the zero of energy V_0 is appropriately shifted and the oscillator frequency is regarded as having an infinitesimal negative imaginary part that is taken to zero at the end of the calculation. This formulation is very useful when computing these types of matrix elements in field theory, for which the Hamiltonian resembles a harmonic oscillator for sufficiently weak couplings.

21 Path integrals for fields

This section extends the path integral discussion of the previous chapter to quantum fields. At one level this is very simple to do to the extent that (appropriately regulated) quantum fields are just the quantum mechanics of a very large but finite number of degrees of freedom. The goal is to arrive at a framework that is much more convenient to work with (for some purposes) than are the operator calculations used in the rest of these notes.

21.1 Scalar fields

Relativistic scalar fields are a good starting point: they are the simplest relativistic fields but also are complicated enough to illustrate the relative simplicity of path-integral methods.

[100] This is the Hamiltonian of (20.2.21) after using $k = m\omega^2$ and adding an arbitrary constant V_0 to the energy.

Regarded as a quantum mechanical system a scalar field $\phi(\mathbf{x},t)$ corresponds to the quantum variable $Q^a(t)$ where a should be thought of as running over all possible positions $\mathbf{x}$. With this identification all sums over a become integrations over $\mathbf{x}$.

Following the discussion of §13, we take the lagrangian for a real scalar field to be

$$L = -\int \mathrm{d}^3x \Big[\tfrac{1}{2}\,\partial_\mu\Phi\,\partial^\mu\Phi + V(\Phi)\Big] = \int \mathrm{d}^3x \Big[\tfrac{1}{2}\,\dot\Phi^2 - \tfrac{1}{2}(\nabla\Phi)^2 - V(\Phi)\Big] \tag{21.1.1}$$

where $\dot\Phi := \partial_t\Phi$ and for much of the discussion to follow the form of the potential $V(\Phi)$ can be left arbitrary. The canonical momentum is then defined by

$$\Pi(\mathbf{x},t) := \frac{\delta L}{\delta\dot\Phi(\mathbf{x},t)} = \frac{\partial\mathcal{L}}{\partial\dot\Phi(\mathbf{x},t)} = \dot\Phi\,, \tag{21.1.2}$$

where $L = \int \mathrm{d}^3x\,\mathcal{L}$ defines the lagrangian density $\mathcal{L}$. The Hamiltonian then becomes the local quantity $H = \int \mathrm{d}^3x\,\mathcal{H}$ with

$$\mathcal{H}(\Phi,\Pi) = \Pi(\mathbf{x},t)\,\dot\Phi(\mathbf{x},t) - \mathcal{L} = \tfrac{1}{2}\Pi^2 + \tfrac{1}{2}(\nabla\Phi)^2 + V(\Phi)\,. \tag{21.1.3}$$

The fields are time dependent because we work in the Heisenberg picture, for which the usual equal-time commutation relations in this case are

$$[\Phi(\mathbf{x},t)\,,\Pi(\mathbf{y},t)] = i\,\delta^3(\mathbf{x}-\mathbf{y})\,. \tag{21.1.4}$$

The field eigenvalues and eigenvectors are similarly denoted

$$\Phi(\mathbf{x},t)\,|\phi(\mathbf{x}),t\rangle = \phi(\mathbf{x},t)\,|\phi(\mathbf{x}),t\rangle \qquad \text{and} \qquad \Pi(\mathbf{x},t)\,|\mathfrak{p}(\mathbf{x}),t\rangle = \mathfrak{p}(\mathbf{x},t)\,|\mathfrak{p}(\mathbf{x}),t\rangle\,, \tag{21.1.5}$$

though to avoid notational clutter in what follows we write $|\phi(\mathbf{x}),t\rangle$ as $|\{\phi\},t\rangle$.

21.1.1 Path integral construction

The path integral construction now follows very closely the development in §20.1. Standard arguments ensure that (21.1.4) implies

$$\langle\{\phi\},t|\{\mathfrak{p}\},t\rangle = \mathcal{N}\,\exp\left[i\int \mathrm{d}^3x\;\phi(\mathbf{x},t)\,\mathfrak{p}(\mathbf{x},t)\right]\,, \tag{21.1.6}$$

where $\mathcal{N}$ is a field-independent normalization constant. Repeating earlier steps shows that for infinitesimal time differences $t' = t + \mathrm{d}t$ we have

$$\begin{aligned}\langle\{\phi\},t+\mathrm{d}t|\{\mathfrak{p}\},t\rangle &= \langle\{\phi\},t|\,e^{-iH(\Phi,\Pi)\mathrm{d}t}\,|\{\mathfrak{p}\},t\rangle \\ &= \mathcal{N}\,\exp\left\{i\int \mathrm{d}^3x\Big[\phi\,\mathfrak{p} - \mathcal{H}(\phi,\mathfrak{p})\,\mathrm{d}t\Big]\right\}\,,\end{aligned} \tag{21.1.7}$$

where the fields in the final equality are all evaluated at spacetime position $(\mathbf{x},t)$.

Conversion to initial field eigenstates is done as in (20.1.7) though the required momentum integral must be separately performed at each spatial position; which is to say that it becomes a functional integral over all possible configurations $\mathfrak{p}(\mathbf{x})$:

$$\begin{aligned}\langle\{\phi\},t+\mathrm{d}t|\{\tilde{\phi}\},t\rangle &= \int \mathcal{D}\mathfrak{p}(\mathbf{x})\ \langle\{\phi\},t|\,e^{-iH(\Phi,\Pi)\mathrm{d}t}\,|\{\mathfrak{p}\},t\rangle\,\langle\{\mathfrak{p}\},t|\{\tilde{\phi}\},t\rangle \\ &= \int \mathcal{D}\mathfrak{p}(\mathbf{x})\ \exp\left\{i\int \mathrm{d}^3x\Big[\mathfrak{p}(\phi-\tilde{\phi})-\mathcal{H}(\phi,\mathfrak{p})\mathrm{d}t\Big]\right\}. \qquad (21.1.8)\end{aligned}$$

This process is repeated for other time steps obtained by dividing the finite time difference $T := t_f - t_i > 0$ into a series of times, t_k, spaced by a short interval of width $\mathrm{d}t$ and integrating over all possible field configurations $\phi(\mathbf{x},t_k)$ for each intermediate step.

In the limit of an infinite number of steps this leads to the analog of (20.1.9):

$$\begin{aligned}&\langle\{\phi_f\},t_f|\{\phi_i\},t_i\rangle \qquad (21.1.9)\\ &\quad= \int_{\phi_i}^{\phi_f}\mathcal{D}\phi(\mathbf{x},t)\int\mathcal{D}\mathfrak{p}(\mathbf{x},t)\ \exp\left\{i\int_{t_i}^{t_f}\mathrm{d}t\,\mathrm{d}^3x\Big[\mathfrak{p}(\mathbf{x},t)\,\dot{\phi}(\mathbf{x},t)-\mathcal{H}[\phi(\mathbf{x},t),\mathfrak{p}(\mathbf{x},t)]\Big]\right\},\end{aligned}$$

where now the functional integral is over all field configurations in space and time, subject to the temporal boundary conditions

$$\phi(\mathbf{x},t_i)=\phi_i(\mathbf{x}) \qquad \text{and} \qquad \phi(\mathbf{x},t_f)=\phi_f(\mathbf{x})\,, \qquad (21.1.10)$$

while all values of $\mathfrak{p}(\mathbf{x},t_f)$ and $\mathfrak{p}(\mathbf{x},t_i)$ are integrated over.

Because the functional integral is over all functions of position and time it becomes an integral over all functions $\phi(x)$ of spacetime position $x^\mu = (\mathbf{x},t)$. To avoid notational clutter the functional integral measure is from here on just denoted $\mathcal{D}\phi$ rather than $\mathcal{D}\phi(x)$ or $\mathcal{D}\phi(\mathbf{x},t)$.

21.1.2 Integrating out the momenta

For this particular system the Hamiltonian (21.1.3) is quadratic in the momenta $\Pi(\mathbf{x},t)$ and so the momenta can be explicitly integrated out, following the steps of §20.1.2.

The functional integral to be evaluated is

$$J := \int \mathcal{D}\mathfrak{p}(x)\ \exp\left\{i\int_{t_i}^{t_f}\mathrm{d}^4x\Big[\mathfrak{p}\dot{\phi}-\tfrac{1}{2}\,\mathfrak{p}^2-\tfrac{1}{2}(\nabla\phi)^2-V(\phi)\Big]\right\}, \qquad (21.1.11)$$

which is gaussian and so can be evaluated using the arguments of §20.1.1. The saddle point of the exponent is in this case given by $\overline{\mathfrak{p}}(x)=\dot{\phi}(x)$ and so the functional integral evaluates to

$$J = K\exp\left\{i\int_{t_i}^{t_f}\mathrm{d}^4x\,\Big[\tfrac{1}{2}\dot{\phi}^2(x)-\tfrac{1}{2}(\nabla\phi)^2-V(\phi)\Big]\right\}, \qquad (21.1.12)$$

where K is a constant to be determined later (if needed). We are led in this way to the following updated version of (20.1.11):

$$\begin{aligned}\langle\{\phi_f\},t_f|\{\phi_i\},t_i\rangle &= \int_{\phi_i}^{\phi_f}\mathcal{D}\phi(\mathbf{x},t)\ \exp\left\{-i\int_{t_i}^{t_f}\mathrm{d}^4x\left[\tfrac{1}{2}\partial_\mu\phi\,\partial^\mu\phi+V(\phi)\right]\right\}\\ &= \int_{\phi_i}^{\phi_f}\mathcal{D}\phi(\mathbf{x},t)\ \exp\left\{i\int_{t_i}^{t_f}\mathrm{d}^4x\,\mathcal{L}(\phi,\dot\phi)\right\}\,,\end{aligned}\tag{21.1.13}$$

where the constant K is again absorbed into the definition of the measure and the last equality recognizes the integrand as the relativistic Klein-Gordon lagrangian density (21.1.1).

It is here that we begin to reap the rewards of path-integral quantization. Eq. (21.1.13) is very attractive as a starting point for subsequent calculations because it gives the time evolution purely in terms of the *Lagrangian density* rather than the Hamiltonian. As a result the conditions required for invariance under the Lorentz transformations of special relativity are much more transparent, because this only demands that $\mathcal{L}$ transform like a scalar field. This is to be contrasted with the more complicated transformation properties of the Hamiltonian and Hamiltonian density that were found in earlier sections – see the discussion in §12.5, §13.4 and §16.1 for example – and yet were still consistent with the Lorentz-invariance of the S-matrix.

21.1.3 Time-ordered correlators

A final step is required before real calculations can begin because our interest is usually in time-ordered correlation functions evaluated in the vacuum, as opposed to transition amplitudes between field eigenstates. To fix this we next repeat the steps of §20.6 to identify the path integral representation for time-ordered correlators.

The first step is to evaluate expectations of operators, and repeating the arguments leading to (20.6.4) leads to the useful formula

$$\begin{aligned}&\langle\{\phi_f\},t_f|T\Big\{\mathcal{O}_n[\Phi(x_n)]\cdots\mathcal{O}_1[\Phi(x_1)]\Big\}|\{\phi_i\},t_i\rangle\\ &\qquad=\int_{\phi_i}^{\phi_f}\mathcal{D}\phi(x)\ \mathcal{O}_n[\phi(x_n)]\cdots\mathcal{O}_1[\phi(x_1)]\exp\left\{i\int_{t_i}^{t_f}\mathrm{d}^4x\ \mathcal{L}(\phi)\right\}\,,\end{aligned}\tag{21.1.14}$$

where again $\mathcal{L}(\phi)$ is as given in (21.1.13) and the functional integration is over all field configurations $\phi(x)$ satisfying the boundary condition (21.1.10):

$$\phi(\mathbf{x},t_i)=\phi_i(\mathbf{x})\qquad\text{and}\qquad\phi(\mathbf{x},t_f)=\phi_f(\mathbf{x})\,.\tag{21.1.15}$$

It is here that we see the second benefit of path-integral methods (from the point of view of relativistic systems). Notice that the path-integral representation shows that the time-ordering appearing in expressions like (21.1.14) explicitly commute with differentiation,

in the sense that it implies for instance

$$\begin{aligned}\langle\{\phi_f\},t_f|T\Big\{\partial_\mu\Phi(x_2)\,\partial_\nu\Phi(x_1)\Big\}|\{\phi_i\},t_i\rangle \qquad (21.1.16)\\ &= \int_{\phi_i}^{\phi_f}\mathcal{D}\phi(x)\;\partial_\mu\phi(x_2)\,\partial_\nu\phi(x_1)\exp\left\{i\int_{t_i}^{t_f}\mathrm{d}^4x\;\mathcal{L}(\phi)\right\}\\ &= \langle\{\phi_f\},t_f|\frac{\partial^2}{\partial x_2^\mu\partial x_1^\nu}\,T\Big\{\Phi(x_2)\,\Phi(x_1)\Big\}|\{\phi_i\},t_i\rangle\,.\end{aligned}$$

As is discussed at some length in §12.5, this property is *not* true for the naive time-ordering operation as defined in (3.2.17), since it omits the Lorentz-noncovariant local Schwinger terms like those appearing in (12.5.10) or (12.5.12). Instead we see that the path integral directly gives the manifestly Lorentz covariant T^* time ordering defined in (12.5.17) that drops these terms.

An audacious claim made in §12.5 now sounds much more plausible. §12.5 argued that non-covariant Schwinger terms coming from naive time ordering systematically cancel non-covariant terms in the Hamiltonian to leave a covariant perturbative series that is 'as if' $\mathcal{H}_{\rm int} = -\mathcal{L}_{\rm int}$ and all time ordering were covariant T^* orderings. The path integral derivation of the perturbative expansion makes this more transparent because the path integral itself (for the theories of interest) only explicitly involves the lagrangian and the T^* product from the get-go.

21.2 Vacuum state and Feynman boundary conditions

There is one more step required to obtain path-integral representations for the time-ordered products arising in earlier chapters when perturbatively evaluating scattering amplitudes: we must convolve expressions like (21.1.14) with the vacuum wave-functional, $\Psi_v[\phi,t] = \langle\{\phi\},t|\Omega\rangle$, describing the field's ground state (evaluated at $t=t_i$ and $t=t_f$) and then take the limits $t_f\to\infty$ and $t_i\to-\infty$. We perform this convolution here following the procedures followed in §20.6.

For perturbative scattering calculations the wave-functional required in the remote past is the one for the free no-particle state $|0\rangle$ that agrees with the ground state $|\Omega,\text{in}\rangle\!\rangle$ – *c.f.* eq. (3.3.5) – in the limit $t_i\to-\infty$. And in the remote future it is the free no-particle state $\langle 0|$ that agrees with $\langle\!\langle\Omega,\text{out}|$ – *c.f.* eq. (3.3.6) – in the limit $t_f\to\infty$. The good news is that these are the no-particle states for the free fields at these times, and so – as described all the way back in §2 – are defined by the condition $\mathfrak{a}^{\rm in}_{\mathbf{p}}|0\rangle = 0$ and $\langle 0|\mathfrak{a}^{\rm out\,\star}_{\mathbf{p}} = 0$ where $\mathfrak{a}_{\mathbf{p}}$ is the appropriate particle destruction operator.

For free real scalar fields the relation between $\Phi(\mathbf{x},t)$, $\Pi(\mathbf{x},t)$ and $\mathfrak{a}_{\mathbf{p}}$ is given by expres-

sions like (12.1.8), which state

$$\Phi(x) = \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \Big[\mathfrak{a}_{\mathbf{p}}\, e^{ip\cdot x} + \mathfrak{a}^\star_{\mathbf{p}}\, e^{-ip\cdot x} \Big] \tag{21.2.1}$$
$$\Pi(x) = \partial_t \Phi(x) = \int \frac{\mathrm{d}^3p}{\sqrt{(2\pi)^3 2\varepsilon(p)}} \Big[-i\varepsilon(p)\, \mathfrak{a}_{\mathbf{p}}\, e^{ip\cdot x} + i\varepsilon(p)\, \bar{\mathfrak{a}}^\star_{\mathbf{p}}\, e^{-ip\cdot x} \Big] ,$$

where $\varepsilon(p) = \sqrt{p^2 + m^2}$ is the asymptotic free-particle energy. These can be solved to give $\mathfrak{a}_{\mathbf{p}}$ as a function of Φ and Π:

$$\mathfrak{a}_{\mathbf{p}} = e^{i\varepsilon(p)t} \int \frac{\mathrm{d}^3x}{\sqrt{(2\pi)^3 2\varepsilon(p)}}\, e^{-i\mathbf{p}\cdot\mathbf{x}} \Big[\varepsilon(p)\, \Phi(\mathbf{x},t) + i\Pi(\mathbf{x},t) \Big] . \tag{21.2.2}$$

The free vacuum wave-functional is then obtained in the field eigenbasis in the same way that the harmonic oscillator wave-function is obtained in the position basis, by representing

$$\Phi(\mathbf{x}) \to \phi(\mathbf{x}) \qquad \text{and} \qquad i\Pi(\mathbf{x}) \to \frac{\delta}{\delta\phi(\mathbf{x})} . \tag{21.2.3}$$

The condition $\mathfrak{a}_{\mathbf{p}}|0\rangle = 0$ then implies the vacuum wave-functional $\Psi_v[\phi(\mathbf{x})] = \langle\{\phi\}|0\rangle$ must satisfy

$$\int \mathrm{d}^3x\, e^{-i\mathbf{p}\cdot\mathbf{x}} \left[\frac{\delta\Psi_v}{\delta\phi(\mathbf{x})} + \varepsilon(p)\, \phi(\mathbf{x})\, \Psi_v \right] = 0 , \tag{21.2.4}$$

and (because we know how things work for the simple harmonic oscillator) this can be solved by making a gaussian ansatz

$$\Psi_v[\phi(\mathbf{x})] = \mathcal{N} \exp\left\{ -\tfrac{1}{2} \int \mathrm{d}^3x \int \mathrm{d}^3y\, \mathcal{K}(\mathbf{x},\mathbf{y})\, \phi(\mathbf{x})\, \phi(\mathbf{y}) \right\} , \tag{21.2.5}$$

and substituting this into (21.2.4). The result is a condition on $\mathcal{K}(\mathbf{x},\mathbf{y})$ whose solution is

$$\mathcal{K}(\mathbf{x},\mathbf{y}) = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\, \varepsilon(p)\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} . \tag{21.2.6}$$

From here on the steps precisely follow those leading up to (20.6.8) in §20.6. These lead to

$$\begin{aligned} &\langle\Omega,\mathrm{out}|T\Big\{\mathcal{O}_n[\Phi(x_n)]\cdots\mathcal{O}_1[\Phi(x_1)]\Big\}|\Omega,\mathrm{in}\rangle \\ &\quad = \int \mathcal{D}\phi(x)\; \mathcal{O}_n[\phi(x_n)]\cdots\mathcal{O}_1[\phi(x_1)]\; \exp\left\{ i\int_{-\infty}^{\infty}\mathrm{d}t \left[\int \mathrm{d}^3x\, \mathcal{L}(\phi) \right.\right. \\ &\qquad\qquad \left.\left. +\tfrac{1}{2}i\epsilon \int \mathrm{d}^3x \int \mathrm{d}^3y\, \mathcal{K}(\mathbf{x},\mathbf{y})\, \phi(\mathbf{x},t)\, \phi(\mathbf{y},t)\, e^{-\epsilon|t|} \right] \right\} , \end{aligned} \tag{21.2.7}$$

where constant overall factors are absorbed into the integration measure and the limit $\epsilon \to 0^+$ is taken at the end of the calculation. The vacuum wave-functional is here put inside the time integral using the identity (20.6.7), giving the last term in the exponent of (21.2.7).

As we shall see, this last term eventually turns into the small imaginary part in the particle mass, $m^2 \to m^2 - i\delta$, appearing in the integrand for Feynman propagators for fields (such as encountered in (12.4.16), (15.7.15) and (16.2.10)). To see how this happens notice that for a free lagrangian – where $\mathcal{L}(\phi) = -\frac{1}{2}(\partial_\mu\phi\,\partial^\mu\phi + m^2\phi^2)$ – the momentum space version of the exponent in (21.2.7) is

$$-\tfrac{1}{2}\int \mathrm{d}^3x(\partial_\mu\phi\,\partial^\mu\phi + m^2\phi^2) + \tfrac{1}{2}i\epsilon\int \mathrm{d}^3x\int \mathrm{d}^3y\;\mathcal{K}(\mathbf{x},\mathbf{y})\,\phi(\mathbf{x},t)\,\phi(\mathbf{y},t)\,e^{-\epsilon|t|} \qquad (21.2.8)$$
$$= -\tfrac{1}{2}\int \frac{\mathrm{d}^3p}{(2\pi)^3}\Big[p^2 + m^2 - i\epsilon\,\varepsilon(p)\,e^{-\epsilon|t|}\Big]\tilde{\phi}(\mathbf{p},t)\,\tilde{\phi}(-\mathbf{p},t)\,,$$

in which we use the definition

$$\phi(\mathbf{x},t) = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\,\tilde{\phi}(\mathbf{p},t)\,e^{i\mathbf{p}\cdot\mathbf{x}}\,, \qquad (21.2.9)$$

together with (21.2.6). This shows that the combination $\epsilon\,\varepsilon(p)\,e^{-\epsilon|t|}$ plays the same role as δ: it is a strictly positive infinitesimal that gives a small negative imaginary part to the particle mass that is ultimately taken to zero at the end of the calculation.

21.3 Perturbative methods

We are now in a position to set up the path-integral version of the perturbative calculation of scattering matrix elements for a self-interacting real scalar field, for which we take the lagrangian (21.1.1) with $V(\phi)$ not purely quadratic in the field. We assume $V(\phi)$ is bounded from below and has a minimum for some $\phi = \phi_0$. It is convenient to shift the field $\phi \to \phi - \phi_0$ so that the new variable vanishes at the minimum, so

$$V(\phi) = V_0 + \tfrac{1}{2}m^2\phi^2 + \tfrac{1}{3}g\phi^3 + \tfrac{1}{4}\lambda\phi^4 + \cdots\,. \qquad (21.3.1)$$

In this case the lagrangian density can be expanded in powers of ϕ with

$$-\mathcal{L} = V_0 + \tfrac{1}{2}\,\partial_\mu\phi\,\partial^\mu\phi + \tfrac{1}{2}\,m^2\phi^2 + \tfrac{1}{3}g\phi^3 + \tfrac{1}{4}\lambda\phi^4 + \cdots\,, \qquad (21.3.2)$$

and so the action can be split into an 'unperturbed' part (containing all terms with two powers of ϕ or less) and an 'interaction' part (including all cubic and higher terms): $S[\phi] = S_0[\phi] + S_{\text{int}}[\phi]$ with

$$S_0[\phi] = -\int \mathrm{d}^4x\Big[V_0 + \tfrac{1}{2}\,\partial_\mu\phi\,\partial^\mu\phi + \tfrac{1}{2}\,m^2\phi^2\Big]$$
$$\text{and}\qquad S_{\text{int}} = -\int \mathrm{d}^4x\Big[\tfrac{1}{3}g\phi^3 + \tfrac{1}{4}\lambda\phi^4 + \cdots\Big]\,. \qquad (21.3.3)$$

The idea is to compute correlation functions and transition amplitudes within the saddle-point approximation wherein the functional integrand is expanded in the (assumed small) non-quadratic interactions contained in S_{int}.

21.4 Fermions

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21.5 Electromagnetism

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21.6 Generating functionals

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21.7 Integrating out heavy degrees of freedom

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A Refreshers on useful tools

This appendix gathers together some topics that are normally seen in a physics program but which might need refreshing for this course.

A.1 Fundamental units

This appendix collects together a list of useful conversions between conventional units and fundamental units (with energies measured in eV).

1. Length and Time

$1/M_p\ (= G/\hbar c)^{\frac{1}{2}}$	=	8.1897×10^{-29}	c^2/eV	=	1.6161×10^{-35}	m$c/\hbar$
$1/m_p$	=	1.0658×10^{-9}	c^2/eV	=	2.1031×10^{-16}	m$c/\hbar$
1 fm	=	5.06773×10^{-9}	$\hbar c$/eV	=	$\cdot 10^{-15}$	m
$1/m_e$	=	1.957×10^{-6}	c^2/eV	=	3.8616×10^{-13}	m$c/\hbar$
$a_0\ (= 1/\alpha m_e)$	=	2.6818×10^{-4}	c^2/eV	=	5.2918×10^{-11}	m$c/\hbar$
1 A	=	5.06773×10^{-4}	$\hbar c$/eV	=	$\cdot 10^{-10}$	m
1 nm	=	5.06773×10^{-3}	$\hbar c$/eV	=	$\cdot 10^{-9}$	m
1 μm	=	5.06773	$\hbar c$/eV	=	$\cdot 10^{-6}$	m
1 cm	=	5.06773×10^{4}	$\hbar c$/eV	=	0.01	m
1 m	=	5.06773×10^{6}	$\hbar c$/eV	=	1	m
1 km	=	5.06773×10^{9}	$\hbar c$/eV	=	$\cdot 10^{3}$	m
1 sec	=	1.51927×10^{15}	$\hbar$/eV	=	2.99792×10^{8}	m/c
1 min	=	9.11562×10^{16}	$\hbar$/eV	=	1.79875×10^{10}	m/c
1 hr	=	5.46937×10^{18}	$\hbar$/eV	=	1.07925×10^{12}	m/c
1 day	=	1.31265×10^{20}	$\hbar$/eV	=	2.59020×10^{13}	m/c
1 yr	=	4.795×10^{22}	$\hbar$/eV	=	9.461×10^{15}	m/c
1 pc	=	1.564×10^{23}	$\hbar c$/eV	=	3.08568×10^{16}	m
1 kpc	=	1.564×10^{26}	$\hbar c$/eV	=	3.08568×10^{19}	m
1 Mpc	=	1.564×10^{29}	$\hbar c$/eV	=	3.08568×10^{22}	m

2. Microscopic Energy and Mass

1 eV	=	$\cdot 10^{-9}$	GeV	=	5.06773×10^{6} $\hbar c/\mathrm{m}$
1 keV	=	$\cdot 10^{-6}$	GeV	=	5.06773×10^{9} $\hbar c/\mathrm{m}$
1 MeV	=	$\cdot 10^{-3}$	GeV	=	5.06773×10^{12} $\hbar c/\mathrm{m}$
1 GeV	=	1	GeV	=	5.06773×10^{15} $\hbar c/\mathrm{m}$
αm_e	=	3.7289×10^{-6}	GeV/c^2	=	1.8897×10^{10} $\hbar/\mathrm{m}c$
m_e	=	5.10999×10^{-4}	GeV/c^2	=	2.5896×10^{12} $\hbar/\mathrm{m}c$
	=	9.10939×10^{-28}	g		
m_p	=	0.938272	GeV/c^2	=	4.75491×10^{15} $\hbar/\mathrm{m}c$
	=	1.67262×10^{-24}	g		
	=	1.83615×10^{3}	m_e		
$M_p = (\hbar c/G)^{\frac{1}{2}}$	=	1.22105×10^{19}	GeV/c^2	=	6.1879×10^{34} $\hbar/\mathrm{m}c$
	=	2.17671×10^{-5}	g		
	=	1.30138×10^{19}	m_p		
$\hat{M}_p = (\hbar c/8\pi G)^{\frac{1}{2}}$	=	2.43564×10^{18}	GeV/c^2	=	1.23431×10^{34} $\hbar/\mathrm{m}c$
	=	4.34191×10^{-6}	g		
	=	2.59588×10^{18}	m_p		

3. Ordinary Units Expressed Microscopically

1 g	=	5.60959×10^{23}	GeV/c^2	=	2.84279×10^{39}	$\hbar$/mc
1 kg	=	5.60959×10^{26}	GeV/c^2	=	2.84279×10^{42}	$\hbar$/mc
1 Joule = 1 kg m^2/s^2	=	6.24151×10^{9}	GeV	=	3.16303×10^{25}	$\hbar c$/m
1 erg = 1 g cm^2/s^2	=	6.24151×10^{2}	GeV	=	3.16303×10^{18}	$\hbar c$/m
$= \cdot 10^{-7}$ J						
1 Newton = 1 kg m/s^2	=	1.23162×10^{-6}	GeV$^2/\hbar c$	=	3.16303×10^{25}	$\hbar c$/m^2
	=	1.23162×10^{12}	eV$^2/\hbar c$			
1 dyne = 1 g cm/s^2	=	1.23162×10^{-11}	GeV$^2/\hbar c$	=	3.16303×10^{20}	$\hbar c$/m^2
$= \cdot 10^{-5}$ N	=	1.23162×10^{7}	eV$^2/\hbar c$			
1 Watt = 1 J/s	=	4.10824×10^{-15}	GeV$^2/\hbar$	=	1.05507×10^{17}	$\hbar c^2$/m^2
	=	4.10824×10^{3}	eV$^2/\hbar$			
1 Hz = 1/s	=	6.5821×10^{-25}	GeV/$\hbar$	=	3.3356×10^{-9}	c/m
1 Kelvin	=	8.61742×10^{-14}	GeV/k_B	=	4.36707×10^{2}	$\hbar c$/mk_B
	=	8.61742×10^{-5}	eV/k_B	=	1/11604.4	eV/k_B

4. Electromagnetic Units

1 Coulomb	=	6.24151×10^{18}	e			
1 Volt = 1 J/C	=	1	eV/e	=	5.06773×10^{6}	$\hbar c$/me
	=	$\cdot 10^{-9}$	GeV/e			
1 Farad = 1 C/V	=	6.24151×10^{18}	e^2/eV	=	1.23162×10^{12}	m$e^2/\hbar c$
1 Ampere = 1 C/s	=	4.10824×10^{3}	eV$e/\hbar$	=	2.08194×10^{10}	ec/m
1 Ohm = 1 V/A	=	2.43413×10^{-4}	$\hbar/e^2$			
1 Mho = 1/Ohm	=	4.10824×10^{3}	$e^2/\hbar$			
1 Weber = 1 V s	=	1.51927×10^{15}	$\hbar/e$			
1 Tesla = 1 Weber/m^2	=	59.1572	eV$^2/\hbar ec^2$	=	1.51927×10^{15}	$\hbar/e$m^2
1 Gauss = $\cdot 10^{-4}$ Tesla	=	5.91572×10^{-3}	eV$^2/\hbar ec^2$	=	1.51927×10^{11}	$\hbar/e$m^2
$\phi_0 = 2\pi\hbar/e$	=	6.28319	$\hbar/e$	=	4.13567×10^{-15}	Weber
				=	$1/(2.418 \times 10^{14}\ )$	Weber
$\epsilon_0 = 8.854 \times 10^{-12}$ F/m	=	10.905	$e^2/\hbar c$			
$\mu_0 = 4\pi \times 10^{-7}$ N/A^2	=	0.0917012	$\hbar/ce^2$		$\epsilon_0\mu_0 = 1/c^2$	
$\alpha = e^2/(4\pi\epsilon_0\hbar c)$	=	7.2974×10^{-3}			$1/\alpha = 137.036$	

A.2 Method of Lagrange multipliers

Suppose one wishes to minimize or maximize a function $h(x, y)$ of two independent variables, x and y. This is relatively easy to do, by finding those $x = x_m$ and $y = y_m$ that make the partial derivatives of h vanish:

$$\left(\frac{\partial h}{\partial x}\right)_{x_m,y_m} = \left(\frac{\partial h}{\partial y}\right)_{x_m,y_m} = 0\,. \tag{A.2.1}$$

For instance suppose x and y locally describe local coordinates for the surface of the earth and $h(x, y)$ describes the local height of the terrain for some part of the earth's surface. Then x_m and y_m might pick out the highest and lowest points of the terrain in the local area.

A more complicated problem is to minimize h subject to a constraint that relates x and y. For instance, suppose a road crosses the terrain with a route described by the curve $c(x, y) = 0$ for some function $c(x, y)$. Then a constrained problem might ask for the highest or lowest point of the terrain that is encountered by someone who moves only along this road. This is not necessarily found by (A.2.1) unless x_m and y_m happen by chance also to satisfy $c(x_m, y_m) = 0$.

In principle this constrained problem can be solved by solving the constraint $c(x, y) = 0$ to find the function $y = \mathfrak{y}(x)$ that satisfies $c(x, \mathfrak{y}(x)) \equiv 0$ as an identity for all x. For instance if $c(x, y) = x^2 + y^2 - 1$ then the constraint $c(x, y) = 0$ implies $x^2 + y^2 = 1$, a condition solved by $y = \mathfrak{y}(x) = \pm\sqrt{1 - x^2}$. Once this constraint is solved then evaluating $h(x, y)$ along this curve gives a function of the single independent variable x: $\mathfrak{h}(x) := h(x, \mathfrak{y}(x))$ that expresses the values for $h(x, y)$ seen along the curve. The minima of $\mathfrak{h}(x)$ are then found (as usual) by setting to zero the derivative of h restricted to lie along this curve:

$$\left(\frac{\mathrm{d}\mathfrak{h}(x)}{\mathrm{d}x}\right)_{x_c} = \left(\frac{\partial h}{\partial x}\right)_{x_c,\mathfrak{y}(x_c)} + \left(\frac{\mathrm{d}\mathfrak{y}}{\mathrm{d}x}\right)_{x_c} \left(\frac{\partial h}{\partial y}\right)_{x_c,\mathfrak{y}(x_c)} = 0\,. \tag{A.2.2}$$

The method of lagrange multipliers is just a simpler way to obtain x_c without having to explicitly solve for the curve $y = \mathfrak{y}(x)$. The idea is instead to minimize the quantity

$$f(x, y, \lambda) := h(x, y) + \lambda\, c(x, y) \tag{A.2.3}$$

with respect to all three independent variables x, y and λ. This leads to the following three equations:

$$\frac{\partial f}{\partial x} = \frac{\partial h}{\partial x} + \lambda\frac{\partial c}{\partial x} = 0\,, \quad \frac{\partial f}{\partial y} = \frac{\partial h}{\partial y} + \lambda\frac{\partial c}{\partial y} = 0 \quad \text{and} \quad \frac{\partial f}{\partial \lambda} = c = 0\,, \tag{A.2.4}$$

whose solutions can be denoted x_l, y_l and λ_l. Lagrange's claim is that (x_l, y_l) coincide with (x_c, y_c) and so the solutions to (A.2.4) agree with those of (A.2.2).

To see why this is so first notice that the third equation in (A.2.4) states that $c(x_l, y_l) = 0$ and so $y_l = \mathfrak{y}(x_l)$ lies on the constraint curve. Next, notice that the derivative of $\mathfrak{y}(x)$ is related

to those of $c(x, y)$, using the fact that $c(x, \mathfrak{y}(x)) \equiv 0$ is an identity for all x, and so remains true once differentiated. Differentiating this with respect to x using the chain rule leads to the conclusion (also true for all x)

$$\frac{\partial c}{\partial x} + \frac{\partial c}{\partial y}\frac{\mathrm{d}\mathfrak{y}}{\mathrm{d}x} = 0 \quad \text{and so} \quad \left(\frac{\mathrm{d}\mathfrak{y}}{\mathrm{d}x}\right)_{x_l} = -\left(\frac{\partial c/\partial x}{\partial c/\partial y}\right)_{x_l,y_l} . \tag{A.2.5}$$

Finally taking the following linear combination of the first two equations of (A.2.4) and using (A.2.5) leads to the inference

$$\begin{aligned} 0 &= \left(\frac{\partial f}{\partial x}\right)_{x_l,y_l,\lambda_l} + \left(\frac{\mathrm{d}\mathfrak{y}}{\mathrm{d}x}\right)_{x_l}\left(\frac{\partial f}{\partial y}\right)_{x_l,y_l,\lambda_l} \\ &= \left(\frac{\partial f}{\partial x}\right)_{x_l,y_l,\lambda_l} - \left(\frac{\partial c/\partial x}{\partial c/\partial y}\right)_{x_l,y_l,\lambda_l}\left(\frac{\partial f}{\partial y}\right)_{x_l,y_l,\lambda_l} \\ &= \left(\frac{\partial h}{\partial x} + \lambda\frac{\partial c}{\partial x}\right)_{x_l,y_l,\lambda_l} - \left(\frac{\partial c/\partial x}{\partial c/\partial y}\right)_{x_l,y_l,\lambda_l}\left(\frac{\partial h}{\partial y} + \lambda\frac{\partial c}{\partial y}\right)_{x_l,y_l,\lambda_l} \\ &= \left(\frac{\partial h}{\partial x} + \frac{\mathrm{d}\mathfrak{y}}{\mathrm{d}x}\frac{\partial h}{\partial y}\right)_{x_l,y_l,\lambda_l} , \end{aligned} \tag{A.2.6}$$

which shows that (x_l, y_l) automatically satisfy (A.2.2) and so $(x_l, y_l) = (x_c, y_c)$, as claimed.

A.3 Review of vector calculus

This appendix contains a (very short) review of the basic facts of multivariate vector calculus (in three spatial dimensions) used in the main text.

The gradient of a scalar field is perhaps the simplest vector derivative to define. Consider a scalar field $\phi(\mathbf{x})$ that returns a real number for each position throughout space. (Temperature as a function of position is an example of such a scalar field.) A vector field can be built from its derivatives:

$$\nabla\phi := \frac{\partial\phi}{\partial x}\,\mathbf{e}_x + \frac{\partial\phi}{\partial y}\,\mathbf{e}_y + \frac{\partial\phi}{\partial z}\,\mathbf{e}_z\,, \tag{A.3.1}$$

where $\{x, y, z\}$ are the three Cartesian coordinates and $\mathbf{e}_i$ point along the three Cartesian axes so that $\mathbf{x} = x\,\mathbf{e}_x + y\,\mathbf{e}_y + z\,\mathbf{e}_z$. This transforms under rotation the way the notation suggests: it is a 3-dimensional vector. Geometrically, the vector $\nabla\phi(\mathbf{x})$ points in the direction along which ϕ increases the most quickly starting at the given point $\mathbf{x}$.

A vector field,

$$\mathbf{A}(\mathbf{x}) = A_x(\mathbf{x})\,\mathbf{e}_x + A_y(\mathbf{x})\,\mathbf{e}_y + A_z(\mathbf{x})\,\mathbf{e}_z\,, \tag{A.3.2}$$

is a vector that is specified independently at each position throughout space. For physical applications its component functions are usually imagined to be smooth enough that it can be differentiated as many times as needed.

There is more than one way to combine derivatives with vector fields, and in particular given a vector field $\mathbf{A}(\mathbf{x})$ one can always define a scalar field by taking the 'divergence':

$$\operatorname{div}\mathbf{A} := \nabla\cdot\mathbf{A} := \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}\,. \tag{A.3.3}$$

This is a scalar in the sense that if $\{x', y', z'\}$ are rotations of $\{x, y, z\}$ then the formula for $\nabla\cdot\mathbf{A}$ is precisely the same as above, but using the primed coordinates: $\nabla\cdot\mathbf{A} = \partial_{x'}A_{x'} + \partial_{y'}A_{y'} + \partial_{z'}A_{z'}$.

A second combination of derivatives – the 'curl' – of a vector field transforms as a vector, and is defined by

$$\operatorname{curl}\mathbf{A} := \nabla\times\mathbf{A} := \left(\frac{\partial A_y}{\partial z} - \frac{\partial A_z}{\partial y}\right)\mathbf{e}_x + \left(\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z}\right)\mathbf{e}_y + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\mathbf{e}_z\,. \tag{A.3.4}$$

A straightforward application of the definitions shows that the following two identities are true for any multiply differentiable scalar and vector fields. The symmetry of a second derivative — *e.g.* $\partial^2\phi/\partial x\partial y = \partial^2\phi/\partial y\partial x$ — implies the curl of a gradient vanishes:

$$\nabla\times(\nabla\phi) = 0\,, \tag{A.3.5}$$

for any $\phi(\mathbf{x})$. The inverse of this is also locally true: if a vector $\mathbf{A}$ satisfies $\nabla\times\mathbf{A} = 0$ in some region around a point $\mathbf{x}$ then it is also true that there exists a scalar ϕ such that $\mathbf{A} = \nabla\phi$, at least in a sufficiently small region around $\mathbf{x}$.

A similar statement for the second derivative of a vector field states that the divergence of a curl vanishes:

$$\nabla\cdot(\nabla\times\mathbf{A}) = 0\,, \tag{A.3.6}$$

for any $\mathbf{A}(\mathbf{x})$. Besides being sufficient this is also (locally) necessary: if a vector field satisfies $\nabla\cdot\mathbf{A} = 0$ in some region about a point $\mathbf{x}$ then there exists another vector field $\mathbf{C}$ such that $\mathbf{A} = \nabla\times\mathbf{C}$, at least in some sufficiently small region around $\mathbf{x}$.

Applying a divergence to a gradient similarly gives the Laplace operator:

$$\nabla\cdot(\nabla\phi) = \nabla^2\phi := \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2}\,, \tag{A.3.7}$$

while a simple calculation (again simply using the definitions) shows that applying a curl to a curl gives

$$\nabla\times(\nabla\times\mathbf{A}) = \nabla(\nabla\cdot\mathbf{A}) - \nabla^2\mathbf{A}\,. \tag{A.3.8}$$

Vector identities, such as (A.3.5) through (A.3.8), are often easier to prove using notation where a vector's components are listed with indices. That is, if the basis vectors $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ are collectively written $\mathbf{e}^i$ with $i = x, y, z$ then a vector $\mathbf{v} = v_i\,\mathbf{e}_i$ (with the Einstein summation convention enforced, wherein repeated indices represent a sum over the entire range of the relevant index) can be represented by its components v_i.

In this language $\nabla\phi$ has components $\partial_i\phi$ and $\nabla \times \mathbf{v}$ has components $\epsilon_{ijk}\partial_j v_k$ where ϵ_{ijk} is the completely antisymmetric (Levi-Civita) symbol that is antisymmetric under the interchange of any pair of indices and is normalized so that $\epsilon_{xyz} = +1$. This tensor satisfies a useful identity (from which expressions like (A.3.8) are easily derived):

$$\epsilon_{ijk}\,\epsilon_{abc} = \delta_{ia}\,\delta_{jb}\,\delta_{kc} \pm (5 \text{ other permutations}) \tag{A.3.9}$$

where δ_{ij} is the usual Kronecker delta that is unity if $i = j$ and zero otherwise. This last identity can be proven by verifying that both sides agree on the symmetry of their indices and checking specific values for a, b, c, i, j, k. A second pair of identities comes from contracting the above with Kronecker deltas:

$$\epsilon_{ijk}\,\epsilon_{abc}\,\delta^{ia} = \delta_{jb}\,\delta_{kc} - \delta_{jc}\,\delta_{kb} \quad \text{and} \quad \epsilon_{ijk}\,\epsilon_{abc}\,\delta^{ia}\,\delta^{jb} = 2\,\delta_{kc} \tag{A.3.10}$$

and so on.

B Representations of the Poincaré algebra

This appendix describes the representations of Lorentz and Poincaré transformations that are used in the main body of the text. There are two kinds of representations that naturally arise: the unitary representations that describe their action on states in the quantum Hilbert space, and the finite-dimensional (and non-unitary) representations that describe their action on fields. Each is considered in turn in its own subsection.

B.1 Unitary representations on particle states

For particle states we choose to diagonalize the mutually commuting operators P^μ, so that $P^\mu|k,\sigma\rangle = k^\mu|k,\sigma\rangle$, for which the eigenvalue is assumed either to be time-like ($k \cdot k = \eta_{\mu\nu}k^\mu k^\nu < 0$) or null ($k \cdot k = 0$). It is easy to show that $[J^{\mu\nu}, P_\lambda P^\lambda] = 0$ and because of this the eigenvalue $k \cdot k$ of P^2 is Lorentz invariant. It follows that all inertial observers necessarily agree on whether $k \cdot k < 0$ or $k \cdot k = 0$. The only other Lorentz-invariant quantity that can be built using the eigenvalue k^μ is the sign k^0, which distinguishes 4-vectors that point into the future from those that point into the past. All physical states are assumed to have $k^0 > 0$.

Any two 4-momenta that share the same values for the two invariants $k \cdot k$ and k^0 are always related by some Lorentz transformation, Λ. The strategy for finding the representations of Poincaré transformations on these states therefore is to choose a standard momentum, k^μ, consistent with these two invariants, and find the representations of all of the elements of the 'little group' that preserves this standard momentum. The effect of any other transformation not within this little group is then simply then to change k^μ away from its standard form. The kinds of standard representations that are possible differ for null and time-like particles, so each of these is considered separately below.

B.1.1 Massive Particles

Massive particles are those whose four-momentum is timelike: $k \cdot k = -m^2 < 0$. It is always possible to choose an inertial frame, the rest frame, in which k^μ takes the standard form:

$$k^0 = m > 0 \quad \text{and} \quad \mathbf{k} = 0\,. \tag{B.1.1}$$

The mass parameter m^2 can be used to label states since it is an eigenvalue of the operator $P^\mu P_\mu$, and this commutes with all of the Poincaré generators. Any other momentum, p^μ, is related to the standard momentum by: $p^\mu = L^\mu{}_\nu(\mathbf{p}/m)k^\nu$, where $L(\mathbf{p}/m)$ is the Lorentz transformation given explicitly by:

$$\begin{aligned} L^i{}_j(\mathbf{p}/m) &= \delta_{ij} + (\gamma - 1)p_i p_j/\mathbf{p}^2 \\ L^i{}_0(\mathbf{p}/m) = L^0{}_i(\mathbf{p}/m) &= p_i/m \\ L^0{}_0(\mathbf{p}/m) &= \gamma \end{aligned} \tag{B.1.2}$$

Here $\gamma = p^0/m = \sqrt{\mathbf{p}^2 + m^2}/m = (1 - \mathbf{v}^2)^{-1/2}$.

The subgroup of proper Lorentz transformations that preserve this standard form for k^μ is the group of rotations in space: $\Lambda^i{}_j = R^i{}_j$, $\Lambda^0{}_i = \Lambda^i{}_0 = 0$, and $\Lambda^0{}_0 = 1$, with $R^T R = 1$ and $\det R = 1$. States with $p^\mu = k^\mu$ must therefore fall into representations of this group:

$$U(R)|k,\sigma\rangle = \sum_{\sigma'} D^{(j)}_{\sigma',\sigma}(R)|k,\sigma'\rangle \tag{B.1.3}$$

Here $D^{(j)}(R_1)D^{(j)}(R_2) = D^{(j)}(R_1 R_2)$ are the same $(2j+1)\times(2j+1)$ matrices that represent rotations in nonrelativistic quantum mechanics, and so $2j$ an integer and $\sigma = -j, -j+1, ..., j$. Infinitesimally, for $R = 1+\omega$ we have $D^{(j)}(1+\omega) = 1 + \frac{i}{2}\omega^{ik}J^{(j)}_{ik}$. The matrices $J^{(j)}_{ik} = \epsilon^{ikl}J^{(j)}_l$ are given explicitly by:

$$\begin{aligned} \left[J^{(j)}_3\right]_{\sigma'\sigma} &= \sigma\delta_{\sigma'\sigma} \\ \left[J^{(j)}_1 \pm iJ^{(j)}_2\right]_{\sigma'\sigma} &= \sqrt{(j \mp \sigma)(j \pm \sigma + 1)}\,\delta_{\sigma',\sigma\pm1} \\ \left[(J^{(j)})^2\right]_{\sigma'\sigma} &= j(j+1)\delta_{\sigma'\sigma}\,. \end{aligned} \tag{B.1.4}$$

A state of arbitrary four-momentum is defined by: $|p,\sigma\rangle = N(\mathbf{p}/m)U(L(\mathbf{p}/m))|k,\sigma\rangle$, where the function, $N(\mathbf{p}/m)$, is chosen to satisfy the (noncovariant) normalization condition $\langle p,\sigma|p',\sigma'\rangle = \delta^3(\mathbf{p}-\mathbf{p}')\delta_{\sigma\sigma'}$. Its Lorentz-transformation properties are then given by:

$$\begin{aligned} U(\Lambda)|p,\sigma\rangle &= N(\mathbf{p}/m)U(\Lambda L(\mathbf{p}/m))|k,\sigma\rangle \\ &= N(\mathbf{p}/m)U(L(\Lambda\mathbf{p}/m))U(L(\Lambda\mathbf{p}/m)^{-1}\Lambda L(\mathbf{p}/m))|k,\sigma\rangle \end{aligned} \tag{B.1.5}$$

Here $(\Lambda p)^\mu = \Lambda^\mu{}_\nu p^\nu$. Now, the combination $W(\Lambda, \mathbf{p}/m) = L(\Lambda\mathbf{p}/m)^{-1}\Lambda L(\mathbf{p}/m)$, called a Wigner rotation, is a member of the little group that preserves k^μ and so is an ordinary spatial rotation. To see this notice that:

$$\begin{aligned} W(\Lambda, \mathbf{p}/m)k &= L(\Lambda\mathbf{p}/m)^{-1}\Lambda L(\mathbf{p}/m)k \\ &= L(\Lambda\mathbf{p}/m)^{-1}\Lambda p \\ &= k \end{aligned} \tag{B.1.6}$$

This allows the transformation law for $|p,\sigma\rangle$ to be written:

$$\begin{aligned} U(\Lambda)|p,\sigma\rangle &= N(\mathbf{p}/m)U(L(\Lambda\mathbf{p}/m))U(W(\Lambda,\mathbf{p}/m))|k,\sigma\rangle \\ &= N(\mathbf{p}/m)U(L(\Lambda\mathbf{p}/m))\sum_{\sigma'} D^{(j)}_{\sigma'\sigma}(W(\Lambda,\mathbf{p}/m))|k,\sigma'\rangle \\ &= \frac{N(\mathbf{p}/m)}{N(\Lambda\mathbf{p}/m)}\sum_{\sigma'} D^{(j)}_{\sigma'\sigma}(W(\Lambda,\mathbf{p}/m))|\Lambda p,\sigma'\rangle \end{aligned} \tag{B.1.7}$$

The momentum-dependence of the normalization is easily determined:

$$\begin{aligned} \delta^3(\mathbf{p}-\mathbf{p}')\delta_{\sigma'\sigma} &= \langle p',\sigma'|p,\sigma\rangle \\ &= \langle p',\sigma'|U^{-1}(\Lambda)U(\Lambda)|p,\sigma\rangle \\ &= \frac{N(\mathbf{p}'/m)^*}{N(\Lambda\mathbf{p}'/m)^*}\frac{N(\mathbf{p}/m)}{N(\Lambda\mathbf{p}/m)} \\ &\quad \sum_{\lambda',\lambda} D^{(j)*}_{\lambda'\sigma'}(W(\Lambda,\mathbf{p}'/m))D^{(j)}_{\lambda\sigma}(W(\Lambda,\mathbf{p}/m))\langle\Lambda p',\lambda'|\Lambda p,\lambda\rangle \\ &= \delta^3(\Lambda\mathbf{p}-\Lambda\mathbf{p}')\frac{N(\mathbf{p}'/m)^*}{N(\Lambda\mathbf{p}'/m)^*}\frac{N(\mathbf{p}/m)}{N(\Lambda\mathbf{p}/m)} \\ &\quad \sum_{\lambda',\lambda} D^{(j)}_{\sigma'\lambda'}(W^{-1}(\Lambda,\mathbf{p}'/m))D^{(j)}_{\lambda\sigma}(W(\Lambda,\mathbf{p}/m))\delta_{\lambda'\lambda} \\ &= \delta^3(\Lambda\mathbf{p}-\Lambda\mathbf{p}')\left|\frac{N(\mathbf{p}/m)}{N(\Lambda\mathbf{p}/m)}\right|^2 D^{(j)}_{\sigma'\sigma}(W^{-1}(\Lambda,\mathbf{p}'/m)W(\Lambda,\mathbf{p}/m)) \\ &= \delta^3(\Lambda\mathbf{p}-\Lambda\mathbf{p}')\left|\frac{N(\mathbf{p}/m)}{N(\Lambda\mathbf{p}/m)}\right|^2 \delta_{\sigma'\sigma} \end{aligned} \tag{B.1.8}$$

Now for any function $f(p)$:

$$\int \mathrm{d}^4p\ \delta(p^2+m^2)\theta(p^0)f(p) = \int \frac{d^3p}{2\varepsilon(\mathbf{p})}\ f(\mathbf{p}, p^0=\varepsilon(\mathbf{p})) \tag{B.1.9}$$

where $\varepsilon(\mathbf{p}) = \sqrt{\mathbf{p}^2+m^2}$ and $\theta(x)$ denotes the usual step function. This implies that $\mathrm{d}^3p/\varepsilon(\mathbf{p})$ is Lorentz-invariant and so $\delta^3(\mathbf{p}-\mathbf{p}')\varepsilon(\mathbf{p})$ must also be a Lorentz scalar. Since the combination $\delta^3(\mathbf{p}-\mathbf{p}')/|N(\mathbf{p}/m)|^2$ is invariant, as shown above, choose $N(\mathbf{p}/m) = \sqrt{m/\varepsilon(\mathbf{p})}$.

The final representation of any Lorentz transformation is then given by

$$U(\Lambda)|p,\sigma\rangle = \sqrt{\frac{\varepsilon(\Lambda\mathbf{p})}{\varepsilon(\mathbf{p})}} \sum_{\sigma'} D^{(j)}_{\sigma'\sigma}[W(\Lambda,\mathbf{p}/m)]|\Lambda p,\sigma'\rangle \tag{B.1.10}$$

with $D^{(j)}$ and W as defined above.

B.1.2 Massless Particles

Massless particle states are those whose momenta are future-directed null four-vectors: $p^2 = 0$. Just as for timelike vectors, any such null vector can be expressed as the Lorentz transform of a standard vector: $p^\mu = \mathcal{L}^\mu{}_\nu(\mathbf{p}/\kappa)k^\nu$ where

$$k^0 = k^3 = \kappa > 0 \quad \text{and} \quad k^1 = k^2 = 0\,. \tag{B.1.11}$$

$\mathcal{L}^\mu{}_\nu(\mathbf{p}/\kappa)$ is given explicitly by $\mathcal{L} = RB$ where B is a boost along the 3-axis, chosen to doppler shift κ to $|\mathbf{p}|$, and R is a rotation from the 3-axis to the direction of $\mathbf{p}$.

The little group which preserves the form of this standard vector, k^μ, is the three-parameter set of transformations $S(a,b)R(\theta)$ where $R(\theta)$ is a rotation about the 3-axis:

$$R(\theta) = \begin{pmatrix} 1 & & & \\ & \cos\theta & -\sin\theta & \\ & \sin\theta & \cos\theta & \\ & & & 1 \end{pmatrix} \tag{B.1.12}$$

and $S(a,b)$ is a boost in the 1-2 plane together with a rotation about the axis perpendicular to the boost in the 1-2 plane:

$$S(a,b) = \begin{pmatrix} 1+c & a & b & -c \\ a & 1 & 0 & -a \\ b & 0 & 1 & -b \\ c & a & b & 1-c \end{pmatrix} \tag{B.1.13}$$

with $c = (a^2+b^2)/2$.

The proof that this does indeed form the little group goes as follows: First, $R(\theta)$ and $S(a,b)$ are members of the little group by explicit calculation. To see that they exhaust the little group, suppose that Λ satisfies: $\Lambda k = k$. Consider, then, $l' = \Lambda l$, where l^μ is the timelike vector : $l^0 = M$, $\mathbf{l} = 0$. l'^μ has components $\mathbf{l}'$ and $l'^0 = \sqrt{\mathbf{l}'^2 + M^2}$, and satisfies:

$$-\kappa M = k^\mu l_\mu = k^\mu l'_\mu = \kappa(l_3 - \sqrt{\mathbf{l}'^2 + M^2}) \tag{B.1.14}$$

This implies that $l_3 = (l_1^2 + l_2^2)/2M$. Defining $a = l_1/M$, $b = l_2/M$ and $c = l_3/M = (a^2+b^2)/2$ shows that Λ and $S(a,b)$ both give l'^μ when acting on l^μ. $S^{-1}(a,b)\Lambda$ must therefore be in

the little group of both l^μ and k^μ and so is a rotation about the 3-axis: $R(\theta)$. It follows that $\Lambda = S(a,b)R(\theta)$ as claimed.

Matrix multiplication gives the group multiplication law:

$$S(a,b)S(c,d) = S(a+c, b+d) \tag{B.1.15}$$

$$R(\theta)S(a,b)R^{-1}(\theta) = S(a\cos\theta - b\sin\theta, b\cos\theta + a\sin\theta). \tag{B.1.16}$$

This means that the $S(a,b)$ form an invariant abelian subgroup. The finite-dimensional unitary representations of the little group can be constructed from those of this subgroup. Claim: the representations can only be unitary and finite-dimensional if $U[S(a,b)] = 1$. To see this choose a basis of states that diagonalize the mutually commuting generators, A and B, of the invariant abelian subgroup $U[S(a,b)] = \exp(iaA+ibB)$. That is, choose $A|\alpha,\beta\rangle = \alpha|\alpha,\beta\rangle$ and $B|\alpha,\beta\rangle = \beta|\alpha,\beta\rangle$. Then the group relation:

$$U[R(\theta)]\exp(iaA+ibB)U^{-1}[R(\theta)] = \exp[i(a\cos\theta - b\sin\theta)A + i(b\cos\theta + a\sin\theta)B] \tag{B.1.17}$$

implies:

$$U[R(\theta)]AU^{-1}[R(\theta)] = A\cos\theta + B\sin\theta \tag{B.1.18}$$

$$\text{and} \quad U[R(\theta)]BU^{-1}[R(\theta)] = B\cos\theta - A\sin\theta. \tag{B.1.19}$$

The action of $U[R(\theta)]$ on the basis $|\alpha,\beta\rangle$ is therefore:

$$\begin{aligned} A(U[R(\theta)]|\alpha,\beta\rangle) &= U[R(\theta)]U^{-1}[R(\theta)]AU[R(\theta)]|\alpha,\beta\rangle \\ &= U[R(\theta)](A\cos\theta - B\sin\theta)|\alpha,\beta\rangle \\ &= (\alpha\cos\theta - \beta\sin\theta)U[R(\theta)]|\alpha,\beta\rangle \end{aligned} \tag{B.1.20}$$

and similarly:

$$B(U[R(\theta)]|\alpha,\beta\rangle) = (\beta\cos\theta + \alpha\sin\theta)U[R(\theta)]|\alpha,\beta\rangle \tag{B.1.21}$$

$$\text{so:} \quad U[R(\theta)]|\alpha,\beta\rangle = |\alpha\cos\theta - \beta\sin\theta, \beta\cos\theta + \alpha\sin\theta\rangle. \tag{B.1.22}$$

Rotations generate a continuous one-parameter family of states labelled by the eigenvalues $(\alpha\cos\theta - \beta\sin\theta, \beta\cos\theta + \alpha\sin\theta)$. The representation can be finite-dimensional only if $\alpha = \beta = 0$. For this choice $U[S(a,b)]$ is trivial, as claimed.

For massive particles, states in the rest frame are completely characterized by the integer or half-integer eigenvalue, λ, of J_3. Notice that only one value of λ appears in each representation for massless particles, since all raising and lowering operators are represented by the unit operator. If Λ is in the little group, $U(\Lambda)|k,\lambda\rangle = \exp(i\lambda\Theta(\Lambda))|k,\lambda\rangle$ for some angle $\Theta(\Lambda)$. For a generic momentum state: $|p,\lambda\rangle = \mathcal{N}(\mathbf{p}/\kappa)U(\mathcal{L}(\mathbf{p}/\kappa))|k,\lambda\rangle$, with $p^\mu = \mathcal{L}^\mu{}_\nu k^\nu$,

the transformation becomes:

$$\begin{aligned} U(\Lambda)|p,\lambda\rangle &= \mathcal{N}(\mathbf{p}/\kappa)U(\Lambda\mathcal{L}(\mathbf{p}/\kappa))|k,\lambda\rangle \\ &= \mathcal{N}(\mathbf{p}/\kappa)U(\mathcal{L}(\Lambda\mathbf{p}/\kappa))U(\mathcal{W}(\Lambda,\mathbf{p}/\kappa))|k,\lambda\rangle \\ &= \frac{\mathcal{N}(\mathbf{p}/\kappa)}{\mathcal{N}(\Lambda\mathbf{p}/\kappa)}e^{i\lambda\Theta(\mathcal{W})}|\Lambda p,\lambda\rangle. \end{aligned} \tag{B.1.23}$$

Here the Wigner rotation $\mathcal{W}(\Lambda,\mathbf{p}/\kappa) \equiv \mathcal{L}^{-1}(\Lambda\mathbf{p}/\kappa)\Lambda\mathcal{L}(\mathbf{p}/\kappa)$ is a member of the little group. The normalization condition $\langle p,\lambda|p',\lambda'\rangle = \delta^3(\mathbf{p}-\mathbf{p}')\delta_{\lambda\lambda'}$ is consistent with $\mathcal{N}(\mathbf{p}/\kappa) = \sqrt{\kappa/\varepsilon(\mathbf{p})}$, where $\varepsilon(\mathbf{p}) = |\mathbf{p}|$ for massless particles.

B.2 Finite-dimensional representations for fields

The unitary representations of the Poincaré group described in the previous section give the action of Poincaré transformations on quantum states, and are unitary but infinite-dimensional (because there are an infinite number of possible values allowed for the momentum eigenvalue p^μ). But these are not the only representations that come up when combining quantum mechanics with special relativity. The other important class of representations that arise are the finite-dimensional ones, which it turns out are not unitary.[101] These representations play a role in describing how fields transform under Poincaré transformations, and they must be finite-dimensional if they are to involve only a finite number of fields.

The goal is to construct finite-dimensional matrices, $D(\Lambda)$, that represent Lorentz transformations inasmuch as they obey the same group multiplication rule as do the group elements themselves:

$$D(\Lambda_1)\,D(\Lambda_2) = D(\Lambda_1\Lambda_2)\,. \tag{B.2.1}$$

As is often the case, a simple way to construct these matrices in the general case is to first construct matrices that perform the same function when restricted to transformations that are infinitesimally close to the unit matrix. That is, find matrices $\mathcal{J}^{\mu\nu}$ that have the property that if $\Lambda^\mu{}_\nu = \delta^\mu_\nu + \omega^\mu{}_\nu + \cdots$ then

$$D(1+\omega) = \mathbb{I} + \frac{i}{2}\,\omega_{\mu\nu}\,\mathcal{J}^{\mu\nu} + \cdots\,, \tag{B.2.2}$$

where $\mathbb{I}$ denotes the unit matrix and the ellipses denote terms that are order $\mathcal{O}(\omega^2)$ or smaller.

Notice the similarity of this equation to (11.2.4), which defines the Lorentz generator $J^{\mu\nu}$, and is reproduced again here for convenience:

$$U(1+\omega,0) = 1 + \frac{i}{2}\omega_{\mu\nu}J^{\mu\nu} + \cdots\,. \tag{B.2.3}$$

[101] There are no representations of the Lorentz group that are both finite dimensional *and* unitary, as it happens. It is a theorem that representations that are both finite-dimension and unitary can only exist for *compact* groups, of which the Lorentz group is not one.

Although similar in spirit, the main difference is that the hermitian operators $J^{\mu\nu}$ act in the infinite-dimensional Hilbert space of quantum states while the (not in general unitary) matrices $\mathcal{J}^{\mu\nu}$ are finite-dimensional.

The requirement that the matrices $D(\Lambda)$ reproduce the group multiplication law impose conditions on the matrices $\mathcal{J}^{\mu\nu}$. Indeed, repeating the same arguments that show that group multiplication implies that the $J^{\mu\nu}$ must satisfy the algebra (11.2.7), implies in the present case that the matrices $\mathcal{J}^{\mu\nu}$ must satisfy

$$\left[\mathcal{J}^{\mu\nu}, \mathcal{J}^{\lambda\rho}\right] = i(\mathcal{J}^{\mu\lambda}\eta^{\nu\rho} - \mathcal{J}^{\nu\lambda}\eta^{\mu\rho} + \mathcal{J}^{\nu\rho}\eta^{\mu\lambda} - \mathcal{J}^{\mu\rho}\eta^{\nu\lambda}). \tag{B.2.4}$$

The construction of a set of matrices that satisfy this algebra is based on a simple trick that allows (B.2.4) to be rewritten in a way that resembles the $O(3)$ algebra of ordinary rotations. This is done by rewriting the commutation relations (B.2.4) in terms of the following combinations of the $\mathcal{J}^{\mu\nu}$:

$$\mathcal{J}_i := \frac{1}{2}\epsilon_{ijk}\mathcal{J}^{jk} \quad \text{and} \quad \mathcal{K}_i := \mathcal{J}_{i0}. \tag{B.2.5}$$

These have the interpretation of being the three generators of rotations in space, $\mathcal{J}_i$, and the generators of the Lorentz *boosts*, $\mathcal{K}_i$ that relate observers that move relative to one another with constant velocity.

In terms of the six generators $\mathcal{J}_i$ and $\mathcal{K}_i$ (with $i = 1, 23$) the algebra (B.2.4) becomes:

$$[\mathcal{J}_i, \mathcal{J}_k] = i\epsilon_{ik\ell}\mathcal{J}_\ell\,, \quad [\mathcal{J}_i, \mathcal{K}_k] = i\epsilon_{ik\ell}\mathcal{K}_\ell \quad \text{and} \quad [\mathcal{K}_i, \mathcal{K}_k] = -i\epsilon_{ik\ell}\mathcal{J}_\ell. \tag{B.2.6}$$

The trick consists of recognizing that if $\mathcal{K}_k$ is replaced in (9.2.3) by $i\mathcal{K}_k$ then only the last relation changes sign, giving the algebra of $O(4)$ (*i.e.* 4×4 orthogonal matrices). However, the commutation relations of the group $SO(4)$ the same as for the group $SU(2) \times SU(2)$, where $SU(2)$ is the group of 2×2 unitary matrices with unit determinant. This means that its matrix representations can be built from those of $SU(2)$, if these are known. But these *are* known because $SU(2)$ has the same algebra as rotations in 3-dimensional space and so its representations are simply the familiar representations of spin encountered in single-particle quantum mechanics.

B.2.1 The (A, B) classification

To make this connection between the Lorentz group and $SU(2) \times SU(2)$ more explicit define:

$$\mathcal{A}_k := \frac{1}{2}(\mathcal{J}_k + i\mathcal{K}_k) \quad \text{and} \quad \mathcal{B}_k := \frac{1}{2}(\mathcal{J}_k - i\mathcal{K}_k)\,, \tag{B.2.7}$$

in terms of which the algebra (B.2.6) becomes:

$$[\mathcal{A}_k, \mathcal{A}_\ell] = i\epsilon_{k\ell m}\mathcal{A}_m\,, \quad [\mathcal{B}_k, \mathcal{B}_\ell] = i\epsilon_{k\ell m}\mathcal{B}_m \quad \text{and} \quad [\mathcal{A}_k, \mathcal{B}_\ell] = 0\,. \tag{B.2.8}$$

Clearly the $\mathcal{A}_k$ and $\mathcal{B}_l$'s commute with one another and each separately satisfies the rotational $SU(2)$ algebra.

The finite-dimensional representation matrices $\mathcal{A}$ (and similarly for $\mathcal{B}$) are therefore simply the usual angular-momentum matrices. The states in these representations are therefore labelled by their eigenvalues, A, for the 'total spin' and their eigenvalues, a, for the 'third-component of angular momentum':

$$\mathcal{A}_3|A,a\rangle = a|A,a\rangle \quad \text{and} \quad \mathcal{A}^2|A,a\rangle = A(A+1)|A,a\rangle\,, \tag{B.2.9}$$

where $2A$ is an arbitrary non-negative integer and a runs through the values $a = -A, -A+1, ..., A-1, A$. The resulting representation matrices are therefore $(2A+1)$-dimensional. The corresponding eigenvalues for $\mathcal{B}^2$ and $\mathcal{B}_3$ are similarly denoted by B and b respectively.

The upshot of all of this is that the finite-dimensional representations of the Lorentz group can therefore be classified by a pair of numbers (A,B), where $2A$ and $2B$ are both non-negative integers that correspond to the 'spin' of the representation matrices that are used for $\mathcal{A}_k$ and $\mathcal{B}_k$. The fields in these representations are labelled by a pair of indices $m = (a,b)$, where $a = -A, -A+1, \cdots, A-1, A$ and $b = -B, -B+1, \cdots, B-1, B$, on which the transformation matrices $D_{mn}(\Lambda) = D_{ab,a'b'}(\Lambda)$ act reducibly, as

$$\sum_n D_{mn}(\Lambda)\,\psi_n = \sum_{a'b'} D_{ab,a'b'}(\Lambda)\,\psi_{a'b'}\,. \tag{B.2.10}$$

The dimension of the corresponding representation matrices is therefore $D = (2A+1)(2B+1)$.

The explicit matrices $\mathcal{J}_k$ and $\mathcal{K}_k$ whose exponentials give the D's are given by the $(2A+1)$-dimension generators $\mathcal{A}_k$ and the $(2B+1)$-dimensional generators $\mathcal{B}_k$ of the two $SU(2)$'s by

$$\begin{aligned} [\mathcal{J}_k]_{ab,a'b'} &= ([\mathcal{A}_k]_{aa'}\,\delta_{bb'} + \delta_{aa'}\,[\mathcal{B}_k]_{bb'}) \\ [\mathcal{K}_k]_{ab,a'b'} &= -i\,([\mathcal{A}_k]_{aa'}\,\delta_{bb'} - \delta_{aa'}\,[\mathcal{B}_k]_{bb'})\,. \end{aligned} \tag{B.2.11}$$

Because $\mathcal{A}_k$ and $\mathcal{B}_k$ are Hermitian, so must be the rotation generators $\mathcal{J}_k$. $\mathcal{K}_k$ on the other hand is antiHermitean and so the representation is not unitary. Notice also that the representation that is conjugate of the (A,B) representation is the (B,A) representation.

The required matrices for finite proper Lorentz transformations are then simply obtained by exponentiating these generators. For example, if the Lorentz-transformation parameters are chosen to be the rotation and boost angles, θ_k and ϕ_k, so that $\Lambda = \exp[i\vec{\theta}\cdot\mathbf{J} + i\vec{\phi}\cdot\mathbf{K}]$, then

$$\begin{aligned} D^{(A,B)}_{ab,a'b'}[\Lambda] &= \exp\left[i\vec{\theta}\cdot\vec{\mathcal{J}}^{(A,B)} + i\vec{\phi}\cdot\vec{\mathcal{K}}^{(A,B)}\right] \\ &= \left[\exp\Big((i\vec{\theta}+\vec{\phi})\cdot\vec{\mathcal{A}}^{(A)}\Big)\right]_{aa'}\left[\exp\Big((i\vec{\theta}-\vec{\phi})\cdot\vec{\mathcal{B}}^{(B)}\Big)\right]_{bb'}. \end{aligned} \tag{B.2.12}$$

Connection to more familiar representations

It is perhaps worth making explicit contact between this general framework of fields $\psi_{ab}(x)$, transforming in the (A, B) representation and the handful of commonly used low-dimension representations, like 4-vectors and antisymmetric tensors. Recall when doing so that the dimension of (A, B) representation is $D = (2A + 1)(2B + 1)$. A list of translations between the lowest-dimensional versions of this general classification of the Lorentz representations and more conventional ways of writing these representations is given in the main text in Table 2.

The scalar representation is the simplest one, because it is the trivial 1-dimensional representation that corresponds to $A = B = 0$ and so $D = (2A+1)(2B+1) = 1$. In this case there are no indices (a, b) and so $\psi(x) = \phi(x)$.

The $(\frac{1}{2}, 0)$ and $(0, \frac{1}{2})$ representations are the next smallest, with $D = (2A+1)(2B+1) = 2$. These respectively correspond to left- and right-handed spinors, which we can label by $(\psi_L)_a(x)$ and $(\psi_R)_{\bar{a}}(x)$. These are the upper and lower two component parts[102] of the 4-component Dirac spinor encountered in later sections.

The $(\frac{1}{2}, \frac{1}{2})$ representation has dimension $D = (2A+1)(2B+1) = 4$, and corresponds to a 4-vector. The precise connection can be seen from the rules of combining angular momenta, since these tell us that $(\frac{1}{2}, \frac{1}{2})$ can be obtained as the product $(\frac{1}{2}, 0) \otimes (0, \frac{1}{2})$. This shows that the connection between $V_\mu(x)$ and $\psi_{a\bar{c}}(x)$ is given by

$$\psi_{a\bar{c}}(x) = V_\mu(x)\,(\epsilon\,\sigma^\mu)_{a\bar{c}}\,, \tag{B.2.13}$$

where $\epsilon := i\tau^2$, $\sigma^0 = -i\mathbb{I}$ and $\sigma^k = -i\tau^k$ where $\mathbb{I}$ is the 2×2 unit matrix and τ^k are the standard three Pauli matrices. The $(\sigma^\mu)_{a\bar{c}}$ are the appropriate Clebsch-Gordan coefficients for this decomposition.

Similarly, since the rules for combining angular momentum imply $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$, the representation $(1, 0)$ can be obtained as the symmetric product $(\frac{1}{2}, 0) \otimes (\frac{1}{2}, 0)$ — and similarly for $(0, 1)$ as $(0, \frac{1}{2}) \otimes (0, \frac{1}{2})$. Explicitly, Table 2 gives the $(1, 0)$ and $(0, 1)$ representations as the self-dual and anti-self-dual parts of an antisymmetric tensor, $F_{\mu\nu} = -F_{\nu\mu}$, with the explicit connection again given in terms of Pauli matrices by

$$\psi_{ac}(x) = \psi_{ca}(x) = F_{\mu\nu}(\epsilon\,[\sigma^\mu\,, \overline{\sigma}^\nu])_{ac} \tag{B.2.14}$$

where ϵ is as above and $\overline{\sigma}^0 = -i\mathbb{I}$ and $\overline{\sigma}^k = +i\tau^k$.

C Relativistic fields

This appendix identifies how the compatability of Lorentz transformation properties determines how any given particle can be represented in terms of fields.

[102] For aficionados, this is so in a basis where γ_5 is diagonal.

C.1 Which fields can represent which particles?

We have seen in the main text that the condition that the Hamiltonian be local (*i.e.* the integral over space of a local Hamiltonian density) requires creation and annihilation operators to appear within it through local fields, that have the general form

$$A_n(\mathbf{x},t) = \sum_\sigma \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\; u_n(\mathbf{p},\sigma)\, a_{\mathbf{p}\sigma}\; e^{-i\varepsilon(p)t + i\mathbf{p}\cdot\mathbf{x}}\,, \tag{C.1.1}$$

where $a_{\mathbf{p}\sigma}$ is the destruction operator for a spin-j particle. This appendix solves the problem of deriving the form for the coefficient functions $u_n(\mathbf{p},\sigma)$ under the assumption that the fields $A_n(\mathbf{x},t)$ transform linearly under Poincaré transformations:

$$U(\Lambda)A_n(x)U^\star(\Lambda) = \sum_m D_{nm}(\Lambda^{-1})A_m(\Lambda x)\,, \tag{C.1.2}$$

where $U(\Lambda)$ denotes the representation of the Lorentz transformation on quantum states, whose unitarity implies $U^\star = U^{-1}$.

As argued in the main text, this condition implies that the matrices, D_{mn}, satisfy the same group multiplication law as do the unitary operators $U(\Lambda)$: $D(\Lambda_1)D(\Lambda_2) = D(\Lambda_1\Lambda_2)$. For representations involving a finite number of fields this implies the D_{mn}'s must be one of the finite-dimensional representations derived in Appendix B.2.

C.1.1 Consistency Conditions

Before pursuing the representations of the Lorentz group further it is important to recognize that requirement (C.1.2) severely constrains the form of the mode functions, $u_n(\mathbf{k},\sigma)$. This is because the transformation properties of the destruction operators, $a(\mathbf{k},\sigma)$, are determined by the transformation rules derived in the previous chapter for the single-particle states. In fact, the constraints on $u_m(\mathbf{k},\sigma)$ are so severe that they completely determine their dependence on their arguments, $\mathbf{p}$, and σ.

To see this in detail recall the transformation law (11.2.14) for massive particle states. (The results for massless particles are given at the end of this section.) If all of the other particles in a generic many-particle state are labelled by α, then:

$$U(\Lambda)|\mathbf{k},\sigma;\alpha\rangle = \left\{\sqrt{\frac{\varepsilon(\Lambda k)}{\varepsilon(k)}}\sum_{\sigma'} D^{(j)}_{\sigma'\sigma}\left[W(\Lambda,\mathbf{k}/m)\right]|\Lambda\mathbf{k},\sigma'\rangle\right\}U(\Lambda)|\alpha\rangle. \tag{C.1.3}$$

Now, since $|\mathbf{k},\sigma;\alpha\rangle = a^\star_{\mathbf{k}\sigma}|\alpha\rangle$, with a similar relation for $|\Lambda\mathbf{k},\sigma;\alpha\rangle$, and since equation (C.1.3) holds for all states $|\alpha\rangle$, it follows that:

$$U(\Lambda)\; a^\star_{\mathbf{k},\sigma}U^\star(\Lambda) = \sqrt{\frac{\varepsilon(\Lambda k)}{\varepsilon(k)}}\sum_{\sigma'} D^{(j)}_{\sigma'\sigma}\left[W(\Lambda,\mathbf{k}/m)\right]\; a^\star_{\Lambda\mathbf{k},\sigma'}. \tag{C.1.4}$$

Therefore:

$$U(\Lambda)\, a_{\mathbf{k},\sigma} U^{-1}(\Lambda) = \sqrt{\frac{\varepsilon(\Lambda k)}{\varepsilon(k)}} \sum_{\sigma'} D^{(j)*}_{\sigma'\sigma} \left[W(\Lambda, \mathbf{k}/m)\right]\; a_{\Lambda\mathbf{k},\sigma'}. \tag{C.1.5}$$

This allows us to compute explicitly how $A_n(x)$ must transform under Lorentz transformations:

$$\begin{aligned} U(\Lambda) A_n(x) U^\star(\Lambda) &= c \sum_\sigma \int \mathrm{d}^3k\; u_n(\mathbf{k},\sigma) \left[U(\Lambda)\; a_{\mathbf{k},\sigma} U^\star(\Lambda)\right] e^{ik\cdot x} \\ &= c \sum_{\sigma\sigma'} \int \mathrm{d}^3k \sqrt{\frac{\varepsilon(\Lambda k)}{\varepsilon(k)}}\; D^{(j)*}_{\sigma'\sigma} \left[W(\Lambda, \mathbf{k}/m)\right] u_n(\mathbf{k},\sigma)\, a_{\Lambda\mathbf{k},\sigma'}\; e^{ik\cdot x}, \end{aligned} \tag{C.1.6}$$

where c is a normalization constant.

On the other hand from eqs. (C.1.1) and (C.1.2)

$$\begin{aligned} U(\Lambda) A_n(x) U^\star(\Lambda) &= \sum_m D_{nm}(\Lambda^{-1}) A_m(\Lambda x) \\ &= c \sum_m D_{nm}(\Lambda^{-1}) \sum_\sigma \int \mathrm{d}^3k\; u_m(\mathbf{k},\sigma)\, a_{\mathbf{k},\sigma}\; e^{ik\cdot(\Lambda x)}. \end{aligned} \tag{C.1.7}$$

In order to better compare eq. (C.1.7) with (C.1.6) relabel the integration variables in (C.1.7) by: $\mathbf{k} \to \Lambda\mathbf{k}$ and $\sigma \to \sigma'$, and use the properties that $k\cdot x$ and $\mathrm{d}^3\mathbf{k}/\varepsilon(k)$ are Lorentz invariants, so

$$(\Lambda k)\cdot(\Lambda x) = k\cdot x \quad \text{and} \quad \mathrm{d}^3(\Lambda\mathbf{k}) = \frac{\mathrm{d}^3(\Lambda k)}{\varepsilon(\Lambda k)}\, \varepsilon(\Lambda k) = \frac{\mathrm{d}^3 k}{\varepsilon(k)}\, \varepsilon(\Lambda k). \tag{C.1.8}$$

Eq. (C.1.7) then becomes

$$U(\Lambda) A_n(x) U^\star(\Lambda) = c \sum_m D_{nm}(\Lambda^{-1}) \sum_{\sigma'} \int \mathrm{d}^3k\; \frac{\varepsilon(\Lambda k)}{\varepsilon(k)}\; u_m(\Lambda\mathbf{k},\sigma')\, a_{\Lambda\mathbf{k},\sigma'}\; e^{ik\cdot x}. \tag{C.1.9}$$

Finally, equating the coefficients of $a_{\Lambda\mathbf{k},\sigma'}\, e^{ik\cdot x}$ in this last equation and in (C.1.6) gives the following condition on $u_m(\mathbf{k},\sigma)$:

$$\sum_\sigma D^{(j)*}_{\sigma'\sigma} \left[W(\Lambda, \mathbf{k}/m)\right] u_n(\mathbf{k},\sigma) = \sum_m \sqrt{\frac{\varepsilon(\Lambda k)}{\varepsilon(k)}} D_{nm}(\Lambda^{-1}) u_m(\Lambda\mathbf{k},\sigma'). \tag{C.1.10}$$

C.1.2 Solutions

This last relation is the principal result that governs the form of $u_m(\mathbf{k},\sigma)$. The remainder of this section is devoted to solving it for the unknown functions $u_n(\mathbf{k},\sigma)$. The first step in doing so is to rewrite it in an equivalent form. To this end consider the following two special cases of eq. (C.1.10):

1. Suppose first we choose $\mathbf{k} = 0$ and $\Lambda = L(\mathbf{p}/m)$. Recalling the definition of the Wigner rotation:

$$W(\Lambda, \mathbf{k}/m) = L^{-1}(\Lambda \mathbf{k}/m)\ \Lambda\ L(\mathbf{k}/m). \tag{C.1.11}$$

we see that in this case $W(\Lambda, \mathbf{k}/m)$ is the identity transformation:

$$W(\Lambda, \mathbf{k}/m) = L^{-1}(\mathbf{p}/m)\ L(\mathbf{p}/m)\ \mathbf{1} = \mathbf{1}. \tag{C.1.12}$$

As a result eq. (C.1.10) reduces to:

$$u_n(\mathbf{k} = 0, \sigma') = \sqrt{\frac{\varepsilon(p)}{m}} \sum_m D_{nm}\left[L^{-1}(\mathbf{p}/m)\right]\ u_m(\mathbf{p}, \sigma'), \tag{C.1.13}$$

or, equivalently:

$$u_m(\mathbf{p}, \sigma) = \sqrt{\frac{m}{\varepsilon(p)}} \sum_n D_{mn}\left[L(\mathbf{p}/m)\right]\ u_n(\mathbf{0}, \sigma). \tag{C.1.14}$$

In the particular case where the fields transform trivially under Lorentz transformations, $D_{mn} \equiv \delta_{mn}$, we have the solution: $u_m(\mathbf{k}) = \sqrt{m/\varepsilon(k)}\ u_m(\mathbf{0})$, and so $u_m(\mathbf{k}) = c/\sqrt{\varepsilon(k)}$ for some constant, c.

2. As our second special case of eq. (C.1.10), again choose $\mathbf{k} = \mathbf{0}$, but this time choose Λ to be in the little group of spatial rotations: $\Lambda = R^{-1}$. In this case $\Lambda\mathbf{k} = \mathbf{k} = \mathbf{0}$ and the relevant Wigner rotation is $W = \Lambda = R^{-1}$. Remembering that the matrices $D^{(j)}_{\sigma'\sigma}$ are unitary, eq. (C.1.10) reduces to:

$$\sum_\sigma D^{(j)}_{\sigma\sigma'}(R)\ u_n(\mathbf{0}, \sigma) = \sum_m D_{nm}(R)\ u_m(\mathbf{0}, \sigma'). \tag{C.1.15}$$

The two special cases, eqs. (C.1.14) and (C.1.15), give complementary information about the wavefunctions, $u_m(\mathbf{k}, \sigma)$. Eq. (C.1.14) determines the wavefunction in a general frame, $u_m(\mathbf{k}, \sigma)$, in terms of the result in the rest frame, $u_m(\mathbf{0}, \sigma)$. Eq. (C.1.15), on the other hand, is a restriction purely on $u_m(0, \sigma)$.

The main claim now is that the two special cases, eqs. (C.1.14) and (C.1.15), are *equivalent* to the original condition, eq. (C.1.10). It therefore suffices to solve eq. (C.1.15) and to use (C.1.14) to extend the result to an arbitrary frame. To establish the equivalence we now derive eq. (C.1.10) using only eqs (C.1.14) and (C.1.15).

Define, then, X to be the left-hand-side of eq. (C.1.10):

$$X \equiv \sum_\sigma D^{(j)*}_{\sigma'\sigma}\left[W(\Lambda, \mathbf{k}/m)\right] u_n(\mathbf{k}, \sigma). \tag{C.1.16}$$

Using first eq. (C.1.14) and then (C.1.15) in X gives:

$$\begin{aligned} X &= \sum_{\sigma m} D^{(j)*}_{\sigma'\sigma}\left[W(\Lambda,\mathbf{k}/m)\right]\sqrt{\frac{m}{\varepsilon(k)}}D_{nm}\left[L(\mathbf{k}/m)\right]u_m(\mathbf{0},\sigma) \\ &= \sqrt{\frac{m}{\varepsilon(k)}}\sum_{\ell m} D_{nm}\left[L(\mathbf{k}/m)\right]D_{m\ell}\left[W^{-1}(\Lambda,\mathbf{k}/m)\right]u_\ell(\mathbf{0},\sigma') \\ &= \sqrt{\frac{m}{\varepsilon(k)}}\sum_{\ell} D_{n\ell}\left[L(\mathbf{k}/m)\;W^{-1}(\Lambda,\mathbf{k}/m)\right]u_\ell(\mathbf{0},\sigma'). \end{aligned} \tag{C.1.17}$$

Using the definition of W now gives:

$$\begin{aligned} L(\mathbf{k}/m)\;W^{-1}(\Lambda,\mathbf{k}/m) &= L(\mathbf{k}/m)\;L^{-1}(\mathbf{k}/m)\;\Lambda^{-1}\;L(\Lambda\mathbf{k}/m) \\ &= \Lambda^{-1}\;L(\Lambda\mathbf{k}/m), \end{aligned} \tag{C.1.18}$$

which, when used in eq. (C.1.17), allows X to be written as:

$$\begin{aligned} X &= \sqrt{\frac{m}{\varepsilon(k)}}\sum_{m\ell} D_{nm}(\Lambda^{-1})\;D_{m\ell}\left[L(\Lambda\mathbf{k}/m)\right]u_\ell(\mathbf{0},\sigma') \\ &= \sqrt{\frac{\varepsilon(\Lambda k)}{\varepsilon(k)}}\sum_{m} D_{nm}(\Lambda^{-1})\;u_m(\Lambda\mathbf{k},\sigma'), \end{aligned} \tag{C.1.19}$$

which may be recognized as the right-hand-side of eq. (C.1.10). This establishes the equivalence of eqs. (C.1.14) and (C.1.15) with eq. (C.1.10).

The plan now is as follows: Knowledge of the particle type fixes the representation matrices $D^{(j)}_{\sigma'\sigma}(R)$. The choice of representation for the field similarly specifies the $D_{mn}(\Lambda^{-1})$'s. Given these representations we then solve eq. (C.1.15) for $u_m(\mathbf{0},\sigma)$, and then use eq. (C.1.14) to find $u_n(\mathbf{k},\sigma)$.

The conditions quoted in the main text for the existence of solutions can be seen from the main obstruction equation: eq. (C.1.15). To see what this implies recall that eq. (B.2.12) implies that the reprentation matrix for a pure rotation — *i.e.* one for which $\vec{\phi}=0$ — within an (A,B) Lorentz representation is :

$$D_{mn}(R) = D^{(A,B)}_{ab,a'b'}(R) = D^{(A)}_{aa'}(R)\;D^{(B)}_{bb'}(R). \tag{C.1.20}$$

Consequently eq. (C.1.15) reduces for pure rotations to the statement

$$\sum_{\sigma} D^{(j)}_{\sigma\sigma'}(R)\;u_n(\mathbf{0},\sigma) = \sum_{a'b'} D^{(A)}_{aa'}(R)\;D^{(B)}_{bb'}(R)\;u_m(\mathbf{0},\sigma'). \tag{C.1.21}$$

This condition has a simple interpretation. It state that $u_{ab}(\mathbf{0},\sigma)$ — which *a priori* transforms *reducibly* as the product of a spin A and a spin B representation

$$A\otimes B = \bigoplus_{j=|A-B|}^{A+B} j, \tag{C.1.22}$$

actually transforms irreducibly as spin j under rotations. In other words, it projects out the spin-j part from the above sum. $u_{ab}(\mathbf{0},\sigma)$ must therefore be the *Clebsch-Gordan coefficient* for the appearance of spin j within the product of two spins A and B: $A\otimes B \to j$. Eq. (C.1.22) shows that this can only happen when j takes one of the following values

$$j \in \Big\{ A+B, \quad A+B-1, \quad \cdots \quad |A-B|+1, \quad |A-B| \Big\}\,. \tag{C.1.23}$$

Otherwise (for massive particles) no solution exists.

C.1.3 Consistency: massless particles

Arguments that are identical to those just given imply the same condition, eq. (C.1.10), on the wavefunctions, $u_m(\mathbf{k},\lambda)$, for fields representing massless particles. The only changes required arise in the specialization to eqs. (C.1.14) and (C.1.15). For massless particles we specialize instead to the standard frame in which the particle's four-momentum is: $k^\mu = (\kappa,0,0,\kappa)$ and choose either $\Lambda = \mathcal{L}(\mathbf{p}/\kappa)$ or $\Lambda = \mathcal{R}$ with $\mathcal{R}$ in the little group of k^μ. In this case the analogues for eqs. (C.1.14) and (C.1.15) become:

$$u_m(\mathbf{p},\lambda) = \sqrt{\frac{\kappa}{\varepsilon(p)}} \sum_n D_{mn}\left[\mathcal{L}(\mathbf{p}/\kappa)\right]\; u_n(k,\lambda), \tag{C.1.24}$$

$$\text{and}: \quad e^{i\lambda\Theta(\mathcal{R})}\; u_n(k,\lambda) = \sum_m D_{nm}(\mathcal{R})\; u_m(k,\lambda) \tag{C.1.25}$$

Eqs. (C.1.24) and (C.1.25) together encode all of the restrictions that $u_n(\mathbf{k},\lambda)$ must satisfy for massless states, and it is again (C.1.25) that restricts the kinds of helicities that can be represented by a given type of field. In particular, as is shown in more detail in §C.2.2, because the matrix $D_{nm}(\Theta)$ in this case simply represents the rotation as a phase $e^{i(B-A)\Theta}$ the condition (C.1.25) can only be satisfied if the helicity λ satisfies

$$\lambda = B - A\,. \tag{C.1.26}$$

C.2 Mode functions for general spin

The above consistency conditions can now be solved explicitly to construct the mode functions $u_m(\mathbf{k},\sigma)$ appropriate for massive particles with any spin (or to construct $u_m(\mathbf{k},\lambda)$ for massless particles of any helicity) for any allowed field representation. Since the solutions differ significantly in their character according to whether or not the particles have a nonzero mass, we treat each separately.

C.2.1 Massive Particles

Suppose now a massive spin-j particle is represented by a field transforming in the (A,B) representation of the Lorentz group, for which we write its components as $A_m(x) = A_{ab}(x)$.

Recall that the consistency condition (C.1.15) reduces in this case to:

$$\sum_{\sigma} D^{(j)}_{\sigma\sigma'}(R)\; u_n(\mathbf{0},\sigma) = \sum_{a'b'} D^{(A)}_{aa'}(R)\; D^{(B)}_{bb'}(R)\; u_m(\mathbf{0},\sigma')\,, \tag{C.2.1}$$

whose interpretation, whose interpretation was that $u_{ab}(\mathbf{0},\sigma)$ contains the spin-j part from the product of a spin A and spin B. $u_{ab}(\mathbf{0},\sigma)$ must therefore be the *Clebsch-Gordan coefficient* for the reduction: $A\otimes B \to j$. If j does lie within the range given in (C.1.23) then the solution for $u_{ab}(\mathbf{0},\sigma)$ is unique up to normalization and is given by the Clebsch-Gordan coefficient:

$$u_{ab}(\mathbf{0},\sigma) = C_{AB}(j,\sigma;a,b), \qquad \text{if } |A-B| \le j \le A+B. \tag{C.2.2}$$

The next step is to use eq. (C.1.14) to construct $u(\mathbf{k},\sigma)$ in a general frame. Consider first the special case where the particle moves parallel to the z-axis. In this case the particle four-momentum is: $k^\mu = (\varepsilon(k),0,0,k)$. The standard boost to this frame from rest has the form

$$\begin{aligned} B^\mu{}_\nu(\phi) &\equiv L^\mu{}_\nu(\mathbf{k}/m) \\ &= \begin{pmatrix} \cosh\phi & 0 & 0 & \sinh\phi \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \sinh\phi & 0 & 0 & \cosh\phi \end{pmatrix}. \end{aligned} \tag{C.2.3}$$

for which the arguments of §11.1.3 show

$$\cosh\phi = \frac{\varepsilon(k)}{m} \quad \text{and} \quad \sinh\phi = \frac{k}{m}. \tag{C.2.4}$$

In order to find the representation of this transformation its generator must be constructed using

$$\omega^\mu{}_\nu := \left.\frac{\mathrm{d}B^\mu{}_\nu}{\mathrm{d}\phi}\right|_{\phi=0} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{C.2.5}$$

and so

$$B^\mu{}_\nu(\phi) = \exp\left[\frac{i}{2}\phi\,\omega_{\mu\nu}J^{\mu\nu}\right] = \exp\left[i\phi J^{30}\right] = \exp\left[-i\phi K_3\right]. \tag{C.2.6}$$

Not surprisingly the required generator is a boost along the z-axis.

Generalizing to an arbitrary direction requires the boost parameter $\vec{\phi} = \phi\,\hat{\mathbf{k}}$ for $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$. It follows that

$$D[L(\mathbf{k}/m)] = \exp\left[-i\phi\,\hat{\mathbf{k}}\cdot\vec{\mathcal{K}}\right], \tag{C.2.7}$$

with ϕ given by (C.2.4). Using these results in eq. (C.1.14) then gives the general solution for $u_{ab}(\mathbf{k},\sigma)$:

$$u_{ab}(\mathbf{k},\sigma) = \sqrt{\frac{m}{\varepsilon(k)}} \sum_{a'b'} \left[\exp\left(-\phi\,\hat{\mathbf{k}}\cdot\vec{\mathcal{A}}^{(A)}\right)\right]_{aa'} \left[\exp\left(+\phi\,\hat{\mathbf{k}}\cdot\vec{\mathcal{B}}^{(B)}\right)\right]_{bb'} C_{AB}(j,\sigma;a',b')\,, \tag{C.2.8}$$

where $\mathcal{A}_i$ and $\mathcal{B}_i$ are repectively the explicit angular mometum matrices for spins A and B.

The Massless Limit

It is instructive to examine the massless limit of the massive result, eq. (C.2.8), since it foreshadows the result obtained in the next section for massless particles.

To this end consider a particle moving along the z-axis with momentum k, since this becomes the standard frame used above when defining the Lorentz representation for a massless particle. In this case the four-momentum is $k^\mu = (\varepsilon(k),0,0,k)$ and the boost required in eq. (C.2.8) reduces to:

$$\left[\hat{\mathbf{k}}\cdot\vec{\mathcal{K}}^{(A,B)}\right]_{ab,a'b'} = \left[\mathcal{K}_3^{(A,B)}\right]_{ab,a'b'} = -i(a-b)\;\delta_{aa'}\;\delta_{bb'}. \tag{C.2.9}$$

The massive mode-function of (C.2.8) then becomes

$$u_{ab}(k\,\mathbf{e}_z,\sigma) = \sqrt{\frac{m}{\varepsilon(k)}}\; e^{-\phi\,a}\; e^{+\phi\,b}\; C_{AB}(j,\sigma;a,b), \tag{C.2.10}$$

with

$$e^{\phi} = \cosh\phi + \sinh\phi = \frac{\varepsilon(k)+k}{m} \quad \text{and} \quad e^{-\phi} = \cosh\phi - \sinh\phi = \frac{\varepsilon(k)-k}{m}. \tag{C.2.11}$$

Using these to eliminate ϕ, the final expression for $u_{ab}(k\,\mathbf{e}_z,\sigma)$ becomes

$$u_{ab}(k\,\mathbf{e}_z,\sigma) = \sqrt{\frac{m}{\varepsilon(k)}}\; \left(\frac{\varepsilon(k)-k}{m}\right)^a \left(\frac{\varepsilon(k)+k}{m}\right)^b C_{AB}(j,\sigma;a,b). \tag{C.2.12}$$

Now consider the ultrarelativistic limit for which $m \ll k$. Since $\varepsilon(k) = k + \mathcal{O}(m^2/2k)$ in this limit we have $(\varepsilon(k)-k)/m \to 0$ and $(\varepsilon(k)+k)/m \to \infty$. At face value eq. (C.2.12) therefore diverges as the mass tends to zero. There is, however, freedom to normalize u_{ab} conveniently so we may choose the normalization to vanish with m in such a way as to produce a finite result. Since this normalization must be independent of a and b only the most singular term in eq. (C.2.12) survives. The most singular contribution is that for which a is as negative as possible and b is as positive as possible. That is, $a = -A$ and $b = +B$.

The resulting limit is:

$$\lim_{m\to 0} u_{ab}(k\,\mathbf{e}_z,\sigma) = c\;k^{B-\frac{1}{2}}\; C_{AB}(j,\sigma;-A,B)\;\delta_{a,-A}\;\delta_{b,B}\,, \tag{C.2.13}$$

where c is an undetermined normalization constant. Now, the Clebsch-Gordan coefficient vanishes unless $\sigma = a+b$, and in this frame σ coincides with the helicity. It follows, then, that a field in representation (A,B) of the Lorentz group can represent a massless particle of helicity λ only if the helicity satisfies $\lambda = B - A$, as claimed in eq. (C.1.26).

C.2.2 Massless Particles

This section repeats the previous analysis for massless particles. The starting point is the consistency condition (C.1.25), that states

$$e^{i\lambda\Theta(\mathcal{R})}\; u_n(k,\lambda) = \sum_m D_{nm}(\mathcal{R})\; u_m(k,\lambda). \tag{C.2.14}$$

This expression is to be solved for $u_n(\lambda) := u_n(k,\lambda)$.

The first step in doing so is to construct the matrices for the little-group elements within the (A,B) representation. Recall to this end that a generic element of the little group may be written as the product $S(a,b)R(\theta)$, in which $S(a,b)$ is the boost:

$$S(a,b) = \begin{pmatrix} 1+c & a & b & -c \\ a & 1 & 0 & -a \\ b & 0 & 1 & -b \\ c & a & b & 1-c \end{pmatrix} \tag{C.2.15}$$

with $c = (a^2+b^2)/2$. $R(\theta)$, on the other hand, is a rotation about the z-axis,

$$R(\theta) = \begin{pmatrix} 1 & & & \\ & \cos\theta & -\sin\theta & \\ & \sin\theta & \cos\theta & \\ & & & 1 \end{pmatrix} \tag{C.2.16}$$

In order to construct the matrix representations for these Lorentz transformations it is necessary to find their generators, which are

$$\left.\frac{\mathrm{d}R}{\mathrm{d}\theta}\right|_{\theta=0} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{C.2.17}$$

while

$$\left.\frac{\mathrm{d}S}{\mathrm{d}a}\right|_{a=b=0} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \left.\frac{\mathrm{d}S}{\mathrm{d}b}\right|_{a=b=0} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{C.2.18}$$

From these expressions we read off the Lorentz parameters:

$$\omega^0{}_1 = \omega^1{}_0 = \omega^3{}_1 = -\omega^1{}_3 = a\,, \quad \omega^0{}_2 = \omega^2{}_0 = \omega^3{}_2 = -\omega^2{}_3 = b \tag{C.2.19}$$

and $\omega^1{}_2 = -\omega^2{}_1 = \theta$.

The consistency condition on $u_n(\lambda)$ therefore explicitly becomes

$$e^{i\theta\lambda}\, u_m(\lambda) = \sum_n \Big[\exp\left[ia(\mathcal{J}_2 - \mathcal{K}_1) - ib(\mathcal{J}_1 + \mathcal{K}_2) + i\theta\mathcal{J}_3\right]\Big]_{mn}\, u_n(\lambda), \tag{C.2.20}$$

a condition that must hold for all a, b, θ and λ. Eq. (C.2.20) is therefore equivalent to the following three properties:

$$\sum_n (\mathcal{J}_2 - \mathcal{K}_1)_{mn}\ u_n(\lambda) = \sum_n (\mathcal{J}_1 + \mathcal{K}_2)_{mn}\ u_n(\lambda) = 0\,, \tag{C.2.21}$$

and

$$\sum_n (\mathcal{J}_3)_{mn}\ u_n(\lambda) = \lambda\, u_m(\lambda). \tag{C.2.22}$$

The first two of these conditions express the reasonable requirement that the boosts be trivially represented, $D_{mn}[S(a,b)] = \delta_{mn}$, in accord with what was found for their representation on particle states. Once expressed in terms of the generators, **A** and **B** these conditions are equivalent to the requirement that $u_n(\lambda)$ be annihilated by the lowering operator: $\mathcal{A}_- = (\mathcal{A}_1 - i\mathcal{A}_2)$ and by the raising operator: $\mathcal{B}_+ = (\mathcal{B}_1 + i\mathcal{B}_2)$. For an (A,B) representation these conditions require that $u_{ab}(\lambda)$ be proportional to $\delta_{a,-A}\ \delta_{b,B}$ as indicated by the massless limit taken in the previous section:

$$u_{ab}(\lambda) = c\,\delta_{a,-A}\ \delta_{b,B}. \tag{C.2.23}$$

The final condition, eq. (C.2.22), further implies that $u_m(\lambda)$ must also be the eigenvector of $(\mathcal{J}_3)_{ab,a'b'} = (a+b)\delta_{aa'}\delta_{bb'}$ having eigenvalue λ. This clearly implies that λ must be related to A and B by $\lambda = a + b = B - A$ if there is to be any solution at all for $u_{ab}(\lambda)$, as claimed in eq. (C.1.26).

The result for arbitrary momentum is finally given by eq. (C.1.24), which states

$$\begin{aligned} u_m(\mathbf{p},\lambda) &= \sqrt{\frac{\kappa}{E_p}} \sum_{a'b'} D^{(A)}_{aa'}\left[\mathcal{L}(\mathbf{p}/\kappa)\right]\ D^{(B)}_{bb'}\left[\mathcal{L}(\mathbf{p}/\kappa)\right]\ u_{a'b'}(\lambda) \\ &= c\sqrt{\frac{\kappa}{E_p}} D^{(A)}_{a,-A}\left[\mathcal{L}(\mathbf{p}/\kappa)\right]\ D^{(B)}_{b,B}\left[\mathcal{L}(\mathbf{p}/\kappa)\right]. \end{aligned} \tag{C.2.24}$$

This completes the derivation of the mode functions appropriate in the general case where an arbitrary field representation represents a particle with general spin.

C.3 Microcausality for general spin

This section repeats the construction of the antiparticle contribution to a field — given in §11.4.1 for scalar fields representing spinless particles — for the case of general field representation (A,B) and general spin j. Although the algebra is somewhat more cumbersome the result again establishes crossing symmetry between particle and antiparticle as well as the spin-statistics connection.

Motivated by the discussion of §11.4.1 for spinless particles, consider the following *ansatz* for the relativistic field, $\psi_n(x)$, that represents an arbitrary spin particle and its antiparticle:

$$\psi_n(x) = \sum_\sigma \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}} \left[u_n(\mathbf{p},\sigma)\; a_{\mathbf{p},\sigma}\; e^{ip\cdot x} + v_n(\mathbf{p},\sigma)\; \overline{a}^\star_{\mathbf{p},\sigma}\; e^{-ip\cdot x} \right]. \tag{C.3.1}$$

C.3.1 Antiparticle mode functions

The first problem is to determine the function $v_n(\mathbf{p},\sigma)$ that is required by consistency of this equation with the Lorentz-transformation properties of the fields. The main result to be established on the next few pages is that $v_n(\mathbf{p},\sigma)$ and $u_n(\mathbf{p},\sigma)$ can be related by

$$v_n(\mathbf{p},\sigma) = \xi(-)^{j-\sigma} u_n(\mathbf{p},-\sigma), \tag{C.3.2}$$

in which the complex number ξ corresponds to an to-be-determined relative normalization.

In order to establish eq. (C.3.2) the plan is first to demonstrate that the combination $(-)^{j-\sigma}\; a^\star_{\mathbf{p},-\sigma}$ transforms in precisely the same way as does $a_{\mathbf{p},\sigma}$ under Lorentz transformations. This relation may be derived by comparing the transformation properties of $a^\star_{\mathbf{p},\sigma}$ with those of $a_{\mathbf{p}\sigma}$, as given in (11.3.8) and (11.3.9) of the main text:

$$\begin{aligned} U(\Lambda)\, a^\star_{\mathbf{p},\sigma}\, U^{-1}(\Lambda) &= \sqrt{\frac{\varepsilon(\Lambda p)}{\varepsilon(p)}} \sum_{\sigma'} D^{(j)}_{\sigma'\sigma}\left[W(\Lambda,\mathbf{p}/m)\right]\; a^*(\Lambda\mathbf{p},\sigma') \\ U(\Lambda)\, a_{\mathbf{p},\sigma}\, U^{-1}(\Lambda) &= \sqrt{\frac{\varepsilon(\Lambda p)}{\varepsilon(p)}} \sum_{\sigma'} D^{(j)*}_{\sigma'\sigma}\left[W(\Lambda,\mathbf{p}/m)\right]\; a(\Lambda\mathbf{p},\sigma'). \end{aligned} \tag{C.3.3}$$

The first step in the derivation is to relate $D^{(j)}_{\sigma'\sigma}$ to its complex conjugate: $D^{(j)*}_{\sigma'\sigma}$. Our conventions for $SU(2)$ representations are given in eq. (B.1.4), where it is shown that the matrix representations of $J_\pm = J_1 \pm iJ_2$ and J_3 are real. This implies that of the Hermitian generators J_1 and J_3 are real and symmetric while J_2 is imaginary and antisymmetric. The representation matrices for the generators therefore satisfy

$$(\mathcal{J}_1^*, \mathcal{J}_2^*, \mathcal{J}_3^*) = (\mathcal{J}_1, -\mathcal{J}_2, \mathcal{J}_3). \tag{C.3.4}$$

Notice that reflection of J_2 with the other two generators fixed may also be accomplished by performing an 180° rotation about the y-axis followed by a complete reflection of all three directions: $\mathcal{J}_i \to -\mathcal{J}_i$. That is to say, complex conjugation is equivalent in its effect on the generators, $\mathbf{J}$, to the following similarity transformation,

$$\mathbf{J}^* = -e^{i\pi J_2}\; \mathbf{J}\; e^{-i\pi J_2}. \tag{C.3.5}$$

The implications of this last result for the exponentiated transformations $D^{(j)}_{nm}$ may be determined using the general result: $f(SAS^{-1}) = Sf(A)S^{-1}$ that is satisfied for any well-defined matrix function — as may be established using the Taylor expansion for the function,

$f(A)$. The result is

$$\left[\exp(i\vec{\theta}\cdot\mathbf{J})\right]^* = \exp\left(ie^{i\pi J_2}\,\vec{\theta}\cdot\mathbf{J}e^{-i\pi J_2}\right) = e^{i\pi J_2}\ \left[\exp(i\vec{\theta}\cdot\mathbf{J})\right]\ e^{-i\pi J_2}. \tag{C.3.6}$$

Mathematically this shows that complex conjugation is an *inner automorphism* of $SU(2)$.

In terms of the representation matrices this becomes

$$D^*(R) = D\left(e^{i\pi J_2}\right)\ D(R)\ D\left(e^{-i\pi J_2}\right), \tag{C.3.7}$$

so we require $D\left(e^{\pm i\pi J_2}\right)$ in order to completely relate $D^*(R)$ to $D(R)$. The representation of $e^{i\pi J_2}$ may be simply determined in the spin-j representation as follows. First, since it represents a 180° rotation about the y-axis its action must flip the z-component of spin. It therefore follows that

$$D\left(e^{i\pi J_2}\right)_{\sigma'\sigma} = \eta(\sigma)\delta_{\sigma',-\sigma}, \tag{C.3.8}$$

where $\eta(\sigma)$ must be both real—since J_2 is imaginary—and a phase—because $D\left(e^{i\pi J_2}\right)$ is unitary. Clearly therefore $\eta(\sigma)$ is simply a sign. The sign may be fixed from the known value for a 340^o rotation: $D\left(e^{2i\pi J_2}\right) = (-)^{2j}$ from which we derive

$$\eta(\sigma)\eta(-\sigma) = (-)^{2j}. \tag{C.3.9}$$

This has as its solution: $\eta(\sigma) = (-)^{j+\sigma}$, and so

$$\begin{aligned} & D\left(e^{+i\pi J_2}\right)_{\sigma'\sigma} = (-)^{j+\sigma}\delta_{\sigma',-\sigma} \\ \text{so}: \quad & D\left(e^{-i\pi J_2}\right)_{\sigma'\sigma} = (-)^{j+\sigma}\delta_{\sigma,-\sigma'} = (-)^{-j-\sigma}\delta_{\sigma,-\sigma'}. \end{aligned} \tag{C.3.10}$$

The derivation of this last equation uses the fact that $2(j+\sigma)$ is an even number and so therefore $(-)^{j\pm\sigma} = (-)^{-j\mp\sigma}$. The same reasoning also implies $(-)^{\sigma'\pm\sigma} = (-)^{-\sigma'\mp\sigma}$.

Putting these expressions together then gives the desired expression relating $D(R)$ to $D^*(R)$:

$$D^{(j)}_{\sigma'\sigma}(R) = (-)^{\sigma-\sigma'}D^{(j)*}_{-\sigma',-\sigma}(R) = (-)^{j+\sigma}D^{(j)*}_{-\sigma',-\sigma}(R)(-)^{-j-\sigma'}, \tag{C.3.11}$$

and using this in the transformation law for $a^\star_{\mathbf{p}\sigma}$ then gives

$$\begin{aligned} U(\Lambda)\left[(-)^{j-\sigma}\ a^\star_{\mathbf{p},-\sigma}\right]U^{-1}(\Lambda) &= (-)^{j-\sigma}\sqrt{\frac{\varepsilon(\Lambda p)}{\varepsilon(p)}}\ \sum_{\sigma'} D^{(j)}_{\sigma',-\sigma}[W(\Lambda,\mathbf{p}/m)]\ a^\star_{\mathbf{p},\sigma'} \\ &= \sqrt{\frac{\varepsilon(\Lambda p)}{\varepsilon(p)}}\ \sum_{\sigma'}(-)^{-j-\sigma'}\ D^{(j)*}_{-\sigma',\sigma}[W(\Lambda,\mathbf{p}/m)]\ a^\star_{\mathbf{p},\sigma'} \\ &= \sqrt{\frac{\varepsilon(\Lambda p)}{\varepsilon(p)}}\ \sum_{\sigma'}(-)^{j-\sigma'}\ D^{(j)*}_{\sigma'\sigma}[W(\Lambda,\mathbf{p}/m)]\ a^\star_{\mathbf{p},-\sigma'}, \end{aligned} \tag{C.3.12}$$

in which the identity $(-)^{-j+\sigma'} = (-)^{j-\sigma'}$ is used in obtaining the last equality. Comparing this last expression to (C.3.3) (or (11.3.8)) gives the result that was to be proven: the operators $(-)^{j-\sigma}a^\star_{\mathbf{p},-\sigma}$ and $a_{\mathbf{p},\sigma}$ transform in the same way.

The final step in establishing eq. (C.3.2) then follows by relabelling $\sigma \to -\sigma$ in the sum appearing in eq. (C.3.1) and then multiplying by unity in the form $[(-)^{j-\sigma}]^2$. The equivalence of the transformation law for $(-)^{j-\sigma}\overline{a}^\star_{\mathbf{p},-\sigma}$ with that of $\overline{a}_{\mathbf{p},\sigma}$ together with the uniqueness of the mode functions for particles of given transformation properties then implies that $[v_n(\mathbf{p},-\sigma)(-)^{j-\sigma}]$ must be proportional to $u_n(\mathbf{p},\sigma)$. This proves the claim made in eq. (C.3.2).

Combining eqs. (C.3.1) and (C.3.2) gives the final general expansion law for a relativistic field

$$\psi_n(x) = \sum_\sigma \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\, u_n(\mathbf{p}\sigma)\Big[a_{\mathbf{p},\sigma}\, e^{ip\cdot x} + \xi(-)^{j-\sigma}\, \overline{a}^\star_{\mathbf{p}\sigma}\, e^{-ip\cdot x}\Big]. \tag{C.3.13}$$

C.3.2 Crossing Symmetry and the Spin-Statistics Connection

Having established the proper form for the field operators, $\psi_n(x)$, dictated by Lorentz covariance the next step is to compute the commutation relations of the field with its adjoint at spacelike separations. We are interested in the conditions under which this vanishes. For bosons (or fermions) we compute the commutator (or anticommutator) as in §11.4.

Consider, then, two fields $\psi^{AB}_{ab}(x)$, and $\psi^{\widetilde{A}\widetilde{B}}_{\tilde{a}\tilde{b}}(y)$, that both represent the same particle type (such as a particle of mass m and spin j). Their (anti) commutator is:

$$\Big[\psi^{AB}_{ab}(x), \psi^{\widetilde{A}\widetilde{B}\star}_{\tilde{a}\tilde{b}}(y)\Big]_\mp = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\left[\frac{m}{\varepsilon(p)}\,\Pi^{AB\widetilde{A}\widetilde{B}}_{ab\tilde{a}\tilde{b}}(\mathbf{p})\right]\Big[e^{ip\cdot(x-y)} \mp \xi\tilde{\xi}^*\, e^{-ip\cdot(x-y)}\Big], \tag{C.3.14}$$

which writes the polarization sum as

$$\Pi^{AB\widetilde{A}\widetilde{B}}_{ab\tilde{a}\tilde{b}}(\mathbf{p}) := \frac{\varepsilon(p)}{m}\sum_\sigma u^{AB}_{ab}(\mathbf{p},\sigma)\; u^{*\widetilde{A}\widetilde{B}}_{\tilde{a}\tilde{b}}(\mathbf{p},\sigma). \tag{C.3.15}$$

This function is evaluated in detail below, but the only property it has on which the remainder of the argument is based is its behaviour when $\mathbf{p} \to -\mathbf{p}$. As is shown below — and suppressing the various indices for clarity — $\Pi(\mathbf{p})$ may be written in the general form

$$\Pi(\mathbf{p}) = P_1(\mathbf{p}) + \varepsilon(p)\; P_2(\mathbf{p}) \tag{C.3.16}$$

in which $P_1(\mathbf{p})$ and $P_2(\mathbf{p})$ are polynomials in $\mathbf{p}$ with the following symmetry properties

$$P_1(-\mathbf{p}) = (-)^{2(A+\widetilde{B})}P_1(\mathbf{p}) \quad \text{and} \quad P_2(-\mathbf{p}) = -(-)^{2(A+\widetilde{B})}P_2(\mathbf{p}). \tag{C.3.17}$$

Returning now to commutator (C.3.14), focus on spacelike separation $x-y$ and choose the frame in which $x^0 = y^0 = t$. Then

$$\Big[\psi(\mathbf{x},t), \tilde{\psi}^\star(\mathbf{y},t)\Big]_\mp = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\, \frac{m}{\varepsilon(p)}\Big[\Pi(\mathbf{p}) \mp \xi\tilde{\xi}^*\Pi(-\mathbf{p})\Big]. \tag{C.3.18}$$

Using the symmetry property for $\Pi(\mathbf{p})$ given in eqs. (C.3.17) then gives

$$\Big[\psi(x),\tilde{\psi}^\star(y)\Big]_\mp = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\, \frac{m}{\varepsilon(p)} \Big[P_1(\mathbf{p})\left(1\mp(-)^{2(A+\widetilde{B})}\xi\tilde{\xi}^*\right) \\ +\varepsilon(p)P_2(\mathbf{p})\left(1\pm(-)^{2(A+\widetilde{B})}\xi\tilde{\xi}^*\right)\Big]\,. \tag{C.3.19}$$

Of these, because of the cancellation of $\varepsilon(p)$ the second term can be written in position space as being proportional to

$$\int \frac{\mathrm{d}^3p}{(2\pi)^3} P_2(\mathbf{p})\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} = P_2(-i\nabla)\delta^3(\mathbf{x}-\mathbf{y}) \tag{C.3.20}$$

and consequently vanishes for $\mathbf{x}\neq\mathbf{y}$. (The delta-function divergence at $\mathbf{x}=\mathbf{y}$ will eventually need to be handled, because it does come back to bite us later.)

The result for spacelike $x-y$ with $\mathbf{x}\neq\mathbf{y}$ therefore becomes

$$\Big[\psi(x),\tilde{\psi}^\star(y)\Big]_\mp = P_1(-i\nabla)\int \frac{\mathrm{d}^3p}{(2\pi)^3}\,\frac{m}{\varepsilon(p)}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\Big[1\mp(-)^{2(A+\widetilde{B})}\xi\tilde{\xi}^*\Big]\,, \tag{C.3.21}$$

and so if this is to vanish we must impose

$$\pm(-)^{2(A+\widetilde{B})}\xi\tilde{\xi}^* = 1. \tag{C.3.22}$$

This is the condition required to enforce microcausality in the general case.

To understand the implications of (C.3.22) consider first the special case where both fields, $\psi(x)$ and $\tilde{\psi}(x)$, transform in the same Lorentz representation: $A=\widetilde{A}$ and $B=\widetilde{B}$. In this case the modulus and phase of condition (C.3.22) gives two real conditions

$$(i)\quad |\xi|=1 \qquad \text{and} \qquad (ii)\quad \pm\,(-)^{2(A+B)} = 1. \tag{C.3.23}$$

Condition (i) is the general expression of crossing symmetry, as was found for scalar fields earlier. It implies that for *all* fields the particle and anti-particle parts enter into all interaction with equal strength.

Condition (ii) contains the *spin-statistics* theorem. To see this notice that the spin j must lie in the range $j\in\{|A-B|,\cdots,A+B\}$ and so j differs from $A+B$ by an integer. It follows that $(-)^{2(A+B)}$ is the same as $(-)^{2j}$. As a result condition (ii) may be rewritten

$$\pm(-)^{2j} = \pm(-)^{2(A+B)} = 1. \tag{C.3.24}$$

Keeping in mind that the initial sign, $\pm$, is determined by the particle's statistics — with the upper sign applying for bosons and the lower sign applying for fermions — it follows that all integer-spin particles must satisfy Bose statistics while all half-odd-integer spin particles must be fermions.

Consider next the general case of eq. (C.3.22) but take the fields $\psi(x)$ and $\tilde{\psi}(x)$ as not being identical. In this case, using the spin-statistics connection eq. (C.3.24) to write $\pm(-)^{2A} = (-)^{2B}$, eq. (C.3.22) becomes

$$(-)^{2(B+\tilde{B})}\xi\tilde{\xi}^* = 1. \tag{C.3.25}$$

Since $\tilde{\xi}$ is a phase, its inverse is $\tilde{\xi}^{-1} = \tilde{\xi}^*$. This allows eq. (C.3.25) to be written more suggestively as

$$\xi_0 := (-)^{2B}\xi = (-)^{2\tilde{B}}\tilde{\xi}. \tag{C.3.26}$$

The content of this last condition is that ξ_0 is a phase that is independent of the kind of field used to describe the particle in question. It can therefore be absorbed into the definition of the creation operator, $\overline{a}^*_{\mathbf{p}\sigma}$, for the antiparticle.

There are two cases that need to be considered separately, depending on whether or not the particle and antiparticle are distinct. On one hand, if $a_{\mathbf{p}\sigma} \neq \overline{a}_{\mathbf{p}\sigma}$ then ξ_0 may be simply absorbed into $\overline{a}_{\mathbf{p}\sigma}$. On the other hand, if $a_{\mathbf{p}\sigma} = \overline{a}_{\mathbf{p}\sigma}$ then the phase of the particle and antiparticle creation operators are related to one another. In this case redefine $a_{\mathbf{p}\sigma} \to \xi_0^{\frac{1}{2}}\, a_{\mathbf{p}\sigma}$, which implies that $a^* \to \xi_0^{-\frac{1}{2}}\, a^*_{\mathbf{p}\sigma}$. Then ξ_0 becomes simply an overall factor that can be absorbed into the overall normalization of $\psi(x)$.

In either case this shows there is no loss of generality in choosing the convention $\xi_0 = 1$. As a result we then have $\xi = (-)^{2B}$ and the field expansion of eq. (C.3.1) finally becomes:

$$\psi^{(A,B)}_{ab}(x) = \sum_\sigma \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\, u_{ab}(\mathbf{p},\sigma)\left[a_{\mathbf{p}\sigma}\, e^{ip\cdot x} + (-)^{2B}(-)^{j-\sigma}\, \overline{a}^\star_{\mathbf{p}\sigma}\, e^{-ip\cdot x}\right]. \tag{C.3.27}$$

Properties of $\Pi(\mathbf{p})$

This section is completes the argument by computing the properties of the function $\Pi(\mathbf{p})$ that arose in the previous section. We prove in particular property (C.3.17) concerning its symmetry under the reflection: $\mathbf{p} \to -\mathbf{p}$.

The starting point is to insert expression (C.2.8) for $u_{ab}(\mathbf{p},\sigma)$ (repeated here)

$$u_{ab}(\mathbf{k},\sigma) = \sqrt{\frac{m}{\varepsilon(k)}} \sum_{a'b'} \left[\exp\left(-\phi\,\hat{\mathbf{k}}\cdot\vec{\mathcal{A}}^{(A)}\right)\right]_{aa'} \left[\exp\left(+\phi\,\hat{\mathbf{k}}\cdot\vec{\mathcal{B}}^{(B)}\right)\right]_{bb'} C_{AB}(j,\sigma;a',b'). \tag{C.3.28}$$

into definition (10.3.15) for $\Pi(\mathbf{p})$, leading to

$$\begin{aligned}\Pi^{AB\tilde{A}\tilde{B}}_{ab\tilde{a}\tilde{b}}(\mathbf{p}) &\equiv \frac{\varepsilon(p)}{m}\sum_\sigma u^{AB}_{ab}(\mathbf{p},\sigma)\, u^{*\tilde{A}\tilde{B}}_{\tilde{a}\tilde{b}}(\mathbf{p},\sigma) \qquad\qquad (C.3.29)\\ &= \sum_{a'b'\tilde{a}'\tilde{b}'} C_{AB}(j,\sigma;a',b')\, C_{\tilde{A}\tilde{B}}(j,\sigma;\tilde{a}'\tilde{b}') \left[\exp\left(-\phi\,\hat{\mathbf{p}}\cdot\vec{\mathcal{A}}^{(A)}\right)\right]_{aa'} \left[\exp\left(+\phi\,\hat{\mathbf{p}}\cdot\vec{\mathcal{B}}^{(B)}\right)\right]_{bb'}\\ &\qquad\qquad \times \left[\exp\left(-\phi\,\hat{\mathbf{p}}\cdot\vec{\mathcal{A}}^{(\tilde{A})}\right)\right]^*_{\tilde{a}\tilde{a}'} \left[\exp\left(+\phi\,\hat{\mathbf{p}}\cdot\vec{\mathcal{B}}^{(\tilde{B})}\right)\right]^*_{\tilde{b}\tilde{b}'}.\end{aligned}$$

This form is not easy to use since it involves many factors of the relatively complicated exponential matrices. It is therefore convenient to use some of the properties of $SU(2)$ to reduce things down to an expression involving a single exponential.

The first step in evaluating this expression for $\Pi(\mathbf{p})$ is to use the following Clebsch-Gordan identity:

$$\sum_{\sigma} C_{AB}(j,\sigma;a',b')\, C_{\widetilde{A}'\widetilde{B}'}(j,\sigma;\tilde{a}',\tilde{b}') = \sum_{\ell\nu}(2j+1)(-)^{A+\tilde{A}-\nu-\tilde{b}'-\tilde{a}'} W(A,B,\tilde{B},\tilde{A},j,\ell) \times C_{A\widetilde{B}}(\ell,\nu;a',-\tilde{b}')\, C_{B\widetilde{A}}(\ell,-\nu;b',-\tilde{a}'), \tag{C.3.30}$$

in which $W(A,B,\tilde{B},\tilde{A},j,\ell)$ is known as a *Racah coefficient*. This identity expresses the fact that there are two ways to think about the scalar that is constructed from the tensor product of two given representations, (A,B) and $(\tilde{B},\tilde{A})$. The scalar may either be thought of as being the product of the rotational scalars that are within the reduction of each separate representation, (A,B) and $(\tilde{B},\tilde{A})$, or it may equivalently be constructed by first building scalars from $A\otimes\tilde{B}$ and from $B\otimes\tilde{A}$ and then multiplying these. The above identity gives the relation between these two ways of thinking about the scalars so obtained.

The complex conjugates of the Lorentz matrices that appear in eq. (C.3.29) may be rewritten using the identity (C.3.11) which in the present instance becomes:

$$\Big[\exp(\pm\phi\,\hat{\mathbf{p}}\cdot\mathbf{J})\Big]^*_{aa'} = (-)^{a'-a}\Big[\exp(\mp\phi\,\hat{\mathbf{p}}\cdot\mathbf{J})\Big]_{-a,-a'}. \tag{C.3.31}$$

(The extra sign change did not appear in the exponent for the rotations considered earlier because of the additional factor of i that is present in that case.)

The final useful identity to be used is

$$\sum_{\nu'}\Big[\exp\Big(-\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\Big)\Big]_{\nu\nu'} C_{A\widetilde{B}}(\ell,\nu';a,-\tilde{b}) = \sum_{a',\tilde{b}'}\Big[\exp\Big(-\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(A)}\Big)\Big]_{aa'}\Big[\exp\Big(-\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(B)}\Big)\Big]_{\tilde{b},\tilde{b}'} C_{A\widetilde{B}}(\ell,\nu;a',-\tilde{b}') \tag{C.3.32}$$

which just expresses that the Clebsch-Gordan coefficient projects out all but the 'spin-ℓ' part of the rotation.

Putting all of these identities into eq. (C.3.29) gives

$$\Pi^{AB\widetilde{A}\widetilde{B}}_{ab\tilde{a}\tilde{b}}(\mathbf{p}) = \sum_{\ell\nu\nu'b'\tilde{a}'}\Big[\exp\Big(+\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\tilde{A})}\Big)\Big]_{-\tilde{a},-\tilde{a}'}\Big[\exp\Big(+\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(B)}\Big)\Big]_{bb'} \times(2j+1)(-)^{A+\tilde{A}-\nu-\tilde{a}-\tilde{b}}\, W(A,B,\tilde{B},\tilde{A},j,\ell) \times C_{B\widetilde{A}}(\ell,-\nu;b',-\tilde{a}')\, C_{A\widetilde{B}}(\ell,\nu';a,-\tilde{b})\Big[\exp\Big(-\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\Big)\Big]_{\nu\nu'}. \tag{C.3.33}$$

Using identity (10.3.32) once more to do the sum over $\tilde{a}'$ and $\tilde{b}'$ then gives

$$\Pi^{AB\tilde{A}\tilde{B}}_{ab\tilde{a}\tilde{b}}(\mathbf{p}) = \sum_{\ell\nu\nu'\nu''} \left[\exp\left(+\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right]_{-\nu,-\nu''} \left[\exp\left(-\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right]_{\nu\nu'} \tag{C.3.34}$$
$$\times(2j+1)(-)^{A+\tilde{A}-\nu-\tilde{a}-\tilde{b}}\, W(A,B,\tilde{B},\tilde{A},j,\ell)$$
$$\times C_{A\tilde{B}}(\ell,\nu';a,-\tilde{b})C_{B\tilde{A}}(\ell,-\nu'';b,-\tilde{a}).$$

The final step is to use (C.3.31) and the fact that $\exp(-\phi\hat{\mathbf{p}}\mathbf{J})$ is Hermitian to write

$$\left[\exp\left(\phi\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right]_{-\nu,-\nu''} = (-)^{\nu-\nu''}\ \left[\exp\left(-\phi\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right]^*_{\nu\nu''} = (-)^{\nu-\nu''}\ \left[\exp\left(-\phi\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right]_{\nu''\nu}. \tag{C.3.35}$$

At this point the sum over ν can be performed since it is simply matrix multiplication, leaving

$$\Pi^{AB\tilde{A}\tilde{B}}_{ab\tilde{a}\tilde{b}}(\mathbf{p}) = \sum_{\ell\nu'\nu''} \left[\exp\left(-2\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right]_{\nu'',\nu'} (2j+1)(-)^{A+\tilde{A}-\nu''-\tilde{a}-\tilde{b}} \tag{C.3.36}$$
$$\times W(A,B,\tilde{B},\tilde{A},j,\ell)\ C_{A\tilde{B}}(\ell,\nu';a,-\tilde{b})\ C_{B\tilde{A}}(\ell,-\nu'';b,-\tilde{a})\,.$$

This is the final form with which to demonstrate property (C.3.17).

The trick is to re-express the exponential in terms of the momentum $\mathbf{p}$. To do so use the fact that the matrix $2\hat{\mathbf{p}}\cdot\mathbf{J}$ has integer eigenvalues, which allows use of the following expansions — *c.f.* Gradshteyn and Ryzhik page 28 item (1-332). For k an even integer the following multiple-angle identities are true:

$$\sinh(k\phi) = k\,\cosh\phi\left[\sinh\phi + \frac{k^2-2^2}{3!}\sinh^3\phi + \right.$$
$$\left. + \frac{(k^2-2^2)(k^2-4^2)}{5!}\sinh^5\phi + \cdots\right] \tag{C.3.37}$$
$$\text{and}\quad \cosh(k\phi) = 1 + \frac{k^2}{2!}\sinh^2\phi + \frac{k^2(k^2-2^2)}{4!}\sinh^4\phi +$$
$$+\frac{k^2(k^2-2^2)(k^2-4^2)}{6!}\sinh^6\phi + \cdots,$$

while for k an odd integer the analogous expansions are

$$\sinh(k\phi) = k\left[\sinh\phi + \frac{k^2-1^2}{3!}\sinh^3\phi + \frac{(k^2-1^2)(k^2-3^2)}{5!}\sinh^5\phi + \cdots\right]$$
$$\cosh(k\phi) = \cosh\phi\left[1 + \frac{k^2-1^2}{2!}\sinh^2\phi + \frac{(k^2-1^2)(k^2-3^2)}{4!}\sinh^4\phi + \cdots\right]. \tag{C.3.38}$$

Notice that the right-hand side in all four of these expansions are polynomials in $\cosh\phi$ and $\sinh\phi$ because the series that appears in each case terminates after a finite number of terms.

Combining these allow the exponentials that appear in $\Pi(\mathbf{p})$ to be expanded in a terminating series in powers of $\cosh\phi$ and $\sinh\phi$, with

$$e^{-k\phi} = 1 + \frac{k}{2}\sinh\phi\,(k\sinh\phi - 2\cosh\phi) + \sum_{r=1}^{\frac{1}{2}(k-2)} \frac{k(k^2-2^2)\cdots(k^2-(2r)^2)}{(2r+2)!}\sinh^{2r+1}\phi\,[k\sinh\phi - (2r+2)\cosh\phi]\,, \tag{C.3.39}$$

for k even, while for k odd one instead finds

$$e^{-k\phi} = (\cosh\phi - k\sinh\phi) + \sum_{r=1}^{\frac{1}{2}(k-1)} \frac{(k^2-1^2)\cdots(k^2-(2r-1)^2)}{(2r+1)!}\sinh^{2r}\phi\,[(2r+1)\cosh\phi - k\sinh\phi]\,. \tag{C.3.40}$$

These expansions can be applied as matrix equations with the integer k replaced by $2\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}$ because this matrix has integer eigenvalues. Using the relations (C.2.4) — *i.e.* $\cosh\phi = \varepsilon(p)/m$ and $\sinh\phi = |\mathbf{p}|/m$, one then finds for 2ℓ even

$$\left[\exp\left(-2\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right] = 1 + \frac{2\mathbf{p}\cdot\mathbf{J}^{(\ell)}}{m}\left[\frac{\mathbf{p}\cdot\mathbf{J}^{(\ell)} - \varepsilon(p)}{m}\right] + \sum_{r=1}^{\ell-1} \frac{(2\mathbf{p}\cdot\mathbf{J}^{(\ell)})\left[(2\mathbf{p}\cdot\mathbf{J}^{(\ell)})^2 - 2^2\mathbf{p}^2\right]\cdots\left[(2\mathbf{p}\cdot\mathbf{J}^{(\ell)})^2 - (2r)^2\mathbf{p}^2\right]}{(2r+2)!\;\; m^{2r+1}} \times\left\{\frac{2\mathbf{p}\cdot\mathbf{J}^{(\ell)} - (2r+2)\varepsilon(p)}{m}\right\}, \tag{C.3.41}$$

while for 2ℓ odd

$$\left[\exp\left(-2\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right] = \left(\frac{\varepsilon(p) - 2\mathbf{p}\cdot\mathbf{J}^{(\ell)}}{m}\right) + \sum_{r=1}^{\ell-\frac{1}{2}} \frac{[(2\mathbf{p}\cdot\mathbf{J}^{(\ell)})^2 - \mathbf{p}^2]\cdots[(2\mathbf{p}\cdot\mathbf{J}^{(\ell)})^2 - (2r-1)^2\mathbf{p}^2]}{(2r+1)!\;\; m^{2r}} \times\left\{\frac{(2r+1)\varepsilon(p) - (2\mathbf{p}\cdot\mathbf{J}^{(\ell)})}{m}\right\}. \tag{C.3.42}$$

These are finally in a form that allows their behaviour as $\mathbf{p}\to-\mathbf{p}$ to be made explicit. For 2ℓ even (C.3.41) implies

$$\left[\exp\left(-2\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right] = P_1^{(\ell)}(\mathbf{p}) + \varepsilon(p)\,P_2^{(\ell)}(\mathbf{p}), \tag{C.3.43}$$

where $P_1^{(\ell)}(\mathbf{p})$ and $P_2^{(\ell)}(\mathbf{p})$ are polynomials that satisfy

$$P_1^{(\ell)}(-\mathbf{p}) = P_1^{(\ell)}(\mathbf{p}) \quad\text{and}\quad P_2^{(\ell)}(-\mathbf{p}) = -P_2^{(\ell)}(\mathbf{p}) \qquad (2\ell \text{ even}). \tag{C.3.44}$$

Similarly, for 2ℓ odd one instead finds

$$\left[\exp\left(-2\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right] = P_1^{(\ell)}(\mathbf{p}) + E_p P_2^{(\ell)}(\mathbf{p}), \tag{C.3.45}$$

where

$$P_1^{(\ell)}(-\mathbf{p}) = -P_1^{(\ell)}(\mathbf{p}) \quad \text{and} \quad P_2^{(\ell)}(-\mathbf{p}) = P_2^{(\ell)}(\mathbf{p}) \qquad (2\ell \text{ odd}). \tag{C.3.46}$$

Expressions (C.3.44) and (C.3.46) may be summarized for all ℓ as

$$\left[\exp\left(-2\phi\,\hat{\mathbf{p}}\cdot\mathbf{J}^{(\ell)}\right)\right]_{\nu\nu'} = \left[P_1^{(\ell)}(\mathbf{p})\right]_{\nu\nu'} + \varepsilon(p)\ \left[P_2^{(\ell)}(\mathbf{p})\right]_{\nu\nu'}, \tag{C.3.47}$$

with

$$\left[P_1^{(\ell)}(-\mathbf{p})\right]_{\nu\nu'} = (-)^{2\ell}\ \left[P_1^{(\ell)}(\mathbf{p})\right]_{\nu\nu'} \quad \text{and} \quad \left[P_2^{(\ell)}(-\mathbf{p})\right]_{\nu\nu'} = -(-)^{2\ell}\ \left[P_2^{(\ell)}(\mathbf{p})\right]_{\nu\nu'}. \tag{C.3.48}$$

Furthermore, the dependence on 2ℓ in these last expressions may be exchanged for dependence on $2(A+\tilde{B})$ since the Clebsch-Gordan coefficient guarantees their equality $\pmod 2$. This is because the Clebsch-Gordan coefficient vanishes unless $\ell \in \{|A-\tilde{B}|, |A-\tilde{B}+1, \cdots, A+\tilde{B}-1, A+\tilde{B}\}$. One of the consequences of this is $A+\tilde{B}$ differs from ℓ by an integer, and so $(-)^{2\ell} = (-)^{2(A+\tilde{B})}$. It also follows that the symmetry of the polynomials $P_1^{(\ell)}$ and $P_2^{(\ell)}$ is the same for all terms in the sum over ℓ that appear in the expression for Π. That is

$$\begin{aligned} \Pi^{AB\tilde{A}\tilde{B}}_{ab\tilde{a}\tilde{b}}(\mathbf{p}) &= \left[P_1^{AB\tilde{A}\tilde{B}}\right]_{ab\tilde{a}\tilde{b}}(\mathbf{p}) + \varepsilon(p)\ \left[P_2^{AB\tilde{A}\tilde{B}}\right]_{ab\tilde{a}\tilde{b}}(\mathbf{p}) \\ \text{with}: \quad P_1(-\mathbf{p}) &= (-)^{2(A+\tilde{B})}\ P_1(\mathbf{p}) \\ \text{and}: \quad P_2(-\mathbf{p}) &= -(-)^{2(A+\tilde{B})}\ P_2(\mathbf{p}). \end{aligned} \tag{C.3.49}$$

as is claimed in eq. (C.3.17).

C.4 C, P, T for general spin

This Appendix works out how improper Lorentz transformations and charge conjugation are represented on local fields transforming in a general (A, B) representation, and in particular finds the consequences of microcausality for these transformations.

C.4.1 Charge Conjugation

Charge conjugation is defined as the operation that interchanges particles with their antiparticles without changing their momentum or components of spin,

$$a^\star_{\mathbf{p}\sigma}|0\rangle \to \eta_c\, \overline{a}^\star_{\mathbf{p}\sigma}|0\rangle, \tag{C.4.1}$$

in which η_c is a phase that can differ according to the type of particle that is involved. The action of $\mathcal{C}$ on many-particle states is to similarly replace all particles in the state by the corresponding antiparticles. The no-particle state, $|0\rangle$, is chosen to be invariant.

Since its definition acts linearly (or possibly antilinearly) on states, it may be represented in the Hilbert space by an operator, $\mathcal{C}$, and (C.4.1) implies

$$\mathcal{C}\; a_{\mathbf{p}\sigma}\; \mathcal{C}^{-1} = \eta_c^*\; \overline{a}_{\mathbf{p}\sigma} \quad \text{and} \quad \mathcal{C}\; \overline{a}_{\mathbf{p}\sigma}\; \mathcal{C}^{-1} = \bar{\eta}_c^* a_{\mathbf{p}\sigma}. \tag{C.4.2}$$

The charge-conjugation phases for particle and antiparticle, η_c and $\bar{\eta}_c$, need not *a priori* have been related, although they do turn out to be related by causality, as is demonstrated below.

Because it is defined not to change any of the particle labels such $\mathbf{k}$ or σ, charge conjugation commutes with Poincaré transformations, and so in particular

$$\mathcal{C}\; U(\Lambda = 1, a)\; \mathcal{C}^{-1} = U(\Lambda = 1, a), \tag{C.4.3}$$

and this in turn implies

$$\mathcal{C}\; iP^0\; \mathcal{C}^{-1} = iP^0. \tag{C.4.4}$$

Consistency of this last equation with the Hamiltonian, $H = P^0$, having a spectrum that is bounded from below implies that $\mathcal{C}$ cannot be antilinear and so must be represented a linear transformation.

Microcausality implies that $a_{\mathbf{p}\sigma}$ and $\overline{a}_{\mathbf{p}\sigma}$ appear in H only together in the combination $\psi_{ab}(x)$, and the next paragraphs derive how $\psi_{ab}(x)$ transforms rule and what its consistency implies for the relation between η_c and $\bar{\eta}_c$.

Using (C.4.2) in the field expansion (C.3.13) with the mode functions from (C.2.8) implies

$$\begin{aligned}\mathcal{C}\; \psi_{\,ab}(x)\; \mathcal{C}^{-1} = \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}} \sqrt{\frac{m}{E_p}} \sum_{a'b'\sigma} \Big[\exp\Big(-\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(A)}\Big)\Big]_{aa'} \Big[\exp\Big(+\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(B)}\Big)\Big]_{bb'} \\ \times C_{AB}(j,\sigma;a',b') \left[\overline{a}_{\mathbf{p}\sigma}\; \eta_c^* e^{ipx} + (-)^{2B}(-)^{j-\sigma}\bar{\eta}_c\; a^*_{\mathbf{p},-\sigma}\; e^{-ipx}\right].\end{aligned} \tag{C.4.5}$$

Now, since the expansion of $\psi_{ab}(x)$ in terms of creation and annihilation operators is unique up to normalization consistency with Lorentz transformation properties requires that the phase η_c only enter as an overall common factor in this expression, which is only possible if

$$\bar{\eta}_c = \eta_c^*. \tag{C.4.6}$$

If particle and antiparticle should be identical then this last condition implies $\eta_c = \eta_c^* = \pm 1$ (but not otherwise).

Using (C.4.6), the transformation rule for the field becomes

$$\mathcal{C}\; \psi_{ab}(x)\; \mathcal{C}^{-1} = \eta_c^*\; \tilde{\psi}_{ab}(x), \tag{C.4.7}$$

in which $\tilde{\psi}_{ab}(x)$ is by definition given by the standard expansion for a field, *e.g.* (C.3.13), but in which $a_{\mathbf{p}\sigma} \leftrightarrow \overline{a}_{\mathbf{p}\sigma}$ are interchanged:

$$\tilde{\psi}_{ab}(x) = \sum_\sigma \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}}\; u_{ab}(\mathbf{p}\sigma) \Big[\overline{a}_{\mathbf{p},\sigma}\; e^{ip\cdot x} + \xi(-)^{j-\sigma}\; a^\star_{\mathbf{p}\sigma}\; e^{-ip\cdot x}\Big]. \tag{C.4.8}$$

Notice that because $\psi_{ab}(x)$ depends on $a_{\mathbf{p}\sigma}$ but on the adjoint $\overline{a}^\star_{\mathbf{p}\sigma}$ this means that $\tilde{\psi}_{ab}(x)$ transforms in the (B,A) representation whenever $\psi_{ab}(x)$ transforms in the (A,B) representation. Consequently it can be described as a transformation that takes ψ_{ab} to $\psi^\star_{ab}$. To see this explicitly we therefore now establish the precise connection between this Hermitian conjugate field and $\tilde{\psi}_{ab}(x)$.

Taking the adjoint of (C.3.13) with the mode functions from (C.2.8) gives

$$\psi^\star_{ab}(x) = \sum_{a'b'\sigma} \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}} \sqrt{\frac{m}{E_p}} \left[\exp\left(-\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(A)}\right)\right]^*_{aa'} \left[\exp\left(+\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(B)}\right)\right]^*_{bb'} \times C_{AB}(j,\sigma;a',b')\Big[a^\star_{\mathbf{p}\sigma}\, e^{-ip\cdot x} + (-)^{2B}(-)^{j-\sigma}\overline{a}_{\mathbf{p},-\sigma}\, e^{ip\cdot x}\Big]. \tag{C.4.9}$$

This may be simplified by relabelling $a' \to -a'$, $b' \to -b'$ and $\sigma \to -\sigma$; and using the identities (C.3.11) as well as $C_{AB}(j,\sigma;a',b') = C_{BA}(j,-\sigma;-b',-a')$, leading to

$$\psi^\star_{ab}(x) = \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}} \sqrt{\frac{m}{E_p}} \sum_{a'b'\sigma} \left[\exp\left(-\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(B)}\right)\right]_{-b,b'} \left[\exp\left(+\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(A)}\right)\right]_{-a,a'} \times (-)^{a+a'}(-)^{b+b'} C_{BA}(j,\sigma;b',a')\Big[(-)^{2B}(-)^{j+\sigma}\,\overline{a}_{\mathbf{p}\sigma}\, e^{ip\cdot x} + a^\star_{\mathbf{p},-\sigma}\, e^{-ip\cdot x}\Big]. \tag{C.4.10}$$

Finally use $(-)^{j+\sigma} = (-)^{-j-\sigma}$ and so — since the Clebsch-Gordan coefficient vanishes unless $\sigma = a' + b'$: $(-)^{j+\sigma} = (-)^{-j-a'-b'}$, to find the final expression

$$\left[\psi^{AB}_{ab}(x)\right]^\star = (-)^{2B-j+a+b}\tilde{\psi}^{BA}_{-b,-a}(x) = (-)^{2B+j-a-b}\tilde{\psi}^{BA}_{-b,-a}(x). \tag{C.4.11}$$

Here superscripts like 'AB' are meant to emphasize the representation in which the corresponding field transforms.

Combining this with (C.4.7) the expression for the action of charge conjugation on the field operators becomes

$$\mathcal{C}\;\psi_{\,ab}(x)\;\mathcal{C}^{-1} = \eta_c^*(-)^{2A-j-a-b}\;\psi^\star_{-b,-a}(x). \tag{C.4.12}$$

C.4.2 Parity

The action of parity on single particle states found in (11.2.30) implies (for massive particle states) the transformation rule for creation and annihilation operators is

$$\mathcal{P}\; a_{\mathbf{p}\sigma}\; \mathcal{P}^{-1} = \eta_p^*\; a_{-\mathbf{p},\sigma} \quad \text{and} \quad \mathcal{P}\; \overline{a}_{\mathbf{p}\sigma}\; \mathcal{P}^{-1} = \bar{\eta}_p^*\; \overline{a}_{-\mathbf{p},\sigma}. \tag{C.4.13}$$

The implications of microcausality for the parity phases, $\bar{\eta}_p$ and η_p, can be obtained in the same manner as was done for charge-conjugation above. Because parity also turns out to map the (A,B) representation onto the (B,A) representation, in this section the representation of ψ is denoted explicitly, using a superscript: $\psi^{AB}_{ab}(x)$.

Direct application of transformation rule (C.4.13) to the field expansion (11.4.35) — or to (C.3.27) — gives, after changing integration variable $\mathbf{p} \to -\mathbf{p}$

$$\mathcal{P}\,\psi^{AB}_{ab}(x)\,\mathcal{P}^{-1} = \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\sqrt{\frac{m}{E_p}}\sum_{a'b'\sigma'}\Big[\exp\Big(+\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(A)}\Big)\Big]_{aa'}\Big[\exp\Big(-\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(B)}\Big)\Big]_{bb'} \tag{C.4.14}$$
$$\times C_{AB}(j,\sigma;a',b')\Big[\eta^*_p\,a_{\mathbf{p},\sigma}\,e^{ipx_p} + (-)^{2B}(-)^{j-\sigma}\,\overline{a}^{\star}_{\mathbf{p},-\sigma}\,\bar{\eta}_p\,e^{-ipx_p}\Big].$$

where $x^\mu_p := P^\mu{}_\nu x^\nu = (x^0, -\mathbf{x})$ denotes the parity-transformed coordinate. Next, use the identity $C_{AB}(j,\sigma;a',b') = (-)^{A+B-j}\,C_{BA}(j,\sigma;b',a')$. After doing so this expression has the same form as the original expansion of $\psi^{AB}_{ab}(x)$, eq. (C.3.27), in which the coefficient of $a_{\mathbf{p}\sigma}$ is $(-)^{A+B-j}\eta^*_p$ and that of $(-)^{2A}(-)^{j-\sigma}\overline{a}^*_{\mathbf{p}\sigma}$ is $\bar{\eta}_p(-)^{3B-A-j}$.

Two conclusions can be drawn from the this. First, we see that the condition of causality implies that particle and antiparticle parity phases are related by

$$\eta_p = (-)^{2B-2A}\,\bar{\eta}^*_p = (-)^{2(B+A)}\bar{\eta}^*_p = (-)^{2j}\bar{\eta}^*_p. \tag{C.4.15}$$

Second, the field transformation property is

$$\mathcal{P}\,\psi^{AB}_{ab}(x)\,\mathcal{P}^{-1} = (-)^{A+B-j}\eta^*_p\,\psi^{BA}_{ba}(x_p). \tag{C.4.16}$$

Notice that in the special case of self-conjugate particles, for which $a_{\mathbf{p}\sigma} = \overline{a}_{\mathbf{p}\sigma}$, condition (C.4.15) implies $\eta_p = \overline{\eta}_p = (-)^{2j}$, so for self-conjugate bosons the parity phase must be real, $\eta_p = \pm 1$, while for self-conjugate — or *majorana* — fermions it is imaginary, $\eta_p = \pm i$.

C.4.3 Time Reversal

Finally, the action on the fields of time reversal, $\mathcal{T}$, is governed by the transformation property

$$\mathcal{T}\,a_{\mathbf{p}\sigma}\,\mathcal{T}^{-1} = \eta^*_t(-)^{j-\sigma}\,a_{-\mathbf{p},-\sigma} \quad \text{and} \quad \mathcal{T}\,\overline{a}_{\mathbf{p}\sigma}\,\mathcal{T}^{-1} = \bar{\eta}^*_t(-)^{j-\sigma}\,\overline{a}_{-\mathbf{p},-\sigma}. \tag{C.4.17}$$

that is inherited from the transformation (11.2.30) of particle states. Since $\mathcal{T}$ must be antiunitary (see the discussion below (11.2.21)) the phase η_t can be be absorbed into the definition of the creation operator, $a_{\mathbf{p}\sigma}$.

As was done for C and P, this section now shows how $\bar{\eta}_t$ to η_t are related to one another by microcausality so that $\mathcal{T}$ can be defined to act on $\psi_{ab}(x)$. The fields transform according to

$$\mathcal{T}\,\psi_{ab}(x)\,\mathcal{T}^{-1} = \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\sqrt{\frac{m}{E_p}}\sum_{a'b'\sigma}\Big[\exp\Big(-\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(A)}\Big)\Big]^*_{aa'}\Big[\exp\Big(+\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(B)}\Big)\Big]^*_{bb'} \tag{C.4.18}$$
$$\times C_{AB}(j,\sigma;a',b')\left[e^{-ip\cdot x}\,\eta^*_t(-)^{j-\sigma}\,a_{-\mathbf{p},-\sigma} + (-)^{2B}(-)^{j-\sigma}(-)^{j+\sigma}\,\overline{a}^{\star}_{-\mathbf{p},\sigma}\,\bar{\eta}_t\,e^{ip\cdot x}\right].$$

Next use identity (C.3.11), change the integration variable from $\mathbf{p} \to -\mathbf{p}$, relabel the summations $a' \to -a'$, $b' \to -b'$ and $\sigma \to -\sigma$. Finally, use the Clebsch-Gordan identity:

$C_{AB}(j,\sigma,a',b') = (-)^{A+B-j}\, C_{AB}(j,-\sigma;-a',-b')$. The result is

$$\begin{aligned}\mathcal{T}\,\psi_{\,ab}(x)\,\mathcal{T}^{-1} = \int \frac{\mathrm{d}^3p}{(2\pi)^{3/2}}\sqrt{\frac{m}{E_p}}\sum_{a'b'\sigma}\Big[\exp\Big(\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(A)}\Big)\Big]_{-a,a'}(-)^{a+a'} \\ \times\Big[\exp\Big(+\theta\hat{\mathbf{p}}\cdot\mathbf{J}^{(B)}\Big)\Big]_{-b-b'}(-)^{b+b'}(-)^{A+B-j}\;C_{AB}(j,\sigma;a',b') \\ \times\Big[\eta_t^*(-)^{j+\sigma}\;e^{ip\cdot x_t}\;a_{\mathbf{p}\sigma}+\bar\eta_t(-)^{2B}(-)^{j-\sigma}\;\overline{a}^{\star}_{\mathbf{p},-\sigma}\;e^{-ip\cdot x_t}\Big].\end{aligned} \tag{C.4.19}$$

where the time-reversed coordinate is $x_t^\mu := T^\mu{}_\nu x^\nu = (-x^0,\mathbf{x})$.

Comparing the coefficient, $(-)^{A+B+a+b}\eta_t^*$, of $a_{\mathbf{p}\sigma}$ with the corresponding coefficient, $\bar\eta_t(-)^{A+B+a+b}$, of $(-)^{2B}(-)^{j-\sigma}\overline{a}^{\star}_{\mathbf{p},-\sigma}$ implies the relation between η_t and $\overline{\eta}_t$ is

$$\bar\eta_t = \eta_t^*\,, \tag{C.4.20}$$

which uses the relation $\sigma = a' + b'$ that is enforced by the Clebsch-Gordan coefficient. The field transformation law therefore becomes

$$\mathcal{T}\,\psi_{\,ab}(x)\,\mathcal{T}^{-1} = \eta_t^*(-)^{A+B-a-b}\;\psi_{-a,-b}(x_t). \tag{C.4.21}$$

D Lagrangian and Hamiltonian methods

A key role in both classical and quantum physics is played by a system's action, particularly for relativistic systems. This appendix is meant as a brief reminder of how this key quantities are motivated and defined, since lagrangian and Hamiltonian methods are often not encountered in modern undergraduate physics curricula. Particular attention is paid to the case where the underlying degrees of freedom are fields.

D.1 Lagrangian mechanics

A basic starting point is the reformulation of classical mechanics in terms of arbitrary coordinates. Consider, for example, the Newtonian equations of motion

$$m\ddot{\mathbf{x}} = -\nabla V\,, \tag{D.1.1}$$

for a particle with position $\mathbf{x}(t)$ moving under the influence of a conservative force with potential energy $V(\mathbf{x})$. The observation is that these equations are equivalent to those obtained by asking for the trajectory that extremizes the time integral of the difference between its kinetic and potential energy (called the system's 'action'):

$$S[\mathbf{x}(\tau)] = \int_{t_0}^{t}\mathrm{d}\tau\;\Big[\frac{m}{2}\,\dot{\mathbf{x}}\cdot\dot{\mathbf{x}} - V(\mathbf{x})\Big] \tag{D.1.2}$$

subject to the boundary conditions $\mathbf{x}(t_0) = \mathbf{x}_0$ and $\mathbf{x}(t) = \mathbf{x}$ (where – as usual – $\dot{\mathbf{x}}$ denotes $\mathrm{d}\mathbf{x}/\mathrm{d}t$). The integrand of the action is a rotational scalar called the system's 'lagrangian',

$L = L(\mathbf{x}, \dot{\mathbf{x}})$, defined to be the difference between the kinetic and potential energy evaluated along any trajectory.

The observation that the equations of motion follow from this action principle is a useful one because the value of the action being computed is a functional of the trajectory along which the integral is evaluated, and does not depend on which coordinates are used to describe this trajectory. And changing coordinates in the integral of a scalar function like L is much easier than doing so directly with vector equations of motion like (D.1.1).

To see why the equations of motion can be obtained in this way, explicitly perform the variation by evaluating $S[\mathbf{x}(\tau)]$ at a pair of nearby trajectories, $\mathbf{x}(\tau)$ and $\mathbf{x}(\tau) + \delta\mathbf{x}(\tau)$ that share their initial and final values, $\delta\mathbf{x}(t_0) = \delta\mathbf{x}(t) = 0$. The stationary configuration is the one for which $\delta S := S[\mathbf{x} + \delta\mathbf{x}] - S[\mathbf{x}]$ vanishes for arbitrary choice of $\delta\mathbf{x}(\tau)$.

To see what it means for $S[\mathbf{x}(\tau)]$ to be stationary under variations, expand the integrand in powers of $\delta\mathbf{x}$ and stop at linear order. Stationarity is equivalent to requiring the term linear in $\delta\mathbf{x}$ must vanish for arbitrary choices of $\delta\mathbf{x}(\tau)$, which requires:

$$\begin{aligned} 0 = \delta S &:= \int_{t_0}^{t} \mathrm{d}\tau \, \left\{ \left[\frac{m}{2} (\dot{\mathbf{x}} + \delta\dot{\mathbf{x}}) \cdot (\dot{\mathbf{x}} + \delta\dot{\mathbf{x}}) - V(\mathbf{x} + \delta\mathbf{x}) \right] - \left[\frac{m}{2} \, \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} - V(\mathbf{x}) \right] \right\}_{\text{linear in } \delta\mathbf{x}} \\ &= \int_{t_0}^{t} \mathrm{d}\tau \, \Big[m\dot{\mathbf{x}} \cdot \delta\dot{\mathbf{x}} - \delta\mathbf{x} \cdot \nabla V \Big] = \Big[m\dot{\mathbf{x}} \cdot \delta\mathbf{x} \Big]_{t_0}^{t} - \int_{t_0}^{t} \mathrm{d}\tau \, \Big[m\ddot{\mathbf{x}} + \nabla V \Big] \cdot \delta\mathbf{x} \,, \end{aligned} \tag{D.1.3}$$

where the last line performs an integration by parts to trade $\delta\dot{\mathbf{x}}$ for $\delta\mathbf{x}$. Requiring this to vanish for all possible $\delta\mathbf{x}(\tau)$ provided only that $\delta\mathbf{x}(t) = \delta\mathbf{x}(t_0) = 0$ then requires the coefficient of $\delta\mathbf{x}$ to vanish within the integral, and this implies the equations of motion (D.1.1).

As mentioned earlier, from a purely pragmatic standpoint, rephrasing the equations of motion in this way has the advantage that it simplifies the derivation of the equations of motion in non-Cartesian coordinates. For example imagine changing variables from $x^i(t)$ to $q^a(t)$ [for example, for spherical coordinates one might have $\{x^i\} = \{x, y, z\}$ and $\{q^a\} = \{r, \theta, \phi\}$]. In these new coordinates the kinetic and potential energies are $T = \frac{1}{2} m \, \delta_{ij} \dot{x}^i \dot{x}^i = \frac{1}{2} m \, \mathcal{G}_{ab}(q) \dot{q}^a \dot{q}^b$ and $V = V(x) = V(q)$, where $V(q) = V(x(q))$ and the quantity in the kinetic term is $\mathcal{G}_{ab}(q) = \delta_{ij} \, (\partial x^i / \partial q^a)(\partial x^j / \partial q^b)$. The action therefore becomes

$$S = \int_{t_0}^{t} \mathrm{d}\tau \, \left[\frac{m}{2} \, \mathcal{G}_{ab}(q) \, \dot{q}^a \dot{q}^b - V(q) \right] . \tag{D.1.4}$$

The condition $\delta S = 0$ then reads

$$\begin{aligned} 0 = \delta S &:= \int_{t_0}^{t} \mathrm{d}\tau \, \left\{ \left[\frac{m}{2} \mathcal{G}_{ab}(q + \delta q)(\dot{q}^a + \delta\dot{q}^a)(\dot{q}^b + \delta\dot{q}^b) - V(q + \delta q) \right] \right. \\ &\qquad \left. - \left[\frac{m}{2} \, \mathcal{G}_{ab}(q) \, \dot{q}^a \dot{q}^b - V(q) \right] \right\}_{\text{linear in } \delta q} \\ &= \int_{t_0}^{t} \mathrm{d}\tau \, \left[m\mathcal{G}_{ab}(q) \delta\dot{q}^a \dot{q}^b + \frac{m}{2} \delta q^c \partial_c \mathcal{G}_{ab}(q) \dot{q}^a \dot{q}^b - \delta q^a \partial_a V(q) \right] \\ &= \Big[m\mathcal{G}_{ab}(q) \dot{q}^a \delta q^b \Big]_{t_0}^{t} + \int_{t_0}^{t} \mathrm{d}\tau \, \left\{ -\frac{\mathrm{d}}{\mathrm{d}t} \Big[m\mathcal{G}_{ab}(q) \dot{q}^b \Big] + \frac{m}{2} \partial_a \mathcal{G}_{bc}(q) \dot{q}^b \dot{q}^c - \partial_a V(q) \right\} \delta q^a \,, \end{aligned} \tag{D.1.5}$$

where ∂_a denotes $\partial/\partial q^a$.

This shows that the equations of motion, written in terms of the coordinates q^a, are

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t}\Big[m\mathcal{G}_{ab}(q)\dot{q}^b\Big] - \frac{m}{2}\partial_a\mathcal{G}_{bc}(q)\dot{q}^b\dot{q}^c + \partial_a V(q) \\ &= m\mathcal{G}_{ab}(q)\ddot{q}^b + m\Lambda_{abc}(q)\,\dot{q}^b\dot{q}^c + \partial_a V(q)\,, \end{aligned} \tag{D.1.6}$$

where $\Lambda_{abc}(q)$ is the following combination of derivatives of $\mathcal{G}_{ab}(q)$

$$\Lambda_{abc} := \frac{1}{2}\left[\partial_b\mathcal{G}_{ac} + \partial_c\mathcal{G}_{ab} - \partial_a\mathcal{G}_{bc}\right] \tag{D.1.7}$$

called the 'Christoffel symbol of the first kind' for the 'metric' $\mathcal{G}_{ab}$.

This can be solved to give an equation for $\ddot{q}^a$ once the matrix $\mathcal{G}^{ab}$ that is the inverse to $\mathcal{G}_{ab}$ is found. That is, given a matrix of coefficients $\mathcal{G}^{ab}$ that satisfies $\mathcal{G}^{ab}\mathcal{G}_{bc} = \delta^a{}_c$, the above equations of motion imply

$$m\Big(\ddot{q}^a + \Gamma^a_{bc}(q)\,\dot{q}^b\dot{q}^c\Big) + \mathcal{G}^{ab}\partial_b V(q) = 0\,, \tag{D.1.8}$$

where the 'Christoffel symbol of the second kind' is defined by

$$\Gamma^a_{bc} := \mathcal{G}^{ad}\Lambda_{dbc} := \frac{1}{2}\mathcal{G}^{ad}\Big(\partial_b\mathcal{G}_{dc} + \partial_c\mathcal{G}_{db} - \partial_d\mathcal{G}_{bc}\Big)\,. \tag{D.1.9}$$

More generally, for an arbitrary lagrangian $L = L(q^a\,\dot{q}^a)$ the variation of the action is

$$\delta S = \int_{t_0}^{t}\mathrm{d}\tau\left[\frac{\partial L}{\partial\dot{q}^a}\,\delta\dot{q}^a + \frac{\partial L}{\partial q^a}\,\delta q^a\right] = \left[\frac{\partial L}{\partial\dot{q}^a}\,\delta q^a\right]_{t_0}^{t} + \int_{t_0}^{t}\mathrm{d}\tau\left[-\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{\partial L}{\partial\dot{q}^a}\right) + \frac{\partial L}{\partial q^a}\right]\delta q^a\,, \tag{D.1.10}$$

and this vanishes for arbitrary $\delta q^a(\tau)$ subject to the boundary condition $\delta q^a(t_0) = \delta q^a(t) = 0$ when $q^a(\tau)$ satisfies the following Lagrangian equations of motion

$$-\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{\partial L}{\partial\dot{q}^a}\right) + \frac{\partial L}{\partial q^a} = 0\,. \tag{D.1.11}$$

D.2 Hamiltonian mechanics

The Hamiltonian formulation of mechanics starts from the above Lagrangian formulation, but treats 'positions' q^a and 'velocities' $\dot{q}^a$ independently in order to rewrite things in terms of first-order differential equations rather than second-order ones. More formally, this is done by defining the canonical momentum $p_a(\tau)$ for each variable $q^a(\tau)$ using the definition

$$p_a(\tau) := \frac{\partial L}{\partial\dot{q}^a}\,. \tag{D.2.1}$$

Given this definition the system's Hamiltonian $H(q^a, p_b)$ is defined from its Lagrangian $L(\dot{q}^a, q^b)$ by

$$H(q,p) := p_a\,\dot{q}^a - L[q,\dot{q}(q,p)] \tag{D.2.2}$$

where the dependence of L on $\dot{q}^a$ is traded for a dependence on q^a and p_b by inverting[103] (D.2.1).

In terms of these the action can be written $S = \int \mathrm{d}\tau \ [p_a \, \dot{q}^a - H]$ and so the condition that it be stationary with respect to arbitrary small variations δq^a and δp_b becomes

$$\begin{aligned} \delta S &= \int_{t_0}^{t} \mathrm{d}\tau \left[\delta p_a \, \dot{q}^a + p_a \, \delta \dot{q}^a - \frac{\partial H}{\partial q^a} \, \delta q^a - \frac{\partial H}{\partial p_a} \, \delta p_a \right] \\ &= \Big[p_a \delta q^a \Big]_{t_0}^{t} + \int_{t_0}^{t} \mathrm{d}\tau \left[\left(\dot{q}^a - \frac{\partial H}{\partial p_a} \right) \delta p_a - \left(\dot{p}_a + \frac{\partial H}{\partial q^a} \right) \delta q^a \right] . \end{aligned} \tag{D.2.3}$$

Requiring this to vanish for any $\delta q^a(\tau)$ and $\delta p_a(\tau)$ subject to the boundary condition $\delta q^a(t_0) = \delta q^a(t) = 0$ then implies Hamilton's first-order reformulation of Newton's equations of motion

$$\dot{q}^a = \frac{\partial H}{\partial p_a} \quad \text{and} \quad \dot{p}_a = -\frac{\partial H}{\partial q^a} \, . \tag{D.2.4}$$

Notice in particular that $p_a(\tau)$ is conserved for any q^a that does not appear at all in $H(q,p)$.

Hamiltonian methods are very useful when passing to the quantum version of a theory, because in this version the commutation relations are very easy to state:

$$\Big[q^a, \, p_b \Big] = i \delta^a_b \, . \tag{D.2.5}$$

This is particularly useful when quantizing systems of fields.

D.3 Applications to fields

All of the above can be generalized to the situation where the dynamical variables are fields rather than coordinates. In the discussion provided above the label 'a' in q^a was a discrete label that runs over the number of independent variables (which might be n times N for N particles moving in n spatial dimensions, say). For a field we instead imagine $a \to \{a, \mathbf{x}\}$ to label both the independent fields and position in space. So trajectories $q^a(t)$ instead become $\psi^a(\mathbf{x}, t)$, where $a = 1, \ldots, N$ now labels the independent fields in the problem. Otherwise the above description proceeds much as before.

D.3.1 Lagrangian formulation

Locality is built in by demanding that the system's Lagrangian L be given as an integral over $\mathbf{x}$ of a Lagrangian density,

$$L = \int \mathrm{d}^3 x \ \mathcal{L}[\psi^a, \dot{\psi}^a] \, , \tag{D.3.1}$$

[103] In the simplest version of the formalism it is assumed that these equations are invertible and so that $\dot{q}^a(q,p)$ can be found. This is sometimes not possible, such as when the system is subject to constraints, in which case a generalization is necessary of the procedure described here.

and it is usually true for the cases of interest that L can be expanded in powers of derivatives of ψ^a, such as in

$$\mathcal{L} = \frac{1}{2}\,\mathcal{G}_{ab}(\psi)\,\dot{\psi}^a\,\dot{\psi}^b - \frac{1}{2}\,\mathcal{H}_{ab}(\psi)\,\nabla\psi^a\cdot\nabla\psi^b - V(\psi)\,. \tag{D.3.2}$$

The action then has the following local form

$$S = \int \mathrm{d}t\; L = \int \mathrm{d}^4x\; \mathcal{L}(\psi^a, \dot{\psi}^a, \nabla\psi^a)\,. \tag{D.3.3}$$

With this choice the classical equations of motion are obtained by requiring S be stationary under arbitrary variations $\delta\psi^a(\mathbf{x},t)$, leading to the condition

$$\begin{aligned} 0 = \delta S &= \int_{\mathcal{R}} \mathrm{d}^4x\; \left[\frac{\partial\mathcal{L}}{\partial\dot{\psi}^a}\,\delta\dot{\psi}^a + \frac{\partial\mathcal{L}}{\partial\nabla\psi^a}\cdot\delta\nabla\psi^a + \frac{\partial\mathcal{L}}{\partial\psi^a}\,\delta\psi^a\right] \\ &= \int_{\mathcal{R}} \mathrm{d}^3x\left[\frac{\partial\mathcal{L}}{\partial\dot{\psi}^a}\,\delta\psi^a\right]_{t_0}^{t_f} + \int \mathrm{d}t \oint_{\partial\mathcal{R}} \mathrm{d}^2x\; \left[\mathbf{n}\cdot\frac{\partial\mathcal{L}}{\partial\nabla\psi^a}\right]\delta\psi^a \\ &\qquad + \int_{\mathcal{R}} \mathrm{d}^4x\; \left\{-\partial_t\left[\frac{\partial\mathcal{L}}{\partial\dot{\psi}^a}\right] - \nabla\cdot\left[\frac{\partial\mathcal{L}}{\partial\nabla\psi^a}\right] + \frac{\partial\mathcal{L}}{\partial\psi^a}\right\}\delta\psi^a\,, \end{aligned} \tag{D.3.4}$$

where the spatial integration is over a volume $\mathcal{R}$ with boundary $\partial\mathcal{R}$ on which $\mathbf{n}$ is the outward-pointing unit normal. If (for example) this is to vanish for all variations for which $\delta\psi^a$ vanishes on $\partial\mathcal{R}$ for all times and vanishes throughout $\mathcal{R}$ at the initial and final times then the coefficient of $\delta\psi^a(\mathbf{x},t)$ in the last line must vanish, leading to the field equations

$$-\partial_t\left[\frac{\partial\mathcal{L}}{\partial\dot{\psi}^a}\right] - \nabla\cdot\left[\frac{\partial\mathcal{L}}{\partial\nabla\psi^a}\right] + \frac{\partial\mathcal{L}}{\partial\psi^a} = 0\,. \tag{D.3.5}$$

For example, for the lagrangian density

$$\mathcal{L}(\psi,\dot{\psi},\nabla\psi) = \frac{1}{2}\,Z_{ab}(\psi)\,\dot{\psi}^a\,\dot{\psi}^b - \frac{1}{2}\,Y_{ab}(\psi)\,\nabla\psi^a\cdot\nabla\psi^b - V(\psi) \tag{D.3.6}$$

these equation of motion become

$$-\partial_t\Big[Z_{ab}(\psi)\,\dot{\psi}^b\Big] + \nabla\cdot\Big[Y_{ab}(\psi)\,\nabla\psi^b\Big] + \frac{\partial V}{\partial\psi^a} = 0\,. \tag{D.3.7}$$

In the special case where Z_{ab} and Y_{ab} do not depend on ψ this has the simple form

$$-Z_{ab}\,\partial_t^2\psi^b + Y_{ab}\,\nabla^2\psi^b + \frac{\partial V}{\partial\psi^a} = 0\,. \tag{D.3.8}$$

D.3.2 Hamiltonian formulation

The Hamiltonian formulation is obtained in precisely the same was as was done for simple mechanical system. Starting with the Lagrangian density $\mathcal{L}(\psi,\dot{\psi},\nabla\psi)$ the canonical momentum fields are defined by

$$\Pi_a(\mathbf{x},t) = \frac{\partial\mathcal{L}}{\partial\dot{\psi}^a(\mathbf{x},t)}\,. \tag{D.3.9}$$

With this definition, and assuming the Lagrangian has the local form (D.3.1), the Hamiltonian also is local: $H = \int \mathrm{d}^3x\, \mathcal{H}$ with

$$\mathcal{H} = \Pi_a\, \dot{\psi}^a - \mathcal{L}\,. \tag{D.3.10}$$

For example, for the special case (D.3.6) the momentum becomes

$$\Pi_a = Z_{ab}(\psi)\dot{\psi}^b \quad \text{and so} \quad \dot{\psi}^a = Z^{ab}(\psi)\,\Pi_b \tag{D.3.11}$$

where Z^{ab} is the inverse matrix for Z_{ab}. Similarly

$$\mathcal{H} = \Pi_a\, \dot{\psi}^a - \mathcal{L} = \frac{1}{2}\, Z^{ab}(\psi)\,\Pi_a\,\Pi_b + \frac{1}{2}\, Y_{ab}\,\nabla\psi^a\cdot\nabla\psi^b + V(\psi)\,. \tag{D.3.12}$$

In the quantum system the quantization condition is similarly

$$\Big[\psi^a(\mathbf{x},t)\,,\Pi_b(\mathbf{y},t)\Big] = i\delta^a_b\,\delta^3(\mathbf{x}-\mathbf{y})\,. \tag{D.3.13}$$

Other reading

Eventually put here are a few textbooks on quantum field theory....

1. David Griffiths, *Introduction to Elementary Particles*, Wiley-VCH, 2010.

2. Ernest Henley and Alejandro Garcia, *Subatomic Physics*, Wiley-VCH, 2010.

Here is a selection of textbooks on relativistic quantum field theory.

1. C.P. Burgess and G.D. Moore, *The Standard Model: A Primer*, Cambridge University Press (2007).

Other useful references (to be completed...)

References

[1] C.P. Burgess, *Introduction to Effective Field Theory*, Cambridge University Press (2020).