Material for 6007ESC

Part Q: Introductory Quantum Electrodynamics

Term II, 2021

24 Contact Hours

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incorporating material from long ago

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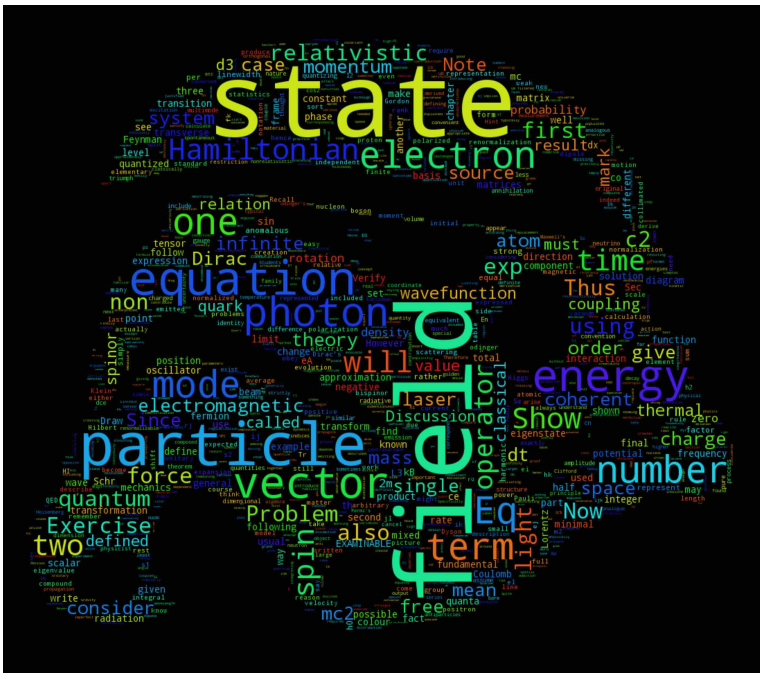


Contents

Introduction

Quantum electrodynamics is the theory of the interaction of charged particles with the electromagnetic field, treating both as quantum systems. It is probably the most successful theory of all time, in terms of the range and precision of phenomena it can predict.

The aim of this Part of the 6007ESC course is to introduce you to some of the fundamental concepts and techniques of this theory, as well as putting it in the context of the relativistic quantum field theory of the "standard model".

The material presented here is not found in any one text book. In fact, some of the material is not found in any text book that I am aware of. That said, the following books may be useful to you

1. F. Mandl and G. Shaw, *Quantum Field Theory* (Wiley, Chichester, 1993).

2. R. Loudon, *The Quantum Theory of Light* (Oxford University Press, Oxford, 1983).

3. C. Cohen-Tannoudji, J. Dupont Roc and G. Grynberg, *Photons and Atoms: An Introduction to Quantum Electrodynamics* (Wiley, New York, 1989).

Many other books may be useful also; feel free to browse. But you may well find the presentation to be quite different from mine.

These notes give a fairly complete overview of the theory of non-relativistic quantum electrodynamics, and an introduction to the relativistic theory. Some sections (or subsections) are labelled

NON-EXAMINABLE.

They contain a few detailed derivations that are mainly intended as a resource for future reference by you. We will go through these derivations relatively quickly in class and you should gain some insight into the theory from them. Shorter passages of the same character appear between horizontal lines, labelled **Aside** and in italics. In general, it is more important to understand the new quantum mechanics than the vector calculus.

Students are strongly advised to attend class because additional, important & assessable material will be delivered by me, as working on the whiteboard, in an interactive manner, particularly in relation to the questions marked for **discussion**. Students should read several pages ahead for each 2-hour class, and work through the **exercises** (if able) and think about the discussion points.

Assessment

Assessment for this part of the course will comprise 55% of the total for 6007ESC, which I will say comprises 55 points for clarity. At least 16 of these points, and at most 32 of these points, will come from **problems**, as follows:

- There are four problem sets, as indicated in the table below. Students should submit at least 4 points of problems per group.
- Students submitting x points of problems for a problem set with $x < 4$, will be marked on these x points and receive a mark of zero for the remaining $4 - x$ points for that chapter.
- Students may submit at most 8 points of problems from any set for marking.

The points assigned to each exercise are in the table below, and students may choose any ones to submit, subject to the restrictions above. Each problem set is due at 5pm ONE WEEK (to the day) after the class covering the last problem in that set. The remaining points for this part of the course (i.e. at least 23, and up to 39) come from an end-of-term exam. Students are advised to study ALL exercises and problems, as well as the material in the notes and the material presented and discussed in class, as preparation for this exam. I will give out a practice exam with worked solution closer to the exam.

Chapter	Problem. #	Points
1	1	2.5
	2	3
	3	2
	4	3
	5	2
	6	2
		14.5
2	1	2
	2	2
	3	1.5
	4	2
	5	1.5
	6	1.5
	7	2
	8	1.5
3	1	2
	2	1
		17
3	3	1
	4	1
5	1	2
	2	2
	3	2
	4	3
	5	2.5
		13.5
6	1	1.5
	2	2
	3	2
	4	1.5
7	1	2
8	1	1
	2	1
		11
TOTAL		55

Table 1: Problem Sets, Problems, and Points Associated

1 Quantization of the Electromagnetic Field

1.1 Harmonic Oscillator Revision

Although the photon is commonly referred to as an elementary particle of light, it is quite different from elementary particles such as electrons and quarks. There is no such thing as a photon wavefunction, although there are some text books which describe the electric field in those terms. This is quite wrong. The electric field is a real field which exists in real space, not a probability amplitude which exists in Hilbert space. The relation between the electric field and the photon should become clear later, but for now the following description will have to do: A photon is an elementary excitation of a mode of the quantized electromagnetic field. In that sense it is analogous to an excitation of a quantized particle in a harmonic potential. That is, the discreteness of the electromagnetic field energy (photons) is present for the same reason as the discreteness of the energy levels of a particle in a potential well. For this reason it is useful first to review the quantized harmonic oscillator.

Discussion 1.1 *What is special about the harmonic oscillator (i.e. a quadratic potential) in terms of its quantized energy levels? How might this be relevant to photons?*

The energy of a classical harmonic oscillator is of course

$$E = \tfrac{1}{2}m\omega^2 q^2 + \tfrac{1}{2}m\dot{q}^2 \tag{1.1.1}$$

$$= \frac{\hbar\omega}{2}\left(X^2 + \omega^{-2}\dot{X}^2\right) \tag{1.1.2}$$

the second line, despite the appearance of $\hbar$, is still classical as I have merely defined a dimensionless position

$$X = \sqrt{\frac{m\omega}{\hbar}}\, q. \tag{1.1.3}$$

Now in the Hamiltonian formulation we have $p = m\dot{q}$ so that

$$H = \frac{m\omega^2 q^2}{2} + \frac{p^2}{2m} \tag{1.1.4}$$

$$= \frac{\hbar\omega}{2}(X^2 + Y^2), \tag{1.1.5}$$

where I have also defined a dimensionless momentum

$$Y = \omega^{-1}\dot{X} = \sqrt{\frac{1}{m\omega\hbar}}\, p\,. \tag{1.1.6}$$

In quantizing the harmonic oscillator we have $p \to \hat{p}$, which in the position basis has the representation $-i\hbar\frac{\partial}{\partial q}$. This means that for an arbitrary quantum state $|\psi\rangle$,

$$\langle q|\hat{p}|\psi\rangle = -i\hbar\frac{\partial}{\partial q}\langle q|\psi\rangle = -i\hbar\psi'(q), \tag{1.1.7}$$

where $\psi(q) = \langle q|\psi\rangle$ is called the position wavefunction. Thus $Y \to \hat{Y} \sim -i\frac{\partial}{\partial X}$. These imply the commutation relations

$$[\hat{q}, \hat{p}] = i\hbar \Longrightarrow [\hat{X}, \hat{Y}] = i. \tag{1.1.8}$$

Now we define (non-Hermitian) *lowering* and *raising* operators

$$a = 2^{-1/2}(\hat{X} + i\hat{Y}), a^\dagger = 2^{-1/2}(\hat{X} - i\hat{Y}). \tag{1.1.9}$$

(Note that for convenience we do not use hats for these.) Then we can rewrite the Hamiltonian as

$$\hat{H} = \hbar\omega \left(a^\dagger a + aa^\dagger\right)/2. \tag{1.1.10}$$

Exercise 1.1 *From the commutation relations of $\hat{X}$ and $\hat{Y}$, show that*

$$[a, a^\dagger] = 1, \tag{1.1.11}$$

and hence that $\hat{H} = \hbar\omega \left(a^\dagger a + \frac{1}{2}\right)$.

It is simple to show that the state $|\psi_0\rangle$ with wavefunction

$$\psi_0(X) = \langle X|\psi_0\rangle \propto \exp(-X^2/2) \tag{1.1.12}$$

is an eigenstate of a with eigenvalue 0, by working in the X-basis:

$$\begin{aligned} \langle X|(\hat{X} + i\hat{Y})|\psi_0\rangle &= \left[X + i\left(-i\frac{\partial}{\partial X}\right)\right]\psi_0(X) \\ &= (X - X)\exp(-X^2/2) = 0 = \langle X|0|\psi_0\rangle. \end{aligned} \tag{1.1.13}$$

From this it is easy to show that the eigenvalues $a^\dagger a$ are the non-negative integers, as follows. To begin, recall that the eigenvalues of an Hermitian operator are real numbers. Then,

Problem 1.1 (2.5 marks) *(In three parts)*

1. *Show that any operator of the form $\hat{A}^\dagger\hat{A}$ has only non-negative real numbers for its eigenvalues.*
   Hint*: Postulate the negation, that there exists a $|\psi\rangle$ such that $\hat{A}^\dagger\hat{A}|\psi\rangle = -r|\psi\rangle$, for r positive. Establish a contradiction by considering $\langle\psi|\hat{A}^\dagger\hat{A}|\psi\rangle = (\langle\psi|\hat{A}^\dagger)(\hat{A}|\psi\rangle)$*

2. *Say $g \geq 0$ is an eigenvalue of $a^\dagger a$, with corresponding eigenstate $|g\rangle$. Consider the (unnormalized) state $|\psi\rangle = a^\dagger|g\rangle$, and show that it is an eigenstate of $a^\dagger a$ with eigenvalue $g + 1$.*
   Hint*: Consider the commutator $[a^\dagger a, a^\dagger]$ to rewrite the expression you get.*

3. *Now consider $a|g\rangle$, and show in a similar way that it is an eigenstate of $a^\dagger a$ with eigenvalue $g - 1$, as long as $a|g\rangle \neq 0$. Explain why that last condition is necessary.*

Now because $a|\psi_0\rangle = 0$, $|\psi_0\rangle$ is an eigenstate of $a^\dagger a$ with eigenvalue 0. Therefore by part 2 of the problem, all positive integers are eigenvalues of $a^\dagger a$ too. Can there be any other eigenvalues? No, because if there were, by part 3, if we started with some putative non-integer eigenstate $|g\rangle$ with $g = m - r$, with m a strictly positive integer and $0 < r < 1$, then applying the operator a to this $m + 1$ times, one would get to a state with eigenvalue $g' = m - r - m = -r$, which is negative. But this is impossible from part 1 of the problem.

Thus we have derived the eigenvalues of the harmonic oscillator as $\hbar\omega\left(n + \frac{1}{2}\right)$, with n a non-negative integer. The corresponding unnormalized eigenstates are $|\psi_n\rangle$, which we will denote $|n\rangle$ when normalized. These states have an integer number of elementary excitations of the vibration of the particle. They are therefore sometimes called *vibron* number states, that is, states with a definite number of vibrons.

1.2 Heisenberg and Schrödinger pictures Revision

An isolated quantum system will undergo reversible evolution governed by its Hamiltonian (that is, energy) operator $\hat{H}$. There are two basic ways of describing this time evolution, called the Schrödinger picture (SP) and the Heisenberg picture (HP). In the former, the state of the system changes and operators are unchanging, while in the latter the state is time-independent and the operators time-dependent.

The SP evolution of the state vector is the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle. \tag{1.2.1}$$

The solution of this equation is

$$|\psi(t)\rangle = \hat{U}(t,0)|\psi(0)\rangle \tag{1.2.2}$$

where $\hat{U}$ is a unitary operator ($\hat{U}^\dagger = \hat{U}^{-1}$) given by

$$\hat{U}(t,0) = \exp(-i\hat{H}t/\hbar). \tag{1.2.3}$$

In the HP, the equation of motion for an arbitrary operator $\hat{A}$ is

$$\frac{\partial}{\partial t}\hat{A}(t) = (i\hbar)^{-1}[\hat{A}(t), \hat{H}]. \tag{1.2.4}$$

Note that, because $\hat{H}$ commutes with itself at a particular time t, the Hamiltonian operator is one operator that is always the same in the HP and SP. The solution of the HP equation is

$$\hat{A}(t) = \hat{U}^\dagger(t,0)\hat{A}(0)\hat{U}(t,0). \tag{1.2.5}$$

Exercise 1.2 *Show this using Eq. (1.2.3).*

The two pictures are equivalent because all expectation values are identical:

$$\begin{aligned}\langle\psi|\hat{A}(t)|\psi\rangle &= \langle\psi|\hat{U}^\dagger(t,0)\hat{A}(0)\hat{U}(t,0)|\psi\rangle \\ &= \langle\psi(t)|\hat{A}|\psi(t)\rangle.\end{aligned} \tag{1.2.6}$$

Here the placement of the time-argument t indicates which picture we are in.

We can also allow for an explicitly time-dependent Hamiltonian $\hat{H}_t$ (in the SP) as would arise from a classical external modulation of the system. In this case $\hat{H}(t) = \hat{U}(t,0)\hat{H}_t\hat{U}^\dagger(t,0)$ in the HP is not necessarily the same as $\hat{H}_t$ in the SP. In this case the solutions are still Eq. (1.2.2) and Eq. (1.2.5), but the expression for the unitary operator is much more complicated:

$$\hat{U}(t,0) = I + \sum_{n=1}^{\infty}(i\hbar)^{-n}\int_0^t ds_n \hat{H}_{s_n}\int_0^{s_n} ds_{n-1}\hat{H}_{s_{n-1}}\cdots\int_0^{s_2} ds_1\hat{H}_{s_1} \tag{1.2.7}$$

Problem 1.2 (3 marks) *From the Schrödinger equation (1.2.1), with $\hat{H} \to \hat{H}_t$, derive the differential equation for $\hat{U}(t,0)$, and show that Eq. (1.2.7) solves it, for the initial condition $\hat{U}(0,0) = I$. Show also that $\hat{U}^\dagger(t,0)\hat{U}(t,0) = I$, by showing that this quantity is a constant of motion and has the appropriate initial value. Finally show that $\hat{U}(t,0)\hat{U}^\dagger(t,0)$ is also a constant of motion, but only* because *it has the appropriate initial value, of I. (These equations should hold, of course, because $\hat{U}(t,0)$ should be unitary, with $\hat{U}^\dagger = \hat{U}^{-1}$.)*

In the case that $\hat{H}$ is time-independent, Eq. (1.2.7) reduces to Eq. (1.2.3).

Exercise 1.3 *Show this.*

1.3 The Classical Electromagnetic Field

1.3.1 Maxwell's Equations

Not surprisingly, we begin with Maxwell's equations. Superficially this might seem similar to considering Schrödinger's equation, but it must be remembered that Schrödinger's equation is an equation for a wavefunction with the usual probability interpretation in quantum mechanics. Maxwell's equations are equations of motion for the *classical* electromagnetic field. They are

$$\boldsymbol{\nabla}\cdot\mathbf{E} = \rho/\epsilon_0\,, \tag{1.3.1}$$

$$\boldsymbol{\nabla}\times\mathbf{B} = \frac{1}{c^2}\left[\mathbf{j}/\epsilon_0 + \frac{\partial\mathbf{E}}{\partial t}\right]\,, \tag{1.3.2}$$

$$\boldsymbol{\nabla}\cdot\mathbf{B} = 0\,, \tag{1.3.3}$$

$$\boldsymbol{\nabla}\times\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t}\,. \tag{1.3.4}$$

Here ϵ_0 is the permittivity of free space, and the permeability μ_0 has been replaced using the identity $\mu_0\epsilon_0 = c^{-2}$.

Eqn(1.3.3) and eqn(1.3.4) are automatically satisfied by introducing the potentials ϕ and $\mathbf{A}$, so that

$$\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}\,,\ \mathbf{E} = -\boldsymbol{\nabla}\phi\ - \frac{\partial\mathbf{A}}{\partial t}\,. \tag{1.3.5}$$

Eqn(1.3.1) and eqn(1.3.2) then become

$$-\nabla^2\phi - \frac{\partial}{\partial t}\boldsymbol{\nabla}\cdot\mathbf{A} = \rho/\epsilon_0\,, \qquad (1.3.6)$$

$$\left(\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right)\mathbf{A} + \boldsymbol{\nabla}\left(\frac{\partial\phi}{\partial t} + c^2\boldsymbol{\nabla}\cdot\mathbf{A}\right) = \mathbf{j}/\epsilon_0\,. \qquad (1.3.7)$$

Here the identity $\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\ = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\ ) - \nabla^2$ has been used.

1.3.2 The Coulomb Gauge

The potentials are not determined uniquely, since the replacements

$$\phi \to \phi' = \phi + \dot{f}\,,\ \mathbf{A} \to \mathbf{A}' = \mathbf{A} - \boldsymbol{\nabla} f\,, \qquad (1.3.8)$$

for arbitrary $f(\mathbf{r},t)$, leave the fields unaltered. (Here the notations $\dot{f}$, $\frac{\partial f}{\partial t}$ and $\partial_t f$ will be used interchangeably.) This is known as a *gauge transformation*. It can be shown that we can choose the gauge such that

$$\boldsymbol{\nabla}\cdot\mathbf{A} = 0. \qquad (1.3.9)$$

This is known as the *Coulomb* or *radiation* gauge. In this gauge, Maxwell's equations become a wave equation for $\mathbf{A}$:

$$\left(\partial_t^2 - c^2\nabla^2\right)\mathbf{A} = \mathbf{j}/\epsilon_0 - \boldsymbol{\nabla}\dot{\phi}\,, \qquad (1.3.10)$$

where $\partial_t \equiv \frac{\partial}{\partial t}$, and Poisson's equation for ϕ:

$$\nabla^2\phi = -\rho/\epsilon_0. \qquad (1.3.11)$$

The latter has the solution (with the boundary condition that ϕ vanishes at infinity).

$$\phi(\mathbf{r},t) = \frac{1}{4\pi\epsilon_0}\int \mathrm{d}^3\mathbf{x}\frac{\rho(\mathbf{x},t)}{|\mathbf{r}-\mathbf{x}|}. \qquad (1.3.12)$$

Exercise 1.4 *For a single charge q at position $\mathbf{q}$, verify that this gives the usual Coulomb's law.*

In the Coulomb gauge the vector potential $\mathbf{A}$ is what is known as a *transverse* field, because $\boldsymbol{\nabla}\cdot\mathbf{A} = 0$. It can be shown that an arbitrary vector field can be split into transverse and longitudinal parts. For example, the current density

$$\mathbf{j} = \mathbf{j}^\perp + \mathbf{j}^\parallel\ ;\ \ \boldsymbol{\nabla}\cdot\mathbf{j}^\perp = 0\ ,\ \ \boldsymbol{\nabla}\times\mathbf{j}^\parallel = \mathbf{0}. \qquad (1.3.13)$$

These components are everywhere orthogonal:

$$\mathbf{j}^\perp\cdot\mathbf{j}^\parallel \equiv 0. \qquad (1.3.14)$$

Discussion 1.2 *How would you explain the concepts of transverse and longitudinal fields to your grandmother?*

Now using $\boldsymbol{\nabla} \times \boldsymbol{\nabla} \equiv 0$ one can split Eq. (1.3.10) into transverse and longitudinal parts. This gives a wave equation with sources for $\mathbf{A}$

$$\left(\partial_t^2 - c^2\nabla^2\right)\mathbf{A} = \mathbf{j}^{\perp}/\epsilon_0 \tag{1.3.15}$$

and the following identity

$$\mathbf{j}^{\parallel}/\epsilon_0 = \boldsymbol{\nabla}\dot{\phi}. \tag{1.3.16}$$

This last equation, with Eq. (1.3.11), and the fact that $\boldsymbol{\nabla}\cdot\mathbf{j}^{\parallel} = \boldsymbol{\nabla}\cdot\mathbf{j}$ then imply the continuity equation

$$\dot{\rho} + \boldsymbol{\nabla}\cdot\mathbf{j} = 0. \tag{1.3.17}$$

If the continuity equation is taken for granted, the only independent equations are then the wave equation with sources (1.3.15) and Poisson's equation (1.3.11). We will return to these equations in Chapter 4.

1.3.3 Free Fields

Now consider the case of fields with no current sources: $\mathbf{j}^{\perp} = \mathbf{0}$. Then $\mathbf{A}$ satisfies the pure wave equation

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right)\mathbf{A} = 0, \tag{1.3.18}$$

which has propagating solutions so $\mathbf{A}$ is not necessarily zero. It will be convenient to represent the field by a discrete set of variables rather than a continuum, so we shall assume that the field is confined to a cube of side L with the origin at one corner. Assuming periodic boundary conditions (this is an arbitrary assumption), we consider standing waves, with wavevectors

$$\mathbf{k} = \frac{2\pi}{L}\left(l, m, n\right)^T, \tag{1.3.19}$$

where l, m, n are integers, and two ($\lambda \in \{1, 2\}$) transverse polarization vectors

$$\boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda} \;:\; \boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda}\cdot\mathbf{k} = 0\;,\;\; \boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda}\cdot\boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda'} = \delta^{\lambda,\lambda'}. \tag{1.3.20}$$

We can thus write the solution in terms of dimensionless coefficients $X_{s,\mathbf{k}}^{\lambda}$ and $X_{c,\mathbf{k}}^{\lambda}$ as

$$\mathbf{A}(\mathbf{x}, t) = \sum_{\mathbf{k},\lambda} \boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda}\sqrt{\frac{2\hbar}{\epsilon_0 c|\mathbf{k}|L^3}}\;\left[X_{s,\mathbf{k}}^{\lambda}(t)\sin(\mathbf{k}\cdot\mathbf{x}) + X_{c,\mathbf{k}}^{\lambda}(t)\cos(\mathbf{k}\cdot\mathbf{x})\right] \tag{1.3.21}$$

Once again, the presence of $\hbar$ here is just a convenient normalization. Because sin and cos remain the same (up to a sign change) when the sign of their arguments are reversed, the modes with wavenumbers $\mathbf{k}$ and $-\mathbf{k}$ are actually the same mode. Thus to avoid redundancy it is necessary that the sum over all $\mathbf{k}$ actually be only one half of all possible $\mathbf{k}$. If some particular $\mathbf{k}$ appears in the sum, then the opposite-pointing one, $-\mathbf{k}$, should not. We can impose this restriction by demanding for example that in Eq. (1.3.19), $l \geq 0$.

Now the electric field can be split into transverse and longitudinal parts

$$\mathbf{E}^{\perp} = -\dot{\mathbf{A}} \tag{1.3.22}$$

$$\mathbf{E}^{\parallel} = -\boldsymbol{\nabla}\phi \tag{1.3.23}$$

From the above expression (1.3.21) we get

$$\mathbf{E}^{\perp}(\mathbf{x},t) = -\frac{\partial}{\partial t}\mathbf{A} = -\sum_{\mathbf{k},\lambda} \boldsymbol{\varepsilon}^{\lambda}_{\mathbf{k}} \sqrt{\frac{2\hbar}{\epsilon_0 c|\mathbf{k}|L^3}} \left[\dot{X}^{\lambda}_{s,\mathbf{k}} \sin(\mathbf{k}\cdot\mathbf{x}) + \dot{X}^{\lambda}_{c,\mathbf{k}} \cos(\mathbf{k}\cdot\mathbf{x})\right] \tag{1.3.24}$$

$$\mathbf{B}(\mathbf{x},t) = \boldsymbol{\nabla}\times\mathbf{A} = \sum_{\mathbf{k},\lambda} \check{\mathbf{k}} \times \boldsymbol{\varepsilon}^{\lambda}_{\mathbf{k}} \sqrt{\frac{2|\mathbf{k}|\hbar}{\epsilon_0 c L^3}} \left[X^{\lambda}_{s,\mathbf{k}} \cos(\mathbf{k}\cdot\mathbf{x}) - X^{\lambda}_{c,\mathbf{k}} \sin(\mathbf{k}\cdot\mathbf{x})\right] \tag{1.3.25}$$

where $\check{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$. From Eq. (1.3.12), $\mathbf{E}^{\parallel}$ can be expressed directly in terms of the charge density ρ.

Problem 1.3 (2 marks) *Show that for an arbitrary scalar function f and constant vector $\boldsymbol{n}$,*

$$\boldsymbol{\nabla} f(\mathbf{k}\cdot\mathbf{x}) = \mathbf{k}\, f'(\mathbf{k}\cdot\mathbf{x}) \tag{1.3.26}$$

$$\boldsymbol{\nabla}\cdot[\boldsymbol{n} f(\mathbf{k}\cdot\mathbf{x})] = \mathbf{k}\cdot\boldsymbol{n}\, f'(\mathbf{k}\cdot\mathbf{x}) \tag{1.3.27}$$

$$\boldsymbol{\nabla}\times[\boldsymbol{n} f(\mathbf{k}\cdot\mathbf{x})] = \mathbf{k}\times\boldsymbol{n}\, f'(\mathbf{k}\cdot\mathbf{x}) \tag{1.3.28}$$

From the last, show Eq. (1.3.25).

Now since $\mathbf{E}^{\perp}\cdot\mathbf{E}^{\parallel} = 0$, the electromagnetic energy density (i.e. energy per unit volume) can be split up as

$$\frac{\epsilon_0}{2}\left(|\mathbf{E}|^2 + c^2|\mathbf{B}|^2\right) = \frac{\epsilon_0}{2}\left(\mathbf{E}^{\perp}\cdot\mathbf{E}^{\perp} + c^2\mathbf{B}\cdot\mathbf{B} + \mathbf{E}^{\parallel}\cdot\mathbf{E}^{\parallel}\right) \tag{1.3.29}$$

The last term corresponds to the Coulomb energy density, which can be expressed in terms of the charge density ρ alone and so need not be considered independently of the matter fields which give rise to $\mathbf{E}^{\parallel}$. We will return to it in Chapter 4. But the radiation field can store energy independent of any charges:

$$E = \int_0^L \mathrm{d}x \int_0^L \mathrm{d}y \int_0^L \mathrm{d}z\, \frac{\epsilon_0}{2}\left(\mathbf{E}^{\perp}\cdot\mathbf{E}^{\perp} + c^2\mathbf{B}\cdot\mathbf{B}\right). \tag{1.3.30}$$

From the above expressions we find

$$E = \sum_{\mathbf{k},\lambda}\sum_{m=s,c} \frac{\hbar\omega_{\mathbf{k}}}{2}\left[\left(X^{\lambda}_{m,\mathbf{k}}\right)^2 + \omega_{\mathbf{k}}^{-2}\left(\dot{X}^{\lambda}_{m,\mathbf{k}}\right)^2\right], \tag{1.3.31}$$

where we have defined $\omega_{\mathbf{k}} = c|\mathbf{k}|$, and m stands for mode (sin or cos). Thus we see that the radiation field consists of an infinite sum of independent harmonic oscillators of frequencies $\omega_{\mathbf{k}}$.

Problem 1.4 (3 marks) *Verify Eq. (1.3.31). Your expression should initially contain double sums of the form $\sum_{\mathbf{k},\lambda,m}\sum_{\mathbf{k}',\lambda',m'}$, and the integrals will yield Kronecker δ functions which reduce these to the single sums in Eq. (1.3.31). If you do the calculation in detail for the $c^2|\mathbf{B}|^2$ term, you can just sketch how it will work for the $|\mathbf{E}^{\perp}|^2$ term.*

1.4 Quantizing the Electromagnetic Field

We now write $Y^{\lambda}_{m,\mathbf{k}} = \omega_{\mathbf{k}}^{-1}\dot{X}^{\lambda}_{m,\mathbf{k}}$ to get the Hamiltonian form of the energy

$$H = \sum_{\mathbf{k},\lambda,m} \frac{\hbar\omega_{\mathbf{k}}}{2}\left[\left(X^{\lambda}_{m,\mathbf{k}}\right)^2 + \left(Y^{\lambda}_{m,\mathbf{k}}\right)^2\right]. \tag{1.4.1}$$

When this is quantized we have, as in Sec. 1.1,

$$[\hat{X}^{\lambda}_{m,\mathbf{k}}, \hat{Y}^{\lambda'}_{m',\mathbf{k}'}] = i\delta_{\mathbf{k},\mathbf{k}'}\delta_{\lambda,\lambda'}\delta_{m,m'}. \tag{1.4.2}$$

Using these relations, the following identity

$$[\hat{C}^2, \hat{D}] = \hat{C}[\hat{C}, \hat{D}] + [\hat{C}, \hat{D}]\hat{C}, \tag{1.4.3}$$

and the Heisenberg equation of motion (1.2.4), we get these equations in the HP:

$$\frac{d}{dt}\hat{X}^{\lambda}_{m,\mathbf{k}} = \omega_{\mathbf{k}}\hat{Y}^{\lambda}_{m,\mathbf{k}} \tag{1.4.4}$$

$$\frac{d}{dt}\hat{Y}^{\lambda}_{m,\mathbf{k}} = -\omega_{\mathbf{k}}\hat{X}^{\lambda}_{m,\mathbf{k}}. \tag{1.4.5}$$

Problem 1.5 (2 marks) *Verify Eq. (1.4.3) and Eq. (1.4.4). Don't forget to use dummy variables in the sum.*

These are as expected for a Harmonic oscillator and are consistent with the above definition of $\hat{Y}^{\lambda}_{\mathbf{k}}$. They also imply

$$\frac{d^2}{dt^2}\hat{X}^{\lambda}_{m,\mathbf{k}} = -\omega^2_{\mathbf{k}}\hat{X}^{\lambda}_{m,\mathbf{k}}. \tag{1.4.6}$$

From this it is easy to show that the original expression for the vector potential (1.3.21) is indeed a solution of Maxwell's wave equation (1.3.18).

Problem 1.6 (2 marks) *Verify the last sentence above.*

We have thus completed the quantization of the free electromagnetic field, without mentioning the word photon.

We can introduce the photon concept simply by defining an annihilation operator for each mode of the field

$$a^{\lambda}_{m,\mathbf{k}} = 2^{-1/2}\left(\hat{X}^{\lambda}_{m,\mathbf{k}} + i\hat{Y}^{\lambda}_{m,\mathbf{k}}\right), \tag{1.4.7}$$

exactly analogously to Sec. 1.1. Then the field Hamiltonian can be written

$$\hat{H} = \sum_{\mathbf{k},\lambda,m} \hbar\omega_{\mathbf{k}}\left[\hat{n}^{\lambda}_{m,\mathbf{k}} + \tfrac{1}{2}\right], \tag{1.4.8}$$

where $\hat{n}^{\lambda}_{m,\mathbf{k}} = (a^{\lambda}_{m,\mathbf{k}})^{\dagger}a^{\lambda}_{m,\mathbf{k}}$. Here the *photon* annihilation and creation operators obey

$$\left[a^{\lambda}_{m,\mathbf{k}}, (a^{\lambda'}_{m',\mathbf{k}'})^{\dagger}\right] = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\lambda,\lambda'}\delta_{m,m'}. \tag{1.4.9}$$

We have thus arrived at a description with a similar structure to the field-theory description of a system of noninteracting bose particles. (It describes bosons, not fermions, because there is no limit to the number of photons in a mode.) However, instead of quantizing the particles and then constructing the field, we have quantized the field and found the "particles" (photons). I prefer to maintain a distinction between particles such as electrons, and quanta such as photons. One can be misled if thinking of photons as particles that it should be possible to write down a wavefunction $\psi(x)$ for a single photon with $|\psi(x)|^2$ interpretable as a photon density. This is not possible. If one wished to introduce a wavefunction representation, it would be a function

$$\psi(\{X^\lambda_{m,\mathbf{k}}\}) = \psi(X^1_{s,\mathbf{k}_1}, X^2_{s,\mathbf{k}_1}, X^1_{c,\mathbf{k}_1}, X^2_{c,\mathbf{k}_1}, X^1_{s,\mathbf{k}_2}, X^2_{s,\mathbf{k}_2}, \ldots) \quad (1.4.10)$$

of the infinite set of canonical coordinates $X^\lambda_{m,\mathbf{k}}$. Remember these coordinates are *not* the positions of photon with momentum $\hbar\mathbf{k}$ *et cetera*. They are the amplitudes of the vector potential for the field mode with wavenumber $\mathbf{k}$ *et cetera*.

Finally, we can now write expressions for the quantized electromagnetic fields $\hat{\mathbf{A}}$ and $\hat{\mathbf{E}}^\perp = -\dot{\hat{\mathbf{A}}} = i[\hat{\mathbf{A}}, \hat{H}]/\hbar$ in terms of the annihilation and creation operators. The result is

$$\hat{\mathbf{A}}(\mathbf{x}) = \sum_{\mathbf{k},\lambda} \boldsymbol{\varepsilon}^\lambda_{\mathbf{k}} \sqrt{\frac{\hbar}{\epsilon_0 \omega_{\mathbf{k}} L^3}} \left\{ [a^\lambda_{s,\mathbf{k}} + (a^\lambda_{s,\mathbf{k}})^\dagger] \sin(\mathbf{k}\cdot\mathbf{x}) + [a^\lambda_{c,\mathbf{k}} + (a^\lambda_{c,\mathbf{k}})^\dagger] \cos(\mathbf{k}\cdot\mathbf{x}) \right\} \quad (1.4.11)$$

$$\hat{\mathbf{E}}^\perp(\mathbf{x}) = \sum_{\mathbf{k},\lambda} \boldsymbol{\varepsilon}^\lambda_{\mathbf{k}} \sqrt{\frac{\hbar\omega_{\mathbf{k}}}{\epsilon_0 L^3}}\, i \left\{ [a^\lambda_{s,\mathbf{k}} - (a^\lambda_{s,\mathbf{k}})^\dagger] \sin(\mathbf{k}\cdot\mathbf{x}) + [a^\lambda_{c,\mathbf{k}} - (a^\lambda_{c,\mathbf{k}})^\dagger] \cos(\mathbf{k}\cdot\mathbf{x}) \right\} \quad (1.4.12)$$

1.4.1 NON-EXAMINABLE Field Commutation Relations

From the above equations it can be show that

$$[\hat{A}_j(\mathbf{r}), \hat{A}_l(\mathbf{r}')] = 0 \quad (1.4.13)$$

$$[\hat{E}^\perp_j(\mathbf{r}), \hat{E}^\perp_l(\mathbf{r}')] = 0 \quad (1.4.14)$$

$$[\hat{A}_j(\mathbf{r}), \hat{E}^\perp_l(\mathbf{r}')] = \frac{-i\hbar}{\epsilon_0} \frac{2}{L^3} \sum_{\mathbf{k},\lambda} (\boldsymbol{\varepsilon}^\lambda_{\mathbf{k}})_j (\boldsymbol{\varepsilon}^\lambda_{\mathbf{k}})_l \left(\sin \mathbf{k}\cdot\mathbf{r} \, \sin \mathbf{k}\cdot\mathbf{r}' + \cos \mathbf{k}\cdot\mathbf{r} \, \cos \mathbf{k}\cdot\mathbf{r}' \right) \quad (1.4.15)$$

Using $\sum_\lambda (\boldsymbol{\varepsilon}^\lambda_{\mathbf{k}})_l (\boldsymbol{\varepsilon}^\lambda_{\mathbf{k}})_j + \check{k}_j \check{k}_l = \delta_{jl}$ enables us to write

$$[\hat{A}_j(\mathbf{r}), \hat{E}^\perp_l(\mathbf{r}')] = (-i\hbar/\epsilon_0) \delta^\perp_{jl}(\mathbf{r} - \mathbf{r}'), \quad (1.4.16)$$

where the symbol $\delta^\perp_{jl}(\mathbf{r} - \mathbf{r}')$ is known as the *transverse* δ function, and can be defined by

$$\delta^\perp_{jl}(\mathbf{x}) = \frac{1}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}} \left(\delta_{jl} - \check{k}_j \check{k}_l \right). \quad (1.4.17)$$

It is so-named because is picks out the transverse part of a vector field $\mathbf{C}(\mathbf{x})$:

$$\int d^3\mathbf{r} C_j(\mathbf{r}) \delta^{\perp}_{jk}(\mathbf{x}-\mathbf{r})\mathbf{e}_k = \mathbf{C}^{\perp}(\mathbf{x}). \tag{1.4.18}$$

This is as opposed to the usual δ function for vector fields,

$$\delta_{jl}(\mathbf{x}) = \delta_{jl}\frac{1}{(2\pi)^3}\int \mathrm{d}^3\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{1.4.19}$$

which is defined so that it picks out the whole vector field $\mathbf{C}(\mathbf{x})$,

$$\int d^3\mathbf{r} C_j(\mathbf{r}) \delta_{jk}(\mathbf{x}-\mathbf{r})\mathbf{e}_k = \mathbf{C}(\mathbf{x}). \tag{1.4.20}$$

Here, and in the below, I am using the **Einstein summation convention** for repeated indices.

To see that (1.4.16) is equivalent to the definition in Eq. (1.4.15) requires that we remember that the fields are defined only in the region $0 \leq x, y, z \leq L$, and taking the limit $L \to \infty$. The result using the transverse δ function is superior because it is independent of the mode functions used to quantize the field. The results (1.4.13)–(1.4.16) will be used later. These equations mean that one could measure $\mathbf{A}$ at all points in space, or measure $\mathbf{E}$ at all points in space, but one could not simultaneously measure both of them at all points in space.

2 Quantum States of the EM Radiation Field

2.1 Single-Mode Pure States

For simplicity, consider a single sin mode of the electromagnetic field with spatial frequency $\mathbf{k}$ and polarization vector $\boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda}$. Strictly, a mode like this extends over the entire universe. However in practice we often consider *quasimodes* which have a similar variation in space but which are confined to a particular part of the universe. For example, a "standing wave" between two mirrors (a Fabry-Perot cavity) is strictly a quasimode, but is often referred to as a mode, and I will follow that usage at times.

In either case, the mode under consideration has a single co-ordinate, $\hat{X} = \hat{X}_{s,\mathbf{k}}^{\lambda}$, proportional to the amplitude of the vector potential $\mathbf{A}$ in that mode. As described in Sec. 1.4 it is possible to represent the state of the field as a wavefunction $\psi(X)$, in this case of just a single co-ordinate X. This is formally analogous to the wavefunction of a single particle, but remember X here is *not* the position of a photon or any other particle. It is describing the $\mathbf{A}$-field in that mode. We can define the eigenstates of the operator $\hat{X} = (a + a^{\dagger})/\sqrt{2}$ as $|X\rangle$ in which case we have

$$\psi(X) = \langle X|\psi\rangle\,. \tag{2.1.1}$$

Note that strictly $\psi(X)$ is a probability *density* amplitude, not a probability amplitude. That is, $|\psi(X)|^2$ is a probability density, normalized as $\int dX|\psi(X)|^2 = 1$, not a probability. Indeed, $|X\rangle$ (or $\langle X|$) are not strictly states at all; they cannot be normalized. This means that it is not possible to prepare the field in the state $|X\rangle$. In this chapter we are concerned with physical states, and we will discuss how some of them can be prepared.

2.1.1 Number States

The first states we will consider are eigenstates of the Hamiltonian $\hat{H} = \hbar\omega(a^{\dagger}a + \frac{1}{2})$ for this single mode. The eigenstates of $\hat{H}$ are the eigenstates $|n\rangle$ of $a^{\dagger}a$. Since $a^{\dagger}a$ can be interpreted as the photon number operator, these are known as photon number eigenstates, or more simply, *number states*. They are also known as *Fock states*, after the Russian Soviet physicist Vladimir Fock.

It was shown in Sec. 1.1 that the number states $|n\rangle$ satisfies

$$|n\rangle \propto (a^{\dagger})^n|0\rangle \tag{2.1.2}$$

where $|0\rangle$ is the *vacuum* state, the state with no excitations. That is, $a^{\dagger}$ (the creation operator) raises the number of photons by one. Similarly, a lowers it by one. However, we require the number states to be normalized, so that

$$\langle n|m\rangle = \delta_{nm}. \tag{2.1.3}$$

Now since $|n\rangle$ is an eigenstate of $a^{\dagger}a$ of eigenvalue n,

$$\langle n|\left[a^{\dagger}a|n\rangle\right] = n\,\langle n|n\rangle = n. \tag{2.1.4}$$

However we also have

$$\left[\langle n|a^\dagger\right]\left[a|n\rangle\right] = \langle\psi|\psi\rangle\,, \tag{2.1.5}$$

where $|\psi\rangle = a|n\rangle \propto |n-1\rangle$. Therefore the constant of proportionality must be

$$|\psi\rangle = a|n\rangle = e^{i\phi}\sqrt{n}|n-1\rangle \tag{2.1.6}$$

for some phase ϕ. We choose the convention that $\phi = 0$, so that

$$a|n\rangle = \sqrt{n}|n-1\rangle. \tag{2.1.7}$$

With this convention it can be shown similarly that

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{2.1.8}$$

Exercise 2.1 *Show this from Eq. (2.1.7). (Hint: consider the Fock-basis matrix elements for a.) Show also that the above two equations are consistent with $|n\rangle$ being an eigenstate of $a^\dagger a$.*

Note that a acting on the vacuum state $|0\rangle$ produces nothing, a null state.

Exercise 2.2 *Show that the normalized number state is*

$$|n\rangle = (n!)^{-1/2}(a^\dagger)^n|0\rangle.$$

You might expect that by considering a large n number state, we could get back to the classical limit of fields with definite (or at least near-definite) values. Actually, this does not happen; for a system in a number state the average value of the electric and magnetic fields is always zero.

Exercise 2.3 *Show that these average values are zero.*

Discussion 2.1 *What is a simple way to understand this? Consider a phase space diagram (i.e. a plot in the X-Y plane) for a harmonic oscillator. From Eq. (1.1.5), what does a constant-energy curve look like? What are the constant energy states in quantum mechanics? Draw a picture you would associate with a Fock state $|n\rangle$.*

2.1.2 Coherent States

The electromagnetic field does not have to be in an eigenstate of the Hamiltonian (in fact, it is quite difficult to prepare a mode of the field in a number state, except for the number zero). Moreover, by considering other states we can obtain a classical limit. The easiest way is by the *coherent* state.

A coherent state can be defined in numerous equivalent ways, but the simplest is that it is an eigenstate (a *right* eigenstate, to be precise) of the annihilation operator:

$$a|\alpha\rangle = \alpha|\alpha\rangle \tag{2.1.9}$$

where α is any complex number (remember a is not an Hermitian operator). There are no such right eigenstates of the creation operator $a^\dagger$.

Problem 2.1 (2 marks) *Prove this last sentence, using a proof by contradiction. That is, assume that there exists states $|\beta\rangle$ such that $a^\dagger|\beta\rangle = \beta|\beta\rangle$. Consider the inner product $\langle n|(a^\dagger)^{n+1}|\beta\rangle$ and hence show that, for $\beta \neq 0$, the inner product of $|\beta\rangle$ with any number state is zero. Explain why this is a contradiction. How can you derive a contradiction for the $\beta = 0$ case?*

It is easy to find an expression for $|\alpha\rangle$ in terms of the number states as follows. In general we have

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle. \tag{2.1.10}$$

Since $a|\alpha\rangle = \alpha|\alpha\rangle$ we get

$$\sum_{n=0}^{\infty} \sqrt{n}c_n|n-1\rangle = \sum_{n=0}^{\infty} \alpha c_n|n\rangle. \tag{2.1.11}$$

In the first sum the $n = 0$ term does not contribute because of the $\sqrt{n}$. Therefore we can change the limits of the sum to $n = 1 \cdots \infty$, then change variables from n to $m = n - 1$ to get

$$\sum_{m=0}^{\infty} \sqrt{m+1}c_{m+1}|m\rangle = \sum_{n=0}^{\infty} \alpha c_n|n\rangle \tag{2.1.12}$$

Equating the co-efficients of the number states on both sides we get the recursion relation

$$c_{n+1} = \frac{\alpha}{\sqrt{n+1}}c_n. \tag{2.1.13}$$

Thus $c_1 = \alpha c_0$, $c_2 = \alpha c_1/\sqrt{2} = \alpha^2 c_0/\sqrt{2}$ *et cetera* so that

$$c_n = \frac{\alpha^n}{\sqrt{n!}}c_0. \tag{2.1.14}$$

To normalize the state we require

$$1 = \sum_n |c_n|^2 = |c_0|^2 \sum_n \frac{\left(|\alpha|^2\right)^n}{n!}. \tag{2.1.15}$$

The final sum is simply the series expansion for the exponential $\exp\left(|\alpha|^2\right)$. Thus $|c_0|^2 = \exp\left(-|\alpha|^2\right)$ and without loss of generality we can take $c_0 = \exp\left(-|\alpha|^2/2\right)$. Thus we have

$$|\alpha\rangle = \exp\left(-|\alpha|^2/2\right) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle, \tag{2.1.16}$$

showing that eigenstates of a do exist.

In a coherent state the mean value of $a = 2^{-1/2}(\hat{X} + i\hat{Y})$ is obviously the eigenvalue α.

Exercise 2.4 *From this, show that for a coherent state $\bar{X}_\alpha \equiv \langle\alpha|\hat{X}|\alpha\rangle = \sqrt{2}\Re[\alpha]$, and $\bar{Y}_\alpha \equiv \langle\alpha|\hat{Y}|\alpha\rangle = \sqrt{2}\Im[\alpha]$.*

Problem 2.2 (2 marks) *Show that for a coherent state* $\langle\alpha|(\hat{X}-\bar{X}_\alpha)^2|\alpha\rangle = 1/2$*, and* $\langle\alpha|(\hat{Y}-\bar{Y}_\alpha)^2|\alpha\rangle = 1/2$*. Hence show that a coherent state is a* minimum uncertainty state*, saturating Heisenberg's uncertainty principle for conjugate observables,*

$$\sigma(X)\sigma(Y) \geq |[\hat{X},\hat{Y}]/2|.$$

Discussion 2.2 *From the above, if you were to represent* $|\alpha\rangle$ *on a phase-space plot, where would you centre it? Would you draw it as a point? If not, why not, and how would you represent it? Think of the value of* $\sigma^2(X)+\sigma^2(Y)$*.*

For α non-zero the coherent state has a non-zero mean photon number:

$$\langle\alpha|a^\dagger a|\alpha\rangle = |\alpha|^2\langle\alpha|\alpha\rangle = |\alpha|^2. \tag{2.1.17}$$

Here we have used $\langle\alpha|a^\dagger = (a|\alpha\rangle)^\dagger = (\alpha|\alpha\rangle)^\dagger = \langle\alpha|\alpha^*$. Thus $|\alpha|^2$ is a measure of the amount of excitation of the harmonic oscillator, while argα is the phase of excitation. The state $|0\rangle$ (where here 0 is the value of α) is the same state as the state $|0\rangle$ (where here 0 is the value of n). In other words, the vacuum state is both a coherent state and a number state.

Exercise 2.5 *Verify this.*

Discussion 2.3 *Compare your picture of* $|\alpha\rangle$ *with* $\alpha = 0$ *with your picture of* $|n\rangle$ *with* $n = 0$*, quantitatively (i.e. with marks on the axes).*

In quantum mechanics a coherent state does not have a definite amount of excitation of the oscillator, because it is not a number eigenstate. The photon number distribution (the probability for measuring a certain photon number) for a coherent state is just $|c_n|^2$, which is a *Poissonian* distribution of mean $|\alpha|^2$:

$$P_n = |\langle n|\alpha\rangle|^2 = e^{-|\alpha|^2}\frac{\left(|\alpha|^2\right)^n}{n!} \tag{2.1.18}$$

This distribution has the property that the variance is equal to the mean. That is,

$$\sigma^2(n) = \left\langle (a^\dagger a)^2\right\rangle - \left\langle a^\dagger a\right\rangle^2 = |\alpha|^2 \tag{2.1.19}$$

Problem 2.3 (1.5 mark) *Verify this, either from the distribution (2.1.18) or directly from the coherent state using the commutation relations for* a *and* $a^\dagger$*.*

Discussion 2.4 *Draw a phase-space diagram, including a coherent state* $|\alpha\rangle$ *with* $|\alpha| \gg 1$*, and various number states* $|n\rangle$*, that illustrates why* $\sigma(n) \sim |\alpha|$ *for a coherent state.*

Unlike a number state, a field in a coherent state can have a mean field. Specifically, if all of the other modes are in the vacuum state then

$$\left\langle \hat{\mathbf{E}}(\mathbf{x}) \right\rangle = \mathbf{E}_0(\mathbf{x}) \frac{\left\langle -ia + ia^\dagger \right\rangle}{2} = \mathbf{E}_0(\mathbf{x}) \frac{\langle \alpha | (-ia + ia^\dagger) | \alpha \rangle}{2} = \mathbf{E}_0(\mathbf{x}) \Im[\alpha]. \tag{2.1.20}$$

Here $\mathbf{E}_0(\mathbf{x})$ is proportional to the mode function of the single mode in the coherent state. For the quantization procedure used in Chapter 1 this may for example be equal to

$$\mathbf{E}_0(\mathbf{x}) = \boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda} \sqrt{\frac{\hbar \omega_{\mathbf{k}}}{\epsilon_0 L^3}}\, 2 \sin(\mathbf{k} \cdot \mathbf{x}) \tag{2.1.21}$$

This quantity can roughly be thought of as the electric field of one photon, because for a coherent state $\alpha = i$, which has a mean occupation of one photon ($|\alpha|^2 = 1$), $\left\langle \hat{\mathbf{E}}(\mathbf{x}) \right\rangle = \mathbf{E}_0(\mathbf{x})$.

Discussion 2.5 *Does the $1/\sqrt{L^3}$ factor make sense to you? If one wanted to see the effect of a single photon on some matter (e.g. an atom) how might one do that?*

Because a is not an Hermitian operator, the coherent states are not orthogonal. In fact it can be shown that

$$|\langle \alpha | \alpha' \rangle|^2 = \exp(-|\alpha - \alpha'|^2). \tag{2.1.22}$$

If α and α' are very different (as they would be if they represent two macroscopically distinct fields) then the two coherent states are very nearly orthogonal. Another consequence of their nonorthogonality is that the coherent states form an *overcomplete* basis. Whereas for number states we have

$$\sum_n |n\rangle\langle n| = I, \tag{2.1.23}$$

the identity, for coherent states we have

$$\int \mathrm{d}^2\alpha |\alpha\rangle\langle\alpha| = \pi I. \tag{2.1.24}$$

Problem 2.4 (2 marks) *Show this using the expansion (2.1.16). For the integral over the complex plane, consider using polar coordinates. The result $n! = \int_0^\infty dx x^n e^{-x}$ may be useful.*

Unlike number states, coherent states are not eigenstates of the Hamiltonian. However, they have the nice property that they remain coherent states under the free Hamiltonian $\hat{H} = \hbar\omega a^\dagger a$. (Note that here we have dropped the $\frac{1}{2}\hbar\omega$, because this is just a constant. This is a convenient practice in all that follows, and simply amounts to setting the energy to be zero when there are no photons present.) The amplitude $|\alpha|$ of the states remain the same; only the phase changes at rate ω (as expected):

$$\exp(-i\hat{H}t/\hbar)|\alpha\rangle = |e^{-i\omega t}\alpha\rangle \tag{2.1.25}$$

Problem 2.5 (1.5 marks) *Show this, using Eq. (2.1.16). Note that* $|e^{-i\omega t}\alpha\rangle$ *is NOT the same as* $e^{-i\omega t}|\alpha\rangle$.

Discussion 2.6 *What does this evolution look like in phase space? Are you surprised?*

2.2 Single Mode Mixed States

2.2.1 Mixed States

All of the states considered so far have been pure states. That is, states which can be represented by a state vector

$$|\psi\rangle = \sum_n \psi_n |n\rangle \tag{2.2.1}$$

This state can also be represented by a *state matrix*

$$\rho = \sum_{n,m} \rho_{n,m} |n\rangle\langle m| = |\psi\rangle\langle\psi|, \tag{2.2.2}$$

where

$$\rho_{n,m} = \psi_n \psi_m^*. \tag{2.2.3}$$

The object ρ is sometimes also called a density operator. Using it, the expectation values of an operator $\hat{O}$ can be written

$$\left\langle \hat{O} \right\rangle = \mathrm{Tr}[\hat{O}\rho], \tag{2.2.4}$$

where the trace of an operator is defined as

$$\mathrm{Tr}[\hat{A}] = \sum_n \langle n|\hat{A}|n\rangle \tag{2.2.5}$$

using any complete basis $\{|n\rangle\}$ (such as the number states). This can be seen as follows:

$$\begin{aligned}
\mathrm{Tr}[\hat{O}\rho] &\equiv \sum_n \langle n|\hat{O}\rho|n\rangle && (2.2.6)\\
&= \sum_{n,m} \langle n|\hat{O}|m\rangle\langle m|\rho|n\rangle && (2.2.7)\\
&= \sum_{n,m} \langle n|\hat{O}|m\rangle \rho_{m,n} && (2.2.8)\\
&= \sum_{n,m} \langle n|\hat{O}|m\rangle \psi_m \psi_n^* && (2.2.9)\\
&= \sum_{n,m} \langle\psi|n\rangle \langle n|\hat{O}|m\rangle \langle m|\psi\rangle && (2.2.10)\\
&= \langle\psi|\hat{O}|\psi\rangle = \left\langle \hat{O} \right\rangle. && (2.2.11)
\end{aligned}$$

The big advantage of the state matrix formalism is that we can represent mixed states. These are states which are in a classical probabilistic

mixture of different pure states If the system were in state $|\psi^1\rangle$ with probability p_1 and in state $|\psi^2\rangle$ with probability p_2 then the average value of an operator O would clearly be

$$\left\langle \hat{O} \right\rangle = p_1 \langle \psi^1 | \hat{O} | \psi^1 \rangle + p_2 \langle \psi^2 | \hat{O} | \psi^2 \rangle. \tag{2.2.12}$$

This result is also obtained from the formula

$$\left\langle \hat{O} \right\rangle = \mathrm{Tr}[\rho \hat{O}] \tag{2.2.13}$$

if we define the state matrix for the mixed state by

$$\rho = p_1 |\psi^1\rangle\langle\psi^1| + p_2 |\psi^2\rangle\langle\psi^2|. \tag{2.2.14}$$

Exercise 2.6 *Show this. Note that there is no requirement for ψ^1 and ψ^2 to be orthogonal.*

In general a state matrix can be written as

$$\rho = \sum_\mu p_\mu |\psi^\mu\rangle\langle\psi^\mu|, \tag{2.2.15}$$

where $p_\mu \geq 0$ and $\sum_\mu p_\mu = 1$. This gives

$$\rho_{nm} = \sum_\mu p_\mu \psi_n^\mu (\psi_m^\mu)^*. \tag{2.2.16}$$

From the Schrödinger equation (1.2.1) for the state vector, it is easy to show that the analogous equation of motion for the state matrix is

$$(i\hbar)\frac{\partial}{\partial t}\rho(t) = [\hat{H}_t, \rho(t)]. \tag{2.2.17}$$

Note that this is different (and has a different interpretation) from the Heisenberg picture equation of motion Eq. (1.2.4) for an operator $\hat{A}(t)$.

As a special example of Eq. (2.2.13), the normalization of a state matrix is

$$1 = \mathrm{Tr}[\rho] = \sum_n \rho_{nn}. \tag{2.2.18}$$

For pure states it can be shown that

$$\mathrm{Tr}[\rho^2] = \mathrm{Tr}[|\psi\rangle\langle\psi|\psi\rangle\langle\psi|] = \mathrm{Tr}[|\psi\rangle\langle\psi|] = \langle\psi|\psi\rangle = 1. \tag{2.2.19}$$

For a general mixed state

$$0 < \mathrm{Tr}[\rho^2] < 1, \tag{2.2.20}$$

and this quantity is a measure of how pure the state is.

Exercise 2.7 *Prove Eq. (2.2.20). Assume a finite dimensional system for simplicity.*

2.2.2 Single-Mode Thermal States

Mixed states arise often in nature because of uncontrollable fluctuations, such as thermal noise which arises when the system is coupled to a heat bath at finite temperature. A single mode of the electromagnetic field coupled to such a bath comes to an equilibrium mixed state called a single mode thermal state. From statistical mechanics we know that the probability for the system to occupy a state of energy E is proportional to $\exp(-E/k_BT)$. For a single harmonic oscillator we know the energy states $|n\rangle$ have eigenvalues $\hbar\omega n$. Therefore the single mode thermal state has the state matrix

$$\rho = \sum_{n=0}^{\infty} p_n |n\rangle\langle n|, \tag{2.2.21}$$

where $p_n = Z^{-1}\exp(-\hbar\omega n/k_BT)$, where Z is the partition function (needed for normalization) given by

$$Z = \sum_{n=0}^{\infty} r^n = \frac{1}{1-r}, \tag{2.2.22}$$

where $r = \exp(-\hbar\omega/k_BT)$. Thus the full expression is

$$\rho_{\rm th} = [1-\exp(-\hbar\omega/k_BT)]\sum_{n=0}^{\infty}\exp(-n\hbar\omega/k_BT)|n\rangle\langle n|. \tag{2.2.23}$$

From Eq. (2.2.23) it is easy to show that the mean photon number of a SMT state is

$$\begin{aligned}
\left\langle a^\dagger a\right\rangle &= \sum_{n=0}^{\infty} p_n n \;=\; (1-r)\sum_{n=0}^{\infty} r^n n && (2.2.24)\\
&= r(1-r)\sum_{n=0}^{\infty} r^{n-1} n \;=\; r(1-r)\frac{\partial}{\partial r}\sum_{n=0}^{\infty} r^n && (2.2.25)\\
&= r(1-r)\frac{\partial}{\partial r}\frac{1}{1-r} = \frac{r}{1-r} && (2.2.26)
\end{aligned}$$

That is,

$$\bar{n}_{\rm th}(\omega) = \frac{1}{\exp(\hbar\omega/k_BT)-1} \tag{2.2.27}$$

This should be familiar as Planck's formula.

$$\bar{E}_{\rm th}(\omega) = \frac{\hbar\omega}{\exp(\hbar\omega/k_BT)-1}. \tag{2.2.28}$$

We can then rewrite a SMT state as follows, with $\bar{n} = \bar{n}_{\rm th}(\omega)$,

$$\rho_{\rm th}\left(\bar{n}\right) = \frac{1}{1+\bar{n}}\sum_{n=0}^{\infty}\left(\frac{\bar{n}}{\bar{n}+1}\right)^n |n\rangle\langle n|. \tag{2.2.29}$$

Following a similar procedure to that use to derive the mean, it can be shown that the photon-number variance of a SMT state is

$$\sigma^2 \equiv \left\langle (a^\dagger a)^2\right\rangle - \left\langle a^\dagger a\right\rangle^2 = \bar{n}^2 + \bar{n}. \tag{2.2.30}$$

Problem 2.6 (1.5 marks) *Show this.*

Thus in contrast to a coherent state, where for $|\alpha|^2 \gg 1$ the standard-deviation σ in the photon number is much less than the mean, for a thermal state the standard-deviation is always larger than the mean. That is, the photon number is not very well defined for a thermal state.

The SMT state can also be expressed in terms of coherent states as

$$\rho_{\rm th}(\bar{n}) = \frac{1}{\pi\bar{n}} \int \mathrm{d}^2\alpha \exp(-|\alpha|^2/\bar{n}) |\alpha\rangle\langle\alpha|. \tag{2.2.31}$$

Problem 2.7 (2 marks) *Show this. Use* $\int dx\, x^n e^{-\gamma x} = \gamma^{-(n+1)} n!$

This is an example of how mixed states can always be represented in (infinitely many) different ways as an ensemble of pure states.

Discussion 2.7 *Draw two phase-space diagrams that show how these two different ensembles can give the same mixed state. Use a pencil and use different pressure to represent different weights given to various states.*

2.2.3 Single-Mode Laser States

Another example of a single mode mixed state is the state inside a laser cavity. It is sometimes stated in textbooks that the state of the laser mode is a coherent state $|\alpha\rangle$. While the coherent state does have the same photon statistics as the state of an ideal laser cavity mode, it is not strictly correct to say that it is in a coherent state. The reason is that whenever a laser is turned on, the *phase* of the field $\arg\alpha$ cannot be predicted beforehand. Rather, it takes on a random value. Furthermore, that value changes randomly (diffuses) on a time scale of $\tau_{\rm coh} = 1/\Gamma$, called the coherence time. Here Γ is the phase diffusion rate. We will discuss this phenomenon in some detail in Sec. 3.3.3.

Thus unless we use another coherent source (another laser) to keep track of the phase of the laser, it will turn into a mixture of all possible phases. We can write the state corresponding to this as

$$\rho_{\rm laser} = \int \frac{d\phi}{2\pi} |\sqrt{\mu}\, e^{i\phi}\rangle\langle\sqrt{\mu}\, e^{i\phi}|, \tag{2.2.32}$$

where here $|\sqrt{\mu}\, e^{i\phi}\rangle$ is a a coherent state. Equivalently, this state is equal to

$$\rho_{\rm laser}(\mu) = \sum_{n=0}^{\infty} e^{-\mu} \frac{\mu^n}{n!} |n\rangle\langle n|. \tag{2.2.33}$$

Here $\mu = |\alpha|^2$ is the mean photon number of the laser mode.

Problem 2.8 (1.5 marks) *Show that equations (2.2.33) and (2.2.32) are equivalent.*

Discussion 2.8 *Draw two phase-space diagrams that show how these two different ensembles can give the same mixed state. Use different depth of shading to represent different weights given to various states.*

2.3 Multimode Field States

The first step to defining multimode field state is to define a basis. It is most convenient to use the number states for each mode. For example, in a hypothetical 3-mode system a joint number state would be denoted

$$|\{n_\kappa\}\rangle = |n_1\, n_2\, n_3\rangle \equiv |n_1\rangle_1 \otimes |n_2\rangle_2 \otimes |n_3\rangle_3, \tag{2.3.1}$$

and the infinite basis set would be

$$\begin{aligned} \{ \quad & |0\,0\,0\rangle, \\ & |1\,0\,0\rangle, |0\,1\,0\rangle, |0\,0\,1\rangle, \\ & |2\,0\,0\rangle, |0\,2\,0\rangle, |0\,0\,2\rangle, |1\,1\,0\rangle, \cdots \\ & \cdots \ \} \end{aligned} \tag{2.3.2}$$

For a full description of the electromagnetic field we have to consider an infinite number of modes. For that we have to consider states

$$|\{n_\kappa\}\rangle = \bigotimes_\kappa |n_\kappa\rangle_\kappa \equiv |n_1\rangle_1 \otimes |n_2\rangle_2 \otimes |n_3\rangle_3 \cdots, \tag{2.3.3}$$

where here κ is the mode label which is meant to include $\mathbf{k}$ (the propagation vector), m (whether it is a sin or cos mode) and λ (labelling the polarization direction), and the product is an infinite product. In this case the basis set is doubly infinite in size. The first member of the basis set is the *vacuum state* $|0\,0\,0\cdots\rangle$.

A general pure state of the multimode field can be written

$$|\psi\rangle = \sum_{\{n_\kappa\}} c_{\{n_\kappa\}} |\{n_\kappa\}\rangle = \sum_{N=0}^{\infty} \sum_{\{n_\kappa : \sum_\kappa n_\kappa = N\}} c_{\{n_\kappa\}} |\{n_\kappa\}\rangle. \tag{2.3.4}$$

That is, we have to sum over all possible total photon numbers, and sum over all the possible ways each total photon number can be distributed between an infinite number of modes. A general mixed state can be written

$$\rho = \sum_{\{n_\kappa\},\{m_\kappa\}} \rho_{\{n_\kappa\},\{m_\kappa\}} |\{n_\kappa\}\rangle\langle\{m_\kappa\}|. \tag{2.3.5}$$

Fortunately the states we will write down explicitly are much less general than this. Specifically, they will all have the structure

$$\rho = \bigotimes_\kappa \rho_\kappa \equiv \rho_1 \otimes \rho_2 \otimes \cdots \tag{2.3.6}$$

where

$$\rho_\kappa = \sum_n P_\kappa(n) |n\rangle_\kappa \langle n|_\kappa \tag{2.3.7}$$

That is, there are no correlations between the state of each mode, and each mode is in a mixture of number states. We will now see how this arises naturally with thermal light.

2.3.1 Thermal Light

The total energy of the multimode system is the sum of the energy of the individual modes:

$$\hat{H} = \sum_{\mathbf{k},\lambda,m} \hbar\omega_{\mathbf{k}} \left(a^{\lambda}_{m,\mathbf{k}}\right)^{\dagger} a^{\lambda}_{m,\mathbf{k}} = \sum_{\kappa} \hbar\omega_{\kappa} a^{\dagger}_{\kappa} a_{\kappa}. \tag{2.3.8}$$

Thus the eigenstates of $\hat{H}$ are just the joint multi-mode number states $|\{n_\kappa\}\rangle$. In thermal equilibrium the probability of being in such a state factorizes:

$$P(\{n_\kappa\}) \propto \exp(-\sum_{\kappa} \hbar\omega_\kappa n_\kappa / k_B T) = \prod_{\kappa} \exp(-\hbar\omega_\kappa n_\kappa / k_B T) \tag{2.3.9}$$

Thus the total state matrix for multimode thermal light just factorizes into the single-mode thermal states:

$$\rho = \bigotimes_{\kappa} \rho^{\kappa}_{\mathrm{th}} \left(\bar{n}_{\mathrm{th}}(\omega_\kappa)\right) \tag{2.3.10}$$

where $\bar{n}_{\mathrm{th}}(\omega_\kappa)$ is defined in Eq. (2.2.27) and, as before,

$$\rho_{\mathrm{th}}\left(\bar{n}\right) = \frac{1}{1+\bar{n}} \sum_{n=0}^{\infty} \left(\frac{\bar{n}}{\bar{n}+1}\right)^{n} |n\rangle\langle n|. \tag{2.3.11}$$

3 Quantum Properties of Laser Light

3.1 From Thermal Light towards Laser Light

Thermal light is the sort of light that comes out an old-fashioned (incandescent) light bulb. This chapter is devoted to teasing out how this is different from the sort of light most physics experiments use these days, laser light.

Discussion 3.1 *What is the difference between light-bulb light and laser light? Write down the words, or simple ideas, that come to mind.*

3.1.1 Collimated Polarized Thermal Light

Because all modes are populated, thermal light is isotropic. That is, it propagates in all directions equally. Also, it is unpolarized: for each $\mathbf{k}$ both polarizations λ are equally populated. One of the aims of this chapter is to compare thermal light with laser light, in order to understand what is special about the light produced by a laser. The first obvious property of laser light which contrasts with thermal light is that it is not isotropic. Rather, it propagates in a single direction, and it is usually polarized. In this section we consider thermal light which has been collimated (so as to make it unidirectional) and polarized.

In order to consider unidirectional light it is convenient to change modes from the standing waves used in Chapter 1, e.g. Eq. (1.4.11), to traveling waves. In these new modes we can drop the m subscript and retain the $\mathbf{k}$ and λ labels. This halves the number of modes, but we double it by allowing $\mathbf{k}$ to take on all possible values, not just those with $k_x \geq 0$. The vector potential and electric fields for a free field are

$$\hat{\mathbf{A}}(\mathbf{x}) = \sum_{\mathbf{k},\lambda} \boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda} \sqrt{\frac{\hbar}{2\epsilon_0 \omega_{\mathbf{k}} L^3}} \left(a_{\mathbf{k}}^{\lambda} e^{i\mathbf{k}\cdot\mathbf{x}} + (a_{\mathbf{k}}^{\lambda})^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{x}} \right), \quad (3.1.1)$$

$$\hat{\mathbf{E}}^{\perp}(\mathbf{x}) = \sum_{\mathbf{k},\lambda} \boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda} \sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2\epsilon_0 L^3}} \left(i a_{\mathbf{k}}^{\lambda} e^{i\mathbf{k}\cdot\mathbf{x}} - i(a_{\mathbf{k}}^{\lambda})^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{x}} \right), \quad (3.1.2)$$

where $\mathbf{k}$ can point in any direction:

$$\mathbf{k} = \frac{2\pi}{L}(l,m,n) \ : \ l,m,m \in \{-\infty \cdots, -2, -1, 0, 1, 2, \cdots \infty\}. \quad (3.1.3)$$

Problem 3.1 (2 marks) *Determine the new mode operators $\{a_{\mathbf{k}}^{\lambda}\}$ in terms of the old ones $\{a_{m,\mathbf{k}}^{\lambda}\}$. Check that the new ones obey the expected commutation relations, $[a_{\mathbf{k}'}^{\lambda'}, a_{\mathbf{k}}^{\lambda\dagger}] = \delta_{\mathbf{k}',\mathbf{k}}\delta^{\lambda,\lambda'}$.*

Collimating the thermal light emitted by a blackbody source (by passing it through a series of finite apertures) will lead, in the ideal limit, to a field with $\mathbf{k}$ vectors in a single direction. Thus $\mathbf{k}$ can be replaced by $k = (2\pi/L)l$, with l a positive integer. Polarizing it will

eliminate the need for the polarization vector and index λ. The energy of the field thus becomes

$$\hat{H} = \sum_k \hbar c k a_k^\dagger a_k, \tag{3.1.4}$$

and the state of the collimated polarized thermal field is

$$\rho = \bigotimes_k \rho_{\rm th}^k \left(\bar{n}_{\rm th}(ck)\right), \tag{3.1.5}$$

where the single-mode thermal state is as before. Here we have included only those modes propagating in the desired direction. The other modes would ideally be in the vacuum state.

Because the light is collimated, the energy density (which scales as $(k_B T)^4/(\hbar c)^3$ for an isotropic thermal field) is not a sensible quantity to consider. Rather, we should calculate the energy per unit length in the direction of propagation. This yields

$$\frac{\left\langle \hat{H} \right\rangle}{L} = \frac{1}{L}\sum_k \hbar c k \bar{n}_{\rm th}(ck) \tag{3.1.6}$$

$$= \frac{\hbar c}{2\pi}\sum_k (\Delta k) k \bar{n}_{\rm th}(ck), \tag{3.1.7}$$

where $\Delta k = 2\pi/L$ is the separation of k modes. In the limit $L \to \infty$ this separation becomes infinitesimal and the sum can be converted to an integral, $\sum_k (\Delta k) \to \int_0^\infty dk$. The result is

$$\frac{\left\langle \hat{H} \right\rangle}{L} = \frac{\pi}{12}\frac{(k_B T)^2}{\hbar c}. \tag{3.1.8}$$

Exercise 3.1 *Show this. Hint:* $\int_0^\infty dx\, x/(e^x - 1) = \pi^2/6$.

Since the light is propagating in one direction, it is natural to convert this result to the energy per unit time, or power in the collimated beam:

$$P = \frac{\left\langle \hat{H} \right\rangle c}{L} = \frac{\pi}{12}\frac{(k_B T)^2}{\hbar}. \tag{3.1.9}$$

This can now be easily compared to the power of the output of a laser, which is typically of order 100 milliwatts.

Exercise 3.2 *Find the temperature of the blackbody required to produce a collimated, polarized output of this power.*

Discussion 3.2 *How does this compare to the temperature of the surface of the sun? What conclusion do you draw from this?*

You might be curious as to how much of the light would be thrown away in this collimation process. The answer depends on the size of the source. The larger the source, the more spatially incoherent it is, and the more severe the collimation has to be be. The Stefan–Boltzmann law says that a blackbody source of area A, at temperature T, has a radiative power of

$$P_{\text{total}} = \frac{\pi^2}{60} \frac{A\,(k_B T)^4}{c^2 \hbar^3} \tag{3.1.10}$$

Exercise 3.3 *A light-bulb filament has an area of about 15 mm^2. Using this, calculate what proportion of total power must be thrown away in the collimation process above, assuming the beam is derived from the light-bulb as discussed above.*

3.1.2 Monochromatic Collimated Polarized Thermal Light

As well as being unidirectional and polarized, laser light is close to monochromatic. That is, almost all of the power is at approximately the same frequency. This property can be achieved from collimated polarized thermal light by passing it through a frequency filter (such as a series of Fabry-Perot etalons) described by $f(\omega)$. To mimic the frequency spread of a typical laser, we can take the filter function to be *Lorentzian*, with

$$f(\omega) = \frac{(\Gamma/2)^2}{(\Gamma/2)^2 + (\omega - \omega_0)^2}, \tag{3.1.11}$$

where ω_0 is the mean frequency and $\Gamma \ll \omega_0$ is the linewidth (Full Width at Half Maximum Height). (Note that this Γ is the same as the phase diffusion rate mentioned in Sec 2.2.3). This changes $\bar{n}_{\text{th}}(\omega)$ to

$$\bar{n}_{\text{f}}(\omega) = \bar{n}_{\text{th}}(\omega) f(\omega) \simeq \bar{n}_{\text{th}}(\omega_0) f(\omega). \tag{3.1.12}$$

Discussion 3.3 *Draw a plot showing both $\bar{n}_{\text{th}}(\omega)$ and $f(\omega)$. Do you see why the '$\simeq$' in Eq. (3.1.12) is justified, at least if we are only interested in light at optical frequencies?*

The state of the filtered light is thus

$$\rho = \bigotimes_k \rho_{\text{th}}^k \left(\bar{n}_{\text{f}}(\omega)\right). \tag{3.1.13}$$

The power in this filtered collimated polarized thermal light is

$$\frac{\left\langle \hat{H} \right\rangle c}{L} = \frac{c}{L} \sum_k \hbar c k \bar{n}_{\text{f}}(ck). \tag{3.1.14}$$

In the limit $\Gamma \ll \omega_0$ this can be evaluated as

$$P = \bar{n}_{\text{th}}(\omega_0) \hbar \omega_0 \Gamma / 4 \tag{3.1.15}$$

Exercise 3.4 *Show this. Hint* $\int_{-\infty}^{\infty} dx/(1+x^2) = \pi$. *Justify all approximations made.*

For high temperatures ($k_B T \gg \hbar\omega_0$) this is simply

$$P = k_B T \Gamma/4 \tag{3.1.16}$$

This enables easy comparison with a moderately high-quality laser, with an output power of order 100 milliwatts (as above) and a linewidth Γ of order 10^7 s^{-1}.

Exercise 3.5 *Find the temperature of the blackbody required to produce a collimated, polarized, frequency-filtered output of this power and linewidth. Would it be feasible to filter this radiation with optical devices? If it were feasible, what proportion of the total power (3.1.10) would be discarded, if the original source were a light bulb filament of area 15 mm*^{2}*?*

Discussion 3.4 *What conclusion do you draw from this?*

3.2 Laser Light

We have seen that it would be completely impractical to try to produce a beam with the same power and linewidth of a laser beam by collimating, polarizing, and filtering a thermal beam. Even if it could be done, the result would still not be equivalent to a laser beam. The remaining difference is essentially the same difference between a single mode thermal state and a single mode laser state. The former has a very poorly defined photon number, while the latter can have a very well-defined photon number. In the multimode case, the filtered collimated polarized thermal beam would have large, slow (at rate Γ) intensity variations over time, whereas a laser beam has very small intensity variations.

For an ideal laser beam, the number of photons with a given frequency is the same as that for the filtered collimated thermal beam, (3.1.12), but because there is no thermal origin we replace $\bar{n}_{\rm th}(\omega_0)$ by a real parameter which we will call ν:

$$\bar{n}_{\rm laser}(\omega) = \nu \frac{(\Gamma/2)^2}{(\Gamma/2)^2 + (\omega - \omega_0)^2}. \tag{3.2.1}$$

Because all of the significantly populated frequency modes are close in frequency to ω_0, if we multiply by $\hbar\omega$ we also get the *energy* in each frequency. For this reason, $\bar{n}_{\rm laser}(\omega)$ is often called the *spectrum* of the laser. One might guess that, in the ideal limit where the state of the laser cavity mode is given by Eq. (2.2.33), the only difference between the collimated filtered thermal light and the laser light would be that each k-mode of the laser output would be in a single-mode laser state. Actually [1] it cannot be of this form, and moreover there seems to be no simple way to write down its state in terms of these modes.

[1] See H. M. Wiseman, "How many principles does it take to change a light bulb ... into a laser?" Physica Scripta **91**, 033001 (2016).

Nevertheless we can draw a simple relation between the single-mode distribution Eq. (2.2.33) and the output of an ideal laser: both have a Poissonian distribution for photon number. Specifically, since P is the power and $\hbar\omega_0$ the energy per photon, $P/\hbar\omega_0$ is the *photon flux* of the laser, in photons per unit time. Thus if we count the number of photons in the ideal laser output beam for a time τ, the result will be a random variable N with a mean $\bar{N} = (P/\hbar\omega_0)\tau$, and a standard deviation of $\sqrt{\bar{N}}$, which is much less than $\bar{N}$ if the latter is large. By contrast, if the beam were derived from a thermal source then on time scales τ up to Γ^{-1} the standard deviation in N would be of the same order as the mean $\bar{N}$.

As discussed already, for a laser, the linewidth Γ is due almost entirely to phase diffusion, not intensity fluctuations. That is, the coherence time, $1/\Gamma$, can be thought of as the time for the phase of the laser to become fairly randomized. Thus

$$P/(\hbar\omega_0\Gamma) = \nu/4 \tag{3.2.2}$$

measures the number of photons which come out of the laser which are coherent (that is, which have roughly the same phase, in some sense). Here ν is the dimensionless number defining the spectral peak occupation number in Eq. (3.2.1). It is the fact that this number is very large in a typical laser which makes it difficult to produce a similar beam from a thermal source.

Exercise 3.6 *Calculate, to the nearest order of magnitude, the number of photons emitted from a laser per coherence time with the typical parameters used above, and for a typical optical frequency.*

Problem 3.2 (1 marks) *Revisiting Exercise 3.5, show that the proportion of power that would be kept in the attempt to produce laser-like light by collimating and filtering light from a very(!) hot light bulb filament is*

$$\frac{P}{P_{\text{total}}} = \frac{15}{4\pi^4} \times \frac{\lambda_0^2}{A} \times \frac{\Gamma}{\omega_0} \times \frac{1}{\nu^3}. \tag{3.2.3}$$

Here A is the area of the filament, $\lambda_0 = 2\pi c/\omega_0$ is the peak wavelength of the filtered beam, and P_{total} is as in Eq. (3.1.10). Evaluate each of the four factors here (separated by $\times$ symbols), and show that by far the most important (i.e. by far the smallest) is the last of them.

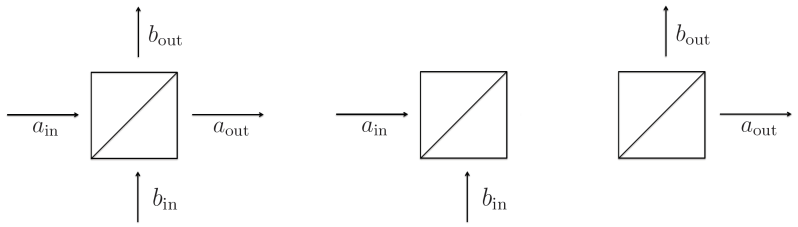
Discussion 3.5 *From what you have now learned, what are the four principle differences between light-bulb light and laser light?*

3.3 The Generation of Laser Light

We have seen that one of the crucial factors that makes laser light hard to mimic with thermal sources is the large size of ν, the mean number of coherent photons in the beam. In this section we will show how a laser can produce such a large ν. But before we get there, some preliminary calculations are necessary to do with coherent states.

3.3.1 Preliminary: the beam-splitter evolution

A beam-splitter is a device which takes two optical inputs and produces two outputs. Traditionally, it is described as a "half-silvered mirror" but there are many physical devices which functionally act as a beam splitter. It is easiest to define it mathematically as a reversible operation acting on two modes which linearly mixes their fields. By a 'mode' here we mean a harmonic oscillator mode. Because of the common physical set up of a beam-splitter, the modes before the beam splitter are called the input or 'in' modes, and those after are called the output or 'out' modes; see Fig. 3.1. Conceptually, it is very important not to think of the input and output modes as existing at the same time. There are always only two modes. There is just a 'before' state (and location) of the two modes, and an 'after' state and location.



"All at once" diagram. Before diagram. After diagram.

Figure 3.1: An optical beam-splitter. Left diagram: the wrong way to think about it. Right two diagrams: the right way to think about it.

Classically, we can describe the action of a beam-splitter by how it transforms the phasor variable (a complex number) describing the harmonic oscillator (e.g. $a = (X + iY)/\sqrt{2}$)

$$\begin{pmatrix} a_{\rm out} \\ b_{\rm out} \end{pmatrix} = \begin{pmatrix} t & r \\ r & t \end{pmatrix} \begin{pmatrix} a_{\rm in} \\ b_{\rm in} \end{pmatrix}. \tag{3.3.1}$$

Here t and r are complex numbers called respectively the transmissivity and reflectivity of the beam-splitter. These obey

$$|r|^2 + |t|^2 = 1 \; ; \;\; t r^* + r t^* = 0. \tag{3.3.2}$$

For example, if the transmissivity $t = 1$ then we simply have $a_{\rm out} = a_{\rm in}$ and $b_{\rm out} = b_{\rm in}$ (no change in the modes), and if reflectivity $r = 1$ then we simply have $a_{\rm out} = b_{\rm in}$ and $b_{\rm out} = a_{\rm in}$ (swapping the modes). Something non-trivial happens only if neither $|t|$ nor $|r|$ equals one. A 50:50 beam-splitter is the case where the transmittance $\mathscr{T} = |t|^2$ and reflectance $\mathscr{R} = |r|^2$ both equal 0.5.

Exercise 3.7 *Is it permissible to choose $t = r = 1/\sqrt{2}$? Why?*

The device is called a beam-*splitter* because classically we often have the situation where there is light only in one mode. That is, we set $b_{\rm in} = 0$, for example, so that $a_{\rm in}$ is *split* into the two output modes:

$$a_{\rm out} = t\, a_{\rm in} \; ; \;\; b_{\rm out} = r a_{\rm in}. \;\; \text{(classical beam-}\textit{splitter}\text{)}. \tag{3.3.3}$$

Exactly the same equations (3.3.1) apply in quantum mechanics for the mode annihilation operators $\hat{a}$ and $\hat{b}$. (Recall that typically we don't even put a hat on these operators, but we are doing so here for emphasis).

Exercise 3.8 *Show that this evolution preserves photon number, i.e.,*

$$a_{\rm out}^\dagger a_{\rm out} + b_{\rm out}^\dagger b_{\rm out} = a_{\rm in}^\dagger a_{\rm in} + b_{\rm in}^\dagger b_{\rm in}. \tag{3.3.4}$$

Here we would regard the mapping (3.3.1) as a discrete-time *Heisenberg picture evolution*, from the 'before' time to the 'after' time. That is,

$$\hat{a}_{\rm out} \equiv \hat{a}(t_{\rm after}) \; ; \;\; \hat{a}_{\rm in} \equiv \hat{a}(t_{\rm before}) \quad etc. \tag{3.3.5}$$

Of course the modes themselves may physically move in space between these two times, as per Fig. 3.1. But that is just the free evolution that would happen even if the beam-splitter were absent. That is, Eq. (3.3.1) is describing the change in quantum state (not the locations) of the modes that occurs as a consequence of $\mathscr{r} \neq 0$.

Now in the quantum case, we *cannot* use Eq. (3.3.3). That is, even if there is "no light" in one of the input modes, we cannot think of the action as being just splitting one mode into two. That is because the vacuum state ("no light") is still a quantum state with uncertainties in variables (such as $\hat{X}$ and $\hat{Y}$) which cannot be ignored. To put it another way, to maintain unitary evolution it is necessary to use the full transformation (3.3.1) with the constraints (3.3.2). That is, there exists a unitary operator $\hat{U}$ on the joint Hilbert space of both modes, such that

$$\hat{a}(t_{\rm after}) \equiv \hat{U}^\dagger \hat{a}(t_{\rm before}) \hat{U} = \mathscr{t}\, \hat{a}(t_{\rm before}) + \mathscr{r}\, \hat{b}(t_{\rm before}). \tag{3.3.6}$$

We will not write $\hat{U}$ down explicitly, as we don't actually need it.

Exercise 3.9 *What is the corresponding equation for $\hat{b}$?*

The action of the beam-splitter is very simple to describe in the Heisenberg picture, in terms of the annihilation operators. It is much more complicated to describe in the Schrödinger picture. Even if each input mode is independently prepared in states $|\psi_a\rangle$ and $|\psi_b\rangle$, say, these **do not** transform as

$$\hat{U}\left[|\psi_a(t_{\rm before})\rangle \otimes |\psi_b(t_{\rm before})\rangle\right] = |\psi_a(t_{\rm after})\rangle \otimes |\psi_b(t_{\rm after})\rangle. \tag{3.3.7}$$

Rather, the output (after) state will be *entangled* between the two modes, and cannot be written as a tensor produce of two pure states[2]:

$$\hat{U}\left[|\psi_a(t_{\rm before})\rangle \otimes |\psi_b(t_{\rm before})\rangle\right] = |\Psi_{ab}(t_{\rm after})\rangle. \tag{3.3.8}$$

However, there is one special class of states for which Eq. (3.3.7) *does* apply. These are the *coherent* states. That is, if $|\psi_a(t_{\rm before})\rangle = |\alpha_{\rm in}\rangle$ and $|\psi_b(t_{\rm before})\rangle = |\beta_{\rm in}\rangle$, then the output state does factorize:

$$\hat{U}\left[|\alpha_{\rm in}\rangle \otimes |\beta_{\rm in}\rangle\right] = |\alpha_{\rm out}\rangle \otimes |\beta_{\rm out}\rangle, \tag{3.3.9}$$

[2]We will cover entanglement more in a later chapter.

where

$$\begin{pmatrix} \alpha_{\rm out} \\ \beta_{\rm out} \end{pmatrix} = \begin{pmatrix} t & r \\ r & t \end{pmatrix} \begin{pmatrix} \alpha_{\rm in} \\ \beta_{\rm in} \end{pmatrix}, \tag{3.3.10}$$

which is the same mathematical transformation as the annihilation operators undergo.

Problem 3.3 (1 mark) *Prove Eqs. (3.3.9) and (3.3.10).*
Hint*: remember that the coherent states are the unique (right)-eigenstates of the annihilation operator. Show that the state* $\hat{U}\left[|\alpha_{\rm in}\rangle \otimes |\beta_{\rm in}\rangle\right]$ *is an eigenstate of both* $\hat{a} \otimes I$ *and* $I \otimes \hat{b}$*, and find the eigenvalues.*
Further hint*: premultiply the expression you are considering by* $\hat{U}\hat{U}^\dagger$*. Why is it permissible to do this?*

For the purposes of describing a laser (which we are gradually making our way towards), it is useful to consider the case where one of the inputs, b, is a vacuum state, and $\mathcal{T} \ll 1$, so that $\mathcal{R} = 1 - \mathcal{T}$ is close to 1. Then to a first approximation we can choose $r = \exp(-\mathcal{T}/2)$ and $t = i\sqrt{\mathcal{T}}$.

Exercise 3.10 *Show that this satisfies Eq. (3.3.2) to first order in* $\mathcal{T}$*.*

In this case, to a zeroth approximation the modes just swap, so it is convenient to relabel the outputs $a \leftrightarrow b$ so that the b mode stays close to vacuum. That is, the output coherent amplitudes are

$$\begin{pmatrix} \beta_{\rm out} \\ \alpha_{\rm out} \end{pmatrix} = \begin{pmatrix} i\mathcal{T}^{1/2} & e^{-\mathcal{T}/2} \\ e^{-\mathcal{T}/2} & i\mathcal{T}^{1/2} \end{pmatrix} \begin{pmatrix} \alpha_{\rm in} \\ 0 \end{pmatrix} = \begin{pmatrix} i\mathcal{T}^{1/2}\alpha_{\rm in} \\ e^{-\mathcal{T}/2}\alpha_{\rm in} \end{pmatrix}. \tag{3.3.11}$$

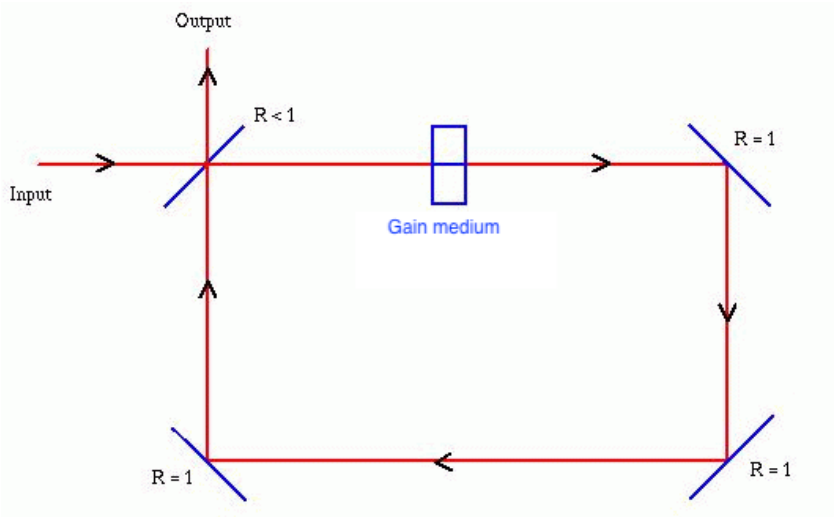


Figure 3.2: An optical cavity for a laser, showing 'input' and 'output' in a potentially misleading way, as per Fig. 3.1.

In all of the above, the time difference $\tau = t_{\rm after} - t_{\rm before}$ didn't play any explicit role. But there are situations where it does, namely when the beam-splitter is actually one mirror of a cavity. See Fig. 3.2, ignoring the

gain medium for the moment. To think about this the right way, imagine the input divided into many pieces of length $c\tau$, travelling towards the mirror at speed c, and identically sized pieces of the output travelling away from the mirror at speed c. When the leading edge of one piece of the input reaches the mirror, it undergoes the beam-splitter evolution over the next time interval of duration τ, and becomes the newest piece of the output. That is, for any given piece, it is either input (before the beam-splitter evolution) or output (after the beam-splitter evolution). It does not exist as input and output at the same time.

Note that we don't divide the path of the light inside the ring-cavity into many pieces. We treat it as a single mode. This makes sense if the Transmittance $\mathscr{T} = 1 - \mathscr{R}$ of the output mirror is very small, as we can choose τ equal to the round-trip time of the cavity, τ_{round}. (This is not a necessary choice, but it makes the discussion simple.) Thus, in every time interval of duration τ, all the light in the cavity bounces off the output mirror (the beam-splitter). Now for a laser, the input is just the vacuum state, and we will assume (see later for more discussion) that the laser cavity mode is in a coherent state $|\alpha(t)\rangle$ at time t. The laser mode (because it does a full round trip in the time τ) does not change, so it does not make sense to talk about an 'input' and 'output' coherent states for this mode, but rather the coherent state for a single spatially fixed mode at different times. Thus from Eq. (3.3.11), the evolution in the time interval $[t, t+\tau)$ is described by:

$$\begin{aligned} \beta_{\text{out}}(t) &= i\sqrt{\kappa\tau}\alpha(t) && (3.3.12) \\ \alpha(t+\tau) &= e^{-\kappa\tau/2}\alpha(t). && (3.3.13) \end{aligned}$$

Here, the time argument t for $\beta_{\text{out}}(t)$ indicates that this is the coherent amplitude of the bit of the field (of length $c\tau$) that began interacting with the cavity mode at time t, and we have defined a *loss rate* $\kappa = \mathscr{T}/\tau_{\text{round}}$.

Discussion 3.6 *Looking at the exponential term in Eq. (3.3.13), why would we define the loss rate as $\kappa = \mathscr{T}/\tau_{\text{round}}$, rather than half that? Is κ only the loss rate when the cavity mode is a coherent state, or does it always apply?*

You might be wondering what happened to the oscillation of the phase, the $e^{-i\omega_0\tau}$ that you would expect to see in the evolution of the coherent amplitude forward in time by a duration τ. One answer is that if $c\tau$ is the round-trip length of the cavity, then it contains an exact number of wavelengths $\lambda = c2\pi/\omega_0$, and hence $\omega_0\tau$ is an exact multiple of 2π. But really, we are just ignoring this phase factor because we know we could always put it back at the end if we wanted to.

3.3.2 Preliminary: harmonic oscillator phase

As we just discussed, the annihilation operator $\hat{a} = (\hat{X} + i\hat{Y})/\sqrt{2}$ is the quantum equivalent of the classical phasor $a = (X + iY)/\sqrt{2}$. The term 'phasor' suggests phase, and that's because classically we would write

$$a = re^{i\phi}\ ;\ \ r = \sqrt{X^2 + Y^2}\ ;\ \ \phi = \arctan(Y/X). \qquad (3.3.14)$$

In the quantum case, the analogous expression for r is perfectly fine:

$$\hat{r} = \sqrt{\hat{X}^2 + \hat{Y}^2} = \sqrt{2\hat{n} + 1}. \tag{3.3.15}$$

But $\arctan(\hat{Y}/\hat{X})$ is problematic, because $\hat{Y}$ and $\hat{X}$ do not commute so this expression is not even Hermitian. In fact, there is no way to define a phase operator acting on the Hilbert space of a quantum harmonic oscillator.

Aside 3.1 *Even though there is no way to write a phase operator, we can still consider phase measurements, and even 'perfect' (or 'canonical', as they are called) phase measurements. The probability distribution for the outcome of such a measurement on a pure state $|\psi\rangle$ is*

$$P_\psi(\phi) = \frac{1}{2\pi} \left| \sum_{n=0}^{\infty} e^{in\phi} \langle n|\psi\rangle \right|^2. \tag{3.3.16}$$

From this you can see that phase and number are related by a Fourier transform, but it is a discrete Fourier transform (unlike the continuous one that relates position and momentum).

The problem with defining phase is not really an issue for classical-like states with a well defined mean field, such as coherent states. For example, consider a coherent state with α real, large, and positive. Then $\arctan(\hat{Y}/\hat{X})$ can be approximated by

$$\hat{\phi} = \hat{Y}/(\sqrt{2}|\alpha|). \tag{3.3.17}$$

Exercise 3.11 *Justify this. Consider both the mean and standard deviations in $\hat{X}$ and $\hat{Y}$. Draw a phase-space diagram to illustrate.*

Thus in this case $\left\langle \hat{\phi} \right\rangle = 0$ and the variance in the phase for the coherent state is

$$V(\hat{\phi}) = 1/(4|\alpha|^2), \tag{3.3.18}$$

which is a good approximation for any coherent state with $|\alpha|^2 \gg 1$.

3.3.3 Deriving the Laser Linewidth

Now we have the basics from which to understand how a laser generates the output described in Sec. 3.2. For this we have to consider the gain medium illustrated in Fig. 3.2. Whole courses are given on how laser gain is achieved. Here we only need to note that it can be achieved using thermal radiation (at a perfectly reasonable temperature) to create excited-state atoms, for example. If the excited–ground transition has approximately the same frequency as the cavity mode of interest, ω_0, then the atoms can give up their excitation into the laser mode. This would typically be described as *stimulated emission*, meaning that the rate of excitation, g, is proportional to the number of photons plus one:

$$g = G\left\langle aa^\dagger \right\rangle = G(\langle \hat{n} \rangle + 1). \tag{3.3.19}$$

(Note: we are not deriving this here, just stating it. Yes it is weird that g is bigger than G, but that's the standard notation.) The plus one is sometimes called the spontaneous component. When this model applies, the combination of gain and loss (at rate κ) leads to the following differential equation for the mean photon number.

$$\frac{d}{dt}\langle\hat{n}\rangle = G(\langle\hat{n}\rangle + 1) - \kappa\langle\hat{n}\rangle . \tag{3.3.20}$$

Exercise 3.12 *Show that this gives steady-state mean photon number*

$$\langle\hat{n}\rangle_{\rm ss} = \frac{G}{\kappa - G}. \tag{3.3.21}$$

What happens if $G > \kappa$?

Although we will not show it, if this model applied, the steady-state quantum state is a *single-mode thermal* (SMT) state, as in Eq. (2.2.29), with this mean.

As discussed in Sec. 2.2.3, a SMT state is not what we want for an ideal laser. We want a SML state (2.2.33) in steady state. Thus, Eq. (3.3.19) must not describe an ideal laser. The reason is that for an ideal laser, we have $G > \kappa$ and $\langle\hat{n}\rangle$ grows until it is much larger than some photon number, n_s. At this point the 'stimulation' is so strong that every atom gives up its excitation to the laser mode almost as soon as it is excited. Thus the rate of gain is limited by the number of atoms (and their excitation rate) and becomes independent of the number of photons in the laser mode. This is called *gain saturation* (and n_s is the saturation photon number). In the ideal limit this is very simply modelled by taking the gain g to be constant:

$$g \approx Gn_s. \tag{3.3.22}$$

Under this model, the differential equation for the mean photon number is

$$\frac{d}{dt}\langle\hat{n}\rangle = Gn_s - \kappa\langle\hat{n}\rangle . \tag{3.3.23}$$

That is, the gain looks entirely 'spontaneous'! This gives the steady state

$$\langle\hat{n}\rangle_{\rm ss} = \mu \equiv \frac{Gn_s}{\kappa}. \tag{3.3.24}$$

Moreover, it can be shown that this gain process does lead to the SML state, which can be represented either as a mean-μ Poissonian mixture of number states (2.2.33) or an all-phase mixture of coherent states with $|\alpha|^2 = \mu$ (2.2.32).

But what we are really interested in, for a laser, is not the state of the cavity mode, but rather the properties of the output beam, in particular what the parameters ν and Γ in the spectrum (3.2.1) are. Recall that earlier we stated that Γ is the phase diffusion rate, while $\nu = 4P/(\hbar\omega_0\Gamma)$ is 4 times the number of photons per coherence time $(1/\Gamma)$ in the beam. See Fig. 3.3.

Say hypothetically that the laser cavity mode is in a coherent state $|\alpha\rangle$ with $|\alpha|^2 = \mu$ (a). Its phase variance is $V(\phi) = 1/4\mu$. In time dt, its

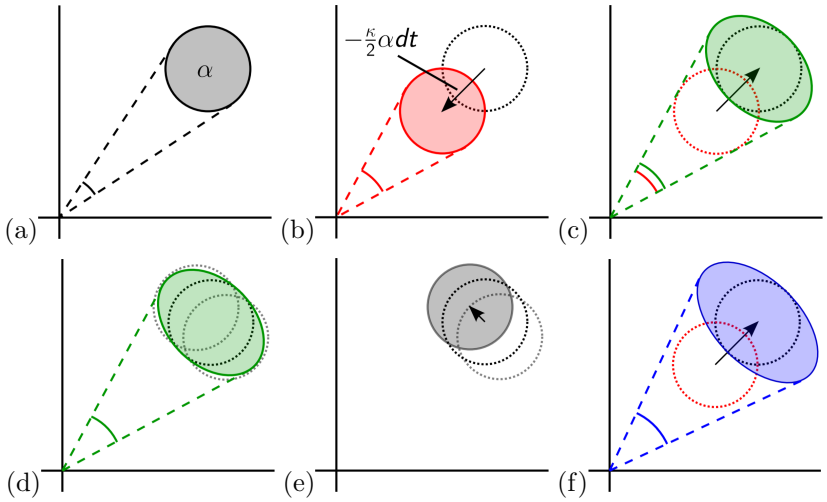


Figure 3.3: Laser phase diffusion. See text for details.

amplitude decreases: $|\alpha\rangle \to |\alpha e^{-\kappa\, dt/2}\rangle$ (b). That is, $\langle\hat{n}\rangle \to \mu(1-\kappa\, dt)$ so $V(\phi) \to 1/[4\mu(1-\kappa\, dt)]$. That is, the phase variance *increases* by

$$dV(\phi) = \frac{\kappa dt}{4\mu}. \tag{3.3.25}$$

Now without an external phase reference (i.e., in this case, another laser) it is impossible to *decrease* the phase variance of a harmonic oscillator.

Discussion 3.7 *Do you believe this? Think about it in terms of a clock.*

The best possible gain would be one that restores $\langle\hat{n}\rangle \to \mu$ *without increasing* $V(\phi)$ (c). But if it maintains the Poissonian photon number distribution, then this means the amplified state will be a *mixture* of coherent states with the same intensity $|\alpha|^2 = \mu$ as originally but with different phases (d). In other words, the evolution is equivalent to the state remaining in a coherent state with $|\alpha| = \sqrt{\mu}$ but with ϕ undergoing a random walk (e). Specifically, this type of continuous random walk is sometimes called Brownian motion, and is a type of diffusion process with the technical name of a *Weiner process*. Its characteristic is that its variance increases linearly in time, as per Eq. (3.3.25). Now the actual standard process of saturated gain in an ideal laser, described in the text above Eq. (3.3.22), is not the "best possible" gain. It does not add amplify without increasing the phase variance. Rather, as it amplifies, it adds the same amount of phase noise as did the loss process it is compensating for (f). Thus, the total phase diffusion rate is double that of Eq. (3.3.25):

$$\frac{dV(\phi)}{dt} = \Gamma_{\text{ideal}} \equiv \frac{\kappa}{2\mu}. \tag{3.3.26}$$

This is the first parameter we sought to derive: the linewidth of a standard laser in ideal conditions. We see that in a time scale of order Γ^{-1} the wandering in the phase of the laser becomes substantial – of

order one radian – which is why this is the coherence time of the laser. And this amount of deviation of the phase from its average value (of $\phi_0 + \omega_0 t$) in time $t \sim \Gamma^{-1}$ is what we would expect if the frequency of the laser was not exactly ω_0 but could be, roughly, $\omega \pm \Gamma$.

Exercise 3.13 *Convince yourself of this.*

That is why Γ does turn up as the width of the laser spectrum (3.2.1). Note that $\Gamma \ll \kappa$ and, for a given cavity set-up (a fixed κ), the larger μ, the steady-state mean photon number is, the smaller the linewidth will become. This is known as *gain-narrowing*, because the stronger the gain g, the larger μ will be and the narrow the spectrum will be.

Now we turn to the second parameter in the spectrum (3.2.1), $\nu/4$, the number of photons in a coherence time. From Eq. (3.3.12), the number of photons in a piece of output beam of duration dt is $\kappa|\alpha|^2 dt$. (This makes sense as it is exactly the number of photons lost in the loss process.) Therefore the number in a coherence time is

$$\frac{\nu}{4} = \frac{\kappa|\alpha|^2}{\Gamma} = 2\mu^2, \tag{3.3.27}$$

where the last expression is for $\Gamma = \Gamma_{\text{ideal}}$. That is, the number of coherent photons in the beam scales as the *square* of the number of photons stored in the laser cavity. In typical lasers, Γ is bigger than Γ_{ideal} because there are other physical processes that introduce phase noise, but still ν is typically much bigger than μ. That explains, via Eq. (3.2.3), why it would be so hard to create a source with the same spectrum as a laser by collimating and filtering thermal light. And remember, even if we could do that, we would not have the property that we see here for an ideal laser, from Eq. (3.3.12) again, that the number of photons in any piece of beam is always exactly Poissonian.

Problem 3.4 (1 marks) *Show that if you have a variable n_1 with Poissonian statistics, and an* independent *variable n_2 with Poissonian statistics, that the variable $n = n_1 + n_2$ is also Poissonian.*
Hint*: You can get full marks by just showing that the variance–mean relation of the Poisson distribution is satisfied. You can get a bonus mark by calculating the complete distribution.*
Further hint*: For independent variables, $\langle f(n_1)g(n_2)\rangle = \langle f(n_1)\rangle \langle g(n_2)\rangle$ for arbitrary functions f and g.*

Discussion 3.8 *What do you think is the relevance of this to the properties of the laser output beam?*

4 Quantum Electrodynamics

4.1 The minimal coupling Hamiltonian

So far we have only considered the quantum theory of radiation in the absence of sources. To include classical sources we just have to add a new term to the Hamiltonian of the field. However in reality the sources are charged particles: electrons, protons *etc.*. These particles not only affect the field as sources, they are affected by it through the Lorentz force. If the field is quantized then the particles must be quantized as well if they are to be affected by the field. Of course we already know how to describe particles (at least nonrelativistically), using the free particle Hamiltonian operator. But now we need to add a *coupling* Hamiltonian which will produce both the source terms in the quantized Maxwell's equations, but also the Lorentz force for the particles.

The Hamiltonian which does both of these jobs is called the *minimal coupling* Hamiltonian. First consider the classical Hamiltonian for a *noninteracting* particle and field

$$H = H_0(\mathbf{v}) = \int \frac{\epsilon_0}{2}\left(|\mathbf{E}^\perp|^2 + c^2|\boldsymbol{\nabla}\times\mathbf{A}|^2\right)\mathrm{d}^3\mathbf{x} + \frac{1}{2m}|m\mathbf{v}|^2 + V(\mathbf{r}), \tag{4.1.1}$$

where $\mathbf{v}$ is the velocity and $V(\mathbf{r})$ is a nonelectromagnetic potential (such as a gravitational potential). The procedure to introduce the minimal coupling is

$$H = H_0(\mathbf{v}) + q\phi(\mathbf{r}), \tag{4.1.2}$$

$$\mathbf{p} = \mathbf{p}_0(\mathbf{v}) + q\mathbf{A}(\mathbf{r}). \tag{4.1.3}$$

Here $\mathbf{p}_0(\mathbf{v}) = m\mathbf{v}$, and q is the charge of the particle. The concept of adding a scalar potential to the Hamiltonian is familiar, but what is probably less familiar is adding a vector potential to the momentum. In the presence of a vector potential the momentum $\mathbf{p}$ of the particle (which still becomes the operator $-i\hbar\boldsymbol{\nabla}$ when quantized) is not equal to $m\mathbf{v}$. However, the kinetic energy is still equal to $(m/2)\mathbf{v}^2$ as in H_0. Thus, from Eq. (4.1.2) and Eq. (4.1.3), the new Hamiltonian, expressed in terms of the momentum $\mathbf{p}$, is

$$H = \int \frac{\epsilon_0}{2}\left(|\mathbf{E}^\perp|^2 + c^2|\boldsymbol{\nabla}\times\mathbf{A}|^2\right)\mathrm{d}^3\mathbf{x} + \frac{1}{2m}|\mathbf{p} - q\mathbf{A}(\mathbf{r})|^2 + q\phi(\mathbf{r}) + V(\mathbf{r}). \tag{4.1.4}$$

The additional term, the coupling, can be split off as

$$H_\mathrm{I} = q\left[\frac{1}{2m}\left(-\mathbf{p}\cdot\mathbf{A}(\mathbf{r}) - \mathbf{A}(\mathbf{r})\cdot\mathbf{p} + q|\mathbf{A}(\mathbf{r})|^2\right) + \phi(\mathbf{r})\right]. \tag{4.1.5}$$

Obviously only charged particles are coupled to the field.

4.2 NON-EXAMINABLE The Lorentz Force

The first task is to show that the coupling term does produce the Lorentz force on the charged particle. To show this the free Hamiltonian of the

field is irrelevant so we can work with

$$H = \frac{1}{2m}|\mathbf{p} - q\mathbf{A}(\mathbf{r})|^2 + q\phi(\mathbf{r}) + V(\mathbf{r}) \quad (4.2.1)$$

$$= \frac{1}{2m}\left(p_j - qA_j(\mathbf{r})\right)\left(p_j - qA_j(\mathbf{r})\right) + q\Phi(\mathbf{r}) + V(\mathbf{r}) \quad (4.2.2)$$

Here the Einstein summation convention for repeated indices is being used, and Φ is a classical scalar potential. We cannot consider the proper quantum expression for ϕ in terms of the charge distribution (1.3.12) because this would involve other particles and we wish to consider only a single particle for he moment.

First, we treat this as classical Hamiltonian. Then, ignoring $V(\mathbf{r})$, the equations of motion (Hamilton's equations) following from this are

$$\dot{r}_j = \frac{\partial H}{\partial p_j} = \frac{1}{m}\left(p_j - qA_j(\mathbf{r})\right) = v_j \,, \quad (4.2.3)$$

$$\dot{p}_j = -\frac{\partial H}{\partial r_j} = -q\frac{\partial \Phi}{\partial r_j} + \frac{q}{m}\left(p_l - qA_l(\mathbf{r})\right)\frac{\partial A_l}{\partial r_j} \,. \quad (4.2.4)$$

The first of these simply confirms the relation between the velocity and the momentum expressed in Eq. (4.1.3). The second can be rewritten

$$\dot{\mathbf{p}} = -q\boldsymbol{\nabla}\Phi + q\left(\boldsymbol{\nabla}\mathbf{A}\right)\cdot\mathbf{v}. \quad (4.2.5)$$

where the last term means $v_l\mathbf{e}_j\left[\frac{\partial}{\partial r_j}A_l(\mathbf{r})\right]$. That is, the ∇ acts only on the $\mathbf{A}$.

Now consider the total rate of change of the mechanical momentum

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \dot{\mathbf{p}} - q\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t}. \quad (4.2.6)$$

Here $\mathrm{d}f/\mathrm{d}t$ is the *total* derivative of a field f, as opposed to the partial derivative $\dot{f}$. For example, if f were a function $f(t,s)$ then we would have

$$\mathrm{d}f/\mathrm{d}t = \frac{\partial}{\partial t}f + (\frac{\partial}{\partial t}s)(\frac{\partial}{\partial s}f) \equiv \partial_t f + (\partial_t s)(\partial_s f).$$

In the current example $\mathbf{A}$ is a function $\mathbf{A}(t,\mathbf{r})$ and $\partial_t r_j = v_j$. Using this, and Eq. (4.2.5), gives

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \left[-q\boldsymbol{\nabla}\Phi + q(\boldsymbol{\nabla}\mathbf{A})\cdot\mathbf{v}\right] - q\left[\frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{A}\right]$$

$$= -q\left(\boldsymbol{\nabla}\Phi + \frac{\partial}{\partial t}\mathbf{A}\right) - q\left[(\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{A} - \boldsymbol{\nabla}(\mathbf{v}\cdot\mathbf{A})\right], \quad (4.2.7)$$

Using the identity $\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = (\mathbf{a}\cdot\mathbf{b})\mathbf{c} - (\mathbf{a}\cdot\mathbf{c})\mathbf{b}$ and the relations

$$\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A} \,,\; \mathbf{E} = -\boldsymbol{\nabla}\Phi \; - \frac{\partial \mathbf{A}}{\partial t} \,, \quad (4.2.8)$$

we get finally

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = q[\mathbf{E} + \mathbf{v}\times\mathbf{B}] \,. \quad (4.2.9)$$

This is the Lorentz force, which we know to be correct for a classical particle in an electromagnetic field.

Exactly the same result would be obtained if the Hamiltonian in Eq. (4.2.1) were treated as a quantum operator, and, instead of Hamilton's equations, Heisenberg's equations

$$\dot{\hat{\mathbf{r}}} = (i/\hbar)[\hat{H}, \hat{\mathbf{r}}] \tag{4.2.10}$$
$$\dot{\hat{\mathbf{p}}} = (i/\hbar)[\hat{H}, \hat{\mathbf{p}}] \tag{4.2.11}$$

were used. This completes the demonstration that the minimal coupling Hamiltonian correctly describes the effect of the field on a particle.

4.3 NON-EXAMINABLE Radiation Sources

The next step is to show that the minimal coupling Hamiltonian gives the correct source terms for the radiation field. For this we have to consider many particles indexed by a greek superscript, so the total Hamiltonian is

$$\begin{aligned}\hat{H} &= \int \frac{\epsilon_0}{2}\left(|\hat{\mathbf{E}}^{\perp}|^2 + c^2|\boldsymbol{\nabla}\times\hat{\mathbf{A}}|^2\right)\mathrm{d}^3\mathbf{x} \\ &\quad + \sum_{\zeta}\left[\frac{1}{2m^{\zeta}}|\hat{\mathbf{p}}^{\zeta} - q^{\zeta}\hat{\mathbf{A}}(\hat{\mathbf{r}}^{\zeta})|^2 + \frac{1}{2}q^{\zeta}\hat{\phi}(\hat{\mathbf{r}}^{\zeta}) + V(\hat{\mathbf{r}}^{\zeta})\right].\end{aligned} \tag{4.3.1}$$

The position and momentum operators for the many particles obey

$$[\hat{p}_j^{\zeta}, \hat{r}_l^{\eta}] = -i\hbar\delta_{jl}\delta^{\zeta\eta} \tag{4.3.2}$$

Here $\hat{\phi}$ is expressed in terms of the particle positions:

$$\hat{\phi}(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\int \mathrm{d}^3\mathbf{r}\frac{\hat{\rho}(\mathbf{r})}{|\mathbf{r}-\mathbf{x}|} = \frac{1}{4\pi\epsilon_0}\sum_{\eta}\frac{q^{\eta}}{|\hat{\mathbf{r}}^{\eta}-\mathbf{x}|} \tag{4.3.3}$$

where the following

$$\hat{\rho}(\mathbf{r}) = \sum_{\eta} q^{\eta}\delta(\mathbf{r}-\hat{\mathbf{r}}^{\eta}) \tag{4.3.4}$$

has been used. Any classical (i.e. with a source external and irrelevant to the system) scalar potential can be included in $V(\mathbf{r})$.

4.3.1 Coulomb Energy

Before dealing with the radiation sources, we will show that the Coulomb energy

$$\hat{H}_{\mathrm{Coulomb}} = \frac{1}{2}\sum_{\zeta} q^{\zeta}\hat{\phi}(\hat{\mathbf{r}}^{\zeta}) \tag{4.3.5}$$

can be expressed in terms of the longitudinal electric field. There is a factor of 1/2 in this expression not included in the original minimal

coupling Hamiltonian in order to avoid counting the Coulomb energy between particles twice. Substituting the above expression (4.3.3) gives

$$\hat{H}_{\rm Coulomb} = \frac{1}{2}\sum_\zeta q^\zeta \frac{1}{4\pi\epsilon_0}\sum_\eta \frac{q^\eta}{|\hat{\mathbf{r}}^\eta - \hat{\mathbf{r}}^\zeta|} \quad (4.3.6)$$

$$= \frac{1}{4\pi\epsilon_0}\sum_{\zeta>\eta} \frac{q^\zeta q^\eta}{|\hat{\mathbf{r}}^\eta - \hat{\mathbf{r}}^\zeta|} \quad (4.3.7)$$

Strictly the infinite self-Coulomb energy when $\zeta = \eta$, [which is in Eq. (4.3.6) but which has been omitted in Eq. (4.3.7)] needs to be included to calculate the exact relativistic quantum dynamics of the system, but it will not be important in our treatment.

Now the energy (4.3.5) can be re-expressed as

$$\hat{H}_{\rm Coulomb} = \frac{1}{2}\int \mathrm{d}^3\mathbf{x}\hat{\rho}(\mathbf{x})\hat{\phi}(\mathbf{x}) \quad (4.3.8)$$

From Eq. (1.3.11) this can be written as

$$\hat{H}_{\rm Coulomb} = -\frac{\epsilon_0}{2}\int \mathrm{d}^3\mathbf{x}\hat{\phi}(\mathbf{x})\nabla^2\hat{\phi}(\mathbf{x}) = -\frac{\epsilon_0}{2}\int \mathrm{d}^3\mathbf{x}\hat{\phi}(\mathbf{x})\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\hat{\phi}(\mathbf{x}) \quad (4.3.9)$$

Using integration by parts and assuming that $\hat{\phi}(\mathbf{x})$ vanishes at infinity as it will if our system is finite, we get

$$\hat{H}_{\rm Coulomb} = \frac{\epsilon_0}{2}\int \mathrm{d}^3\mathbf{x}\boldsymbol{\nabla}\hat{\phi}(\mathbf{x})\cdot\boldsymbol{\nabla}\hat{\phi}(\mathbf{x}) = \frac{\epsilon_0}{2}\int \mathrm{d}^3\mathbf{x}\left|\hat{\mathbf{E}}^\parallel(\mathbf{x})\right|^2 \quad (4.3.10)$$

Thus the Coulomb energy is exactly the non-radiative part of the electromagnetic field energy.

4.3.2 Radiation Sources

Ignoring the Coulomb energy and free Hamiltonian of the particles, the radiation field Hamiltonian is

$$\hat{H} = \hat{H}_{\rm free} + \hat{H}_{\rm source} \quad (4.3.11)$$

where

$$\hat{H}_{\rm free} = \int \frac{\epsilon_0}{2}\left(|\hat{\mathbf{E}}^\perp|^2 + c^2|\boldsymbol{\nabla}\times\hat{\mathbf{A}}|^2\right)\mathrm{d}^3\mathbf{x} \quad (4.3.12)$$

$$\hat{H}_{\rm source} = \sum_\zeta \frac{1}{2m^\zeta}\left[-2q^\zeta\hat{\mathbf{p}}^\zeta\cdot\hat{\mathbf{A}}(\hat{\mathbf{r}}^\zeta) + \left(q^\zeta\hat{\mathbf{A}}(\hat{\mathbf{r}}^\zeta)\right)^2\right] \quad (4.3.13)$$

Here the ordering of $\hat{\mathbf{p}}$ and $\hat{\mathbf{A}}$ does not matter, even in the quantum case where $\hat{\mathbf{p}}^\zeta \sim -i\hbar\boldsymbol{\nabla}^\zeta$, because $\boldsymbol{\nabla}\cdot\hat{\mathbf{A}} = 0$. Consider a single particle:

$$\langle\mathbf{r}|\hat{\mathbf{p}}\cdot\hat{\mathbf{A}}(\hat{\mathbf{r}})|\psi\rangle = \langle\mathbf{r}|\hat{p}_j\hat{A}_j(\hat{\mathbf{r}})|\psi\rangle = -i\hbar\frac{\partial}{\partial r_j}\left[\hat{A}_j(\mathbf{r})\langle\mathbf{r}|\psi\rangle\right] \quad (4.3.14)$$

$$= 0 - i\hbar\hat{A}_j(\mathbf{r})\frac{\partial}{\partial r_j}\langle\mathbf{r}|\psi\rangle = \langle\mathbf{r}|\hat{A}_j(\hat{\mathbf{r}})\hat{p}_j|\psi\rangle \quad (4.3.15)$$

$$= \langle\mathbf{r}|\hat{\mathbf{A}}(\hat{\mathbf{r}})\cdot\mathbf{p}|\psi\rangle. \quad (4.3.16)$$

We have shown in Sec. 1.4 that $\hat{H}_{\rm free}$ implies

$$\partial_t \partial_t \hat{\mathbf{A}} = c^2 \nabla^2 \hat{\mathbf{A}}, \tag{4.3.17}$$

which is the source-free Maxwell equation. To find the effect of the source we need to go back a step and find

$$\partial_t \hat{\mathbf{A}} = (i/\hbar)[\hat{H}_{\rm free} + \hat{H}_{\rm source}, \hat{\mathbf{A}}] \tag{4.3.18}$$

Now since $\hat{H}_{\rm source}$ is a function of $\hat{\mathbf{A}}$, which commutes with itself at different positions [see Eq. (1.4.13)], we have

$$\begin{aligned}
\partial_t \hat{\mathbf{A}}(\mathbf{r}) &= (i/\hbar)[\hat{H}_{\rm free}, \hat{\mathbf{A}}(\mathbf{r})] \\
&= (i\epsilon_0/2\hbar) \int \left[|\hat{\mathbf{E}}^\perp(\mathbf{x})|^2 + c^2 |\boldsymbol{\nabla} \times \hat{\mathbf{A}}(\mathbf{x})|^2, \hat{\mathbf{A}}(\mathbf{r}) \right] \mathrm{d}^3\mathbf{x} \\
&= (i\epsilon_0/2\hbar) \int \left[|\hat{\mathbf{E}}^\perp(\mathbf{x})|^2, \hat{\mathbf{A}}(\mathbf{r}) \right] \mathrm{d}^3\mathbf{x} \\
&= (i\epsilon_0/2\hbar) \int 2\hat{E}_j^\perp(\mathbf{x}) (i\hbar/\epsilon_0) \delta_{jl}^\perp(\mathbf{x}-\mathbf{r}) \mathbf{e}_l \mathrm{d}^3\mathbf{x}\,,
\end{aligned} \tag{4.3.19}$$

where both Eq. (1.4.13) and Eq. (1.4.16) have been used, and where $\mathbf{e}_l$ is the unit vector in the l direction. We have also used the handy operator identity (1.4.3).

Now because $\hat{\mathbf{E}}^\perp$ is a transverse vector field, integrating over all space with the transverse δ function is equivalent to integrating with a normal δ function (see Eq. (1.4.20)). The result is thus

$$\partial_t \hat{\mathbf{A}}(\mathbf{r}) = -\hat{\mathbf{E}}^\perp(\mathbf{r}), \tag{4.3.20}$$

which is as it should be since this was the original definition of $\hat{\mathbf{E}}^\perp$! Now, we find

$$\partial_t \partial_t \hat{\mathbf{A}} = (i/\hbar)[\hat{H}_{\rm free} + \hat{H}_{\rm source}, \partial_t \mathbf{A}] \tag{4.3.21}$$

$$= (i/\hbar)[\hat{H}_{\rm free} + \hat{H}_{\rm source}, -\hat{\mathbf{E}}^\perp] \tag{4.3.22}$$

Recall that $\mathbf{a} \times \mathbf{b} \equiv \epsilon_{ijk} \mathbf{e}_i a_j b_k$, where

$$\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1 \tag{4.3.23}$$

$$\epsilon_{132} = \epsilon_{213} = \epsilon_{321} = -1 \tag{4.3.24}$$

$$\text{all other } \epsilon_{ijk} = 0 \tag{4.3.25}$$

Thus

$$(i/\hbar)[\hat{H}_{\rm free}, -\hat{\mathbf{E}}^\perp(\mathbf{r})] = (i\epsilon_0/2\hbar) \int [c^2 \epsilon_{ijk}\epsilon_{lmk} \partial_i \hat{A}_j(\mathbf{x}) \partial_l \hat{A}_m(\mathbf{x}), -\hat{E}_n^\perp(\mathbf{r}) \mathbf{e}_n] \mathrm{d}^3\mathbf{x} \tag{4.3.26}$$

Using the relation $\epsilon_{ijk}\epsilon_{lmk} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{lj}$ and the commutation relations, this can be evaluated as

$$(i\epsilon_0/2\hbar) 2(i\hbar/\epsilon_0) c^2 \int [\partial_i \delta_{jn}^\perp(\mathbf{x}-\mathbf{r}) \mathbf{e}_n][\partial_i \hat{A}_j(\mathbf{x})] - [\partial_i \delta_{jn}^\perp(\mathbf{x}-\mathbf{r}) \mathbf{e}_n][\partial_j \hat{A}_i(\mathbf{x})] \mathrm{d}^3\mathbf{x} \tag{4.3.27}$$

Now integrating by parts, using the periodic boundary conditions to cancel the boundary terms, and using the fact that $\hat{\mathbf{A}}$ is a transverse vector field [so that integrating $A_j(\mathbf{r})$ with $\delta^\perp_{jn}(\mathbf{r})$ simply returns the field $A_n(\mathbf{r})$, and so that $\partial_i\partial_n\hat{A}_i(\mathbf{r}) = 0$] gives

$$\begin{aligned}(i/\hbar)^2[\hat{H}_{\rm free},[\hat{H}_{\rm free},\hat{\mathbf{A}}(\mathbf{r})]] &= c^2\partial_i\partial_i\hat{A}_n(\mathbf{r})\mathbf{e}_n \\ &= c^2\nabla^2\hat{\mathbf{A}}(\mathbf{r}). \end{aligned} \tag{4.3.28}$$

This result is as expected, giving the source free wave equation (4.3.17) as derived earlier.

The final step is to calculate

$$\begin{aligned}[\hat{H}_{\rm source},-\hat{\mathbf{E}}^\perp(\mathbf{x})] &= \sum_\zeta \frac{1}{2m^\zeta}\left[-2q^\zeta\hat{\mathbf{p}}^\zeta\cdot\hat{\mathbf{A}}(\hat{\mathbf{r}}^\zeta) + \left(q^\zeta\right)^2|\hat{\mathbf{A}}(\hat{\mathbf{r}}^\zeta)|^2, -\hat{\mathbf{E}}^\perp(\mathbf{x})\right] \\ &= (i\hbar/\epsilon_0)\sum_\zeta \frac{1}{2m^\zeta}\left[-2q^\zeta\hat{\mathbf{p}}^\zeta\cdot\mathbf{e}_i\delta^\perp_{ij}(\mathbf{x}-\hat{\mathbf{r}}^\zeta)\mathbf{e}_j\right. \\ &\qquad \left. + 2(q^\zeta)^2\hat{\mathbf{A}}(\hat{\mathbf{r}}^\zeta)\cdot\mathbf{e}_i\delta^\perp_{ij}(\mathbf{x}-\hat{\mathbf{r}}^\zeta)\right], \end{aligned} \tag{4.3.29}$$

where we have used Eq. (1.4.3). Now using

$$\hat{\mathbf{v}}^\zeta = \left(\hat{\mathbf{p}}^\zeta - q^\zeta\hat{\mathbf{A}}(\hat{\mathbf{r}}^\zeta)\right)/m^\zeta \tag{4.3.30}$$

we can rewrite this as

$$(i/\hbar)[\hat{H}_{\rm source},-\hat{\mathbf{E}}^\perp] = \frac{1}{\epsilon_0}\sum_\zeta \hat{\mathbf{v}}^\zeta\cdot\mathbf{e}_i\delta^\perp_{ij}(\mathbf{x}-\hat{\mathbf{r}}^\zeta)\mathbf{e}_j q^\zeta \tag{4.3.31}$$

Thus, combining the evolution from the free and source Hamiltonians we obtain

$$\partial_t\partial_t\hat{\mathbf{A}} = c^2\nabla^2\hat{\mathbf{A}} + \hat{\mathbf{j}}^\perp/\epsilon_0, \tag{4.3.32}$$

which is the wave equation with sources, as desired. In this equation,

$$\hat{\mathbf{j}}^\perp(\mathbf{x}) = \sum_\zeta \hat{\mathbf{v}}^\zeta\cdot\mathbf{e}_i\delta^\perp_{ij}(\mathbf{x}-\hat{\mathbf{r}}^\zeta)\mathbf{e}_j q^\zeta \tag{4.3.33}$$

is the transverse part of the current density. The operator ordering here is unimportant because $\mathbf{e}_i\delta^\perp_{ij}(\mathbf{x}-\hat{\mathbf{r}}^\zeta)\mathbf{e}_j$ is transverse and so commutes with $\hat{p}^\zeta \sim -i\hbar\boldsymbol{\nabla}$. If we were to ignore the operator nature of $\hat{\mathbf{v}}$ we could write the total current density as

$$\mathbf{j}(\mathbf{x}) = \sum_\zeta \mathbf{v}^\zeta\cdot\mathbf{e}_i\delta_{ij}(\mathbf{x}-\mathbf{r}^\zeta)\mathbf{e}_j q^\zeta = \sum_\zeta \mathbf{v}^\zeta\delta(\mathbf{x}-\mathbf{r}^\zeta)q^\zeta. \tag{4.3.34}$$

from which Eq. (4.3.33) is easy to understand as the transverse part.

4.4 Interpretation of the Minimal Coupling Hamiltonian

We restate the coupling term which arises from the minimal coupling method, once again concentrating on a single particle for simplicity.

$$\hat{H}_{\rm I} = q\hat{\phi}(\hat{\mathbf{r}}) + \frac{-q\hat{\mathbf{p}}\cdot\hat{\mathbf{A}}(\hat{\mathbf{r}})}{m} + \frac{q^2|\hat{\mathbf{A}}(\hat{\mathbf{r}})|^2}{2m}. \tag{4.4.1}$$

Recall the expression for $\hat{\mathbf{A}}$ in terms of annihilation and creation operators (1.4.11) — it is of the form

$$\hat{\mathbf{A}}(\hat{\mathbf{r}}) = \sum_\kappa \mathbf{u}_\kappa(\hat{\mathbf{r}})(a_\kappa + a_\kappa^\dagger). \tag{4.4.2}$$

By concentrating on the operators in this expression, and ignoring constants, and the vector nature of the vectors, we can understand better the basic action of the interaction Hamiltonian, and represent it by diagrams (which I will draw during lectures). Remember that it is the action of the Hamiltonian operator on a state $|\psi\rangle$ that generates the change of the state into the future. It is helpful to separate out the interaction Hamiltonian into three terms.

The first is

$$\hat{H}_{\rm I,0} \sim \hat{\phi}(\hat{r}) \tag{4.4.3}$$

Remember the first hat here is because of other electrons the one with position r is interacting with. Thus this describes an instantaneous Coulomb repulsion — both the particle under consideration and all the other charged particles in the universe are altered by the action of this term. This term does not involve photons at all.

The next term is

$$\hat{H}_{\rm I,1} \sim \hat{p}\sum_\kappa u_\kappa(\hat{r}) \otimes (\hat{a}_\kappa + \hat{a}_\kappa^\dagger). \tag{4.4.4}$$

Here I have put a hat on a_κ to emphasize that it is an operator (even though conventionally we omit it). This operator changes the state of the particle [due to the presence both of the $\hat{p}$ operator and the $\hat{r}$ operator inside $u_\kappa(\hat{r})$] and, at the same time, either creates ($\hat{a}^\dagger$) or destroys ($\hat{a}$) a photon in one of the modes κ. (Here, saying "either ... or" and "in one of the modes" is loose talk for what is actually a grand superposition of creating and destroying a photon, across all modes .)

The final term is

$$\hat{H}_{\rm I,2} \sim |\hat{A}(\hat{r})|^2 \tag{4.4.5}$$

$$\sim \sum_{\kappa,\kappa'} u_\kappa(\hat{r})u_{\kappa'}(\hat{r}) \otimes (\hat{a}_\kappa\hat{a}_{\kappa'} + \hat{a}_\kappa\hat{a}_{\kappa'}^\dagger + \hat{a}_\kappa^\dagger\hat{a}_{\kappa'} + \hat{a}_\kappa^\dagger\hat{a}_{\kappa'}^\dagger). \tag{4.4.6}$$

This operator changes the state of the particle [due to the presence of the $\hat{r}$ operator inside $u_\kappa(\hat{r})$] and, at the same time, either creates photons in two modes, or creates a photon in one mode and destroys on in another, or destroys photons in two modes. (Again, saying "either ... or" *etc.* is loose talk for a grand superposition of actions.) We will see in Chapter 5 that this term is a result of the non-relativistic approximation.

Discussion 4.1 *What do you think the 0, 1, and 2 subscripts stand for in the above? How will it be reflected in the diagrams we draw?*

5 Examples of QED processes

5.1 Radiative Transitions in Atoms

Atomic energy levels are not infinitely sharp, but have a finite width, called the *natural linewidth*. More precisely, the energy of the photon emitted by a spontaneous transition between two levels need not be exactly the energy difference of the levels. This can be thought of as a consequence of the energy-time uncertainty relation

$$\Delta E \Delta t \approx \tfrac{1}{2}\hbar \ : \tag{5.1.1}$$

the shorter-lived the atomic state, the less well-defined its energy and the greater the natural linewidth. If there was no uncertainty in the energy difference between the levels, the atom would not decay at all.

There is an uncertainty in the energy levels of an atom because the atomic Hamiltonian is not the full Hamiltonian of the system. Rather, as we have seen, there is a coupling between any charged particle and the electromagnetic field. Thus the explanation for radiative atomic transitions is to be sought in the minimal coupling Hamiltonian introduced in the preceding chapter. In this chapter we will see how the spontaneous emission rate between two levels of an atom can be calculated from first principles, by making lots of approximations.

5.1.1 The Non-Relativistic Approximation

Let us consider the situation in which the radiation field interacts with just electrons in a bound states in an atom. This applies to the case of a one-electron atom (or an effectively one-electron atom) in which $\Phi(\hat{\mathbf{r}})$ can be treated as a $c-$number due to the nucleus (or nucleus and inner core of electrons). As in all the theory we have considered so far, we use a *non-relativistic Hamiltonian*. This Hamiltonian, for the two systems of electron and radiation field, is

$$\hat{H} = \hat{H}_{\rm el} \otimes \hat{I} + \hat{I} \otimes \hat{H}_{\rm rad} + \hat{H}_{\rm I}. \tag{5.1.2}$$

The first term, $\hat{H}_{\rm el}$, is the non-relativistic Hamiltonian for the electron bound to the atom:

$$\hat{H}_{\rm el} = \frac{\hat{\mathbf{p}}^2}{2m} + \Phi(\hat{\mathbf{r}}) = \sum_j E_j |j\rangle\langle j|. \tag{5.1.3}$$

Here $E_j, |j\rangle$ are the eigenvalues and eigenstates of $\hat{H}_{\rm el}$, found by solving Schrödinger's equation.

The second term is the energy of the radiation field,

$$\hat{H}_{\rm rad} = \int \mathrm{d}^3\mathbf{x} \frac{\epsilon_0}{2}\left(|\hat{\mathbf{E}}^\perp|^2 + c^2|\hat{\mathbf{B}}|^2\right) = \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k}} \left(a^\lambda_{\mathbf{k}}\right)^\dagger a^\lambda_{\mathbf{k}}. \tag{5.1.4}$$

The third term is the interaction between these two systems, which we split into two parts:

$$\hat{H}_{\rm I} = \hat{H}_{\rm I,1} + \hat{H}_{\rm I,2} \tag{5.1.5}$$

where

$$\hat{H}_{\mathrm{I},1} = \left(\frac{e}{m}\right) \hat{\mathbf{A}}(\hat{\mathbf{r}})\cdot\hat{\mathbf{p}}, \tag{5.1.6}$$

$$\hat{H}_{\mathrm{I},2} = \left(\frac{e^2}{2m}\right) |\hat{\mathbf{A}}(\hat{\mathbf{r}})|^2. \tag{5.1.7}$$

These describe one and two-photon processes respectively, as noted in Sec. 4.4.

5.1.2 Single-photon Transition Approximation

Radiative transitions in an atom are dominated by $\hat{H}_{\mathrm{I},1}$, unless it is a forbidden transition with zero dipole moment. Quantitatively, the effects of $\hat{H}_{\mathrm{I},2}$ are typically smaller than those of $\hat{H}_{\mathrm{I},1}$ by a factor of

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137} \text{ (the } \textit{fine structure constant}\text{)}. \tag{5.1.8}$$

(This means, as we will see later, that in terms of the decay rate it is a factor of α^2.)

5.1.3 Electric Dipole Approximation

Recall that the vector potential $\hat{\mathbf{A}}$ is defined in terms of annihilation and creation operators for photons of definite momenta in Eq. (3.1.1). We make the further approximation that

$$e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} = e^{i\mathbf{k}\cdot\mathbf{r}_0}\ , \tag{5.1.9}$$

where $\mathbf{r}_0$ is the position of the centre of the atom. That is, we consider $\mathbf{r}$ as $\mathbf{r}_0+\delta\mathbf{r}$, where $\delta\mathbf{r}$ is the displacement of the electron from the centre of the atom, and use the approximation $\exp(i\mathbf{k}\cdot\delta\mathbf{r}) = 1$. This is justified by the fact that the wavelength of the light emitted (or absorbed) by atoms is much greater than the linear dimensions of the atom. (Typically, $r_{\mathrm{atom}} \approx 1$Å while $\lambda/2\pi \approx 10^3$Å). Under this *dipole approximation*, we can replace $\hat{\mathbf{A}}(\mathbf{r})$ in Eq. (5.1.6) by

$$\hat{\mathbf{A}} = \sum_{\mathbf{k},\lambda} \boldsymbol{\varepsilon}^{\lambda}_{\mathbf{k}} \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}L^3}}\ \left(a^{\lambda}_{\mathbf{k}} + (a^{\lambda}_{\mathbf{k}})^{\dagger}\right), \tag{5.1.10}$$

where we have taken $\mathbf{r}_0 = \mathbf{0}$ without loss of generality.

Problem 5.1 (2 marks) *Use these first-year quantum mechanical ingredients: the Coulomb force law between a proton and an electron; the circular orbits of radius r and speed v that would result classically; de Broglie's standing wave condition $2\pi r = nh/mv$; the resulting (classically calculated) radii r_n and energies E_n of these orbits; and Bohr's formula for photon emission $h\nu_{n',n} = E_{n'} - E_n$ $(n' > n)$. Show that for a transition between neighbouring levels $n' = n+1$ and n, $k\bar{r} \leq (3/4)\alpha$, where $\bar{r}$ is the geometric mean of r_n and r_{n+1} and $k = 2\pi\nu_{n+1,n}/c$. What conclusion do you draw?*

The electron operator $\hat{\mathbf{p}}$ can be written in the atomic state basis as

$$\hat{\mathbf{p}} = \sum_{jl} |j\rangle\langle j|\hat{\mathbf{p}}|l\rangle\langle l|. \tag{5.1.11}$$

Thus the interaction Hamiltonian can be taken to be

$$\hat{H}_{\mathrm{I},1} = \frac{e}{m}\sum_{\mathbf{k}\lambda jl}\left(\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}L^3}\right)^{\frac{1}{2}} \boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda}\cdot\langle j|\hat{\mathbf{p}}|l\rangle\left[\left(a_{\mathbf{k}}^{\lambda}\right) + \left(a_{\mathbf{k}}^{\lambda}\right)^{\dagger}\right]|j\rangle\langle l|. \tag{5.1.12}$$

To continue we note that $\hat{\mathbf{p}} = im[\hat{H}_{\mathrm{el}}, \hat{\mathbf{r}}]/\hbar$, so that $\langle j|\hat{\mathbf{p}}|l\rangle$ can be written in terms of the dipole matrix element:

$$\langle j|\hat{\mathbf{p}}|l\rangle = \frac{im}{\hbar}\langle j|[\hat{H}_{\mathrm{el}}, \hat{\mathbf{r}}]|l\rangle = imE_{jl}\langle j|\hat{\mathbf{r}}|l\rangle/\hbar\,, \tag{5.1.13}$$

where $E_{jl} = E_j - E_l$. We then have

$$\hat{H}_{\mathrm{I},1} = i\sum_{\mathbf{k}\lambda jl}\left(\hbar 2\epsilon_0\omega_{\mathbf{k}}L^3\right)^{-1/2}\boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda}\cdot\mathbf{d}_{jl}E_{jl}[\left(a_{\mathbf{k}}^{\lambda}\right) + \left(a_{\mathbf{k}}^{\lambda}\right)^{\dagger}]|j\rangle\langle l|, \tag{5.1.14}$$

where $\mathbf{d}_{jl} = e\langle j|\mathbf{r}|l\rangle$ is the *electric dipole moment* for the $l \to j$ transition. In wavefunction terms, this is

$$\mathbf{d}_{jl} = e\int d^3\mathbf{r}\,\phi_j^*(\mathbf{r})\mathbf{r}\phi_l(\mathbf{r}). \tag{5.1.15}$$

Discussion 5.1 *What advantage is there in doing this work to get rid of $\langle j|\hat{\mathbf{p}}|l\rangle$ but introduce $\langle j|\hat{\mathbf{r}}|l\rangle$? Can you use Eq. (5.1.15) and what you remember of electron orbital theory to say something about atomic transitions in specific cases?*

5.1.4 Rotating-Wave Approximation

We may simplify this further by noting that the "energy non-conserving terms" in eqn(5.1.14) — those where the atom makes a transition to a lower energy level by absorbing a photon, or to a higher energy level by emitting a photon — will not contribute significantly to the process we are describing. Dropping these terms is called making the *rotating wave approximation* (RWA) or *secular approximation*, and gives

$$\hat{H}_{\mathrm{I},1} \approx \sum_{\mathbf{k},\lambda,E_l<E_j}\left(\hbar 2\epsilon_0\omega_{\mathbf{k}}L^3\right)^{-1/2}\boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda}\cdot\mathbf{d}_{jl}E_{jl}[-i\left(a_{\mathbf{k}}^{\lambda}\right)^{\dagger}|l\rangle\langle j| + i(a_{\mathbf{k}}^{\lambda})|j\rangle\langle l|]\,, \tag{5.1.16}$$

The RWA Hamiltonian means that either the atom can make a transition to a lower energy level by emitting a photon, or to a higher energy level by absorbing a photon. The term "rotating-wave approximation" will be explained below.

Discussion 5.2 *Should not energy be conserved without our having to make alterations to the theory? What energy do we mean when we talk about "energy non-conserving terms"? Why would it make sense to concentrate on this energy?*

5.1.5 Two-level Assumption

We assume that initially the field has no photons in it (the vacuum field), and that the atom is initially in a non-degenerate excited state $|e\rangle$. We also assume that there is only a single lower-energy state, the ground state $|g\rangle$, to which it can make a transition by emitting a photon. We define the energy of the ground state to be 0 and the excited state energy to be $\hbar\omega_e$. The initially excited atom in a vacuum field will, we expect, spontaneously decay to the ground state. That is, there is a transition, due to the interaction Hamiltonian Eq. (5.1.16), from an initial state $|i\rangle = |e, \{0\}\rangle$ to a final state $|f_{\mathbf{k}}^{\lambda}\rangle = |g, 1_{\mathbf{k}}^{\lambda}\rangle$ in which a photon of momentum $\mathbf{k}$ and polarization λ has been emitted. The ket $|1_{\mathbf{k}}^{\lambda}\rangle$ is short for the ket $|00\cdots00100\cdots\rangle$ in the Fock basis, where the 1 appears as the photon number of the mode $\mathbf{k}, \lambda$. In principle, the interaction Hamiltonian Eq. (5.1.16) would allow transitions from $|f_{\mathbf{k}}^{\lambda}\rangle$ to a state $|e', \{0\}\rangle$, where $|e'\rangle$ is an excited state of *higher* energy than $|e\rangle$. However, another RWA-type ("energy conservation") approximation would rule this out.

Discussion 5.3 *What terms in the Hamiltonian would you discard when applying this approximation?*

Because the interaction Hamiltonian describes a one-photon process, the states $|i\rangle$ and $|f_{\mathbf{k}}^{\lambda}\rangle$ are the only states we need consider. Thus the state of the atom-field system at time t can be expanded as

$$|\psi(t)\rangle = c_e(t)\exp(-i\omega_e t)|i\rangle + \sum_{\mathbf{k},\lambda} c_{\mathbf{k}}^{\lambda}(t)\exp(-i\omega_{\mathbf{k}}t)|f_{\mathbf{k}}^{\lambda}\rangle\,, \qquad (5.1.17)$$

with $c_e(0) = 1$ and all $c_{\mathbf{k}}^{\lambda}(0) = 0$.

Discussion 5.4 *Why do you think I included the factors* $\exp(-i\omega_e t)$ *and* $\exp(-i\omega_{\mathbf{k}}t)$*, rather than just allowing them to be included in* $c_e(t)$ *and* $c_{\mathbf{k}}^{\lambda}(t)$*?*

Now the combined state of the system obeys Schrödinger's equation which is, ignoring $\hat{H}_{\mathrm{I},2}$,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \left(\hat{H}_{\mathrm{el}} + \hat{H}_{\mathrm{rad}} + \hat{H}_{\mathrm{I},1}\right)|\psi(t)\rangle \qquad (5.1.18)$$

Subsitituting Eq. (5.1.17) into this equation, the left-hand-side evaluates to

$$i\hbar\left[(\dot{c}_e - i\omega_e c_e)\exp(-i\omega_e t)|i\rangle + \sum_{\mathbf{k},\lambda}\left(\dot{c}_{\mathbf{k}}^{\lambda} - i\omega_{\mathbf{k}}c_{\mathbf{k}}^{\lambda}\right)\exp(-i\omega_{\mathbf{k}}t)|f_{\mathbf{k}}^{\lambda}\rangle\right], \qquad (5.1.19)$$

while the three Hamiltonians on the right-hand-side give the three terms

$$\hbar\omega_e c_e\exp(-i\omega_e t)|i\rangle + \sum_{\mathbf{k},\lambda}\hbar\omega_{\mathbf{k}}c_{\mathbf{k}}^{\lambda}\exp(-i\omega_{\mathbf{k}}t)|f_{\mathbf{k}}^{\lambda}\rangle + \hat{H}_{\mathrm{I},1}|\psi(t)\rangle. \qquad (5.1.20)$$

Cancelling common terms on both sides, and acting upon the remaining terms with $\langle f^\lambda_{\mathbf{k}}|$ and $\langle i|$ respectively gives

$$\exp(-i\omega_{\mathbf{k}}t)i\hbar\frac{\mathrm{d}c^\lambda_{\mathbf{k}}}{\mathrm{d}t} = \langle f^\lambda_{\mathbf{k}}|\hat{H}_{\mathrm{I},1}|\psi(t)\rangle \quad (5.1.21)$$

$$\exp(-i\omega_e t)i\hbar\frac{\mathrm{d}c_e}{\mathrm{d}t} = \langle i|\hat{H}_{\mathrm{I},1}|\psi(t)\rangle \quad (5.1.22)$$

Discussion 5.5 *This simplifies greatly using* $\langle i|\hat{H}_{\mathrm{I},1}|i\rangle = \langle f^\lambda_{\mathbf{k}}|\hat{H}_{\mathrm{I},1}|f^{\lambda'}_{\mathbf{k}'}\rangle = 0$. *What is a physical reason that these quantities vanish?*

Denoting the matrix element $\langle f^\lambda_{\mathbf{k}}|\hat{H}_{\mathrm{I},1}|i\rangle$ by $\kappa^\lambda_{\mathbf{k}}$ we thus obtain

$$\frac{\mathrm{d}c^\lambda_{\mathbf{k}}}{\mathrm{d}t} = (-i/\hbar)\kappa^\lambda_{\mathbf{k}}c_e(t)\exp(-i(\omega_e-\omega_{\mathbf{k}})t) \quad (5.1.23)$$

$$\frac{\mathrm{d}c_e}{\mathrm{d}t} = (-i/\hbar)\sum_{\mathbf{k},\lambda}\kappa^{\lambda *}_{\mathbf{k}}c^\lambda_{\mathbf{k}}(t)\exp(i(\omega_e-\omega_{\mathbf{k}})t)\,. \quad (5.1.24)$$

These equations are exact given the approximate Hamiltonian Eq. (5.1.16). If the RWA had not been made there would be terms oscillating as $\exp\big(i(\omega_e+\omega_{\mathbf{k}})t\big)$. These average to zero over any significant time scale because they are oscillating at twice the optical frequency. Hence the name (and justification) of the rotating-wave approximation.

Eq. (5.1.23) can be formally integrated to give

$$c^\lambda_{\mathbf{k}}(t) = \frac{-i}{\hbar}\kappa_{\mathbf{k}}\int_0^t c_e(t')\exp(-i(\omega_e-\omega_{\mathbf{k}})t')\mathrm{d}t'\,. \quad (5.1.25)$$

Substituting this into Eq. (5.1.24) gives the *integro-differential equation*

$$\frac{\mathrm{d}c_e}{\mathrm{d}t} = -\frac{1}{\hbar^2}\sum_{\mathbf{k},\lambda}|\kappa^\lambda_{\mathbf{k}}|^2\int_0^t c_e(t')\exp(-i(\omega_e-\omega_{\mathbf{k}})(t'-t))\mathrm{d}t'\,. \quad (5.1.26)$$

5.1.6 Continuum limit

To proceed further, note that as the normalization volume L^3 becomes infinite, the final states $|f^\lambda_{\mathbf{k}}\rangle$ become infinitely closely spaced in energy. Also note that the integral in Eq. (5.1.26) depends only on the frequency $\omega_{\mathbf{k}} = c|\mathbf{k}|$ of the emitted photon, not its direction $\check{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$ or polarization $\lambda = 1, 2$. (Here I use a $\check{}$ to represent a unit vector, rather than the usual $\hat{}$, to avoid confusion with the notation for an operator.) Thus we can make the replacement:

$$\sum_{\mathbf{k},\lambda}|\kappa^\lambda_{\mathbf{k}}|^2 \to \sum_\lambda\frac{1}{2}\int\frac{\mathrm{d}\Omega(\check{\mathbf{k}})}{4\pi}\int\mathrm{d}\omega_f\,\rho(\omega_f)\,|\kappa^\lambda(\check{\mathbf{k}},\omega_f)|^2. \quad (5.1.27)$$

Here $d\Omega(\check{\mathbf{k}})$ is the solid angle element $d\phi\sin\theta d\theta$ for $\mathbf{k}$ parametrized by the Euler angles ϕ and θ, while $\rho(\omega_f)\mathrm{d}\omega_f$ is the mode density of the emitted (final) frequency ω_f. These are normalized so that $\int\frac{\mathrm{d}\Omega(\check{\mathbf{k}})}{4\pi} = 1$

and $\int_0^\omega \mathrm{d}\omega_f \rho(\omega_f) = N(\omega)$, the number of modes with frequency less than or equal to ω. The mode count includes a factor of two for the two polarizations, which is why the $\frac{1}{2}$ has appeared in the polarization sum, to cancel it. Thus we have

$$\frac{\mathrm{d}c_e}{\mathrm{d}t} = -\frac{1}{\hbar^2}\sum_\lambda \frac{1}{2} \int \frac{\mathrm{d}\Omega(\check{\mathbf{k}})}{4\pi} \int_0^\infty \mathrm{d}\omega_f |\kappa^\lambda(\check{\mathbf{k}},\omega_f)|^2 \rho(\omega_f) \int_0^t c_e(t') e^{-i(\omega_e-\omega_f)(t'-t)} \mathrm{d}t'. \tag{5.1.28}$$

5.1.7 Markovian (Memoryless) Approximation

A systematic solution to this can be developed using Laplace transform techniques. However, a simple approximation allows us to get a direct estimate of the spontaneous emission rate and hence the linewidth. We note that the exponential in the integrand

$$f(t,\omega_f) \equiv \int_0^t c_e(t') e^{-i(\omega_e-\omega_f)(t'-t)} \mathrm{d}t' \tag{5.1.29}$$

is rapidly oscillating (as a function of t') except for $\omega_f \approx \omega_e$. Thus $f(t,\omega_f)$ will average to zero except in the region $\omega_f \approx \omega_e$. This is physically reasonable too: it says that the frequency of the emitted photon is close to the transition frequency of the atom. Since the coupling constant $|\kappa^\lambda(\check{\mathbf{k}},\omega_f)|^2$ and mode density $\rho(\omega_f)$ are slowly varying functions of ω_f,[3] we can replace them by their values at the resonant frequency $\omega_f = \omega_e$. Also, we can extend the lower limit of the ω_f-integral to $-\infty$ without greatly changing the value of the integral. This gives

$$\frac{\mathrm{d}c_e}{\mathrm{d}t} \approx -\frac{1}{\hbar^2}\rho(\omega_e)\overline{|\kappa_0|^2} \int_{-\infty}^\infty \mathrm{d}\omega_f \int_0^t \mathrm{d}t'\, c_e(t') e^{-i(\omega_e-\omega_f)(t'-t)}\,, \tag{5.1.30}$$

where I have defined an average coupling constant

$$\overline{|\kappa_0|^2} = \sum_\lambda \frac{1}{2} \int \frac{\mathrm{d}\Omega(\check{\mathbf{k}})}{4\pi}\, |\kappa^\lambda(\check{\mathbf{k}},\omega_e)|^2. \tag{5.1.31}$$

Now we can change the order of the integrals in Eq. (5.1.30), and change variables to $s = \omega_f - \omega_e$ to get

$$\frac{\mathrm{d}c_e}{\mathrm{d}t} \approx -\frac{1}{\hbar^2}\overline{|\kappa_0|^2}\rho(\omega_e) \int_0^t \mathrm{d}t'\, c_e(t') \int_{-\infty}^\infty \mathrm{d}s\, e^{-is(t'-t)}\,. \tag{5.1.32}$$

But the second integral, over s, is the standard complex Fourier representation of the Dirac delta function:

$$2\pi\delta(t'-t) = \int_{-\infty}^\infty e^{-is(t'-t)} \mathrm{d}s\,. \tag{5.1.33}$$

This makes the integral over t' trivial, if we remember that for a smooth function $g(t)$, $\int^t \delta(t-t')g(t')dt' = \frac{1}{2}g(t)$. Thus

$$\frac{\mathrm{d}c_e}{\mathrm{d}t} \approx -\frac{\gamma}{2} c_e(t)\,, \tag{5.1.34}$$

[3] In *structured media* such as photonic band-gaps, this assumption may not be valid, in which case the Markovian approximation is a poor one.

where the spontaneous decay rate γ is

$$\gamma = \frac{2\pi\overline{|\kappa_0|^2}\rho(\omega_e)}{\hbar^2} \ . \tag{5.1.35}$$

Discussion 5.6 *Why would I define γ this way? Why not as half this quantity so that the right-hand-side of Eq. (5.1.34) would be simply $-\gamma c_e(t)$? Think about the solution of Eq. (5.1.34) and what it means physically.*

5.1.8 Evaluating the spontaneous decay rate

To fully evaluate this, we need the mode density $\rho(\omega_e)$ and the average coupling coefficient $\overline{|\kappa_0|^2}$. These can be found as follows.

$$\rho(\omega_e) = \frac{\mathrm{d}N(\omega)}{\mathrm{d}\omega}|_{\omega=\omega_e}, \tag{5.1.36}$$

where $N(\omega)$ is the number of modes with frequency less than ω. Recall that with a normalization volume of L^3, $\mathbf{k} = (2\pi/L)(l,m,n) = (2\pi/L)(\nu_1,\nu_2,\nu_3)$. The number of modes is thus

$$\begin{aligned} N(\omega) &= \sum_{(\nu_1,\nu_2,\nu_3) \text{ such that } (2\pi c/L)^2(\nu_1^2+\nu_2^2+\nu_3^2)<\omega^2} \ \sum_{\lambda=1,2} 1 \\ &\approx 2 \times \frac{4}{3}\pi(L\omega/2\pi c)^3 \end{aligned} \tag{5.1.37}$$

Thus

$$\rho(\omega_e) = \frac{L^3\omega_e^2}{\pi^2 c^3}. \tag{5.1.38}$$

Next,

$$\kappa_{\mathbf{k}}^{\lambda} = \langle f_{\mathbf{k}}^{\lambda}|\hat{H}_{\mathrm{I},1}|i\rangle = i\left(\hbar 2\epsilon_0\omega_e L^3\right)^{-1/2} E_e \boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda}\cdot\mathbf{d}, \tag{5.1.39}$$

where $E_e = \hbar\omega_e$ (remember E_g is taken to be 0), and $\mathbf{d} = \mathbf{d}_{eg}$.

Exercise 5.1 *Show Eq. (5.1.39).*

Thus we have

$$|\kappa^{\lambda}(\check{\mathbf{k}},\omega_e)|^2 = \hbar\omega_e(2\epsilon_0 L^3)^{-1}d^2\cos^2\theta, \tag{5.1.40}$$

where θ is the angle between the polarization vector of the mode and the dipole vector $\mathbf{d} = d\hat{\mathbf{d}}$ of the atom. Thus the average in Eq. (5.1.31) is

$$\overline{|\kappa_0|^2} = \hbar\omega_e(2\epsilon_0 L^3)^{-1}d^2\,\overline{\cos^2\theta}, \tag{5.1.41}$$

where

$$\overline{\cos^2\theta} = \frac{\int_0^{2\pi}d\phi\int_0^{\pi}\sin\theta d\theta\cos^2\theta}{\int_0^{2\pi}d\phi\int_0^{\pi}\sin\theta d\theta} = \frac{1}{2}\int_{-1}^{1}dx x^2 = \frac{1}{3}. \tag{5.1.42}$$

The final expression for the total spontaneous emission rate is thus

$$\gamma = \frac{\omega_e^3 d^2}{3\pi\epsilon_0 c^3 \hbar}. \tag{5.1.43}$$

Note that the normalization volume L^3 has disappeared from this expression.

Discussion 5.7 *Do you think this is significant, or just the way things turned out? Why?*

5.1.9 Fermi's Golden Rule

For a typical atom, γ is of the order of $10^8 s^{-1}$ or smaller, which is much less than the transition frequency which is of order $10^{15} s^{-1}$. This difference in time scales is what justifies the rotating wave approximation. The ratio can be expressed as follows:

$$\frac{\gamma}{\omega_e} = \frac{4}{3}\alpha \left(\frac{|\langle e|\mathbf{r}|g\rangle|}{\lambda/2\pi} \right)^2. \tag{5.1.44}$$

Now the fine structure constant α (see Eq. (5.1.8)) is small, and was used to ignore $\hat{H}_{\mathrm{I},2}$. Also, we have used the fact that the wavelength λ is much greater than the displacement of the electron $|\langle e|\mathbf{r}|g\rangle|$ in making the dipole approximation. In fact, using problem 5.1 in Sec. 5.1.3, we can say that $\gamma/\omega_e \sim \alpha^3$. Thus all of the approximations are justified by the smallness of α. Indeed, this is why QED is such a good theory for calculating with (compared to other quantum field theories we will meet in Chapter 6).

This result for spontaneous emission is one application of a general theory of irreversible processes in QM. The irreversibility arises from the fact that there are many final states into which the system may evolve, so the chances of it finding its way back into its initial state is negligible. By taking the continuum limit (by using a density of states $\rho(\omega)$), true irreversibility is obtained. It applies to any scattering problem in which the particles (or quanta as in this case) are scattered into an infinite region of free space. The general result, known as Fermi's golden rule, is that the rate of the irreversible process is

$$\gamma_{i\to f} = 2\pi \overline{|V_{fi}|^2} \rho(E_f)/\hbar, \tag{5.1.45}$$

where V_{fi} is the amplitude of the interaction Hamiltonian matrix element taking the initial state i to final state f, and $\rho(E_f)$ is the density of final states as a function of of energy.

5.1.10 The Lamb shift and Renormalization

A more careful calculation of the radiative process in atoms agrees with this result for the emission rate, but shows that there is in addition a frequency shift Δ_{L}, the *Lamb shift*, due to emission and reabsorption of virtual photons, so that

$$\frac{\mathrm{d}c_e}{\mathrm{d}t} = -\left(\frac{\gamma}{2} + i\Delta_{\mathrm{L}}\right) c_e(t)\,, \tag{5.1.46}$$

and hence

$$c_e(t) = \exp\left[-\left(\frac{\gamma}{2} + i\Delta_{\rm L}\right)t\right] \ . \tag{5.1.47}$$

A naive calculation of $\Delta_{\rm L}$ returns the value infinity; to obtain a finite answer requires relativistic QED and the theory of *renormalization*.

Basically, the naive calculation gives the shift in the energy of an atomic level due to coupling to the infinite number of electromagnetic modes in the vacuum state. But these infinite number of modes in fact give an infinite energy shift to a *free* electron — it can be thought of as giving it an infinite mass (since $E_0 = mc^2$). Since we know electrons do not have an infinite mass, we assume the electron actually has an infinite *negative* mass to begin with, such that this infinite positive mass contribution from the electromagnetic field is almost cancelled, leaving over just the usual finite mass of the electron. (There are an awful lot of mathematical tricks in this as you might imagine). This is called *mass-renormalization*. Now this infinite negative mass also cancels the infinity in the naive calculation of the energy of the electron in the atom, but what is left over is not only the usual electron mass term, but also an additional small energy shift, which is the Lamb shift. The calculation of the Lamb shift by Bethe in 1947 was the first triumph of renormalization theory.

5.1.11 The Spectrum

To find the linewidth, we just substitute the solution eqn(5.1.47) back into eqn(5.1.25), to get

$$c^\lambda_{\mathbf{k}}(t) = \frac{\kappa^\lambda_{\mathbf{k}}/\hbar}{\omega_e - \omega_{\mathbf{k}} + \Delta_{\rm L} - i\frac{\gamma}{2}} \left\{\exp[-i(\omega_e - \omega_{\mathbf{k}} + \Delta_{\rm L})t - \frac{\gamma}{2}t] - 1\right\} \ . \tag{5.1.48}$$

The emission spectrum $S(\mathbf{k})$ can be defined as the probability for the photon to be emitted with propagation vector $\mathbf{k} = (\omega_{\mathbf{k}}/c)\check{\mathbf{k}}$. This includes both direction and frequency information. Using the approximation Eq. (5.1.40), the spectrum is given by

$$\begin{aligned} S(\check{\mathbf{k}}, \omega_{\mathbf{k}}, \lambda) &= \lim_{t\to\infty} |c^\lambda_{\mathbf{k}}(t)|^2 = \frac{|\kappa^\lambda(\check{\mathbf{k}}, \omega_e)|^2/\hbar^2}{(\omega_e - \omega_{\mathbf{k}} + \Delta_{\rm L})^2 + (\gamma/2)^2} \\ &= \frac{\omega_e (2\epsilon_0 L^3\hbar)^{-1} d^2 \cos^2\theta}{(\omega_e - \omega_{\mathbf{k}} + \Delta_{\rm L})^2 + (\gamma/2)^2} \ . \end{aligned} \tag{5.1.49}$$

That is, the spectrum is a Lorentzian, peaked at $\omega_e + \Delta_{\rm L}$, with linewidth (FWHMH) γ. This is exactly the linewidth expected from the simple uncertainty principle argument outlined at the beginning of this section, taking Δt to be the lifetime $1/\gamma$ and $\Delta E = \hbar\Delta\omega$ using the HWHMW, $\gamma/2$, for $\Delta\omega$. The fact that $\gamma \ll \omega_e$ (as found above) then justifies the use of the RWA and dipole approximations, since the spectrum derived here indicates that only modes with frequencies within a few linewidths of ω_e have a significant probability of containing a photon.

Note that the dipole radiation distribution, proportional to $\cos^2\theta$, is incorporated, following from Eq. (5.1.40). Recall that θ is the angle between the atomic dipole and the photon polarization vector.

Discussion 5.8 *Draw a diagram showing* $\mathbf{d}$, $\mathbf{k}$, *two suitable* $\boldsymbol{\varepsilon}_{\mathbf{k}}^{\lambda}$*s, and* θ*. In what directions will the atom* not *emit any light? (Your answer should ring a bell from 2nd and 3rd year physics.)*

It might be thought strange that the normalization volume L^3 appears on the RHS of Eq. (5.1.49), but that is because we have assumed that the photon propagation vectors $\mathbf{k}$ can be differentiated no matter how small the difference between them. More realistically we can consider the probability for the photon to be emitted in a small solid angle $\sin\theta \mathrm{d}\theta\mathrm{d}\phi$ and small frequency range $\mathrm{d}\omega$, which equals

$$S(\omega,\theta,\phi)\rho(\omega_e)\mathrm{d}\omega\frac{\sin\theta\mathrm{d}\theta\mathrm{d}\phi}{4\pi} = \frac{\gamma}{2\pi}\frac{3\cos^2\theta}{(\omega_e-\omega+\Delta_{\mathrm{L}})^2+(\gamma/2)^2}\mathrm{d}\omega\frac{\sin\theta\mathrm{d}\theta\mathrm{d}\phi}{4\pi} \tag{5.1.50}$$

Problem 5.2 (2 marks) *Show this and verify that it integrates to unity. Discuss any approximations made.*

5.2 Thomson scattering

In Thomson scattering a photon with propagation vector $\mathbf{k}_i$ and polarization $\boldsymbol{\varepsilon}_{\mathbf{k}_i}^{\lambda_i}$ is scattered by a free electron with initial momentum $\mathbf{p}_i$. After the scattering process the electron has momentum $\mathbf{p}_f$ while the scattered photon has propagation vector $\mathbf{k}_f$ and polarization $\boldsymbol{\varepsilon}_{\mathbf{k}_f}^{\lambda_f}$. For convenience we can always transform to a frame where the initial momentum of the electron is $\mathbf{p}_i = \mathbf{0}$. In that frame, the nonrelativistic QED Hamiltonian can be used as long as $\hbar\omega_i \ll mc^2$, where m is the rest mass of the electron. We will assume this to be the case.

Problem 5.3 (2 marks) *Show from conservation of free energy* ($H_{\mathrm{el}}+H_{\mathrm{rad}} = |\mathbf{p}|^2/2m+\hbar c|\mathbf{k}|$) *and of momentum* ($\mathbf{p}+\hbar\mathbf{k}$) *that if* $\mathbf{p}_i = \mathbf{0}$ *then*

$$\frac{\omega_i-\omega_f}{\omega_i} \le \frac{2\hbar\omega_i}{mc^2}. \tag{5.2.1}$$

Note that this is just an argument involving c-numbers (scalars and vectors).

Thus, since we have assumed $\hbar\omega_i \ll mc^2$, the exercise shows that the change in the energy of the photon is negligible in this scattering process. From this it follows that we can assume $\omega_i \approx \omega_f$ (*elastic scattering*).

Exercise 5.2 *Show that* $\hat{H}_{\mathrm{I},1}$ *does not contribute to the scattering process according to Fermi's golden rule (which is really a first-order perturbation result). Draw Feynman diagrams to illustrate this.*

Problem 5.4 (3 marks) *Show that the amplitude* V_{fi} *(between initial and final states that are* different — $\mathbf{k}_i \neq \mathbf{k}_f$ etc.*) is therefore given by*

$$V_{fi} = \langle \mathbf{p}_f, 1_{\mathbf{k}_f}^{\lambda_f}|\hat{H}_{\mathrm{I},2}|\mathbf{p}_i, 1_{\mathbf{k}_i}^{\lambda_i}\rangle \tag{5.2.2}$$

$$= \frac{e^2\hbar}{2m\epsilon_0 L^3}(\boldsymbol{\varepsilon}_{\mathbf{k}_i}^{\lambda_i}\cdot\boldsymbol{\varepsilon}_{\mathbf{k}_f}^{\lambda_f})\langle \mathbf{p}_f+\hbar\mathbf{k}_f|\mathbf{p}_i+\hbar\mathbf{k}_i\rangle(\omega_i\omega_f)^{-1/2}, \tag{5.2.3}$$

where (for $\alpha = i, f$) $\omega_\alpha = c|\mathbf{k}_\alpha|$ and the states $|\mathbf{p}_\alpha + \hbar\mathbf{k}_\alpha\rangle$ are momentum eigenstates of the electron. Hint: show first that $e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}|\mathbf{p}\rangle = |\mathbf{p} + \hbar\mathbf{k}\rangle$ by considering the momentum eigenstate in the position representation.

Problem 5.5 (2.5 marks) *Consider for the moment $\mathbf{p}_f$ fixed. Show using Fermi's golden rule (in a similar way to the radiative transition problem, where the final photon states to be averaged over are states with 1 photon in some mode $\mathbf{k}_f, \boldsymbol{\varepsilon}_{\mathbf{k}_f}^{\lambda_f}$) that the probability of scattering into the final state per unit time is*

$$\gamma_{i\to f} = 2\pi r_0^2 \delta_{\mathbf{p}_f + \hbar\mathbf{k}_f, \mathbf{p}_i + \hbar\mathbf{k}_i} \frac{c}{L^3} \frac{4}{3} \tag{5.2.4}$$

where you will need to use $\omega_i = \omega_f$, and where

$$r_0 = \frac{e^2}{4\pi\epsilon_0 mc^2} \approx 2.8 \times 10^{-15}\text{m} \tag{5.2.5}$$

is known as the "classical electron radius". Hint: $\langle\mathbf{p}|\mathbf{p}'\rangle = \delta_{\mathbf{p},\mathbf{p}'}$.

In Eq. (5.2.4), the rate $\gamma_{i\to f}$ still contains the normalization volume L^3, and in the limit $L^3 \to \infty$ the rate goes to zero. That is because our initial state contained one photon and in the limit $L^3 \to \infty$ that photon (which is spread over all space) has a zero probability of hitting the electron. To obtain a quantity with a physical interpretation it is necessary to divide $\gamma_{i\to f}$ by the beam intensity which this single photon represents. Since the speed of the photon is c, and the length of the volume is L, the "flow rate" of photons in the beam is c/L photons per second. Since the cross section of the beam is L^2, the beam intensity is c/L^3 photons per second per square meter.

Exercise 5.3 *Show that the rate of scattering, normalized relative to the beam intensity, and summed over all possible final electron momenta $\mathbf{p}_f$ is*

$$\sigma = \frac{8\pi}{3} r_0^2. \tag{5.2.6}$$

Discussion 5.9 *How can σ be interpreted, and why?*

6 Relativistic QM: Preliminaries

6.1 Spin

6.1.1 Rotations

Spin was a surprising feature of quantum mechanics, with no classical analogue. However, it is intimately related to rotations, so we begin by reviewing rotations. These form a *group*[4] of transformations denoted $SO(3)$, whose elements are 3×3 matrices R which are *S*pecial ($\det(R) = 1$) and *O*rthogonal ($R^T R = I$). In index notation, the latter equation is (note that the order of the indices here matter!):

$$R_j{}^i R^j{}_k = \delta^i_k \ . \tag{6.1.1}$$

Here we are using the Einstein summation convention — if an an index appears twice, once "upstairs" and once "downstairs", it is summed over. For finite square matrices (as we are dealing with here), this equation also implies $R^i{}_j R_k{}^j = \delta^i_k$; that is, $RR^T = I$. Under a rotation of the frame of reference, a vector transforms as

$$r^i \to r^{i'} = R^{i'}_j \ r^j. \tag{6.1.2}$$

Rotations preserve the scalar product between two vectors $\mathbf{q}$ and $\mathbf{r}$:

$$\mathbf{q}\cdot\mathbf{r} = \delta_{ij} q^i r^j = q^1 r^1 + q^2 r^2 + q^3 r^3. \tag{6.1.3}$$

Exercise 6.1 *Using Eq. (6.1.1), show that the scalar product (6.1.3) is invariant under a rotation of axes.*

This invariance is what defines the structure of Euclidean space, and the matrix δ_{ij} is known as the metric tensor for Euclidean space.

An arbitrary 3×3 matrix has 9 elements. The restriction of Eq. (6.1.1) gives six equations these must satisfy (only six because $R^T R$ is automatically a symmetric matrix). Moreover, these restrictions imply that $\det(R) = \pm 1$, so that the requirement that $\det(R) = 1$ is not an independent restriction (it simply rules out spatial reflection). Thus R can be specified by three real numbers, which can be represented by a vector $\mathbf{w}$ known as the **twist vector**, where the rotation is by an angle $\theta = |\mathbf{w}|$ around the axis $\check{\mathbf{w}}$. (Note again I use a $\check{}$ to represent a unit vector, rather than the usual $\hat{}$, to avoid confusion with the notation for an operator.) For example, if $\mathbf{w} = \theta \mathbf{e}_3$ (a rotation around the z-axis), then

$$R = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{6.1.4}$$

[4] A group G is a set of elements $\{T\}$ which can be 'multiplied' satisfying: i) G contains the identity I; ii) G is closed $[\forall T, T' \in G, T'T \in G]$; iii) G is invertible $[\forall T \in G \exists T' \in G : T'T = I]$; iv) G is associative $[\forall T, T', T'' \in G, T(T'T'') = (TT')T'']$.

6.1.2 Spinors

The most important case of spin is $s = \frac{1}{2}$, for two reasons. First, particles of all other spins (including zero spin) can be made from a compound of spin half particles. Second, as we will see, all fundamental *particles* are spin half. (Here I am maintaining the distinction between particles such as electrons and quanta such as photons.)

A spin-half particle is described by a two-dimensional Hilbert space, and so spin is represented by 2×2 matrices. Because they are so important, they are given a special name, the Pauli matrices. Specifically,

$$\hat{\mathbf{S}} = \tfrac{1}{2}\hbar\boldsymbol{\sigma}, \tag{6.1.5}$$

where the three Pauli matrices are[5]

$$\boldsymbol{\sigma} = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right)^T . \tag{6.1.6}$$

The Pauli matrices obey the following relations

$$\sigma_i\sigma_j = \sqrt{-1}\,\epsilon_{ijk}\sigma_k + \delta_{ij}I\,; \tag{6.1.7}$$

From this it may be shown that, for any vectors $\mathbf{A}$ and $\mathbf{B}$,

$$(\boldsymbol{\sigma}\cdot\mathbf{A})(\boldsymbol{\sigma}\cdot\mathbf{B}) \;=\; I\mathbf{A}\cdot\mathbf{B} + i\boldsymbol{\sigma}\cdot(\mathbf{A}\times\mathbf{B}). \tag{6.1.8}$$

Note that $\boldsymbol{\sigma}\cdot\mathbf{v}$, for any vector $\mathbf{v}$, is a 2×2-matrix.

Problem 6.1 (1.5 marks) *Check (6.1.7) for any four of the nine cases. Show that Eq. (6.1.8) follows from (6.1.7).*

Aside 6.1 *Here's a cute thing you can do with the above relations: writing Maxwell's equations (yes, all four) as a single 2×2 complex matrix equation, as here: (This is related to Clifford algebra; see later.)*

$$\big[\,\tfrac{1}{c}\tfrac{\partial}{\partial t} - \boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\,\big]\big[\,\boldsymbol{\sigma}\cdot(\mathbf{E} - i\mathbf{B})\,\big] = \big[\,\rho + \tfrac{1}{c}\boldsymbol{\sigma}\cdot\mathbf{j}\,\big]/\epsilon_0. \tag{6.1.9}$$

A spin half particle has only two orthogonal spin states. Ignoring the spatial dependence of the wavefunction for the present, we can write the system state in terms of the eigenstates of σ_3:

$$|\xi\rangle = \xi_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \xi_{-1} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \xi_1 \\ \xi_{-1} \end{pmatrix}. \tag{6.1.10}$$

In the relativistic theory there is not as simple a relation between the components of the wavefunction and the value of the spin. For this reason, it is simpler now to label the states instead as 1 and 2:

$$|\xi\rangle = \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}. \tag{6.1.11}$$

[5]Note that I will generally not use the $\hat{}$ symbol on Pauli operators and certain related operators that we will see in the relativistic setting. This is for three reasons. First, they are usually represented as matrices, so it should be easy to remember that they do not commute. Second, as well as representing quantum quantities, these matrices also have other applications, as we will see. Third, the quantum quantities they represent have no close classical analogues, so no confusion is likely.

This object is called a *spinor*. If we wish to describe the system relative to a different set of coordinates, rotated relative to the original axes by twist vector $\mathbf{w}$, it can be shown that the state transforms to

$$|\xi'\rangle = S_{\mathbf{w}}|\xi\rangle \equiv \exp(-i\tfrac{1}{2}\mathbf{w}\cdot\boldsymbol{\sigma})|\xi\rangle. \tag{6.1.12}$$

Writing $\mathbf{w} = \theta\check{\mathbf{w}}$ we find

$$S_{\mathbf{w}} = I\cos\frac{\theta}{2} - i\check{\mathbf{w}}\cdot\boldsymbol{\sigma}\sin\frac{\theta}{2}. \tag{6.1.13}$$

Problem 6.2 (2 marks) *Derive Eq. (6.1.13) from Eq. (6.1.12) and show that Eq. (6.1.13) preserves the norm of the state (that is, preserves* $|\xi_1|^2 + |\xi_2|^2$*).*
Hint: *First show that* $\sigma^2 = I$*, where* $\sigma = \check{\mathbf{w}}\cdot\boldsymbol{\sigma}$*, then expand the exponential in an infinite Taylor series.*

The group of transformations of the form (6.1.13) is called the group $SU(2)$. Here 2 indicates that the elements operate in a two dimensional linear space, U that they are unitary ($S^\dagger_{\mathbf{w}}S_{\mathbf{w}} = I$), and S that they are 'special'[6] ($\det(S_{\mathbf{w}}) = 1$). The two-component state on which they act is called a *spinor*. A spinor is an object distinct from scalars, vectors, tensors *etc.*, because of its manner of transformation (6.1.12). Spinors are fundamental to the study of elementary particles. It is obvious from Eq. (6.1.13) that a rotation of $\theta = 2\pi$ yields a phase factor of -1. More generally, a rotation of $\theta + 2\pi$ is identical with a rotation of θ and a sign change. That is, there is a two-to-one mapping from $SU(2)$ to $SO(3)$, the group of rotations in three dimensions.

6.1.3 Spinors and Vectors

The mapping between the $SU(2)$ group and the group of rotations can be made explicit. First, from any given spinor $|\xi\rangle$ we can define a 3-vector $\mathbf{h} = (h_1, h_2, h_3)^T$ according to the following:

$$\mathbf{h} = \langle\xi|\boldsymbol{\sigma}|\xi\rangle. \tag{6.1.14}$$

From this, if $|\xi\rangle$ is normalized, then $\mathbf{h}$ is a unit vector.

Exercise 6.2 *Show this by first working out* $\mathbf{h}$ *in terms of* ξ_1 *and* ξ_2*.*

This unit vector (technically a pseudovector) can be thought of as the mean spin of the spin-$\frac{1}{2}$ particle[7]. Moreover, any unit vector can be represented in this way.

Now the identification (6.1.14) by itself is of no great significance. The crucial point is that the matrices on both sides transform identically

[6] This last fact follows from the fact that the "generators" $\boldsymbol{\sigma}$ are traceless

[7] This vector is in fact a useful representation for any two-level quantum system, and is usually called the Bloch vector. It even generalizes to a two-level system in a mixed state, via $\mathbf{h} = \mathrm{tr}[\rho\boldsymbol{\sigma}]$. That is, there is a one-to-one relation between the Bloch vector and the state matrix ρ, allowing that for a mixed state $|\mathbf{h}| \leq 1$.

under rotations. That is, if you calculate the transformed vector from (6.1.14),

$$\mathbf{h}' = \langle \xi' | \boldsymbol{\sigma} | \xi' \rangle = \langle \xi | S_{\mathbf{w}} \boldsymbol{\sigma} S_{\mathbf{w}}^{\dagger} | \xi \rangle, \tag{6.1.15}$$

you get the same answer as from ordinary 3-dimensional rotation,

$$\mathbf{h}' = R_{\mathbf{w}} \mathbf{h}. \tag{6.1.16}$$

Exercise 6.3 *Verify the equality for a rotation around the* $\mathbf{e}_3$ *axis.*

The conclusion we may draw from the above correspondence is that spinors are something like the square root of a vector.

We can rewrite the above relation between $R_{\mathbf{w}}$ and $S_{\mathbf{w}}$ just in terms of $|\xi\rangle$ as:

$$R_{\mathbf{w}} \langle \xi | \boldsymbol{\sigma} | \xi \rangle = \langle \xi | S_{\mathbf{w}} \boldsymbol{\sigma} S_{\mathbf{w}}^{\dagger} | \xi \rangle \tag{6.1.17}$$

In the first term, we can take $R_{\mathbf{w}}$ inside (it is a 3x3 matrix, remember — nothing to do with the 2-dimensional Hilbert space where the spinors live), to get $\langle \xi | R_{\mathbf{w}} \boldsymbol{\sigma} | \xi \rangle$. But since the relation is true for all states $|\xi\rangle$ the operators themselves must be equal:

$$R_{\mathbf{w}} \boldsymbol{\sigma} = S_{\mathbf{w}} \boldsymbol{\sigma} S_{\mathbf{w}}^{\dagger}. \tag{6.1.18}$$

Fundamentally, the reason for the close relationships between rotations in 3 dimensions and the $SU(2)$ group is that the Pauli matrices satisfy a *Clifford algebra*

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2\delta_{ij} I \tag{6.1.19}$$

appropriate for the Euclidean metric tensor δ_{ij} in 3 dimensions. Equations (6.1.18) and (6.1.19) are the ones we will generalise later to the relativistic case.

6.1.4 NON-EXAMINABLE Combining Spins (Revision)

It was stated above that particles of all spins can be formed by combining spin half particles. This is now demonstrated for the case of spin 0 and spin 1, which can be formed from two spin half particles. Let the two basis spinors of one each particle be denoted $|u\rangle$ for the $+1$ eigenstate of σ_3, and $|d\rangle$ for the -1 eigenstate, and let a and b denote the particle. Then one possibility for the four basis states for the compound system is

$$|u_a u_b\rangle, |u_a d_b\rangle, |d_a u_b\rangle, |d_a d_b\rangle. \tag{6.1.20}$$

Here $|u_a u_b\rangle = |u_a\rangle \otimes |u_b\rangle$ *etc.* This defines the tensor product of the two Hilbert spaces, as the larger Hilbert space spanned by the basis vectors (6.1.20). We can thus expand an arbitrary state of the joint system as

$$|\psi\rangle = c_{uu}|u_a u_b\rangle + c_{ud}|u_a d_b\rangle + c_{du}|d_a u_b\rangle + c_{dd}|d_a d_b\rangle. \tag{6.1.21}$$

The two particles are said to be not entangled if $|\psi\rangle = |\xi^a\rangle|\xi^b\rangle$. In this case

$$c_{uu} = \xi_1^a \xi_1^b \ , \ c_{ud} = \xi_1^a \xi_2^b \ , \ c_{du} = \xi_2^a \xi_1^b \ , \ c_{dd} = \xi_2^a \xi_2^b, \tag{6.1.22}$$

where ξ_1 and ξ_2 are as defined by Eq. (6.1.10). In general, this is not the case, and the two particles are said to be entangled.

Now the spin operator for the compound system is

$$\mathbf{S}_c = \mathbf{S}_a + \mathbf{S}_b. \tag{6.1.23}$$

Although these two matrices are added, it must be remembered that they act in different Hilbert spaces. A more complete notation for the addition of $\mathbf{S}_a$ and $\mathbf{S}_b$ is

$$\mathbf{S}_c = \mathbf{S}_a \otimes I_b + I_a \otimes \mathbf{S}_b, \tag{6.1.24}$$

where I is the identity operator as above and $\otimes$ is known as the direct product or tensor product. In the tensor product, each element of the first matrix is replaced by itself multiplied by the entire second matrix. Thus the dimension of the tensor product of two matrices is equal to the product of the dimensions of the two matrices. Thus $\mathbf{S}_c$ is a 3-vector of 4×4 matrices. Explicitly,

$$\mathbf{S}_c = \frac{\hbar}{2}\left(\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix}, \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix}\right)^T \tag{6.1.25}$$

where the state vector on which this would act is $(c_{uu}, c_{ud}, c_{du}, c_{dd})^T$. The spin-squared operator for the system is

$$\mathbf{S}_c^2 = \hbar^2 \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}. \tag{6.1.26}$$

From the result for the $z-$component of $\mathbf{S}_c/\hbar$ it is evident that the spin in that direction can either take the values $-1, 0, 1$, as expected from adding values of $\frac{1}{2}$ or $-\frac{1}{2}$. This eigenvalue we will denote in the usual way as m. The eigenvalues of $\mathbf{S}_c^2/\hbar^2$ are 2 and 0. Since they are defined to be $s(s+1)$ where s is the total spin, we have $s = 0$ or 1, also as expected. Therefore we can find a new basis $|s, m\rangle$ of the joint system in terms of joint eigenvalues of $\mathbf{S}_c^2$ and the $\mathbf{e}_3 \cdot \mathbf{S}_c$. First the single $s = 0$ state (called the *singlet*) is

$$\sqrt{2}|0, 0\rangle = |ud\rangle - |du\rangle. \tag{6.1.27}$$

The three $s = 1$ states (forming the *triplet*) are

$$|1, 1\rangle = |uu\rangle \ , \ \sqrt{2}|1, 0\rangle = |ud\rangle + |du\rangle \ , \ |1, -1\rangle = |dd\rangle. \tag{6.1.28}$$

Evidently states with $m = 0$ are entangled states with respect to the original particles. In fact, they are precisely those sorts of states used by Bell to prove the nonlocality inherent in quantum mechanics.

We can write the two-particle wavefunction (6.1.21) using the s, m basis as

$$|\psi\rangle = c_s|0, 0\rangle + c_x(|1, 1\rangle - |1, -1\rangle)/\sqrt{2} + c_y i(|1, 1\rangle + |1, -1\rangle)/\sqrt{2} + c_z(-|1, 0\rangle) \tag{6.1.29}$$

From the results of the preceding exercise, it can be shown that, under rotations, c_s transforms as a scalar and (c_x, c_y, c_z) as a vector. It is thus clear why spin zero particles are sometimes called scalar particles, and spin one particles vector particles.

6.1.5 The Spin-Statistics Relation

A scalar is a rank-zero tensor, and a vector is a rank-one tensor. A spin two particle would be a rank-two tensor particle because its components could be arranged into a matrix which transformed as a rank-two tensor. A spin $\frac{3}{2}$ particle would transform as a vector whose 3 components each were spinors. The relation between the nature of the object that is the wavefunction (spinorial, vectorial *etc.*), and the value of the spin s, reinforces the idea that a spinor is like a tensor of rank $\frac{1}{2}$ (that is, the square root of a vector in some sense). In general, a spin-s particle has a wavefunction that transforms as a rank-s tensor.

If we accept that all fundamental particles are fermions of spin half (which will be justified in the next chapter), the spin-statistics theorem for particles also follows from the analysis here. Any particle with integer spin n must be composed of an even number $2n$ of fermions. Swapping two such compound particles swaps $2n$ fermions, so that the total effect is to multiply the wavefunction by $(-1)^{2n} = 1$. That is to say, an integer spin particle must be a boson. Conversely, a half integer spin particle made up of an odd number of fermions must be a fermion.

6.2 Relativity and Quantum Mechanics

6.2.1 Summary of relativistic notation

A coordinate 4-vector is denoted by $x = (x^0, x^1, x^2, x^3) = (ct, \mathbf{x})$. (We use greek-letter indices for 4-vectors and latin-letter indices for 3-vectors.) Under a Lorentz transformation from frame S to frame S'

$$x^\mu \to x^{\mu'} = \Lambda^{\mu'}{}_{\nu}\, x^\nu \,, \tag{6.2.1}$$

where the Einstein summation convention is again being used. The Lorentz transformations includes frames that are rotated relative to one another, and frames that are moving at a constant velocity $\mathbf{v}$ relative to one another (called boosts). For example, for a boost by speed $\mathbf{v} = v\mathbf{e}_3$ (in the z direction),

$$\Lambda = \begin{pmatrix} \gamma & 0 & 0 & -\gamma v/c \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\gamma v/c & 0 & 0 & \gamma \end{pmatrix}, \tag{6.2.2}$$

where $\gamma = (1 - v^2/c^2)^{-\frac{1}{2}}$.

In a relativistic theory, physical quantities should transform under Lorentz transformations in well-defined ways. The simplest case is **scalar** quantities, which do not change at all, such as the rest mass of a particle. The next simplest case is a **vector** such as the coordinate vector x

itself. The quantities q^μ are components of a 4-vector (technically, a *contravariant* 4-vector). if they transform in the same way as a coordinate vector, that is, if

$$q^\mu \to q^{\mu'} = \Lambda^{\mu'}{}_\nu \; q^\nu \; . \tag{6.2.3}$$

Conventionally we associate a contravariant 4-vector with the 3-vector sharing the same symbol: $q^\mu = (q^0, \mathbf{q})^\mu$. That is, the 3-vector part $\mathbf{q}$ is (q^1, q^2, q^3).

It is convenient to define the *covariant* version of a contravariant 4-vector by

$$q_\mu = g_{\mu\nu} q^\nu, \tag{6.2.4}$$

where $g_{00} = 1$, $g_{0j} = 0$, $g_{ij} = -\delta_{ij}$. (N.B. Greek indices run from 0 to 3, Latin from 1 to 3.) In other notation, the matrix $g^{\mu\nu}$ equals $\mathrm{diag}(1, -1, -1, -1)$. That is, if $q^\mu = (q^0, \mathbf{q})^\mu$ then the covariant 4-vector is $q_\mu = (q^0, -\mathbf{q})_\mu$. A contravariant vector transforms as

$$q_\mu \to q_{\mu'} = \Lambda_{\mu'}{}^{\nu} \; q_\nu \; . \tag{6.2.5}$$

Note that the derivative with respect to the components of a contravariant vector automatically gives a covariant vector:

$$\partial_\mu \equiv \frac{\partial}{\partial x^\mu} \leftrightarrow \left(\tfrac{1}{c}\partial_t, \boldsymbol{\nabla}\right) . \tag{6.2.6}$$

and vice versa ($\partial^\mu = \frac{\partial}{\partial x_\mu}$).

The covariant–contravariant notation allows us to write the analogue of a scalar product for 3-vectors by

$$q.r \equiv q_\mu r^\mu = q^\mu g_{\mu\nu} r^\nu = q^0 r^0 - \mathbf{q}\cdot\mathbf{r} \tag{6.2.7}$$

Just as rotations leave the scalar product of Euclidean geometry unchanged, Lorentz transformations leave the scalar product of 4-vectors unchanged. This requirement implies that

$$\Lambda^{\mu'}{}_\nu \Lambda_{\mu'}{}^\lambda = g^\lambda_\nu, \tag{6.2.8}$$

which is the matrix $\mathrm{diag}(1, 1, 1, 1)$. (Compare with Eq. (6.1.1).) In particular, the "length" (it may be imaginary) of a 4-vector is a scalar (the same in all reference frames), where the "squared length" is

$$q.q = q^\mu q_\mu = (q^0)^2 - \mathbf{q}\cdot\mathbf{q} \, ; \tag{6.2.9}$$

Equation (6.2.8) is the only restriction that need be placed on the matrix $\Lambda^{\mu'}{}_\nu$ for it to represent a Lorentz transformation, but we will follow the common convention of also assuming that $\det(\Lambda) = 1$, just as for rotation matrices, and also that $\Lambda^0{}_0 > 0$ (this rules out reversing the arrow of time). Equation (6.2.8) gives 10 equations restricting the elements of Λ, so that the number of free elements is 6. These can be determined from a twist vector $\mathbf{w}$ and a boost vector $\mathbf{v}$.

Exercise 6.4 *Verify that the example (6.2.2) satisfies Eq. (6.2.8).*

Proper time τ for an arbitrary path in space-time is the time as measured by a clock following that path. By definition it is a scalar (unchanged by changing frames) and for an infinitesimal path is given by

$$c^2(d\tau)^2 = dx_\mu dx^\mu = c^2dt^2 - |d\mathbf{x}|^2. \tag{6.2.10}$$

(This follows because if the clock is at rest relative to the moving frame, $d\mathbf{x} = \mathbf{0}$ relative to that frame, so $d\tau = dt$.) That is,

$$d\tau = dt\sqrt{1 - |d\mathbf{x}/dt|^2/c^2} = dt/\gamma, \tag{6.2.11}$$

where γ as defined above is the usual time-dilation factor.

The 4-velocity u is then defined by

$$u^\mu = \frac{dx^\mu}{d\tau} = (c\gamma, \mathbf{v}\gamma)\,, \tag{6.2.12}$$

It follows that

$$u.u = u_\mu u^\mu = \frac{dx_\mu}{d\tau}\frac{dx^\mu}{d\tau} = \frac{c^2(d\tau)^2}{(d\tau)^2} = c^2. \tag{6.2.13}$$

The 4-momentum is then defined as

$$p^\mu = mu^\mu = (p_0, \mathbf{p})^\mu, \tag{6.2.14}$$

where m is the *rest mass*. From the definition of u^μ it follows

$$\mathbf{p} = m\mathbf{v}\gamma. \tag{6.2.15}$$

For low velocities $\gamma \approx 1$, so that $\mathbf{p}$ is approximately the Newtonian momentum, and we refer to it as the 3-momentum. Note also that from Eq. (6.2.13), $p.p = m^2c^2$. So far, we don't know what p_0 is, but $p.p = p_0^2 - |\mathbf{p}|^2$, so

$$p_0 = \sqrt{m^2c^2 + |\mathbf{p}|^2} \tag{6.2.16}$$

Expanding this by Taylor series, and writing $E = cp_0$, we have

$$E = mc^2 + \frac{|\mathbf{p}|^2}{2m} + \cdots, \tag{6.2.17}$$

so we identify this as the energy (rest energy plus kinetic energy).

Note that it is also possible to express the energy as

$$E = \mathbf{p}\cdot\mathbf{v} + \gamma^{-1}mc^2, \tag{6.2.18}$$

Problem 6.3 (2 marks) *Verify the approximation Eq. (6.2.17). Also verify the exact expression Eq. (6.2.18) and expand it to get the same approximation.*

6.2.2 Quantizing time?

The striking new feature of relativity is that it replaces Galileian space-time, in which space and time are distinct entities, by Minkowskian space-time, in which they are inextricably linked. In putting quantum mechanics on a relativistic footing it might therefore be thought that we should quantize time, so that $t \to \hat{t}$ in the same way that $\mathbf{x} \to \hat{\mathbf{x}}$. Some further thought shows that this is untenable.

In non-relativistic quantum mechanics, we are not actually quantizing space when we put $\mathbf{x} \to \hat{\mathbf{x}}$. Rather, we are quantizing a property of the system which happens to equal the position of the particle in space. If there are many particles, we must quantize the position of each one individually: $\mathbf{x}_i \to \hat{\mathbf{x}}_i$, but there is still only one time. In relativistic mechanics, whatever frame we happen to be working in, the system state in configuration space is still defined by the position of each of the particles $\mathbf{x}_i$ at a particular time t. It makes no sense to have an operator $\hat{t}_i$ for each particle; what is the average time for a particle? The usual structure of non-relativistic QM is based on a time evolution equation

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle, \tag{6.2.19}$$

for a single time t. The effect of the Minkowskian space-time in relativistic QM is that t depends on one's frame of reference, and hence that the wavefunction will transform differently from in non-relativistic QM.

6.3 The Klein-Gordon Equation

The obvious guess for how to make Schrödinger's equation relativistically invariant is as follows. The Schrödinger equation for a particle in an external potential $V(\mathbf{x})$ with wave function $\psi(\mathbf{x})$,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\,, \tag{6.3.1}$$

can be obtained from the Newtonian equation for total energy,

$$E = \frac{|\mathbf{p}|^2}{2m} + V\,, \tag{6.3.2}$$

by the identification

$$E \to i\hbar\frac{\partial}{\partial t}\,,\ \mathbf{p} \to -i\hbar\boldsymbol{\nabla}\,. \tag{6.3.3}$$

We may make the same identification in the relativistic energy equation (for a free particle)

$$E^2 = m^2c^4 + c^2|\mathbf{p}|^2\,, \tag{6.3.4}$$

to give the *Klein-Gordon equation* for a (scalar) wave function ϕ:

$$(i\hbar\frac{\partial}{\partial t})^2\phi = (i\hbar\nabla)^2c^2\phi + m^2c^4\phi\,. \tag{6.3.5}$$

This can be rearranged as

$$(\partial_\mu \partial^\mu + k_{\rm C}^2)\phi = 0\,, \tag{6.3.6}$$

where $k_{\rm C} = mc/\hbar$ is the *Compton wavenumber*. That is, $k_{\rm C} = 2\pi/\lambda_{\rm C}$, where $\lambda_{\rm C} = h/mc$ is the Compton wavelength.

Exercise 6.5 *Verify that Eq. (6.3.6) and Eq. (6.3.5) are the same.*

This equation was suggested independently by no fewer than 5 authors in 1926 (the same year as Schrödinger published his non-relativistic equation), and Schrödinger himself actually wrote it down in 1925, before switching to the nonrelativistic Schrödinger equation because he could not get sensible answers from it. For no particularly good reason, it has come to be known under the name of two of those authors, Klein and Gordon.

6.3.1 Problems with the Klein-Gordon equation

For the Schrödinger equation we have the probability density

$$\rho(\mathbf{x}, t) = \psi^*(\mathbf{x}, t)\psi(\mathbf{x}, t) \tag{6.3.7}$$

and probability current density

$$\mathbf{j}(\mathbf{x}, t) = -\frac{i\hbar}{2m}(\psi^*(\mathbf{x}, t)\boldsymbol{\nabla}\psi(\mathbf{x}, t) - \psi(\mathbf{x}, t)\boldsymbol{\nabla}\psi^*(\mathbf{x}, t))\,. \tag{6.3.8}$$

In hindsight, the first of these is a fundamental part of quantum mechanics (the probability density to find, at time t, the particle at position $\mathbf{x}$). In 1926 this was not obvious at all. The probability current is such that probability is locally conserved:

$$\frac{\partial}{\partial t}\rho + \boldsymbol{\nabla}\cdot\mathbf{j} = 0. \tag{6.3.9}$$

Problem 6.4 (1.5 marks) *Show that Eq. (6.3.9) is satisfied.*

Defining $j = (c\rho, \mathbf{j})$, the above conservation law has a relativistic form

$$\partial_\mu j^\mu = 0\,. \tag{6.3.10}$$

This can be derived from the Klein-Gordon equation by choosing

$$j^\mu = \frac{i\hbar}{2mc}(\phi^*\partial^\mu\phi - \phi\partial^\mu\phi^*)\,. \tag{6.3.11}$$

However this has

$$\rho = j^0/c = \frac{i\hbar}{2mc^2}(\phi^*\frac{\partial\phi}{\partial t} - \phi\frac{\partial\phi^*}{\partial t})\,, \tag{6.3.12}$$

which does not equal $|\phi|^2$ as it would if ϕ were a wavefunction. In fact, this j^0/c is not even positive definite (i.e. it can be negative).

This problem with the KG equation arise from two (related) fundamental problems The first is that it is second-order in time, and hence is not of the form (6.2.19). The second is that it is an equation for a scalar field $\phi(x)$, that is, $\phi'(x') = \phi(x)$ under all Lorentz transformations. This means that $|\phi(x)|^2$ is also a scalar. But relativistically, the density $|\psi(x)|^2$ of a wavefunction should be the time component of a 4-vector. That is needed so that $\int d^3\mathbf{x}|\psi(x)|^2$ is a scalar (equal to one if the wavefunction is normalized). In a moving frame $d^3\mathbf{x} = dx\,dy\,dz$ shrinks by a factor of γ^{-1} due to Lorentz contraction, so that $|\psi(x)|^2$ must increase by a factor γ, as indeed it would if it were the 0-component of a 4-vector.

Of course, these criticisms do not imply that there is anything wrong with the Klein-Gordon equation *per se*. It is simply that it cannot be interpreted as an evolution equation for the wavefunction of a quantum particle. It is possible in fact to reinterpret $\phi(x)$ as a classical field (which can be quantized just like the electromagnetic field), as we will discuss in Chap. 8. In this case, ρ and $\mathbf{j}$ appear as *charge* density and current, so that negative density is not a difficulty.

6.3.2 A peek at the solution

In the next Chapter we will introduce a relativistic equation for a wavefunction of a quantum particle that does not suffer from the above problems, Dirac's equation. Before proceeding, it may be good for us to have a peek at the end result, as Dirac derived it,

$$(-i\gamma^\nu\partial_\nu + k_{\mathrm{C}})\psi = 0, \tag{6.3.13}$$

where $k_{\mathrm{C}} = mc/\hbar$ as above, and the γ^ν will be explained below. This equation was derived by Dirac in 1928. Unlike the Klein-Gordon equation, Dirac's equation is a work of genius, and nobody else was even close to deriving it at the time that he did.

7 Relativistic Quantum Mechanics: Dirac

7.1 The Dirac Equation: Derivation

7.1.1 First Derivation

Since we require $|\psi(x)|^2$ to be the 0-component of a 4-vector, it is evident that $\psi(x)$ itself must be something like the square root of a 4-vector. In Sec. 6.1.3 we saw that a spinor is something like the square root of a 3-vector, which gives us hope that a relativistic theory based on spinors will work.

Inspired by Eq. (6.1.8), we can rewrite Eq. (6.3.4) as

$$E^2/c^2 - (\boldsymbol{\sigma}\cdot\mathbf{p})^2 = m^2c^2, \tag{7.1.1}$$

which can be factorized as

$$(I_2E/c - \boldsymbol{\sigma}\cdot\mathbf{p})\,(I_2E/c + \boldsymbol{\sigma}\cdot\mathbf{p}) = I_2m^2c^2. \tag{7.1.2}$$

If ξ is the spinor wavefunction for a relativistic electron, it evidently obeys

$$(i\hbar\partial_0 + i\hbar\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\,(i\hbar\partial_0 - i\hbar\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\,\xi = m^2c^2\xi, \tag{7.1.3}$$

which is simply the KG equation for each component.

Now define a new spinor η as

$$mc\eta = (i\hbar\partial_0 - i\hbar\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\,\xi \tag{7.1.4}$$

Then we have

$$mc\xi = (i\hbar\partial_0 + i\hbar\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\,\eta. \tag{7.1.5}$$

We can make these two coupled equations one equation by defining a 4-component wavefunction

$$\psi = \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \xi_1 \\ \xi_2 \\ \eta_1 \\ \eta_2 \end{pmatrix}. \tag{7.1.6}$$

This wavefunction is known as a *bispinor* or *Dirac spinor*. Note that it is *not* a 4-vector. Now if we define a 4-vector of 4×4 matrices

$$\gamma^0 = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix},\ \boldsymbol{\gamma} = \begin{pmatrix} \mathbf{0} & -\boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{pmatrix}. \tag{7.1.7}$$

then Eqs. (7.1.4) and (7.1.5) are equivalent to the single equation,

$$(-i\hbar\gamma^\mu\partial_\mu + mc)\psi(x) = 0. \tag{7.1.8}$$

which is Dirac's equation as already stated in Eq. (6.3.13).

Exercise 7.1 *Show this equivalence.*

7.1.2 Second Derivation (Minkowskian Clifford Algebra)

A quicker, but perhaps less enlightening, path to Dirac's equation is via the Minkowskian Clifford algebra. Recall that non-relativistically the Pauli matrices could be used to define a 3-dimensional Euclidean Clifford Algebra using the symmetrized product

$$\tfrac{1}{2}\{\sigma_i, \sigma_j\} = \delta_{ij}, \tag{7.1.9}$$

where here the curly brackets indicate an anticommutator. The relativistic analogue is a set of four basis matrices γ_μ satisfying

$$\tfrac{1}{2}\{\gamma_\mu, \gamma_\nu\} = g_{\mu\nu}. \tag{7.1.10}$$

In an analogy to the non-relativistic $\boldsymbol{\sigma}\cdot\mathbf{h} = \sum_j \sigma_j h_j$, here we define a "slash" notation (due to Feynman) for a 4-vector

$$\not{A} \equiv \gamma_\mu A^\mu. \tag{7.1.11}$$

Then it follows that for arbitrary 4-vectors that

$$A.B \equiv A_\mu B^\mu = \tfrac{1}{2}\{\not{A}, \not{B}\}, \tag{7.1.12}$$

which is the analogue of the non-relativistic $\mathbf{a}\cdot\mathbf{b} = \frac{1}{2}\{\boldsymbol{\sigma}\cdot\mathbf{a}, \boldsymbol{\sigma}\cdot\mathbf{b}\}$. Note that it is to be understood that the left-hand-side of both of these equations (the Minkowski and the Euclidean) multiplies an identity matrix of the appropriate (see below) dimension.

Exercise 7.2 *Verify that the γ^μ as defined in Eq. (7.1.7) do obey the anticommutation relations Eq. (7.1.10). You can assume Eq. (7.1.9).*

In particular, the relativistic relation between energy and momentum

$$p.p = m^2c^2 \tag{7.1.13}$$

(recall $p.p$ means $p_\mu p^\mu$) can be rewritten as $(\not{p})^2 = I_4 m^2 c^2$. This will be satisfied as an operator equation if every wavefunction satisfies $\not{p}\psi = mc\psi$. Introducing the usual quantum-mechanical relation $p_\mu \to i\hbar\partial_\mu$ makes this constraint

$$(-i\not{\partial} + k_{\mathrm{C}})\psi = 0 \tag{7.1.14}$$

which is Dirac's equation in its most succinct form.

Exercise 7.3 *Verify that $p_\mu \to i\hbar\partial_\mu$ is indeed the usual quantum-mechanical relation for energy and momentum.*

In this derivation, the γ matrices need not be 4×4. However it can be shown that this is the minimum size of any set of matrices which satisfy the Minkowskian Clifford algebra (7.1.10). In the same way, the minimum size of the Pauli matrices (2×2) is set by the Euclidean Clifford algebra.

Discussion 7.1 *What would happen if we lived in a world with two (rather than three) spatial dimensions?*

Even if we choose 4-dimensional matrices, there is no reason that the γ matrices must be the same as those used above (7.1.7). In fact, Dirac's original choice was

$$\gamma^0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \boldsymbol{\gamma} = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & \mathbf{0} \end{pmatrix}, \tag{7.1.15}$$

This is known as the Dirac-Pauli representation, and will be used in all that follows unless otherwise stated. The previous representation is known as the chiral representation, for reasons we will not explore.

Exercise 7.4 *Verify that the γ^μ as defined in Eq. (7.1.15) also obey the anticommutation relations Eq. (7.1.10).*

7.2 The Dirac Equation: Properties

7.2.1 Hamiltonian form

So far we have written the state of a Dirac particle as a bispinor wavefunction $\psi(\mathbf{x}, t)$, but we can also write it as a ket:

$$|\psi(t)\rangle = \int d^3\mathbf{x}\, \psi(\mathbf{x}, t) \otimes |\mathbf{x}\rangle \tag{7.2.1}$$

That is, it is a vector in the Hilbert space which is the usual Hilbert space for a scalar particle, in *tensor product* with the 4-dimensional bispinor Hilbert space. When we write $\psi(x)$ as above and below, $x = (ct, \mathbf{x})$ and $\psi(x) = \langle \mathbf{x}|\psi(t)\rangle$ is still a vector in the 4-dimensional bispinor Hilbert space, and is a function of a the 3-position $\mathbf{x}$ as well as time. Then we can rewrite the Dirac equation as

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle\,, \tag{7.2.2}$$

$$\hat{H} = c\hat{\boldsymbol{\alpha}}\cdot\hat{\mathbf{p}} + \hat{\beta}mc^2\,, \tag{7.2.3}$$

where

$$\hat{\boldsymbol{\alpha}} = \gamma^0\boldsymbol{\gamma} = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{pmatrix}, \tag{7.2.4a}$$

$$\hat{\beta} = \gamma^0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}. \tag{7.2.4b}$$

Exercise 7.5 *Show that this is equivalent to Eq. (7.1.14).*

Compare Eq. (7.2.2) to that other expression (6.2.18) for the relativistic energy

$$E = \mathbf{v}\cdot\mathbf{p} + \gamma(\mathbf{v})^{-1}mc^2, \tag{7.2.5}$$

where $\gamma(\mathbf{v})^{-1} = \sqrt{1 - |\mathbf{v}|^2/c^2}$ as usual. This suggests that we may expect $c\hat{\boldsymbol{\alpha}}$ to play a role analogous to the velocity, and $\hat{\beta}$ to γ^{-1}. Although the former analogue works well, $\hat{\beta}$ just as often takes on the role of γ, since $\hat{\beta}^2 = 1$.

7.2.2 Probability density

Consider now the probability density

$$\rho(x) = \psi^\dagger(x)\psi(x) \equiv |\psi_1(x)|^2 + |\psi_2(x)|^2 + |\psi_3(x)|^2 + |\psi_4(x)|^2 \,. \quad (7.2.6)$$

Note that this does not denote a mixed state as in Chap. 2. It is just a non-neagative real-valued function of position and time. One might think that this is all that is required, but that is not so. If we have succeeded in deriving a true relativistic version of Schrödinger's equation, then ρ should transform in the way a probability density should transform, relativistically, as discussed in Sec. 6.3.1. We will not show this explicitly, but we will discuss how it would be shown in the next section. Meanwhile, we also have to show that probability is conserved locally.

Exercise 7.6 Carefully *considering*

$$i\hbar\frac{\partial\psi}{\partial t} = (c\hat{\boldsymbol{\alpha}}\cdot\hat{\mathbf{p}} + \hat{\beta}mc^2)\psi$$

and the Hermitian adjoint of this equation, show that

$$i\hbar\frac{\partial\rho}{\partial t} = i\hbar\left(\frac{\partial\psi^\dagger}{\partial t}\psi + \psi^\dagger\frac{\partial\psi}{\partial t}\right) \quad (7.2.7)$$

$$= -i\hbar c\left[(\boldsymbol{\nabla}\psi)^\dagger\cdot\hat{\boldsymbol{\alpha}}^\dagger\psi + \psi^\dagger\hat{\boldsymbol{\alpha}}\cdot\boldsymbol{\nabla}\psi\right] . \quad (7.2.8)$$

Since $\hat{\boldsymbol{\alpha}} = \hat{\boldsymbol{\alpha}}^\dagger$, we can write this as a continuity equation

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{j} = 0\,, \quad (7.2.9)$$

by defining the probability current to be

$$\mathbf{j} = c\psi^\dagger\hat{\boldsymbol{\alpha}}\psi\,, \quad (7.2.10)$$

as expected if $c\hat{\boldsymbol{\alpha}}$ is the velocity. So, assuming that the 4-current j^μ correctly transforms as a 4-vector (see below) we *can* take Eq. (7.2.6) as defining a probability density. The probability current 4-vector $j = (c\rho, \mathbf{j})$ is then

$$j^\mu = \psi^\dagger(c, c\hat{\boldsymbol{\alpha}})^\mu\psi = c\psi^\dagger\gamma^0\gamma^\mu\psi\,. \quad (7.2.11)$$

7.2.3 NON-EXAMINABLE Lorentz Transformation

Recall that under a rotation by a twist vector $\mathbf{w}$, an ordinary (two-component) spinor translates according to

$$\xi' = \exp(-i\tfrac{1}{2}\mathbf{w}\cdot\boldsymbol{\sigma})\xi, \quad (7.2.12)$$

which is actually a completely general unitary transformation on a spinor (apart from a missing global phase factor). Now a Lorentz transformation has 6 parameters ($\mathbf{v}$ and $\mathbf{w}$), which is another way of seeing why we

need two spinors in the relativistic case. The Lorentz transformation of the bispinor is most easily expressed using the chiral representation of Sec. 7.1.1. It is:

$$\begin{pmatrix} \xi' \\ \eta' \end{pmatrix} = S(\mathbf{w}, \boldsymbol{\zeta}) \begin{pmatrix} \xi \\ \eta \end{pmatrix}, \tag{7.2.13}$$

where

$$S(\mathbf{w}, \boldsymbol{\zeta}) = \begin{pmatrix} \exp[-i\frac{1}{2}(\mathbf{w} + i\boldsymbol{\zeta})\cdot\boldsymbol{\sigma}] & 0 \\ 0 & \exp[-i\frac{1}{2}(\mathbf{w} - i\boldsymbol{\zeta})\cdot\boldsymbol{\sigma}] \end{pmatrix}. \tag{7.2.14}$$

Here $\boldsymbol{\zeta}$ is called the *rapidity* and is related to the boost velocity $\mathbf{v}$ by

$$\zeta_i = \operatorname{artanh}(v_i/c) = \tfrac{1}{2}\log\left(\frac{c+v_i}{c-v_i}\right). \tag{7.2.15}$$

One can actually derive Eq. (7.2.14) from basic properties of the Lorentz group, and moreover one can then use this transformation equation to derive Dirac's equation itself. But we will not go into those details. Note that in the case of no boost, the transformation above is the usual spinor rotation applied to both spinors in the Dirac bispinor. This is the same in any bispinorial representation of the Dirac equation. The general expression is

$$S(\mathbf{w}, \boldsymbol{\zeta}) = \exp(-\tfrac{1}{2} i\omega_{\mu\nu}\eta^{\mu\nu}) \tag{7.2.16}$$

where, the parameters are encoded in an antisymmetric tensor $\omega_{\mu\nu}$ according to $\omega_{ij} = \epsilon_{ijk}w_k$ and $-\omega^{0i} = \omega_{0i} = \zeta_i$, and the 6 independent "generators" $\eta^{\mu\nu}$ are each a 4x4 operator in bispinor space

$$\eta^{\mu\nu} = \frac{i}{4}[\gamma^\nu, \gamma^\mu], \tag{7.2.17}$$

so that S is also such an operator, as required.

Note also that it can be shown that under the general transformation (7.2.16), the 4-current j^μ correctly transforms as a 4-vector:

$$j^{\mu'} = \Lambda(\boldsymbol{\zeta}, \mathbf{w})^{\mu'}{}_\nu j^\nu. \tag{7.2.18}$$

Here $\Lambda(\boldsymbol{\zeta}, \mathbf{w})$ is the Lorentz transformation matrix parametrized by the twist vector $\mathbf{w}$ and the rapidity vector $\boldsymbol{\zeta}$. To be specific,

$$\Lambda(\boldsymbol{\zeta}, \mathbf{w}) = \exp(-\tfrac{1}{2} i\omega_{\mu\nu}\Upsilon^{\mu\nu}). \tag{7.2.19}$$

Here $\omega_{\mu\nu}$ is as above, while the 6 independent "generators" $\Upsilon_{\mu\nu}$ are each a rank-2 tensor

$$[\Upsilon_{\mu\nu}]^\alpha{}_\beta = i(g^\alpha_\mu g_{\nu\beta} - g_{\mu\beta}g^\alpha_\nu). \tag{7.2.20}$$

so that Λ ends up being a rank-2 tensor as required.

We can now exhibit the relativistic generalisation of Eq. (6.1.18), reproduced here but written explicitly with the 3-space indices:

$$[R_\mathbf{w}]^j{}_k\, \sigma^k = S_\mathbf{w}\, \sigma^j\, S^\dagger_\mathbf{w} \tag{7.2.21}$$

The generalisation is:

$$[\Lambda_{(\boldsymbol{\zeta},\mathbf{w})}]^\mu{}_\nu \gamma^\nu = S_{(\mathbf{w},\boldsymbol{\zeta})}\, \gamma^\mu\, S^\dagger_{(\mathbf{w},\boldsymbol{\zeta})}. \tag{7.2.22}$$

Due to its complexity we will not show this explicitly.

7.2.4 Motion of a free Dirac particle

Working now in the Heisenberg picture, and using the Dirac Hamiltonian Eq. (7.2.3), the velocity of the electron is

$$\hat{\mathbf{v}} = \frac{d\hat{\mathbf{r}}}{dt} = \frac{-i}{\hbar}[\hat{\mathbf{r}}, \hat{H}] = c\hat{\boldsymbol{\alpha}}, \tag{7.2.23}$$

as expected from previous results. Note that components of $\hat{\boldsymbol{\alpha}} = \{\hat{\alpha}_1, \hat{\alpha}_2, \hat{\alpha}_3\}$ do not commute with one another, and that each has eigenvalues ± 1.

Problem 7.1 (2 marks) *Verify the statements in the preceding sentence.*

This means that the velocity can be perfectly measured only in one direction at a time, and that the result of such a perfect measurement would be the speed of light! In practice one cannot measure velocity instantaneously, and it is usually inferred from a time-of-flight measurement, involving a (necessarily imperfect) initial position measurement and a final position measurement, as

$$\hat{\mathbf{v}}_{\text{inferred}}(t_\text{i}) = \frac{\hat{\mathbf{r}}_\text{f} - \hat{\mathbf{r}}_i}{t_\text{f} - t_\text{i}}. \tag{7.2.24}$$

It can be shown that for a sufficiently imperfect initial position measurement,

$$\lim_{t_\text{f}\to\infty} \hat{\mathbf{v}}_{\text{inferred}}(t_\text{i}) = \frac{c^2\hat{\mathbf{p}}(t_i)}{\hat{H}(t_i)}. \tag{7.2.25}$$

This is as expected for a classical relativistic particle, and can take values from 0 to c in any direction.

Exercise 7.7 *Show that this is indeed what is expected classically.*

Discussion 7.2 *Why must the first position measurement be imperfect?*

7.3 The Dirac Equation: Solutions

7.3.1 Momentum eigenstates

We start from the Hamiltonian form of the Dirac equation:

$$i\hbar\frac{\partial\psi}{\partial t}(x) = [c\hat{\boldsymbol{\alpha}}\cdot(-i\hbar\boldsymbol{\nabla}) + \hat{\beta}mc^2]\psi(x)\,. \tag{7.3.1}$$

Dirac originally suggested this equation for a free electron, so we expect to be able to find plane wave solutions, corresponding to a well-defined momentum $\mathbf{p}$:

$$\psi(x) = \exp\left(\frac{-ip.x}{\hbar}\right)u(\mathbf{p})\,, \tag{7.3.2}$$

where recall that $p.x$ is another notation for $p^\mu x_\mu$, which equals $Et - \mathbf{p}\cdot\mathbf{x}$, while $u(\mathbf{p})$ is a bispinor that is independent of space and time. If we substitute this in as a trial solution, we get

$$Eu(\mathbf{p}) = (c\hat{\boldsymbol{\alpha}}\cdot\mathbf{p} + \hat{\beta}mc^2)u(\mathbf{p})\,. \tag{7.3.3}$$

It is now an algebraic problem to find possible forms of $u(\mathbf{p})$. We can exploit the block form of the Dirac-Pauli representation of $\hat{\boldsymbol{\alpha}}$ and $\hat{\beta}$ by introducing the two-component (non-relativistic) spinors $\chi_{\rm A}$ and $\chi_{\rm B}$:

$$u(\mathbf{p}) = \begin{pmatrix} \chi_{\rm A}(\mathbf{p}) \\ \chi_{\rm B}(\mathbf{p}) \end{pmatrix} . \tag{7.3.4}$$

Now the Dirac equation in terms of $\chi_{\rm A}, \chi_{\rm B}$ is

$$\left\{ E - c \begin{pmatrix} 0 & \boldsymbol{\sigma}\cdot\mathbf{p} \\ \boldsymbol{\sigma}\cdot\mathbf{p} & 0 \end{pmatrix} - \begin{pmatrix} mc^2 & 0 \\ 0 & -mc^2 \end{pmatrix} \right\} \begin{pmatrix} \chi_{\rm A} \\ \chi_{\rm B} \end{pmatrix} = 0 , \tag{7.3.5}$$

or, rearranging,

$$(E - mc^2)\chi_{\rm A} = c\boldsymbol{\sigma}\cdot\mathbf{p}\chi_{\rm B} \tag{7.3.6a}$$
$$(E + mc^2)\chi_{\rm B} = c\boldsymbol{\sigma}\cdot\mathbf{p}\chi_{\rm A} . \tag{7.3.6b}$$

Exercise 7.8 *Show that for these two equations to be consistent, the usual relativistic energy-momentum relation $E^2 = c^2|\mathbf{p}|^2 + m^2c^4$ must hold. (This is just the reverse of how we derived the Dirac equation in the first place.)*

Note that for each value of $\mathbf{p}$, negative energies as well as positive energies are still allowed: $E = \pm\sqrt{c^2|\mathbf{p}|^2 + m^2c^4}$. In fact, these occur twice each (4 eigenvalues for a 4×4 matrix). Thus we can roughly understand why the Dirac particle is described by a *bi*spinor as being because there is an extra binary variable (not present classically) saying whether the particle has positive energy or negative energy. Negative energies could also exist classically, but do not pose a problem as classical energy must vary continuously, so an electron starting with $E > mc^2$ could never reach a negative energy state. Quantum mechanics, however, allows particles to jump from one state to another, so an electron in a positive energy state may make a transition to a negative energy one, despite the intervening band of impossible energies ($-mc^2 < E < +mc^2$).

7.3.2 Particles and Holes

It might be thought that the existence of negative energy states is a problem with the Dirac theory. From Eq. (7.2.25), a negative energy (or *anomalous*) electron would move in the opposite direction to its momentum, which has never been observed. Also, since there is no lower limit to the negative energies, the system would be unstable as electrons could keep losing energy, while going faster and faster in the "wrong" direction.

In fact, the anomalous states are one of the triumphs of the Dirac theory. Dirac realized that these problems would be solved if one assumed that the universe were full of electrons in the anomalous states. For a finite normalization volume L^3 the number of anomalous states is infinite but countable, so it is possible to imagine them all being filled. The infinite negative charge and negative energy resulting from this "Dirac

sea" would not be observable because it is equally spread everyhwere in space. Of course creating this sea would not be possible if electrons were bosons (as bosons can never "fill" an energy level), and we can also view this as a proof of why electrons (and other fundamental particles) must be fermions. Any extra electrons would be forced into the usual positive energy states and would appear as usual electrons. Any *holes* (i.e. missing electrons) in the anomalous states would appear as missing negative energy, missing negative momentum (that is, in the opposite direction to the velocity), and missing negative charge. That is, it would appear as a electron with positive energy, positive momentum (in the same direction as the velocity) and *positive* charge. In other words, it would be an *anti-electron* or *positron*. See Fig. 7.1 and the table below.

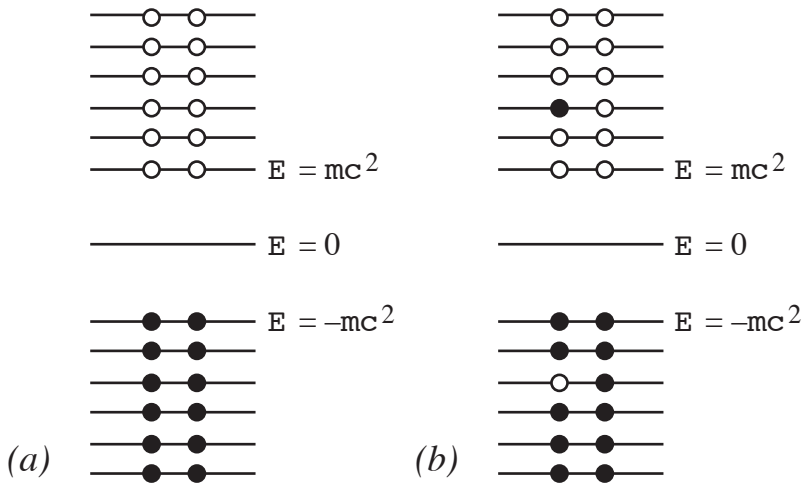


Figure 7.1: The Dirac sea of anomalous electrons *(a)* in the ground state and *(b)* after the creation of one electron-positron pair.

Table 2: Antiparticles are holes in the Dirac sea.

Particle	Velocity	Momentum	Energy	Charge
electron (e)	$\longrightarrow$	$m\gamma\times\longrightarrow$	$> mc^2$	$-e$
anomalous electron (æ)	$\longrightarrow$	$m\gamma\times\longleftarrow$	$< -mc^2$	$-e$
positron (missing æ)	$\longrightarrow$	$m\gamma\times\longrightarrow$	$> mc^2$	$+e$

If an anomalous electron is given enough energy to turn it into an ordinary electron, this creates a hole (a positron) and an ordinary electron. This is the phenomenon of pair creation. The amount of energy required is at least $2mc^2$ (the energy gap). This is exactly as expected for creating two particles each with rest mass m.

The prediction of antiparticles by Dirac in 1930 was one of the many triumphs of his equation, and positrons were first observed in 1932. This explanation of antiparticles relies on the exclusion principle, and so implies that electrons must be fermions. More generally, it requires that

all fundamental particles (being spin half) must be fermions. This is part of the proof of the spin-statistics theorem, which will be discussed in greater detail in the next chapter.

7.3.3 Non-relativistic behaviour

The occupation of the negative energy states does not affect low-energy electron dynamics, again because of the exclusion principle — the electron cannot make a transition to a full state. For $|\mathbf{p}| \ll E/c$ with $E > 0$ we can take

$$\frac{c|\mathbf{p}|}{E + mc^2} \ll 1 \tag{7.3.7}$$

$$E \approx mc^2 \,. \tag{7.3.8}$$

Then from Eqs. (7.3.6a) and (7.3.6b), χ_{B} will be much smaller than χ_{A}. Thus in this limit, we can ignore χ_{B} and use only χ_{A}. This simple non-relativistic limit is the principal attraction of the standard Dirac-Pauli representation. It is obviously consistent with the standard non-relativistic description of electrons using spinors (i.e. not a bispinor). We will derive the non-relativistic equation for χ_{A} after we have included the coupling to the electromagnetic field, in the next chapter.

8 Relativistic QED and the Standard Model

8.1 Dirac's Relativistic QED

8.1.1 The minimal coupling

Recall that the minimal coupling Hamiltonian arises from the replacement

$$H = H_0(\mathbf{v}) + q\phi(\mathbf{r}), \tag{8.1.1}$$
$$\mathbf{p} = \mathbf{p}_0(\mathbf{v}) + q\mathbf{A}(\mathbf{r}). \tag{8.1.2}$$

In the relativistic case, these are combined in the 4-vector transformation

$$p^\mu = p_0^\mu + qA^\mu, \tag{8.1.3}$$

where $A^\mu = (\phi/c, \mathbf{A})$ is the 4-vector potential. The Dirac equation for an electron (with charge $q = -e$) coupled to a field is thus

$$[-i\partial\!\!\!/ + (-e/\hbar)A\!\!\!/(x) + \lambda\!\!\!^{-}_{\mathrm{C}}{}^{-1}]\psi(x) = 0 \tag{8.1.4}$$

In the Hamiltonian formulation, the Dirac Hamiltonian changes into

$$\hat{H} = \hat{H}_{\mathrm{el}} + \hat{H}_{\mathrm{I}} \tag{8.1.5}$$

where $\hat{H}_{\mathrm{el}} = c\hat{\boldsymbol{\alpha}}\cdot\hat{\mathbf{p}} + \hat{\beta}mc^2$ and

$$\hat{H}_{\mathrm{I}} = -e\hat{\phi}(\hat{\mathbf{r}}) + ec\hat{\boldsymbol{\alpha}}\cdot\hat{\mathbf{A}}(\hat{\mathbf{r}}). \tag{8.1.6}$$

Here we have included a quantized field. In contrast to the nonrelativistic expression in Eq. (4.4.1), there are just two terms in $\hat{H}_{\mathrm{I}}$. The first does not involve photons, while the other involves the annihilation or creation of a single photon. Once again the electron is not created or destroyed, but may change state. However, in Dirac theory an electron can change state from positive to negative energy states (or vice versa) via the electromagnetic field. This is observable as the annihilation (or creation) of electron-positron pairs.

Discussion 8.1 *How do you think the two-photon $\hat{H}_{I,2}$ in the nonrelativistic case arises if fundamentally there is only $\hat{H}_{I,1}$ involving photons? Draw some diagrams.*

8.1.2 The Dyson Series

Consider a system of charged particles (labelled by l) interacting with the electromagnetic field. The total Hamiltonian is

$$\hat{H} = \hat{H}_0 + \hat{V}, \tag{8.1.7}$$

where $\hat{H}_0$ is the total "free Hamiltonian":

$$\hat{H}_0 = \sum_l \left[c\hat{\boldsymbol{\alpha}}_l\cdot\hat{\mathbf{p}}_l + \hat{\beta}_l m_l c^2\right] + \int \frac{\epsilon_0}{2}\left(|\hat{\mathbf{E}}^\perp(\boldsymbol{x})|^2 + c^2|\hat{\mathbf{B}}(\boldsymbol{x})|^2\right)\mathrm{d}^3\boldsymbol{x} \tag{8.1.8}$$

and $\hat{V}$ is the total "interaction Hamiltonian",

$$\hat{V} = \frac{1}{4\pi\epsilon_0}\frac{1}{2}\sum_{l \neq l'} \frac{q_l q_{l'}}{|\hat{\mathbf{r}}_l - \hat{\mathbf{r}}_{l'}|} + \sum_l q_l c\hat{\boldsymbol{\alpha}}_l \cdot \hat{\mathbf{A}}(\hat{\mathbf{r}}_l). \tag{8.1.9}$$

The free Hamiltonian is easy to deal with — it describes particles that propagate with constant momentum (we showed this in Sec. 7.3.1) and a collection of Harmonic oscillators for the field (we showed this in Sec. 1.3.3). That is to say, the unitary evolution

$$\hat{U}_0(t,0) \equiv \exp(-i\hat{H}_0 t/\hbar) \tag{8.1.10}$$

is easy to apply to any initial state. By contrast the interaction Hamiltonian is very difficult to deal with, as it describes electrons interacting with eachother, or interacting with photons in the field. For this reason it is very difficult to work out the action of the full unitary evolution

$$\hat{U}(t,0) \equiv \exp[-i(\hat{H}_0 + \hat{V})t/\hbar]. \tag{8.1.11}$$

It is however possible to develop an approximation to $\hat{U}(t,0)$ that can be applied. First note that for *any* operators $\hat{H}_0$ and $\hat{V}$,

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,0) = [\hat{H}_0 + \hat{V}]\hat{U}(t,0) \tag{8.1.12}$$

$$i\hbar\frac{\partial}{\partial t}\hat{U}_0(t,0) = \hat{H}_0\hat{U}_0(t,0), \tag{8.1.13}$$

and (taking the Hermitian adjoint of the last equation)

$$-i\hbar\frac{\partial}{\partial t}\hat{U}_0^\dagger(t,0) = \hat{U}_0^\dagger(t,0)\hat{H}_0 \tag{8.1.14}$$

Now consider the following unitary operator:

$$\hat{u}(t,0) \equiv \hat{U}_0^{-1}(t,0)\hat{U}(t,0) = \hat{U}_0^\dagger(t,0)\hat{U}(t,0), \tag{8.1.15}$$

so that $\hat{U}(t,0) = \hat{U}_0(t,0)\hat{u}(t,0)$. This obeys the following differential equation:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{u}(t,0) &= \left(i\hbar\frac{\partial}{\partial t}\hat{U}_0^\dagger(t,0)\right)\hat{U}(t,0) + \hat{U}_0^\dagger(t,0)\left(i\hbar\frac{\partial}{\partial t}\hat{U}(t,0)\right) \\ &= -\hat{U}_0^\dagger(t,0)\hat{H}_0\hat{U}(t,0) + \hat{U}_0^\dagger(t,0)(\hat{H}_0 + \hat{V})\hat{U}(t,0) \\ &= \hat{U}_0^\dagger(t,0)\hat{V}\hat{U}_0(t,0)\hat{u}(t,0). \end{aligned} \tag{8.1.16}$$

That is to say, $\hat{u}(t,0)$ is a unitary evolution operator that would result from a *time-dependent* Hamiltonian

$$\hat{v}(t) = \hat{U}_0^\dagger(t,0)\hat{V}\hat{U}_0(t,0). \tag{8.1.17}$$

Now we know from Sec. 1.2 that the unitary operator resulting from a time-dependent Hamiltonian is

$$\hat{u}(t,0) = I + \sum_{n=1}^{\infty}(i\hbar)^{-n}\int_0^t ds_n \hat{v}(s_n)\int_0^{s_n} ds_{n-1}\hat{v}(s_{n-1})\cdots\int_0^{s_2} ds_1\hat{v}(s_1). \tag{8.1.18}$$

Expanding this out and substituting in Eq. (8.1.17), we have the full evolution

$$\begin{aligned}\hat{U}(t,0) &= \hat{U}_0(t,0) \\ &+ (i\hbar)^{-1}\int_0^t ds_1 \hat{U}_0(t,s_1)\hat{V}\hat{U}_0(s_1,0) \\ &+ (i\hbar)^{-2}\int_0^t ds_2 \int_0^{s_2} ds_1 \hat{U}_0(t,s_2)\hat{V}\hat{U}_0(s_2,s_1)\hat{V}\hat{U}_0(s_1,0) \\ &+ (i\hbar)^{-3}\int_0^t ds_3 \int_0^{s_3} ds_2 \int_0^{s_2} ds_1 \hat{U}_0(t,s_3)\hat{V}\hat{U}_0(s_3,s_2)\hat{V}\hat{U}_0(s_2,s_1)\hat{V}\hat{U}_0(s_1,0) \\ &+ \cdots. \end{aligned} \tag{8.1.19}$$

Problem 8.1 (1 mark) *Show this.*

This is known as a *Dyson expansion* after the work of British physicist Freeman Dyson in the 1940s. The zeroth-order term is where the electrons and photons don't interact. The first order term is where they freely evolve up to time s_1, then interact, then freely evolve from time s_1 to t, and we have to integrate over all possible interaction times s_1. You can tell the story for the higher-order terms.

8.1.3 Feynman Diagrams

There is one-to-one relation between terms in the Dyson exansion, and Feynman diagrams, named after the simultaneous work of American physicist Richard Feynman. In these diagrams, free evolution corresponds to lines (wiggly for photons and straight for electrons), while interactions correspond to vertices. The minimal coupling Hamiltonian gives "three-line vertices", two straight and one wiggly.[8] Thus as well as giving a picture of quantum interactions, Feynman diagrams are actually a tool for figuring out what the relevant terms in the Dyson expansion are. A Feynman diagram with n vertices is a contribution to the nth order term in the Dyson expansion. Fermi's golden rule comes out from using just the first order term in the Dyson expansion.

Exercise 8.1 *Draw all Feynman diagrams of nth order for $n = 0, 1,$ and 2.*

Exercise 8.2 *Which of these Feynman diagrams corresponding to Thomson scattering? (Note that there are two, unlike the non-relativistic case where there is one first-order diagram.)*

You might wonder how to include antiparticles in Feynman diagrams, since the description in terms of a hole in the Dirac sea would require drawing in all the infinite number of lines for anomalous electrons in the sea, which is obviously not practical. It turns out there is a much simpler

[8] Because of the gauge we are working in there are direct electron-electron "four-line" vertices from the Coulomb Hamiltonian. In other gauges these sorts of vertices don't occur, but there are other complications.

way: we put arrows indicating direction on the lines for electrons. An arrow oriented up the page (in the positive time direction) corresponds to an electron e, while one pointing down corresponds to a positron $\bar{\text{e}}$. Apart from this, the rules are exactly the same — there is only one type of vertex, where one wiggly line and two straight lines meet, but their orientation and (for the electron lines) time-orientation are arbitrary.

Exercise 8.3 *Using these conventions, draw the first-order Feynman diagram for pair creation, where a photon "turns into" an electron plus a positron.*

Note that second- and higher-order Feynman diagrams can include *loops*. The lines (straight or wiggly) which appear only inside a loop are interpreted in terms of *virtual particles*, as opposed to the the "real" particles (photons included here) which enter and exit the "interaction region". Feynman actually took seriously the idea that a positron is an electron travelling backwards in time, and even suggested that there was only one electron in the universe, which travelled around, forwards and backwards in time, simulating all the electrons and positrons we see. Most physicists think this is a silly idea.

8.2 The nonrelativistic limit

For simplicity, we will now treat the field classically (which just means dropping the hats on the field). Then the two-component equations for fixed energy E, Eq. (7.3.6), become

$$\begin{aligned}(E+e\phi-mc^2)\chi_{\text{A}} &= c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}}+e\mathbf{A})\chi_{\text{B}} &\text{(8.2.1a)}\\ (E+e\phi+mc^2)\chi_{\text{B}} &= c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}}+e\mathbf{A})\chi_{\text{A}}\,. &\text{(8.2.1b)}\end{aligned}$$

In the non-relativistic regime $\chi_{\text{A}} \gg \chi_{\text{B}}$, so we aim for an equation for χ_{A} only.

$$\begin{aligned}&(E+e\phi+mc^2)(E+e\phi-mc^2)\chi_{\text{A}}\\ &\quad= (E+e\phi+mc^2)c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}}+e\mathbf{A})\chi_{\text{B}}\\ &\quad= c\left(\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}}+e\mathbf{A})(E+e\phi+mc^2)+[e\phi,c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}]\right)\chi_{\text{B}}\\ &\quad\approx c^2\left(\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}}+e\mathbf{A})\right)^2\chi_{\text{A}}\,, &\text{(8.2.2)}\end{aligned}$$

where the last line follows if we neglect the commutator (see discussion below).

Discussion 8.2 *Why is* $[e\phi, c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}]$ *non-zero in general?*

From the properties of the Pauli matrices (6.1.8),

$$\begin{aligned}&\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}}+e\mathbf{A})\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}}+e\mathbf{A})\\ &\quad= |(\hat{\mathbf{p}}+e\mathbf{A})|^2+i\boldsymbol{\sigma}\cdot[(\hat{\mathbf{p}}+e\mathbf{A})\times(\hat{\mathbf{p}}+e\mathbf{A})]\\ &\quad= |(\hat{\mathbf{p}}+e\mathbf{A})|^2+i\boldsymbol{\sigma}\cdot[(\hat{\mathbf{p}}\times e\mathbf{A}(\hat{\mathbf{r}}))+(e\mathbf{A}(\hat{\mathbf{r}})\times\hat{\mathbf{p}})]\\ &\quad= |(\hat{\mathbf{p}}+e\mathbf{A})|^2+\hbar\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}\times e\mathbf{A}(\hat{\mathbf{r}}))\\ &\quad= |(\hat{\mathbf{p}}+e\mathbf{A})|^2+\hbar e\boldsymbol{\sigma}\cdot\mathbf{B}\,. &\text{(8.2.3)}\end{aligned}$$

We can write $E = mc^2 - e\phi + E_{\rm K}$, and for the non-relativistic regime in which $E_{\rm K} \ll mc^2$ we then have

$$(E + e\phi + mc^2)(E + e\phi - mc^2) \approx 2E_{\rm K}mc^2 \,, \tag{8.2.4}$$

and hence

$$E_{\rm K}\chi_{\rm A} \approx \left(\frac{1}{2m}|(\hat{\mathbf{p}} + e\mathbf{A})|^2 + \frac{\hbar e}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}\right)\chi_{\rm A} \,. \tag{8.2.5}$$

Finally, introducing the total non-relativistic energy $\Delta E = E - mc^2 = E_K - e\phi$, we have

$$\Delta E\chi_{\rm A} \approx \left(\frac{1}{2m}|(\hat{\mathbf{p}} + e\mathbf{A})|^2 - e\phi + \frac{\hbar e}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}\right)\chi_{\rm A} \,. \tag{8.2.6}$$

The term we neglected to obtain Eq. (8.2.2) is of relative size $e\phi'\lambda_{\rm C}/mc^2$, the change in the potential energy of the electron across the Compton wavelength of the electron compared to its rest energy.

Problem 8.2 (1 mark) *Evaluate $\lambda_{\rm C}$, and compare it to the Borh radius, and to the "classical electron radius" r_0. How large a voltage (give the answer in Volts!) would invalidate the approximation used to obtain Eq. (8.2.2)?*

Since $\lambda_{\rm C}$ is so small, this potential energy change is typically much smaller than the rest mass energy. If it is not, then this whole approach fails; physically, such strong fields lead to pair creation.

Equation (8.2.6) is just the time-independent Schrödinger equation for a non-relativistic charged particle in an electromagnetic field, plus the $-\boldsymbol{\mu}\cdot\mathbf{B}$ term for a magnetic moment, with

$$\boldsymbol{\mu} = \frac{-e\hbar}{2m}\boldsymbol{\sigma} \,. \tag{8.2.7}$$

In terms of the electron spin,

$$\boldsymbol{\mu} = \frac{-e}{m}\mathbf{S} \,. \tag{8.2.8}$$

Now, for a classical charged particle in a closed orbit of angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, the effective magnetic moment would be

$$\boldsymbol{\mu}_{\rm classical} = \frac{q}{2m}\mathbf{L} \tag{8.2.9}$$

Aside 8.1 *To see this, consider a constant magnetic field. First we show that we can write $\mathbf{A} = -\frac{1}{2}\mathbf{r} \times \mathbf{B}$. Remembering that $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$:*

$$\begin{aligned}
\boldsymbol{\nabla} \times \mathbf{A} &= -\frac{1}{2}\epsilon_{jkl}\mathbf{e}_j\frac{\partial}{\partial r_k}\epsilon_{lmn}r_m B_n \;=\; -\frac{1}{2}\mathbf{e}_j B_n \epsilon_{jkl}\epsilon_{lmn}\frac{\partial}{\partial r_k}r_m \\
&= -\frac{1}{2}\mathbf{e}_j B_n \epsilon_{jkl}\epsilon_{lmn}\delta_{km} \;=\; +\frac{1}{2}\mathbf{e}_j B_n \epsilon_{jkl}\epsilon_{nkl} \\
&= +\frac{1}{2}\mathbf{e}_j B_n 2\delta_{kl} \;=\; \mathbf{B}
\end{aligned} \tag{8.2.10}$$

Next, we consider a perturbatively small $\mathbf{B}$ *and the energy shift it produces. Recall from Eq. (4.1.5) that the minimal coupling Hamiltonian produces (for a classical particle) is*

$$H_{\rm I} = q\left[\frac{1}{m}\left(-\mathbf{p}\cdot\mathbf{A}(\mathbf{r}) + q|\mathbf{A}(\mathbf{r})|^2\right) + \phi(\mathbf{r})\right]. \tag{8.2.11}$$

We are not concerned with $\phi(\mathbf{r})$*, and in the perturbative approach we can discard the term which is second-order in* $\mathbf{B}$*. Using* $\mathbf{A} = -\frac{1}{2}\mathbf{r}\times\mathbf{B}$ *gives*

$$H_{\rm I} = +\frac{q}{2m}\mathbf{p}\cdot(\mathbf{r}\times\mathbf{B}) = -\frac{q}{2m}\mathbf{B}\cdot(\mathbf{r}\times\mathbf{p}) = -\boldsymbol{\mu}_{\rm classical}\cdot\mathbf{B}, \tag{8.2.12}$$

where we have used the properties of the triple product.

So quantum spin angular momentum gives a contribution to the magnetic moment twice as large as the same amount of orbital angular momentum. This is another triumph of Dirac's equation, as the so-called anomalous g factor of the electron was a mystery at the time (1928). The extra factor of 2 is sometimes called the Landé g-factor. (The full theory of QED predicts small corrections to this, beginning with a term of $O(\alpha)$; the corrections have been experimentally confirmed to more than 13 decimal places, making the g-factor of the electron one of the most precisely predicted of all physical quantities.)

8.3 NON-EXAMINABLE Fundamental Particles

We have argued above that the only good relativistic wavefunction is the Dirac bispinor. This means that all fundamental particles should, like electrons,

1. be spin-half particles
2. be Fermions
3. have antiparticles of opposite charge
4. have a magnetic moment of (approximately) $2\times(\hbar/2)(q/2m)$, where q is the charge and m the mass.

Electrons and neutrinos (which are neutral) certainly obey these rules. What about the heavier constituents of matter? Protons and neutrons both obey all of the above rules, except for the last. The magnetic moment of a proton is about $2.8\times e/4m_p$, while that of a neutron (which should be zero since it is neutral) is about $-1.9\times e/4m_n$. This suggests that protons and neutrons are not fundamental particles.

From the accumulated evidence of many experiments it became generally accepted in the early 1970s that nucleons (protons and neutrons) are compound particles made up of quarks. For example, deep (very high energy) inelastic scattering of electrons off protons are consistent with the presence of point-like particles inside the proton. As far as anyone knows, quarks (named by Murray Gell-Mann) are fundamental particles like electrons and neutrinos. Two sorts of quarks are needed to

explain protons and neutrons, up quarks u (with charge $+\frac{2}{3}e$) and down quarks d (with charge $-\frac{1}{3}e$). A proton is the compound particle uud and the neutron the compound particle ddu. The orbital motion of quarks within a nucleon explains why the magnetic moment of nucleons is not simply related to their charge and spin. One of the recent triumphs of the quark model is the calculation of these magnetic moments to good agreement with experiment.

Like electrons and neutrinos, quarks have antiquarks represented as $\bar{\mathrm{u}}, \bar{\mathrm{d}}$. In addition to electrical charge, quarks have another sort of charge, called *colour charge*. This charge has three values, called r, g, b for red, green, blue. These are so-called because a mixture of all three gives white w, representing a lack of colour charge. The three quarks in a nucleon always have colours such that the nucleon is colour-neutral. Antiquarks have the anti-colour values c, m, y for cyan, magenta, yellow (these are the colours opposite red, green, blue on a colour wheel). In a *meson* (which is composed of a quark and an anti-quark), a colour is always paired with its anti-colour, so that mesons are also colour neutral. The fundamental particles which make up the matter of ordinary experience are summarized in table 3

Table 3: The first family of fundamental particles

Particle	E. Charge	Colour Charge	Lepton #	Baryon #
e	-e	w	1	0
$\bar{\mathrm{u}}$	$-(2/3)e$	c, m, y	0	$-1/3$
d	$-(1/3)e$	r, g, b	0	$1/3$
$\nu, \bar{\nu}$	0	w	± 1	0
$\bar{\mathrm{d}}$	$(1/3)e$	c, m, y	0	$-1/3$
u	$(2/3)e$	r, g, b	0	$1/3$
$\bar{\mathrm{e}}$	e	w	-1	0

Leptons, meaning light ones, comprise electrons and neutrinos. Baryons, meaning heavy ones, comprise quarks and all of the particles quarks make up. Lepton number and baryon number are important quantum numbers because they are conserved. That is, although it turns out that the number of electrons, for example, is not conserved in subatomic interactions, the total lepton number of the universe is conserved. In some sense this means that a neutrino and an electron are really the same particle, just in different states. Similarly, it means that an up quark and a down quark are in some sense just different states of the same particle. But leptons and baryons are distinct (as far as we know). A typical subatomic interaction which conserves lepton and baryon number is β decay:

$$\mathrm{n} \rightarrow \mathrm{p} + \mathrm{e} + \bar{\nu}.$$

Since p=uud and n=ddu, what is really going on is

$$\mathrm{d} \rightarrow \mathrm{u} + \mathrm{e} + \bar{\nu}.$$

Note that this also conserves electric charge and colour charge (the two quarks must be the same colour).

Counting all of the particles in the above table, including their possible colours, gives a total of 16. This already seems like quite a lot of elementary particles. However, nature is not satisfied with this. Instead, she has replicated the above structure two more times. The three groups of this structure are called families. The first family given above accounts for all of ordinary matter. The second family has higher mass and the third family higher still. Counting all three families gives a grand total of 48 elementary particles. These particles, with their often whimsical names, are summarized in table 4.

Table 4: The three families of fundamental particles

Family #1 (normal)	Family # 2 (heavy)	Family # 3 (super-heavy)
electron e	muon μ	tauon τ
up quark u	strange quark s	top quark t
down quark d	charmed quark c	bottom quark b
e-neutrino ν_{e}	μ-neutrino ν_μ	τ-neutrino ν_τ

8.4 NON-EXAMINABLE Other Quanta

The list of elementary particles given above does not include photons for the reasons explained in Chapters 1 and 3: photons are quanta arising from quantizing the electromagnetic field, not particles that have to be quantized. The electromagnetic field is of course not the only force field in nature. Three others are known: the weak force, the strong force, and gravity. Gravity was of course the first force to be mathematically described. It is also the only one which has not been successfully quantized. Gravity is intimately connected with space and time, as Einstein showed. All other fields are quantized by *assuming* a certain space-time metric.

The strong and weak force fields can both be quantized in a similar manner to the electromagnetic force fields, and each gives rise to quanta which are bosons. However, they are much more complicated. Firstly, each field has a number of different quanta (three for the the weak force, eight for the strong force) compared to just one sort of electromagnetic quanta (photons). Secondly, the force-carrying quanta are massive, so that influences do not propagate at a constant speed. This is the reason that the strong and the weak forces are said to be finite range forces. The range of the force is roughly equal to the Compton wavelength $\lambda_{\mathrm{C}} = h/mc$ of the force-carrying "particle". (This can be shown by considering a radial, time-independent solution $\phi(r)$ of the Klein-Gordon equation.) Thirdly, the strong and weak fields couple to themselves, not just to matter fields. (The weak field also couples to the electromagnetic field because the weak field is itself charged.) Fourthly, the self-coupling of the strong and weak fields can be quartic in the fields (a Feynman vertex with four edges, not three edges as in relativistic QED coupling).

Because of these complications we will not consider the details of the strong or weak forces. Table 5 summarizes the quanta of these forces

(and electromagnetism), and how they couple to matter.

Table 5: The three known quantized forces of nature.

Force	Quanta	Symbols	Action
Electromag.	Photons	γ	couples to electric charge
Strong	Gluons	$g^1 \dots g^8$	couples to colour charge
Weak	IVBs	W^+,W^-,Z^0	transmutes particles

Note that the action of the weak force, transmuting particles, is what causes interactions such as β decay. Such interactions take place relatively rarely, which is why this is known as the weak force. The name of the force carrier, IVB, stands for intermediate vector boson.

The strong force is what holds the quarks together in nucleons. It also holds the nucleons together in a nucleus. Since nucleons are white (colour neutral), the bonding of nucleons is really just a residual strong force. That is, the strong nuclear force is analogous to the van-der-Waals forces of electromagnetic origin which hold together neutral atoms or molecules in condensed matter. The residual strong force in the nucleus of an atom is many orders of magnitude stronger than the electromagnetic force between the nucleus and the electrons. This gives an idea as to how strong the strong force really is.

In addition to these force-fields, there exists another fundamental field. This is the Higgs field, named after British physicist Peter Higgs, who along with several other physicists, predicted it in the early 1960s. This field has some unusual properties, but when it is quantized in the usual way it has low-energy excitations that are evenly spaced in energy, like other fields, and these excitations are identified as the Higgs boson. The Higgs field is believed to couple to all particles and fields (except the electromagnetic field), giving all the particles and quanta their masses (see below). The Higgs boson was experimentally observed in 2013. The Higgs boson itself is one of the most massive of the elementary particles/quanta (only the top quark is more massive), with a mass about 250,000 times that of the electron.

The discovery of the Higgs means that all of the elements of the so-called *standard model* of particle physics have been observed. This term was introduced by Stephen Weinberg in 1967, who was one of the theoreticians who helped complete the model. But neither he nor anyone else expected at the time that it would still be the most successful model for particle physics, more than half a century later. This is a source of considerable frustration for new generations of particle physicists.

8.5 NON-EXAMINABLE Renormalization revisited

Recall from Sec. 5.1.10 that if one goes beyond the first-order calculation (Fermi's golden rule), one finds an infinite energy shift for the atom. This calculation (which physicists first tried to perform in the 1930s) corresponds to a second-order term in Dyson's expansion. As explained in that earlier section, performing this calculation for an unbound electron also gives an infinite energy shift even to a free electron.

it can be shown that this is equivalent to adding an infinite contribution Δm to the electron's mass, coming from the interaction with the continuum of electromagnetic vacuum modes. We deal with this by *mass renormalization* — we give the electron an infinite negative mass m_{bare}, called the *bare mass* to start with. This is chosen to cancel the infinite contribution to the energy of the unbound electron, leaving only the *physical* mass $m_{\text{physical}} = m_{\text{bare}} + \Delta m \approx 10^{-30}\text{kg}$.

Of course if $\Delta m \to \infty$ one cannot simply say $m_{\text{bare}} = -\infty + m_{\text{physical}}$ — that is a meaningless equation. Rather, one must deal with finite quantities the whole way, and then take a limit at the end. This is a tricky business, and is known as *regularization*. One type of regularization is *dimensional regularization*, in which we assumes that space is $3-\delta$ dimensional. For $\delta > 0$, the integrals in Dyson's expansion actually converge, and we can take the limit $\delta \to 0$ at the end.

You might think that these infinities are an artefact of truncating the Dyson expansion, and that if we kept all orders that the infinites would cancel out and the result would be finite. In fact this is not the case. Each higher-order term in the Dyson expansion generates its own infinite terms, and they add up rather than cancel. All of these infinites are actually due to *loops* in the corresponding Feynman diagrams, which are explained in terms of *virtual particles*, as opposed to the the "real" particles (photons included here) that enter or exit the interaction region. Thankfully, all of these loops generate the same sort of infinities, so they can all be cancelled by using the trick of mass renormalization.

One final comment should be made about mass renormalization: the standard model is only renormalizable if the bare masses of all the particles is zero. This sounds crazy, since I said above that renormalization with regularization sets the bare mass to a very large negative value. The trick is to get an *effective* bare mass which is nonzero (and in fact, very large and negative) by coupling the zero-mass particles to another massless field. This is the Higgs field (or fields). The Higgs field is special in that it interacts with itself in such a way that its lowest energy state is not like the vacuum state $|0\rangle$ with zero mean field, but rather something like a coherent state $|\alpha\rangle$, with a large mean field. This gives rise to an effective mass both for the Higgs field itself, and to all other fields or particles it interacts with. If the Higgs field did not exist, then the standard model could not explain why elementary particles have mass[9]. This is why the Higgs field was predicted to exist.

As it turns out, mass renormalization is not the whole story. Not only the mass of the electron (or whatever particle we are considering) must be renormalized, but so too must ϵ_0, which sets the scale of the electromagnetic field energy — see Eq. (8.1.8). And finally (for QED), so too must the coupling constant q (the charge) between the particle and the field. Like mass, the infinite contributions to these quantities come from Feynman loops, and every term in the Dyson expansion can be dealt with by using a regularization procedure with suitable values of m_{bare}, $(\epsilon_0)_{\text{bare}}$, and q_{bare}.

[9] If an electron's bare mass were exactly zero, the corrections to its mass through couplings to the EM vacuum field would also be zero, so its physical mass would remain zero. Hence the Higgs field is necessary to give it some mass to start with.

The other interactions in the standard model can be dealt with in a similar way — by renormalizing a finite number of parameters. This is what we mean by saying the theory is renormalizable. Other field theories are not renormalizable — each term in the Dyson expansion throws up a *different sort* of infinity, so one must introduce an infinite number of parameters in the theory in order to calculate anything.

These days, most physicists think of renormalization in the following way. It does not mean that the electron really has an infinite negative bare mass, for instance. Rather it means that on a small enough length scale (or high enough energy scale), quantum field theory breaks down. We may never know what theory applies at very small length scales — it may be a theory of strings of length $\sim 10^{-43}$m, or it may be something not yet dreamt of. But at the "everyday" length scales of high energy physics ($\sim 10^{-12}$m or greater) the details of the "theory of everything" will be invisible. What will *emerge* is an *effective field theory*, which, like the standard model, will necessarily be renormalizable, as non-renormalizable theories will get either stronger and stronger at lower energies (which contradicts what we see) or weaker and weaker at lower energies (and so become irrelevant to physics) [10]. The fact that neutrinos have been discovered to have nonzero masses, albeit very small, is evidence that the standard model is only an effective field theory; if it were fundamental then neutrinos should be massless.

8.6 The spin-statistics theorem

The spin-statistics theorem has been stated a number of times already, but now that we have completed our look at elementary particles and fields it is worth revisiting. That is because explaining the spin-statistics connection is one of the triumphs of relativistic quantum mechanics and quantum field theory. Another triumph is the prediction of antiparticles, and that is part of the spin-statistics theorem.

To reiterate, the spin-statistics connection is that

> All particles having half-integer spins are fermions, while all particles and quanta having integer spin are bosons.

This is an observed fact of nature. Assuming relativity and quantum mechanics to be correct it can be proven (and thus becomes a theorem). The rigorous proof was first constructed by Pauli. We can understand it more heuristically in three steps as follows.

[10] Gravity seems to be an exception. Einstein's field equations, when quantized, are non-renormalizable. On the other hand, gravity is extraordinarily weak compared to the other forces, about 10^{-42} times weaker. It may be an anomalous non-renormalizable low-energy "relic" of the true "theory of everything", which gets weaker with scale (unlike renormalizable theories). We feel the effect of this extraordinarily weak force only because there is only one sort of gravitational "charge". That is, masses add up to give perceptible gravitational fields in the vicinity of stars and planets, unlike electrical and other charges which tend to cancel in bulk.

1. Elementary particles are spin-half fermions. (See Chap. 7)
   (a) The only relativistically invariant object which can be interpreted as a particle wavefunction is the Dirac bispinor.
   (b) The particles described by the Dirac bispinor are spin-half.
   (c) The Dirac equation has anomalous (negative energy) solutions which would make all dynamics unstable unless particles were prevented from occupying these states.
   (d) The only way particles can be prevented from occupying negative energy states is if they are (almost) full already.
   (e) The anomalous states can only be full if the particles are fermions (obeying the Pauli exclusion principle).
2. Compound particles composed of elementary spin-half fermions obey the theorem (see Sec. 6.1.4)
   (a) A compound particle composed of an odd number of fermions is a fermion; one composed of an even number is a boson.
   (b) A compound particle composed of an odd number of spin-$\frac{1}{2}$ particles has half-integer spin; one composed of an even number has integer spin.
3. Elementary quanta for force-fields behave like integer spin bosons
   (a) Quantizing a classical field results in a description of quanta analogous to that of bose particles (there is no restriction on the number of "particles" per mode.) (see Chap. 1).
   (b) The fundamental objects in relativity are integer-rank tensors (scalars, 4-vectors, 4×4-tensors etc.) and half-integer-rank tensors (spinors, spinors of vectors etc.)
   (c) A classical field must be an integer-rank tensor, because a classical spinor field would have an energy density which is not bounded below (see Sec. 7.3.2).
   (d) A tensor field of rank r transforms in the same way as a particle wavefunction of spin r (see Sec. 6.1.4).