



ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

Department of Physics and Astronomy "A. Righi"

Theoretical Physics

Relativistic Quantum Mechanics and Path Integrals

Lectures held by
Prof. Fiorenzo Bastianelli

Notes by
Gioele Mancino

Academic Year 2025/2026

Contents

1 Group Theory	3
1.1 Review of Linear Algebra	4
1.2 Definition of a Group	10
1.3 Representations	12
1.4 Lie Groups and Lie Algebras	26
1.5 Special relativity and the Lorentz group	36
2 Relativistic Quantum Mechanics	41
2.1 Schrödinger equation	44
2.2 Klein Gordon Equation	48
2.3 Dirac Equation	62
2.4 Integer Spin Particles	95
3 Path Integrals	103
3.1 Canonical Quantization	106
3.2 Path Integrals in Phase Space	108
3.3 Path Integrals in Configuration Space	111
3.4 Correlation Functions	117
3.5 Perturbative Expansion	129
3.6 Path Integrals for Fermions	135
Appendices	155
A Notation and Conventions	155
B Theoretical insights	157

Introduction

The unification of Quantum Mechanics and Special Relativity represents one of the most significant milestones in theoretical physics. While non-relativistic quantum mechanics successfully describes atomic spectra and low-energy phenomena, it fails to respect the fundamental symmetries of spacetime imposed by Einstein's theory.

In this course, we reconstruct quantum theory from first principles to ensure Lorentz covariance. We will see that imposing relativistic constraints is not merely a formal correction; it leads to profound physical consequences, including the emergence of intrinsic spin, the necessity of antiparticles, and the CPT theorem. Furthermore, we will move beyond the canonical operator formalism to introduce the Path Integral approach, which provides the most transparent framework for understanding symmetries, gauge theories, and the deep connection between quantum field theory and statistical mechanics.

Symmetry as a Guiding Principle

In theoretical physics, dynamics is often dictated by symmetry. Before writing down equations of motion, we must understand the mathematical language of symmetries: **Group Theory** will be the subject of Chapter 1.

We will focus on Lie groups and Lie algebras, specifically the Lorentz group $SO(3, 1)$ and the unitary groups $SU(N)$. A central insight of this course is that elementary particles are not just objects that "have" properties; they are defined mathematically as **irreducible representations** of the spacetime symmetry group. This geometric perspective allows us to classify particles by their spin and mass before we even discuss their dynamics.

Relativistic Wave Equations

The Schrödinger equation is structurally non-relativistic, treating space and time on unequal footings (first-order in time, second-order in space). To restore covariance, we must construct new wave equations.

In the second chapter, we systematically derive the equations governing different spin sectors:

- The **Klein-Gordon equation** for scalar particles (spin 0).
- The **Dirac equation** for fermions (spin 1/2), which naturally explains the origin of the gyromagnetic factor $g = 2$ and the existence of antimatter.
- The **Proca and Maxwell equations** for vector bosons (spin 1).

We will analyze the discrete symmetries (Parity, Time Reversal, Charge Conjugation) of these fields and confront the difficulties of the "single-particle" interpretation, which inevitably points towards the necessity of a many-body field theory.

The Path Integral Formalism

While the canonical quantization method (imposing commutation relations) is rigorous, it can be cumbersome for relativistic systems. In the third chapter, we introduce Richard Feynman's **Path Integral** formulation.

This approach reimagines quantum mechanics not as the evolution of a state vector in Hilbert space, but as a sum over all possible classical histories, weighted by the action phase $e^{iS/\hbar}$. This formalism is particularly powerful for:

1. **Perturbation Theory:** It allows for a systematic derivation of Feynman diagrams and correlation functions.
2. **Symmetries:** It makes the preservation of symmetries (like gauge invariance) manifest in the measure of integration.
3. **Fermions:** We will introduce **Grassmann numbers** (anticommuting variables) to extend the path integral to fermionic fields.

Finally, by performing a "Wick rotation" to imaginary time ($t \rightarrow -i\tau$), we will demonstrate the isomorphism between the quantum path integral and the partition function of Statistical Mechanics, revealing the unity between quantum fluctuations and thermal fluctuations.

Prerequisites: *Familiarity with the Lagrangian and Hamiltonian formalisms of Classical Mechanics, standard Quantum Mechanics, and the basic tenets of Special Relativity is required.*

1 | Group Theory

Group theory is a powerful mathematical language that describes the invariance properties of physical systems. These notes provide a concise introduction to group theory, focusing on developing the tensorial language used by physicists. The main concepts of Lie groups are introduced, which are essential for following many courses in the master's program in physics.

1.1 | Review of Linear Algebra

Consider a vector space V with a basis of vectors $|e_i\rangle$, so that an arbitrary vector $|v\rangle \in V$ can be expressed as:

$$|v\rangle = v^i |e_i\rangle,$$

where repeated indices are summed over (Einstein summation convention), with $i = 1, 2, \dots, \dim V$; assuming the basis to exist, we can denote the vector $|v\rangle$ just by its components v^i , i.e. its projection on the basis vectors. We assume V to be finite-dimensional and use Dirac's bra-ket notation.

1.1.1 | Linear Operators

A linear operator A maps vectors to vectors:

$$\begin{aligned} A : V &\longrightarrow V, \\ |v\rangle &\longrightarrow |v'\rangle = A|v\rangle. \end{aligned} \tag{1.1.1}$$

Using linearity, the transformed vector becomes:

$$|v'\rangle = A|v\rangle = A(v^i |e_i\rangle) = v^i A|e_i\rangle = v^i |e'_i\rangle = v^i A^j_i |e_j\rangle = A^i_j v^j |e_i\rangle = v'^i |e_i\rangle,$$

where we have set $|e'_i\rangle = A|e_i\rangle = A^j_i |e_j\rangle$, since the transformed vectors of the basis can be expressed as linear combinations of the original basis. In the second line, we have renamed indices to extract the components v'^i of the transformed vector, which reads $|v'^i\rangle = v'^i |e_i\rangle$. This identifies the matrix elements A^i_j and shows how it operates on the components of the vector:

$$v'^i = A^i_j v^j.$$

Physicist's Notation

Physicists often use only the components v^i to indicate the vector $|v\rangle$, assuming that a basis (or reference frame) has been chosen. Thus, the **linear transformation** above is often written in the form

$$\boxed{v'^i = A^i_j v^j}. \tag{1.1.2}$$

where A^i_j are the matrix entries that perform the linear transformation on the column vector with components v^j . Note that the second index of the matrix is summed over with the index of the vector components (summation convention on repeated indices). This linear transformation can be expressed in matrix language using column vectors and matrices. Considering the example of a two-dimensional vector space V ($|v\rangle \in V$, $\dim V = 2$), where indices can take only two values, we write:

$$v = \begin{pmatrix} v^1 \\ v^2 \end{pmatrix}, \quad A = \begin{pmatrix} A^1_1 & A^1_2 \\ A^2_1 & A^2_2 \end{pmatrix}, \quad \boxed{v' = Av}$$

where the first index (conventionally written as an upper index) is the row index, while the second index (conventionally written as a lower index) is the column index.

1.1.2 | Matrix Multiplication

Since we will use extensively square matrices, most of the time interpreted as linear operators acting on a vector space, let us review some of their properties. For square matrices, one can define a product and several other operations. We review these operations using 2×2 matrices, as the extension to higher dimensions is straightforward. The product of two such matrices $C = AB$ is defined by the *row-by-column multiplication rule*:

$$C = \begin{pmatrix} C_1^1 & C_1^2 \\ C_2^1 & C_2^2 \end{pmatrix} = \begin{pmatrix} A_1^1 & A_1^2 \\ A_2^1 & A_2^2 \end{pmatrix} \begin{pmatrix} B_1^1 & B_1^2 \\ B_2^1 & B_2^2 \end{pmatrix} = \begin{pmatrix} A_1^1 B_1^1 + A_1^2 B_2^1 & A_1^1 B_1^2 + A_1^2 B_2^2 \\ A_2^1 B_1^1 + A_2^2 B_2^1 & A_2^1 B_1^2 + A_2^2 B_2^2 \end{pmatrix}$$

Each matrix entry can be written more compactly as:

$$C^i_j = \sum_{k=1}^2 A^i_k B^k_j,$$

or using Einstein's convention as:

$$C^i_j = A^i_k B^k_j. \quad (1.1.3)$$

Note that matrix multiplication is non-commutative: $A^i_k B^k_j \neq B^i_k A^k_j$, meaning $AB \neq BA$. However, $A^i_k B^k_j = B^k_j A^i_k$ since numbers commute.

Matrix product is associative:

$$(AB)C = A(BC) = ABC,$$

so brackets may be omitted without ambiguity.

1.1.3 | Dual Space

The dual space \tilde{V} of a vector space V is defined as the space of linear maps that produce a number from any vector $|v\rangle \in V$. An element of the dual space $\langle w| \in \tilde{V}$ is defined by its action on the vectors $|v\rangle \in V$:

$$\begin{aligned} \langle w| : V &\longrightarrow \mathbb{R}, \\ |v\rangle &\longrightarrow \langle w|v\rangle \in \mathbb{R}, \end{aligned} \quad (1.1.4)$$

where we use Dirac's bra-ket notation. (Although we use \mathbb{R} here, similar definitions apply to complex numbers \mathbb{C} used in quantum mechanics.) The set of all such elements defines the dual space \tilde{V} , which is itself a vector space.

Expanding a dual vector using a dual basis $\langle \tilde{e}^i|$:

$$\langle w| = w_i \langle \tilde{e}^i|,$$

where the dual basis is chosen such that:

$$\langle \tilde{e}^i|e_j\rangle = \delta^i_j = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases}$$

with δ^i_j being the Kronecker delta. The action on a vector becomes:

$$\langle w|v\rangle = (w_i \langle \tilde{e}^i|)(v^j |e_j\rangle) = w_i v^j \langle \tilde{e}^i|e_j\rangle = w_i v^j \delta^i_j = w_i v^i,$$

that is:

$$\langle w|v\rangle = w_i v^i.$$

In component notation, the index position indicates whether we are considering a vector (upper indices, e.g., v^i) or a dual vector (lower indices, e.g., w_i). In general relativity, vectors with upper indices are called **contravariant**, while dual vectors with lower indices are called **covariant**. Note how the basis vectors and dual basis vectors have opposite index positions with respect to the components of vectors and dual vectors: $|e_i\rangle$ has a lower index, while $\langle\tilde{e}^i|$ has an upper index.

The **scalar** quantity $w_i v^i$ obtained by contracting a dual vector with a vector is invariant under changes of basis, as vectors are independent of the basis in which they are expanded. Let us consider a change of basis in V :

$$|e_i\rangle \rightarrow |e'_i\rangle = B_i^j |e_j\rangle,$$

where B_i^j represents an invertible matrix B . An arbitrary vector $|v\rangle$ can be expressed in both bases as:

$$|v\rangle = v^i |e_i\rangle = v'^i |e'_i\rangle.$$

The new components v'^i are related to the old components v^i by:

$$v'^i = A^i_j v^j,$$

where the transformation matrix A satisfies:

$$A^i_j B_i^k = \delta_j^k.$$

In matrix notation, this corresponds to $A^T B = \mathbb{I}$, and thus $A = (B^{-1})^T$.

Similarly, the dual basis vectors transform as:

$$\langle\tilde{e}'^i| = A^i_j \langle\tilde{e}^j|,$$

to maintain the orthonormality condition $\langle\tilde{e}'^i|e'_j\rangle = \delta_j^i$, while the components of dual vectors transform as:

$$w'_i = B_i^j w_j.$$

One can now verify the invariance of the scalar product:

$$\langle w|v\rangle = w_i v^i = w'_i v'^i. \quad (1.1.5)$$

This shows that the scalar product can be computed independently using either the primed or unprimed components. In detail:

$$\begin{aligned} w'_i v'^i &= (B_i^k w_k)(A^i_l v^l) = B_i^k A^i_l w_k v^l \\ &= (B^T A)^k_l w_k v^l = \delta_l^k w_k v^l = w_k v^k = w_i v^i, \end{aligned}$$

where we used $B^T = A^{-1}$ and renamed summed indices.

The vector spaces V and \tilde{V} are isomorphic, being of the same dimensions. However, this isomorphism is not unique: a *canonical isomorphism*, relating a vector of V to a vector of the dual space \tilde{V} in a unique way, can be established if there is a metric defined on the original vector space V .

Without a metric, there is no preferred way to relate vectors and dual vectors. Let us explore this important concept in the next section.

1.1.4 | Metric and Canonical Isomorphism

The vector spaces V and \tilde{V} are isomorphic, being of the same dimension. However, this isomorphism is not unique. A canonical isomorphism can be established if there is a metric defined on V : We define a metric g as a bilinear function mapping two vectors to a real number:¹

$$\begin{aligned} g : V \times V &\longrightarrow \mathbb{R}, \\ |w\rangle, |v\rangle &\longrightarrow g(|w\rangle, |v\rangle), \end{aligned} \tag{1.1.6}$$

so that $g(|w\rangle, |v\rangle) \in \mathbb{R}$. The metric is linear in both entries:

$$g(|w\rangle, |v\rangle) = g(w^i |e_i\rangle, v^j |e_j\rangle) = w^i v^j g(|e_i\rangle, |e_j\rangle) \equiv w^i v^j g_{ij},$$

where we set $g_{ij} \equiv g(|e_i\rangle, |e_j\rangle)$. The components g_{ij} form the metric tensor, which we assume to be invertible. Note the index structure: metric components carry two lower indices.

Having a metric, we can define a canonical isomorphism between V and \tilde{V} . Given a vector $|w\rangle \in V$, we identify its dual $\langle w| \in \tilde{V}$ by:

$$\langle w| = g(|w\rangle, \cdot),$$

which operates as:

$$\langle w|v\rangle \equiv g(|w\rangle, |v\rangle) \in \mathbb{R}.$$

Expanding using linearity:

$$\langle w|v\rangle = g(|w\rangle, |v\rangle) = g(w^i |e_i\rangle, v^j |e_j\rangle) = w^i v^j g(|e_i\rangle, |e_j\rangle) = w^i v^j g_{ij} = w_i v^i,$$

where in the last step we recognize the components $w_i = g_{ij} w^j$ of the dual vector $\langle w|$ with respect to the dual basis $\langle \tilde{e}^i |$.

When the metric is positive definite, one often considers an orthonormal basis where:

$$g_{ij} = \langle e_i | e_j \rangle = \delta_{ij}.$$

Note that g_{ij} can be written as a matrix, but its index structure shows it cannot be interpreted as a linear operator on V . Rather, it acts on the product $V \times V$ and may be interpreted as a tensor belonging to the space $\tilde{V} \otimes V$.

To summarize, in physicist's notation, the vector w^i (the covector v_i) is related to the dual vector w_i (to the vector v^i) by lowering (raising) its index with the metric:

$w_i = g_{ij} w^j, \quad v^i = g^{ij} v_j.$

(1.1.7)

The inverse relation for indices raising uses the inverse metric $g^{ij} = (g^{-1})^{ij}$, which satisfies:

$$g^{ij} g_{jk} = \delta^i_k,$$

so that $w^i = g^{ij} w_j$.

The canonical isomorphism between V and \tilde{V} depends on the introduction of a metric, a fact heavily utilized in general relativity since the metric tensor $g_{\mu\nu}$ allows raising and lowering indices of tensors defined on spacetime and encodes its geometric properties (such as its curvature).

¹The metric does not need to be *positive definite*, as in the case of the Minkowski metric in spacetime, since it can have an indefinite signature.

Example (Euclidean space). The Euclidean space E_N of N dimensions can be considered as a vector space with coordinates $x \in \mathbb{R}^N$ if we pick an origin. It is endowed with a scalar product that defines a metric:

$$s^2 = x^T x = x^T \mathbb{I} x = \delta_{ij} x^i x^j,$$

which exposes the Euclidean metric tensor δ_{ij} . This metric relates the vector x^i to its dual vector x_i by $x_i = \delta_{ij} x^j$. In this case, vectors and dual vectors can be identified numerically.

Example (Minkowski space). The Minkowski space M_4 of 4 dimensions with coordinates $x \in \mathbb{R}^4$ has a scalar product:

$$s^2 = x^T \eta x = \eta_{\mu\nu} x^\mu x^\nu = -(x^0)^2 + (x^1)^2 + (x^2)^2 + (x^3)^2,$$

where the metric $\eta_{\mu\nu}$ has components $\eta_{00} = -1$, and $\eta_{11} = \eta_{22} = \eta_{33} = 1$:

$$\eta = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \leftrightarrow \eta_{\mu\nu}.$$

We use Greek indices $\mu = 0, 1, 2, 3$, with 0 indicating the time-like direction (for space-like directions we will use $i = 1, 2, 3$). The Minkowski metric is not positive definite but allows mapping vectors x^μ to dual vectors $x_\mu = \eta_{\mu\nu} x^\nu$, so the scalar product becomes $s^2 = x^\mu x_\mu$. Note that $x^\mu \neq x_\mu$ in this case, but $x_\mu x^\mu = x^\mu x_\mu$.

Complex spaces. Similar definitions extend to complex vector spaces like the Hilbert space of quantum mechanics, with \mathbb{R} replaced by \mathbb{C} . Let us describe \mathbb{C}^N , considered as a complex vector space of N complex dimensions. Its dual space, denoted $\tilde{\mathbb{C}}^N$, is defined as the space of linear maps $\langle w |$ from \mathbb{C}^N to \mathbb{C} :

$$\begin{aligned} \langle w | : \mathbb{C}^N &\longrightarrow \mathbb{C} \\ |z\rangle &\longrightarrow \langle \tilde{w} | z \rangle = \tilde{w}_i z^i \end{aligned}$$

where the components z^i and \tilde{w}_i are all complex numbers. A canonical map relating the two spaces is obtained by introducing a complex metric defined by the scalar product:

$$s^2 = z^\dagger z = z_i^* z^i,$$

where $z \in \mathbb{C}^N$ has components z^i for $i = 1, \dots, N$, with z_i^* denoting their complex conjugates.

1.1.5 | Transposition of Matrices

To introduce transposition, let us first consider a matrix with lower indices only. Setting:

$$A = \begin{pmatrix} A_{11} & A_{21} \\ A_{12} & A_{22} \end{pmatrix},$$

we define the transposed matrix by exchanging rows and columns:

$$A^T = \begin{pmatrix} A_{11}^T & A_{12}^T \\ A_{21}^T & A_{22}^T \end{pmatrix} = \begin{pmatrix} A_{11} & A_{21} \\ A_{12} & A_{22} \end{pmatrix},$$

i.e.,

$$A_{ij}^T = A_{ji},$$

which means precisely exchanging rows with columns.

For products of matrices, we have the important properties:

$$\begin{cases} (AB)^T &= B^T A^T \\ (AB)^{-1} &= B^{-1} A^{-1} \\ \det(AB) &= \det A \det B, \end{cases} \quad (1.1.8)$$

where we recall that the inverse of a matrix exists only if its determinant is nonvanishing.

To familiarize ourselves with index notation, consider how the product $A = B^T C$ is written with indices:

$$A_{ij} = B_{ik}^T C_{kj} = B_{ki} C_{kj},$$

where in the last expression, we use the entries of B rather than those of B^T . This example shows that one must be careful in reconstructing matrix products from index expressions.

Similarly, we define the transpose of an operator A with index structure $A^i{}_j$ as follows:

$$(A^T)_i{}^j = A^j{}_i.$$

This shows that A^T cannot be interpreted as a linear operator on the original vector space V , but rather as an operator acting on the dual space \tilde{V} . The index structure of A^T precisely reflects this.

In Euclidean space (with metric δ_{ij}), one often identifies A and A^T numerically, but this is not generally correct in spaces with nontrivial metrics (the trivial metric δ_{ij} let us identify higher and lower indices objects, since it acts as the identity).

1.2 | Definition of a Group

Let us define a group $G = \{g\}$ as a set of elements g that satisfy the following properties:

1. **Composition law:** Given $g_1, g_2 \in G$, then $g_1 \cdot g_2 = g_3 \in G$.
2. **Identity element:** There exists $e \in G$ such that $g \cdot e = e \cdot g = g$, for all $g \in G$.
3. **Inverse element:** For each $g \in G$, there exists $g^{-1} \in G$ such that $g \cdot g^{-1} = g^{-1} \cdot g = e$.
4. **Associativity:** $(g_1 \cdot g_2) \cdot g_3 = g_1 \cdot (g_2 \cdot g_3)$ for all $g_1, g_2, g_3 \in G$.

Groups are fundamental mathematical structures that describe symmetries in various physical systems. The elements of a group can represent transformations, such as rotations or reflections, that leave certain properties of a system invariant.

1.2.1 | Types of Groups

We can classify groups into different types based on their properties and structure.

- **Discrete groups:** Contain a finite number of elements. For example, the group $Z_2 \equiv \{1, -1\}$ with the usual multiplication law defines a group with two elements.
- **Lie groups:** Groups with an infinite number of elements, where the elements depend continuously on certain parameters. For example, rotations around the z -axis of our three-dimensional space form a Lie group whose elements are parameterized by an angle $\theta \in [0, 2\pi]$. For Lie groups, one can consider infinitesimal transformations leading to the concept of Lie algebras, which are essential in understanding the structure of the groups.
- **Abelian groups:** Groups whose elements commute under the composition law: $g_1 \cdot g_2 = g_2 \cdot g_1$ for every $g_1, g_2 \in G$. If this does not happen, the group is said to be **non-abelian**.

Example (Discrete groups).

- The **cyclic group** Z_n : The finite group generated by the powers of an element a , $Z_n = \{e, a, a^2, \dots, a^{n-1}\}$, with the condition that $a^n = a^0 = e$. It is isomorphic to the n -th roots of unity $e^{\frac{2\pi i}{n}k}$, with $k = 0, 1, \dots, n - 1$. It is an abelian group for any n .
- The **symmetric group** S_n : The group of permutations of n objects, containing $n!$ elements. One can check that $S_2 = Z_2$, while S_3 contains six elements and is the simplest example of a non-abelian group.

Example (Lie groups).

- $GL(N, \mathbb{R}) = \{g \in \mathbb{R}^{N \times N} \mid \det g \neq 0\}$ **general linear group**: the group of real $N \times N$ matrices with determinant $\neq 0$.
- $SL(N, \mathbb{R}) = \{g \in GL(N, \mathbb{R}) \mid \det g = 1\}$ **special linear group**: the group of real $N \times N$ matrices with determinant = 1.
- $O(N) = \{g \in GL(N, \mathbb{R}) \mid g^T g = \mathbb{I}\}$ **orthogonal group**: the group of real orthogonal $N \times N$ matrices. It describes the invariances of the scalar product $x^T x$ with $x \in \mathbb{R}^N$.

- $\mathrm{SO}(N) = \{g \in \mathrm{O}(N) \mid \det g = 1\}$ **special orthogonal group**: the group of real orthogonal $N \times N$ matrices with determinant = 1.
- $\mathrm{GL}(N, \mathbb{C}) = \{g \in \mathbb{C}^{N \times N} \mid \det g \neq 0\}$ **general linear group**: the group of complex $N \times N$ matrices with determinant $\neq 0$.
- $\mathrm{SL}(N, \mathbb{C}) = \{g \in \mathrm{GL}(N, \mathbb{C}) \mid \det g = 1\}$ **special linear group**: the group of complex $N \times N$ matrices with determinant = 1.
- $\mathrm{U}(1) = \{z \in \mathbb{C} \mid |z| = 1\} = \{e^{i\theta} \mid \theta \in [0, 2\pi]\}$ **unitary group**: the group of phases. It describes the invariances of the product z^*z with $z \in \mathbb{C}$.
- $\mathrm{U}(N) = \{g \in \mathrm{GL}(N, \mathbb{C}) \mid g^\dagger g = \mathbb{I}\}$ **unitary group**: the group of unitary $N \times N$ matrices. It describes the invariances of the scalar product $z^\dagger z$ with $z \in \mathbb{C}^N$.
- $\mathrm{SU}(N) = \{g \in \mathrm{U}(N) \mid \det g = 1\}$ **special unitary group**: the group of unitary $N \times N$ matrices with determinant = 1.

There are important relationships between these groups, for example:

$$\begin{aligned} U(1) &\cong SO(2), \\ O(N) &= Z_2 \otimes SO(N), \\ U(N) &= U(1) \otimes SU(N). \end{aligned}$$

These isomorphisms and decompositions reveal the underlying structure of these symmetry groups and are fundamental in many physical applications.

1.3 | Representations

We now introduce the concept of group representation. A *representation* of an abstract group G is a “realization” of the multiplicative relations of the group G in a corresponding group of square matrices, where the product is given by the usual matrix multiplication. These matrices must be thought of as *linear operators* that act on a *vector space* V , whose dimension is called the *dimension of the representation*.

Explicitly, a representation is given by a mapping:

$$\begin{aligned} R : G &\longmapsto \text{Square Matrices,} \\ g &\longmapsto R(g), \end{aligned}$$

such that:

1. $R(g_1)R(g_2) = R(g_1 \cdot g_2)$.
2. $R(e) = \mathbb{I}$, where \mathbb{I} is the identity matrix.

From these properties, it also follows that $R(g^{-1})R(g) = R(e) = \mathbb{I}$, hence $R(g^{-1}) = R^{-1}(g)$ exists. Associativity is automatic because matrix multiplication is associative. Thus, all the properties of the group are explicitly realized by the matrices of a representation.

By thinking of the matrices of a representation as operators that act on a vector space V of dimension N , the matrices are $N \times N$ matrices, and that is why the representation is said to be of dimension N .

Example (Representation of Z_2). As a very simple example of a representation, consider the cyclic group $Z_2 = \{e, a\}$ with the relation that $a^2 = e$. Then, a simple two-dimensional representation is given by the following 2×2 matrices:

$$R(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad R(a) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}.$$

It is easily checked that the matrices of this representation satisfy all the properties of the abstract group $Z_2 = \{e, a\}$. As we shall understand soon, this representation is reducible, as it contains two copies of the more simple representation defined in terms of 1×1 matrices, i.e., numbers:

$$R(e) = 1, \quad R(a) = -1.$$

1.3.1 | Classification of Representations

At this point, the problem arises of studying how many and what kinds of representations of a given group possibly exist. In particular, it is useful to know which are their dimensions. This problem is of great importance for physical applications because the “vectors” of a representation (generically called “tensors”) are conveniently used to describe physical quantities associated with models where G acts as a symmetry group.

Defining Representation

In the list of Lie groups introduced in the previous examples, we have used matrices to define the groups. Thus, these matrices give rise immediately to a particular representation: the *defining representation* (also called the *fundamental representation*).

The elements of the group in the defining representation naturally perform transformations on vectors belonging to a vector space V , the space on which the matrices act as linear operators. Let v^a denote the components of a vector in V . The matrix $R(g)$, which represents the element g of the abstract group G , transforms this vector as follows:

$$v^a \xrightarrow{g \in G} v'^a = [R(g)]_b^a v^b,$$

where, as usual, $[R(g)]_b^a$ describes, as the indices a and b vary, the elements of the matrix $R(g)$. The row index a is the first index and is conventionally placed in the upper position, and the column index b is the second index and is conventionally placed in the lower position.

In this way, the vectors in the vector space V are transformed by operations associated with the group G . Repeated indices are summed over all their possible values, and the convention is used that in the sum, one index is in the upper position and the other one in the lower position.

Equivalent Representations

In general, *equivalent* representations are defined as those that are related by similarity transformations: $R(g)$ and $\tilde{R}(g)$ are equivalent representations if:

$$\tilde{R}(g) = A R(g) A^{-1} \quad \forall g \in G,$$

where A is a matrix independent of g . This equivalence relation allows us to consider equivalent representations as essentially the same representation. Indeed, the similarity transformation simply represents a change of basis in the vector space V : the matrices of the different equivalent representations identify the same linear operator expressed in different bases.

Reducible and Irreducible Representations

A *reducible* representation is a representation equivalent to a representation whose matrices are block diagonal. For example, $R(g)$ is reducible if:

$$\tilde{R}(g) = A R(g) A^{-1} = \left(\begin{array}{c|c|c} R_1(g) & 0 & 0 \\ \hline 0 & R_2(g) & 0 \\ \hline 0 & 0 & R_3(g) \end{array} \right) \quad \forall g \in G,$$

for an appropriate matrix A . It is said that $R(g)$ is reducible to the three representations $R_1(g)$, $R_2(g)$, $R_3(g)$. In this example, the vector space V on which the reducible representation $R(g)$ acts is naturally decomposed as a direct sum of the three vector spaces on which the representations $R_1(g)$, $R_2(g)$, $R_3(g)$ act, i.e., $V = V_1 \oplus V_2 \oplus V_3$. This reducibility is thus written as:

$$R(g) = R_1(g) \oplus R_2(g) \oplus R_3(g).$$

An *irreducible* representation is a representation that cannot be decomposed as above².

In the classification of the possible representations of a group G , it is useful to consider only inequivalent irreducible representations, as all other representations follow from them. Given a fixed integer N , it is not guaranteed that an irreducible representation of dimension N exists. In general, only for certain values of N will there be representations of a fixed group G (sometimes even more than one with the same dimension).

²For some groups, there can exist reducible representations of a particular type, formed by upper triangular matrices, but we overlook this subtlety in a first exposition to group theory, as the simplest groups we are interested in do not show such a phenomenon.

Unitary Representations

A *unitary* representation is a representation in terms of unitary matrices (operators). Unitary representations are very useful in applications of quantum mechanics, where the symmetries of a quantum system are described by unitary operators acting in the Hilbert space (an infinite-dimensional vector space endowed with a positive-definite norm).

Derived Representations

Given the defining representation $R(g)$ that acts on the vector space V , which corresponds to transforming vectors with upper indices, we can immediately construct three other representations:

- $R(g)^*$, the **complex conjugate** representation acting on V^* .
- $R(g)^{-1T}$, the **inverse transposed** representation acting on the dual space \tilde{V} .
- $R(g)^{-1\dagger}$, the **inverse Hermitian conjugate**³ representation acting on \tilde{V}^* .

We could not have an inverse representation without transposing, since when taking the inverse of a product of matrices, the order of the matrices is reversed:

$$(AB)^{-1} = (B^{-1}A^{-1})^T = A^{-1T}B^{-1T},$$

and the same is true for the inverse Hermitian conjugate representation (again the order of the matrices is reversed two times to ensure the correct properties of the representation).

The vectors on which these representations act have follow a precise index structure by convention⁴, respectively:

- Vectors with “upper indices” v^a (vectors in the space V).
- Vectors with “dotted upper indices” $v^{\dot{a}}$ (vectors in the complex conjugate space V^*).
- Vectors with “lower indices” v_a (vectors in the dual space \tilde{V}).
- Vectors with “dotted lower indices” $v_{\dot{a}}$ (vectors in the complex conjugate dual space \tilde{V}^*).

In formulae:

$$\begin{aligned} R(g) : \quad v^a &\xrightarrow{g \in G} v'^a = [R(g)]_b^a v^b, \quad v \in V \\ R(g)^* : \quad v^{\dot{a}} &\xrightarrow{g \in G} v'^{\dot{a}} = [R(g)^*]_{\dot{b}}^{\dot{a}} v^{\dot{b}}, \quad v \in V^* \\ R(g)^{-1T} : \quad v_a &\xrightarrow{g \in G} v'_a = [R(g)^{-1T}]_a^b v_b, \quad v \in \tilde{V} \\ R(g)^{-1\dagger} : \quad v_{\dot{a}} &\xrightarrow{g \in G} v'_{\dot{a}} = [R(g)^{-1\dagger}]_{\dot{b}}^{\dot{a}} v_{\dot{b}}, \quad v \in \tilde{V}^*. \end{aligned} \tag{1.3.1}$$

It is immediate to verify that these are representations of the group G if $R(g)$ is one. The different index structure associated with these matrices reflects the fact that they are operators acting on different vector spaces.

Remark. Note that there may be groups for which some of these representations are equivalent to each other:

- For real representations, $R(g)^* \cong R(g)$ and $R(g)^{-1\dagger} \cong R(g)^{-1T}$.

³Given a matrix R , its Hermitian conjugate (or adjoint) R^\dagger is defined as the complex conjugate of the transpose, $R^\dagger = R^{T*}$.

⁴More information about dotted indices can be found in Appendix A.

- For unitary representations, $R(g)^{-1\dagger} \cong R(g)$ and $R(g)^{-1T} \cong R(g)^*$ (since $R(g)^\dagger = R(g)^{-1}$).
- For orthogonal representations, $R(g)^{-1T} \cong R(g)$ and $R(g)^{-1\dagger} \cong R(g)^*$ (since $R(g)^T = R(g)^{-1}$).
- For unitary and real representations, all four representations are equivalent to each other (for example, for the group $SO(N)$).

1.3.2 | Invariant Quantities and Index Contractions

Invariant quantities under the action of the group G can be obtained by taking the scalar product between vectors with upper indices (sometimes called contravariant) and those with lower indices (sometimes called covariant), whether dotted or undotted. One can verify the following identities:

$$\begin{aligned} v_a w^a &\xrightarrow{g \in G} v'_a w'^a = v'^T w' = (R(g)^{-1T} v)^T R(g) w = v^T R(g)^{-1} R(g) w = v^T w = v_a w^a, \\ x_{\dot{a}} y^{\dot{a}} &\xrightarrow{g \in G} x'_{\dot{a}} y'^{\dot{a}} = x'^T y' = (R(g)^{-1\dagger} x)^T R(g)^* y = x^T R(g)^{-1*} R(g)^* y = x^T y = x_{\dot{a}} y^{\dot{a}}. \end{aligned}$$

In general, it makes no group-theoretic sense to contract indices of the vectors described above in any other way (“contracting” refers to the operation of equating two indices and summing over all possible values that these indices can assume). For example, the quantities $v^a w_a$ or $x^{\dot{a}} y_{\dot{a}}$ are not invariant under the action of the group G , and contracting indices of different nature (for example, $v^a y_{\dot{a}}$) is not even defined.

1.3.3 | Tensors and Tensor Representations

Other representations can be obtained from the tensor product of the previously described representations. By definition, these representations act on “tensors,” which are elements of vector spaces obtained from the tensor product of copies of V , V^* , \tilde{V} , and \tilde{V}^* . Therefore, tensors, by definition, have a certain number of upper and lower indices, with transformation properties defined by the nature associated with those indices.

For example, a tensor $F^{ab}{}^{\dot{c}}{}_{\dot{e}}$ is, by definition, an object with N^5 components that transform exactly like the product of the components of the previously defined vectors (tensor product):

$$F^{ab}{}^{\dot{c}}{}_{\dot{e}} \sim v^a u^b w_c x^{\dot{c}} y_{\dot{e}}.$$

Thus, the tensor $F^{ab}{}^{\dot{c}}{}_{\dot{e}}$ represents (the components of) an element of a vector space of dimension N^5 (because each index can take N values; it corresponds to an element of the vector space $V \otimes V \otimes \tilde{V} \otimes V^* \otimes \tilde{V}^*$ and we can write $F^{ab}{}^{\dot{c}}{}_{\dot{e}} \in V \otimes V \otimes \tilde{V} \otimes V^* \otimes \tilde{V}^*$).

Tensor Transformation Law

Under the action of the group G , the tensor transforms as follows:

$$F'^{ab}{}^{\dot{c}}{}_{\dot{e}} = [R(g)]^a_f [R(g)]^b_g [R(g)^{-1T}]_c{}^h [R(g)^*]^{\dot{c}}{}_{\dot{m}} [R(g)^{-1\dagger}]_{\dot{e}}{}^{\dot{n}} F^{fg}{}_{h}{}^{\dot{m}}.$$

This linear transformation law identifies a representation of dimension N^5 (the N^5 components are mixed among themselves by an $N^5 \times N^5$ matrix, implicitly defined by the above formula, thus providing a representation of the group).

Reducibility of Tensor Representations

Typically, tensors correspond to reducible representations, i.e., are transformed by reducible representations. The problem of decomposing representations into irreducible ones now arises. One way to decompose a representation is to study the tensors on which they act. A first decomposition operation is to separate the tensors by considering their symmetry properties under permutations of indices of the same nature (it is, therefore, useful to know the properties of the permutation group of n objects, i.e., the symmetric group S_n).

For example, the tensor T^{ab} can be separated into its symmetric part ($S^{ab} = S^{ba}$) and its anti-symmetric part ($A^{ab} = -A^{ba}$) as follows:

$$T^{ab} = \underbrace{\frac{1}{2}(T^{ab} + T^{ba})}_{S^{ab}} + \underbrace{\frac{1}{2}(T^{ab} - T^{ba})}_{A^{ab}}.$$

It is easy to convince oneself that the symmetric and antisymmetric parts with distinct symmetries do not mix under group transformations. Indeed, one can calculate the transformed symmetric part under an arbitrary group transformation and verify that it remains symmetric:

$$\begin{aligned} S^{ab} &\xrightarrow{g \in G} S'^{ab} = [R(g)]_c^a [R(g)]_d^b S^{cd} \\ &= [R(g)]_c^a [R(g)]_d^b S^{dc} \\ &= [R(g)]_d^b [R(g)]_c^a S^{dc} = S'^{ba}. \end{aligned}$$

Similarly, one can verify that the antisymmetric part remains antisymmetric:

$$\begin{aligned} A^{ab} &\xrightarrow{g \in G} A'^{ab} = [R(g)]_c^a [R(g)]_d^b A^{cd} \\ &= [R(g)]_c^a [R(g)]_d^b (-A^{dc}) \\ &= -[R(g)]_d^b [R(g)]_c^a A^{dc} = -A'^{ba}. \end{aligned}$$

Thus, symmetric parts and antisymmetric parts are never mixed by group transformations, so the tensor representation identified by the tensor T^{ab} is reducible. In a compact notation, we can denote the representation that transforms the tensor $T^{ab} \sim T$ as $R_T(g)$, by grouping all the tensorial indices of different nature and position with a single multi-index, so that:

$$\begin{aligned} T^{ab} &\xrightarrow{g \in G} T^A, \quad T'^A = [R_T(g)]_B^A T^B, \\ [R_T(g)]_B^A &= [R(g)]_k^a [R(g)]_f^b [R(g)^{-1}]_c^l [R(g)^*]_m^d [R(g)^{-1}]_e^n. \end{aligned}$$

This representation is reducible:

$$\begin{pmatrix} S' \\ A' \end{pmatrix} = \underbrace{\begin{pmatrix} R_S(g) & 0 \\ 0 & R_A(g) \end{pmatrix}}_{R_T(g)} \begin{pmatrix} S \\ A \end{pmatrix},$$

where $T \sim \begin{pmatrix} S \\ A \end{pmatrix}$ indicates the decomposition into symmetric and antisymmetric parts.

These parts may be further reduced if there are other invariant operations (such as the possibility of taking scalar products of vectors and covectors in different representations as seen in 1.3.2). For the simpler representations, it is easy to study any further reducibility on a case-by-case basis.

Invariant Tensors

Note that the Kronecker delta tensors δ_a^b and $\delta_{\dot{b}}^{\dot{a}}$, which are the matrix elements of the identity operators, remain invariant under group transformations if their indices are transformed according to their nature. For example:

$$\begin{aligned}\delta_a^b &\xrightarrow{g \in G} (\delta')_b^a = [R(g)]_c^a [R(g)^{-1T}]_b^d \delta_d^c \\ &= [R(g)]_c^a [R(g)^{-1T}]_b^c \\ &= [R(g)]_c^a [R(g)^{-1}]_b^c \\ &= [R(g)R(g)^{-1}]_b^a = \delta_b^a.\end{aligned}\tag{1.3.2}$$

These are called *invariant tensors*. In contrast, δ_{ab} does not identify any invariant tensor (unless there are special relations between the various types of indices): if we define a tensor that coincides with δ_{ab} in a “reference frame”, under a group transformation (a “change of reference frame”) the components of the tensor change value.

The existence and number of invariant tensors depend on the group G under consideration. For example:

- The group $SO(N)$ admits an invariant tensor defined by the completely antisymmetric symbol $\epsilon^{a_1 \dots a_N}$, where the indices are those of the fundamental representation. This follows from the unitary determinant of the matrices in $SO(N)$.
- Similarly, the group $SU(N)$ admits the invariant tensors given by the completely antisymmetric symbols $\epsilon^{a_1 \dots a_N}$ and $\epsilon_{a_1 \dots a_N}$.

1.3.4 | Representations of $SO(N)$

We describe here the simplest representations of $SO(N)$, the **special orthogonal group** of real $N \times N$ matrices:

$$SO(N) = \{\text{real } N \times N \text{ matrices } R \mid R^T R = \mathbb{I}, \det R = 1\}.$$

This is the group that leaves invariant the scalar product of vectors $\vec{v}, \vec{w} \in \mathbb{R}^N$, defined by $\vec{v} \cdot \vec{w} = \delta_{ab} v^a w^b$, where the metric δ_{ab} is recognized to be an invariant tensor (indices up and down are equivalent for $SO(N)$, so that $\delta_{ab} = \delta_a^b$, and we already know that δ_a^b is an invariant tensor).

Remember that the group $SO(N)$ describes rotations in an N -dimensional real vector space. The condition $\det R = 1$ ensures that we are considering only proper rotations (excluding reflections).

Since this is a real and orthogonal group, upper and lower, dotted and undotted indices are equivalent, thus we have four equivalent ways of representing a vector:

$$v^a \sim v_a \sim v^{\dot{a}} \sim v_{\dot{a}}.$$

Invariance of the scalar product. More directly, using matrix notation, we compute:

$$\begin{aligned}v' &= Rv, \quad w' = Rw \\ \vec{v} \cdot \vec{w} &= v^T w \quad \rightarrow \quad v'^T w' = (Rv)^T R w = v^T R^T R w = v^T w.\end{aligned}$$

Equivalently, using components:

$$\begin{aligned} v'_a &= R_{ab}v_b, \quad w'_a = R_{ab}w_b \\ \vec{v} \cdot \vec{w} = v_a w_a &\rightarrow v'_a w'_a = R_{ab}v_b R_{ac}w_c = v_b R_{ab}R_{ac}w_c = v_b \underbrace{R_{ba}^T R_{ac}}_{\delta_{bc}} w_c = v_b w_b = v_a w_a, \end{aligned}$$

where we used again the fact that upper and lower indices are equivalent.

Defining representation. Thus, the defining representation (also called vector representation) acts on the vectors v^a . As already described, the four basic representations are all equivalent as $v^a \sim v_a \sim v^{\dot{a}} \sim v_{\dot{a}}$. We denote this representation by N , i.e., by its dimension.

The tensor product $N \otimes N$ identifies the tensor representation that acts on tensors with two indices T^{ab} and thus corresponds to a representation of dimension N^2 . It is a reducible representation. To extract the irreducible representations that it contains, we proceed as follows.

Decomposing the tensor representation. We have already seen that the tensor T^{ab} can be separated into the symmetric part S^{ab} (of dimension $\frac{N(N+1)}{2}$) and the antisymmetric part A^{ab} (of dimension $\frac{N(N-1)}{2}$).

The symmetric part is still reducible because one can construct a scalar (an invariant under the group transformations) by taking its trace:

$$S \equiv \delta_{ab}S^{ab} = S^a_a.$$

It is easily seen that this is a scalar, as we already know that the contraction of an upper index with a lower index produces a scalar:

$$S \xrightarrow{g \in SO(N)} S' = S$$

It identifies a trivial one-dimensional representation: $R_{\text{scal}}(g) = 1$. We can separate the trace from the symmetric tensor S^{ab} in the following way:

$$S^{ab} = \underbrace{S^{ab} - \frac{1}{N}\delta^{ab}S}_{\hat{S}^{ab}} + \frac{1}{N}\delta^{ab}S$$

where we have defined the traceless symmetric tensor \hat{S}^{ab} (which satisfies $\hat{S}^a_a = 0$).⁵ Thus, collecting all pieces, we have succeeded in separating the tensor T^{ab} into its irreducible parts:

$$T^{ab} = \frac{\delta^{ab}}{N}S + A^{ab} + \hat{S}^{ab}$$

They transform independently without ever mixing. Indicating the irreducible representations with their respective dimensions, the above translates into the following expression:

$$N \otimes N = 1 \oplus \frac{N(N-1)}{2} \oplus \left(\frac{N(N+1)}{2} - 1 \right)$$

It can be shown that there are no further reductions. The representation acting on antisymmetric tensors with two indices A^{ab} , the $\frac{N(N-1)}{2}$, is also called the **adjoint representation**: its dimension

⁵We have divided by N since the trace involves summing over N components, and for the delta in particular, $\delta_a^a = N$, since it is the trace of the identity $N \times N$ matrix.

corresponds to the number of independent parameters of the group, given by the angles describing the rotations in the a - b planes (with $a \neq b$).

In summary, for $\mathrm{SO}(N)$, we understand that there exist the following irreducible representations, indicated by their dimension:

$$1, \quad N, \quad \frac{N(N-1)}{2}, \quad \left(\frac{N(N+1)}{2} - 1 \right), \quad \dots$$

where 1 is the trivial representation (the scalar), N is the vector representation (also called defining or fundamental), the $\frac{N(N-1)}{2}$ is the adjoint representation, the $\frac{N(N+1)}{2} - 1$ is the traceless symmetric representation, etc.

Example ($\mathrm{SO}(3)$ case and quantum mechanics). In the specific case of $\mathrm{SO}(3)$, the irreducible tensor decomposition becomes:

$$3 \otimes 3 = 1 \oplus 3 \oplus 5.$$

We see that in this special case, the adjoint representation coincides with the vector representation (the defining representation): the dimensions are the same, and a full proof is simple to produce. Translated into the language of quantum mechanics, this formula tells us that combining spin 1 (the vector representation “3”) with another spin 1 yields spin 0 (the “1” representation, the scalar), spin 1 (again the “3” representation), and spin 2 (the “5” representation).

Equivalently, defining the quantum numbers l by setting $n = 2l + 1$ for $n = 1, 3, 5, \dots$, this relation can be written as:

$$(l=1) \otimes (l=1) = (l=0) \oplus (l=1) \oplus (l=2)$$

which is the formula for adding quantum angular momenta. In quantum mechanics, orbital angular momentum is quantized and is fixed by an integer quantum number $l = 0, 1, 2, 3, \dots$, indicating that the projection of the angular momentum along a fixed axis can only take $2l + 1$ values. The $(2l + 1)$ -representation is the one acting on the traceless, symmetric tensor with l indices, $\hat{S}^{a_1 a_2 \dots a_l}$.

The electron orbiting the nucleus can have angular momentum with $l = 0$ (S orbital), angular momentum with $l = 1$ (P orbital), angular momentum with $l = 2$ (D orbital), etc. Continuing with the study of angular momentum in quantum mechanics, one discovers that intrinsic angular momenta (spins) are characterized by integer and half-integer values of the quantum number, i.e., $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$. The rules for composing angular momentum in quantum mechanics correspond precisely to the decomposition of a tensor product into irreducible representations mentioned above.

Strictly speaking, the representations with half-integer spin (spinors) are not truly representations of the $\mathrm{SO}(N)$ group, as they are double valued (a rotation of 2π is not the identity but minus the identity). They are representations of the covering group as well as of the $\mathrm{SO}(N)$ Lie algebra, a concept that we shall introduce shortly.

Example ($\mathrm{SO}(4)$ and Lorentz group $\mathrm{SO}(3, 1)$).

In the case of $\mathrm{SO}(4)$, or the Lorentz group $\mathrm{SO}(3, 1)$, the irreducible tensor decomposition becomes:

$$4 \otimes 4 = 1 \oplus 6 \oplus 9.$$

The 6-dimensional representation is the adjoint representation. It is the one that acts on the electromagnetic field, which indeed has six independent components that are mixed under Lorentz transformations. The electromagnetic field is described by an antisymmetric tensor with two indices $F^{\mu\nu}$.

In the case of the Lorentz group, upper and lower indices are equivalent, and the Minkowski metric is used to pass from one to the other (the metric describes the similarity transformation that connects the two representations).

1.3.5 | Representations of $SU(N)$

Consider now $SU(N)$, the special unitary group of $N \times N$ matrices:

$$SU(N) = \{ \text{complex } N \times N \text{ matrices } U \mid U^\dagger U = \mathbb{I}, \det U = 1 \}.$$

This is the group that preserves the inner product of vectors $\vec{v}, \vec{w} \in \mathbb{C}^N$ defined by⁶ $\vec{v}^* \cdot \vec{w} = v^a w^a \sim v_a w^a = \delta^a_b v^b w^a$, where $*$ denotes the complex conjugate. The metric δ^a_b is an invariant tensor, as we have seen in eq. (1.3.2).

Starting from the fundamental representation, N (corresponding to the vectors v^a), we immediately obtain another representation, the **antifundamental representation** (or complex conjugate of the fundamental, transforming the vectors $v^a \sim v_a$), which is denoted by \bar{N} . Note that, unlike the case of $SO(N)$, here not all indices are equivalent: the representation is unitary ($U^\dagger U = \mathbb{I}$), thus we have $v^a \sim v_a$ transforming in N , while $v^a \sim v_a$ transforming in \bar{N} .

Invariance of the scalar product. Using matrix notation, we compute:

$$\begin{aligned} v' &= Uv, & w' &= Uw \\ \vec{v}^* \cdot \vec{w} &= v^\dagger w & \rightarrow & v'^\dagger w' = (Uv)^\dagger Uw = v^\dagger U^\dagger Uw = v^\dagger w. \end{aligned}$$

Equivalently, using components:

$$\begin{aligned} v'^a &= U^a_b v^b, & w'^a &= U^a_b w^b \\ \vec{v}^* \cdot \vec{w} &= v_a w^a & \rightarrow & v'_a w'^a = (U^a_b v^b)^* U^a_c w^c = v_b U^b_a U^a_c w^c = v_b \underbrace{U^b_a U^a_c}_{\delta^b_c} w^c = v_a w^a, \end{aligned}$$

where we used $U^b_a \sim U^a_b = (U^a_b)^\dagger$, thus we have seen that this representation preserves the scalar product among daggered and undaggered vectors.

Decomposing the tensor representation. Now, let's find other irreducible representations by considering the tensor product:

$$N \otimes N = \frac{N(N+1)}{2} \oplus \frac{N(N-1)}{2},$$

which corresponds to the decomposition of the tensor T^{ab} into its symmetric and antisymmetric parts, $T^{ab} = S^{ab} + A^{ab}$, now an exhaustive decomposition.⁷ Hence, we have discovered the existence of two new representations and know their dimensions.

⁶Remember that, since the representation is unitary we have $R(g)^{-1T} \cong R(g)^*$, thus $v^a \sim v_a$ (the adjoint is equivalent to the inverse).

⁷Note that it is not possible to take traces to form scalars on these tensors because δ_{ab} is not an invariant tensor for $SU(N)$: to see this, simply transform the tensor δ_{ab} as dictated by the structure of its indices and see that it is not invariant. The invariant tensors would be δ^a_b and δ_a^b : $\delta_a^b = U^\dagger U \delta_a^b = \delta_a^b$.

Consider now:

$$N \otimes \bar{N} = 1 \oplus (N^2 - 1),$$

which corresponds to the decomposition of the tensor T_b^a into its trace part (the scalar) and its traceless part. This is possible because we know that contracting a raised index with a lowered index produces a scalar. In formulas, this separation is written as:

$$T_b^a = \frac{\delta_b^a}{N} T + \hat{T}_b^a,$$

where $T \equiv T_a^a$ and $\hat{T}_b^a \equiv T_b^a - \frac{1}{N} \delta_b^a T$. Note that the tensor δ_b^a is an invariant tensor (it corresponds to the metric of the complex vector space \mathbb{C}^N). Thus, we have discovered the existence of the representation of dimension $N^2 - 1$, the so-called **adjoint representation**.

One can consider other invariant tensors of $SU(N)$, such as the completely antisymmetric tensors with N indices, $\epsilon_{a_1 a_2 \dots a_N}$ and $\epsilon^{a_1 a_2 \dots a_N}$ (this can be demonstrated using the fact that the group matrices have determinants equal to one), which can be used to study the reduction (or equivalence) of other tensorial representations.

In summary, for $SU(N)$, we have seen that there exist the following irreducible representations:

$$1, \quad N, \quad \bar{N}, \quad N^2 - 1, \quad \frac{N(N-1)}{2}, \quad \frac{N(N+1)}{2}, \quad \frac{\bar{N}(N-1)}{2}, \quad \frac{\bar{N}(N+1)}{2},$$

where 1 is the trivial representation (the scalar), N is the fundamental representation (or defining), \bar{N} is the antifundamental (complex conjugate of the fundamental), and $N^2 - 1$ is the adjoint representation (which is real) etc.

Example ($SU(2)$ case and quantum mechanics). Let's make this explicit for the case of $SU(2)$. We have:

$$2 \otimes 2 = 1 \oplus 3, \quad 2 \otimes \bar{2} = 1 \oplus 3, \tag{1.3.3}$$

where 2 is the fundamental representation (acting on vectors v^a), $\bar{2}$ is the antifundamental representation (acting on vectors $v^{\bar{a}} \sim v_a$), 1 is the scalar representation, and 3 is the adjoint representation (acting on traceless tensors T_b^a).

These formulas suggest that perhaps 2 and $\bar{2}$ are *equivalent representations*, i.e. $\bar{2} \sim 2$. This is indeed the case: using the invariant tensor ϵ_{ab} we may relate the two representations by setting $w_a = \epsilon_{ab} v^b$, then under a group transformation we see that:

$$w'_a = \epsilon'_{ab} v'^b = \epsilon_{ab} v'^b$$

which indicates that, up to a change of basis given by the ϵ_{ab} tensor, the vectors v^a and w_a transform in the same way. Here, we used the fact that ϵ_{ab} is an invariant tensor. The explicit proof is as follows: if $U \in SU(2)$ then:

$$\epsilon'^{ab} = U_c^a U_d^b \epsilon^{cd} = k \epsilon^{ab}, \quad \epsilon^{ab} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

for some coefficient k . This follows from the fact that an antisymmetric tensor transforms into another antisymmetric one, and from antisymmetric 2×2 matrix having only one independent component (otherwise the coefficient k would have been a vector or a matrix). To determine k , we calculate:

$$\epsilon'^{12} = U_c^1 U_d^2 \epsilon^{cd} = U_1^1 U_2^2 - U_2^1 U_1^2 = \det U = 1, \quad U \in SU(2),$$

where we constructed the determinant of the matrix U using the Levi-Civita symbol ϵ^{cd} . Comparing with $\epsilon'^{12} = k\epsilon^{12}$, we find $k = 1$ and $\epsilon'^{ab} = \epsilon^{ab}$, and thus w_a transforms in the same way as v^a (up to a change of basis), confirming that $\bar{2} \sim 2$.

Translating (1.3.3) into the language of quantum mechanics, it means that combining spin $\frac{1}{2}$ (the representation “2”) with itself yields spin 0 (the representation “1”, the scalar) and spin 1 (the representation “3”). Indeed, defining $j = 2s + 1$ for $s = 0, \frac{1}{2}, 1$, this relation can be equivalently written as:

$$(j = \frac{1}{2}) \otimes (j = \frac{1}{2}) = (j = 0) \oplus (j = 1).$$

The group $SU(2)$ describes space rotations, including the possibility of having half-integer spins associated with fermionic particles. In mathematical terms, one says that the group $SU(2)$ is the universal cover of the group $SO(3)$.

Example (SU(3) case and quark model). Now, let us make explicit also the case of $SU(3)$. It has physical applications both as the **flavor symmetry group** $SU(3)_{\text{flavor}}$ which mixes the three “flavors” of quarks (up, down, strange), and as **color symmetry group** $SU(3)_{\text{color}}$ which mixes the three colors of each quark (conventionally red, green, blue). We have:

$$3 \otimes \bar{3} = 1 \oplus 8 \tag{1.3.4}$$

where 3 is the fundamental representation (acting on vectors $v^a \sim v_a$), $\bar{3}$ is the antifundamental representation (acting on vectors $v^{\dot{a}} \sim v_{\dot{a}}$), 1 is the scalar representation, and 8 is the adjoint representation (acting on traceless tensors T_b^a).

In $SU(3)_{\text{flavor}}$, 3 and $\bar{3}$ correspond to the up, down, and strange quarks and their antiquarks:

$$q^a = \begin{pmatrix} u \\ d \\ s \end{pmatrix} \sim 3, \quad \bar{q}_a = \begin{pmatrix} \bar{u} \\ \bar{d} \\ \bar{s} \end{pmatrix} \sim \bar{3}.$$

Flavor symmetry means that we can redefine flavors through $SU(3)$ group transformations without changing anything in the description of physical phenomena: $SU(3)_{\text{flavor}}$. In the static quark model of mesons, which are hadrons composed of bound states of quark-antiquark ($q\bar{q}$), the symmetry implies that only singlets or octets of flavor can emerge. The *mesonic octet* containing the pions is the main example: there are eight mesons with identical properties, and one could not distinguish them from each other if the symmetry were exact (same masses, same spin, etc.). In reality, the symmetry is only approximate, so there are some small differences (e.g., they have slightly different mass, also they have different charges and electromagnetism violates this symmetry).

Another application concerns the color of quarks and is associated with another $SU(3)$ group, called $SU(3)_{\text{color}}$. Each quark flavor has three colors (red, green, blue); for example, for the up quark, we can group them in a vector:

$$u^a = \begin{pmatrix} u^{\text{red}} \\ u^{\text{green}} \\ u^{\text{blue}} \end{pmatrix} \sim 3, \quad \bar{u}_a = \begin{pmatrix} \bar{u}^{\text{red}} \\ \bar{u}^{\text{green}} \\ \bar{u}^{\text{blue}} \end{pmatrix} \sim \bar{3},$$

where the colors associated with the antiquarks are called anticolors (antired, antigreen, antiblue).

Color symmetry means that we can redefine colors through SU(3) group transformations without changing anything (color symmetry is exact). The information contained in the relation (1.3.4) is that it is possible to combine the colors of a quark with the colors of an antiquark (the anticolors) to form a colorless state (the scalar) or states with eight possible different color combinations: indeed, quark/antiquark of the same flavor can combine into a photon (the scalar, or singlet, of color) or into a gluon (there are eight different possibilities, so that one says that the gluons form an octet of color).

Moreover:

$$3 \otimes 3 = 6 \oplus \bar{3}.$$

The possible ambiguity in understanding whether the tensor A^{ab} , which has three components, corresponds to 3 or $\bar{3}$ is resolved in favor of the latter option considering that $A^{ab} \sim A^{ab}\epsilon_{abc} \sim V_c$ (since ϵ_{abc} is an invariant tensor for SU(3)). This relation in $SU(3)_{\text{color}}$ tells us that combining the colors of two quarks is not possible to obtain a colorless state (the scalar).

With a bit more effort, one can also deduce (considering the symmetries of the tensor T^{abc}) that:

$$3 \otimes 3 \otimes 3 = 1 \oplus 8 \oplus 8 \oplus 10 \quad (1.3.5)$$

where the 1 corresponds to the completely antisymmetric part of T^{abc} , the 10 to the completely symmetric part of T^{abc} , and the two 8s to parts of the tensor with mixed symmetry. In applications in the static quark model of **baryons**, hadrons composed of bound states of three quarks (qqq), the symmetry $SU(3)_{\text{flavor}}$ predicts that families of similar particles can only exist with 1, 8, or 10 components (not all need to exist: some combinations might not appear for other reasons). There are several octets (the 8), like the eight baryons, which have similar properties concerning the strong interactions (a particular octet contains the proton and the neutron). Their antiparticles also form octets. There is also a famous decuplet of baryons, whose wave functions are symmetric in the flavors of the three constituent quarks. These wave functions transform into the 10 of SU(3) under flavor symmetry transformations (the corresponding anti-baryons group into $\bar{10}$). Applying the relation (1.3.5) to color, the fact that the 1 appears on the right side is interpreted as the possibility of combining the colors of three quarks to form a colorless state (e.g., the proton is made of three quarks; in general mesons and baryons must be color scalars due to a dynamical process called *color confinement*).

1.3.6 | Representations of U(1)

Let us also consider the case of representations of the group U(1), which also plays a significant role in physics. The group U(1) is the group of phases:

$$U(1) = \{e^{i\theta} \mid \theta \in [0, 2\pi]\}.$$

It can be shown that all its irreducible unitary representations are one-dimensional complex representations which are characterized by an integer number, positive or negative, called the “charge”. The defining representation represents an element of the group U(1) with the phase $e^{i\theta}$ which “rotates” naturally a complex one-dimensional vector v ($v \in \mathbb{C}$, where \mathbb{C} denotes the field of complex numbers, which we interpret here as a one-dimensional complex vector space):

$$v \xrightarrow{g \in U(1)} v' = e^{i\theta} v, \quad v \in \mathbb{C}.$$

Thus, the vector space of the defining representation is one-dimensional and complex, and the matrices of the representation are complex 1×1 matrices (i.e., complex numbers).

Objects that transform as tensor products of the defining representation:

$$v_{(q)} \sim \underbrace{vv \cdots v}_{q \text{ times}} = v^q$$

with q an integer give rise to the *representation of charge q* :

$$v_{(q)} \xrightarrow{g \in U(1)} v'_{(q)} = e^{iq\theta} v_{(q)}.$$

The number q can also be negative, as seen by tensoring the antifundamental representation acting on \bar{v} , but it remains an integer. Thus, all irreducible representations of $U(1)$ are one-dimensional and characterized by an integer q , called the **charge of the representation**.⁸

The tensor product of a representation with charge q_1 with a representation with charge q_2 yields the representation with charge $q_1 + q_2$. The symmetry group $U(1)$ is used in physics when there are *quantized additive quantum numbers*. Since all its representations are one-dimensional, to distinguish the various inequivalent representations, one indicates the charge q of the representation rather than its dimension.

What has been analyzed so far also allows us to interpret the possible charges (**generalized charges**, such as electric charge, color charge, etc.) of particles and associate them with a representation of the corresponding symmetry group. For example, the Standard Model of elementary particles contains the symmetry group $SU(3) \times SU(2) \times U(1)$, called the **gauge symmetry group**. The fermions of the Standard Model have generalized charges under these groups.

We can indicate these charges using a notation of the form $(SU(3), SU(2))_{U(1)}$, where for the non-abelian groups ($SU(N)$) we specify the representation by its corresponding dimension, while for the abelian part we use the $U(1)$ charge, called **hypercharge** Y . Anticipating that fermions can be decomposed into right-handed (R) and left-handed (L) fermions, with possibly different charges, one has so far discovered in nature elementary fermions with the following charges:

⁸Not to be confused with the dimension of the representation, which is always 1.

$\begin{pmatrix} \nu_e^L \\ e^L \end{pmatrix}$	ν_e^R	e^R	$\begin{pmatrix} u^L \\ d^L \end{pmatrix}$	u^R	d^R
$\begin{pmatrix} \nu_\mu^L \\ \mu^L \end{pmatrix}$	ν_μ^R	μ^R	$\begin{pmatrix} c^L \\ s^L \end{pmatrix}$	c^R	s^R
$\begin{pmatrix} \nu_\tau^L \\ \tau^L \end{pmatrix}$	ν_τ^R	τ^R	$\begin{pmatrix} t^L \\ b^L \end{pmatrix}$	t^R	b^R
$(1, 2)_{-\frac{1}{2}}$	$(1, 1)_0$	$(1, 1)_{-1}$	$(3, 2)_{\frac{1}{6}}$	$(3, 1)_{\frac{2}{3}}$	$(3, 1)_{-\frac{1}{3}}$

Table 1.1: From this classification we can deduce the properties of the elementary fermions of the Standard Model under the gauge symmetry group $SU(3) \times SU(2) \times U(1)$. The left table contains the leptons (electron, muon, tau, and their corresponding neutrinos), while the right table contains the quarks (up, down, charm, strange, top, bottom). The left-handed fermions are grouped into doublets of $SU(2) = 2$, since they can interact weakly, while the right-handed ones are singlets, scalars of the weak interaction ($SU(2) = 1$). Leptons do not feel the strong interaction, so they are singlets of $SU(3) = 1$ (and thus colorless), while quarks transform in the fundamental representation of $SU(3) = 3$, since they feel the strong interaction. The hypercharge Y under $U(1)$ is indicated as a subscript, and it is related to the electric charge as explained in the text.

The group $SU(3)$ is called the **color group**, and the quarks transform in the fundamental representation (3) , and thus have three “colors”, while the corresponding antiparticles, the antiquarks, transform in the complex conjugate representation $(\bar{3})$, and thus have three “anticolors”. Leptons do not feel the strong force and, therefore, are singlets under the color group.

The group $SU(2)$ is called the **weak isospin group**, and the $SU(2)$ doublets have been written above in the form of column vectors: they transform in the two-dimensional representation (2) , and thus have weak isospin $I = \frac{1}{2}$, with the third component $I_3 = \frac{1}{2}$ for the upper element of the vector and $I_3 = -\frac{1}{2}$ for the lower one. Note that the 2 is equivalent to the $\bar{2}$, both identifying the same representation with weak isospin equal to $\frac{1}{2}$.

$U(1)$ is the **hypercharge group**. If we denote by Y the hypercharge of a particle, the corresponding electric charge Q is given by

$$Q = I_3 + Y$$

where I_3 denotes the third component of the weak isospin. From the above table, one may extract which are the electric charges of these elementary particles.

1.4 | Lie Groups and Lie Algebras

A Lie group is, by definition, a group whose elements depend continuously on some parameters. By studying the infinitesimal group transformations, i.e., those transformations that differ slightly from the identity, one obtains the so-called Lie algebra of the group, an algebra that summarizes essential information about the group. In particular, the Lie algebra captures the non-abelian structure of the group. To introduce these topics, we first study some of the simplest yet most commonly used groups in physics and then list general properties and definitions.

1.4.1 | SO(2)

Consider the familiar group of rotations in two-dimensional Euclidean space, the group SO(2) of real orthogonal 2×2 matrices with determinant equal to 1. These matrices generate the transformations of a vector

$$\vec{x} \rightarrow \vec{x}' = R\vec{x}$$

or in tensor notation $x'^i = R^i_j x^j$ with $i, j = 1, 2$. This is the defining (or vector) representation. The rotations that mix the two components of the vector $\vec{x} = (x, y) = (x^1, x^2)$ depend on an angle θ and can be written as

$$R(\theta) = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} \xrightarrow{\theta \rightarrow 0} \begin{pmatrix} 1 & \theta \\ -\theta & 1 \end{pmatrix} = 1 + i\theta T \quad (1.4.1)$$

where the matrix T is the operator that “generates” the infinitesimal part of the transformation

$$T = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (1.4.2)$$

The imaginary unit i in (1.4.1) is conventional but allows us to present the generator T as a Hermitian matrix (whose eigenvalues are real).

The group is abelian: its elements commute

$$R(\theta_1)R(\theta_2) = R(\theta_2)R(\theta_1),$$

and thus

$$[T, T] = 0, \quad (1.4.3)$$

where $[., .]$ denotes the commutator ($[A, B] = AB - BA$). This is called the Lie algebra of SO(2). In general, the Lie algebra of a group is generated by the commutators of its infinitesimal generators, and it can be proven that if the commutator of the generators is non zero then the group is non-abelian.

Exponential map. Finite transformations can be obtained by iterating infinitesimal transformations (if the parameter θ is not infinitesimal, consider θ with n large enough to make it infinitesimal). Then, one can write⁹

$$[R(\theta)] \approx \left[R\left(\frac{\theta}{n}\right) \right]^n \approx (1 + i\frac{\theta}{n}T)^n \sim \left(e^{i\frac{\theta}{n}T} \right)^n = e^{i\theta T} = \mathbb{I} \cos(\theta) + iT \sin(\theta), \quad (1.4.4)$$

⁹In the end, if one expands the exponential map as a Taylor series, it can be recognized the final expression, since the generator T is idempotent: $T^2 = \mathbb{I}$. Thus it appears only on the odd powers of the expansion, while the even powers give rise to the identity matrix.

which reproduces the finite transformation in (1.4.1). The notation $e^{i\theta T}$, which contains the infinitesimal generator T and the continuous Lie parameter θ of the group, is the **exponential representation** of the elements of the group $\text{SO}(2)$. It generalizes to arbitrary Lie groups.

Here, we have obtained the Lie algebra of the group $\text{SO}(2)$ (1.4.3) by considering the defining representation of $\text{SO}(2)$, which is enough to recognize its abstract Lie algebra. Then, one can study the various representations of the $\text{SO}(2)$ Lie algebra in terms of other matrices and classify inequivalent representations.

Note that by defining the complex number $z = x + iy$, the $\text{SO}(2)$ transformation of (x, y) takes the form of $\text{U}(1)$ a phase transformation:

$$\begin{aligned} z' &= x' + iy' = (x \cos(\theta) + y \sin(\theta)) + i(-x \sin(\theta) + y \cos(\theta)) \\ &= (\cos(\theta) - i \sin(\theta))(x + iy) = e^{-i\theta} z. \end{aligned}$$

The groups $\text{SO}(2)$ and $\text{U}(1)$ are equivalent, $\text{SO}(2) \cong \text{U}(1)$.

1.4.2 | $\text{SO}(3)$

Consider now the group of rotations in three-dimensional space, the group $\text{SO}(3)$ of real orthogonal 3×3 matrices with determinant equal to 1. These matrices generate transformations of a three-dimensional vector $\vec{x} \rightarrow \vec{x}' = R\vec{x}$. Consider the rotations around the three Cartesian axes with coordinates $(x, y, z) = (x^1, x^2, x^3)$

$$\begin{aligned} R_x(\theta_x) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta_x) & \sin(\theta_x) \\ 0 & -\sin(\theta_x) & \cos(\theta_x) \end{pmatrix} = 1 + \theta_x \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} + \dots \\ R_y(\theta_y) &= \begin{pmatrix} \cos(\theta_y) & 0 & -\sin(\theta_y) \\ 0 & 1 & 0 \\ \sin(\theta_y) & 0 & \cos(\theta_y) \end{pmatrix} = 1 + \theta_y \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} + \dots \\ R_z(\theta_z) &= \begin{pmatrix} \cos(\theta_z) & \sin(\theta_z) & 0 \\ -\sin(\theta_z) & \cos(\theta_z) & 0 \\ 0 & 0 & 1 \end{pmatrix} = 1 + \theta_z \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \dots \end{aligned}$$

so that the generators T^i of the infinitesimal transformations are given by

$$T^1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad T^2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad T^3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (1.4.5)$$

The corresponding Lie algebra is easily computed by calculating the commutators of the matrices just identified

$$[T^i, T^j] = i\epsilon^{ijk}T^k, \quad (1.4.6)$$

where ϵ^{ijk} is the Levi-Civita antisymmetric tensor defined by $\epsilon^{123} = 1$ and antisymmetric under the exchange of any pair of indices.

The right-hand side is not zero, indicating that the group is non-abelian (the group elements do not commute). The constants ϵ^{ijk} are called the **structure constants** of the $\text{SO}(3)$ group

because they encode the non-abelian structure of the group. A finite element of the group can be parameterized in exponential form as

$$R(\vec{\theta}) = e^{i\vec{\theta} \cdot \vec{T}} = e^{i\theta_i T^i}, \quad (1.4.7)$$

where θ_i are the independent parameters of the group (a rotation of angle $\theta = \sqrt{\vec{\theta} \cdot \vec{\theta}}$ around the axis of the unit vector $\hat{n} = \vec{\theta}/\theta$).

To understand the role of the Lie algebra, let us study the product

$$R(\vec{\alpha})R(\vec{\beta})R^{-1}(\vec{\alpha})R^{-1}(\vec{\beta}),$$

that would be the identity of an abelian group (which have commuting operators, thus we could swap the positions of the elements and simplify them with their inverse). For infinitesimal parameters and working at the linear order in both $\vec{\alpha}$ and $\vec{\beta}$:

$$\begin{cases} R(\vec{\alpha}) = \mathbb{I} + A = \mathbb{I} + i\alpha_i T^i, \\ R(\vec{\beta}) = \mathbb{I} + B = \mathbb{I} + i\beta_i T^i, \end{cases}$$

one finds

$$\begin{aligned} R(\vec{\alpha})R(\vec{\beta})R^{-1}(\vec{\alpha})R^{-1}(\vec{\beta}) &= (\mathbb{I} + A)(\mathbb{I} + B)(\mathbb{I} - A)(\mathbb{I} - B) \\ &= \mathbb{I} + A^2 + B^2 - A^2 - B^2 + AB - BA + \dots \\ &= \mathbb{I} + [A, B], \end{aligned}$$

and since $A = i\alpha_i T^i$, $B = i\beta_i T^i$, we have (up to second order corrections):

$$\begin{aligned} R(\vec{\alpha})R(\vec{\beta})R^{-1}(\vec{\alpha})R^{-1}(\vec{\beta}) &= \mathbb{I} + [i\alpha_i T^i, i\beta_j T^j] \\ &= \mathbb{I} - \alpha_i \beta_j [T^i, T^j] = \mathbb{I} + i\gamma_k T^k, \end{aligned}$$

which is nonvanishing for the non-abelian group SO(3):¹⁰ the Lie algebra captures the non-commutative structure of the Lie group. In addition, one understands that the result must correspond to an infinitesimal group transformation, just like the left-hand side, so that the commutator $[T^i, T^j]$ must be proportional to a generator, as indeed verified in (1.4.6):

$$\gamma_k = -\alpha_i \beta_j f^{ij}_k,$$

where the constants f^{ij}_k are identified with the structure constants of the group, which in this case are recognized to be $f^{ij}_k \sim \epsilon^{ijk}$.

We have obtained the Lie algebra using the defining representation, and now we can consider it as the abstract Lie algebra of the group SO(3) and study its different irreducible representations, as done for the representations of the group. From the representations of the group studied previously, one obtains the corresponding representations of the associated Lie algebra. Conversely, exponentiating the matrices of a representation of the Lie algebra yields finite transformations that provide a representation of the group.¹¹

SO(3) and quantum mechanics. Let us comment on the SO(3) Lie algebra and relate it to known topics studied in quantum mechanics. In equation (1.4.6), we recognize the algebra of the

¹⁰We have shown how this products can be rewritten as a rotation of an angle $\vec{\gamma}$: $\mathbb{I} + i\gamma_k T^k \sim R(\vec{\gamma})$.

¹¹Except for possible topological obstructions that might prevent the representation from being truly single-valued. This situation is exemplified by the spinor representations of SO(3), which, as we will see later, are true representations (i.e., single-valued representations) of the SU(2) group only.

quantum angular momentum operator. Renaming $T^i \rightarrow L^i$, we recognize the familiar algebra of the angular momentum (in units of $\hbar = 1$)

$$[L^i, L^j] = i\epsilon^{ijk}L^k.$$

The study of its irreducible unitary representations is solved explicitly using the methods of quantum mechanics: the known result is that these irreducible representations are those given by the spherical harmonics $|l, m\rangle \sim Y_{lm}$, which for fixed l form a basis of the spin- l representation. It is $(2l + 1)$ -dimensional, as for fixed l the possible values of m are $2l + 1$:

$$Y'_{lm} = [R_{(l)}(\theta)]_m^n Y_{ln}, \quad l \text{ fixed}, \quad m, n \in [-l, -l + 1, \dots, 0, \dots, l - 1, l].$$

In the case of spinorial representations (i.e., with half-integer spin, i.e., with $l \rightarrow j$ and j half-integer), a rotation by 2π (which for $\text{SO}(3)$ coincides with the identity) is represented by the matrix $-\mathbb{I}$, and thus we speak of a 2-valued representation (one needs to rotate by another 2π to get back to the identity). As we will see, these spinorial representations are true representations of the $\text{SU}(2)$ group, which has the same Lie algebra as $\text{SO}(3)$ and therefore has the same local structure but different global properties.

Hints on generalization. To appreciate future developments (such as the Lie algebras of $\text{SO}(N)$ and $\text{SO}(N, M)$), let's rewrite the matrices identifying the generators in the vector representation (1.4.5) and the corresponding Lie algebra in (1.4.6) in an alternative way. We can rename the generator T^1 as T^{23} , as it generates a rotation in the 2-3 plane, and so on: $T^2 \equiv T^{31}$, $T^3 \equiv T^{12}$. The matrix elements in (1.4.5) can be written as

$$(T^1)^i_j \equiv (T^{23})^i_j = -i(\delta^{2i}\delta^3_j - \delta^{3i}\delta^2_j),$$

and similarly for T^{31} and T^{12} . Thus, the general expression obtained is

$$(T^{kl})^i_j = -i(\delta^{ki}\delta^l_j - \delta^{li}\delta^k_j),$$

which can be used to recalculate the Lie algebra of $\text{SO}(3)$. Rewritten on this basis, the Lie algebra (1.4.6) becomes

$$[T^{kl}, T^{mn}] = -i\delta^{lm}T^{kn} + i\delta^{km}T^{ln} + i\delta^{ln}T^{km} - i\delta^{kn}T^{lm}.$$

Note the presence of the Euclidean (inverse) metric δ^{ij} in this relation. Written in this form, the Lie algebra is valid for the generic group $\text{SO}(N)$, provided that the indices range from 1 to N. There are thus $\frac{1}{2}N(N - 1)$ independent generators. Moreover, by replacing the metric δ^{ij} with a Minkowski metric η^{ij} , appropriate for a spacetime with N spatial and M temporal dimensions, one obtains the Lie algebra of $\text{SO}(N, M)$.

1.4.3 | $\text{U}(1)$

Consider the group $\text{U}(1) = \{e^{i\theta} \mid \theta \in [0, 2\pi]\}$, the group of phases defined via its defining representation. For infinitesimal transformations (up to second order corrections in θ) we have:

$$e^{i\theta} = 1 + i\theta,$$

where the infinitesimal generator is given by $T = 1$ (we can think of it as a 1×1 matrix), which produces the Abelian Lie algebra of the $\text{U}(1)$ group given by the commutator

$$[T, T] = 0. \tag{1.4.8}$$

In the charge q representation, where the element $e^{i\theta}$ is represented by $e^{iq\theta}$, the infinitesimal generator is represented by $T = q$ and satisfies the same Lie algebra (1.4.8). Therefore, we can think of the Lie algebra $[T, T] = 0$ as the abstract Lie algebra corresponding to the $U(1)$ group, which is represented by different matrices in different representations. Since the irreducible representations of the $U(1)$ group are all one-dimensional, all these matrices are 1×1 matrices and thus are simply numbers. In the charge q representation, the generator of $U(1)$ is represented by $T = q$. It is also common to use the notation Q (which often denotes a charge) instead of T for the generator of the $U(1)$ group. The groups $U(1)$ and $SO(2)$ identify the same Abelian Lie group, as already described.

1.4.4 | $SU(2)$

Let's now analyze the group $SU(2)$, the group of 2×2 unitary matrices with unit determinant:

$$SU(2) = \{U \text{ complex matrices } 2 \times 2 \mid U^\dagger = U^{-1}, \det U = 1\}.$$

We can write the matrices that differ infinitesimally from the identity matrix as

$$U = 1 + iT, \quad T^i_j \ll 1.$$

Now, the requirement of unitarity $U^\dagger = U^{-1}$, along with the infinitesimal form above of U

$$\begin{cases} U^\dagger &= 1 - iT^\dagger, \\ U^{-1} &= 1 - iT, \end{cases} \quad \text{with } U^\dagger = U^{-1},$$

implies that the matrices T must be Hermitian:

$$T^\dagger = T,$$

while the requirement for unit determinant, $\det U = 1 + i \operatorname{Tr} T = 1$,¹² implies that these matrices must be traceless:

$$\operatorname{Tr} T = 0.$$

A basis of Hermitian traceless 2×2 matrices is given by the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (1.4.9)$$

so we can express an arbitrary matrix T as a linear combination of the σ^a :

$$T = \theta_a \frac{\sigma^a}{2} = \theta_a T^a, \quad T^a = \frac{1}{2} \sigma^a, \quad a = 1, 2, 3, \quad (1.4.10)$$

The normalization has been chosen to satisfy

$$\operatorname{Tr}(T^a T^b) = \frac{1}{2} \delta^{ab}, \quad (1.4.11)$$

With this normalization, the infinitesimal generators $T^a = \frac{1}{2} \sigma^a$ give rise to the following $SU(2)$ Lie algebra:

$$[T^a, T^b] = i \epsilon^{abc} T^c, \quad (1.4.12)$$

¹²Intuitively, when computing the determinant of $I + \epsilon$, where ϵ is a small matrix, the determinant is approximately $1 + \operatorname{Tr} \epsilon$ (since all the components out of the diagonal are infinitesimal).

which is recognized to coincide with the Lie algebra of $\text{SO}(3)$ in (1.4.6). This shows that locally they are similar (they have the same structure constants), although globally there are differences: using the language of differential geometry, we can say that the group $\text{SU}(2)$ is a double cover of the group $\text{SO}(3)$. This difference is seen explicitly in the defining representation of $\text{SU}(2)$ (the spin- $\frac{1}{2}$ or 2 representation).

A finite rotation is obtained by exponentiating infinitesimal transformations to make them finite:

$$U(\vec{\theta}) = \exp(i\theta_a T^a). \quad (1.4.13)$$

In particular, a finite rotation around the z -axis is obtained by choosing $\theta^3 = \theta$ and $\theta^1 = \theta^2 = 0$, to find a matrix $U_3(\theta)$ given by

$$\begin{aligned} U_3(\theta) &= e^{i\theta T^3} = e^{i\theta \frac{\sigma^3}{2}} = \sum_{n=0}^{\infty} \frac{(i\frac{\theta}{2}\sigma^3)^n}{n!} = \mathbb{I} \cos(\theta/2) + i\sigma^3 \sin(\theta/2) \\ &= \begin{pmatrix} \cos(\theta/2) + i \sin(\theta/2) & 0 \\ 0 & \cos(\theta/2) - i \sin(\theta/2) \end{pmatrix} = \begin{pmatrix} e^{i\theta/2} & 0 \\ 0 & e^{-i\theta/2} \end{pmatrix}, \end{aligned}$$

where again we have used the idempotent property of the Pauli matrices, $(\sigma^3)^2 = \mathbb{I}$ to group the even and odd powers of the expansion separately.

Setting $\theta = 2\pi$ gives the transformation

$$U_3(\theta = 2\pi) = -\mathbb{I},$$

which does not coincide with the identity in $SU(2)$. The identity transformation is obtained only for $\theta = 4\pi$. As known from quantum mechanics, all irreducible unitary representations of $SU(2)$ are characterized by a quantum number j that can be either an integer or a half-integer. They are of dimension $2j + 1$.

Historical Note: Pauli introduced the matrices in (1.4.9) to describe the electron's spin, defining the spin operator $\vec{S} = \frac{1}{2}\vec{\sigma}$, which acts on a two-component wave function (spinor).

1.4.5 | $\text{SU}(3)$

The same analysis performed to extract the infinitesimal generators of $SU(2)$ applies also to the general $SU(N)$ group, whose generators are then seen to be traceless, Hermitian, $N \times N$ matrices. There are $N^2 - 1$ of such matrices, so that there are $N^2 - 1$ independent Lie parameters for the group $SU(N)$. In particular, the eight infinitesimal generators of $SU(3)$ in the fundamental representation are given by the Gell-Mann matrices λ^a , which form a basis of Hermitian 3×3 traceless matrices (generalizing the Pauli matrices σ^a for $SU(2)$):

$$T^a = \frac{1}{2}\lambda^a, \quad a = 1, \dots, 8, \quad (1.4.14)$$

where the Gell-Mann matrices are

$$\begin{aligned}\lambda^1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda^2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda^3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ \lambda^4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & \lambda^5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, & \lambda^6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \\ \lambda^7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, & \lambda^8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix},\end{aligned}\tag{1.4.15}$$

where λ^3 and λ^8 are diagonal (and λ^8 is not uniquely defined). The maximal number of simultaneously diagonalizable generators is called the rank of the group. The rank of $SU(3)$ is 2, while the rank of $SU(N)$ is $N - 1$. The above matrices are normalized so that

$$\text{Tr}(T^a T^b) = \frac{\delta^{ab}}{2},\tag{1.4.16}$$

just as was done for $SU(2)$, see eq. (1.4.11). An arbitrary element of the $SU(3)$ group in the fundamental representation is thus described by 3×3 matrices of the form

$$U(\theta) = e^{i\theta_a T^a},\tag{1.4.17}$$

where θ^a with $a = 1, \dots, 8$ are the eight parameters of the group. By calculating the Lie algebra, one finds the structure constants f^{abc} that correspond to the $SU(3)$ group:

$$[T^a, T^b] = if^{abc} T^c.\tag{1.4.18}$$

They are antisymmetric and given by:

$$f^{123} = 1, \quad f^{147} = -f^{156} = f^{246} = f^{257} = f^{345} = -f^{367} = \frac{1}{2}, \quad f^{458} = f^{678} = \frac{\sqrt{3}}{2}$$

while all other f^{abc} not related to these by permuting indices are zero. This group has important applications in the description of color associated with strong interactions and in the quark model that classifies the hadrons composed of the three lightest flavors of quarks (up, down, strange).

1.4.6 | General Case

We summarize for arbitrary Lie groups what was illustrated above through examples. A Lie group is, by definition, a group of transformations that depend continuously on some parameters. By studying the infinitesimal transformations of the group, i.e., transformations that differ only slightly from the identity, we recognize the generators, operators that “generate” the infinitesimal transformations (and by repetition finite transformations). They identify the so-called Lie algebra of the group, which summarizes information about the group.

In general, an element $g(\theta)$ of a Lie group G (or, more precisely, of the component connected to the identity) can be parametrized by an **exponential map** in the following way:

$$g(\theta) = e^{i\theta_a T^a}, \quad a = 1, \dots, \dim G,\tag{1.4.19}$$

where the parameters θ_a are real numbers that parametrize the various elements of the group. They are chosen so that for $\theta_a = 0$ one gets the identity $g = \mathbb{I}$. The operators T^a are the **generators**

of the group. Considering the group as a group of $N \times N$ matrices for some N (for example, the defining representation), the generators are also $N \times N$ matrices. They generate infinitesimal transformations when $\theta_a \ll 1$. Simply expand the exponential function in a Taylor series and keep the lowest order terms:

$$g(\theta) = 1 + i\theta_a T^a + \dots$$

By studying the relations that capture the composition properties of the group using infinitesimal transformations (which are generically non-commutative), one obtains the **Lie algebra** of the group G :

$$[T^a, T^b] = if^{ab}_c T^c. \quad (1.4.20)$$

The constants f^{ab}_c are called **structure constants** of the group and characterize it. Groups with the same Lie algebra may only differ in their topology but are locally similar. It is useful to mention the **Jacobi identities**:

$$f^{ab}_d f^{dc}_e + f^{bc}_d f^{da}_e + f^{ca}_d f^{db}_e = 0, \quad (1.4.21)$$

which are quadratic relations satisfied by the structure constants and emerge as a consequence of the operatorial Jacobi identities (given by the associativity of the operator product):

$$[[T^a, T^b], T^c] + [[T^b, T^c], T^a] + [[T^c, T^a], T^b] = 0. \quad (1.4.22)$$

We have indeed:

$$\begin{aligned} [[T^a, T^b], T^c] &= if^{ab}_d [T^d, T^c] = if^{ab}_d (if^{dc}_e T^e) = -f^{ab}_d f^{dc}_e T^e, \\ [[T^b, T^c], T^a] &= -f^{bc}_d f^{da}_e T^e, \\ [[T^c, T^a], T^b] &= -f^{ca}_d f^{db}_e T^e, \end{aligned}$$

so that summing these three expressions and imposing (1.4.22) leads to (1.4.21), and the identities are null since expliciting all the commutators in the operatorial identity leads to a vanishing sum.

The structure constants can be used to define the **adjoint representation** $T_{(A)}^a$ of the Lie algebra, given by the formula:

$$(T_{(A)}^a)_c^b = -if^{ab}_c. \quad (1.4.23)$$

It is verified to be a representation of the Lie algebra thanks to the Jacobi identities:

$$(T_{(A)}^a)_g^d (T_{(A)}^b)_f^g - (T_{(A)}^b)_g^d (T_{(A)}^a)_f^g = if^{ab}_c (T_{(A)}^c)_f^d,$$

which, substituting the definition of the adjoint representation, is equivalent to (1.4.21):

$$\begin{aligned} -f^{ad}_g f^{bg}_f + f^{bd}_g f^{ag}_f &= f^{ab}_c f^{cd}_f \\ \rightarrow f^{ab}_g f^{gd}_f + f^{bd}_g f^{ga}_f + f^{da}_g f^{gb}_f &= 0, \end{aligned}$$

after renaming indices appropriately and using the antisymmetry of the structure constants in the first two indices. It is a real representation because the structure constants are real numbers, and it is a representation of dimension equal to the dimension of the group, since the indices $a, b, c = 1, \dots, \dim G$.

Finally, it is useful to mention the **Baker-Campbell-Hausdorff formula** for the product of exponentials of two linear operators A and B :

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,[A,B]]-\frac{1}{12}[B,[A,B]]+\dots} \quad (1.4.24)$$

where the dots indicate higher-order terms, always expressible in terms of commutators. This formula shows that the knowledge of the Lie algebra is sufficient to reconstruct the (generally non-commutative) product of the elements of the corresponding Lie group.

To summarize, let us list and review some of the main definitions and properties of Lie algebras:

- (i) $g = e^{i\theta_a T^a} \in G, \quad a = 1, \dots, \dim G.$
- (ii) $[T^a, T^b] = if^{ab}_c T^c.$
- (iii) $\text{Tr}\left(T_{(F)}^a T_{(F)}^b\right) = \gamma^{ab}$ (generators in the fundamental representation).
- (iv) $[[T^a, T^b], T^c] + [[T^b, T^c], T^a] + [[T^c, T^a], T^b] = 0 \Rightarrow f^{ab}_d f^{dc}_e + f^{bc}_d f^{da}_e + f^{ca}_d f^{db}_e = 0.$
- (v) $f^{abc} = f^{ab}_d \gamma^{dc}$ (completely antisymmetric tensor).

Point (i) describes the *exponential parametrization* of an arbitrary element of the group that is connected to the identity. The index a takes as many values as the dimensions of the group. An element of the group is parametrized by the parameters θ_a with $a = 1, \dots, \dim G$.

Point (ii) corresponds to the *Lie algebra* satisfied by the infinitesimal generators T^a . The structure constants f^{ab}_c are antisymmetric on indices a and b and characterize the group G .

Point (iii) identifies (the inverse of) a metric γ^{ab} called the “**Killing metric**”. This metric is positive-definite only for compact and simple Lie groups, such as $SU(N)$ or $SO(N)$. Being positive, it is often normalized to the Kronecker delta: $\gamma^{ab} = \delta^{ab}$.

Point (iv) amounts to the so-called “*Jacobi identities*” satisfied by the structure constants. They can be used to construct the adjoint representation of the Lie algebra. Denoting by $(T_{(A)}^a)^b_c$ the matrix elements of the generators of the adjoint representation $T_{(A)}$, we have $(T_{(A)}^a)^b_c = -if^{ab}_c$. The Jacobi identities imply that this is a representation. It is real and of dimension equal to the dimension of the group since the indices $a, b, c = 1, \dots, \dim G$. By exponentiation, it gives rise to a representation of the group.

In point (v), the Killing metric is used to raise an index of the structure constants. Then, f^{abc} are completely antisymmetric in all indices: antisymmetry in the indices a and b is obvious from (ii), while antisymmetry in the indices b and c is deduced by taking the trace of the Jacobi identities in (iv) and using (ii) and (iii):

$$\begin{aligned} \text{Tr}([T^a, T^b]T^c) &= if^{ab}_d \text{Tr}(T^d T^c) = if^{ab}_d \frac{\gamma^{dc}}{2} = \frac{i}{2} f^{abc} \\ &= \text{Tr}(T^a T^b T^c) - \text{Tr}(T^b T^a T^c) = \text{Tr}(T^c T^a T^b) - \text{Tr}(T^c T^a T^b) \\ &= -\text{Tr}([[T^a, T^c], T^b]) = -\frac{i}{2} f^{acb}, \end{aligned}$$

where we have used the cyclicity property of the trace, thus proving antisimmetry in the indices b and c . By combining the two antisymmetries, one finds that f^{abc} is completely antisymmetric.

Finally, we conclude with the statement of a theorem which we shall not prove:

Theorem 1.1. *The unitary irreducible representations of compact groups are finite-dimensional, while the unitary representations of non-compact groups must be infinite-dimensional.*

Thus, compact groups such as $SO(N)$ and $SU(N)$ have unitary finite-dimensional irreps. Non-compact groups, such as the Lorentz group $SO(3, 1)$ and the Poincaré group $ISO(3, 1)$, have unitary

representations that must be infinite-dimensional. For applications in relativistic field theory, it is useful to have some knowledge of:

- The finite-dimensional representations of the Lorentz group. They are not unitary and are used to label the quantum fields that define a given relativistic QFT.
- The unitary representations of the Poincaré group, which are infinite-dimensional and are realized in the Hilbert space of quantum field theories via unitary operators.

1.5 | Special relativity and the Lorentz group

Let us review the main points of special relativity, keeping in mind group theory applied to the Lorentz group $\text{SO}(3, 1)$. The standard Lorentz transformation that relates the spacetime coordinates of two inertial frames in relative motion with constant velocity v along the x axis are given by

$$\begin{pmatrix} ct' \\ x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}$$

where $\beta = \frac{v}{c}$ and $\gamma = \frac{1}{\sqrt{1-\beta^2}}$. Taking the relative velocity v to be positive, we see that $0 < \beta < 1$ and $1 < \gamma < \infty$. Denoting by x the column 4-vector with components x^μ

$$x^\mu = \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix},$$

we can write more compactly the Lorentz transformation in the equivalent forms as

$$x' = \Lambda x, \quad x'^\mu = \Lambda^\mu_\nu x^\nu.$$

This transformation is seen to leave invariant the light cone at the origin. More generally, it leaves invariant the modulus square of the 4-vector x^μ , which is defined in the following way

$$s^2 = -c^2 t^2 + x^2 + y^2 + z^2 = x^T \eta x = \eta_{\mu\nu} x^\mu x^\nu = x^\mu x_\mu,$$

where η is the Minkowski metric

$$\eta = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (1.5.1)$$

It is also used to lower indices on vectors and tensors.

The general Lorentz group is defined as the group of linear transformations that leave invariant the scalar s^2 :

$$s'^2 = x'^T \eta x' = x^T \Lambda^T \eta \Lambda x = x^T \eta x \implies \Lambda^T \eta \Lambda = \eta,$$

or equivalently, in components

$$s'^2 = \eta_{\mu\nu} x'^\mu x'^\nu = \eta_{\mu\nu} \Lambda^\mu_\rho \Lambda^\nu_\sigma x^\rho x^\sigma = \eta_{\mu\nu} x^\mu x^\nu \implies \eta_{\mu\nu} \Lambda^\mu_\rho \Lambda^\nu_\sigma = \eta_{\rho\sigma}.$$

This invariance allows us to define the *group of Lorentz transformations* as

$$O(3, 1) = \{\text{real } 4 \times 4 \text{ matrices } \Lambda \mid \Lambda^T \eta \Lambda = \eta\} \quad (1.5.2)$$

This group contains the space-inversion (the parity transformation P) as well as time-inversion (the time reversal T), which can be eliminated from the group by defining the **proper orthochronous Lorentz group**

$$SO^+(3, 1) = \{\text{real } 4 \times 4 \text{ matrices } \Lambda \mid \Lambda^T \eta \Lambda = \eta, \det \Lambda = 1, \Lambda^0_0 \geq 1\}, \quad (1.5.3)$$

also called the restricted Lorentz group. By relativistic invariance, one generically refers to an invariance under the latter; parity and time reversal are usually treated separately.

Tensors are defined as usual for the Lorentz group. They are used to describe physical quantities and their transformation properties under changes of inertial frames. An example is the 4-momentum p^μ :

$$p^\mu = (p^0, \vec{p}) = \left(\frac{E}{c}, \vec{p} \right) = \left(\frac{mc}{\sqrt{1 - \beta^2}}, \frac{m\vec{v}}{\sqrt{1 - \beta^2}} \right),$$

that transforms as a 4-vector and whose modulus square satisfies

$$p^\mu p_\mu = -m^2 c^2.$$

This last relation states that

$$E^2 = p^2 c^2 + m^2 c^4,$$

the well-known relativistic energy-momentum relation.

Similarly, the electric and magnetic fields \vec{E} and \vec{B} are recognized to be the components of an antisymmetric tensor field $F_{\mu\nu}$:

$$F^{\mu\nu} = \begin{pmatrix} 0 & E_x & E_y & E_z \\ -E_x & 0 & B_z & -B_y \\ -E_y & -B_z & 0 & B_x \\ -E_z & B_y & -B_x & 0 \end{pmatrix},$$

here written using Gaussian or Heaviside-Lorentz units. Under a Lorentz transformation, the electromagnetic tensor transforms according to the tensor laws as

$$F'^{\mu\nu} = \Lambda^\mu_\alpha \Lambda^\nu_\beta F^{\alpha\beta}.$$

From it, one can construct the scalar

$$F^{\mu\nu} F_{\mu\nu} = 2(B^2 - E^2),$$

which is proportional to the free Lagrangian of the electromagnetic field.

The *space-time derivatives* naturally form a vector with a lower index

$$\partial_\mu = \left(\frac{1}{c} \frac{\partial}{\partial t}, \nabla \right) \equiv \frac{\partial}{\partial x^\mu},$$

so that $\partial_\mu x^\mu$ is a scalar (i.e., $\partial^\mu x_\mu = \partial'_\mu x'^\mu = 4$).

Then, the inhomogeneous Maxwell's equations are written in a covariant form as

$$\partial_\mu F^{\mu\nu} = -\frac{1}{c} J^\nu,$$

where $J^\mu = (J^0, \vec{J}) = (c\rho, \vec{J})$ is the 4-vector charge-current density. The homogeneous Maxwell's equations take instead the following covariant form

$$\partial_\lambda F_{\mu\nu} + \partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} = 0. \quad (1.5.4)$$

The last equation can be integrated by introducing a four-potential A^μ and setting

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu.$$

It solves automatically eq. (1.5.4), as all terms cancel two by two. For this reason, using the last equation as a definition of the electromagnetic field, equation (1.5.4) becomes an identity often called Bianchi identity. The integration is not unique, since the potential A^μ can be transformed by a **gauge transformation** to a new potential A'^μ :

$$A'_\mu(x) = A_\mu(x) + \partial_\mu \alpha(x),$$

without changing the electromagnetic field tensor $F^{\mu\nu}$, as the gauge symmetry keeps the electromagnetic field invariant. Here $\alpha(x)$ is an arbitrary scalar function vanishing at infinity.

1.5.1 | Finite Dimensional Representations of the Lorentz Group

First, it is useful to derive the Lie algebra of the Lorentz group. For infinitesimal transformations, we can write

$$\Lambda^\mu_\nu = \delta^\mu_\nu + \omega^\mu_\nu, \quad |\omega^\mu_\nu| \ll 1, \quad (1.5.5)$$

and imposing the condition that defines Lorentz transformations ($\eta_{\rho\sigma} = \eta_{\mu\nu}\Lambda^\mu_\rho\Lambda^\nu_\sigma$), we obtain that $\omega_{\mu\nu}$ must satisfy the antisymmetric condition

$$\omega_{\mu\nu} = -\omega_{\nu\mu},$$

(indices are lowered as usual, $\omega_{\mu\nu} = \eta_{\mu\rho}\omega^\rho_\nu$). Thus, they contain six independent parameters identified with the $\omega_{\mu\nu}$ with fixed indices $\mu < \nu$.

Then, in matrix notation, we can re-write an arbitrary infinitesimal Lorentz transformation by making explicit the infinitesimal parameters that multiply the corresponding generators

$$\Lambda = 1 + \frac{1}{2}\omega_{\mu\nu}M^{\mu\nu}. \quad (1.5.6)$$

The six matrices $M^{\mu\nu}$ with $\mu < \nu$ are the independent generators of the Lorentz group. In the defining representation (the “four-vector” representation), they are given by

$$(M^{\mu\nu})^\rho_\sigma = -i(\eta^{\mu\rho}\delta^\nu_\sigma - \eta^{\nu\rho}\delta^\mu_\sigma), \quad (1.5.7)$$

so that eq. (1.5.6) reproduces eq. (1.5.5). For example, some of these generators can be written explicitly as

$$M^{12} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad M^{01} = \begin{pmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

where M_{12} generates infinitesimal rotations around the z -axis, while M_{01} generates a boost along the x -axis.

Although it might seem tedious, it is straightforward to calculate the Lie algebra

$$[M^{\mu\nu}, M^{\rho\sigma}] = -i(\eta^{\mu\rho}M^{\nu\sigma} - \eta^{\nu\rho}M^{\mu\sigma} + \eta^{\nu\sigma}M^{\mu\rho} - \eta^{\mu\sigma}M^{\nu\rho}). \quad (1.5.8)$$

This is also valid for any generic group $\text{SO}(N, M)$ if one identifies $\eta_{\mu\nu}$ with the corresponding metric: in particular, to obtain $\text{SO}(3)$ one sets $\eta_{\mu\nu} \rightarrow \delta_{ij}$ and defining $J^i = \epsilon^{ijk}M^{jk}$ one recovers the form of the $\text{SO}(3)$ Lie algebra given in eq.(1.4.6) with $T^i = J^i$.

Returning to the specific case of $\text{SO}(3, 1)$, one can rewrite the algebra in a more useful form that allows us to deduce immediately its finite-dimensional representations. Separating the indices into time and space parts $\mu = (0, i)$, and defining the following basis for the generators of the Lorentz group

$$J^i = \frac{1}{2}\epsilon^{ijk}M^{jk}, \quad K^i = M^{i0},$$

the Lie algebra (1.5.8) can be rewritten as

$$[J^i, J^j] = i\epsilon^{ijk}J^k, \quad [J^i, K^j] = i\epsilon^{ijk}K^k, \quad [K^i, K^j] = -i\epsilon^{ijk}J^k, \quad (1.5.9)$$

where the generators J^i generate the spatial rotation subgroup $\text{SO}(3)$, while K^i generate boosts. Finally, defining the complex linear combinations

$$N^i = \frac{1}{2}(J^i - iK^i), \quad \bar{N}^i = \frac{1}{2}(J^i + iK^i) \quad (1.5.10)$$

the algebra can be rewritten as

$$[N^i, N^j] = i\epsilon^{ijk}N^k, \quad [\bar{N}^i, \bar{N}^j] = i\epsilon^{ijk}\bar{N}^k, \quad [N^i, \bar{N}^j] = 0, \quad (1.5.11)$$

which shows that the algebra of $\text{SO}(3, 1)$ is equivalent to that of $\text{SU}(2) \times \text{SU}(2)$, up to different hermiticity relations (arising because $\text{SO}(3, 1)$ is not compact, while $\text{SU}(2)$ is). Since $\text{SO}(3, 1)$ reduces to two independent copies of $\text{SU}(2)$, the well-known finite-dimensional representations of the latter can be used to find the finite-dimensional representations of $\text{SO}(3, 1)$: they are classified by two integer or half-integer numbers (j_1, j_2) corresponding to the representations of the two subgroups $\text{SU}(2)$ generated by N^i and \bar{N}^i . Furthermore, recalling (1.5.10), the spin operator corresponds to $J^i = N^i + \bar{N}^i$, so that the highest spin content of the representation is given by $j = j_1 + j_2$. These representations are finite-dimensional but are not unitary due to the necessity of taking complex combinations of the generators in (1.5.10).

In quantum field theory, fields with these Lorentz representations are used to describe particles with fixed spin, for example

$$\begin{aligned} (0, 0) &\longrightarrow \text{scalar } \phi \\ (\frac{1}{2}, 0) &\longrightarrow \text{left-handed Weyl fermion } \psi_L \sim \xi^a \\ (0, \frac{1}{2}) &\longrightarrow \text{right-handed Weyl fermion } \psi_R \sim \bar{\eta}^{\dot{a}} \\ (\frac{1}{2}, 0) \oplus (0, \frac{1}{2}) &\longrightarrow \text{Dirac fermion } \psi \sim \psi^\alpha \\ (\frac{1}{2}, \frac{1}{2}) &\longrightarrow \text{spin-1 field } A^\mu \end{aligned}$$

Just as $\text{SO}(3) \rightarrow \text{SU}(2)$ allows to view the spinorial representations of $\text{SO}(3)$ as single-valued representations of $\text{SU}(2)$, a similar phenomenon happens for $\text{SO}(3, 1) \rightarrow \text{SL}(2, \mathbb{C})$: the Lie algebras of $\text{SO}(3, 1)$ and $\text{SL}(2, \mathbb{C})$ coincide and the latter is the covering group of the former.

1.5.2 | Unitary Representations of the Poincaré Group

The Poincaré group extends the Lorentz group with spacetime translations. It transforms the position four-vector as follows

$$x^\mu \rightarrow x'^\mu = \Lambda^\mu_\nu x^\nu + a^\mu$$

where Λ^μ_ν describes a Lorentz transformation and a^μ a spacetime translation. This group is sometimes referred to as the $\text{ISO}(3, 1)$ group, the inhomogeneous special orthogonal group, where the inhomogeneity refers to the translations.

The Lie algebra of the Poincaré group can be written as

$$\begin{aligned}[P^\mu, P^\nu] &= 0, \quad [M^{\mu\nu}, P^\alpha] = -i(\eta^{\nu\alpha} P^\mu - \eta^{\mu\alpha} P^\nu), \\ [M^{\mu\nu}, M^{\rho\sigma}] &= -i(\eta^{\mu\rho} M^{\nu\sigma} - \eta^{\nu\rho} M^{\mu\sigma} + \eta^{\nu\sigma} M^{\mu\rho} - \eta^{\mu\sigma} M^{\nu\rho}),\end{aligned}\tag{1.5.12}$$

where P^μ are the generators of the translations and $M^{\mu\nu}$ are the generators of the Lorentz transformations¹³.

Its unitary irreducible representations are infinite-dimensional and have been classified by Wigner in 1939. They are classified according to the values of the so-called Casimir operators $P^2 = P^\mu P_\mu$ and $W^2 = W^\mu W_\mu$, where

$$W_\mu = \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} P^\nu M^{\rho\sigma}$$

is the so-called **Pauli-Lubanski vector**. It is seen, using equations (1.5.12), that P^2 and W^2 commute with all elements of the Poincaré algebra: they are invariant under infinitesimal transformations of the Poincaré group. Thus, they take constant values inside an irreducible representation, just like J^2 takes a constant value inside a fixed representation of the rotation group with generators J^i . The unitary representations of the Poincaré group are classified by the following values of the Casimir operators:

- $P^2 = -m^2 < 0$, $W^2 = m^2 s(s+1)$ with $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$: it corresponds to quantum particles of mass m and spin s . This unitary representation is associated with a Hilbert space that contains the allowed states of a relativistic particle with mass m and spin s .
- $P^2 = 0$, $W^2 = 0$ and with $W^\mu = \pm s P^\mu$ where $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$: massless particles with helicity s .
- $P^2 = 0$, $W^2 = \kappa^2 > 0$: massless “particles” with infinitely many states of “polarization” that can vary continuously: they do not seem to have any immediate application to field theory (at least at the perturbative level).
- $P^2 = \mu^2 > 0$: tachyonic representations, never used in physics (inconsistent with standard physical interpretations).
- $P^\mu = 0$, $W^\mu = 0$: trivial (scalar) representation \rightarrow vacuum (no particles).

For example, the physical case of mass m and spin s (i.e. the case with $P^2 = -m^2 < 0$ and $W^2 = m^2 s(s+1)$) corresponds to an infinite-dimensional vector space that is constructed as the Hilbert space spanned by vectors of the form

$$|\vec{p}, s_3\rangle, \quad \vec{p} \in \mathbb{R}^3, \quad s_3 = -s, \dots, +s,$$

which are the eigenstates of the linear momentum operator \vec{p} and of the component of the spin operator along the z -axis \hat{S}_3 . Unitary operators representing the Poincaré group transformations act on this infinite-dimensional Hilbert space.

¹³The Lorentz part of this algebra was found previously using the defining representation of the Lorentz group. The Poincaré group, as given above, is not defined in terms of matrices only. A way of finding its Lie algebra is to consider its generators that perform the infinitesimal transformation in a quantum mechanical Hilbert space where $P^\mu = \hat{p}^\mu$ and $M^{\mu\nu} = \hat{x}^\mu \hat{p}^\nu - \hat{x}^\nu \hat{p}^\mu$, with the elementary commutators given by $[\hat{x}^\mu, \hat{p}_\nu] = i\delta_\nu^\mu$. This allows us to deduce the Lie algebra of the Poincaré group given above.

2 | Relativistic Quantum Mechanics

The **Schrödinger equation** is a wave equation for the quantum mechanics of non-relativistic particles. The attempts to generalize it to the relativistic case led historically to the discovery of many different relativistic wave equations (Klein–Gordon, Dirac, Proca–Maxwell, etc.). It soon became clear that all of these wave equations for relativistic particles had some interpretative problems:

- (i) some did not admit a probabilistic interpretation,
- (ii) all of them admitted solutions with negative energy.

These equations are often called “**first quantized**” equations, as they are obtained by quantizing the mechanics of a single relativistic particle.

To solve those problems, eventually, one had to reinterpret them as equations for *classical fields* (just like Maxwell’s equations) that should be quantized anew (hence the name of “**second quantization**” given to the quantum theory of fields). All of the interpretative problems can be solved consistently within the framework of quantum field theory: the quantum fields are seen to describe an arbitrary number of indistinguishable particles (the quanta of the field, like the photons for the electromagnetic field). The relativistic equations mentioned above remain valid, but reinterpreted as equations satisfied by quantum field operators.

The main reason for the interpretative problems of the first quantized equations lies in the fact that relativity allows particles to be created and destroyed by physical processes. It would not be consistent to fix the number of particles and require that number to be conserved. Indeed, let us recall that relativity assigns the energy $E = mc^2$ to a particle of mass m at rest. In the limit $c \rightarrow \infty$, which formally describes the nonrelativistic limit, it would take infinite energy to create a particle. Non-relativistic quantum mechanics can be developed consistently to conserve the number of particles, which is linked to the conservation of probability for those particles to exist somewhere in space. In relativistic quantum mechanics it is impossible to do so: certain processes that carry enough energy may allow the creation of new particles, as observed in nature. This explains the *failure to have a probabilistic interpretation* of the quantum mechanics of a single particle in the relativistic regime.

The other problem, the *presence of negative energy states*, was eventually turned into a prediction: the existence of antiparticles: every particle should have a corresponding antiparticle with the same mass and opposite charges. The existence of antiparticles was experimentally confirmed with the discovery of the positron in 1932, validating the theoretical framework.

Given that the methods of second quantization (alias quantum field theory or QFT) is the natural mathematical framework to study the above properties, why review the historical development? There are many justifications to do so. One reason is that the historical development *clarifies the physical ideas leading to more formal constructions*, such as QFT. A second motivation is that one finds many situations that can be dealt with – often more simply – in the context of relativistic quantum mechanics without the need to turn to more elaborate methods. This happens, for example, if one considers those cases where pair creation is suppressed and the single-particle approximation is applicable. More generally, first-quantized methods, which nowadays go under the name of the *worldline formalism*, are often used as efficient tools to study the scattering of relativistic particles. As a final motivation, one may recall that first-quantized methods for relativistic particles are pedagogically useful for approaching string theory, a model for quantum gravity where particles are generalized to strings. The reason is that string theory has been mostly developed in first-quantization.

The different relativistic wave equations mentioned above correspond to the quantum mechanics of particles with different spin s . There is also a difference if the particle is massive ($m \neq 0$) or massless ($m = 0$) if the spin is $s > 0$. The simplest relativistic equation is the Klein–Gordon equation, that describes scalar particles, i.e., particles of spin $s = 0$. It takes into account the correct relativistic relation between energy and momentum, and thus it contains the essence of all relativistic wave equations (like negative energy solutions that signal the need for antiparticles).

The correct wave equation for a relativistic particle depends crucially on the value of the spin s , some standard names are as follows:

- spin 0 → Klein–Gordon equation
- spin $\frac{1}{2}$ → Dirac equation
- spin 1 ($m \neq 0$) → Proca equation
- spin 1 ($m = 0$) → (free) Maxwell equations
- spin $\frac{3}{2}$ → Rarita–Schwinger equation
- spin 2 → Fierz–Pauli equations (or linearized Einstein eq. fSr $m = 0$).
- spin $s > 2$ → Fierz–Pauli eqs. (for $m \neq 0$) and Fronsdal eqs. (for $m = 0$).

We have anticipated that relativistic particles are classified by their mass m and spin s , where the value of the spin indicates that there are only $2s + 1$ independent physical components of the wave function, describing the possible polarizations of the spin vector along a chosen axis. That is true unless $m = 0$, in which case the wave function describes only two physical components, those with maximum and minimum helicity (helicity is the projection of the spin along the direction of motion). The reduction of the number of degrees of freedom is mathematically achieved by the emergence of gauge symmetries satisfied by the corresponding wave equations, as we shall see in the examples of spin 1 and 2.

The classification just described is due to Wigner, who in 1939 studied the *unitary irreducible representations* of the Poincaré group. The Poincaré group is, by definition, the group of symmetries of relativistic theories, symmetries that must be realized by unitary operators in the Hilbert space of the particle. Different particles have different realizations (i.e., representations) of the symmetry group and **Wigner's theorem** describes the possible different unitary representations

that are allowed by group theory. As anticipated above, a physical way of understanding Wigner's classification is to recall that for a massive particle of spin s , one may always find a reference frame where the particle is at rest. Then, its spin is observed to have the $2s + 1$ physical projections along the z -axis, as familiar from quantum mechanics. Thus, we understand that massive particles of spin s must have $2s + 1$ physical polarizations. On the other hand, a rest frame does not exist if the particle is massless: the particle must travel with the speed of light in any frame. Choosing the direction of motion as the axis where to measure the spin, one finds that only two values of the helicity $h = \pm s$ are possible. Other helicities are not needed, as they would never mix with the previous ones under Poincaré transformations (they could be considered as belonging to different particles, which may or may not exist in a given model. On the contrary, the discrete CPT symmetry requires both helicities $\pm s$ to be present).

In these notes, after a brief review of the Schrödinger equation, we discuss the main properties of the Klein–Gordon and Dirac equations, treated as first quantized wave equations for particles of spin 0 and $\frac{1}{2}$, and then briefly comment on other relativistic free wave equations.

Our main conventions for special relativity are reported in appendix A, and we use the standard definitions for Lorentz and Poincaré groups as in the lecture notes.

2.1 | Schrödinger equation

Crucial milestones in the discovery of quantum mechanics are:

- (1900) the introduction of Planck's constant h to describe the spectrum of black-body radiation;
- (1905) Einstein's use of h to explain the photoelectric effect, by interpreting light as composed of quanta (photons) of energy $E = h\nu$;
- (1913) Bohr's atomic model, where the electron energy levels are quantized as $E_n \sim \frac{1}{n^2}$;
- (1923) de Broglie's hypothesis extending Einstein's idea to matter, suggesting that particles with momentum p exhibit wave-like properties with wavelength $\lambda = \frac{h}{p}$.

At that time, it was still unclear which fundamental laws governed the quantum behavior of subatomic particles. However, de Broglie's assumption provided a natural explanation for Bohr's quantized energy levels: the allowed orbits could be interpreted as those for which an integer number of electron wavelengths fits exactly along the circular trajectory around the nucleus.

De Broglie's wave hypothesis. Inspired by special relativity, de Broglie proposed to associate a periodic wave to every material particle. A periodic wave function characterized by

- $\nu = \frac{1}{T}$, the **frequency** (periodicity in time),
- $|\mathbf{k}| = \frac{1}{\lambda}$, the **wavenumber** (periodicity in space),

has the mathematical form of a plane wave:

$$\psi(\mathbf{x}, t) \sim e^{2\pi i(\mathbf{k} \cdot \mathbf{x} - \nu t)}.$$

This is the simplest possible representation of a wave extending through space and time, with phase $\Phi = 2\pi(\mathbf{k} \cdot \mathbf{x} - \nu t)$.

Invariant formulation of the de Broglie wave. De Broglie assumed that the phase Φ must be invariant under Lorentz transformations. Since the spacetime coordinates form a four-vector $x^\mu = (ct, \mathbf{x})$, the quantities ν/c and \mathbf{k} must also combine into a four-vector:

$$k^\mu = \left(\frac{\nu}{c}, \mathbf{k} \right).$$

If the phase $2\pi k_\mu x^\mu$ is invariant, then both x^μ and k^μ must transform in the same way under Lorentz transformations. At the same time, special relativity tells us that the energy and momentum of a particle form the four-vector

$$p^\mu = \left(\frac{E}{c}, \mathbf{p} \right).$$

In the case of photons, Einstein's relation $E = h\nu$ is already known, and the photon momentum satisfies $\mathbf{p} = h\mathbf{k}$. It was therefore natural for de Broglie to extend this proportionality to all particles by postulating that

$$p^\mu = h k^\mu,$$

with the same universal constant \hbar linking the two four-vectors. From this, the familiar relations follow immediately:

$$E = \hbar\nu, \quad \mathbf{p} = \hbar\mathbf{k}.$$

The second expression implies that any material particle with momentum p has an associated wavelength

$$\lambda = \frac{\hbar}{p}.$$

This was the first step toward the concept of matter waves.

The scalar (Lorentz-invariant) contraction between the four-position and the four-wavevector is

$$x_\mu k^\mu = \mathbf{x} \cdot \mathbf{k} - \nu t.$$

Thus, the plane wave associated with a free particle of definite energy and momentum can be written in a manifestly invariant form as

$$\psi(\mathbf{x}, t) \sim e^{2\pi i x_\mu k^\mu} = e^{2\pi i (\mathbf{k} \cdot \mathbf{x} - \nu t)} = e^{i(\mathbf{p} \cdot \mathbf{x} - Et)/\hbar}. \quad (2.1.1)$$

In this expression, $\mathbf{p} \cdot \mathbf{x} - Et/c^2$ is the standard relativistic scalar product between the four-momentum and the four-position. The exponential phase encodes the oscillatory nature of the particle's quantum state and ensures that the function transforms covariantly under Lorentz transformations. It will be this very function — representing a free particle of definite energy and momentum — that Schrödinger later used as a starting point to search for the differential equation governing its evolution.

From de Broglie's hypothesis to Schrödinger's equation. At this point, Schrödinger asked a fundamental question: *what kind of equation does a de Broglie wave satisfy?* He initially attempted to find such an equation in a fully relativistic form, aiming to describe the electron in the hydrogen atom. However, the resulting energy spectrum did not match the experimental results. Schrödinger then turned to the non-relativistic limit, which provided the correct predictions. (Today, we understand that the discrepancies in the relativistic case were due to neglecting the electron's spin, whose effects compensate for those missing corrections.)

For a free non-relativistic particle, the classical relation between energy and momentum is

$$E = \frac{p^2}{2m}.$$

If we consider the de Broglie plane wave

$$\psi(\mathbf{x}, t) = e^{i(\mathbf{p} \cdot \mathbf{x} - Et)/\hbar},$$

we can check directly which differential equation it satisfies. By acting with the operators $i\hbar \frac{\partial}{\partial t}$ and $-i\hbar \nabla$ on the wave function, we find

$$i\hbar \frac{\partial}{\partial t} \psi = E\psi, \quad -i\hbar \nabla \psi = \mathbf{p}\psi.$$

Combining these relations with the classical energy expression $E = \frac{p^2}{2m}$, we obtain

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = \frac{1}{2m} (-i\hbar \nabla)^2 \psi(\mathbf{x}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}, t).$$

Thus, the de Broglie plane wave automatically satisfies the differential equation

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}, t), \quad (2.1.2)$$

which is precisely the **free Schrödinger equation** for a particle of mass m . In other words, Schrödinger's equation is the dynamical law that has de Broglie's plane waves as its elementary solutions.

Quantization prescription. The above reasoning suggests a simple and general rule for constructing a wave equation starting from a classical mechanical model of a particle. Given a classical expression for the energy as a function of momentum (and possibly position), such as $E = \frac{p^2}{2m}$, one can obtain the corresponding quantum equation by making the substitutions

$$E \longrightarrow i\hbar \frac{\partial}{\partial t}, \quad \mathbf{p} \longrightarrow -i\hbar \nabla,$$

and letting these differential operators act on a wave function $\psi(\mathbf{x}, t)$.

This procedure — which converts classical observables into operators acting on wave functions — defines the **quantization prescription**. When applied to the classical Hamiltonian $H = \frac{p^2}{2m}$, it directly produces the Schrödinger equation for a free particle.

Schrödinger soon extended this idea to include interactions. For example, by considering a charged particle in the electrostatic potential of a nucleus, he replaced the classical energy $E = \frac{p^2}{2m} + V(\mathbf{x})$ and obtained

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right] \psi(\mathbf{x}, t),$$

successfully reproducing Bohr's energy levels for the hydrogen atom. This achievement marked the beginning of modern quantum mechanics.

General form. Although it was first derived for a single non-relativistic particle, Schrödinger's equation can be written in a general and abstract form:

$$i\hbar \frac{\partial}{\partial t} |\psi(\mathbf{x}, t)\rangle = \hat{H} |\psi(\mathbf{x}, t)\rangle, \quad (2.1.3)$$

where \hat{H} is the **Hamiltonian operator** of the system.

In this formulation, the equation becomes a universal dynamical law for all quantum systems, not limited to point particles. The specific form of \hat{H} encodes the physical content of the problem — kinetic energy, external fields, and interactions — while the wave function $|\psi\rangle$ encapsulates the probabilistic state of the system. This single equation thus unifies the dynamics of all non-relativistic quantum phenomena under a common mathematical structure.

2.1.1 | Conservation of probability

When a non-relativistic particle is described by a normalizable wave function $\psi(\mathbf{x}, t)$, the quantity

$$\rho(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2$$

is interpreted as the **probability density** of finding the particle at position \mathbf{x} at time t . (The plane wave considered earlier is not normalizable in infinite space, so in practice one works with *wave packets*, i.e., superpositions of plane waves that are localized in space.)

A crucial property of the Schrödinger equation is that this probability density obeys a **continuity equation**, expressing the conservation of total probability:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0, \quad (2.1.4)$$

where the **probability current density** is given by

$$\mathbf{J} = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*). \quad (2.1.5)$$

This equation is directly analogous to the continuity equation in fluid dynamics or electrodynamics: the change in probability within a given volume is compensated by the flux of probability through its boundary.

Equation (2.1.4) expresses the **conservation of probability**, meaning that at any instant the particle must exist somewhere in space — it cannot be spontaneously created or annihilated in the non-relativistic theory. This can be understood by examining the non-relativistic limit of the relativistic energy-momentum relation:

$$E = \sqrt{p^2 c^2 + m^2 c^4} = mc^2 \sqrt{1 + \frac{p^2}{m^2 c^2}} \approx mc^2 + \frac{p^2}{2m} + \dots$$

In the limit $c \rightarrow \infty$, the rest energy term mc^2 becomes infinitely large, meaning that creating or destroying a massive particle would require an infinite amount of energy. Hence, the number of particles is effectively conserved.

Integrating (2.1.4) over all space shows explicitly that the **total probability**

$$P = \int d^3x \rho(\mathbf{x}, t),$$

is constant in time. Indeed,

$$\frac{dP}{dt} = \int d^3x \frac{\partial \rho}{\partial t} = - \int d^3x \nabla \cdot \mathbf{J} = - \oint_{\partial V} \mathbf{J} \cdot d\mathbf{S} = 0,$$

where the last equality holds if \mathbf{J} vanishes sufficiently fast at infinity ($V \rightarrow \infty$). Therefore, the Schrödinger dynamics preserves the normalization of the wave function:

$$\int |\psi(\mathbf{x}, t)|^2 d^3x = 1.$$

2.2 | Klein Gordon Equation

As discussed previously, the Schrödinger equation arises from the quantization of a *non-relativistic* particle. In complete analogy, the **Klein–Gordon equation** can be obtained by applying the same quantization procedure to a *relativistic* particle (this is often referred to as *first quantization* of the relativistic theory).

However, unlike the Schrödinger equation, the Klein–Gordon equation does not allow for a consistent **probabilistic interpretation** in terms of a positive-definite probability density. This limitation signals that the equation, while formally correct as a relativistic wave equation, cannot be the final description of a single-particle quantum system.

A consistent framework is recovered by interpreting the Klein–Gordon *wave function* as a **classical field** and quantizing this field itself. In this approach—known as **second quantization** or **field quantization**—the field is promoted to an operator acting on a Fock space, describing states with an arbitrary number of identical particles and antiparticles. Historically, this formalism first appeared in the quantization of the electromagnetic field, and it naturally extends to the Klein–Gordon field.

In the language of quantum field theory, the Klein–Gordon field thus represents a system of **spin-0 particles** and their corresponding antiparticles. Nevertheless, even if we restrict ourselves to the first-quantized formulation, the Klein–Gordon equation remains of fundamental importance, as it encapsulates the essential features of the quantum mechanics of relativistic scalar particles and provides the starting point for the construction of quantum field theory.

2.2.1 | Derivation of the Klein-Gordon equation

How can we obtain a relativistic version of the wave equation? A natural starting point is to repeat the same procedure used for the Schrödinger equation, but now employing the **relativistic energy–momentum relation**. For a free relativistic particle of mass m , the four-momentum $p^\mu = (p^0, p^1, p^2, p^3) = (E, \mathbf{p})$ satisfies the **mass-shell condition**

$$p^\mu p_\mu = -m^2 c^2 \quad \Rightarrow \quad E^2 = \mathbf{p}^2 c^2 + m^2 c^4.$$

One could then try to promote this classical relation to a wave equation by using the correspondence

$$E \rightarrow i\hbar \frac{\partial}{\partial t}, \quad \mathbf{p} \rightarrow -i\hbar \nabla.$$

If we apply this substitution directly to the relativistic energy expression $E = \sqrt{\mathbf{p}^2 c^2 + m^2 c^4}$, we obtain

$$i\hbar \frac{\partial}{\partial t} \phi(\mathbf{x}, t) = \sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4} \phi(\mathbf{x}, t).$$

However, this equation involves the *square root of a differential operator*, whose precise meaning is not well defined. Such an operator would introduce **non-local effects**, implying that distant points in space could directly influence each other—an undesirable and physically obscure feature. For this reason, this form was soon abandoned.

A more elegant and mathematically tractable approach was proposed independently by **Oskar Klein** and **Walter Gordon**. Instead of working with the square-root form, they started from the **quadratic** energy–momentum relation

$$E^2 = \mathbf{p}^2 c^2 + m^2 c^4,$$

and replaced E and \mathbf{p} by their corresponding operators. This leads to the **Klein–Gordon equation**:

$$\left(-\frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \nabla^2 - \frac{m^2 c^2}{\hbar^2} \right) \phi(\mathbf{x}, t) = 0. \quad (2.2.1)$$

In a more compact and manifestly relativistic form, it can be written as

$$(\square - m^2) \phi(x) = 0, \quad (2.2.2)$$

where the **d'Alembertian operator** is defined as

$$\square = \partial^\mu \partial_\mu = -\partial_0^2 + \nabla^2.$$

From now on, we adopt **natural units** with $\hbar = c = 1$, so that the equation takes the simple form

$$(\square - m^2) \phi = 0,$$

and the mass m becomes dimensionless, unless otherwise specified.

2.2.2 | Plane wave solutions

The Klein–Gordon equation was constructed precisely to ensure that it admits plane-wave solutions satisfying the correct relativistic dispersion relation between energy and momentum:

$$(\square - m^2) \phi(x) = 0.$$

To find such solutions, let us assume a **plane wave ansatz** of the form

$$\phi_p(x) = e^{ip_\mu x^\mu}, \quad (2.2.3)$$

where p_μ is the four-momentum of the particle. Substituting this expression into the Klein–Gordon equation gives

$$(\partial^\mu \partial_\mu - m^2) e^{ip_\nu x^\nu} = ((ip^\mu)(ip_\mu) - m^2) e^{ip_\nu x^\nu} = -(p^\mu p_\mu + m^2) e^{ip_\nu x^\nu} = 0.$$

This condition is satisfied if the four-momentum p^μ lies on the **mass shell**, that is,

$$p^\mu p_\mu = -m^2 \Rightarrow (p^0)^2 = \mathbf{p}^2 + m^2 \Rightarrow p^0 = \pm E_p, \quad E_p = \sqrt{\mathbf{p}^2 + m^2}.$$

Hence, the Klein–Gordon equation admits both **positive** and **negative energy solutions**. The positive-energy modes correspond to

$$\phi_{\mathbf{p}}^{(+)}(x) = e^{-iE_p t + i\mathbf{p} \cdot \mathbf{x}}, \quad (2.2.4)$$

while the negative-energy modes are given by

$$\phi_{\mathbf{p}}^{(-)}(x) = e^{iE_p t - i\mathbf{p} \cdot \mathbf{x}}. \quad (2.2.5)$$

At first sight, the existence of solutions with $p^0 = -E_p$ seems problematic: if negative-energy states exist, the system could in principle decay indefinitely into lower and lower energy levels, making the theory **unstable**. In the framework of relativistic quantum field theory, however, these modes acquire a consistent interpretation: they correspond to **antiparticles** carrying positive energy but opposite charge or quantum numbers.

The most general solution of the Klein–Gordon equation can therefore be expressed as a linear superposition of all plane waves with both signs of energy:

$$\phi(x) = \int \frac{d^3\mathbf{p}}{(2\pi)^3 2E_p} [a(\mathbf{p}) e^{-iE_p t + i\mathbf{p}\cdot\mathbf{x}} + b^*(\mathbf{p}) e^{iE_p t - i\mathbf{p}\cdot\mathbf{x}}], \quad (2.2.6)$$

and its complex conjugate as

$$\phi^*(x) = \int \frac{d^3\mathbf{p}}{(2\pi)^3 2E_p} [a^*(\mathbf{p}) e^{iE_p t - i\mathbf{p}\cdot\mathbf{x}} + b(\mathbf{p}) e^{-iE_p t + i\mathbf{p}\cdot\mathbf{x}}].$$

Here, $a(\mathbf{p})$ and $b(\mathbf{p})$ are **Fourier coefficients** that determine the relative weight of each momentum mode. The normalization factor $2E_p$ is conventional and chosen so that the coefficients transform as Lorentz scalars. Finally, for a **real scalar field**, where $\phi^* = \phi$, the coefficients of positive- and negative-energy modes coincide:

$$a(\mathbf{p}) = b(\mathbf{p}).$$

2.2.3 | Continuity equation

From the Klein–Gordon equation one can derive a continuity equation, although the associated conserved quantity cannot be interpreted as a probability density. Let us examine this in detail.

A straightforward way to obtain the continuity equation is to multiply the Klein–Gordon equation by the complex conjugate field ϕ^* and subtract from it the complex conjugate equation multiplied by ϕ . One finds:

$$\begin{aligned} \phi^*(\square - m^2)\phi - \phi(\square - m^2)\phi^* &= \phi^*\square\phi - m^2\phi\phi^* - \phi\square\phi^* + m^2\phi\phi^* = \phi^*\partial_\mu\partial^\mu\phi - \phi\partial_\nu\partial^\nu\phi^* \\ &= \partial_\mu(\phi^*\partial^\mu\phi) - \partial_\mu\phi^*\partial^\mu\phi - (\partial_\nu(\phi\partial^\nu\phi^*) - \partial_\nu\phi\partial^\nu\phi^*) \\ &= \partial_\mu(\phi^*\partial^\mu\phi - \phi\partial^\mu\phi^*) = 0, \end{aligned}$$

which is zero because the starting expression vanishes identically (literally the KG equation (??), which is zero, multiplied by something).

We can thus define the four-current

$$J^\mu = \frac{1}{2im}(\phi^*\partial^\mu\phi - \phi\partial^\mu\phi^*), \quad (2.2.7)$$

which satisfies the conservation law $\partial_\mu J^\mu = 0$. The normalization factor is chosen so that J^μ is real and, in the nonrelativistic limit, reproduces the form of the probability current in the Schrödinger theory.

The temporal component reads

$$J^0 = \frac{1}{2im}(\phi^*\partial^0\phi - \phi\partial^0\phi^*),$$

which, while real, is not positive definite. Indeed, both ϕ and its time derivative $\partial_0\phi$ can be freely specified as initial conditions, since the Klein–Gordon equation is second order in time. Therefore, J^0 can take either positive or negative values depending on these data. Evaluating J^0 for plane-wave solutions explicitly yields

$$J^0 = \pm \frac{E_p}{m},$$

confirming that its sign depends on the energy branch chosen.

We thus conclude that the Klein–Gordon equation cannot sustain a probabilistic interpretation in terms of a positive-definite probability density: the quantity J^0 cannot be interpreted as a probability density $\frac{\rho}{c}$.

This difficulty motivated Dirac to search for a different relativistic wave equation that would preserve a positive-definite probability density. He succeeded, but it later became clear that all relativistic wave equations should be reinterpreted as classical field equations to be quantized anew, describing particles of mass m as the quanta of those fields—an idea reminiscent of Einstein’s interpretation of electromagnetic waves in the photoelectric effect.

Historically, this field interpretation was first successfully applied by Yukawa in 1935, who employed the Klein–Gordon field to model nuclear interactions mediated by short-range forces.

2.2.4 | Yukawa potential

Let us now consider the Klein–Gordon equation in the presence of a static, point-like source:

$$(\square - m^2)\phi(x) = g \delta^3(\mathbf{x}),$$

where the source is located at the origin of the coordinate system and g characterizes the strength of its coupling to the Klein–Gordon field. Since the source is static, we can look for a time-independent solution, in which case the equation reduces to

$$(\nabla^2 - m^2)\phi(\mathbf{x}) = g \delta^3(\mathbf{x}). \quad (2.2.8)$$

This equation can be solved by Fourier transform, yielding the so-called *Yukawa potential*:

$$\phi(r) = \frac{g}{4\pi} \frac{e^{-mr}}{r}, \quad (2.2.9)$$

where the exponential factor introduces an effective cut-off in the interaction range.

To derive this result, we start by expressing the field as a Fourier transform

$$\phi(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \tilde{\phi}(\mathbf{k}),$$

and recall that the Fourier transform of the Dirac delta distribution is

$$\delta^3(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}}.$$

Substituting these expressions into the equation gives

$$\begin{aligned} \int \frac{d^3\mathbf{k}}{(2\pi)^3} (-k^2 - m^2) e^{i\mathbf{k}\cdot\mathbf{x}} \tilde{\phi}(\mathbf{k}) &= g \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}}, \\ \tilde{\phi}(\mathbf{k}) &= \frac{-g}{k^2 + m^2}. \end{aligned}$$

The inverse transform can then be evaluated explicitly in spherical coordinates ($r = \sqrt{|\mathbf{x}|^2}$):

$$\begin{aligned} \phi(\mathbf{x}) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \frac{-g}{k^2 + m^2} \\ &= -\frac{g}{(2\pi)^3} \int_0^\infty dk \frac{k^2}{k^2 + m^2} \int_{-1}^1 d\cos\theta e^{ikr\cos\theta} \int_0^{2\pi} d\psi \\ &= -\frac{g}{(2\pi)^2} \int_0^\infty dk \frac{k^2}{k^2 + m^2} \left[\frac{e^{ikr} - e^{-ikr}}{ikr} \right], \end{aligned}$$

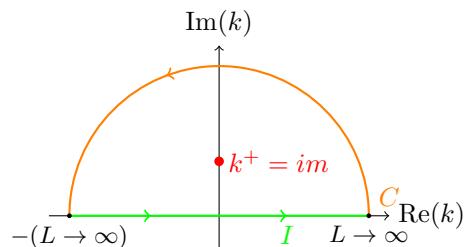
which is the integral of an even function, since the integrand can be expressed in terms of $2 \sin(kr)$. Moreover, by splitting the integral into the terms involving ke^{ikr} and ke^{-ikr} , we observe that the latter, when integrated from $0 \rightarrow \infty$, is identical to the former integrated from $-\infty \rightarrow 0$. Therefore, the integration domain can be extended from $0 \rightarrow \infty$ to $-\infty \rightarrow \infty$ writing

$$\phi(\mathbf{x}) = -\frac{g}{(2\pi)^2 ir} \int_{-\infty}^{\infty} dk \frac{k}{k^2 + m^2} e^{ikr}.$$

It is convenient to study this expression in the complex plane: by closing the contour with an arc C in the upper half-plane, we can integrate on a closed curve and use **Cauchy's residue theorem**:

$$\frac{k}{k^2 + m^2} e^{ikr} = \frac{k}{(k + im)(k - im)} e^{ikr},$$

which has two poles $\bar{k} = \pm im = k^\pm$.

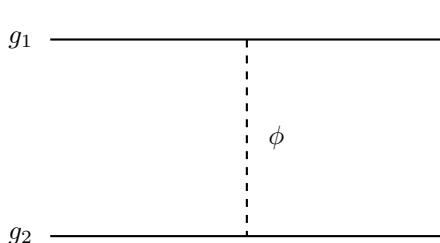


Hence, we obtain:

$$\begin{aligned} \phi(\mathbf{x}) &= -\frac{g}{(2\pi)^2 ir} (2\pi i) \sum_i \text{Res}_i f(k) \Big|_{k^\pm} \\ &= -\frac{g}{2\pi r} \lim_{k \rightarrow im} \frac{ke^{ikr}}{(k + im)(k - im)} (k - im) \\ &= -\frac{g}{2\pi r} \frac{ime^{-mr}}{2im} = -\frac{g}{4\pi r} e^{-mr}. \end{aligned}$$

This potential describes an attractive interaction between sources of the same sign. Its range is finite and characterized by $\lambda \sim \frac{1}{m}$, corresponding to the **Compton wavelength** of a particle of mass m . Hence, the Yukawa potential models *short-range forces*, such as the nuclear force. One can verify that $\phi(\mathbf{x}) = -\frac{g}{4\pi r} e^{-mr}$ satisfies equation (2.2.8) by direct substitution.

Feynman diagrams. A pictorial representation of the interaction between two scalar charges g_1 and g_2 mediated by the exchange of a Klein–Gordon quantum can be represented by the following Feynman-like diagram:



This diagram illustrates the exchange of a virtual scalar quantum between the worldlines of two point particles carrying charges g_1 and g_2 . The resulting interaction potential is

$$V(r) = -\frac{g_1 g_2}{4\pi} \frac{e^{-mr}}{r}, \quad (2.2.10)$$

which is attractive for charges of the same sign.

As we have said, the potential has a characteristic range scaling inversely with the mass of the exchanged particle: the behaviour of a short-range force

$$R \sim \frac{1}{m},$$

which is suppressed exponentially for distances $r \gg R$.

In 1935, Yukawa proposed that nuclear interactions arise from the exchange of a massive scalar particle, later identified as the *meson*. By estimating a typical range $R \sim 1$ fm (comparable to the proton radius), one obtains a mass

$$m \sim 197 \text{ MeV},$$

in remarkable agreement (the same order of magnitude) with the mass of the neutral pion, $m_{\pi^0} \approx 135$ MeV, discovered later in cosmic-ray experiments.

2.2.5 | Green functions and the propagator

The Green functions of the Klein–Gordon (KG) equation play a central role in the quantum interpretation of the scalar field. Although the field $\phi(x)$ satisfies a wave-like equation, we refrain from calling it a *wave function*, since its probabilistic interpretation—in the sense of single-particle quantum mechanics—is not consistent. Instead, the field must be regarded as a quantum operator describing the creation and annihilation of scalar particles.

A specific Green function $G(x - y)$ is associated with the *propagator*, which can be interpreted as the amplitude for a quantum of the field to propagate from a spacetime point y to another point x . The Green function $G(x)$ is defined as the response of the field to a pointlike, instantaneous source of unit strength placed at the origin ($y = 0$). Mathematically, it satisfies the inhomogeneous KG equation

$$(-\square + m^2)G(x) = \delta^{(4)}(x), \quad (2.2.11)$$

where $\square = \partial_\mu \partial^\mu$ is the d'Alembert operator and $\delta^{(4)}(x)$ is the four-dimensional Dirac delta function.

Knowing the Green function, the general solution to the non-homogeneous KG equation

$$(-\square + m^2)\phi(x) = J(x), \quad (2.2.12)$$

where $J(x)$ is an arbitrary external source, can be expressed as

$$\phi(x) = \phi_0(x) + \int d^4y G(x - y)J(y), \quad (2.2.13)$$

where $\phi_0(x)$ is any solution of the corresponding homogeneous KG equation $(-\square + m^2)\phi_0 = 0$. This representation can be easily verified by substituting it back into the differential equation and using the defining property of $G(x)$.

$$\begin{aligned} & (-\square + m^2) \left(\phi_0(x) + \int d^4y G(x - y)J(y) \right) \\ &= (-\square + m^2)\phi_0(x) + (-\square + m^2) \int d^4y G(x - y)J(y) \\ &= \int d^4y (-\square + m^2)G(x - y)J(y) = \int d^4y \delta^{(4)}(x - y)J(y) = J(x). \end{aligned}$$

The Green function thus acts as a *kernel* that “*propagates*” the influence of the source $J(y)$ from each spacetime point y to the observation point x .

Feynman–Stueckelberg prescription

For hyperbolic differential equations such as the Klein–Gordon equation, the Green function is *not unique*: its precise form depends on the boundary (or, equivalently, causality) conditions imposed at infinity. In quantum field theory, the physically meaningful choice is the *causal Green*

function, determined by the **Feynman–Stueckelberg** prescription. This prescription enforces that positive-frequency components (associated with particles of positive energy) propagate forward in time, while negative-frequency components (associated with antiparticles with negative energy) propagate backward in time (changing the sign of their energy). Such a rule guarantees a consistent causal interpretation and unifies the propagation of particles and antiparticles within a single formalism.

The corresponding *Feynman propagator* can be expressed in momentum space as a Fourier transform:

$$G(x) = \int \frac{d^4 p}{(2\pi)^4} e^{ip_\mu x^\mu} \tilde{G}(p) = \int \frac{d^4 p}{(2\pi)^4} \frac{e^{ip_\mu x^\mu}}{p^2 + m^2}, \quad (2.2.14)$$

since $\tilde{G}(p) = 1/(p^2 + m^2)$ follows directly from the Klein–Gordon equation for $G(x)$:

$$\begin{aligned} (-\square + m^2)G(x) &= \delta^{(4)}(x), \\ \int \frac{d^4 p}{(2\pi)^4} (-\square + m^2)e^{ip_\mu x^\mu} \tilde{G}(p) &= \int \frac{d^4 p}{(2\pi)^4} e^{ip_\mu x^\mu}, \\ \int \frac{d^4 p}{(2\pi)^4} (p_\mu p^\mu + m^2)e^{ip_\mu x^\mu} \tilde{G}(p) &= \int \frac{d^4 p}{(2\pi)^4} e^{ip_\mu x^\mu}, \\ \implies \tilde{G}(p) &= \frac{1}{p^2 + m^2}. \end{aligned}$$

From the standpoint of quantum field theory, the Green function—or propagator—encodes both the propagation of *real particles* (on-shell quanta satisfying $p^2 = -m^2$) and the virtual fluctuations (off-shell contributions) that appear in quantum processes. It therefore provides a unified mathematical object describing both the causal structure and the dynamical correlations of the scalar field.

Since this expression contains two poles in the complex plane, one introduces a small imaginary displacement $i\epsilon$ in the denominator to specify how the integration contour should avoid them:

$$G(x) = \int \frac{d^4 p}{(2\pi)^4} \frac{e^{ip_\mu x^\mu}}{p^2 + m^2 - i\epsilon}.$$

The infinitesimal term $-i\epsilon$ (with $\epsilon \rightarrow 0^+$) determines the position of the poles in the complex p^0 -plane and thus implements the causal boundary conditions (Feynman–Stueckelberg) described above. The $i\epsilon$ -term dictates whether a given frequency component propagates forward or backward in time.

More explicitly, the $i\epsilon$ prescription moves the poles of the integrand in a definite direction and therefore fixes the causal behavior of the Green function: positive-energy modes ($p^0 = E_p$) are propagated forward in time, while negative-energy modes ($p^0 = -E_p$) are propagated backward. This is called the *causal* prescription, as it forbids negative-energy states from propagating into the future. In this sense, negative-energy states are reinterpreted as antiparticles with positive energy propagating forward in time. This correspondence follows from the phase relation

$$e^{-i(-E_p)t} = e^{-iE_p(-t)},$$

which shows that a wave moving backward in time with energy $-E_p$ is equivalent to a positive-energy wave propagating forward in time.

Let us now make this interpretation explicit by performing the integral over p^0 in the Green function $G(x - y)$. We also recall that, in quantum field theory, the propagator is defined as

$\Delta(x - y) = -iG(x - y)$. Carrying out the integration, one finds

$$\begin{aligned}\Delta(x - y) &= -iG(x - y) = \int \frac{d^4 p}{(2\pi)^4} \frac{-i}{p^2 + m^2} e^{ip_\mu \cdot (x^\mu - y^\mu)} \\ &= \int \frac{d^3 \mathbf{p}}{(2\pi)^3} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \int \frac{dp^0}{2\pi} \frac{ie^{-ip^0(x^0 - y^0)}}{(p^0 - E_p)(p^0 + E_p)},\end{aligned}$$

where $E_p = \sqrt{\mathbf{p}^2 + m^2}$.

Remark. In the classical theory, the Green function $G(x - y)$ represents the response of the field to a localized source. In quantum field theory, however, $\phi(x)$ becomes an operator, and the relevant physical quantity is the Feynman propagator

$$\Delta(x - y) = \langle 0 | T\{\hat{\phi}(x)\hat{\phi}^\dagger(y)\} | 0 \rangle,$$

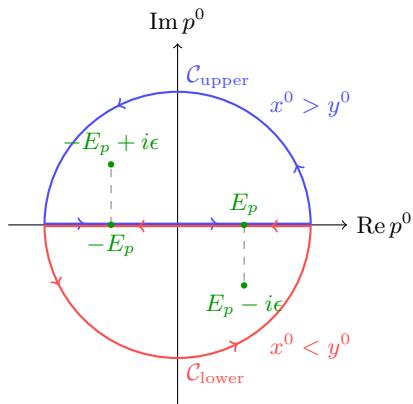
which measures the amplitude for a quantum of the field created at y to be annihilated at x . It satisfies $(-\square + m^2)\Delta(x - y) = i\delta^{(4)}(x - y)$, so that, by convention,

$$\boxed{\Delta(x - y) = -iG(x - y).}$$

This identifies the classical Green function G with the quantum propagator Δ , which encodes the causal and probabilistic structure of the field.

Without the $i\epsilon$ displacement, the poles at $p^0 = \pm E_p$ lie directly on the real axis of the integration contour. To specify how the contour avoids them, we introduce the Feynman prescription:

$$\Delta(x - y) = \int \frac{d^3 \mathbf{p}}{(2\pi)^3} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \int \frac{dp^0}{2\pi} \frac{ie^{-ip^0(x^0 - y^0)}}{(p^0 - E_p + i\epsilon)(p^0 + E_p - i\epsilon)}.$$



The role of the $-i\epsilon$ term is now evident: it prescribes how the poles are displaced. The pole associated with the positive-energy solution is shifted into the lower half-plane ($\text{Im } p^0 < 0$), allowing propagation into the future, while the negative-energy pole is moved into the upper half-plane ($\text{Im } p^0 > 0$), corresponding to backward propagation in time.

By closing the contour with either C_{upper} or C_{lower} , depending on the sign of $x^0 - y^0$, we can apply Cauchy's residue theorem to evaluate the integral:

$$(2\pi i) \lim_{p^0 \rightarrow E_p} \frac{i}{2\pi} \frac{e^{-ip^0(x^0 - y^0)}}{(p^0 + E_p)} = \frac{e^{-iE_p(x^0 - y^0)}}{2E_p}, \quad (2\pi i) \lim_{p^0 \rightarrow -E_p} \frac{i}{2\pi} \frac{e^{-ip^0(x^0 - y^0)}}{(p^0 - E_p)} = \frac{e^{-iE_p(y^0 - x^0)}}{2E_p}.$$

We must now ensure convergence when $|p^0| \rightarrow \infty$. This requires distinguishing two cases according to the sign of the exponential, and hence choosing whether to close the contour with C_{upper} or C_{lower} , depending on the sign of $x^0 - y^0$. Introducing the Heaviside step function

$$\theta(x) = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x < 0, \end{cases}$$

we obtain

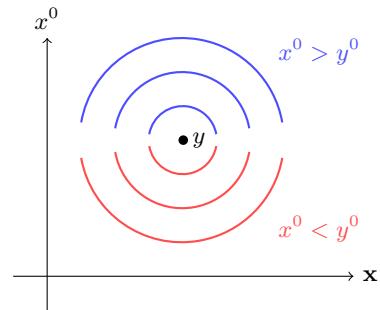
$$\Delta(x - y) = \int \frac{d^3 p}{(2\pi)^3} e^{ip \cdot (x-y)} \left[\theta(x^0 - y^0) \frac{e^{-iE_p(x^0 - y^0)}}{2E_p} + \theta(y^0 - x^0) \frac{e^{-iE_p(y^0 - x^0)}}{2E_p} \right].$$

Since the step functions already encode the time ordering, the propagator can finally be written in the compact form

$$\Delta(x - y) = \int \frac{d^3 p}{(2\pi)^3} e^{ip \cdot (x-y)} \frac{e^{-iE_p|x^0 - y^0|}}{2E_p}.$$

It is now explicit how the propagator with this prescription respects causality: particles with positive energy are propagated forward in time, while antiparticles associated with negative-energy solutions are propagated backward.

Recalling the form of the harmonic oscillator propagator ($\sim e^{-i\omega|t-t'|}/2\omega$), to be reviewed when studying the path integral quantization, one can see how the field ϕ can be interpreted as an infinite collection of harmonic oscillators parameterized by the frequency E_p .



Other prescriptions to displace the poles lead to different Green functions satisfying (2.2.11), which we now rewrite as

$$(-\square_x + m^2)G(x - y) = \delta^4(x - y),$$

with y^μ the spacetime point that supports the external source.

The **retarded Green function** $G_R(x - y)$ is defined to propagate all frequencies excited by the source at the spacetime point y^μ forward in time, so that $G_R(x - y)$ vanishes for $x^0 < y^0$. It is fixed by displacing all the poles below the real p^0 axis.

The **advanced Green function** $G_A(x - y)$ is defined to propagate all frequencies backward in time so that it vanishes for $x^0 > y^0$. It is obtained by displacing the poles above the real p^0 axis.

In the massless case ($m = 0$), and setting again $y^\mu = 0$ for simplicity, one computes the integrals and obtains

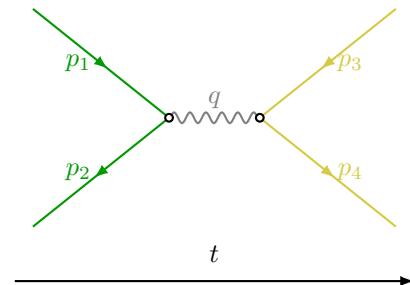
$$G_R(x) = \frac{1}{4\pi r} \delta(t - r), \quad G_A(x) = \frac{1}{4\pi r} \delta(t + r), \quad (2.2.15)$$

where $t = x^0$ and $r = |\mathbf{x}|$, as known from electromagnetism. They can be written in a manifestly Lorentz-invariant form as

$$G_R(x) = \frac{\theta(x^0)}{2\pi} \delta(x^2), \quad G_A(x) = \frac{\theta(-x^0)}{2\pi} \delta(x^2). \quad (2.2.16)$$

Real and virtual particle propagation. The propagator describes how field excitations travel through spacetime, encompassing both *real* and *virtual* particles. Real particles correspond to on-shell modes satisfying the mass-shell condition $p^2 = -m^2$, representing observable quanta that propagate over macroscopic distances.

Virtual particles, instead, are off-shell fluctuations ($p^2 \neq -m^2$) that exist only as intermediate states in interactions. Although they cannot be directly detected, their presence is essential: they mediate forces and account for quantum corrections in perturbation theory. Thus, the propagator unifies the causal motion of real particles and the short-lived virtual exchanges responsible for interactions.



Exercise: Derive the retarded and advanced Green functions in eqs. ((2.2.16)) by performing the momentum integrations.

Exercise: Derive the Yukawa potential by using the propagator and eq. ((2.2.13)), setting $\phi_0 = 0$ and $J(x) = -g \delta^3(\mathbf{x})$.

2.2.6 | Action and Lagrangian formalism

The *action principle* provides a compact and elegant way to express the dynamics of a physical system. Rather than writing equations of motion directly, one defines a single functional quantity — the *action* — whose stationary points correspond to the physical trajectories or field configurations that the system can take. This principle plays a central role not only in classical field theory but also in quantum field theory, where it is essential for the formulation of the *path integral quantization*. A brief review of the action formalism and Noether's theorem is given in Appendix B.

We can verify that the Klein–Gordon (KG) equation for a complex scalar field $\phi(x)$ follows from the action

$$S[\phi, \phi^*] = \int d^4x \mathcal{L}, \quad \mathcal{L} = -\partial_\mu \phi^* \partial^\mu \phi - m^2 \phi^* \phi, \quad (2.2.17)$$

where \mathcal{L} is the *Lagrangian density*, a local function of the fields and their derivatives. It is the Lagrangian density that determines the equations of motion through the *least action principle*, which states that the physical evolution of the field makes the action stationary under arbitrary infinitesimal variations of the fields:

$$\delta S[\phi, \phi^*] \equiv S[\phi + \delta\phi, \phi^* + \delta\phi^*] - S[\phi, \phi^*] = 0. \quad (2.2.18)$$

By varying ϕ and ϕ^* independently and taking the variation inside the integral, one finds:

$$\begin{aligned} \delta S &= \int d^4x (-\partial_\mu \delta\phi^* \partial^\mu \phi - \partial_\mu \phi^* \partial^\mu \delta\phi - m^2 \delta\phi^* \phi - m^2 \phi^* \delta\phi) \\ &= \int d^4x [\delta\phi (\partial^\mu \partial_\mu \phi^* - m^2 \phi^*) + \delta\phi^* (\partial_\mu \partial^\mu \phi - m^2 \phi)], \end{aligned}$$

where we have integrated by parts and discarded surface terms assuming that the variations $\delta\phi$ and $\delta\phi^*$ vanish at infinity.

Since the variations $\delta\phi$ and $\delta\phi^*$ are arbitrary, the integrand must vanish independently for each, we obtain to the Euler–Lagrange equations:

$$\begin{cases} (\square - m^2)\phi(x) &= 0, \\ (\square - m^2)\phi(x)^* &= 0. \end{cases}$$

TODO: Add appendix

These are exactly the Klein–Gordon equations for a complex scalar field and its complex conjugate.

Alternatively, one can express the same result using *functional derivatives*. Writing the variation of the action as

$$\delta S[\phi, \phi^*] = \int d^4x \left(\frac{\delta \mathcal{L}[\phi, \phi^*]}{\delta \phi(x)} \delta \phi(x) + \frac{\delta \mathcal{L}[\phi, \phi^*]}{\delta \phi^*(x)} \delta \phi^*(x) \right) = 0,$$

and imposing suitable boundary conditions (so that surface terms vanish), one obtains the field equations

$$\frac{\delta \mathcal{L}[\phi, \phi^*]}{\delta \phi^*(x)} = (\square - m^2)\phi(x) = 0, \quad \frac{\delta \mathcal{L}[\phi, \phi^*]}{\delta \phi(x)} = (\square - m^2)\phi^*(x) = 0.$$

This formulation is particularly useful in quantum field theory, where the action functional plays the role of the “generator” of the dynamics and symmetries of the theory.

For a *real* scalar field $\phi = \phi^*$, the action is usually written with a conventional normalization factor:

$$S[\phi] = \int d^4x \left(-\frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{m^2}{2} \phi^2 \right),$$

from which we immediately obtain the equation of motion:

$$\frac{\delta S[\phi]}{\delta \phi(x)} = (\square - m^2)\phi(x) = 0.$$

This form highlights the direct analogy between a free scalar field and a collection of independent harmonic oscillators labeled by momentum.

Finally, note that a *complex* scalar field can always be decomposed into two real fields of equal mass. Setting

$$\phi = \frac{1}{\sqrt{2}}(\varphi_1 + i\varphi_2), \quad \phi^* = \frac{1}{\sqrt{2}}(\varphi_1 - i\varphi_2),$$

where φ_1 and φ_2 denote the real and imaginary parts of ϕ , one finds that the Lagrangian density in (2.2.17) becomes

$$\mathcal{L} = -\partial_\mu \phi^* \partial^\mu \phi - m^2 \phi^* \phi = -\frac{1}{2} \partial_\mu \varphi_1 \partial^\mu \varphi_1 - \frac{1}{2} \partial_\mu \varphi_2 \partial^\mu \varphi_2 - \frac{m^2}{2} (\varphi_1^2 + \varphi_2^2). \quad (2.2.19)$$

Hence, a complex scalar field is dynamically equivalent to two independent real Klein–Gordon fields with identical masses. This observation will be useful later when discussing internal symmetries and conserved currents.

2.2.7 | Symmetries

The action formalism provides a powerful framework to connect *symmetries* of a theory—i.e. transformations that leave the action invariant—with corresponding *conservation laws*. This fundamental relation is expressed by **Noether’s theorem**, reviewed in Appendix B.

The free complex Klein–Gordon field possesses two main types of rigid (or *global*) symmetries:

1. **Space–time symmetries**, described by the *Poincaré group*.
2. **Internal symmetries**, associated with the invariance under phase rotations belonging to the group $U(1)$.

The term “rigid” (or equivalently “global”) indicates that these transformations do not depend on the spacetime point x : the same transformation is applied everywhere, unlike the case of *gauge symmetries*, where the transformation parameters are local functions of x .

The global U(1) symmetry. The U(1) symmetry corresponds to phase rotations of the field:

$$\phi(x) \rightarrow \phi'(x) = e^{i\alpha}\phi(x), \quad \phi^*(x) \rightarrow \phi'^*(x) = e^{-i\alpha}\phi^*(x), \quad (2.2.20)$$

where α is a real constant parameter. It is straightforward to verify that under this transformation the action in (2.2.17) remains invariant.¹

$$S[\phi', \phi'^*] = S[\phi, \phi^*].$$

In the real-field basis used in eq. (2.2.19), this symmetry corresponds to ordinary rotations in the plane spanned by (φ_1, φ_2) , i.e. to an SO(2) symmetry.

For infinitesimal transformations ($\alpha \ll 1$), one can expand the exponentials and obtain:

$$\delta_\alpha \phi(x) = \phi'(x) - \phi(x) = i\alpha\phi(x), \quad \delta_\alpha \phi^*(x) = \phi'^*(x) - \phi^*(x) = -i\alpha\phi^*(x), \quad (2.2.21)$$

which again leave the action invariant, $\delta_\alpha S[\phi, \phi^*] = 0$.

From global to local transformations. If we now generalize the transformation parameter to depend on spacetime, $\alpha \rightarrow \alpha(x)$, we obtain *local* U(1) transformations. In this case, the action is no longer invariant, and taking an infinitesimal transformation, the variation becomes

$$\delta_{\alpha(x)} S[\phi, \phi^*] = \int d^4x \partial_\mu \alpha \underbrace{(i\phi^* \partial^\mu \phi - i(\partial^\mu \phi^*)\phi)}_{J^\mu}. \quad (2.2.22)$$

For a constant α , $\partial_\mu \alpha = 0$ and the variation vanishes, confirming that the U(1) symmetry is global. The expression multiplying $\partial_\mu \alpha$ identifies the conserved **Noether current**:

$$J^\mu = i\phi^* \partial^\mu \phi - i(\partial^\mu \phi^*)\phi \equiv i\phi^* \overset{\leftrightarrow}{\partial}^\mu \phi. \quad (2.2.23)$$

By applying the equations of motion, one verifies that this current satisfies the continuity equation

$$\partial_\mu J^\mu = 0.$$

Indeed, since the equations of motion arise from $\delta S = 0$ for arbitrary variations, the variation in (2.2.22) must vanish for all possible choices of $\alpha(x)$, implying $\partial_\mu J^\mu = 0$. This is precisely the mechanism behind Noether's theorem.

The conserved **charge** associated with this current is

$$Q \equiv \int d^3\mathbf{x} J^0 = -i \int d^3\mathbf{x} \phi^* \overset{\leftrightarrow}{\partial}_0 \phi, \quad (2.2.24)$$

which is constant in time. However, Q is not positive definite: this is why, in the context of the Klein–Gordon field, it cannot be interpreted as a probability.

Still, this structure motivates the definition of a *conserved scalar product* between any two solutions χ and ϕ of the Klein–Gordon equation:

$$\langle \chi | \phi \rangle \equiv \int d^3\mathbf{x} i\chi^* \overset{\leftrightarrow}{\partial}_0 \phi.$$

Using the equations of motion, one can verify that this inner product is time-independent.

¹Since we can always factorize the two exponentials out of the derivatives (ϕ and ϕ^* appear multiplied together in the Lagrangian), the invariance holds for any real value of α .

Poincaré symmetries. The other fundamental symmetry of the Klein–Gordon theory is its invariance under the *Poincaré group*, which combines Lorentz transformations and translations:

$$x^\mu \rightarrow x'^\mu = \Lambda_\nu^\mu x^\nu + a^\mu, \quad \phi(x) \rightarrow \phi'(x') = \phi(x), \quad \phi^*(x) \rightarrow \phi'^*(x') = \phi^*(x). \quad (2.2.25)$$

The field ϕ thus transforms as a scalar under Poincaré transformations, and the action is easily verified to be invariant.

To extract the associated conserved quantities, it is convenient to study the *infinitesimal* form of these transformations. For an infinitesimal translation a^μ

$$\begin{aligned} \delta_a \phi(x) &= \phi'(x) - \phi(x) = \phi'(x) - \phi'(x') \\ &= \delta_a \phi'(x) = -(\phi'(x+a) - \phi'(x)) \\ &= -(\phi'(x) + a^\mu \partial_\mu \phi'(x) - \phi'(x)) = -a^\mu \partial_\mu \phi'(x) \end{aligned}$$

where we have Taylor expanded, so that eq. (2.2.25) becomes²

$$\begin{aligned} \delta_a \phi(x) &= -a^\mu \partial_\mu \phi(x), \\ \delta_a \phi^*(x) &= -a^\mu \partial_\mu \phi^*(x). \end{aligned} \quad (2.2.26)$$

If we let the parameter a^μ depend arbitrarily on x , Noether's theorem yields the four corresponding conserved currents — in this case, the components of the **energy–momentum tensor**:

$$\delta_{a(x)} S[\phi, \phi^*] = \int d^4x (\partial_\mu a_\nu) \underbrace{(\partial^\mu \phi^* \partial^\nu \phi + \partial^\nu \phi^* \partial^\mu \phi + \eta^{\mu\nu} \mathcal{L})}_{T^{\mu\nu}}.$$

Here, total derivatives have been neglected, and \mathcal{L} denotes the Lagrangian density from eq. (2.2.17): this result can be obtained considering linearity of the lagrangian, thus we can compute the variation of each term separately and directly in the lagrangian

$$\begin{aligned} \delta_{a(x)} \mathcal{L}[\phi, \phi^*] &= -(\partial_\mu \delta_{a(x)} \phi^*) (\partial^\mu \phi) - (\partial_\mu \phi^*) (\partial^\mu \delta_{a(x)} \phi) - m^2 (\delta_{a(x)} \phi^* \phi + \phi^* \delta_{a(x)} \phi) \\ &= \partial_\mu (a^\nu \partial_\nu \phi^*) (\partial^\mu \phi) + (\partial_\mu \phi^*) \partial^\mu (a^\nu \partial_\nu \phi) + m^2 (a^\nu \partial_\nu \phi^* \phi + \phi^* a^\nu \partial_\nu \phi) \\ &= [(\partial_\mu a_\nu) \partial^\nu \phi^* + a^\nu (\partial_\mu \partial^\nu \phi^*)] \partial^\mu \phi + \partial^\mu \phi^* [(\partial_\mu a_\nu) \partial^\nu \phi + a_\nu (\partial_\mu \partial^\nu \phi)] + m^2 (\cdot) \\ &= (\partial_\mu a_\nu) (\partial^\mu \phi^* \partial^\nu \phi + \partial^\nu \phi^* \partial^\mu \phi) + a_\nu [(\partial_\mu \partial^\nu \phi^*) \partial^\mu \phi + \partial^\mu \phi^* (\partial_\mu \partial^\nu \phi)] + m^2 (\cdot) \\ &= (\partial_\mu a_\nu) (\partial^\mu \phi^* \partial^\nu \phi + \partial^\nu \phi^* \partial^\mu \phi) - \eta^{\mu\nu} \partial_\mu a_\nu (\partial_\mu \phi^* \partial^\mu \phi) + m^2 (\cdot), \end{aligned}$$

where in the last step we have integrated by parts the second term, yielding a total derivative that can be neglected (in the end we are interested only in the action, and we assume boundary terms vanish)

$$a^\nu (\partial_\mu \partial^\nu \phi^*) \partial^\mu \phi = \partial_\nu (\cdot) - \eta^{\nu\lambda} \partial_\lambda a_\nu (\partial_\mu \phi^* \partial^\mu \phi) - a_\nu \partial^\mu \phi^* (\partial_\mu \partial^\nu \phi),$$

from which the final expression follows. Now, rearranging the first mass term with the idea to construct the lagrangian density (multiplied by the Minkowski metric), and a deletion for the remaining mass term, we obtain

$$m^2 (a^\nu \partial_\nu \phi^* \phi) = m^2 \partial_\nu (\cdot) - m^2 \eta^{\nu\lambda} \partial_\lambda a_\nu (\phi^* \phi) - m^2 \phi^* a^\nu \partial_\nu \phi,$$

where again the total derivative can be neglected, leading to the final form of the variation:

$$\delta_{a(x)} \mathcal{L}[\phi, \phi^*] = (\partial_\mu a_\nu) (\partial^\mu \phi^* \partial^\nu \phi + \partial^\nu \phi^* \partial^\mu \phi + \eta^{\mu\nu} \mathcal{L}),$$

²Since the field is multiplied by an infinitesimal displacement a^μ , we can replace ϕ' with ϕ in the last step without affecting the result to first order in a^μ .

from which the variation of the action follows immediately and thus the identification of the energy-momentum tensor:

$$T^{\mu\nu} = \partial^\mu \phi^* \partial^\nu \phi + \partial^\nu \phi^* \partial^\mu \phi + \eta^{\mu\nu} \mathcal{L}. \quad (2.2.27)$$

This tensor is both symmetric and conserved,

$$\partial_\mu T^{\mu\nu} = 0,$$

which, according to Noether's theorem, implies the existence of conserved quantities associated with spacetime translations.

The corresponding conserved four-vector, the Noether charge associated with translations, is given by

$$P^\mu = \int d^3x T^{0\mu},$$

represents the total **four-momentum** of the field. Each component of P^μ is linked to a specific symmetry:

- The temporal component P^0 is conserved in **time translations** and represents the total *energy* of the field.
- The spatial components P^i ($i = 1, 2, 3$) are conserved in **spatial translations** and represent the components of the *momentum vector*.

Explicitly, the **local energy density** is given by

$$\begin{aligned} T^{00} &= 2\partial^0 \phi^* \partial^0 \phi - \eta^{00} (\partial_\lambda \phi^* \partial^\lambda \phi - m^2 \phi^* \phi) \\ &= 2\partial_0 \phi^* \partial_0 \phi + \partial_0 \phi^* \partial^0 \phi + (\nabla \phi^*) \cdot (\nabla \phi) + m^2 \phi^* \phi, \end{aligned}$$

so that we can write

$$\mathcal{E}(x) = \partial_0 \phi^* \partial_0 \phi + (\nabla \phi^*) \cdot (\nabla \phi) + m^2 \phi^* \phi. \quad (2.2.28)$$

The total energy of the field is therefore

$$P^0 \equiv E = \int d^3x T^{00}.$$

This quantity is conserved in time and, for the Klein–Gordon field, it is manifestly *positive definite*.

These results illustrate how the action formalism and Noether's theorem together provide a unified and systematic way to identify the conserved quantities associated with the fundamental symmetries of a field theory.

2.3 | Dirac Equation

Dirac found the correct equation to describe particles of spin $\frac{1}{2}$ by looking for a relativistic wave equation that could admit a probabilistic interpretation and thus be consistent with the principles of quantum mechanics, since the Klein-Gordon equation did not have such an interpretation due to the non positive-definite probability density.

Although a probabilistic interpretation will not be possible in the presence of interactions (eventually, Dirac's wave function must be treated as a classical field to be quantized again in the second quantization), it is useful to retrace the line of thinking that brought Dirac to the formulation of an equation of first order in time.

The Dirac equation takes the form

$$(\gamma^\mu \partial_\mu + m)\psi(x) = 0, \quad (2.3.1)$$

where the wave function $\psi(x)$ has four complex components (it is a so-called Dirac spinor) and the γ^μ are 4×4 matrices. Because the components of the Dirac spinor $\psi(x)$ are not that of a four-vector (they mix differently under Lorentz transformations), it is necessary to use different indices to indicate their components without ambiguities. Here, we use greek indices $\mu, \nu, \dots = 0, 1, 2, 3$ to indicate the components of a four-vector and latin indices $a, b, \dots = 1, 2, 3, 4$ to indicate the components of a Dirac spinor. Equation (2.3.1) is then written more explicitly as

$$\left[(\gamma^\mu)_a^b \partial_\mu + m \delta_a^b \right] \psi_b(x) = 0,$$

and consists of four distinct coupled equations ($a = 1, 2, 3, 4$). Spinorial indices are usually left implicit, and a matrix notation is used instead: γ^μ are matrices and ψ a column vector.

Derivation of the Dirac Equation

The relativistic relation between energy and momentum reads

$$p_\mu p^\mu = -m^2 c^2 \iff E^2 = p^2 c^2 + m^2 c^4,$$

thus, with the correspondence principle

$$E = cp^0 \rightarrow i\hbar \frac{\partial}{\partial t}, \quad \mathbf{p} \rightarrow -i\hbar \nabla \implies p_\mu \rightarrow -i\hbar \partial_\mu,$$

which leads to the Klein-Gordon equation, second order in both time and space derivatives. As a consequence, the KG conserved current density is not positive definite, making difficult a probability density interpretation of the theory.

Dirac proposed an alternative equation, first order in both time and space derivatives, that could overcome these problems. He started from the ansatz

$$E = c\mathbf{p} \cdot \boldsymbol{\alpha} + \beta mc^2, \quad (2.3.2)$$

with $\boldsymbol{\alpha} = (\alpha^1, \alpha^2, \alpha^3)$ and β hermitian matrices to be determined. Squaring both sides and imposing the relativistic relation, one finds the conditions

$$\begin{aligned} E^2 &= (c\mathbf{p} \cdot \boldsymbol{\alpha} + \beta mc^2)(c\mathbf{p} \cdot \boldsymbol{\alpha} + \beta mc^2) \\ &= c^2(p^i \alpha^i)^2 + m^2 c^4 \beta^2 + mc^3 (p^i \alpha^i \beta + \beta p^j \alpha^j) \\ &= m^2 c^4 \frac{1}{2} (\beta \beta + \beta \beta) + c^2 p^i p^j \alpha^i \alpha^j + mc^3 p^i (\alpha^i \beta + \beta \alpha^i) \\ &= m^2 c^4 \frac{1}{2} \{\beta, \beta\} + c^2 p^i p^j \frac{1}{2} (\alpha^i \alpha^j + \alpha^j \alpha^i + \alpha^i \alpha^j - \alpha^j \alpha^i) + mc^3 p^i \{\alpha^i, \beta\}, \end{aligned}$$

where we have recognized the anticommutator $\{ , \}$ and decomposed the product of α matrices into symmetric and antisymmetric parts. Since $p^i p^j \rightarrow \hbar^2 \partial^i \partial^j$ is symmetric in the indices i and j , the antisymmetric part of the product of α matrices vanishes. Thus, we are able to recognize the last anticommutator, before imposing the relativistic relation:

$$E^2 = m^2 c^4 \frac{1}{2} \{ \beta, \beta \} + c^2 p^i p^j \frac{1}{2} \{ \alpha^i, \alpha^j \} + mc^3 p^i \{ \alpha^i, \beta \} = m^2 c^4 + c^2 p^2,$$

hence the relations that the matrices must satisfy:

$$\begin{aligned} \{ \alpha^i, \alpha^j \} &= 2\delta^{ij}\mathbb{I}, \\ \{ \alpha^i, \beta \} &= 0, \\ \{ \beta, \beta \} &= 2\mathbb{I}. \end{aligned} \tag{2.3.3}$$

These relations define the **Clifford Algebra** and cannot be satisfied by numbers, as the first relation implies that α^i cannot commute among themselves. The smallest matrices that can satisfy these relations (minimal solution) are 4×4 **traceless** matrices, which can be constructed in terms of the Pauli matrices σ^i (in equation (1.4.9)) as:

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}, \tag{2.3.4}$$

known as the **Dirac representation** of the Clifford algebra; let us remember that the Pauli matrices are

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and they satisfy the relation $\sigma^i \sigma^j = \delta^{ij}\mathbb{I} + i\epsilon^{ijk}\sigma^k$.

Theorem 2.1. *All four dimensional irreducible representations of the Clifford algebra are unitarily equivalent to the Dirac representation, and thus related by a change of basis; other non trivial representations can be constructed as direct sums of irreducible ones and are thus reducible.*

With the correspondence principle, we can now quantize the ansatz for the energy and thus write the **Dirac equation** in Hamiltonian form:

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = (-i\hbar c \boldsymbol{\alpha} \cdot \nabla + \beta mc^2) \psi(\mathbf{x}, t), \tag{2.3.5}$$

where the operator acting on the right-hand side is the Dirac Hamiltonian, acting on the four-component spinor $\psi(\mathbf{x}, t)$; since $\boldsymbol{\alpha}$ and β are hermitian matrices, the Hamiltonian is hermitian as well and the time evolution is unitary. The Dirac equation can be written in **covariant form**

$$\begin{aligned} \frac{-\beta}{\hbar c} \left(i\hbar \frac{\partial}{\partial t} \right) \psi &= \frac{-\beta}{\hbar c} (-i\hbar c \boldsymbol{\alpha} \cdot \nabla + \beta mc^2) \psi, \\ -i\frac{\beta}{c} \partial_t \psi &= \left(i\beta \boldsymbol{\alpha} \cdot \nabla - \frac{mc}{\hbar} \right) \psi, \\ \left(-i\beta \partial_0 - i\beta \boldsymbol{\alpha} \cdot \nabla + \frac{mc}{\hbar} \right) \psi &= 0, \end{aligned}$$

we can identify components of a scalar product between four-vectors if we define the gamma matrices as

$$\gamma^0 = -i\beta = -i \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}, \quad \gamma^i = -i\beta \alpha^i = \begin{pmatrix} 0 & -i\sigma^i \\ i\sigma^i & 0 \end{pmatrix} \tag{2.3.6}$$

so that the Dirac equation takes the form

$$(\gamma^\mu \partial_\mu + \mu^2) \psi(x) = 0, \quad (2.3.7)$$

with $\mu = \frac{mc}{\hbar}$ the *inverse Compton wavelength* of the particle. The gamma matrices satisfy the clifford algebra relations

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu},$$

where $\eta^{\mu\nu} = \text{diag}(-1, 1, 1, 1)$ is the Minkowski metric tensor. In the Dirac representation, the gamma matrices read³

$$\gamma^0 = -i \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}, \quad \gamma^i = -i \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix},$$

and we can adopt natural units and **Feynman slash notation**

$$\not{A} = \gamma^\mu A_\mu = \gamma_\mu A^\mu,$$

so that $\not{\partial} = \gamma^\mu \partial_\mu$ to write the Dirac equation in a more compact form in natural units ($\hbar = c = 1 \implies \mu = m$):

$$(\gamma^\mu \partial_\mu + \mu) \psi(x) = 0 \iff (\not{\partial} + m) \psi(x) = 0.$$

2.3.1 | Continuity Equation

It is immediate to derive an equation of continuity describing the conservation of a positive definite charge. Dirac tentatively identified the relative charge density, appropriately normalized, with a probability density. Let us see how to get the continuity equation algebraically. Using the hamiltonian form, we multiply eq. (2.3.5) with ψ^\dagger on the left and subtract the hermitian-conjugated equation multiplied by ψ on the right, and obtain (remember that α and β are hermitian matrices)

$$\begin{aligned} i\hbar \psi^\dagger \frac{\partial}{\partial t} \psi + i\hbar c \psi^\dagger \alpha \cdot \nabla \psi - mc^2 \psi^\dagger \beta \psi \\ - i\hbar \frac{\partial}{\partial t} \psi^\dagger \psi - i\hbar c \nabla \psi^\dagger \cdot \alpha \psi + mc^2 \psi^\dagger \beta \psi = 0, \end{aligned}$$

which can be rearranged, after simplifying the mass terms, as the continuity equation

$$\frac{\partial \psi^\dagger \psi}{\partial t} + \nabla \cdot (c \psi^\dagger \alpha \psi) = 0, \quad (2.3.8)$$

identifying the probability density and current density as

$$\rho = \psi^\dagger \psi, \quad \mathbf{J} = c \psi^\dagger \alpha \psi.$$

The probability density is positive definite, overcoming the problem of the Klein-Gordon equation. The current density can be interpreted as the flow of probability per unit area per unit time.

2.3.2 | Plane Wave Solutions

The free equation admits plane wave solutions which contain the phase $e^{ip_\mu x^\mu}$ for propagation in space-time and a polarization $\omega(p)$ for the spin. Inserting in the Dirac equation (2.3.7) a plane

³Note that the minus in the first element of the secnd raw of γ^i does not appear in α : it comes from the product among α and β .

wave ansatz of the form

$$\psi_p(x) \sim \omega(p) e^{ip_\mu x^\mu}, \quad \omega(p) = \begin{pmatrix} \omega_1(p) \\ \omega_2(p) \\ \omega_3(p) \\ \omega_4(p) \end{pmatrix},$$

with p^μ arbitrary four-momentum, one finds conditions on the spinor $\omega(p)$ and on the four-momentum p^μ such that the Dirac equation is satisfied. Plugging the ansatz in the Dirac equation

$$(\not{d} + m) \psi_p(x) = (\gamma^\mu p_\mu + m) \omega(p) e^{ip_\mu x^\mu} = 0,$$

where $\partial_\mu \psi_p = \partial_\mu (\omega(p) e^{ip_\mu x^\mu}) = i p_\mu \omega(p) e^{ip_\mu x^\mu}$, hence we find

$$(i\gamma^\mu p_\mu + m) \omega(p) e^{ip_\mu x^\mu} = 0,$$

which can be multiplied by $(-i\gamma^\nu p_\nu + m)$ on the left to obtain

$$(\not{p}^2 + m^2) \omega(p) e^{ip_\mu x^\mu} = (p_\mu p^\mu + m^2) \omega(p) = 0,$$

since it is easy to show that $\not{p}^2 = p^2$:⁴

$$\begin{aligned} \not{p}^2 &= \gamma^\mu \gamma^\nu p_\mu p_\nu = \frac{1}{2} (\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu + \gamma^\mu \gamma^\nu - \gamma^\nu \gamma^\mu) p_\mu p_\nu \\ &= \frac{1}{2} \{\gamma^\mu, \gamma^\nu\} p_\mu p_\nu = \eta^{\mu\nu} p_\mu p_\nu = p^2 = p_\mu p^\mu, \end{aligned}$$

since the antisymmetric part vanishes due to the symmetry of $p_\mu p_\nu$. Thus, we find the mass-shell condition

$$p_\mu p^\mu + m^2 = 0 \iff E^2 = p^2 + m^2,$$

which is satisfied by both positive and negative energy solutions $E = \pm \sqrt{p^2 + m^2}$, as for Klein-Gordon. The spinor $\omega(p)$ must satisfy the equation

$$(p_\mu p^\mu + m^2) \omega(p) = 0. \quad (2.3.9)$$

Particle at rest. In order to understand the structure of the spinor $\omega(p)$, let us first consider the case of a particle at rest, i.e., $p^\mu = (E, 0, 0, 0)$. In this case, the Dirac equation (2.3.7) with the plane wave ansatz reduces to

$$\begin{aligned} (i\gamma^0 p_0 + m) \omega(p) e^{-ip_0 x^0} &= 0, \\ (-i(-i\beta)E + m) \omega(p) e^{-iEt} &= 0, \\ \beta E \omega(p) &= m \omega(p), \end{aligned}$$

and by multiplying by beta ($\beta^2 = \mathbb{I}$) we get

$$E \omega(p) = \beta m \omega(p) \implies E \omega(p) = \begin{pmatrix} m & 0 & 0 & 0 \\ 0 & m & 0 & 0 \\ 0 & 0 & -m & 0 \\ 0 & 0 & 0 & -m \end{pmatrix} \omega(p),$$

which are the four solutions of the Dirac equation for a particle at rest. The first two solutions correspond to positive energy, while the last two correspond to negative energy. The spinor $\omega(p)$

⁴Here p^2 is not the square of the spatial momentum norm, but the Minkowski norm $p_\mu p^\mu$.

is thus a four-component object, with two independent components for each value of the energy:

$$\begin{aligned} E = m) \quad \psi_1(x) &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{-imt}, & \psi_2(x) &= \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{-imt}, \\ E = -m) \quad \psi_3(x) &= \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{imt}, & \psi_4(x) &= \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{imt}. \end{aligned}$$

The general case with arbitrary momentum can be derived with similar calculations. Alternatively, they can be obtained from a Lorentz transformation applied to the solution above. To use the last method, it is necessary to study explicitly the covariance of the Dirac equation, which we postponed for a while. At this stage, Dirac seemed to have solved the issue regarding the probabilistic interpretation of relativistic quantum mechanics, but was confronted with the existence of apparently unphysical negative energy solutions. Nevertheless, he continued to explore the consequences of his equation, starting by looking at its non-relativistic limit.

2.3.3 | Pauli Equation: Non-Relativistic Limit

To study the non-relativistic limit of the Dirac equation, we reinsert \hbar and c . It is convenient to use the hamiltonian form

$$i\hbar\partial_t\psi(\mathbf{x}, t) = (c\boldsymbol{\alpha} \cdot \mathbf{p} + \beta mc^2)\psi(\mathbf{x}, t),$$

where $\mathbf{p} = -i\hbar\nabla$. We separate the rest energy from the total energy by writing the spinor as

$$\psi(\mathbf{x}, t) = e^{-\frac{i}{\hbar}mc^2t} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix}, \quad (2.3.10)$$

factoring out an expected time dependence due to the rest energy $E = mc^2$, and splitting the Dirac spinor into two two-component spinors φ and χ (choice enforced by the positive / negative energy solutions). Inserting this expression into the Dirac equation (and remembering the expressions for α^i and β in (2.3.4)), we can manipulate it in order to obtain two coupled equations for φ and χ :

$$i\hbar\frac{\partial}{\partial t}e^{-\frac{i}{\hbar}mc^2t} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix} = (-i\hbar c\boldsymbol{\alpha} \cdot \nabla + mc^2\beta) e^{-\frac{i}{\hbar}mc^2t} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix},$$

which computing terms individually gives

$$\begin{aligned} i\hbar\partial_t \left(e^{-\frac{i}{\hbar}mc^2t} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix} \right) &= i\hbar e^{-\frac{i}{\hbar}mc^2t} \left[-\frac{i}{\hbar}mc^2 \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix} + \begin{pmatrix} \partial_t\varphi(\mathbf{x}, t) \\ \partial_t\chi(\mathbf{x}, t) \end{pmatrix} \right], \\ -i\hbar c\boldsymbol{\alpha} \cdot \nabla e^{-\frac{i}{\hbar}mc^2t} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix} &= -i\hbar c e^{-\frac{i}{\hbar}mc^2t} \begin{pmatrix} 0 & \boldsymbol{\sigma} \cdot \nabla \\ \boldsymbol{\sigma} \cdot \nabla & 0 \end{pmatrix} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix}, \\ mc^2\beta e^{-\frac{i}{\hbar}mc^2t} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix} &= mc^2 e^{-\frac{i}{\hbar}mc^2t} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ -\chi(\mathbf{x}, t) \end{pmatrix}. \end{aligned}$$

Finally, simplifying the identical exponential factors, we get to

$$\left[mc^2 \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix} + i\hbar \begin{pmatrix} \partial_t\varphi(\mathbf{x}, t) \\ \partial_t\chi(\mathbf{x}, t) \end{pmatrix} \right] = -i\hbar \begin{pmatrix} 0 & \boldsymbol{\sigma} \cdot \nabla \chi(\mathbf{x}, t) \\ \boldsymbol{\sigma} \cdot \nabla \varphi(\mathbf{x}, t) & 0 \end{pmatrix} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ -\chi(\mathbf{x}, t) \end{pmatrix} + mc^2 \begin{pmatrix} \varphi(\mathbf{x}, t) \\ -\chi(\mathbf{x}, t) \end{pmatrix},$$

which can be separated into the two equations

$$\begin{cases} i\hbar \frac{\partial}{\partial t} \varphi(\mathbf{x}, t) = c\boldsymbol{\sigma} \cdot \mathbf{p} \chi(\mathbf{x}, t), \\ i\hbar \frac{\partial}{\partial t} \chi(\mathbf{x}, t) = c\boldsymbol{\sigma} \cdot \mathbf{p} \varphi(\mathbf{x}, t) - 2mc^2 \chi(\mathbf{x}, t). \end{cases}$$

If we now take the non relativistic limit, where the kinetic energy is much smaller than the rest energy, we can neglect the time derivative in the second equation, obtaining

$$\chi(\mathbf{x}, t) \simeq \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{2mc} \varphi(\mathbf{x}, t),$$

which can be inserted into the first equation to obtain

$$i\hbar \frac{\partial}{\partial t} \varphi(\mathbf{x}, t) = \frac{(\boldsymbol{\sigma} \cdot \mathbf{p})^2}{2m} \varphi(\mathbf{x}, t).$$

Using the identity

$$(\boldsymbol{\sigma} \cdot \mathbf{p})^2 = \mathbf{p}^2 + i\epsilon^{ijk} \sigma^k p^i p^j = \mathbf{p}^2,$$

from the algebra of the Pauli matrices $\sigma^i \sigma^j = \delta^{ij} + i\epsilon^{ijk} \sigma^k$ and the null product of the symmetric momenta operators and the antisymmetric Levi-Civita symbol, we finally obtain the **free Pauli equation** (for a free particle):

$$i\hbar \frac{\partial}{\partial t} \varphi(\mathbf{x}, t) = \frac{\mathbf{p}^2}{2m} \varphi(\mathbf{x}, t). \quad (2.3.11)$$

It is similar to the Schrödinger equation, but the wave function $\varphi(\mathbf{x}, t)$ is a two-component spinor, describing the two possible spin states of a spin- $\frac{1}{2}$ particle.

Electromagnetic Coupling

This analysis can be extended to include the interaction with an external electromagnetic field, introduced via **minimal coupling**:

$$p^\mu \rightarrow \pi^\mu = p^\mu - \frac{e}{c} A^\mu,$$

where $A^\mu = (\phi, \mathbf{A})$ is the four-potential of the electromagnetic field. The Hamiltonian in presence of an external electromagnetic field reads

$$H = \frac{\pi^2}{2m} = \frac{1}{2m} \left(p - \frac{e}{c} A \right)^2,$$

thus we are substituting $E \rightarrow E - e\phi$ and $\mathbf{p} \rightarrow \mathbf{p} - \frac{e}{c}\mathbf{A}$. Starting from the Dirac equation in (2.3.2)⁵ making the minimal substitution, we have

$$E - e\phi = c\boldsymbol{\alpha} \cdot \boldsymbol{\pi} + \beta mc^2 \implies E = c\boldsymbol{\alpha} \cdot \boldsymbol{\pi} + \beta mc^2 + e\phi,$$

thus the Dirac equation in presence of an external electromagnetic field reads

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = (c\boldsymbol{\alpha} \cdot \boldsymbol{\pi} + \beta mc^2 + e\phi) \psi(\mathbf{x}, t).$$

If we repeat the previous analysis for the non-relativistic limit, splitting the spinor and factoring out the rest energy, we obtain

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix} + mc^2 \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix} = c\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \begin{pmatrix} \chi(\mathbf{x}, t) \\ \varphi(\mathbf{x}, t) \end{pmatrix} + mc^2 \begin{pmatrix} \varphi(\mathbf{x}, t) \\ -\chi(\mathbf{x}, t) \end{pmatrix} + e\phi \begin{pmatrix} \varphi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix}.$$

⁵We can invert $\mathbf{p} \cdot \boldsymbol{\alpha} \rightarrow \boldsymbol{\alpha} \cdot \mathbf{p}$ since they act on different spaces, hence they commute.

This leads to the coupled equations

$$\begin{cases} i\hbar \frac{\partial}{\partial t} \varphi(\mathbf{x}, t) = c\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \chi(\mathbf{x}, t) + e\phi \varphi(\mathbf{x}, t), \\ i\hbar \frac{\partial}{\partial t} \chi(\mathbf{x}, t) = c\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \varphi(\mathbf{x}, t) - 2mc^2 \chi(\mathbf{x}, t) + e\phi \chi(\mathbf{x}, t). \end{cases}$$

In the non-relativistic limit, we can neglect again the time derivative in the second equation, along with the term of EM coupling (small with respect to c^2), obtaining again

$$\chi(\mathbf{x}, t) \simeq \frac{\boldsymbol{\sigma} \cdot \boldsymbol{\pi}}{2mc} \varphi(\mathbf{x}, t),$$

which can be inserted into the first equation to obtain

$$i\hbar \frac{\partial}{\partial t} \varphi(\mathbf{x}, t) = \left(\frac{(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^2}{2m} + e\phi \right) \varphi(\mathbf{x}, t).$$

Using the algebra of the Pauli matrices, we can expand $(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^2$ as

$$\begin{aligned} (\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^2 &= \sigma^i \sigma^j \pi_i \pi_j = (\delta^{ij} + i\epsilon^{ijk} \sigma^k) \pi_i \pi_j \\ &= \pi^2 + i\epsilon^{ijk} \sigma_k \pi_i \pi_j = \pi^2 + \frac{i}{2} \epsilon^{ijk} \sigma^k [\pi_i, \pi_j], \end{aligned}$$

since only the antisymmetric part of $\pi_i \pi_j$ contributes to the last term. The commutator of the kinetic momenta can be computed as

$$[\pi_i, \pi_j] = \left[p_i - \frac{e}{c} A_i, p_j - \frac{e}{c} A_j \right] = -\frac{e}{c} ([p_i, A_j] - [p_j, A_i]),$$

which can be applied to a test function $f(\mathbf{x})$ to obtain

$$[p_i, A_j] f(\mathbf{x}) = -i\hbar \partial_i (A_j f(\mathbf{x})) + A_j i\hbar \partial_i f(\mathbf{x}) = -i\hbar (\partial_i A_j) f(\mathbf{x}),$$

so that the commutator $[p_i, A_j] = -i\hbar \partial_i A_j$ and we can continue the computation of $[\pi_i, \pi_j]$ as:

$$[\pi_i, \pi_j] = -\frac{e}{c} ([p_i, A_j] - [p_j, A_i]) = \frac{e i \hbar}{c} (\partial_i A_j - \partial_j A_i).$$

If we now insert this commutator into the previous expression for $(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^2$, we obtain

$$(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^2 = \boldsymbol{\pi}^2 - \frac{e \hbar}{2c} \sigma^k \epsilon^{ijk} (\partial_i A_j - \partial_j A_i),$$

where we can recognize the electromagnetic strength tensor components $F_{ij} = \partial_i A_j - \partial_j A_i$, which can be related to the magnetic field as $B^k = \frac{1}{2} \epsilon^{ijk} F_{ij}$, indeed

$$\epsilon^{ijk} F_{ij} = \epsilon^{ijk} (\partial_i A_j - \partial_j A_i) = B^k - \epsilon^{jik} \partial_j A_i == B^k + \epsilon^{ijk} \partial_i A_j = 2B^k.$$

Thus, we finally obtain

$$(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})^2 = \boldsymbol{\pi}^2 - \frac{e \hbar}{c} \boldsymbol{\sigma} \cdot \mathbf{B},$$

and recognizing the **Pauli spin operator** $\mathbf{S} = \frac{\hbar}{2} \boldsymbol{\sigma}$, we can write the non-relativistic limit of the Dirac equation (Pauli equation) in presence of an external electromagnetic field as

$$i\hbar \frac{\partial}{\partial t} \varphi(\mathbf{x}, t) = \left[\frac{\boldsymbol{\pi}^2}{2m} + e\phi - \frac{e}{mc} \mathbf{S} \cdot \mathbf{B} \right] \varphi(\mathbf{x}, t). \quad (2.3.12)$$

Gyromagnetic factor. The last term in the Pauli equation (2.3.12) describes the interaction between the intrinsic magnetic moment of the particle and the external magnetic field. The magnetic moment operator is defined as

$$\boldsymbol{\mu} = \frac{ge}{2mc} \mathbf{S},$$

where g is the **gyromagnetic factor**. Comparing with the Pauli equation, we find that the gyromagnetic factor for a Dirac particle is $g = 2$. This result was one of the first triumphs of the Dirac equation, as it correctly predicted the gyromagnetic factor of the electron, which had been measured experimentally to be very close to 2.

Classically, when we have electromagnetic coupling, the interacting term of the Hamiltonian is

$$H = -\boldsymbol{\mu} \cdot \mathbf{B},$$

where $\boldsymbol{\mu} = \frac{ge}{2mc} \mathbf{L}$ is the magnetic moment of the particle with orbital angular momentum \mathbf{L} and g expected to be 1. We can see that the intrinsic spin of the electron gives rise to a magnetic moment twice as large as that expected from classical considerations, but we can concile the results by noting that the spin is not a classical angular momentum; considering a constant magnetic field $\mathbf{B} = B\hat{z}$, the vector potential can be chosen as $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$, so that the squared kinetic momentum reads

$$\begin{aligned} \pi^2 &= \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 = \mathbf{p}^2 - \frac{e}{c} (\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + \frac{e^2}{c^2} \mathbf{A}^2, \\ &= \mathbf{p}^2 + \frac{e^2}{c^2} \mathbf{A}^2 - \frac{e}{c} \{ \mathbf{p}, \mathbf{A} \} = \mathbf{p}^2 + \frac{e^2}{c^2} \mathbf{A}^2 - \frac{2e}{c} \mathbf{p} \cdot \mathbf{A} \\ &= \mathbf{p}^2 + \frac{e^2}{c^2} \mathbf{A}^2 - \frac{e}{c} \mathbf{B} \cdot (\mathbf{r} \times \mathbf{p}) = \mathbf{p}^2 + \frac{e^2}{c^2} \mathbf{A}^2 - \frac{e}{c} \mathbf{B} \cdot \mathbf{L}, \end{aligned}$$

where we have used the fact that $\nabla \cdot \mathbf{A} = 0$ for this choice of gauge, so that $\mathbf{p} \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{p}$ and in the end the identity of the triple product $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a})$. Thus, inserting this back into the Pauli equation (2.3.12) gives

$$i\hbar \frac{\partial}{\partial t} \varphi(\mathbf{x}, t) = \left[\frac{\mathbf{p}^2}{2m} + \frac{e^2}{2mc^2} \mathbf{A}^2 + e\phi - \frac{e}{2mc} (\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B} \right] \varphi(\mathbf{x}, t),$$

where we can see that both the orbital angular momentum and the intrinsic spin contribute to the magnetic moment, with gyromagnetic factors $g_L = 1$ and $g_S = 2$ respectively.

2.3.4 | Angular Momentum and Spin

As seen from the non-relativistic limit, the Dirac spinor describes a particle of spin $\frac{1}{2}$, such as the electron. The spin operator acts on the two components of the wave function ψ , and is proportional to the Pauli matrices $\mathbf{S} = \frac{\hbar}{2} \boldsymbol{\sigma}$. This suggests that the full spin operator acting on the four-component Dirac spinor is given (in natural units) in the Dirac representation by

$$\mathbf{S} = \frac{1}{2} \boldsymbol{\Sigma} = \frac{1}{2} \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}, \text{ acting on } \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}.$$

The Σ^i matrices can be expressed in terms of the Pauli matrices as

$$\Sigma^i = -\frac{i}{2} \epsilon^{ijk} \alpha^j \alpha^k, \quad \text{where} \quad \alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}.$$

Example. We can indeed compute Σ^1 as

$$\Sigma^1 = -\frac{i}{2} (\epsilon^{123} \alpha^2 \alpha^3 + \epsilon^{132} \alpha^3 \alpha^2) = -\frac{i}{2} (\alpha^2 \alpha^3 - \alpha^3 \alpha^2),$$

since $\epsilon^{123} = 1$ and $\epsilon^{132} = -1$. Now we can use the fact that the α^i matrices anticommute, $\{\alpha^i, \alpha^j\} = 0$, to write

$$\Sigma^1 = -\frac{i}{2} (2\alpha^2 \alpha^3) = -i\alpha^2 \alpha^3 = \begin{pmatrix} \sigma^1 & 0 \\ 0 & \sigma^1 \end{pmatrix},$$

since from the Pauli algebra $\sigma^2 \sigma^3 = i\sigma^1$.

The orbital angular momentum operator is defined as usual as the operatoral version of the classical expression

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \longrightarrow L^i = \epsilon^{ijk} x^j p^k,$$

while the total angular momentum operator is given by

$$\mathbf{J} = \mathbf{L} + \mathbf{S} \implies J^i = L^i + S^i,$$

which is conserved under rotational symmetry. It is possible to verify that the total angular momentum operator commutes with the Dirac Hamiltonian (appearing in r.h.s. of equation (2.3.5)) in the free particle case:

$$[H_D, J^i] = 0, \quad \text{where } H_D = p^i \alpha^i + \beta m.$$

This can be shown by computing the commutators $[H_D, L^i]$ and $[H_D, S^i]$ separately, using the commutation relations of the angular momentum operators and the properties of the α^i and β matrices. We will start from the orbital part:

$$\begin{aligned} [H_D, L^i] &= [\alpha^l p^l + \beta m, \epsilon^{ijk} x^j p^k] = \alpha^l [p^l, x^j] \epsilon^{ijk} p^k + [\beta m, \epsilon^{ijk} x^j p^k], \\ &= \alpha^l (-i\delta^{lj}) \epsilon^{ijk} p^k = -i\epsilon^{ijk} \alpha^j p^k, \end{aligned}$$

since in the first step we used the null commutators $[p^l, p^k] = 0$ and $[\beta m, x^j] = 0 = [\beta m, p^k]$. Now we can compute the spin part:

$$[H_D, S^i] = [\alpha^l p^l + \beta m, -\frac{i}{4} \epsilon^{ijk} \alpha^j \alpha^k] = -\frac{i}{4} \epsilon^{ijk} p^l [\alpha^l, \alpha^j \alpha^k] - \frac{i}{4} \epsilon^{ijk} [\beta m, \alpha^j \alpha^k],$$

where the second term is zero since β commutes with the α^i matrices and the first term is the only commutator to compute since p^i commutes with α^j . Using the expression $[A, BC] = \{A, B\} C - B \{A, C\}$ we can write

$$\begin{aligned} [H_D, S^i] &= -\frac{i}{4} \epsilon^{ijk} p^l (\{\alpha^l, \alpha^j\} \alpha^k - \alpha^j \{\alpha^l, \alpha^k\}) \\ &= -\frac{i}{4} \epsilon^{ijk} p^l (2\delta^{lj} \alpha^k - 2\delta^{lk} \alpha^j) \\ &= -\frac{i}{2} \epsilon^{ijk} (p^j \alpha^k - p^k \alpha^j) = +i\epsilon^{ijk} \alpha^j p^k, \end{aligned}$$

since the two terms are antisymmetric in j and k . Finally, summing the two contributions we obtain

$$[H_D, J^i] = [H_D, L^i] + [H_D, S^i] = -i\epsilon^{ijk} \alpha^j p^k + i\epsilon^{ijk} \alpha^j p^k = 0,$$

showing that the total angular momentum is conserved in the Dirac theory.

2.3.5 | Hydrogen Atom and Dirac Equation

A crucial test for the Dirac equation was to check its predictions for the quantized energy levels of the hydrogen atom. The problem is exactly solvable. Nevertheless, it is illuminating to study perturbatively the solution for the energy levels and compare it with the non-relativistic solution of the Schrödinger equation. The energies obtained from the Schrödinger, Klein-Gordon, and Dirac equations are

$$\begin{aligned} E_{n,l}^{(S)} &= -\frac{m_e \alpha^2}{2n^2}, \quad \alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \simeq \frac{1}{137}, \\ E_{n,l}^{(KG)} &= m_e \left[1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{n^4} \left(\frac{n}{2l+1} - \frac{3}{8} \right) + O(\alpha^6) \right], \\ E_{n,j}^{(D)} &= m_e \left[1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{n^4} \left(\frac{n}{2j+1} - \frac{3}{8} \right) + O(\alpha^6) \right], \end{aligned}$$

where $n = 1, 2, \dots \infty$ is the principal quantum number, $l > 0$ is the orbital angular momentum quantum number, and $j = l \pm \frac{1}{2}$ is the total angular momentum quantum number. The Schrödinger non-relativistic result has the main quantum number n and degeneration in $l = 0, 1, \dots n-1$ (as $n-l$ must be a strictly positive integer, $n-l > 0$). The degeneration⁶ in l is broken by relativistic effects (“fine structure” effects), but the Klein-Gordon prediction is in contradiction with the experimental results (seen in the Paschen spectroscopic series, the spectral lines in the infrared due to transitions to level $n = 3$ from higher levels): $2l+1$ is an odd integer, but that number is experimentally measured to be even. The prediction from the Dirac equation gives instead a result compatible with experiments since now $2j+1$ is even.⁷

2.3.6 | Properties of Gamma Matrices

The original Dirac equation was written in terms of the α^i and β matrices, but it is often more convenient to use the set of four gamma matrices defined as

$$\gamma^0 = -i\beta, \quad \gamma^i = -i\beta\alpha^i,$$

which are 4×4 traceless matrices⁸ satisfying the **Clifford algebra**

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu},$$

with

$$\begin{aligned} (\gamma^0)^\dagger &= -\gamma^0 \text{ antihermitian,} \\ (\gamma^i)^\dagger &= +\gamma^i \text{ hermitian.} \end{aligned}$$

We can compact the last two properties as

$$(\gamma^\mu)^\dagger = \gamma^0 \gamma^\mu \gamma^0 = -\beta \gamma^\mu \beta,$$

which can be verified separately for $\mu = 0$ and $\mu = i$. One can even prove that they are traceless, $\text{Tr}(\gamma^\mu) = 0$.

⁶There is an additional degeneration in the magnetic quantum number m , common to all three cases.

⁷Additional effects exist but are smaller. The most important ones are the hyperfine structure, due to the interaction of the electron with the magnetic moment of the nucleus, and the “Lamb shift”, which breaks the degeneracy in j , due to quantum corrections obtainable by using the Dirac field as a QFT.

⁸We can reconstruct α^i with $\alpha^i = \gamma^i \gamma^0 = -i\beta \alpha^i (-i\beta) = -\beta \alpha^i \beta = \beta^2 \alpha^i = \alpha^i$.

Example. We will now prove that γ^1 is traceless, the other cases are very similar. Using the anticommutation relations we have $(\gamma^\mu)^2 = \mathbb{I}$ for $\mu = 0, 1, 2, 3$. Thus,

$$\text{Tr}(\gamma^1) = \text{Tr}(\gamma^1 \gamma^2 \gamma^2) = \text{Tr}(\gamma^2 \gamma^1 \gamma^2),$$

where in the last step we used the cyclicity of the trace. If we instead use the anticommutation relation $\{\gamma^1, \gamma^2\} = 0$, we have

$$\text{Tr}(\gamma^2 \gamma^1 \gamma^2) = -\text{Tr}(\gamma^1 \gamma^2 \gamma^2) = -\text{Tr}(\gamma^1),$$

so that, comparing the results we obtain the tracelessness of gamm matrices:

$$\text{Tr}(\gamma^1) = -\text{Tr}(\gamma^1) \implies \text{Tr}(\gamma^1) = 0.$$

Chirality matrix. We have to introduce one last matrix, the **chirality matrix or gamma five**:

$$\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3, \quad (2.3.13)$$

which has the properties

$$\begin{aligned} (\gamma^5)^\dagger &= \gamma^5 && \text{hermiticity,} \\ (\gamma^5)^2 &= \mathbb{I} && \text{idempotency,} \\ \{\gamma^5, \gamma^\mu\} &= 0, \forall \mu && \text{anticommutation with } \gamma^\mu, \\ \text{Tr}(\gamma^5) &= 0 && \text{tracelessness.} \end{aligned}$$

In the Dirac representation, the chirality matrix takes the form

$$\gamma^5 = \begin{pmatrix} 0 & -\mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}.$$

Example. Let's verify the anticommutation relation between γ^5 and γ^3 :

$$\begin{aligned} \{\gamma^5, \gamma^3\} &= i(\gamma^0\gamma^1\gamma^2\gamma^3\gamma^3 + \gamma^3\gamma^0\gamma^1\gamma^2\gamma^3) \\ &= i(\gamma^0\gamma^1\gamma^2 + (-\gamma^0\gamma^1\gamma^2)) = 0, \end{aligned}$$

since $(\gamma^3)^2 = \mathbb{I}$ and γ^3 anticommutes with γ^0, γ^1 , and γ^2 , so we changed the sign three times in the second term.

Chiral projectors. We can use the chirality matrix to define the **chiral projectors**

$$P_R = \frac{1 + \gamma^5}{2}, \quad P_L = \frac{1 - \gamma^5}{2}, \quad (2.3.14)$$

which satisfy the properties of projectors:

$$P_R + P_L = \mathbb{I}, \quad P_L^2 = P_L, \quad P_R^2 = P_R.$$

These projectors can be used to decompose a Dirac spinor into its right-handed and left-handed components:

$$\psi = \psi_R + \psi_L, \quad \text{where} \quad \psi_R = P_R\psi, \quad \psi_L = P_L\psi.$$

These two components have definite chirality, with $\gamma^5\psi_R = +\psi_R$ and $\gamma^5\psi_L = -\psi_L$, and they live in two-dimensional subspaces of the four-dimensional spinor space: they are **Weyl spinors**, which transform under the $(\frac{1}{2}, 0)$ and $(0, \frac{1}{2})$ representations of the Lorentz group independently:

$$\psi \in \left(\frac{1}{2}, 0\right) \oplus \left(0, \frac{1}{2}\right) \implies \psi_R \in \left(\frac{1}{2}, 0\right), \quad \psi_L \in \left(0, \frac{1}{2}\right).$$

Gamma matrices are four dimensional operators acting on Dirac spinors, which are elements of a four-dimensional complex vector space $\psi \in \mathbb{C}^4$. They provide a representation of the Clifford algebra associated with the Minkowski spacetime metric, and they are essential in formulating the Dirac equation and describing the behavior of spin- $\frac{1}{2}$ particles in relativistic quantum mechanics.

It is useful to introduce a complete basis for these linear operators acting on \mathbb{C}^4 . Such a basis is given by the set of $4 \times 4 = 16$ linearly independent matrices:

$$\{\mathbb{I}, \gamma^\mu, \Sigma^{\mu\nu}, \gamma^\mu \gamma^5, \gamma^5\},$$

where $\Sigma^{\mu\nu} = \frac{-i}{4}[\gamma^\mu, \gamma^\nu]$ (with $\mu < \nu$) and we can count $1+4+6+4+1=16$ independent matrices. We can also generalize this complete basis to span any even dimensional space of gamma matrices, i.e. $d = 2k$ with $k \in \mathbb{N}$. In this case, the dimension of the space of linear operators acting on spinors is $2^{2k} = 4^k$, and a complete basis is given by

$$\{\mathbb{I}, \gamma^\mu, \gamma^{\mu\nu}, \gamma^{\mu\nu\rho}, \dots, \gamma^{\mu_1\mu_2\dots\mu_{2k}}\}, \quad \gamma^{\mu_1\mu_2\dots\mu_n} = \frac{1}{n!} \sum_{\sigma \in S_n} \text{sgn}(\sigma) \gamma^{\mu_{\sigma(1)}} \gamma^{\mu_{\sigma(2)}} \dots \gamma^{\mu_{\sigma(n)}},$$

where the totally antisymmetric products of gamma matrices are defined as above, summing over all permutations σ of n indices with the appropriate sign.

Remark. $\gamma^{\mu_1\mu_2\dots\mu_n}$, the totally antisymmetric product of n gamma matrices, works in odd dimensions as well, but in that case the set of gamma matrices is not complete, as there is an additional matrix (the analog of γ^5 in four dimensions) that commutes with all gamma matrices and can be used to construct additional linearly independent matrices. There is then degeneracy in the representation of the Clifford algebra in odd dimensions. Since we cannot define chirality in odd dimensions, this means that Weyl spinors cannot be defined in odd dimensions.

2.3.7 | Covariance Formulation

The Dirac equation, derived from relativistic considerations, is consistent with relativistic invariance. To prove this, it is necessary to show that the equation is invariant in form under a change of inertial frame of reference, generated by a proper and orthochronous Lorentz transformation.

Recall that by Lorentz invariance, one generically refers to the transformations that are continuously connected to the identity, leaving out the discrete transformations of parity P and time reversal T , which are treated separately. Thus, we need to construct the precise transformation of the Dirac spinor $\psi(x)$ under a Lorentz transformation Λ , which may be conjectured to be linear:

$$\psi(x) \xrightarrow{\Lambda} \psi'(x') = S(\Lambda)\psi(x),$$

so that a Lorentz transformation acts as

$$\begin{aligned} (\gamma^\mu \partial_\mu + m) &= 0 &\iff& (\gamma^\mu \partial'_\mu + m) \psi'(x') = 0, \\ x^\mu &\iff& x'^\mu = \Lambda^\mu_\nu x^\nu, \\ \partial_\mu &\iff& \partial'_\mu = (\Lambda^{-1})^\nu_\mu \partial_\nu, \\ \psi(x) &\iff& \psi'(x') = S(\Lambda)\psi(x). \end{aligned}$$

Relating the second reference frame to the first one through the transformation of coordinates, we have

$$(\gamma^\mu \partial'_\mu + m) \psi'(x') = 0 \longrightarrow (\gamma^\mu \Lambda^\nu_\mu \partial_\nu + m) S(\Lambda)\psi(x) = 0,$$

which can be rewritten after multiplying by $S^{-1}(\Lambda)$ from the left as

$$(S^{-1}(\Lambda)\gamma^\mu S(\Lambda)\Lambda_\mu^\nu \partial_\nu + m) \psi(x) = 0.$$

Comparing with the original Dirac equation, we see that they are equivalent if $S(\Lambda)$ satisfies the relation

$$S^{-1}(\Lambda)\gamma^\mu S(\Lambda)\Lambda_\mu^\nu = \gamma^\nu,$$

or equivalently, after multiplying with Λ^ρ_ν , observing that $\Lambda^\rho_\nu \Lambda_\mu^\nu = \delta_\mu^\rho$, and renaming indices,⁹

$$S^{-1}(\Lambda)\gamma^\mu S(\Lambda) = \Lambda_\nu^\mu \gamma^\nu. \quad (2.3.15)$$

This equation defines the spinorial representation of the Lorentz group. We have to show that such a representation exists. Thus we have to consider infinitesimal Lorentz transformations of the form

$$\Lambda_\nu^\mu = \delta_\nu^\mu + \omega_\nu^\mu, \quad \text{with } \omega_{\mu\nu} = -\omega_{\nu\mu},$$

where the antisymmetry of $\omega_{\mu\nu}$ follows from the defining property of Lorentz transformations $\Lambda^T \eta \Lambda = \eta$. We can write the infinitesimal transformation of $S(\Lambda)$ as

$$S(\Lambda) = \mathbb{I} + \frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}, \quad \text{with } \Sigma^{\mu\nu} = \frac{-i}{4}[\gamma^\mu, \gamma^\nu] = -\Sigma^{\nu\mu},$$

where $\Sigma^{\mu\nu}$ are the six independent generators of the spinorial representation of the Lorentz group. Now we can plug these infinitesimal transformations into equation (2.3.15) and verify that it holds to first order in ω :

$$\begin{aligned} S^{-1}(\Lambda)\gamma^\rho S(\Lambda) &= \Lambda_\sigma^\rho \gamma^\sigma, \\ \left(\mathbb{I} - \frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}\right) \gamma^\rho \left(\mathbb{I} + \frac{i}{2}\omega_{\alpha\beta}\Sigma^{\alpha\beta}\right) &= (\delta_\sigma^\rho + \omega_\sigma^\rho) \gamma^\sigma, \\ \frac{i}{2}\omega_{\alpha\beta}[\gamma^\rho, \Sigma^{\alpha\beta}] + O(\omega^2) &= \eta^{\mu\rho}\omega_{\mu\sigma}\gamma^\sigma = \omega_{\alpha\beta}\eta^{\alpha\rho}\gamma^\beta, \\ \frac{i}{2}\omega_{\alpha\beta}[\gamma^\rho, \Sigma^{\alpha\beta}] &= \omega_{\alpha\beta} \frac{\eta^{\alpha\rho}\gamma^\beta - \eta^{\beta\rho}\gamma^\alpha}{2}, \end{aligned}$$

where in the second step we expanded to first order in ω , in the second step we renamed ($\mu \leftrightarrow \alpha$ and $\sigma \leftrightarrow \beta$) and rearranged indices and in the third step we used the antisymmetry of $\omega_{\mu\nu}$ to rewrite the r.h.s. Finally, we have found that the relation (2.3.15) holds if the following commutation relation is satisfied:

$$[\Sigma^{\alpha\beta}, \gamma^\rho] = i(\eta^{\alpha\rho}\gamma^\beta - \eta^{\beta\rho}\gamma^\alpha), \quad (2.3.16)$$

which can be verified using the definition of $\Sigma^{\alpha\beta} = \frac{-i}{4}[\gamma^\alpha, \gamma^\beta]$ in terms of gamma matrices and the Clifford algebra. Thus, we have shown that the spinorial representation of the Lorentz group is well defined and compatible with the transformation properties of the gamma matrices.

To convince ourselves further, we may compute (2.3.16) explicitly for some values of the indices. For example, let us take $\alpha = 1$, $\beta = 2$, and $\rho = 2$:

$$\begin{aligned} [\Sigma^{12}, \gamma^2] &= i(\eta^{12}\gamma^2 - \eta^{22}\gamma^1), \\ [\Sigma^{12}, \gamma^2] &= -\frac{i}{4}[[\gamma^1, \gamma^2], \gamma^2] = -\frac{i}{4}[\gamma^1\gamma^2 - \gamma^2\gamma^1, \gamma^2] \\ &= -\frac{i}{4}(\gamma^1\gamma^2\gamma^2 - \gamma^2\gamma^1\gamma^2 - \gamma^2\gamma^1\gamma^2 + \gamma^2\gamma^2\gamma^1) = -i\gamma^1, \\ i(\eta^{12}\gamma^2 - \eta^{22}\gamma^1) &= i(0 - (+1)\gamma^1) = -i\gamma^1, \end{aligned}$$

⁹Note that Λ_μ^ν acts on vectors with lower indices: it is obtained by raising/lowering indices on Λ_ν^μ , so that it corresponds to the matrix $\eta\Lambda\eta^{-1} = (\Lambda^{-1})^T$. The last relation follows from the defining property $\Lambda^T \eta \Lambda = \eta$. Then, one may check that $\Lambda^\rho_\nu \Lambda_\mu^\nu = [\Lambda(\eta\Lambda\eta^{-1})^T]_\mu^\rho = [\Lambda\Lambda^{-1}]_\mu^\rho = \delta_\mu^\rho$.

as expected; for the other combinations of indices, the verification is similar. Finally, let us remark that this same result can be obtained with the use of the gamma matrix properties and Clifford algebra presented in the previous section:

$$\begin{aligned}
[\Sigma^{\mu\nu}, \gamma^\rho] &= -\frac{i}{4} [[\gamma^\mu, \gamma^\nu], \gamma^\rho] = -\frac{i}{4} ([\gamma^\mu \gamma^\nu, \gamma^\rho] - [\gamma^\nu \gamma^\mu, \gamma^\rho]) \\
[AB, C] &= A\{B, C\} - \{A, C\}B \\
&= -\frac{i}{4} (\gamma^\mu \{\gamma^\nu, \gamma^\rho\} - \{\gamma^\mu, \gamma^\rho\} \gamma^\nu - \gamma^\nu \{\gamma^\mu, \gamma^\rho\} + \{\gamma^\nu, \gamma^\rho\} \gamma^\mu) \\
&= -\frac{i}{4} (2\eta^{\nu\rho}\gamma^\mu - 2\eta^{\mu\rho}\gamma^\nu - 2\eta^{\mu\rho}\gamma^\nu + 2\eta^{\nu\rho}\gamma^\mu) \\
&= -\frac{i}{2} (2\eta^{\nu\rho}\gamma^\mu - 2\eta^{\mu\rho}\gamma^\nu) \\
&= i(\eta^{\mu\rho}\gamma^\nu - \eta^{\nu\rho}\gamma^\mu).
\end{aligned}$$

Now that we know that the spinorial representation of the Lorentz group exists, we can construct finite transformations by exponentiating the infinitesimal ones. Let us take the infinitesimal transformation of $S(\Lambda)$:

$$S(\Lambda) = \mathbb{I} + \frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu},$$

thus, the finite Lorentz transformation of a Dirac spinor is given by repeated application of the infinitesimal transformation, leading to the **exponential form**

$$S(\Lambda) = \exp\left\{\frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}\right\} = \exp\left\{\frac{1}{4}\omega_{\mu\nu}\gamma^\mu\gamma^\nu\right\}, \quad (2.3.17)$$

from antisymmetry of $\omega_{\mu\nu}$.

Example (Rotation around axis). Transformations with $\omega_{12} = -\omega_{21} = \varphi$ and other vanishing produce rotations around the z -axis. If the parameter φ is finite then

$$\omega^\mu{}_\nu = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \varphi & 0 \\ 0 & -\varphi & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \implies \Lambda^\mu{}_\nu = (e^\omega)^\mu{}_\nu = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \varphi & \sin \varphi & 0 \\ 0 & -\sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We obtained this result by exponentiating the matrix $\omega^\mu{}_\nu$: note that even powers of ω have positive sign in the central diagonal block, while odd powers have alternating signs ($e^\omega = e^{\varphi J}$ with $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ the generator of rotations around \hat{z} and $J^2 = -\mathbb{I}$, $J^3 = -J$ and finally $J^4 = \mathbb{I}$). If we take the Taylor expansion of the exponential we find

$$\begin{aligned}
e^{\varphi J} &= \sum_{n=0}^{\infty} \frac{(\varphi J)^n}{n!} = \mathbb{I} \left[1 + \frac{\varphi^2}{2!} J^2 + \frac{\varphi^4}{4!} J^4 + \dots \right] + J \left[\varphi + \frac{\varphi^3}{3!} J^2 + \frac{\varphi^5}{5!} J^4 + \dots \right] \\
&= \cos \varphi \mathbb{I} + \sin \varphi J.
\end{aligned}$$

Thus the result obtained by exponentiating the matrix of Lie parameters is the rotation matrix (even and odd powers in the central diagonal block of $\omega^\mu{}_\nu$).

So we are looking at rotations around \hat{z} . Let's find an expression for $S(\Lambda)$: using the **spinorial**

representation found in (2.3.17) we have

$$\begin{aligned} S(\Lambda) &= \exp\left\{\frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}\right\} = \exp\left\{\frac{1}{4}\omega_{\mu\nu}\gamma^\mu\gamma^\nu\right\} = \exp\left\{\frac{1}{4}\omega_{12}\gamma^1\gamma^2 + \frac{1}{4}\omega_{21}\gamma^2\gamma^1\right\} \\ &= \exp\left\{\frac{\varphi}{2}\gamma^1\gamma^2\right\} = \exp\left\{\frac{\varphi}{2}\begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix}\right\} = \begin{pmatrix} e^{i\frac{\varphi}{2}} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\varphi}{2}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\varphi}{2}} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\varphi}{2}} \end{pmatrix}, \end{aligned}$$

where we used the Dirac representation of the gamma matrices

$$\gamma^1\gamma^2 = i\Sigma^3, \quad \text{with } \Sigma^3 = \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix},$$

and the fact that the exponential of a diagonal matrix is the diagonal matrix of the exponentials of the entries.¹⁰

The transformation is immediately recognized to be unitary, $S^\dagger(\Lambda) = S^{-1}(\Lambda)$. It is also clear that it is a spinorial transformation¹¹, which is **double valued**: the rotation with $\psi = 2\pi$ (that coincides with the identity on vectors) is represented by -1 on the spinors; it is thus necessary to make a rotation of 4π to get back the identity. We should have a double cover of our $\text{SO}(3)$ representation.

The rotation of an angle ϕ around a generic axis $\hat{\mathbf{n}}$ is represented by

$$S(\Lambda) = \begin{pmatrix} \exp\left\{i\frac{\phi}{2}\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}\right\} & 0 \\ 0 & \exp\left\{i\frac{\phi}{2}\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}\right\} \end{pmatrix}, \quad (2.3.18)$$

which is recognized to be unitary as well. Now going back to the non relativistic limit and splitting the representation as in (2.3.10)

$$\psi(x) = e^{-\frac{i}{\hbar}mc^2 t} \begin{pmatrix} \varphi(x) \\ \chi(x) \end{pmatrix},$$

we can see that the $4D$ spinor representation reduces to two copies of the $2D$ spinor representation of $\text{SU}(2)$ acting on non relativistic Pauli spinors, with the spin operator $\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$ acting on each $2D$ subspace:

$$\mathbf{S} = \frac{1}{2} \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}.$$

Example (Boost along axis). We could imagine a pure boost along the x -axis, which would be represented by

$$\omega_{0i} = -\omega_{i0} = \eta$$

so that the finite transformation matrix is

$$\omega^\mu{}_\nu = \begin{pmatrix} 0 & -\eta & 0 & 0 \\ -\eta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \implies \Lambda^\mu{}_\nu = (e^\omega)^\mu{}_\nu = \begin{pmatrix} \cosh \eta & -\sinh \eta & 0 & 0 \\ -\sinh \eta & \cosh \eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

¹⁰It is not difficult to understand why: if $\overline{A} = \text{diag}(a_1, a_2, \dots, a_n)$ then $\overline{A}^2 = \text{diag}(a_1^2, a_2^2, \dots, a_n^2)$ and so on for higher powers; thus the Taylor expansion of the exponential gives the desired result; this explains also where the ones on the diagonal of the exponential come from: $e^0 = 1$.

¹¹The ω matrices are a four vector representation, here acting on a spinor.

where we obtained this result by exponentiating the matrix ω^μ_ν : note that even powers of ω have positive sign in the first diagonal block, while odd powers have always positive sign as well ($e^\omega = e^{\eta K}$ with $K = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$ the generator of boosts along \hat{x} and $K^2 = \mathbb{I}$, $K^3 = K$ and finally $K^4 = \mathbb{I}$). If we take the Taylor expansion of the exponential we find

$$\begin{aligned} e^{\eta K} &= \sum_{n=0}^{\infty} \frac{(\eta K)^n}{n!} = \mathbb{I} \left[1 + \frac{\eta^2}{2!} K^2 + \frac{\eta^4}{4!} K^4 + \dots \right] + K \left[\eta + \frac{\eta^3}{3!} K^2 + \frac{\eta^5}{5!} K^4 + \dots \right] \\ &= \mathbb{I} \cosh \eta + K \sinh \eta. \end{aligned}$$

Thus the result obtained by exponentiating the matrix of Lie parameters is the boost matrix (even and odd powers in the first diagonal block of ω^μ_ν).

This is almost the same case as before, but now space and time coordinates are mixing, it's like a rotation of an imaginary angle (rotating in the first diagonal block of ω). There is not anymore the alternating signs in the expansion, but we recognize the expansion of the hyperbolic functions cosh and sinh; if we then use the relation

$$\gamma^2 + \gamma^2 \beta^2 = 1 \implies \gamma = \cosh \eta, \quad \gamma \beta = \sinh \eta \implies \beta = \tanh \eta,$$

then we can relate the parameter η to the velocity of the boost $\beta = \frac{v}{c}$ and the Lorentz factor $\gamma = (1 - \beta^2)^{-1/2}$ to obtain the usual form of the Lorentz boost along \hat{x} :

$$\Lambda^\mu_\nu = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

If we call η the *rapidity*, it is additive for boosts along the same direction, while velocities are added in a more complicated way. For the **spinorial representation** we have to find $S(\Lambda)$:

$$\begin{aligned} S(\Lambda) &= \exp \left\{ \frac{i}{2} \omega_{\mu\nu} \Sigma^{\mu\nu} \right\} = \exp \left\{ \frac{1}{4} \omega_{\mu\nu} \gamma^\mu \gamma^\nu \right\} = \exp \left\{ \frac{1}{4} \omega_{01} \gamma^0 \gamma^1 + \frac{1}{4} \omega_{10} \gamma^1 \gamma^0 \right\} \\ &= \exp \left\{ \frac{\eta}{4} [\gamma^0, \gamma^1] \right\} = \exp \left\{ \frac{\eta}{4} [(-i\beta), (-i\beta\alpha^1)] \right\} = \exp \left\{ -\frac{\eta}{2} \alpha^1 \right\}, \end{aligned}$$

where, if we now Taylor expand the expression, we find even powers giving the identity, while odd powers give α^1 . Thus in the end we can recognize the hyperbolic functions again:

$$\begin{aligned} \exp \left\{ -\frac{\eta}{2} \alpha^1 \right\} &= \sum_{n=0}^{\infty} \frac{(-\frac{\eta}{2} \alpha^1)^n}{n!} = \mathbb{I} \left[1 + \frac{1}{2!} \left(\frac{\eta}{2} \right)^2 + \frac{1}{4!} \left(\frac{\eta}{2} \right)^4 + \dots \right] \\ &\quad + \alpha^1 \left[-\frac{\eta}{2} + \frac{1}{3!} \left(-\frac{\eta}{2} \right)^3 + \frac{1}{5!} \left(-\frac{\eta}{2} \right)^5 + \dots \right] = \mathbb{I} \cosh \frac{\eta}{2} - \alpha^1 \sinh \frac{\eta}{2}, \end{aligned}$$

to find the final expression for the spinorial representation of a boost along \hat{x} :

$$S(\Lambda) = \mathbb{I} \cosh \frac{\eta}{2} - \alpha^1 \sinh \frac{\eta}{2} = \begin{pmatrix} \cosh \frac{\eta}{2} & 0 & 0 & -\sinh \frac{\eta}{2} \\ 0 & \cosh \frac{\eta}{2} & -\sinh \frac{\eta}{2} & 0 \\ 0 & -\sinh \frac{\eta}{2} & \cosh \frac{\eta}{2} & 0 \\ -\sinh \frac{\eta}{2} & 0 & 0 & \cosh \frac{\eta}{2} \end{pmatrix}.$$

Note that this transformation is not unitary, but satisfies $S^\dagger(\Lambda) = S(\Lambda)$: α^1 is hermitian and computing further, we find the whole representation to be hermitian.

Plane Waves

We want to construct the plane wave solution with the spinorial representation. The previous boost transformation can be written and generalized to find the general plane wave solutions of the Dirac equation for a particle with arbitrary momentum \mathbf{p} . Starting from the shell condition for a free particle

$$E^2 - \mathbf{p}^2 = m^2, \quad p_\mu p^\mu + m^2 = 0,$$

since the four momentum can be written as

$$p^\mu = (E, \mathbf{p}) = (m\gamma, m\beta\gamma), \quad \text{with } p'^\mu = (m, \mathbf{0}),$$

obtained from the rest frame. One can use hyperbolic trigonometric identities (plus the previous results $\gamma = \cosh(\eta)$ and $\beta\gamma = \sinh(\eta)$) to find

$$\begin{aligned} \tanh \frac{\eta}{2} &= \frac{\sinh \eta}{1 + \cosh \eta} = \frac{\beta\gamma}{1 + \gamma} = \frac{|\mathbf{p}|}{E + m}, \\ \cosh \frac{\eta}{2} &= \sqrt{\frac{1}{2} + \frac{1}{2} \cosh(\eta)} = \sqrt{\frac{E + m}{2m}}, \end{aligned}$$

and if we plug them in the previous expression for the Lorentz boost transformation along \hat{x} we can find the following representation:

$$S(\Lambda) = \mathbb{I} \cosh \frac{\eta}{2} - \alpha^1 \sinh \frac{\eta}{2} = \cosh \frac{\eta}{2} \left(\mathbb{I} - \alpha^1 \tanh \frac{\eta}{2} \right) =$$

then generalize to a boost in an arbitrary direction $\hat{v} = \frac{\mathbf{v}}{|\mathbf{v}|}$ by substituting α^1 with

$$\alpha^1 \rightarrow \frac{\boldsymbol{\alpha} \cdot \mathbf{v}}{|\mathbf{v}|} = \frac{\boldsymbol{\alpha} \cdot \boldsymbol{\beta}}{|\boldsymbol{\beta}|}$$

and finally change the direction of the boost $\eta \rightarrow -\eta$ so that by acting on a spinor at rest we get the spinor moving with velocity \mathbf{v} (and momentum \mathbf{p}). The final transformation takes the form

$$S(\Lambda) = \sqrt{\frac{E + m}{2m}} \left(\mathbb{I} + \frac{\boldsymbol{\alpha} \cdot \mathbf{p}}{E + m} \right). \quad (2.3.19)$$

Before applying this transformation to the spinors at rest, we can exploit the product $\boldsymbol{\alpha} \cdot \mathbf{p}$:

$$\boldsymbol{\alpha} \cdot \mathbf{p} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \cdot \mathbf{p} \\ \boldsymbol{\sigma} \cdot \mathbf{p} & 0 \end{pmatrix}, \quad \text{with } \boldsymbol{\sigma} \cdot \mathbf{p} = \begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix} = \begin{pmatrix} p_3 & p^{(-)} \\ p^{(+)} & -p_3 \end{pmatrix},$$

so that the final expression for the spinorial representation of a boost in an arbitrary direction is given by the application to the spinors at rest:

$$\psi_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{-imt}, \quad \psi_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{-imt}, \quad \psi_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{+imt}, \quad \psi_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{+imt},$$

which produce the general plane wave solutions of the Dirac equation. We obtain the **positive energy solutions** (the columns of the matrix $S(\Lambda)$ times the plane wave)

$$\psi_1(x) = \sqrt{\frac{E + m}{2m}} \begin{pmatrix} 1 \\ 0 \\ \frac{p_3}{E+m} \\ \frac{p^{(+)}}{E+m} \end{pmatrix} e^{ip_\mu x^\mu}, \quad \psi_2(x) = \sqrt{\frac{E + m}{2m}} \begin{pmatrix} 0 \\ 1 \\ \frac{p^{(-)}}{E+m} \\ \frac{-p_3}{E+m} \end{pmatrix} e^{ip_\mu x^\mu},$$

and the **negative energy solutions**

$$\psi_3(x) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \frac{p_3}{E+m} \\ \frac{p^+(+)}{E+m} \\ 1 \\ 0 \end{pmatrix} e^{-ip_\mu x^\mu}, \quad \psi_4(x) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \frac{p^(-)}{E+m} \\ \frac{-p_3}{E+m} \\ 0 \\ 1 \end{pmatrix} e^{-ip_\mu x^\mu}.$$

It can be verified by direct substitution that these four spinors are indeed solutions of the Dirac equation $(i\gamma^\mu p_\mu + m)\omega(p) = 0$.

Pseudo Unitarity

The spinorial representation we found for a Lorentz transformation involving spatial rotations (eq. (2.3.18)) is not unitary, $S^\dagger(\Lambda) \neq S^{-1}(\Lambda)$, as seen on the Lorentz boost (eq. (2.3.19)). This is understandable in the light of a theorem according to which unitary irreducible representations of compact groups are finite-dimensional, while those of non-compact groups are infinite-dimensional (this result was expressed in the first chapter, with theorem 1.1).

Lorentz's group is non-compact because of the boosts, however, the spinorial representations are pseudo-unitary in the sense that

$$S^\dagger(\Lambda) = \beta S^{-1}(\Lambda) \beta. \quad (2.3.20)$$

To verify this property, we can start from the hermiticity properties of the gamma matrices:

$$(\gamma^\mu)^\dagger = -\beta \gamma^\mu \beta,$$

which can be verified directly using the Dirac representation of the gamma matrices. From this relation, we can find the hermitian conjugate of the generators of the spinorial representation of the Lorentz group:

$$\begin{aligned} (\Sigma^{\mu\nu})^\dagger &= \left(-\frac{i}{4} [\gamma^\mu, \gamma^\nu] \right)^\dagger = \frac{i}{4} [(\gamma^\nu)^\dagger, (\gamma^\mu)^\dagger] \\ &= \frac{i}{4} [-\beta \gamma^\nu \beta, -\beta \gamma^\mu \beta] = \beta \left(-\frac{i}{4} [\gamma^\mu, \gamma^\nu] \right) \beta = \beta \Sigma^{\mu\nu} \beta, \end{aligned}$$

so that we can compute the hermitian conjugate of the finite transformation (2.3.17):

$$\begin{aligned} S^\dagger(\Lambda) &= \left(\exp \left\{ \frac{i}{2} \omega_{\mu\nu} \Sigma^{\mu\nu} \right\} \right)^\dagger = \exp \left\{ \left(\frac{i}{2} \omega_{\mu\nu} \Sigma^{\mu\nu} \right)^\dagger \right\} = \exp \left\{ -\frac{i}{2} \omega_{\mu\nu} (\Sigma^{\mu\nu})^\dagger \right\} \\ &= \exp \left\{ -\frac{i}{2} \omega_{\mu\nu} \beta \Sigma^{\mu\nu} \beta \right\} = \beta \exp \left\{ -\frac{i}{2} \omega_{\mu\nu} \Sigma^{\mu\nu} \right\} \beta = \beta S^{-1}(\Lambda) \beta, \end{aligned}$$

where in the final steps we could factor out β from the exponentials since it is a diagonal matrix

$$e^\beta = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} = \beta \sum_{n=0}^{\infty} \frac{1}{n!} = \beta e^1,$$

thus proving the pseudo-unitarity relation (2.3.20).

Fermionic Bilinears. We start from the Dirac spinor and we want to find the **Dirac conjugate** of the spinor:

$$\bar{\psi}(x) = \psi^\dagger(x) \beta, \quad (2.3.21)$$

which transforms as

$$\bar{\psi}(x) \rightarrow \bar{\psi}'(x') = S^{-1}(\Lambda)\bar{\psi}(x).$$

Let's show this result:

$$\begin{aligned}\bar{\psi}'(x') &= \psi'^\dagger(x')\beta = (S(\Lambda)\psi(x))^\dagger\beta = \psi^\dagger(x)S^\dagger(\Lambda)\beta \\ &= \psi^\dagger(x)\beta S^{-1}(\Lambda)\beta\beta = \psi^\dagger(x)\beta S^{-1}(\Lambda) = \bar{\psi}(x)S^{-1}(\Lambda).\end{aligned}$$

Thus we have the transformation rules for the Dirac spinor, its hermitian conjugate and its Dirac conjugate:

$$\begin{cases} \psi(x) &\rightarrow \psi'(x') = S(\Lambda)\psi(x), \\ \psi^\dagger(x) &\rightarrow \psi'^\dagger(x') = \psi^\dagger(x)S^\dagger(\Lambda), \\ \bar{\psi}(x) &\rightarrow \bar{\psi}'(x') = \bar{\psi}(x)S^{-1}(\Lambda). \end{cases} \quad (2.3.22)$$

By looking at the transformation rules, one can notice that the bilinear $\bar{\psi}(x)\psi(x)$ form a scalar:

$$\bar{\psi}(x)\psi(x) \rightarrow \bar{\psi}'(x')\psi'(x') = \bar{\psi}(x)S^{-1}(\Lambda)S(\Lambda)\psi(x) = \bar{\psi}(x)\psi(x).$$

Remark. The quantity $\psi^\dagger\psi$ instead is not a scalar but identifies the time component of the four-vector

$$J^\mu = (J^0, \mathbf{J}) = (\psi^\dagger\psi, \psi^\dagger\boldsymbol{\alpha}\psi),$$

which is the current that appears in the continuity equation (2.3.8).

Having introduced the Dirac conjugate, it is now natural to express the probability current in a manifestly covariant form as

$$J^\mu = i\bar{\psi}\gamma^\mu\psi, \quad (2.3.23)$$

which ultimately transforms as a 4-vector:

$$J^\mu \rightarrow J'^\mu = i\bar{\psi}'(x')\gamma^\mu\psi'(x') = i\bar{\psi}(x)S^{-1}(\Lambda)\gamma^\mu S(\Lambda)\psi(x) = \Lambda^\mu_\nu J^\nu,$$

where we used the transformation properties of the spinor and the Dirac conjugate, as well as the relation (2.3.15) for the gamma matrices transformations.

The quantities $\bar{\psi}\psi$ and $\bar{\psi}\gamma^\mu\psi$ are examples of **fermionic bilinears**, quantities that furnish useful expressions for describing the physical properties of the spin 1/2 relativistic particle. Quite generally, using the basis of the spinor space $\Gamma^A = (\mathbb{I}, \gamma^\mu, \Sigma^{\mu\nu}, \gamma^\mu\gamma^5, \gamma^5)$, one may define fermionic bilinears of the form

$$\bar{\psi}\Gamma^A\psi$$

which transform as *scalar*, *vector*, *antisymmetric tensor of rank 2*, *pseudovector*, and *pseudoscalar*, respectively.

We have already discussed the first two cases, so for the pseudoscalar (neglecting for notational simplicity the dependence on the spacetime point), we find

$$(\bar{\psi}\gamma^5\psi)' = \bar{\psi}S^{-1}(\Lambda)\gamma^5S(\Lambda)\psi = \bar{\psi}\gamma^5\psi,$$

that indeed we recognize to be a scalar under proper and orthochronous Lorentz transformations (the adjective “pseudo” refers to a different behavior under spatial reflection, i.e., under a parity transformation).

As the last example, we consider the antisymmetric tensor

$$\begin{aligned} (\bar{\psi} \Sigma^{\mu\nu} \psi)' &= \bar{\psi} S^{-1}(\Lambda) \Sigma^{\mu\nu} S(\Lambda) \psi = \bar{\psi} S^{-1}(\Lambda) \left(-\frac{i}{4} [\gamma^\mu, \gamma^\nu] \right) S(\Lambda) \psi \\ &= -\frac{i}{4} \bar{\psi} [S^{-1}(\Lambda) \gamma^\mu S(\Lambda), S^{-1}(\Lambda) \gamma^\nu S(\Lambda)] \psi \\ &= -\frac{i}{4} \bar{\psi} [\Lambda^\mu{}_\rho \gamma^\rho, \Lambda^\nu{}_\sigma \gamma^\sigma] \psi = \Lambda^\mu{}_\rho \Lambda^\nu{}_\sigma (\bar{\psi} \Sigma^{\rho\sigma} \psi), \end{aligned}$$

where we have used again the transformation properties of the gamma matrices in (2.3.15). Thus, we saw that $\bar{\psi} \Sigma^{\mu\nu} \psi$ transforms as an antisymmetric tensor of rank 2 indeed.

2.3.8 | Discrete Symmetries

In addition to the Lorentz transformations connected to the identity, one can prove the invariance of the free Dirac equation under discrete transformations such as **parity** P (also known as spatial reflection), **time reversal** T , and **charge conjugation** C , which exchanges particles with antiparticles.

Parity

Let us discuss the transformation that reverses the orientation of the spatial axes, i.e., parity

$$\begin{aligned} \mathbf{x} &\xrightarrow{P} \mathbf{x}' = -\mathbf{x}, \\ t &\xrightarrow{P} t' = t, \end{aligned}$$

which in tensorial notation becomes:

$$x^\mu \xrightarrow{P} x'^\mu = P^\mu{}_\nu x^\nu, \quad \text{with } P^\mu{}_\nu = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (2.3.24)$$

This is a discrete operation with $\det P^\mu{}_\nu = -1$. It belongs to the Lorentz group $O(3, 1)$ but is not connected to the identity. Together with the identity, it forms a subgroup isomorphic to $\mathbb{Z}_2 = \{1, -1\}$. Invariance under parity can be studied by conjecturing an appropriate linear transformation of the spinor

$$\psi(x) \xrightarrow{P} \psi'(x') = \mathcal{P}\psi(x),$$

generated by a suitable matrix \mathcal{P} . Requiring invariance in form of the Dirac equation

$$\begin{aligned} (\gamma^\mu \partial_\mu + m) \psi(x) = 0 &\iff (\gamma^\mu \partial'_\mu + m) \psi'(x') = 0, \\ x^\mu &\iff x'^\mu = P^\mu{}_\nu x^\nu, \\ \partial_\mu &\iff \partial'_\mu = (P^{-1})^\nu{}_\mu \partial_\nu, \\ \psi(x) &\iff \psi'(x') = \mathcal{P}\psi(x). \end{aligned}$$

the form of \mathcal{P} is determined. Proceeding as for the Lorentz transformations $S(\Lambda)$ one finds

$$\mathcal{P}^{-1} \gamma^\mu \mathcal{P} P_\mu{}^\nu = \gamma^\nu,$$

or equivalently

$$\mathcal{P} \gamma^\mu \mathcal{P}^{-1} = P^\mu{}_\nu \gamma^\nu = \begin{pmatrix} \gamma^0 \\ -\gamma^i \end{pmatrix}.$$

A matrix \mathcal{P} which respects:

$(\mu = 0)$ commutes with γ^0 :

$$\mathcal{P}\gamma^0\mathcal{P}^{-1} = P_\nu^0\gamma^\nu = P_0^0\gamma^0 = \gamma^0,$$

which implies $\mathcal{P}\gamma^0\mathcal{P}^{-1} = \xi\mathcal{P}\mathcal{P}^{-1}\gamma^0 = \xi\gamma^0$ with $\xi = +1$;

$(\mu = i)$ anticommutes with γ^i :

$$\mathcal{P}\gamma^i\mathcal{P}^{-1} = P_\nu^i\gamma^\nu = P_j^i\gamma^j = -\gamma^i,$$

which implies $\mathcal{P}\gamma^i\mathcal{P}^{-1} = \zeta\mathcal{P}\mathcal{P}^{-1}\gamma^i = \zeta\gamma^i$ with $\zeta = -1$.

Thus \mathcal{P} commutes with γ^0 and anticommutes with γ^i ; a matrix with these properties is γ^0 itself, or equivalently, $\beta = i\gamma^0$. Thus, one may choose

$$\mathcal{P} = \eta_P\beta$$

with η_P a phase fixed by requiring that \mathcal{P}^4 coincides with the identity on fermions (so that the possible choices are $\eta_P = (\pm 1, \pm i)$). For simplicity we choose $\eta_P = 1$, and use the parity transformations

$$\begin{cases} \psi(x) \xrightarrow{P} \psi'(x') = \beta\psi(x), \\ \psi^\dagger(x) \xrightarrow{P} \psi'^\dagger(x') = \psi^\dagger(x)\beta, \\ \bar{\psi}(x) \xrightarrow{P} \bar{\psi}'(x') = \bar{\psi}(x)\beta, \end{cases}$$

since

$$\bar{\psi}'(x') = \psi'^\dagger(x')\beta = (\psi^\dagger(x)\beta)\beta = \bar{\psi}(x)\beta.$$

From these basic rules, one deduces the transformations of the *fermionic bilinears*:

$$\begin{aligned} \bar{\psi}(x)\psi(x) &\xrightarrow{P} \bar{\psi}'(x')\psi'(x') = \bar{\psi}(x)\psi(x) && \text{scalar,} \\ \bar{\psi}(x)\gamma^5\psi(x) &\xrightarrow{P} \bar{\psi}'(x')\gamma^5\psi'(x') = -\bar{\psi}(x)\gamma^5\psi(x) && \text{pseudo-scalar,} \\ \bar{\psi}(x)\gamma^\mu\psi(x) &\xrightarrow{P} \bar{\psi}'(x')\gamma^\mu\psi'(x') = P_\nu^\mu\bar{\psi}(x)\gamma^\nu\psi(x) && \text{(polar) vector,} \\ \bar{\psi}(x)\gamma^\mu\gamma^5\psi(x) &\xrightarrow{P} \bar{\psi}'(x')\gamma^\mu\gamma^5\psi'(x') = -P_\nu^\mu\bar{\psi}(x)\gamma^\nu\gamma^5\psi(x) && \text{(axial) vector,} \\ \bar{\psi}(x)\Sigma^{\mu\nu}\psi(x) &\xrightarrow{P} \bar{\psi}'(x')\Sigma^{\mu\nu}\psi'(x') = P_\rho^\mu P_\sigma^\nu\bar{\psi}(x)\Sigma^{\rho\sigma}\psi(x) && \text{tensor.} \end{aligned} \tag{2.3.25}$$

Chiral properties of spinors. Having understood how parity works, it is time to focus on the reducibility of a Dirac spinor under the restricted Lorentz group $\text{SO}^+(3,1)$. Using the projectors¹²

$$P_L = \frac{1 - \gamma^5}{2}, \quad P_R = \frac{1 + \gamma^5}{2},$$

one can separate the Dirac spinors in their *left and right handed components*

$$\psi = \psi_L + \psi_R, \quad \text{with } \psi_L = P_L\psi = \frac{1 - \gamma^5}{2}\psi, \quad \psi_R = P_R\psi = \frac{1 + \gamma^5}{2}\psi.$$

They constitute the two irreducible spin $\frac{1}{2}$ representations of the Lorentz group contained inside the Dirac spinor. The irreducibility follows from the fact that the Lorentz generators $\Sigma^{\mu\nu}$ commute with the projectors P_L and P_R . Then, also finite transformations commute with the projectors. For example, considering P_L one calculates

$$\Sigma^{\mu\nu}P_L = \left(-\frac{i}{4}[\gamma^\mu, \gamma^\nu]\right)\frac{1 - \gamma^5}{2} = \frac{1 - \gamma^5}{2}\left(-\frac{i}{4}[\gamma^\mu, \gamma^\nu]\right),$$

¹²Hermitian matrices that satisfy $P_{L/R}^2 = P_{L/R}$, $P_L + P_R = \mathbb{I}$, $P_L P_R = 0$, as defined in (2.3.14).

knowing that $\Sigma^{\mu\nu}$ commutes with the projectors since γ^5 commutes with an even number of gamma matrices, and likewise for P_R . The interpretation of this commutativity is that operating with an infinitesimal Lorentz rotation on a chiral spinor of given chirality produces a chiral spinor of the same chirality.

More explicitly, considering infinitesimal transformations, one verifies that the transformed spinor ψ'_L remains left-handed

$$\begin{aligned}\psi_L &\xrightarrow{\text{SO}^+(3,1)} \psi'_L = \left(1 + \frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}\right)\psi_L = \left(1 + \frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}\right)P_L\psi_L \\ &= P_L \left(1 + \frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}\right)\psi_L = P_L\psi'_L.\end{aligned}$$

The same remains true for finite $\text{SO}^+(3,1)$ transformations. Left-handed and right-handed spinors are called Weyl spinors. They identify the two inequivalent, irreducible spinor representations of $\text{SO}^+(3,1)$. Now, let us consider parity. Including parity, the Dirac spinor is not reducible anymore. Parity transforms left-handed spinors into right-handed ones and vice versa. Recalling the form of the parity transformation of a Dirac spinor, $\psi \xrightarrow{P} \psi' = \beta\psi$, one finds that a left-handed spinor is transformed into a right-handed one

$$\begin{aligned}\psi_L &\xrightarrow{P} \psi'_L = \beta\psi_L = \beta\left(\frac{1-\gamma^5}{2}\right)\psi = \left(\frac{1+\gamma^5}{2}\right)\beta\psi = P_R\psi', \\ \psi_R &\xrightarrow{P} \psi'_R = \beta\psi_R = \beta\left(\frac{1+\gamma^5}{2}\right)\psi = \left(\frac{1-\gamma^5}{2}\right)\beta\psi = P_L\psi'.\end{aligned}$$

Both chiralities are needed to realize parity, as parity exchanges two opposite chiralities. Additional remarks: the representations of the Lorentz group are constructed systematically using the fact that its Lie algebra can be written in terms of two commuting $\text{SU}(2)$ subalgebras, $\text{SO}^+(3,1) \sim \text{SU}(2) \times \text{SU}(2)$. Knowing the $\text{SU}(2)$ representations that are familiar from quantum mechanics, one assigns two integer or semi-integer quantum numbers (j, j') to indicate an irreducible representation of the Lorentz group. The irreps $(\frac{1}{2}, 0)$ and $(0, \frac{1}{2})$ correspond to the two inequivalent chiral spinors described above (left-handed and right-handed Weyl spinors). The Dirac spinor forms a **reducible** representation of $\text{SO}^+(3,1)$ given by the direct sum $(\frac{1}{2}, 0) \oplus (0, \frac{1}{2})$. It becomes **irreducible** once considering the group $\text{O}(3,1)$ that includes parity. Chiral theories (theories that are non-invariant under parity) are constructed using Weyl fermions rather than Dirac fermions.

Chiral representation. When dealing with chiral fermions, it is often useful to employ a different representation of the gamma matrices, called the *chiral representation*. A chiral representation is identified by the fact that the chiral matrix γ^5 is diagonal. A chiral representation is given by

$$\gamma^5 = \begin{pmatrix} -\mathbb{I} & 0 \\ 0 & \mathbb{I} \end{pmatrix}, \quad \gamma^0 = i \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}, \quad \gamma^i = -i\beta\alpha^i = \begin{pmatrix} 0 & -i\sigma^i \\ i\sigma^i & 0 \end{pmatrix},$$

where is obtained from the Dirac representation

$$\gamma^5 = \begin{pmatrix} 0 & -\mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}, \quad \gamma^0 = i \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}, \quad \gamma^i = -i\beta\alpha^i = \begin{pmatrix} 0 & -i\sigma^i \\ i\sigma^i & 0 \end{pmatrix},$$

by a similarity transformation (a change of basis) generated by a unitary matrix U such that

$$\gamma_{\text{chiral}}^\mu = U\gamma_{\text{Dirac}}^\mu U^{-1}$$

where

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I} & \mathbb{I} \\ -\mathbb{I} & \mathbb{I} \end{pmatrix}, \quad U^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I} & -\mathbb{I} \\ \mathbb{I} & \mathbb{I} \end{pmatrix}.$$

In the chiral representation, the Lorentz generators $\Sigma^{\mu\nu} = -\frac{i}{4}[\gamma^\mu, \gamma^\nu] = -\frac{i}{2}\gamma^{\mu\nu}$ are given by

$$\Sigma^{0i} = -\frac{i}{2}\gamma^{0i} = \frac{i}{2} \begin{pmatrix} \sigma^i & 0 \\ 0 & -\sigma^i \end{pmatrix}, \quad \Sigma^{ij} = -\frac{i}{2}\gamma^{ij} = \frac{1}{2}\epsilon^{ijk} \begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix}.$$

The block-diagonal form of the Lorentz generators makes evident that they act independently on the chiral parts of a Dirac spinor

$$\psi = \begin{pmatrix} \tilde{\psi}_L \\ \tilde{\psi}_R \end{pmatrix} = \begin{pmatrix} (\tilde{\psi}_L)_a \\ (\tilde{\psi}_R)_{\dot{a}} \end{pmatrix}, \quad a = 1, 2, \dot{a} = \dot{1}, \dot{2},$$

where the two-component chiral spinors (Weyl spinors) are identified by

$$\psi_L = P_L \psi = \begin{pmatrix} \tilde{\psi}_L \\ 0 \end{pmatrix}, \quad \psi_R = P_R \psi = \begin{pmatrix} 0 \\ \tilde{\psi}_R \end{pmatrix}.$$

Helicity. For massless fermions, chirality is correlated to the concept of *helicity*, which we indicate by h . It is defined as the projection of the spin along the direction of motion

$$h = \frac{\mathbf{S} \cdot \mathbf{p}}{|\mathbf{p}|}. \quad (2.3.26)$$

Note that helicity is a Lorentz invariant concept only for massless particles. Let us consider a massless, left-handed fermion $\psi_L = \frac{1-\gamma^5}{2}\psi$, which satisfies $\gamma^5\psi_L = -\psi_L$. Its Dirac equation would read

$$\not{D}\psi_L(x) = \gamma^\mu \partial_\mu \psi_L(x) = 0,$$

which in momentum space (i.e., after a Fourier transform) reads

$$\not{D}\psi_L(p) = \gamma^\mu p_\mu \psi_L(p),$$

with the mass-shell condition $p_\mu p^\mu = 0$. Considering motion along the positive z direction, then $p^0 = p^3$ and $p^1 = p^2 = 0$ (for mass-shell it has the momentum on the z axis and the energy equal to it, $p^\mu = (p, 0, 0, p)$), so that

$$0 = (\gamma^0 p_0 + \gamma^3 p_3)\psi_L(p) = p^0(\gamma^3 - \gamma^0)\psi_L(p) \longrightarrow \gamma^0\psi_L(p) = \gamma^3\psi_L(p).$$

Now, the spin operator¹³

$$S^i = \frac{1}{2}\Sigma^i = -\frac{i}{4}\epsilon^{ijk}\alpha^j\alpha^k = -\frac{i}{4}\epsilon^{ijk}\gamma^j\gamma^k = \frac{1}{2}\epsilon^{ijk}\Sigma^{jk},$$

has a component along the z axis given by

$$S^3 = \frac{1}{2}(\Sigma^{12} - \Sigma^{21}) = \Sigma^{12} = -\frac{i}{4}[\gamma^1, \gamma^2] = -\frac{i}{2}\gamma^1\gamma^2,$$

and measures the helicity h . One computes it as follows

$$\begin{aligned} h\psi_L(p) &= S^3\psi_L(p) = -\frac{i}{2}\gamma^1\gamma^2\psi_L(p) = +\frac{i}{2}\gamma^0\gamma^0\gamma^1\gamma^2\psi_L(p) \\ &= +\frac{i}{2}\gamma^0\gamma^1\gamma^2\gamma^0\psi_L(p) = \frac{i}{2}\gamma^0\gamma^1\gamma^2\gamma^3\psi_L(p) \\ &= -\frac{1}{2}\gamma^5\psi_L(p) = \frac{1}{2}\psi_L(p). \end{aligned}$$

¹³We will use the substitution $\alpha^i\alpha^j = \gamma^0\gamma^i\gamma^0\gamma^j = -\gamma^i(-\mathbb{I})\gamma^j = \gamma^i\gamma^j$.

Thus, ψ_L describes a particle of helicity $h = \frac{1}{2}$. Its antiparticle is described by the charge conjugated field $\psi_{L,c}$ that is right-handed and has helicity $h = -\frac{1}{2}$.

$$\begin{cases} h\psi_L = +\frac{1}{2}\psi_L, \\ h\psi_{L,c} = -\frac{1}{2}\psi_{L,c}, \end{cases} \quad \begin{cases} h\psi_R = -\frac{1}{2}\psi_R, \\ h\psi_{R,c} = +\frac{1}{2}\psi_{R,c}. \end{cases}$$

This statement will become clear after the discussion on charge conjugation.

Time reversal

Let us discuss the transformation that reverses the direction of time, i.e., time reversal

$$\begin{aligned} \mathbf{x} &\xrightarrow{T} \mathbf{x}' = \mathbf{x}, \\ t &\xrightarrow{T} t' = -t, \end{aligned}$$

which in tensorial notation becomes:

$$x^\mu \xrightarrow{T} x'^\mu = T_\nu^\mu x^\nu, \quad \text{with } T_\nu^\mu = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (2.3.27)$$

It is a discrete symmetry with $\det T^{\mu\nu} = -1$. It belongs to $O(3, 1)$ but is not connected to the identity. Together with the identity it forms a subgroup isomorphic to $\mathbb{Z}_2 = \{1, -1\}$. The way time reversal acts on spinors can be found by conjecturing a suitable anti-linear transformation on the spinor

$$\psi(x) \xrightarrow{T} \psi'(x') = \mathcal{T}\psi^*(x),$$

generated by a matrix \mathcal{T} . The complex conjugate is suggested by the non-relativistic limit that links the Dirac equation to the Schrödinger equation. The Schrödinger equation is known to have a time-reversal symmetry that acts by transforming the wave function to its complex conjugate one. Thus, requiring invariance implies the equivalences

$$\begin{aligned} (\gamma^\mu \partial_\mu + m) \psi(x) = 0 &\iff (\gamma^\mu \partial'_\mu + m) \psi'(x') = 0, \\ x^\mu &\iff x'^\mu = T_\nu^\mu x^\nu, \\ \partial_\mu &\iff \partial'_\mu = (T^{-1})_\mu^\nu \partial_\nu, \\ \psi(x) &\iff \psi'(x') = \mathcal{T}\psi^*(x). \end{aligned}$$

Comparing the first equation (transformed Dirac equation, which we multiply further by \mathcal{T}^{-1} from the left) with its complex conjugate, namely $(\gamma^{\mu*} \partial_\mu + m)\psi^*(x) = 0$, one finds

$$\mathcal{T}^{-1} \gamma^\mu (T^{-1})_\mu^\nu \mathcal{T} = \gamma^\nu*,$$

or equivalently

$$\mathcal{T}^{-1} \gamma^\mu \mathcal{T} = T_\nu^\mu \gamma^\nu* = \begin{pmatrix} -\gamma^{0*} \\ \gamma^{1*} \\ \gamma^{2*} \\ \gamma^{3*} \end{pmatrix} = \begin{pmatrix} \gamma^0 \\ -\gamma^1 \\ \gamma^2 \\ -\gamma^3 \end{pmatrix}$$

The last equality is obtained using the explicit Dirac representation of gamma matrices (2.3.6). One needs to find a matrix \mathcal{T} that commutes with γ^0 and γ^2 and anticommutes with γ^1 and γ^3 :

$(\mu = 0)$ commutes with γ^0 :

$$\mathcal{T}^{-1}\gamma^0\mathcal{T} = T_0^0\gamma^{0*} = -\gamma^{0*} = \gamma^0,$$

which implies $[\mathcal{T}, \gamma^0] = 0$;

$(\mu = 2)$ commutes with γ^2 :

$$\mathcal{T}^{-1}\gamma^2\mathcal{T} = T_2^2\gamma^{2*} = \gamma^{2*} = \gamma^2,$$

which implies $[\mathcal{T}, \gamma^2] = 0$;

$(\mu = 1)$ anticommutes with γ^1 :

$$\mathcal{T}^{-1}\gamma^1\mathcal{T} = T_1^1\gamma^{1*} = \gamma^{1*} = -\gamma^1,$$

which implies $\{\mathcal{T}, \gamma^1\} = 0$;

$(\mu = 3)$ anticommutes with γ^3 :

$$\mathcal{T}^{-1}\gamma^3\mathcal{T} = T_3^3\gamma^{3*} = \gamma^{3*} = -\gamma^3,$$

which implies $\{\mathcal{T}, \gamma^3\} = 0$.

This matrix is proportional to $\gamma^1\gamma^3$: it commutes with an even number of gamma matrices with indices different from 1 and 3 (i.e. γ^0 and γ^2). Adding an arbitrary phase η_T one finds

$$\mathcal{T} = \eta_T\gamma^1\gamma^3.$$

For simplicity, one can set $\eta_T = 1$. Note that on spinors $T^2 = -1$ and $T^4 = 1$.

Hole theory. To overcome the problem of negative energy solutions, Dirac developed the theory of holes, abandoning the single-particle interpretation of his wave equation and predicting the existence of antiparticles. He supposed that the vacuum state, defined as the state with the lowest energy, consists of a configuration in which all the negative energy levels are occupied by electrons (the “Dirac sea”): Pauli’s exclusion principle guarantees that no more electrons can be added to the negative energy levels. This vacuum state has, by definition, vanishing energy and charge

$$E_{(\text{vacuum})} = 0, \quad Q_{(\text{vacuum})} = 0.$$

The state with one physical electron consists of an occupied positive energy level on top of the filled Dirac sea

$$E_{(\text{electron})} = E_p > 0, \quad Q_{(\text{electron})} = e < 0,$$

It has a charge $e < 0$ (by convention) and cannot jump to a negative energy level because the negative energy levels are all occupied, and the Pauli principle forbids the jump: the configuration is stable. In addition, one can also imagine a configuration in which a negative energy level lacks its electron: this is a hole in the Dirac sea. It is equivalent to a configuration in which a particle with positive energy and charge $-e$ is present on top of the vacuum. In fact, filling the hole with an electron with negative energy $-E_p$ and charge e gives back the vacuum state with vanishing energy and charge:

$$\begin{aligned} E_{(\text{hole})} + (-E_p) &= E_{(\text{vacuum})} = 0 \implies E_{(\text{hole})} = +E_p > 0, \\ Q_{(\text{hole})} + e &= Q_{(\text{vacuum})} = 0 \implies Q_{(\text{hole})} = -e > 0. \end{aligned}$$

These considerations led Dirac to predict the existence of the positron, the antiparticle of the electron. Moreover, it appears possible to imagine the phenomenon of pair creation: a photon

that interacts with the vacuum can transfer its energy to an electron with negative energy sitting in the Dirac sea and brings it up to positive energy, thus creating an electron and a hole, i.e., an electron/positron pair. This interpretation provides useful physical intuition, though it is not directly applicable to bosonic systems (as Pauli's principle is not valid for bosons). The correct realization of these ideas is implemented in QFT, both for fermions and bosons.

Charge conjugation

The Dirac equation can be coupled to electromagnetism with the minimal substitution

$$p_\mu \rightarrow p_\mu - eA_\mu.$$

It takes the form

$$[\gamma^\mu(\partial_\mu - ieA_\mu) - m]\psi = 0, \quad (2.3.28)$$

and describes particles with charge e and antiparticles with same mass but opposite charge $-e$, as suggested by the hole theory of Dirac. It should be possible to describe the same physics in terms of a Dirac equation for the antiparticles, identifying the original particles as anti-antiparticles. The new equation must take the form

$$[\gamma^\mu(\partial_\mu + ieA_\mu) - m]\psi_c = 0, \quad (2.3.29)$$

where ψ_c denotes the charge conjugation of ψ . The existence of a discrete transformation that links ψ to ψ_c is expected on physical ground, as it describes the same physical situation. This transformation is called *charge conjugation*: it exchanges particles and antiparticles. To identify it, one proceeds as follows, comparing eq. (2.3.29) with the complex conjugate of (2.3.28), which becomes

$$[\gamma^{\mu*}(\partial_\mu + ieA_\mu) - m]\psi^* = 0,$$

so that the correct relative sign between ∂_μ and ieA_μ is achieved. Now, one searches for a matrix \mathcal{A} such that

$$\mathcal{A}\gamma^{\mu*}\mathcal{A}^{-1} = \gamma^\mu \iff \mathcal{A}^{-1}\gamma^\mu\mathcal{A} = \gamma^{\mu*}, \quad (2.3.30)$$

so that the identification

$$\psi_c = \mathcal{A}\psi^* \quad (2.3.31)$$

produces the desired equation. One usually defines

$$\mathcal{A} = \mathcal{C}\beta \quad (2.3.32)$$

with \mathcal{C} the **charge conjugation matrix**. Now it is possible to write equation (2.3.31) in terms of the Dirac conjugate $\bar{\psi} = \psi^\dagger\beta$ as follows:

$$\psi_c = \mathcal{A}\psi^* = \mathcal{C}\beta\psi^* = \mathcal{C}(\psi^\dagger\beta)^T = \mathcal{C}\bar{\psi}^T, \quad (2.3.33)$$

where we have used that β is real and symmetric in the Dirac representation. Then, the problem is to identify the charge conjugation matrix. Recalling that $\gamma^\mu\dagger = -\beta\gamma^\mu\beta$ and taking the transpose, one finds $\gamma^{\mu*} = -\beta\gamma^{\mu T}\beta$, i.e. $\beta\gamma^{\mu*}\beta = -\gamma^{\mu T}$. This way eq. (2.3.31) reduces to the requirement

$$\mathcal{C}\gamma^{\mu T}\mathcal{C}^{-1} = -\gamma^\mu, \quad (2.3.34)$$

which assumes the form

$$\mathcal{C}^{-1}\gamma^\mu\mathcal{C} = -\gamma^{\mu T} = \begin{pmatrix} -\gamma^0 \\ \gamma^1 \\ -\gamma^2 \\ \gamma^3 \end{pmatrix},$$

where we have used the Dirac representation (2.3.6), where γ^0 and γ^2 are symmetric ($\gamma^{0T} = \gamma^0$ and $\gamma^{2T} = \gamma^2$) while γ^1 and γ^3 are antisymmetric ($\gamma^{1T} = -\gamma^1$ and $\gamma^{3T} = -\gamma^3$). Thus \mathcal{C} must anticommute with γ^0 and γ^2 while commuting with γ^1 and γ^3 ; then we may take

$$\mathcal{C} = \gamma^0\gamma^2, \quad \mathcal{C}^T = -\mathcal{C} = -\mathcal{C}^{-1}, \quad (2.3.35)$$

where we have highlighted that \mathcal{C} is antisymmetric and coincides with its inverse:

1. \mathcal{C} is antisymmetric:

$$\mathcal{C} = \gamma^0\gamma^2 = (-i\beta)(-i\beta\alpha^2) = -\alpha^2 = \begin{pmatrix} 0 & -\sigma^2 \\ \sigma^2 & 0 \end{pmatrix},$$

but σ^2 is antisymmetric, so that $\mathcal{C}^T = -\mathcal{C}$;

2. \mathcal{C} is its own inverse:

$$\mathcal{C}\mathcal{C} = \gamma^0\gamma^2\gamma^0\gamma^2 = \gamma^0(-\gamma^0\gamma^2)\gamma^2 = -(\gamma^0)^2(\gamma^2)^2 = (-i\beta\alpha^2)^2 = \mathbb{I} \implies \mathcal{C}^{-1} = \mathcal{C}.$$

Inserting an arbitrary phase η_C , one finds for the charge conjugation transformation of the Dirac spinor

$$\psi \rightarrow \psi_c = \eta_C \mathcal{A} \psi^* = \eta_C \mathcal{C} \bar{\psi}^T = \eta_C \gamma^0 \gamma^2 \bar{\psi}^T,$$

here written in two equivalent ways. The arbitrary phase is usually set to 1 for simplicity. What we have described is not a true symmetry if one keeps the background A_μ fixed. To achieve invariance, one should transform the background as well $A_\mu \xrightarrow{\mathcal{C}} A_\mu^c = -A_\mu$. One names this particular symmetry as “**background symmetry**”: it relates solutions in a given background to solutions in a transformed background. It becomes a true symmetry when also the field A_μ is treated as a dynamical field, subject to its own equations of motion and to the transformation for A_μ given above. This is the charge conjugation symmetry of QED.

Finally, let us show that the charge conjugation of a left-handed spinor is right-handed and vice versa: considering that a left-handed spinor and its Dirac conjugate satisfy

$$\psi_L = P_L \psi_L \rightarrow \bar{\psi}_L = \bar{\psi}_L^T P_R,$$

one finds by a direct computation that $\psi_{L,c}$ is right-handed

$$\psi_{L,c} = \mathcal{C} \bar{\psi}_L^T = \mathcal{C} (\bar{\psi}_L^T P_R)^T = \mathcal{C} P_R^T \bar{\psi}_L^T = P_R \mathcal{C} \bar{\psi}_L^T = P_R \psi_{L,c},$$

where we have used the Dirac basis $\mathcal{C} = \gamma^0\gamma^2$ and $\gamma^{5,T} = \gamma^5$, i.e. $P_R^T = P_R$.

CPT

Although the discrete symmetries C , P , and T of the free theory can be broken by interactions (notably, by the weak interaction), the CPT combination is found to be always valid for theories

which are Lorentz invariant (i.e., invariant under $\text{SO}^+(3,1)$). The theorem that proves this statement is known as the “**CPT theorem**” and will not be proved in generality on these notes. In the case of a Dirac fermion, the CPT transformation takes the form

$$\begin{aligned} x^\mu &\rightarrow x'^\mu = -x^\mu, \\ \psi(x) &\rightarrow \psi_{CPT}(x') = \eta_{CPT}\gamma^5\psi(x), \end{aligned}$$

with η_{CPT} an arbitrary phase and one verifies quite easily the invariance of the free Dirac equation.

We can investigate further

$$\begin{aligned} (\gamma^\mu\partial_\mu + m)\psi(x) &\xrightarrow{CPT} (\gamma^\mu\partial'_\mu + m)\psi_{CPT}(x') = 0, \\ [(\gamma^\mu)(-\partial_\mu) + m]\eta_{CPT}\gamma^5\psi(x) &= 0, \\ \eta_{CPT}\gamma^5[-\gamma^\mu\partial_\mu + m]\psi(x) &= 0, \end{aligned}$$

thus we have found that

$$(\gamma^\mu\partial'_\mu + m)\psi_{CPT}(x') = 0 \implies \gamma^5(\gamma^\mu\partial_\mu + m)\psi(x) = 0.$$

Now let us investigate the intermediate step of the CPT transformation:

$$\psi \xrightarrow{C} \psi_C \xrightarrow{P} \psi_{CP} \xrightarrow{T} \psi_{CPT}.$$

We haev:

1. Charge conjugation:

$$\psi \xrightarrow{C} \psi_C = \mathcal{C}\bar{\psi}^T.$$

2. Parity:

$$\psi_C \xrightarrow{P} \psi_{CP} = \mathcal{C}(\bar{\psi}\gamma^0)^T = \mathcal{C}(i\beta)\bar{\psi}^T = i\mathcal{C}\beta(\psi^\dagger\beta)^T = i\mathcal{C}\beta\beta(\psi^\dagger)^T = i\mathcal{C}\psi^*.$$

3. Time reversal:

$$\psi_{CP} \xrightarrow{T} \psi_{CPT} = i\mathcal{C}(\mathcal{T}\psi^*)^* = i\mathcal{C}(\gamma^1\gamma^3)\psi = i(\gamma^0\gamma^2)(\gamma^1\gamma^3)\psi = \gamma^5\psi.$$

Thus, we have found that the combination of the three discrete transformations produces

$$\psi \xrightarrow{CPT} \psi_{CPT} = \gamma^5\psi,$$

which coincides with the previous result up to an overall phase $\eta_{CPT} = 1$.

TODO: check signs.

2.3.9 | Action and Symmetries

The action is of great value to study symmetries, interactions, and equations of motion. It is also the starting point for quantization, either canonical or through path integrals. To identify an action for the Dirac equation, one ensures Lorentz invariance by taking a scalar lagrangian density. The latter is constructed using the Dirac field ψ and its Dirac conjugate $\bar{\psi} = \psi^\dagger\beta = \psi^\dagger i\gamma^0$, which has the property of transforming in such a way to make the product $\bar{\psi}\psi$ a scalar. Then, one recognizes that a suitable action is given by

$$S[\psi, \bar{\psi}] = \int d^4x \mathcal{L}, \quad \mathcal{L} = -\bar{\psi}(\gamma^\mu\partial_\mu + m)\psi. \quad (2.3.36)$$

It is a Lorentz scalar, and varying $\bar{\psi}$ and ψ independently, one finds that the least action principle indeed produces the Dirac equation and its conjugate

$$\begin{aligned}\delta\bar{\psi}) \quad (\gamma^\mu \partial_\mu + m)\psi(x) &= 0, \\ \delta\psi) \quad \bar{\psi}(x)(\overleftarrow{\partial}_\mu \gamma^\mu - m) &= 0,\end{aligned}$$

We could also work with more complex lagrangians, for instance adding interaction terms. An important example is the coupling to electromagnetism through minimal substitution

$$\mathcal{L} = -\bar{\psi} [\gamma^\mu (\partial_\mu - ieA_\mu) + m] \psi.$$

Symmetries. The symmetries under the Lorentz group have already been described. The symmetries under space-time translations are verified by taking the spinor $\psi(x)$ transforming as a scalar ($\psi(x) \rightarrow \psi'(x') = \psi(x)$ under $x^\mu \rightarrow x'^\mu = x^\mu + a^\mu$ with a^μ constant). The related Noether current gives the energy-momentum tensor. Let us consider in more detail the internal symmetry generated by phase transformations

$$\begin{cases} \psi(x) \longrightarrow \psi'(x) = e^{i\alpha} \psi(x), \\ \bar{\psi}(x) \longrightarrow \bar{\psi}'(x) = e^{-i\alpha} \bar{\psi}(x), \end{cases} \quad (2.3.37)$$

forming the group U(1). It is immediate to check that the action (2.3.36) is invariant. The infinitesimal version reads

$$\begin{cases} \delta\psi(x) = i\alpha\psi(x), \\ \delta\bar{\psi}(x) = -i\alpha\bar{\psi}(x), \end{cases}$$

and extending α to an arbitrary function $\alpha(x)$ we compute the variation of the action

$$\delta_\alpha S[\psi, \bar{\psi}] = - \int d^4x (\partial_\mu \alpha) \underbrace{i\bar{\psi} \gamma^\mu \psi}_{J^\mu} = \int d^4x \alpha(x) \partial_\mu J^\mu,$$

which verifies again the U(1) symmetry (for constant α) (in the last step we performed an integration by parts neglecting the boundary term), obtaining at the same time the Noether current

$$J^\mu = i\bar{\psi} \gamma^\mu \psi, \quad (2.3.38)$$

which is conserved on-shell (i.e., using the equations of motion: $\partial_\mu J^\mu = 0$). This result is enforced by the variation of the lagrangian density, which can be computed as the subtraction of the transformed lagrangian density minus the original one:¹⁴

$$\begin{aligned}\delta_\alpha \mathcal{L} &= -\delta_\alpha \bar{\psi}(\gamma^\mu \partial_\mu + m)\psi - \bar{\psi}(\gamma^\mu \partial_\mu + m)\delta_\alpha \psi \\ &= i\alpha \bar{\psi}(\gamma^\mu \partial_\mu)\psi - i\bar{\psi} \gamma^\mu (\partial_\mu \alpha \psi) \\ &= i\alpha \bar{\psi} \gamma^\mu (\partial_\mu \psi) - i\alpha \bar{\psi} \gamma^\mu (\partial_\mu \psi) - i(\partial_\mu \alpha) \bar{\psi} \gamma^\mu \psi \\ &= -i(\partial_\mu \alpha) \bar{\psi} \gamma^\mu \psi.\end{aligned}$$

As already noticed, the conserved charge density is positive definite

$$J^0 = i\bar{\psi} \gamma^0 \psi = \psi^\dagger \psi = |\psi|^2 \geq 0, \quad (2.3.39)$$

and led Dirac to interpret it as a probability density. In second quantization, it is reinterpreted as the symmetry related to the fermionic number (its charge will count the number of particles

¹⁴The action is linear, thus only the terms proportional to the variations of the fields survive.

minus the number of antiparticles), and in that context, eq. (2.3.39) becomes an operator that is no longer positive definite. In the coupling to electromagnetism, it is related to the electric charge. More generally, a collection of N Dirac fermions with the same Dirac mass is invariant under the group $\mathrm{U}(N) = \mathrm{U}(1) \times \mathrm{SU}(N)$. To see this, let us consider N fermions ψ^i transforming in the fundamental representation of $\mathrm{U}(N)$, the \mathbf{N} representation,

$$\psi^i \rightarrow \psi'^i = U^i_j \psi^j, \quad U \in \mathrm{U}(N).$$

The Dirac conjugates $\bar{\psi}_i$ (that contains the complex conjugate fields) transform in the antifundamental representation of $\mathrm{U}(N)$, the $\overline{\mathbf{N}}$ representation, which can be written as

$$\bar{\psi}_i \rightarrow \bar{\psi}'_i = \bar{\psi}_j (U^{-1})^j_i.$$

Then, the lagrangian

$$\mathcal{L} = -\bar{\psi}_i (\gamma^\mu \partial_\mu + m) \psi^i,$$

is manifestly invariant under $\mathrm{U}(N)$:

$$\mathcal{L}' = -\bar{\psi}_j (U^{-1})^j_i (\gamma^\mu \partial_\mu + m) U^i_k \psi^k = -\bar{\psi}_j \delta^j_k (\gamma^\mu \partial_\mu + m) \psi^k = \mathcal{L}.$$

The infinitesimal variations, considering infinitesimal transformations $U = e^{i\alpha^a T^a} = 1 + i\alpha^a T^a$, read

$$\begin{cases} \delta\psi^i = i\alpha_a (T^a)^i_j \psi^j, \\ \delta\bar{\psi}_i = -i\alpha_a \bar{\psi}_j (T^a)^j_i, \end{cases}$$

where T^a , $a = 1, \dots, N^2$ are the generators of $\mathrm{U}(N)$ in the fundamental representation. Thus the variation of the action, after extending α^a to arbitrary functions $\alpha^a(x)$, gives

$$\begin{aligned} \delta_\alpha S[\psi, \bar{\psi}] &= - \int d^4x \left[-i\alpha_a \bar{\psi}_j (T^a)^j_i (\gamma^\mu \partial_\mu + m) \psi^i + \bar{\psi}_i (\gamma^\mu \partial_\mu + m) i\alpha_a (T^a)^i_k \psi^k \right] \\ &= - \int d^4x (-i)(\partial_\mu \alpha_a) \bar{\psi}_i \gamma^\mu (T^a)^i_j \psi^j = \int d^4x \alpha_a(x) \partial_\mu \underbrace{i\bar{\psi}_i \gamma^\mu (T^a)^i_j \psi^j}_{J^{\mu, a}}, \end{aligned}$$

The corresponding Noether currents

$$J^{\mu, a} = i\bar{\psi}_i \gamma^\mu (T^a)^i_j \psi^j, \quad a = 1, \dots, N^2,$$

are conserved $\partial_\mu J^{\mu, a} = 0$, and are also called **non-Abelian currents**. If the mass vanishes, the internal symmetry becomes larger, and given by the group $\mathrm{U}(2N)$, as left and right-handed fermions transform independently. This fact may be better appreciated and proved keeping in mind the properties of chiral fermions and their charge conjugation.

Action for Chiral Fermions

Often, one analyzes the action rather than the equations of motion to derive general properties of the system. Thus, it is interesting to study the action written in terms of the irreducible chiral components ψ_L and ψ_R and their Dirac conjugates. It takes the form

$$S[\psi_L, \psi_R, \bar{\psi}_L, \bar{\psi}_R] = \int d^4x \left[-\bar{\psi}_L \gamma^\mu \partial_\mu \psi_L - \bar{\psi}_R \gamma^\mu \partial_\mu \psi_R - m(\bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L) \right],$$

which is verified by recalling the properties of the projectors $\psi_{L/R}$, and in particular

$$\begin{aligned}\psi_L &= P_L \psi = \frac{\mathbb{I} - \gamma^5}{2} \psi = \frac{\mathbb{I} - \gamma^5}{2} \psi_L, \\ \bar{\psi}_L &= \psi_L^\dagger \beta = \psi_L^\dagger \frac{\mathbb{I} - \gamma^5}{2} \beta = \psi_L^\dagger \beta \frac{\mathbb{I} + \gamma^5}{2} = \bar{\psi}_L P_R, \\ \gamma^\mu P_{L/R} &= P_{R/L} \gamma^\mu, \quad \gamma^\mu \frac{\mathbb{I} \pm \gamma^5}{2} = \frac{\mathbb{I} \mp \gamma^5}{2} \gamma^\mu.\end{aligned}$$

This form of the action shows that the Dirac mass term m cannot be present for chiral fermions (i.e., in models where one keeps only ψ_L by setting $\psi_R = 0$, or more generally where left-handed fermions are coupled differently to other particles than right-handed fermions). Recall that the Dirac mass term had the property of being invariant under the U(1) phase transformations given in equation (2.3.37)¹⁵

However, there is one more Lorentz invariant mass term that is possible: the **Majorana mass**. It breaks the U(1) symmetry related to the fermion number. It is used in extensions of the standard model that describe conjectured phenomena of neutrinos (such as the double beta decay without emission of neutrinos). It is of the form

$$\mathcal{L}_M = -\frac{M}{2} \psi^T \mathcal{C}^{-1} \psi + \text{h.c.} = -\frac{M}{2} (\psi_L^T \mathcal{C}^{-1} \psi_L + \psi_R^T \mathcal{C}^{-1} \psi_R) + \text{h.c.},$$

where M is the Majorana mass, $\mathcal{C} = \gamma^0 \gamma^2$ is the charge conjugation matrix introduced in eq. (2.3.35), and “h.c.” indicates hermitian conjugation. This term is Lorentz invariant and, therefore, admissible. However, it breaks the U(1) fermion number symmetry of (2.3.37). Lorentz invariance is explicitly verified: under infinitesimal transformations of Lorentz, one has

$$\delta\psi = \frac{i}{2} \omega_{\mu\nu} \Sigma^{\mu\nu} \psi, \quad \delta\psi^T = -\frac{i}{2} \omega_{\mu\nu} \psi^T \Sigma^{\mu\nu T} = -\frac{i}{2} \omega_{\mu\nu} \psi^T \mathcal{C}^{-1} \Sigma^{\mu\nu} \mathcal{C},$$

where the latter expression emerges by considering the properties (2.3.34) of the charge conjugation matrix:

$$\gamma^{\mu T} = -\mathcal{C}^{-1} \gamma^\mu \mathcal{C} \implies \Sigma^{\mu\nu T} = -\mathcal{C}^{-1} \Sigma^{\mu\nu} \mathcal{C}.$$

Thus we find that the Majorana mass term is invariant $\delta\mathcal{L}_M = 0$, as expected. We have to highlight that the Majorana mass term is non-vanishing only for chiral fermions. In fact, using the properties of the projectors $P_{L/R}$ and of the charge conjugation matrix \mathcal{C} , one finds

$$\mathcal{L}_M = \frac{M}{2} \psi^T \mathcal{C}^{-1} \psi + \text{h.c.} = \frac{M}{2} (\psi_L^T \mathcal{C}^{-1} \psi_L + \psi_R^T \mathcal{C}^{-1} \psi_R) + \text{h.c.},$$

and by setting for example $\psi_R = 0$ one finds a non-vanishing mass term for ψ_L .

Finally, let us remember, without going into much detail, that a theory of chiral fermions can be equivalently described in terms of Majorana fermions $\mu(x)$, that is Dirac spinors satisfying a reality condition of the form

$$\mu_c(x) = \mu(x).$$

A Majorana fermion can be decomposed into a Weyl fermion and its charge conjugate:

$$\mu(x) = \psi_L(x) + \psi_{L,c}(x) = \psi_L(x) + \mathcal{C} \bar{\psi}_L^T(x).$$

¹⁵In chiral models where parity is not conserved, there may be several right-handed and left-handed fermions with different charges and even different in numbers. The fermions entering the standard model are, in fact, chiral, in the sense that left-hand fermions have different couplings from their right-handed partners (i.e., different charges). They cannot have Dirac masses, which would not be gauge invariant: the transformation laws of ψ_L under the standard model symmetries ($SU(3) \times SU(2) \times U(1)$) are different from those of ψ_R . The Dirac masses of the standard model emerge as a consequence of the Higgs mechanism for the spontaneous breaking of the $SU(2) \times U(1)$ gauge symmetry.

The Majorana fermion has only two independent degrees of freedom, as $\psi_{L,c}$ is not independent from ψ_L .

Dirac and Majorana masses in scalar theories. By definition, a Majorana fermion is described by a spinor field that satisfies a reality condition of the type $\mu_c(x) = \mu(x)$, often interpret by saying that particles and antiparticles coincide. It describes an electrically uncharged fermion. Indeed the transformation (2.3.37) is no longer a symmetry: it cannot be applied to μ as it does not respect the constraint $\mu_c = \mu$, and the corresponding conserved charge no longer exists. A Majorana fermion possesses half the degrees of freedom of a Dirac fermion. To better understand the physical meaning of Dirac and Majorana mass, it is useful to describe an analogy with scalar particles. As a complex scalar field can be thought of as the combination of two real scalars with the same mass, similarly, a Dirac fermion can be considered as composed of two Majorana fermions with identical masses. The analog of a Majorana fermion is a real scalar field φ , which satisfies $\varphi^* = \varphi$ and a Klein-Gordon equation with mass μ , derivable from the lagrangian

$$\mathcal{L} = -\frac{1}{2} (\partial_\mu \varphi \partial^\mu \varphi + \mu^2 \varphi^2). \quad (2.3.40)$$

Two free real scalar fields φ_1 and φ_2 with different masses μ_1 and μ_2 , are described by the lagrangian

$$\mathcal{L} = -\frac{1}{2} (\partial_\mu \varphi_1 \partial^\mu \varphi_1 + \mu_1^2 \varphi_1^2) - \frac{1}{2} (\partial_\mu \varphi_2 \partial^\mu \varphi_2 + \mu_2^2 \varphi_2^2). \quad (2.3.41)$$

If the masses are identical, $\mu_1 = \mu_2 = m$, the model acquires a SO(2) symmetry that mixes the fields φ_1 and φ_2 , and the lagrangian becomes

$$\mathcal{L} = -\frac{1}{2} (\partial_\mu \varphi_1 \partial^\mu \varphi_1 + \partial_\mu \varphi_2 \partial^\mu \varphi_2 + m^2 (\varphi_1^2 + \varphi_2^2)). \quad (2.3.42)$$

The term $\varphi_1^2 + \varphi_2^2$ is SO(2) invariant, as is the kinetic term. The lagrangian can be written in terms of a complex field ϕ defined by

$$\phi = \frac{\varphi_1 + i\varphi_2}{\sqrt{2}}, \quad \phi^* = \frac{\varphi_1 - i\varphi_2}{\sqrt{2}}, \quad (2.3.43)$$

with φ_1 and φ_2 the real and imaginary part of ϕ , respectively. In this basis, the previous lagrangian (2.3.42) takes the form

$$\mathcal{L} = -\partial_\mu \phi^* \partial^\mu \phi - m^2 \phi^* \phi. \quad (2.3.44)$$

The symmetry $\text{SO}(2) \equiv \text{U}(1)$ becomes $\phi' = e^{i\alpha} \phi$ and $\phi'^* = e^{-i\alpha} \phi^*$, and the corresponding charge is often called “bosonic number” (it acts as the electric charge in a coupling to electromagnetism). Now, resuming what we found:

- (i) A complex scalar field ϕ describes a Dirac fermion, its mass m being the analog of a Dirac mass. It possesses a U(1) symmetry related to the conservation of the bosonic number.
- (ii) A real scalar field φ describes a Majorana fermion, its mass μ being the analog of a Majorana mass. It does not possess any U(1) symmetry.

Two Majorana fields with identical masses form a Dirac fermion, with their identical masses becoming the Dirac mass. A key property of the latter is that it respects the U(1) invariance. We also understand that, by breaking the U(1) invariance, it is possible to introduce a further mass term for ϕ and ϕ^* , directly visible in the φ_1 and φ_2 basis, recall eq. (2.3.41). It can be written in the ϕ and ϕ^* basis as

$$\mathcal{L} = -\partial_\mu \phi^* \partial^\mu \phi - m^2 \phi^* \phi - \frac{M^2}{2} (\phi \phi + \phi^* \phi^*). \quad (2.3.45)$$

The term with M^2 is the analog of a Majorana mass term for a Dirac fermion: it is a mass term that breaks the U(1) invariance, but keeps the lagrangian real. The explicit relationships between the mass terms are given by

$$\begin{cases} \mu_1^2 = m^2 + M^2, \\ \mu_2^2 = m^2 - M^2, \end{cases}$$

Note that M^2 does not have to be positive, while μ_1^2 and μ_2^2 must be positive to have a potential energy limited from below. The physical masses are μ_1 and μ_2 , as they give the location of the poles in the propagators (they are the eigenvalues of the mass matrix). In this analogy, we can reinterpret eq. (2.3.43) as saying that ϕ is the analog of a Weyl fermion and ϕ^* of its conjugate complex, remembering however that for the bosons there is no invariant concept of chirality.

Green functions and propagator. Let us briefly introduce also the Green function and related boundary conditions, for the Dirac equation. The Green function satisfies the equation

$$(\not{\partial}_x + m) S(x - y) = \delta^{(4)}(x - y),$$

formally solved in Fourier transform by

$$S(x - y) = \int \frac{d^4 p}{(2\pi)^4} e^{ip_\mu(x^\mu - y^\mu)} \tilde{S}(p) = \int \frac{d^4 p}{(2\pi)^4} \frac{e^{ip_\mu(x^\mu - y^\mu)}}{i\not{p} + m} = \int \frac{d^4 p}{(2\pi)^4} e^{ip_\mu(x^\mu - y^\mu)} \frac{-i\not{p} + m}{p^2 + m^2}.$$

Appropriate boundary conditions can be implemented by the prescription of how to integrate around the poles (points in momentum space where $p^2 + m^2$ vanishes). The same discussion given for the Klein-Gordon equation applies to the present context. In particular, the propagator is obtained by using the Feynman $i\epsilon$ prescription, and takes the form

$$S(x - y) = \int \frac{d^4 p}{(2\pi)^4} e^{ip_\mu(x^\mu - y^\mu)} \frac{-i\not{p} + m}{p^2 + m^2 - i\epsilon}.$$

The prescription $\epsilon \rightarrow 0^+$ makes it consistent to interpret the quantum fluctuations as corresponding to particles or antiparticles with positive energies that propagate from the past to the future, just as in the case of scalar particles. In QFT, it emerges as the correlation function

$$\langle \psi(x) \bar{\psi}(y) \rangle = -iS(x - y),$$

which propagates a particle from y to x if $x^0 > y^0$, and an antiparticle from x to y if $y^0 > x^0$.

2.4 | Integer Spin Particles

At this point, it is relatively easy to describe relativistic wave equations for particles of spin $s \geq 1$ with non-vanishing mass, modeling them on the Klein-Gordon equation (for bosonic fields of integer spin) and Dirac equation (for fermionic fields of semi-integer spin). They are known as Fierz-Pauli equations. The difficulties lie in the introduction of interactions, a non-trivial and subtle problem that we are not going to discuss in these notes.

2.4.1 | Fierz-Pauli equations

In the massive case of integer spin s (i.e. $s = 0, 1, 2, \dots$ is an integer) the wave function is given by a completely symmetric tensor of rank s , i.e. with s vector indices, $\phi_{\mu_1, \dots, \mu_s}$. It satisfies the KG equation in addition to constraints that impose transversality and the condition of vanishing trace¹⁶

$$\begin{aligned} (\square - m^2)\phi_{\mu_1, \dots, \mu_s} &= 0, \\ \partial^\mu \phi_{\mu, \mu_2, \dots, \mu_s} &= 0, \\ \phi_{\mu, \mu_3, \dots, \mu_s}^\mu &= 0, \end{aligned} \tag{2.4.1}$$

to understand their meaning, it is useful to study plane wave solutions using the ansatz

$$\phi_{\mu_1, \dots, \mu_s}(x) = \epsilon_{\mu_1, \dots, \mu_s}(p) e^{ip_\mu x^\mu}.$$

where the polarization tensor $\epsilon_{\mu_1, \dots, \mu_s}(p)$ describes covariantly the spin orientation. Then, eqs. (2.4.1) reduce to

$$\begin{aligned} p^2 + m^2 &= 0, \\ p^\mu \epsilon_{\mu, \mu_2, \dots, \mu_s}(p) &= 0, \\ \epsilon_{\mu, \mu_3, \dots, \mu_s}^\mu(p) &= 0. \end{aligned}$$

1. The first equation imposes the correct relativistic relation between energy and momentum on the plane wave.
2. The second equation (the transversality condition) eliminates in a covariant way non-physical degrees of freedom: choosing the frame of reference at rest with the particle, where the 4-momentum reduces to $\bar{p}^\mu = (m, 0, 0, 0)$, one recognizes that the independent components of the wave function must have only spatial indices:

$$m\epsilon_{0, \mu_2, \dots, \mu_s}(\bar{p}) = 0 \implies \epsilon_{i_1, i_2, \dots, i_s}(\bar{p}) \neq 0.$$

where the index $\mu = (0, i)$ is split into time and space components. This is due to the fact that The remaining polarizations describe the possible orientations in space of the spin.

3. The third equation (the vanishing trace condition) reduces the components of the polarization tensor to have only those components corresponding to the irreducible representation of spin s , which as known from quantum mechanics form a traceless, completely symmetric tensor of rank s of the rotation group $\text{SO}(3)$. It it has precisely $2s + 1$ independent components corresponding to the $2s + 1$ possible spin projections along a quantization axis.

¹⁶The index notation is to indicate that the unnamed index (μ_1 for the second equation, μ_1 and μ_2 for the third one) can be chosen arbitrarily among μ_1, \dots, μ_s , due to the symmetry of the tensor.

Let us verify the number of polarizations by counting the number of independent components of a fully symmetric tensor with s indices taking only three values¹⁷ (the spatial directions of the frame at rest with the particle) and then subtracting the components associated with the trace of the tensor (to be eliminated to get a vanishing trace)¹⁸

$$\frac{3 \cdot 4 \cdots (3+s-1)}{s!} - \frac{3 \cdot 4 \cdots (3+s-3)}{(s-2)!} = \frac{1}{2}(s+2)(s+1) - \frac{1}{2}s(s-1) = 2s+1.$$

This number is correct and supports the statement that the wave field $\phi_{\mu_1, \dots, \mu_s}$ corresponds to massive quanta of spin s . The calculation is valid for $s \geq 2$ but easily extended to lower s . In the case of a massive particle of half-integer spin $s = n + \frac{1}{2}$ (where n is an integer), the field is a spinor with in addition n symmetrical vector indices: $\psi_{\mu_1, \dots, \mu_s}$. It satisfies a Dirac equation with additional constraints that impose transversality and gamma-tracelessness

$$\begin{aligned} (\gamma^\mu \partial_\mu + m)\psi_{\mu_1, \dots, \mu_s} &= 0, \\ \partial^\mu \psi_{\mu, \mu_2, \dots, \mu_s} &= 0, \\ \gamma^\mu \psi_{\mu, \mu_2, \dots, \mu_s} &= 0, \end{aligned} \tag{2.4.2}$$

We will not discuss these equations any further. In the limit of vanishing mass, the correct field equations must have only two physical polarizations¹⁹ (the two possible helicities $h = \pm s$). This is usually obtained by considering equations with gauge symmetries. They need a more detailed discussion, leading to the so-called *Fronsdal equations*. They will not be presented in these notes except for the case $s = 1, 2$. **Gauge symmetries** are responsible for reducing the number of degrees of freedom (i.e., the number of components of the wave function that satisfies the equations of motion) from $2s+1$, corresponding to a massive particle of spin s , to the 2 components required by massless particles. As said, we will briefly review the case of massless spin 1, which certainly admits non-trivial interactions with fields of spin 0, $\frac{1}{2}$, and 1, as used in the construction of the Standard Model, and briefly mention the case of massless spin 2 (the graviton, the quantum of the gravitational waves). This is done by reviewing first the massive case to better understand differences and similarities. Massless higher spin particles do not seem to admit non-trivial interactions, and they have not found phenomenological applications thus far.

2.4.2 | Proca Equations

Massive particles of spin 1 are described by (2.4.1) with $s = 1$. It is customary to denote the wave function $\phi_\mu(x)$ by $A_\mu(x)$, so that the equations read

$$\begin{aligned} (\square - m^2)A_\mu &= 0, \\ \partial^\mu A_\mu &= 0. \end{aligned} \tag{2.4.3}$$

For this specific case, they are known as **Proca equations**. They can be derived from an action

$$S_P[A_\mu] = \int d^4x \left(-\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2}m^2A_\mu A^\mu \right), \tag{2.4.4}$$

¹⁷The number of independent components of a completely symmetric tensor of rank s in d dimension is $\frac{s!}{d(d+1)(d+2)\dots(d+s-1)}$.

¹⁸A trace can be taken on any two indices, but by symmetry, it is equivalent to taking the trace on the first two indices: the remaining tensor has $s-2$ totally symmetric indices.

¹⁹Recall that one cannot find a frame at rest with the particle, as the particle necessarily travels at the speed of light in all reference frames, and so the counting above must be modified.

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the field strength tensor. Integration by parts brings the action in an alternative form

$$\begin{aligned} S_P[A_\mu] &= \int d^4x - \frac{1}{4} \left((\partial_\mu A_\nu - \partial_\nu A_\mu)(\partial^\mu A^\nu - \partial^\nu A^\mu) - \frac{1}{2} m^2 A_\mu A^\mu \right) \\ &= \int d^4x \left(-\frac{1}{2}(\partial_\mu A_\nu)(\partial^\mu A^\nu) + \frac{1}{2}(\partial_\mu A_\nu)(\partial^\nu A^\mu) - \frac{1}{2} m^2 A_\mu A^\mu \right), \end{aligned}$$

since we could integrate by parts the second term in the second step and neglect boundary terms

$$\frac{1}{2}(\partial_\mu A_\nu)(\partial^\nu A^\mu) = -\frac{1}{2}A_\nu \partial^\nu(\partial_\mu A^\mu) = \frac{1}{2}(\partial_\nu A^\nu)(\partial_\mu A^\mu).$$

The final result

$$S_P[A_\mu] = \int d^4x \left(-\frac{1}{2}(\partial_\nu A_\mu)(\partial^\nu A^\mu) - \frac{1}{2}m^2 A_\mu A^\mu + \frac{1}{2}(\partial_\mu A^\mu)^2 \right)$$

is similar to the action of four Klein-Gordon fields A_μ (given by the first two terms), but with the crucial addition of the third term $(\partial_\mu A^\mu)^2$ with a very precise coefficient. The latter is responsible for the emergence of a constraint that reduces the number of degrees of freedom from 4 to 3. Let us verify this statement. By varying the action with respect to A_μ one finds

$$\begin{aligned} \delta S_P[A_\mu] &= \int d^4x \left(-\frac{1}{2}F_{\mu\nu}\delta F^{\mu\nu} - m^2 A_\nu \delta A^\nu \right) \\ &= \int d^4x \left(-\frac{1}{2}F_{\mu\nu}\partial^\mu \delta A^\nu + \frac{1}{2}F_{\mu\nu}\partial^\nu \delta A^\mu - m^2 A_\nu \delta A^\nu \right) \\ &= \int d^4x \left(+\frac{1}{2}(\partial^\mu F_{\mu\nu})\delta A^\nu - \frac{1}{2}\partial^\nu F_{\mu\nu}\delta A^\mu - m^2 A_\nu \delta A^\nu \right) \end{aligned}$$

where in the last step we integrated by parts and neglected boundary terms. Renaming dummy indices, one finds the **Proca equations of motion**:

$$\frac{\delta S_P[A_\mu]}{\delta A^\nu(x)} = 0 = \partial^\mu F_{\mu\nu} - m^2 A_\nu.$$

They are equivalent to the previous ones in (2.4.3). In fact, the identity $\partial^\mu \partial^\nu F_{\mu\nu}$ implies

$$\partial^\nu \partial^\mu F_{\mu\nu} = \partial^\nu(m^2 A_\nu) = 0,$$

which is zero due to the antisymmetry of $F_{\mu\nu}$ contracted with the symmetric operator $\partial^\mu \partial^\nu$. Thus for $m \neq 0$ one has a constraint

$$\partial^\mu A_\mu = 0.$$

Using this relationship, one rewrites Proca equations found extremizing the lagrangian as four Klein-Gordon equations plus the constraint, as in eq. (2.4.3):

$$\begin{aligned} \partial^\mu F_{\mu\nu} &= \square A_\nu - \partial_\nu(\partial^\mu A_\mu) = \square A_\nu = m^2 A_\nu, \\ \implies &\begin{cases} (\square - m^2)A_\mu = 0, \\ \partial^\mu A_\mu = 0. \end{cases} \end{aligned}$$

The constraint tells that only three of the four components of A_μ are independent, and the equations covariantly describe the three polarizations expected for a particle of spin 1. The invariance of the action and the equations of motion under Lorentz transformations is obvious, with A_μ transforming in the vectorial representation as indicated by its index position

$$\begin{aligned} x^\mu &\rightarrow x'^\mu = \Lambda^\mu_\nu x^\nu, \\ A_\mu(x) &\rightarrow A'_\mu(x') = \Lambda^\nu_\mu A_\nu(x). \end{aligned}$$

Plane wave solutions. Plane wave solutions of the Proca equation are obtained by inserting in (2.4.3) the ansatz

$$A_\mu(x) = \epsilon_\mu(p) e^{ip_\mu x^\mu},$$

to find that:

- the momentum p_μ must satisfy the “mass shell” condition $p_\mu p^\mu = -m^2$ (first equation in (2.4.3)),
- a linear combination of the four independent polarizations must vanish, $p^\mu \epsilon_\mu(p) = 0$ (second equation in (2.4.3)).

The three remaining polarizations describe the three degrees of freedom of a spin 1 particle in a manifestly covariant manner. In the rest frame, the polarization is given by a vector in three-dimensional space (spin 1). Real solutions can be obtained by combining with appropriate Fourier coefficients these physical plane waves. The associated quanta have mass m and spin 1, and antiparticles (corresponding to solutions with negative energies) coincide with the particles (no charge differentiates particles and antiparticles). If one considers a complex Proca field, particles and antiparticles are different: they have opposite charges under a $U(1)$ symmetry, which may be interpreted as the electric charge, and used to describe the W^\pm particles of the Standard Model.

Green Functions and Propagator

It is useful to rewrite the action (2.4.4) using integrations by part to reach the form

$$S_P[A_\mu] = \int d^4x \left(-\frac{1}{2} A_\mu K^{\mu\nu}(\partial) A_\nu \right),$$

obtained as

$$\begin{aligned} S_P[A_\mu] &= \int d^4x \left(-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{2} m^2 A_\mu A^\mu \right) \\ &= \int d^4x \left(-\frac{1}{2} (\partial_\mu A_\nu)(\partial^\mu A^\nu) + \frac{1}{2} (\partial_\mu A_\nu)(\partial^\nu A^\mu) - \frac{1}{2} m^2 A_\mu A^\mu \right) \\ &= \int d^4x \left(\frac{1}{2} A_\nu \square A^\nu - \frac{1}{2} A_\nu \partial^\nu (\partial_\mu A^\mu) - \frac{1}{2} m^2 A_\mu A^\mu \right) \\ &= \int d^4x \left(-\frac{1}{2} A_\mu ((-\square + m^2) \eta^{\mu\nu} + \partial^\mu \partial^\nu) A_\nu \right), \end{aligned}$$

The final expression identifies the differential operator

$$K^{\mu\nu}(\partial) = (-\square + m^2) \eta^{\mu\nu} + \partial^\mu \partial^\nu.$$

Using this notation, the Proca field equations read

$$K^{\mu\nu}(\partial) A_\nu(x) = 0,$$

indeed

$$\begin{aligned} K^{\mu\nu}(\partial) A_\nu(x) &= ((-\square + m^2) \eta^{\mu\nu} + \partial^\mu \partial^\nu) A_\nu(x) = -\square A^\mu + m^2 A^\mu + \partial^\mu (\partial^\nu A_\nu) \\ &= -\partial_\nu \partial^\nu A^\mu + m^2 A^\mu + \partial^\mu (\partial^\nu A_\nu) = \partial_\nu F^{\mu\nu} + m^2 A^\mu \\ &= -\partial_\mu F^{\mu\nu} + m^2 A^\nu = 0, \implies \partial_\mu F^{\mu\nu} = m^2 A^\nu. \end{aligned}$$

The relative Green function $G_{\mu\nu}(x - y)$ by definition satisfies

$$K^{\mu\rho}(\partial_x)G_{\rho\nu}(x - y) = \delta^\mu_\nu \delta^{(4)}(x - y). \quad (2.4.5)$$

It is given in Fourier space by

$$G_{\mu\nu}(x - y) = \int \frac{d^4 p}{(2\pi)^4} \tilde{G}_{\mu\nu}(p) e^{ip_\mu(x^\mu - y^\mu)},$$

where, if we apply the operator $K^{\mu\rho}(\partial_x)$ to the Fourier representation of the Green function, as required in (2.4.5), we find

$$K^{\mu\rho}(\partial_x)G_{\rho\nu}(x - y) = \int \frac{d^4 p}{(2\pi)^4} ((p^2 + m^2)\eta^{\mu\rho} - p^\mu p^\rho) \tilde{G}_{\rho\nu}(p) e^{ip_\mu(x^\mu - y^\mu)},$$

which should be equal to $\delta^\mu_\nu \delta^{(4)}(x - y)$; this implies that the Fourier transform of the Green function must satisfy

$$((p^2 + m^2)\eta^{\mu\rho} - p^\mu p^\rho) \tilde{G}_{\rho\nu}(p) = \delta^\mu_\nu.$$

Indeed, by symmetry the $\tilde{G}_{\mu\nu}(p)$ must have the form

$$\tilde{G}_{\mu\nu}(p) = A(p)\eta_{\mu\nu} + B(p)p_\mu p_\nu,$$

and one finds

$$A(p) = \frac{1}{p^2 + m^2}, \quad B(p) = \frac{A(p)}{m^2}.$$

Quantizing the Proca field with second quantized methods, one finds that the Green function is proportional to the propagator

$$\langle A_\mu(x)A_\nu(y) \rangle = -iG_{\mu\nu}(x - y) = -i \int \frac{d^4 p}{(2\pi)^4} \frac{e^{ip_\mu(x^\mu - y^\mu)}}{p^2 + m^2 - i\epsilon} \left(\eta_{\mu\nu} + \frac{p_\mu p_\nu}{m^2} \right),$$

where $\epsilon \rightarrow 0^+$. It describes as usual the propagation of particles and antiparticles of spin 1. Note that the propagator is singular in the limit of vanishing mass, $m \rightarrow 0$. Massless spin 1 particles require a separate treatment.

2.4.3 | Maxwell Equations

For $m \rightarrow 0$, the Proca action reduces to the Maxwell action

$$S_M[A_\mu] = \int d^4 x \left(-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right), \quad (2.4.6)$$

that correctly describes the relativistic waves associated to massless particles of spin 1 (with helicities $h = \pm 1$): if we compute the variation of the action, we can find the homogeneous Maxwell as equations of motion

$$\delta S_M[A_\mu] = \int d^4 x \left(-\frac{1}{2} F_{\mu\nu} \delta F^{\mu\nu} \right) = \int d^4 x \left(-\frac{1}{2} F_{\mu\nu} (\partial^\mu \delta A^\nu - \partial^\nu \delta A^\mu) \right) [\dots]$$

so that integrating by parts and neglecting boundary terms one finds the equations of motion

$$\partial^\mu F_{\mu\nu} = 0.$$

Using the definition of $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, they can be written as

$$\square A_\nu - \partial_\nu (\partial^\mu A_\mu) = 0. \quad (2.4.7)$$

The other half of Maxwell's equations are automatically solved by having expressed $F_{\mu\nu}$ in terms of the potential A_μ , and take the name of Bianchi identities

$$\partial_\lambda F_{\mu\nu} + \partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} = 0.$$

The novelty of this formulation of a relativistic wave equation for massless spin 1 particles is the presence of a gauge symmetry

$$A_\mu(x) \rightarrow A'_\mu(x) = A_\mu(x) + \partial_\mu \alpha(x), \quad (2.4.8)$$

which leaves the action (2.4.6) unchanged: $F_{\mu\nu}$ is invariant

$$F'_{\mu\nu} = \partial_\mu A'_\nu - \partial_\nu A'_\mu = F_{\mu\nu}.$$

and the full action remains invariant. As we shall see, this fact implies that the action describes only two degrees of freedom instead of three: they correspond to the maximum and minimum spin states when projected along the direction of motion (helicity $h = \pm 1$). The infinitesimal gauge transformation has the same form

$$\delta A_\mu(x) = \partial_\mu \alpha(x),$$

with $\alpha(x)$ taken now as an infinitesimal arbitrary function. We can think of this local symmetry as associated with the U(1) group as one can write (2.4.8) in the form

$$A'_\mu(x) = A_\mu(x) - i \left(e^{-i\alpha(x)} \partial_\mu e^{i\alpha(x)} \right),$$

with $e^{i\alpha(x)} \in \text{U}(1)$ for any spacetime point.

Plane wave solutions. The equations of motion do not have a unique solution (even after fixing initial conditions) because of the gauge symmetry: there is a combination of the dynamical variables that does not have a unique evolution as its time evolution can be changed arbitrarily with a gauge transformation. Keeping this gauge redundancy is very useful to have Lorentz invariance manifest, which is instrumental for introducing interactions in a way consistent with relativistic invariance. The Standard Model is indeed a gauge theory with local symmetry group $SU(3) \times SU(2) \times U(1)$. Gauge invariance can be used to set auxiliary conditions (gauge-fixing conditions) that allow to find physical solutions by eliminating (sometimes only partially) equivalent configurations generated by the gauge symmetry. We choose to partially fix the gauge symmetry by imposing the covariant constraint (Lorenz gauge)

$$\partial^\mu A_\mu(x) = 0. \quad (2.4.9)$$

One may verify that this constraint can always be imposed. This condition does not fix the gauge symmetry completely, but residual gauge transformations are left over, namely those with local parameter $\alpha(x)$ that satisfies $\square \alpha(x) = 0$. In the Lorenz gauge, the equations of motion are simplified to

$$\square A_\mu(x) = 0.$$

and the plane wave solutions are

$$A_\mu(x) = \epsilon_\mu(p) e^{ip_\mu x^\mu} \implies \begin{cases} \square A_\mu(x) = 0 \iff p_\mu p^\mu = 0, \\ \partial^\mu A_\mu(x) = 0 \iff p_\mu \epsilon^\mu(p) = 0. \end{cases}$$

which contain 3 independent polarizations $\epsilon^\mu(p)$, as one is removed by the Lorenz gauge constraint $p_\mu \epsilon^\mu(p) = 0$. Of these three remaining polarizations, the longitudinal one, defined by $\epsilon_\mu(p) = p_\mu$,

does not carry energy and momentum and carries vanishing electromagnetic fields \mathbf{E} and \mathbf{B} . It is gauge equivalent to $A_\mu = 0$ and can be eliminated by a residual gauge transformation, i.e. a gauge transformation that preserves the Lorenz condition (2.4.9). The residual gauge transformations have the form $\delta A_\mu(x) = \partial_\mu \alpha(x)$ with $\alpha(x)$ such that

$$\square \alpha(x) = 0.$$

so that the Lorenz gauge (2.4.9) is not modified. A plane wave $\alpha(x) = -ie^{ip_\mu x^\mu}$ with $p_\mu p^\mu = 0$ for the gauge function identifies a **non-physical solution** of the form

$$A_\mu(x) = \partial_\mu \alpha(x) = p_\mu e^{ip_\mu x^\mu},$$

where the polarization is proportional to p_μ , and it is thus removable by a gauge transformation with the opposite parameter. We conclude that only two independent physical polarizations remain. They can be shown to correspond to the two possible helicities of the photon.

2.4.4 | Spin 2 Particles

The general treatment of spin s can be specialized to the case $s=2$. The dynamical variables are grouped into a symmetric tensor of rank two, $\phi_{\mu\nu}(x)$, which satisfies eq.

$$\begin{aligned} (\square - m^2)\phi_{\mu\nu} &= 0, \\ \partial^\mu \phi_{\mu\nu} &= 0, \\ \phi^\mu_{\mu} &= 0, \end{aligned}$$

and plane wave solutions carry 5 independent polarizations, corresponding precisely to those of a particle of spin 2 ($-2, -1, 0, 1, 2$).

Massless Particles

The previous equations are not sufficient to describe the massless case, as only 2 physical polarizations are expected. They correspond to the maximum and minimum possible helicities of the particle, $h = \pm 2$. Gauge symmetries must be present in a Lorentz covariant description, and they are used to eliminate the non-physical polarizations, just as for spin 1. We indicate the spin 2 field with the symmetric tensor $h_{\mu\nu}(x)$, that in Einstein's theory of gravitation corresponds to the deformation of the Minkowski metric $\eta_{\mu\nu}$ to a curved metric

$$g_{\mu\nu}(x) = \eta_{\mu\nu} + h_{\mu\nu}(x) \quad (2.4.10)$$

Using the notation $h = h^\mu_\mu$ the gauge invariant equations (generalizing those in eq. (2.4.7)) are given by

$$\square h_{\mu\nu} - \partial_\mu \partial^\rho h_{\rho\nu} - \partial_\nu \partial^\rho h_{\rho\mu} + \partial_\mu \partial_\nu h = 0. \quad (2.4.11)$$

They are invariant under the local symmetries

$$\delta h_{\mu\nu}(x) = \partial_\mu \xi_\nu(x) + \partial_\nu \xi_\mu(x), \quad (2.4.12)$$

where $\xi_\mu(x)$ are four arbitrary spacetime functions (they form a vector field). Gauge symmetry is verified by a direct calculation: varying eq. (2.4.11) under (2.4.12) produces a vanishing result

$$\begin{aligned} &\square \delta h_{\mu\nu} - \partial_\mu \partial^\rho \delta h_{\rho\nu} - \partial_\nu \partial^\rho \delta h_{\rho\mu} + \partial_\mu \partial_\nu \delta h \\ &= \square(\partial_\mu \xi_\nu + \partial_\nu \xi_\mu) - \partial_\mu \partial^\rho (\partial_\rho \xi_\nu + \partial_\nu \xi_\rho) - \partial_\nu \partial^\rho (\partial_\rho \xi_\mu + \partial_\mu \xi_\rho) + \partial_\mu \partial_\nu (2\partial^\rho \xi_\rho) \\ &= \square(\partial_\mu \xi_\nu + \partial_\nu \xi_\mu) - \partial_\mu (\square \xi_\nu + \partial_\nu \partial^\rho \xi_\rho) - \partial_\nu (\square \xi_\mu + \partial_\mu \partial^\rho \xi_\rho) + 2\partial_\mu \partial_\nu (\partial^\rho \xi_\rho) = 0. \end{aligned}$$

Let us now study the plane wave solutions to check that there are indeed only two inequivalent polarizations. We use the four gauge symmetries to impose four gauge conditions, known as the **de Donder gauge**

$$\partial^\mu h_{\mu\nu} = \frac{1}{2}\partial_\nu h, \quad (2.4.13)$$

so that the equations (2.4.11) simplify to

$$\square h_{\mu\nu} = 0.$$

In analogy with the massless spin 1 case, we have residual gauge transformations with local parameters $\xi_\mu(x)$ satisfying

$$\square \xi_\mu = 0,$$

indeed we have

$$\square h'_{\mu\nu} = \square h_{\mu\nu} + \partial_\mu \square \xi_\nu + \partial_\nu \square \xi_\mu = 0,$$

so that the truly physical solutions, which cannot be eliminated using gauge transformations, are 2. We calculate 10 (independent components of $h_{\mu\nu}$) $- 4$ (number of constraints in de Donder gauge) $- 4$ (number of solutions that can be eliminated with residual gauge transformations) $= 2$. A more refined analysis shows that these two independent polarizations correspond to the two physical helicities of the gravitational waves $h = \pm 2$. Finally, let us mention that these equations emerge from the linearization of the Einstein equations in vacuum

$$R_{\mu\nu}(g) = 0,$$

where $R_{\mu\nu}(g)$ is the Ricci tensor built from the metric $g_{\mu\nu}(x) = \eta_{\mu\nu} + h_{\mu\nu}(x)$. In the linearization, one keeps only terms linear in $h_{\mu\nu}(x)$. Gauge symmetry is related to the invariance under an arbitrary change of coordinates, suitably linearized.

3 | Path Integrals

Quantization can be introduced in two equivalent ways: - operator formalism (canonical quantization, Hilbert space, linear operators, etc ..) - path integrals (functional integrals).

Path integrals were introduced in quantum mechanics by Feynman in 1948, but until about 1970 they did not meet with much success, and the operatorial methods of canonical quantization were still the most widespread. In 1970, the success of gauge theories in developing the Standard Model of particle physics gave a strong impulse to path integral methods.

Quantization of gauge theories is much more clear and elegant if performed with path integrals. Furthermore, path integrals indicate a way of relating a quantum field theory in D spacetime dimensions ($D - 1$ spaces and 1 time) to the statistical mechanics of a system in D space dimensions. This link has given rise to a way of thinking and defining field theories using statistical mechanics and renormalization group ideas, as introduced by Wilson and others (lattice theories). Nowadays, it is convenient to master both methods: according to the problem at hand, one may find one formalism more convenient than the other, even though they are supposed to be equivalent.

Two-slit experiment. To introduce path integrals, let us follow Feynman and consider the *two-slit experiment* for the electron. The standard treatment used to explain the behavior of an electron which passes through the two slits of a barrier and creates a figure of interference on a screen employs the wave nature of the electron together with the Huygens principle for calculating the interference pattern from the elementary waves that originate from the slits. Feynman proposes an *alternative description*. He suggests to keep thinking of the electron as a particle that however can accomplish both trajectories, each one with a certain “amplitude”. The **total amplitude** A_{tot} is defined as the sum of the single amplitudes, and its square is related to the probability that the electron is revealed at a given point on the screen. Moreover, the **elementary amplitude** for each possible trajectory is related in a simple way to the classical action evaluated on the trajectory itself: Feynman, inspired by previous considerations of Dirac, associates to each trajectory an amplitude of unit norm (so that all trajectories “weigh” democratically the same way) and with phase equal to the value of the action S in units of \hbar .

Thus we can write

$$A_{tot} = A(c_1) + A(c_2) + \dots + A(c_n), \quad A(c_n) = e^{\frac{i}{\hbar} S(c_n)}.$$

thus we linked the total amplitude, which let us study probabilities in our experiments, to a sum of single amplitudes with the same module but different phases

$$A_{tot} = \sum_n e^{\frac{i}{\hbar} S(c_n)}, \quad \Rightarrow \quad P \propto |A_{tot}|^2,$$

and defined by the action (the integral of the lagrangian along the path, for a free particle we have just the kinetic contribution)

$$S[q] = \int_0^T dt \frac{1}{2} m \dot{q}^2.$$

So for a path where we assume $D \gg d$ and simplifying the problem with a constant velocity along the two trajectories, we can write the action for each path as

$$\begin{aligned} S(c_1) &= \int_0^T dt \frac{1}{2} m \dot{q}^2 = \int_0^T dt \frac{1}{2} m \left(\frac{D}{T} \right)^2 = \frac{m}{2} \frac{D^2}{T}, \\ S(c_2) &= \int_0^T dt \frac{1}{2} m \dot{q}^2 = \int_0^T dt \frac{1}{2} m \left(\frac{D+d}{T} \right)^2 = \frac{m}{2} \frac{(D+d)^2}{T} \\ &= \frac{mD^2}{2T} + \frac{md^2}{2T} + \frac{mDd}{T} \sim \frac{mD^2}{2T} + \frac{md^2}{2T} + pd + O(d^2) = S(c_1) + pd + O(d^2), \end{aligned}$$

where in the last term $p = \frac{mD}{T}$ is the momentum of the electron (we have simplified the term $\propto d^2$ since $d \rightarrow 0$). Therefore we can now study the total amplitude

$$A_{tot} = e^{\frac{i}{\hbar} S(c_1)} + e^{\frac{i}{\hbar} S(c_2)} = e^{\frac{i}{\hbar} S(c_1)} \left(1 + e^{\frac{i}{\hbar} pd} \right) = A(c_1) \left(1 + e^{\frac{i}{\hbar} pd} \right),$$

which is associated to a total probability proportional to

$$P \propto |A_{tot}|^2 = |A(c_1)|^2 \left| 1 + e^{\frac{i}{\hbar} pd} \right|^2 = \left| 1 + e^{\frac{i}{\hbar} pd} \right|^2,$$

since $|A(c_1)|^2 = 1$. It is easy to notice that the maximum probability, associated to the maximum amplitude, of revealing the electron on the screen is obtained when the two contributions add up constructively, thus

$$e^{\frac{i}{\hbar} pd} = 1, \quad \Rightarrow \quad \frac{pd}{\hbar} = 2\pi n, \text{ with } n \in \mathbb{N},$$

One can interpret this condition as defining a wavelength $\lambda = \frac{\hbar}{p}$ so that when d contains an integer number of times such wavelengths there is constructive interference. The de Broglie relation is obtained by this rudimentary “path integral” and suggests that it contains the essential elements of quantum mechanics.

The number of slits can be increased, as well as the number of intermediate screens, to have the particle performing all possible paths from the initial point to the final point of observation, thus creating a path integral for the total amplitude.

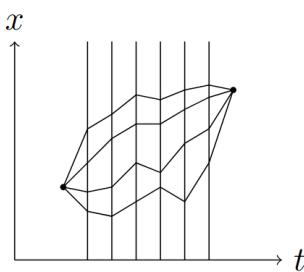


Figure 3.1: Scheme for a rudimental and discretized path integral. The electron can follow all possible paths from the source to the screen, passing ideally through multiple intermediate screens. Each path contributes with an amplitude of unit norm and phase given by the action evaluated on the path itself. The total amplitude is obtained by summing all contributions.

The action is used in an essential way

$$S[q(t)] = \int dt L(q(t), \dot{q}(t)),$$

where the classic path is the one that minimizes the action

$$\delta S = 0, \quad \Rightarrow \quad \frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = 0.$$

In quantum mechanics there is a crucial difference: the transition amplitude is obtained by using the action $S[q]$ **for any possible path**

$$A = \sum_{c_n} e^{\frac{i}{\hbar} S(c_n)} \equiv \int Dq(t) e^{\frac{i}{\hbar} S[q(t)]}.$$

Here we introduce the final notation of the **path integral** or **functional integral**: $S[q]$ is a functional, i.e., a function of the functions $q(t)$, that indicate the possible “paths” of the system, and the symbol $\int Dq$ indicates the formal integration over the space of paths $\{q(t)\}$. Various mathematical subtleties on how to define exactly the path integration are still open. Nevertheless, path integrals have become one of the main tools to study quantum systems.

In this formulation, the classic limit is intuitive: macroscopic systems have large values of the action S in units of \hbar , the quantum of action. Small variations of a path

$$q(t) \rightarrow q(t) + \delta q(t),$$

induce a variation of the action

$$S[q] \rightarrow S[q + \delta q] = S[q] + \delta S[q],$$

which translates in phase variations $i\frac{1}{\hbar}\delta S[q]$ much bigger with respect to $i\pi$ (recall that for such a phase $e^{i\pi} = -1$) and the amplitudes of nearby paths cancel by destructive interference. This happens except at the point in which the action has a minimum, $\delta S = 0$, which identifies the classic trajectory. Trajectories close to the classical one have amplitudes that add up coherently since the phase does not vary: the functional integral, in the end, is dominated by the classic path.

3.1 | Canonical Quantization

Canonical quantization is constructed starting from the hamiltonian formulation of a classical system. It is obtained by lifting its phase space coordinates, the generalized coordinates x^i and conjugate momenta p_i , to linear operators \hat{x}^i and \hat{p}_i that act on a linear space endowed with a positive definite norm, the Hilbert space of physical states \mathcal{H} . The basic operators must satisfy commutation relations required to be equal $i\hbar$ times the value of the corresponding classical Poisson brackets

$$\begin{aligned} [\hat{x}^i, \hat{x}^j] &= [\hat{p}_i, \hat{p}_j] = 0, \\ [\hat{x}^i, \hat{p}_j] &= i\hbar\delta_j^i. \end{aligned} \tag{3.1.1}$$

All classical observables $A(x, p)$, which are functions on phase space, become linear operators $\hat{A}(\hat{x}, \hat{p})$ acting on the Hilbert space \mathcal{H} .

The most important example is given by the hamiltonian function $H(x, p)$, which upon quantization becomes the hamiltonian operator $\hat{H}(\hat{x}, \hat{p})$. The latter generates the time evolution of any state $|\psi\rangle \in \mathcal{H}$ through the Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle. \tag{3.1.2}$$

The corresponding solution is a time-dependent state $|\psi\rangle(t)$ that describes the evolution of the quantum system. This setup is known as the Schrodinger picture of quantum mechanics. It is a formal quantization procedure that becomes operative once one finds an irreducible unitary representation of the operator algebra in eq. (3.1.1).

A mathematical result, known as the Stoneon Neumann theorem, states that in quantum mechanics all irreducible representations of (3.1.1) are unitarily equivalent, so that there is a unique procedure of quantizing a classical system.¹ Historically, this theorem made it clear that the Schrodinger formulation of quantum mechanics was equivalent to the one proposed by Heisenberg with its matrix mechanics (known as the Heisenberg picture).

Let us consider, more specifically, the motion of a nonrelativistic particle in one dimension in the presence of an external potential $V(x)$. The classical dynamics is fixed by the action

$$S[x] = \int dt \left(\frac{m}{2} \dot{x}^2 - V(x) \right).$$

The quantum theory is recognized by first developing the hamiltonian formulation, defined in the phase space with the Poisson bracket structure and phase space action

$$S[x, p] = \int dt (p\dot{x} - H(x, p)), \quad H(x, p) = \frac{p^2}{2m} + V(x),$$

with $\{x, p\} = 1$ and $\{x, x\} = \{p, p\} = 0$.

Now, as prescribed by canonical quantization, the phase space coordinates x and p become fundamental operators \hat{x} and \hat{p} acting on the Hilbert space of physical states \mathcal{H} , satisfying the commutation relations presented by the algebra in eq. (3.1.1) (in this setting there is only one coordinate and one momentum). The hamiltonian function $H(x, p)$ becomes the hamiltonian operator $\hat{H}(\hat{x}, \hat{p})$ acting on \mathcal{H} , responsible for the time evolution of any state $|\psi\rangle \in \mathcal{H}$ through the Schrödinger equation (3.1.2).

¹Up to the problem of resolving ordering ambiguities, often present when one tries to relate the classical hamiltonian $H(x, p)$ to its quantum counterpart $\hat{H}(\hat{x}, \hat{p})$.

Using the coordinate representation, obtained by considering the eigenstates $|x\rangle$ of the position operator \hat{x} , that satisfy $\hat{x}|x\rangle = x|x\rangle$ with real eigenvalues x , and projecting the various states of the Hilbert space onto them to identify the wave functions, one finds the familiar way of realizing quantum mechanics as wave mechanics

$$\begin{aligned} |\psi\rangle &\longrightarrow \psi(x) = \langle x|\psi\rangle, \\ \hat{x} &\longrightarrow x, \quad \langle x|\hat{x}|x'\rangle = x\delta(x-x'), \\ \hat{p} &\longrightarrow -i\hbar\frac{\partial}{\partial x}, \quad \langle x|\hat{p}|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-x'), \\ \hat{H} &\longrightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \end{aligned}$$

Thus the Schrodinger equation (3.1.2) becomes the familiar differential equation for the wave function $\psi(x, t)$

$$i\hbar\frac{\partial}{\partial t}\psi(x, t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x, t).$$

Returning to the Dirac bra and ket notation, let us consider the solution of the Schrödinger equation. Given a ket $|\psi_i\rangle$ that describes the system at initial time t_i , the solution of the Schrödinger equation for time-independent hamiltonians can be written as

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}(t-t_i)}|\psi_i\rangle,$$

satisfying boundary condition $|\psi(t_i)\rangle = |\psi_i\rangle$. The operator $e^{-\frac{i}{\hbar}\hat{H}(t-t_i)}$ is called the evolution operator. The transition amplitude between an initial state $|\psi_i\rangle$ at time t_i and a final state $|\psi_f\rangle$ at time t_f is defined as

$$A = \langle\psi_f|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|\psi_i\rangle = \langle\psi_f|\psi_i\rangle,$$

where the matrix element of the evolution operator are shown to be those transition amplitudes indeed. The transition amplitude contains all the physical information about the quantum system, as it allows one to compute probabilities and expectation values of physical observables.

3.2 | Path Integrals in Phase Space

To derive a path integral expression for the transition amplitudes, we start by inserting twice the identity operator \mathbb{I} , expressed using the eigenstates of the position operator

$$\mathbb{I} = \int dx |x\rangle \langle x|, \quad \text{with } \langle x|x'\rangle = \delta(x - x'),$$

then we can rewrite the transition amplitude derived previously by inserting two of this identity-operators

$$\begin{aligned} A &= \langle \psi_f | e^{-\frac{i}{\hbar} \hat{H}(t_f - t_i)} | \psi_i \rangle = \langle \psi_f | \mathbb{I} e^{-\frac{i}{\hbar} \hat{H}(t_f - t_i)} \mathbb{I} | \psi_i \rangle \\ &= \int dx_i \int dx_f \langle \psi_f | x_f \rangle \langle x_f | e^{-\frac{i}{\hbar} \hat{H}(t_f - t_i)} | x_i \rangle \langle x_i | \psi_i \rangle \\ &= \int dx_i \int dx_f \psi_f^*(x_f) A(x_i, x_f, T) \psi_i(x_i), \end{aligned}$$

where $\psi_i(x_i) = \langle x | \psi_i \rangle$ and $\psi_f(x_f) = \langle x | \psi_f \rangle$ are the wave functions for the initial and final states. This rewriting shows that it is enough to consider the matrix element of the evolution operator between position eigenstates

$$A(x_i, x_f, T) = \langle x_f | e^{-\frac{i}{\hbar} \hat{H}T} | x_i \rangle$$

where $T = t_f - t_i$ is the total propagation time. It satisfies the Schrodinger equation

$$i\hbar \frac{\partial}{\partial T} A(x_i, x_f, T) = \langle x_f | \hat{H}(\hat{x}, \hat{p}) e^{-\frac{i}{\hbar} \hat{H}T} | x_i \rangle = \hat{H}(x_f, \hat{p}_f = -i\hbar \partial_{x_f}) A(x_i, x_f, T),$$

with initial condition $A(x_i, x_f, 0) = \delta(x_i - x_f)$.

We are going to consider quantum hamiltonians of a particle interacting with a generic potential $\hat{V}(\hat{x})$, of the familiar form $\hat{H}(\hat{x}, \hat{p}) = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x})$. The derivation can be extended to more general hamiltonians, but this case is enough to illustrate the main ideas.

We can now proceed to derive the path integral formalism as follows. One can split the transition amplitude $A(x_i, x_f, T)$ in the product of N factors, and insert the completeness relation $N - 1$ times in between the factors

$$\begin{aligned} A(x_i, x_f, T) &= \langle x_f | e^{-\frac{i}{\hbar} \hat{H}T} | x_i \rangle = \langle x_f | \left(e^{-\frac{i}{\hbar} \hat{H} \frac{T}{N}} \right)^N | x_i \rangle \\ &= \langle x_f | e^{-\frac{i}{\hbar} \hat{H}\epsilon} \mathbb{I} e^{-\frac{i}{\hbar} \hat{H}\epsilon} \mathbb{I} \dots e^{-\frac{i}{\hbar} \hat{H}\epsilon} \mathbb{I} e^{-\frac{i}{\hbar} \hat{H}\epsilon} | x_i \rangle \\ &= \int \left(\prod_{k=1}^{N-1} dx_k \right) \langle x_f | e^{-\frac{i\epsilon}{\hbar} \hat{H}} | x_{N-1} \rangle \langle x_{N-1} | e^{-\frac{i\epsilon}{\hbar} \hat{H}} | x_{N-2} \rangle \dots \\ &= \int \left(\prod_{k=1}^{N-1} dx_k \right) \prod_{k=1}^N \langle x_k | e^{-\frac{i\epsilon}{\hbar} \hat{H}} | x_{k-1} \rangle, \end{aligned}$$

where for convenience we have denoted $x_0 = x_i$, $x_N = x_f$, and $\epsilon = \frac{T}{N}$. To evaluate this expression better, it is convenient to use the completeness relation N more times, now expressed in terms of the momentum eigenstates

$$\mathbb{I} = \int \frac{dp}{2\pi\hbar} |p\rangle \langle p|, \quad \text{with } \langle p|p'\rangle = 2\pi\hbar\delta(p - p'),$$

to obtain

$$\begin{aligned} A(x_i, x_f, T) &= \int \left(\prod_{k=1}^{N-1} dx_k \right) \prod_{k=1}^N \langle x_k | \mathbb{I} e^{-\frac{i\epsilon}{\hbar} \hat{H}} | x_{k-1} \rangle \\ &= \int \left(\prod_{k=1}^{N-1} dx_k \right) \prod_{k=1}^N \int \frac{dp_k}{2\pi\hbar} \langle x_k | p_k \rangle \langle p_k | e^{-\frac{i\epsilon}{\hbar} \hat{H}} | x_{k-1} \rangle \\ &= \int \left(\prod_{k=1}^{N-1} dx_k \right) \left(\prod_{k=1}^N \frac{dp_k}{2\pi\hbar} \right) \prod_{k=1}^N \langle x_k | p_k \rangle \langle p_k | e^{-\frac{i\epsilon}{\hbar} \hat{H}} | x_{k-1} \rangle, \end{aligned}$$

which is an exact expression. Note that there is one more integration over momenta than integrations over coordinates, a consequence of choosing coordinate eigenstates as initial and final states in the transition amplitude. Now, one can manipulate this expression further by making approximations that are valid in the limit $N \rightarrow \infty$ (i.e., $\epsilon \rightarrow 0$). The crucial point is the evaluation of the following matrix element in this limit, where we can Taylor expand the exponential in ϵ to obtain

$$\begin{aligned} \langle p | e^{-\frac{i\epsilon}{\hbar} \hat{H}(\hat{x}, \hat{p})} | x \rangle &= \langle p | \left(\mathbb{I} - \frac{i\epsilon}{\hbar} \hat{H}(\hat{x}, \hat{p}) + \dots \right) | x \rangle = \langle p | \left(\mathbb{I} - \frac{i\epsilon}{\hbar} H(x, p) + \dots \right) | x \rangle \\ &= \langle p | x \rangle e^{-\frac{i\epsilon}{\hbar} H(x, p)}, \end{aligned}$$

thus recovering the exponential form with the eigenvalues of the hamiltonian, letting us extract it from the matrix element. These approximations are all valid in the limit of small ϵ . The substitution $\langle p | \hat{H}(\hat{x}, \hat{p}) | x \rangle = \langle p | x \rangle H(x, p)$ follows from the simple structure of the considered hamiltonian, that allows one to act with the momentum operator on the left, and with the position operator on the right, to have the operators replaced by the corresponding eigenvalues. Notice that there is no need for commuting operators inside the hamiltonian, because of the simplicity of the hamiltonian we have considered.

The final result is that all operators are simply replaced by eigenvalues. This way the quantum hamiltonian $\hat{H}(\hat{x}, \hat{p})$ gets replaced by the classical function $H(x, p) = \frac{p^2}{2m} + V(x)$. There exists a mathematically rigorous proof that these manipulations are correct for a wide class of physically interesting potentials $V(x)$ (the “Trotter formula”). We do not review these subtleties, as the physically intuitive derivation given above is enough for our purposes.

and remembering that the wave functions of the momentum eigenstates (the plane waves) are normalized as

$$\langle x | p \rangle = e^{\frac{i}{\hbar} px}, \quad \langle p | x \rangle = (\langle x | p \rangle)^* = e^{-\frac{i}{\hbar} px},$$

following from the normalizations chosen with the two completeness relations, one obtains

$$\langle x_k | p_k \rangle \langle p_k | e^{-\frac{i\epsilon}{\hbar} \hat{H}} | x_{k-1} \rangle = e^{\frac{i}{\hbar} p_k x_k} e^{-\frac{i\epsilon}{\hbar} H(x_{k-1}, p_k)} e^{-\frac{i}{\hbar} p_k x_{k-1}} = e^{\frac{i\epsilon}{\hbar} \left[p_k \frac{x_k - x_{k-1}}{\epsilon} - H(x_{k-1}, p_k) \right]}.$$

up to terms that vanish for $\epsilon \rightarrow 0$. This expression can now be inserted in the last expression for the elements of $A(x_i, x_f, T)$; at this stage, the transition amplitude does not contain any more operators, bras and kets, containing just integrations, though a big number of them, of ordinary functions

$$A(x_i, x_f, T) = \lim_{N \rightarrow \infty} \int \left(\prod_{k=1}^{N-1} dx_k \right) \left(\prod_{k=1}^N \frac{dp_k}{2\pi\hbar} \right) e^{\frac{i\epsilon}{\hbar} \sum_{k=1}^N \left[p_k \frac{x_k - x_{k-1}}{\epsilon} - H(x_{k-1}, p_k) \right]} = \int DxDp e^{\frac{i}{\hbar} S[x, p]}.$$

This is the **path integral in phase space**. One recognizes in the exponent a discretization of the classical phase space action

$$S[x, p] = \int_{t_i}^{t_f} dt (p\dot{x} - H(x, p)), \quad \Rightarrow \quad \sum_{k=1}^N \epsilon \left(p_k \frac{x_k - x_{k-1}}{\epsilon} - H(x_{k-1}, p_k) \right),$$

where $t_f - t_i = T = N\epsilon$ is the total propagation time, with the paths in phase space discretized as

$$\begin{aligned} x(t) &\longrightarrow x_k = x(t_i + k\epsilon), \\ p(t) &\longrightarrow p_k = p(t_i + k\epsilon). \end{aligned}$$

The last way of writing the amplitude is symbolic but suggestive: it indicates the sum over all paths in phase space weighted by the exponential of $\frac{i}{\hbar}$ times the classical action. It depends implicitly on the boundary conditions assigned to the paths $x(t)$. We can compact the notation by writing

$$A(x_i, x_f, T) = \int Dx(t)Dp(t) e^{\frac{i}{\hbar}S[x(t), p(t)]}, \quad (3.2.1)$$

where the symbol $\int Dx(t)Dp(t)$ indicates the formal integration over the space of paths in phase space $\{x(t), p(t)\}$. Various mathematical subtleties on how to define exactly the path integration are still open. Nevertheless, path integrals have become one of the main tools to study quantum systems.

3.3 | Path Integrals in Configuration Space

The path integral in configurations space is easily derived by integrating over the momenta. The dependence on momenta in the exponent of A is at most quadratic and can be eliminated by gaussian integration: if we consider the previous expression for the transition amplitude in phase space

$$A(x_i, x_f, T) = \lim_{N \rightarrow \infty} \int \left(\prod_{k=1}^{N-1} dx_k \right) \left(\prod_{k=1}^N \frac{dp_k}{2\pi\hbar} \right) e^{\frac{i\epsilon}{\hbar} \sum_{k=1}^N \left[p_k \frac{x_k - x_{k-1}}{\epsilon} - \frac{p_k^2}{2m} - V(x_{k-1}) \right]}$$

we can explicitly perform the gaussian integrations over the momenta p_k with

$$\int_{-\infty}^{\infty} dp e^{-\frac{\alpha}{2} p^2} = \sqrt{\frac{2\pi}{\alpha}},$$

which is valid for $\alpha > 0$ and can be generalized by **square completion** to exponents of the type $-\frac{\alpha}{2}p^2 + \beta p$ as follows

$$\begin{aligned} \int_{-\infty}^{\infty} dp e^{-\frac{\alpha}{2}p^2 + \beta p} &= \int_{-\infty}^{\infty} dp e^{-\frac{\alpha}{2}(p^2 - \frac{2\beta}{\alpha}p)} = \int_{-\infty}^{\infty} dp e^{-\frac{\alpha}{2}[(p - \frac{\beta}{\alpha})^2 - (\frac{\beta}{\alpha})^2]} \\ &= e^{\frac{\beta^2}{2\alpha}} \int_{-\infty}^{\infty} dp e^{-\frac{\alpha}{2}(p - \frac{\beta}{\alpha})^2} = e^{\frac{\beta^2}{2\alpha}} \sqrt{\frac{2\pi}{\alpha}}, \end{aligned}$$

performed by shifting the integration variable $p \rightarrow p - \frac{\beta}{\alpha}$ (the differential do not change). Now, extending analytically this expression, we can include complex values of α (see section 3.4.2 for details). Note that the final exponential is the original exponential inside the integral with argument evaluated at the minimum in p (saddle point).

Returning to the path integral, and considering the hamiltonian $H(x, p) = \frac{p^2}{2m} + V(x)$, one completes the squares

$$\begin{aligned} A &= \lim_{N \rightarrow \infty} \int \left(\prod_{k=1}^{N-1} dx_k \right) \frac{1}{(2\pi\hbar)^N} \prod_{k=1}^N \int dp_k e^{\frac{i\epsilon}{\hbar} \sum_{k=1}^N \left[p_k \frac{x_k - x_{k-1}}{\epsilon} - \frac{p_k^2}{2m} - V(x_{k-1}) \right]} \\ &\quad \begin{cases} \alpha = \frac{i\epsilon}{2m\hbar} & \longrightarrow \left(\frac{2\pi\hbar m}{i\epsilon} \right)^{\frac{N}{2}}; \\ \beta = \frac{i}{\hbar} (x_k - x_{k-1}) & \longrightarrow e^{\frac{\beta^2}{2\alpha}} = e^{\frac{im}{2\hbar\epsilon} (x_k - x_{k-1})^2} \text{ inside sum;} \\ \frac{i\epsilon}{\hbar} V(x_{k-1}) & \longrightarrow \text{remains unchanged inside sum;} \end{cases} \\ &= \lim_{N \rightarrow \infty} \int \left(\prod_{k=1}^{N-1} dx_k \right) \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} e^{\frac{i\epsilon}{\hbar} \sum_{k=1}^N \left[\frac{m}{2} \frac{(x_k - x_{k-1})^2}{\epsilon^2} - V(x_{k-1}) \right]}. \end{aligned}$$

where we have implicitly performed the gaussian integrations N times over the momenta. Thus is now possible to write the transition amplitude as

$$A = \lim_{N \rightarrow \infty} \int \left(\prod_{k=1}^{N-1} dx_k \right) \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} e^{\frac{i\epsilon}{\hbar} \sum_{k=1}^N \left[\frac{m}{2} \frac{(x_k - x_{k-1})^2}{\epsilon^2} - V(x_{k-1}) \right]} = \int Dx(t) e^{\frac{i}{\hbar} S[x(t)]}.$$

Our exponent is complex, so the function keeps oscillating; by analytic continuation we can use this results also in the complex case. This is the path integral in configuration space. It contains in the exponent the configuration space action suitably discretized

$$S[x] = \int_{t_i}^{t_f} dt \left(\frac{m}{2} \dot{x}^2 - V(x) \right) \longrightarrow \sum_{k=1}^N \epsilon \left[\frac{m}{2} \frac{(x_k - x_{k-1})^2}{\epsilon^2} - V(x_{k-1}) \right].$$

Again, the last way of writing the path integral in (3.3.1) is symbolic and indicates the formal sum over paths in configuration space, weighted by the exponential of $i\hbar$ times the classical action. The space of paths is given by the space of functions $x(t)$ with boundary values $x(t_i) = x_i$ and $x(t_f) = x_f$. It is an infinite dimensional space. How to perform concretely the path integral over this functional space is defined precisely by the discretization, that approximates a function $x(t)$ by its $N + 1$ values $x_k = x(t_i + \epsilon k)$ at $k = 0, 1, 2, \dots, N$, as shown in fig. 3.

Thus, we have constructed the path integral that computes quantum mechanical amplitudes

$$A = \int Dx(t) e^{\frac{i}{\hbar} S[x(t)]}, \quad (3.3.1)$$

by the sum of all histories of paths weighted by a phase given by the action, with all paths contributing.

3.3.1 | Free Particle

For a free particle ($V(x) = 0$) one may use repeatedly gaussian integration and calculate from eq.

TODO: Add image. (3.3.1) the exact transition amplitude as

$$\begin{aligned} A(x_i, x_f, T) &= \lim_{N \rightarrow \infty} \int \left(\prod_{k=1}^{N-1} dx_k \right) \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} e^{\frac{i\epsilon}{\hbar} \sum_{k=1}^N \left[\frac{m}{2} \frac{(x_k - x_{k-1})^2}{\epsilon^2} \right]} \\ &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{\frac{N-1}{2}} \frac{1}{\sqrt{N}} e^{\frac{i}{\hbar} \frac{m(x_f - x_i)^2}{2T}} \\ &= \sqrt{\frac{m}{2\pi i \hbar T}} e^{\frac{i}{\hbar} \frac{m(x_f - x_i)^2}{2T}} = \langle x_f | e^{-\frac{i}{\hbar} \hat{H} T} | x_i \rangle. \end{aligned}$$

It satisfies the free Schrodinger equation

$$i\hbar \frac{\partial}{\partial T} A(x_i, x_f, T) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_f^2} A(x_i, x_f, T),$$

with initial condition $A(x_i, x_i, 0) = \delta(x_f - x_i)$, since we can compute

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_f^2} \sqrt{\frac{m}{2\pi i \hbar T}} e^{\frac{i}{\hbar} \frac{m(x_f - x_i)^2}{2T}} = \frac{m}{2T^2} (x_f - x_i)^2 A(x_i, x_f, T) = i\hbar \frac{\partial}{\partial T} A(x_i, x_f, T).$$

This way, the path integral has produced a solution of the Schrodinger equation. The result is very suggestive: up to a prefactor, the solution is given by the exponential of $\frac{i}{\hbar}$ times the classical action evaluated on the classical path $S[x]$, i.e., the path that satisfies the classical equations of motion. The free particle case is also quite special: the exact final result is valid for any N , and there is no need to take the limit $N \rightarrow \infty$. The case $N = 1$, which carries no integration at all, is already exact.

A formal but useful way of calculating gaussian path integrals is achieved by working directly in the continuum limit. One does not need the precise definition of the path integral measure but uses only its formal properties, in particular, its translational invariance. The calculation is formal in the sense that one assumes properties of the path integral measure (that eventually must be proven by an explicit regularization and construction, as the one given earlier). The calculation goes as follows. The action is $S[x] = \int_0^T dt \frac{m}{2} \dot{x}^2$, and the classical equations of motion with the boundary conditions are solved by

$$x_{cl}(t) = x_i + \frac{x_f - x_i}{T} t.$$

One can represent a generic path $x(t)$ as the classical path $x_{cl}(t)$ plus quantum fluctuations $q(t)$

$$x(t) = x_{cl}(t) + q(t),$$

where the fluctuations $q(t)$ must vanish at $t = 0$ and $t = T$ to preserve the boundary conditions. One may interpret $x_{cl}(t)$ as the origin in the space of functions. Then, one computes the path integral as follows

$$\begin{aligned} A(x_i, x_f, T) &= \int Dx e^{\frac{i}{\hbar} S[x]} = \int D(x_{cl} + q) e^{\frac{i}{\hbar} S[x_{cl} + q]} \\ &= e^{\frac{i}{\hbar} S[x_{cl}]} \int Dq e^{\frac{i}{\hbar} S[q]} = N e^{\frac{i}{\hbar} S[x_{cl}]} = N e^{\frac{i}{\hbar} \frac{m(x_f - x_i)^2}{2T}}, \end{aligned}$$

where we have used different inputs to solve it:

- The translational invariance of the path integral measure has been used in the form $Dx = D(x_{cl} + q) = Dq$.
- The normalization factor $N = \int Dq e^{\frac{i}{\hbar} S[q]}$ is undetermined by this method, but it is a constant that does not depend on x_i and x_f . Very often, its precise value is not needed, but one can fix it by requiring that the final result satisfies the Schrodinger equation, finding $N = \sqrt{\frac{m}{2\pi i\hbar T}}$.
- The action splits into a classical part plus a quantum part:

$$S[x_{cl} + q] = S[x_{cl}] + S[q] + (\text{linear terms in } q).$$

There is no linear term in $q(t)$ in the action because the function $x_{cl}(t)$ solves the classical equations of motion: for quadratic actions one has $S[x_{cl} + q] = S[x_{cl}] + S[q]$; we can integrate non quadratic terms by parts indeed:

$$\int dt \dot{x}_{cl}\dot{q} = \dot{x}_{cl}q|_0^T - \int dt \ddot{x}_{cl}q = 0,$$

where the first term vanishes because $q(0) = q(T) = 0$, while the second term vanishes because $\ddot{x}_{cl} = 0$ for the free particle (it solves the classical equations of motion).

This method of calculation is very powerful and can be extended to more general cases, as we will see later.

3.3.2 | Euclidean Time and Statistical Mechanics

Quantum mechanics can be related to statistical mechanics by an analytic continuation. We introduce this relation by considering the free particle, with

$$A(x_i, x_f, T) = \int Dx e^{\frac{i}{\hbar} S[x]} = \sqrt{\frac{m}{2\pi i\hbar T}} e^{\frac{i}{\hbar} \frac{m(x_f - x_i)^2}{2T}}.$$

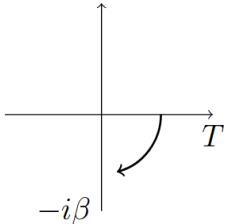
Continuing analytically the time parameter to purely imaginary values by $T \rightarrow -i\beta$ with real β , and setting $\hbar = 1$, the free Schrodinger equation turns into the **heat equation** (or diffusion equation)

$$\frac{\partial}{\partial \beta} A = \frac{1}{2m} \frac{\partial^2}{\partial x_f^2} A.$$

Its fundamental solution, i.e. the solution with boundary condition $A \xrightarrow{\beta \rightarrow 0} \delta(x_f - x_i)$, is given by

$$A = \sqrt{\frac{m}{2\pi\beta}} e^{-\frac{m(x_f - x_i)^2}{2\beta}},$$

and can be obtained from the original expression by the same analytic continuation. This continuation is called “**Wick rotation**”, see figure below.



(?) Why
integration limits
change without
imaginary unit?

The Wick rotation can be performed directly on the path integral to obtain euclidean path integrals. Analytically continuing the time variable $t \rightarrow -i\tau$, one finds that the action with “minkowskian” time (i.e. with a real time t) turns into an “euclidean” action S_E defined by

$$iS[x] = i \int_0^T dt \frac{m}{2} \dot{x}^2 \xrightarrow{dt \rightarrow -i d\tau} -S_E[x] = - \int_0^\beta d\tau \frac{m}{2} \dot{x}^2.$$

In the euclidean action we have defined $\dot{x} = \frac{dx}{d\tau}$, with τ usually called “euclidean time” (or imaginary time). The euclidean action thus defined is positive definite and it appears in the path integral as follows

$$\langle x_f | e^{-\beta \hat{H}} | x_i \rangle = \int Dx e^{-S_E[x]}, \quad (3.3.2)$$

where the crucial difference with respect to the original path integral is *the absence of the imaginary unit i in the exponent*. The operator on the left-hand side is called the “heat kernel” and the path integrals computes its matrix elements. For a free theory, the path integral is truly gaussian, with exponential damping rather than increasingly rapid phase oscillations (now the phase is real). In this form, it coincides with the integral functional introduced by Wiener in the 1920’s to study brownian motion and the heat equation (that explains why eq. (3.3.2) is called the heat kernel).

Such euclidean path integrals are useful in **statistical mechanics**, where β is related to the absolute temperature Θ as $\beta = \frac{1}{k\Theta}$, where k is the Boltzmann’s constant. To see this, let us consider the trace of the evolution operator

$$e^{-\frac{i}{\hbar} \hat{H} T}, \quad e^{-\frac{i}{\hbar} \hat{H} T} |n\rangle = e^{-\frac{i}{\hbar} E_n T} |n\rangle,$$

where we have written it using energy eigenstates (labeled by n if the spectrum is discrete), or equivalently we could use position eigenstates (which are continuous and labeled by x). Since these are two complete bases of the Hilbert space, and its eigenvalues identify the diagonal elements, we can write the trace in either way:

$$Z \equiv \text{Tr}\left(e^{-\frac{i}{\hbar} \hat{H} T}\right) = \sum_n e^{-\frac{i}{\hbar} E_n T} = \int dx \langle x | e^{-\frac{i}{\hbar} \hat{H} T} | x \rangle.$$

This can be Wick rotated $Z \rightarrow Z_E$ (with $T \rightarrow -i\beta$) to obtain the statistical partition function Z_E of the quantum system with hamiltonian \hat{H} . Setting $\hbar = 1$, it reads

$$Z_E = \text{Tr}\left(e^{-\beta \hat{H}}\right) = \sum_n e^{-\beta E_n} = \int dx \langle x | e^{-\beta \hat{H}} | x \rangle. \quad (3.3.3)$$

Again, it is immediate to find a path integral representation of the statistical partition function: one performs a Wick rotation of the path integral action, sets the initial state (at euclidean time

$\tau = 0$) equal to the final state (at euclidean time $\tau = \beta$), and sums over all possible states, as indicated in (3.3.3). The paths become closed, as $x(\beta) = x(0)$, and the partition function becomes

$$Z_E = \text{Tr}\left(e^{-\beta \hat{H}}\right) = \int_{PBC} Dx e^{-S_E[x]},$$

where PBC stands for “periodic boundary conditions”, indicating the sum over all paths that close onto themselves in an euclidean time β . Introduced here for the free theory, the Wick rotation is supposed to be of more general value, relating quantum mechanics to statistical mechanics in the interacting case as well. Even if one is interested in the theory with a real time, nowadays, one often works in the euclidean version of the theory, where factors of the imaginary unit i are absent, and path integral convergence is more easily kept under control. Only at the very end one performs the inverse Wick rotation to read off the result for the theory in real time.

The Wick rotation procedure is better appreciated by first considering the usual time as corresponding to the real line of a complex plane. Then, defining

$$t_\theta = te^{-i\theta},$$

the usual real time appears at $\theta = 0$, while the euclidean time τ appears at $\theta = \frac{\pi}{2}$ as $t_{\frac{\pi}{2}} = -i\tau$. The analytical continuation of all physical quantities is achieved by continually increasing θ from 0 to $\frac{\pi}{2}$, a clockwise rotation of the real axis into the imaginary one. The generalized partition function

$$Z_\theta = \text{Tr}\left(e^{-\frac{i}{\hbar} \hat{H} t_\theta}\right)$$

with a complex time $t_\theta = te^{-i\theta}$ with positive t has a damping factor for all $0 < \theta < \frac{\pi}{2}$ and for all hamiltonians that are bounded from below (up to an inessential overall factor due to the value of the ground state energy, if that happens to be negative).

Similar considerations can be made for path integrals in minkowskian and euclidean times with other boundary conditions. Path integrals in euclidean times are mathematically better defined (one may develop a mathematically well-defined measure theory on the space of functions), at least for quadratic actions and perturbations thereof. Path integral with a minkowskian time are more delicate, and physicists usually use the argument of rapid phase oscillations to deduce that unwanted terms vanish. The Wick rotation suggests a way of defining the path integral in real time starting from the euclidean time one. These points of mathematical rigor are not needed for the applications that we are going to consider, and the derivation of path integrals described previously is enough for our purposes.

3.3.3 | Comments

We have seen that the quantization of a classical system with action $S[x]$ is achieved by the path integral $\int Dx e^{\frac{i}{\hbar} S[x]}$ that computes the transition amplitude.

In the path integral formulation, the classical limit is intuitive: macroscopic systems have large values of action in \hbar units. Macroscopically small variations of paths can still make the phase variations $\frac{\delta S[x]}{\hbar}$ much bigger than π , so that amplitudes of nearby paths cancel by destructive interference. This is true except for variations that make $\delta S[x] = 0$, which is the condition that identifies the classical path. Nearby paths have amplitudes that sum coherently with the classical one, and the path integral is dominated by the classical trajectory.

The notation $\int Dx$ is symbolic and indicates the formal integration over the space of functions $x(t)$. To make it precise, one has to regulate the functional space by making it finite-dimensional

(“regularization”). Then one integrates over the regulated finite-dimensional space, and eventually takes the continuum limit by removing the regularization parameters. If this procedure is done with care, the limit exists and gives the correct transition amplitude. In the previous derivation, we have seen that the space of paths is regulated by approximating the functions $x(t)$ by their $N - 1$ values computed at intermediate points, the x_k ’s with $k = 1, \dots, N - 1$. This makes the space of functions finite dimensional. The action is discretized and evaluated using the approximated functions. At this stage, the integration over the regulated functional space is well-defined. Eventually, one takes the continuum limit ($N \rightarrow \infty$): if the integration measure is chosen appropriately, this limit exists and gives a viable definition of the path integral.

We started from canonical quantization and derived the above discretized form of the space of functions. This regularization is often called **Time Slicing (TS)**. Vice versa, one can start directly with the path integral, regulate it suitably, and use it to construct the quantum theory (Feynman originally started this way). The path integral is used to evaluate a transition amplitude that is seen to satisfy a Schrödinger wave equation. This can be viewed as an alternative approach to quantization. In the regularization procedure of the path integral, one must make several choices, and they may produce different transition amplitudes. For example, in a TS regularization one may discretize the potential term $V(x(t))$ in the action to $V(x_k)$ or $V(x_{k-1})$ or $V(\frac{1}{2}(x_k + x_{k-1}))$. In the present case, this makes no difference, and one obtains the same continuum limit.

These ambiguities are the path integral counterparts of the *ordering ambiguities* of canonical quantization. Ordering ambiguities arise when one must construct a quantum hamiltonian out of a classical one: as \hat{x} and \hat{p} do not commute, it may happen that one must choose an ordering to define the quantum hamiltonian. Different orderings produce different quantum hamiltonians, and thus different quantum theories. Examples of systems where ordering ambiguities arise are the case of a charged particle in a magnetic field and the motion of a particle in a curved space, where the respective hamiltonians are:

$$H = \frac{(\vec{p} - \frac{e}{c}\vec{A}(x))^2}{2m}, \quad H = \frac{1}{2m}g^{ij}(x)p_ip_j.$$

We have introduced path integrals by considering a single degree of freedom. Extension to a finite number of degrees of freedom is immediate, so that quantizing the motion of one or more particles in a finite dimensional space does not pose any new conceptual problem. For example, the motion of a nonrelativistic particle in \mathbb{R}^3 with cartesian coordinates \vec{x} , in the presence of a scalar potential $V(\vec{x})$, is quantized by the following discretized path integral:

$$\int Dx e^{\frac{i}{\hbar}S[x]} = \lim_{N \rightarrow \infty} \int \left(\prod_{k=1}^{N-1} d^3x_k \right) \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{3N}{2}} e^{\frac{i}{\hbar} \sum_{k=1}^N \epsilon \left[\frac{m}{2} \frac{(\vec{x}_k - \vec{x}_{k-1})^2}{\epsilon^2} - V(\vec{x}_{k-1}) \right]},$$

where, of course, the classical action is

$$S[x] = \int_0^T dt \left(\frac{m}{2} \dot{\vec{x}}^2 - V(\vec{x}) \right) = \lim_{N \rightarrow \infty} \sum_{k=1}^N \epsilon \left[\frac{m}{2} \frac{(\vec{x}_k - \vec{x}_{k-1})^2}{\epsilon^2} - V(\vec{x}_{k-1}) \right].$$

Formally, one can also consider the case of an infinite number of degrees of freedom, as appropriate for a field theory. In this case, convergence is not guaranteed, and the removal of the regularization may lead to infinite results. In the class of theories called renormalizable, the infinities can be removed consistently by a *renormalization* procedure that redefines the dynamical variables and the coupling constants, and allows to obtain finite results, at least at the level of perturbation theory.

3.4 | Correlation Functions

Correlation functions are quantities used to describe several physical observables in the quantum theory. They are also useful to develop the perturbative expansion around the solvable gaussian path integral that corresponds to a “free” theory (we include the harmonic oscillator in this class, as it is recognized as the quantum mechanical equivalent of a free Klein-Gordon QFT). For our purposes, we will not spend time explaining the physical meaning of correlation functions, but rather focus on their definition in the path integral formalism and their computation in simple cases: they are powerful tools to extract physical information from the path integral formulation of quantum mechanics and quantum field theory.

As we will see explicitly, this formalism is equivalent to the canonical quantization approach for scalar theories and thus bosonic fields, and we will compute explicitly correlation functions for the KG field. At the end of the chapter we will include the treatment of fermionic fields, which require some additional tools.

Correlation functions are *normalized averages of the product of n dynamical variables, evaluated at different times and weighted by $e^{\frac{i}{\hbar}S}$* , and they implement directly the computation of physical observables through the path integral formalism. In our one-dimensional example, the normalized “n-point correlation function” is defined by

$$\langle x(t_1)x(t_2) \cdots x(t_n) \rangle = \frac{1}{Z} \int Dx x(t_1)x(t_2) \cdots x(t_n) e^{\frac{i}{\hbar}S[x]}, \quad (3.4.1)$$

where $Z = \int Dx e^{\frac{i}{\hbar}S[x]}$ is the normalization factor, also known as the **partition function**, providing $\langle 1 \rangle = 1$ (by definition).

Of particular importance is the 2-point correlation function $\langle x(t_1)x(t_2) \rangle$, often called the propagator. It is understood that correlation functions depend implicitly on the boundary conditions that specify the initial and final states. Very often, especially in quantum field theory, one chooses the initial and final states to be the vacuum state (the state with lowest energy) and considers an infinite propagation time (which also implements the projection onto the ground state). We have considered amplitudes between positions eigenstates, but one can insert any desired state as a boundary state when defining the matrix elements of the evolution operator.

It is often useful to introduce a **generating functional** $Z[J]$ defined by

$$Z[J] = \int Dx e^{\frac{i}{\hbar}(S[x] + \int dt J(t)x(t))}, \quad (3.4.2)$$

where $J(t)$ is an auxiliary external function, known as a **source**. Visually, when we compute the equations of motion, we are adding a source that "pushes" the particle around

$$E(x) = J(x),$$

substantially being a mathematical trick to compute all correlation functions by functional differentiation with respect to the source $J(t)$.

Let's consider a differentiation with respect to the source at time t_1 :

$$\frac{\delta}{\delta J(t_1)} Z[J] = \int Dx x(t_1) e^{\frac{i}{\hbar}(S[x] + \int dt J(t)x(t))},$$

where we have to pay attention to the functional derivative, which acts as a delta function

$$\int dt \frac{\delta J(t)}{\delta J(t_i)} x(t) = \int dt \delta(t - t_i) x(t) = x(t_i). \quad (3.4.3)$$

Continuing this process iterating the functional differentiation n times, we obtain

$$\frac{\delta}{\delta J(t_n)} \cdots \frac{\delta}{\delta J(t_2)} \frac{\delta}{\delta J(t_1)} \rightarrow \left(\frac{i}{\hbar}\right)^n x(t_1)x(t_2) \cdots x(t_n),$$

and then if we apply this to the generating functional and set the source to zero at the end, we obtain

$$\langle x(t_1)x(t_2) \cdots x(t_n) \rangle = \frac{1}{Z} \left(\frac{\hbar}{i}\right)^n \frac{\delta}{\delta J(t_n)} \cdots \frac{\delta}{\delta J(t_2)} \frac{\delta}{\delta J(t_1)} Z[J] \Big|_{J=0}.$$

Alternatively, if we expand the generating functional in powers of the source $J(t)$, we can read off all correlation functions of the theory summed over n as coefficients

$$Z[J] = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i}{\hbar}\right)^n \int dt_1 dt_2 \cdots dt_n \langle x(t_1)x(t_2) \cdots x(t_n) \rangle_U J(t_1)J(t_2) \cdots J(t_n),$$

where this n -point correlation function is non normalized (i.e., without the factor $1/Z$, as indicated by the subscript U). Thus our definition of path integrals is given by the normalized n point correlation functions

$$\langle x(t_1)x(t_2) \cdots x(t_n) \rangle = \frac{1}{Z} \int Dx x(t_1)x(t_2) \cdots x(t_n) e^{\frac{i}{\hbar} S[x]},$$

which can be computed by functional differentiation of the generating functional with respect to the source $J(t)$. It is also easier to compute the correlation functions differentiating the generating functional expanded in powers of the source $J(t)$.

3.4.1 | Comparison with Canonical Quantization

It is useful to compare with the corresponding definition of correlation functions given in canonical quantization. We have employed the **Schrödinger picture** to evaluate the transition amplitude. In this picture operators are time-independent, and states acquire the time dependence by the Schrödinger equation. To state the equivalent definition of the n -point correlation function, given the n times which we have to order

$$t_1, t_2, \dots, t_n \xrightarrow{T} t_{T(1)}, t_{T(2)}, \dots, t_{T(n)},$$

respecting the order $t_{T(1)} \leq t_{T(2)} \leq \cdots \leq t_{T(n)}$, implemented using the time ordering permutations T , we can define the **time-ordered n -point correlation function** as

$$\langle x(t_1)x(t_2) \cdots x(t_n) \rangle = \frac{1}{Z} \langle x_f | e^{-\frac{i}{\hbar} \hat{H}(t_f - t_{T(n)})} \hat{x} e^{-\frac{i}{\hbar} \hat{H}(t_{T(n)} - t_{T(n-1)})} \cdots e^{-\frac{i}{\hbar} \hat{H}(t_{T(2)} - t_{T(1)})} \hat{x} e^{-\frac{i}{\hbar} \hat{H}(t_{T(1)} - t_i)} | x_i \rangle,$$

where the normalization factor $Z = \langle x_f | e^{-\frac{i}{\hbar} \hat{H}(t_f - t_i)} | x_i \rangle$ is the transition amplitude. The time ordering is necessary because operators at different times do not commute in general. One can verify that this definition coincides with the one given in the path integral formalism.

We have to change paradigm to the **Heisenberg picture** to see the equivalence more clearly. In this picture, states are time-independent, and operators acquire the time dependence through the Heisenberg equation of motion

$$i\hbar \frac{d}{dt} \hat{O}_H(t) = [\hat{O}_H(t), \hat{H}], \quad \Rightarrow \quad \hat{O}_H(t) = e^{\frac{i}{\hbar} \hat{H}t} \hat{O} e^{-\frac{i}{\hbar} \hat{H}t},$$

for a time independent hamiltonian \hat{H} . In particular, the position operator in the Heisenberg picture is given by

$$\hat{x}_H(t) = e^{\frac{i}{\hbar} \hat{H} t} \hat{x} e^{-\frac{i}{\hbar} \hat{H} t}, \quad \hat{x}_H(t) |x, t\rangle = x |x, t\rangle.$$

Then, the n-point correlation function can be rewritten as

$$\langle x(t_1)x(t_2)\cdots x(t_n) \rangle = \frac{1}{Z} \langle x_f, t_f | T [\hat{x}_H(t_1)\hat{x}_H(t_2)\cdots\hat{x}_H(t_n)] |x_i, t_i\rangle,$$

where T is the time-ordering operator that rearranges the operators in order of increasing time arguments from right to left. This expression is evidently equivalent to the previous one, and coincides with the path integral definition of the n-point correlation function.

The simplest boundary conditions to consider for correlation functions are given by setting the initial and final states equal to states at infinite past and future times, i.e., $|x_i, t_i\rangle = |x_i, -\infty\rangle$ and $|x_f, t_f\rangle = |x_f, +\infty\rangle$. In this case, one usually assumes that the system is in its ground state at $t = -\infty$, and that the initial and final states coincide with the ground state $|0\rangle$ of the system. In the Schrödinger picture we were more general, since the boundary states were arbitrary position eigenstates computed in the integral.

3.4.2 | Digression on Gaussian Integrals

Gaussian integrals are integrals of exponential functions with quadratic exponents. They are very important in physics, as they appear in the evaluation of path integrals for free theories, and in perturbation theory around free theories. Here we review some basic results on gaussian integrals that will be useful in the following.

The simplest gaussian integral is the one-dimensional integral

$$\int_{-\infty}^{+\infty} \frac{d\phi}{(2\pi)^{\frac{1}{2}}} e^{-\frac{1}{2}K\phi^2} = \frac{1}{\sqrt{K}}, \quad \text{for } K \in \mathbb{R}^+.$$

If we include a linear term in the exponent, we can complete the square writing $-\frac{1}{2}K\phi^2 + J\phi = -\frac{1}{2}K(\phi - \frac{J}{K})^2 + \frac{J^2}{2K}$ and changing the measure $\phi \rightarrow \phi' = \phi - \frac{J}{K}$ to obtain

$$\int_{-\infty}^{+\infty} \frac{d\phi}{(2\pi)^{\frac{1}{2}}} e^{-\frac{1}{2}K\phi^2 + J\phi} = \frac{1}{\sqrt{K}} e^{\frac{J^2}{2K}}, \quad \text{for } K \in \mathbb{R}^+.$$

We used the letters K and J to indicate a “kinetic” term and a “source”, in analogy with the notation used in path integrals. The integral can be generalized to n dimensions as

$$\int \frac{d^n\phi}{(2\pi)^{\frac{n}{2}}} e^{-\frac{1}{2}\phi^i K_{ij}\phi^j} = \det(K_{ij})^{-\frac{1}{2}}$$

and if we include a linear term in the exponent, we have

$$\int \frac{d^n\phi}{(2\pi)^{\frac{n}{2}}} e^{-\frac{1}{2}\phi^i K_{ij}\phi^j + J_i\phi^i} = \det(K_{ij})^{-\frac{1}{2}} e^{\frac{1}{2} J_i (K^{-1})^{ij} J_j}, \quad (3.4.4)$$

where K_{ij} is a symmetric² positive definite matrix, so it is diagonalizable with positive eigenvalues, and $(K^{-1})^{ij} = G^{ij}$ is its inverse. Repeated indices are summed over from 1 to n (Einstein summation convention).

²Since $\phi^i\phi^j$ is also symmetric in $i \leftrightarrow j$.

The first integral is immediate if K_{ij} is diagonal and valid in full generality since K_{ij} is diagonalizable by an orthogonal transformation, which leaves the measure invariant. The last integral is obtained again by square completion. These gaussian integrals are suitable for euclidean path integrals. Moreover, in a hypercondensed notation (to be explained shortly), path integrals look very much like ordinary integrals. Of course, the definition of determinants for infinite dimensional matrices is delicate and requires a regularization procedure.

By analytical extension, one obtains gaussian integrals suitable for quantum mechanics

$$\int \frac{d^n \phi}{(-2\pi i)^{\frac{n}{2}}} e^{\frac{i}{2}\phi^i K_{ij} \phi^j + i J_i \phi^i} = \det(K_{ij})^{-\frac{1}{2}} e^{-\frac{i}{2} J_i G^{ij} J_j}, \quad \text{for } \text{Im}(K_{ij}) > 0, \quad (3.4.5)$$

where the condition on the imaginary part of K_{ij} ensures convergence of the integral (and again $K_{ij} G^{jl} = \delta_i^l$). This condition is usually satisfied in physical applications by adding a small imaginary part to the kinetic term, known as “ $i\epsilon$ prescription” or “**Feynman prescription**”: we replace

$$K_{ij} \rightarrow K_{ij} + i\epsilon \delta_{ij}$$

with $\epsilon > 0$ infinitesimal, which ensures a gaussian damping for $|\phi| \rightarrow \infty$:

$$e^{i\phi^i K_{ij} \phi^j} \rightarrow e^{i\phi^i (K_{ij} + i\epsilon \delta_{ij}) \phi^j} = e^{i\phi^i K_{ij} \phi^j} e^{-\epsilon |\phi|^2} \xrightarrow[|\phi| \rightarrow \infty]{} 0.$$

In a hypercondensed notation, to be explained shortly, these formulae give the formal solution of path integrals of free theories (meaning theories with quadratic actions, in this context) without gauge invariances, in either quantum mechanics or quantum field theory. Gauge invariance would produce a vanishing $\det(K_{ij})$, and one must apply a gauge fixing procedure to obtain a finite answer.

3.4.3 | Hypercondensed Notation and Generating Functionals

To proceed swiftly, it is useful to introduce a hypercondensed notation. It allows us to treat path integrals, including those for field theories, formally as ordinary integrals. The hypercondensed notation is defined by lumping together discrete and continuous indices into a single index, so that a variable ϕ_i can be used as a shorthand notation for the position $x(t)$ of the particle, identifying

$$x(t) \rightarrow \phi^i \implies \begin{cases} x \rightarrow \phi, \\ t \rightarrow i. \end{cases}$$

Similarly, for fields, as the vector quadripotential $A_\mu(x^\nu)$, the hypercondensed notation is obtained by denoting

$$A_\mu(x^\nu) \rightarrow \phi^i \implies \begin{cases} A_\mu \rightarrow \phi, \\ \mu, x^\nu \rightarrow i. \end{cases}$$

where now the index i contains a discrete part (the discrete index $\mu = 0, 1, 2, 3$) and a continuous part (the spacetime coordinates $x^\nu = (x^0, x^1, x^2, x^3) \in \mathbb{R}^4$). Indices may be lowered and raised with a metric, so that one could also write $\phi^i \phi_i = \phi^i g_{ij} \phi^j$, as in the following examples:

$$\begin{aligned} \phi_i \phi^i &= \int dt x(t) x(t) = \int dt \int dt' x(t) \delta(t - t') x(t'), \\ \phi_i \phi^i &= \int d^4 x A_\mu(x) A^\mu(x) = \int d^4 x d^4 y A_\mu(x) \eta^{\mu\nu} \delta^4(x - y) A_\nu(y), \end{aligned}$$

where in the last step we have explicitated the presence of a metric, given by the identity matrix in many cases, though one may consider more general situations (as we did in the second case). Repeated indices are understood to be summed over (the Einstein summation convention). In the first case, the summation includes an integration over time, while in the second case it includes a summation over the discrete index μ and an integration over spacetime.

One must pay attention to simple-looking expressions, as they include integrations or infinite sums, and might not converge. With such a notation at hand, we are ready to review quickly the definition of correlation functions, introduce generating functionals, and present gaussian path integration formulae. We will also describe the Wick's theorem, which gives a simple way of computing all correlation functions in a free theory in terms of the 2-point function only (the propagator).

The path integrals in (3.3.1), reported here for convenience

$$A = \int Dx(t) e^{\frac{i}{\hbar} S[x(t)]} = \lim_{N \rightarrow \infty} \int \left(\prod_{k=1}^{N-1} dx_k \right) \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} e^{\frac{i\epsilon}{\hbar} \sum_{k=1}^N \left[\frac{m}{2} \frac{(x_k - x_{k-1})^2}{\epsilon^2} - V(x_{k-1}) \right]} = Z,$$

after denoting the variables in a hypercondensed notation by ϕ^i , can be written as

$$Z = \int D\phi e^{\frac{i}{\hbar} S[\phi]} \quad (3.4.6)$$

and the n point correlation function (in eq. (3.4.1)) reads

$$\langle \phi^{i_1} \phi^{i_2} \cdots \phi^{i_n} \rangle = \frac{1}{Z[0]} \int D\phi \phi^{i_1} \phi^{i_2} \cdots \phi^{i_n} e^{\frac{i}{\hbar} S[\phi]}. \quad (3.4.7)$$

The generating functional can be written as

$$Z[J] = \int D\phi e^{\frac{i}{\hbar} S[\phi] + J_i \phi^i}, \quad (3.4.8)$$

and generates all correlation functions by differentiation (in hypercondensed notation, functional derivatives look like usual derivatives, but we keep using the symbol δ of functional derivative)

$$\langle \phi^{i_1} \phi^{i_2} \cdots \phi^{i_n} \rangle = \frac{1}{Z} \left(\frac{\hbar}{i} \right)^n \frac{\delta}{\delta J_{i_n}} \cdots \frac{\delta}{\delta J_{i_2}} \frac{\delta}{\delta J_{i_1}} Z[J] \Big|_{J=0}.$$

We can now define the **generating functional of connected correlation functions** $W[J]$ by

$$Z[J] = e^{\frac{i}{\hbar} W[J]}, \quad \Rightarrow \quad W[J] = -i\hbar \ln(Z[J]). \quad (3.4.9)$$

One can prove that it generates “connected” correlation functions by differentiation

$$\langle \phi^{i_1} \phi^{i_2} \cdots \phi^{i_n} \rangle_c = \left(\frac{\hbar}{i} \right)^{n-1} \frac{\delta}{\delta J_{i_n}} \cdots \frac{\delta}{\delta J_{i_2}} \frac{\delta}{\delta J_{i_1}} W[J] \Big|_{J=0}.$$

We will check this statement and its meaning in the free theories (next section). It is also useful to define the **effective action** $\Gamma[\varphi]$ as the Legendre transform of $W[J]$ (analogous to the Legendre transform that relates the Lagrangian and Hamiltonian formalisms in classical mechanics)

$$\Gamma[\varphi] = \min_J \{W[J] - J_i \varphi^i\}, \quad \text{where } \varphi^i = \frac{\delta W[J]}{\delta J_i}, \quad (3.4.10)$$

which is considered as a classical action that includes all quantum corrections. It generates the so-called one-particle irreducible (1PI) correlation functions, though we will not investigate further this particular property. The minimum in J is obtained at $\varphi^i = \frac{\delta W[J]}{\delta J_i}$, furnishing a relation $\varphi^i = \varphi^i(J)$ that must be inverted to obtain $J_i = J_i(\varphi)$ and inserted back into the right-hand side of (3.4.10) to obtain the effective action indeed as a functional of the variable φ^i only.

The last two functionals, $W[J]$ and $\Gamma[\varphi]$, find their main applications in quantum field theory. Equivalent definitions can be given for euclidean path integrals.

3.4.4 | Free Theories

It is useful to study free theories, here meaning theories that have a quadratic action. They provide a simple application of the previous formulae, giving at the same time additional intuition. A free theory is described by a quadratic action

$$S[\phi] = -\frac{1}{2}\phi^i K_{ij} \phi^j,$$

which produces the linear equations of motion $K_{ij} \phi^j = 0$:

$$\begin{aligned} \delta S[\phi] &= -\frac{1}{2}\delta(\phi^i K_{ij} \phi^j) = -\frac{1}{2}(\delta\phi^i K_{ij} \phi^j + \phi^i K_{ij} \delta\phi^j) \\ &= -\frac{1}{2}(\delta\phi^i K_{ij} \phi^j + \delta\phi^j K_{ji} \phi^i) = -\delta\phi^i K_{ij} \phi^j = 0 \quad \forall \delta\phi^i \\ \implies \frac{\delta S[\phi]}{\delta\phi^i} &= K_{ij} \phi^j = 0, \end{aligned}$$

since $K_{ij} = K_{ji}$ is symmetric and the variation $\delta\phi^i$ is arbitrary. We assume K_{ij} invertible, which translates to the fact that there are no gauge symmetries in our model.

As an example, consider the harmonic oscillator (with $m = 1$ for simplicity), whose action is

$$\begin{aligned} S[x] &= \int_{-\infty}^{\infty} dt \left(\frac{\dot{x}^2}{2} - \frac{\omega^2 x^2}{2} \right) = -\frac{1}{2} \int_{-\infty}^{\infty} dt x(t) \left(\frac{d^2}{dt^2} + \omega^2 \right) x(t) \\ &= -\frac{1}{2} \int dt \int dt' x(t) \left[\left(\frac{d^2}{dt^2} + \omega^2 \right) \delta(t - t') \right] x(t') \\ &= -\frac{1}{2} \int dt dt' x(t) K(t, t') x(t'), \end{aligned}$$

where we integrated by parts in the first step and introduced the Dirac delta function $\delta(t - t')$ to expose the ‘‘kinetic matrix’’ $K(t, t') = \left(\frac{d^2}{dt^2} + \omega^2 \right) \delta(t - t')$, thus we can write the action in hypercondensed notation as

$$S[\phi] = -\frac{1}{2}\phi^i K_{ij} \phi^j,$$

general for any free theory.

Denoting $D\phi = \frac{d^n \phi}{(-i2\pi)^{n/2}}$, setting $\hbar = 1$ for simplicity, and using the gaussian result in eq. (3.4.5), one calculates formally the path integral with sources

$$Z[J] = \int D\phi e^{\frac{i}{2}\phi^i K_{ij} \phi^j + i J_i \phi^i} = \det(K_{ij})^{-\frac{1}{2}} e^{-\frac{i}{2} \int J_i G^{ij} J_j}, \quad (3.4.11)$$

where the inverse kinetic matrix $G^{ij} = (K^{-1})^{ij}$ is the **Green’s function** of the theory, satisfying

$$K_{ij} G^{jk} = \delta_i^k.$$

We can now compute all correlation functions by differentiating with respect to the source J_i

$$\langle \phi^{i_1} \phi^{i_2} \dots \phi^{i_n} \rangle = \frac{1}{Z} (-i)^n \frac{\delta}{\delta J_{i_n}} \dots \frac{\delta}{\delta J_{i_2}} \frac{\delta}{\delta J_{i_1}} Z[J] \Big|_{J=0},$$

obtaining for the first few correlation functions (zero, one, and two-point functions)

$$\begin{aligned} \langle 1 \rangle &= 1, \\ \langle \phi^{i_1} \rangle &= 0, \\ \langle \phi^{i_1} \phi^{i_2} \rangle &= -i G^{i_1 i_2}. \end{aligned}$$

The first one is a consequence of the normalization, the second one reflects the symmetry $\phi^i \rightarrow -\phi^i$, and the third one is known as the propagator, which we find proportional to the inverse of the kinetic matrix K_{ij} . We did not pay attention to normalization factors since they simplify with $\frac{1}{Z}$ in this case.

Continuing with the calculation of higher point functions, we see that all correlation functions with an odd number of points vanish, again a consequence of the symmetry $\phi^i \rightarrow -\phi^i$. Those ones with an even number n factorize into a sum of $(n-1)!!$ terms, given by the product of the 2-point functions which connect any two points in all possible ways. This fact is known as the **Wick's theorem**.

$$\begin{aligned} \langle \phi^{i_1} \phi^{i_2} \phi^{i_3} \rangle &= 0, \\ \langle \phi^{i_1} \phi^{i_2} \phi^{i_3} \phi^{i_4} \rangle &= \left(\frac{\hbar}{1}\right)^4 \left(\frac{i}{\hbar}\right)^2 (G^{i_1 i_2} G^{i_3 i_4} + G^{i_1 i_3} G^{i_2 i_4} + G^{i_1 i_4} G^{i_2 i_3}) \\ &= \langle \phi^{i_1} \phi^{i_2} \rangle \langle \phi^{i_3} \phi^{i_4} \rangle + \langle \phi^{i_1} \phi^{i_3} \rangle \langle \phi^{i_2} \phi^{i_4} \rangle + \langle \phi^{i_1} \phi^{i_4} \rangle \langle \phi^{i_2} \phi^{i_3} \rangle, \end{aligned}$$

where one recognizes a general pattern to derive all higher point correlation functions for free theories. The 4-point function is given as the sum of the products of all possible pairings of 2-point functions, and is called disconnected since it factorizes into products of lower order correlation functions. This result is summarized in the following theorem.

Theorem 3.1 (Wick's theorem). *In a free theory with quadratic action $S[\phi] = -\frac{1}{2}\phi^i K_{ij} \phi^j$, all n -point correlation functions with odd n vanish, while those with even n factorize into a sum of $(n-1)!!$ terms, given by the product of the 2-point functions which connect any two points in all possible ways:*

$$\langle \phi^{i_1} \phi^{i_2} \cdots \phi^{i_n} \rangle = \sum_{\{(a,b)\}} \prod_{(a,b)} \langle \phi^{i_a} \phi^{i_b} \rangle,$$

where the sum runs over all possible ways to pair the indices i_1, i_2, \dots, i_n into pairs (a, b) .

The **generating functional of connected correlation functions** $W[J]$ is obtained from eq. (3.4.11) using the definition in eq. (3.4.9):

$$W[J] = \frac{1}{2} J_i G^{ij} J_j - \Lambda, \quad \Lambda = -\frac{i}{2} \ln(\det(K_{ij})) = -\frac{i}{2} \text{Tr}(\ln(K_{ij})),$$

where the constant Λ is an infinite constant that can be regularized and interpreted as the vacuum energy of the free theory. One verifies that it generates a 2-point correlation functions that is connected from³

$$\langle \phi^{i_1} \phi^{i_2} \cdots \phi^{i_n} \rangle_c = (-i)^n \frac{\delta}{\delta J_{i_n}} \cdots \frac{\delta}{\delta J_{i_2}} \frac{\delta}{\delta J_{i_1}} i W[J] \Big|_{J=0}.$$

It is time to start associating Feynman diagrams to these correlation functions. The 2-point connected correlation function is represented by a line connecting two points (it connects them in the spacetime)

$$\langle \phi^{i_1} \phi^{i_2} \rangle_c = -i G^{i_1 i_2} \longrightarrow \bullet \text{---} \bullet,$$

and that is why it is called the propagator. Higher point connected correlation functions vanish in a free theory, so there are no other Feynman rules to introduce at this stage. In interacting theories, vertices will appear, connecting more than two points. For example, the four-point correlation function in an interacting theory would be represented by the sum of the three diagrams

$$\langle \phi^{i_1} \phi^{i_2} \phi^{i_3} \phi^{i_4} \rangle_c \longrightarrow \bullet \text{---} \bullet + \bullet \text{---} \bullet + \bullet \times \bullet,$$

³It also generates a 0-point function, given by $-\Lambda$, that can be shown to be connected as well.

which correspond to the three possible ways of connecting four points with two propagators; that is why it is said to be non-connected. We will see more Feynman rules when treating interacting theories.

Let us also calculate the **effective action**. The minimum in J of eq. (3.4.10) is achieved for

$$\varphi^i = \frac{\delta W}{\delta J_i} = G^{ij} J_j \implies J_i = K_{ij} \varphi^j,$$

so that the effective action reads

$$\Gamma[\varphi] = W[J] - J_i \varphi^i = -\frac{1}{2} \varphi^i K_{ij} \varphi^j + \Lambda, \quad (3.4.12)$$

We see that for a free theory, the effective action $\Gamma[\phi]$ reproduces the original action $S[\phi]$ with an additive constant $-\Lambda$, which could be interpreted as minus a vacuum energy, which is of quantum origin. The latter can be disregarded if gravitational interactions are neglected. In general, the effective action is considered as a classical action that contains the effects of quantization in its couplings (and thus, the effective actions should not be quantized again). Reinserting \hbar by a simple rescaling, we collect here the formulae for a free (gaussian) theory

$$\begin{aligned} S[\phi] &= -\frac{1}{2} \phi^i K_{ij} \phi^j, \\ Z[J] &= \det(K_{ij})^{-\frac{1}{2}} e^{-\frac{i}{2\hbar} J_i G^{ij} J_j}, \\ W[J] &= \frac{1}{2} J_i G^{ij} J_j - \hbar \Lambda, \quad \Lambda = -\frac{i}{2} \ln(\det(K_{ij})), \\ \Gamma[\phi] &= -\frac{1}{2} \varphi^i K_{ij} \varphi^j - \hbar \Lambda = S[\varphi] + \hbar [\text{ corrections }], \end{aligned}$$

with a propagator given by the two point correlation function

$$\langle \phi^i \phi^j \rangle = -i\hbar (K^{-1})^{ij} = -i\hbar G^{ij}.$$

Harmonic Oscillator

Let us work out in more explicit terms the case of a harmonic oscillator with unit mass and frequency ω . The action is

$$S[x] = \int_{-\infty}^{\infty} dt \left(\frac{\dot{x}^2}{2} - \frac{\omega^2 x^2}{2} \right), \quad Z[J] = \int Dx e^{iS[x] + i \int dt J(t)x(t)},$$

where we have computed the path integral to obtain $Z[J]$. We repeat the deduction without using the hypercondensed notation. We consider an infinite propagation time and a transition amplitude between the ground state, classically achieved for $x = 0$. The action in the exponent can be manipulated with an integration by parts without producing boundary terms (imposing that $x(t)$ is in its classical vacuum at initial and final times gives a vanishing boundary term, another justification will be given later on when treating the euclidean version of the problem). Thus, the action takes the form we already computed

$$S[x] = -\frac{1}{2} \int_{-\infty}^{\infty} dt x(t) \left(\frac{d^2}{dt^2} + \omega^2 \right) \delta(t - t') x(t) = \int \int dt dt' x(t) K(t, t') x(t'),$$

where $K(t, t') = \left(\frac{d^2}{dt^2} + \omega^2 \right) \delta(t - t')$ is the differential “kinetic” operator of the harmonic oscillator. We can compute the two point correlation function (the propagator) by

$$\langle x(t) x(t') \rangle = \frac{1}{Z} \left(\frac{\hbar}{i} \right)^2 \frac{\delta}{\delta J(t')} \frac{\delta}{\delta J(t)} Z[J] \Big|_{J=0} = -i\hbar (K^{-1})(t, t') = -i\hbar G(t, t'),$$

where the inverse of K is recognized as the Green function of the differential operator, and it can be conveniently written in a Fourier transform

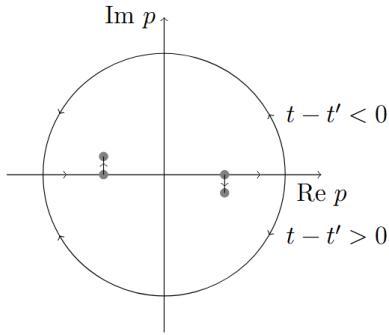
$$G(t, t') = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{e^{-ip(t-t')}}{-p^2 + \omega^2},$$

which can be verified to satisfy the equation

$$\int dt'' K(t, t'') G(t'', t') = \delta(t - t').$$

that in a hypercondensed notation would have been written as $K_{il} G^{lj} = \delta_i^j$. Adding the Feynman $i\epsilon$ prescription⁴ for specifying how to integrate around the poles $p = \pm\omega$, one computes

$$G(t, t') = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{e^{-ip(t-t')}}{-p^2 + \omega^2 - i\epsilon} = -\frac{i}{2\omega} [\theta(t - t') e^{-i\omega(t-t')} + \theta(t' - t) e^{i\omega(t-t')}] = -\frac{i}{2\omega} e^{-i\omega|t-t'|}.$$



The Feynman prescription sends positive frequencies forward in time and negative frequencies backward in time, corresponding to the physical interpretation of particles and antiparticles with positive energies and always propagating forward in time.

Having computed the Green's function, we can write the generating functional in (3.4.11) we can now complete the square (and reducing to the form in (3.4.5)) to obtain an explicit expression for $Z[J]$, which will let us compute all correlation functions of the harmonic oscillator.

Thus defining $\tilde{x}(t) = x(t) - \int dt' G(t, t') J(t')$ to complete the square in the exponent of the path integral, we obtain

$$\begin{aligned} Z[J] &= \int Dx e^{iS[x] + i \int dt J(t)x(t)} = \int Dx e^{-\frac{i}{2} \int \int dt dt' (x(t)K(t,t')x(t') + 2J(t)\delta(t,t')x(t'))} \\ &= \int D\tilde{x} \exp \left(-\frac{i}{\hbar} \int \int dt dt' \tilde{x}(t)K(t,t')\tilde{x}(t') \right) \left[\exp \left(\frac{i}{2\hbar} \int \int dt dt' J(t)G(t,t')J(t') \right) \right] \\ &= Z[0] \exp \left(\frac{i}{2\hbar} \int \int dt dt' J(t)G(t,t')J(t') \right), \end{aligned}$$

where $Z[0] = \int D\tilde{x} e^{\frac{i}{\hbar} S[\tilde{x}]}$ is a normalization constant. We can now compute all correlation functions by differentiating with respect to the source $J(t)$; for example, the two-point function reads

$$\begin{aligned} \langle x(t)x(t') \rangle &= \frac{1}{Z[0]} \left(\frac{\hbar}{i} \right)^2 \frac{\delta}{\delta J(t')} \frac{\delta}{\delta J(t)} Z[J] \Big|_{J=0} \\ &= \left(\frac{\hbar}{i} \right)^2 \frac{\delta}{\delta J(t')} \frac{\delta}{\delta J(t)} \left[\exp \left(\frac{i}{2\hbar} \int \int dt_1 dt_2 J(t_1)G(t_1, t_2)J(t_2) \right) \right] \Big|_{J=0} \\ &= -i\hbar G(t, t') = \frac{\hbar}{2\omega} e^{-i\omega|t-t'|}. \end{aligned}$$

⁴Mathematically, it is seen to arise from requiring that the path integral has a small damping factor $e^{-\frac{i}{\hbar} \int dt x^2(t)}$, obtained by the shift $\omega^2 \rightarrow \omega^2 - i\epsilon$ with $\epsilon \rightarrow 0^+$. Recall the comments made under eq. (3.4.5)

Klein Gordon Field

The quantum field theory of a free Klein-Gordon scalar field can be viewed as a higher-dimensional analog of the harmonic oscillator. The action of a real scalar field $\phi(x)$ is given by

$$S[\phi] = \int d^4x \left(-\frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{1}{2} m^2 \phi^2 \right),$$

where m is the mass of the scalar particle. Integrating by parts and neglecting boundary terms, the action can be rewritten as

$$S[\phi] = -\frac{1}{2} \int d^4x \phi(x) (\square + m^2) \phi(x) = -\frac{1}{2} \int d^4x d^4y \phi(x) K(x, y) \phi(y),$$

where $K(x, y) = (\square + m^2) \delta^4(x-y)$ is the kinetic operator of the Klein-Gordon field, and $\square = \partial_\mu \partial^\mu$ is the d'Alembertian operator.

We can compute the path integral with sources

$$Z[J] = \int D\phi e^{iS[\phi] + i \int d^4x J(x) \phi(x)} = N e^{\frac{i}{2} \int d^4x d^4y J(x) G(x, y) J(y)},$$

where $N = \det(K_{ij})^{-\frac{1}{2}}$ is a normalization constant. The inverse of the kinetic operator K is the Green's function $G(x, y)$ of the Klein-Gordon operator.

We are in $(3+1)$ spacetime dimensions, but if we imagine to be in a $(0+1)$ spacetime dimension, meaning that there is only one time coordinate and no spatial coordinates, the Klein-Gordon field theory reduces to the harmonic oscillator treated previously. Indeed, in this case the action reduces to

$$S[\phi] = \int dt \left(\frac{1}{2} \dot{\phi}^2 - \frac{1}{2} m^2 \phi^2 \right),$$

which is the action of a harmonic oscillator with frequency $\omega = m$ in hypercondensed notation.

If we complete the square in the exponential of the path integral (with the idea to use gaussian integrals to obtain the generator of correlation functions), we obtain

$$\int d^4z K(x, z) G(z, y) = \delta^4(x-y),$$

where we have indeed $(\square_x + m^2) G(x-y) = \delta^4(x-y)$ as the usual equation for the Green's function of the Klein-Gordon operator.

We can now compute the two-point correlation function (the propagator) by

$$\langle \phi(x) \phi(y) \rangle = \frac{1}{Z[0]} (-i)^2 \frac{\delta}{\delta J(y)} \frac{\delta}{\delta J(x)} Z[J] \Big|_{J=0} = -iG(x, y),$$

where the Green's function can be conveniently written in a Fourier transform

$$G(x, y) = \int \frac{d^4p}{(2\pi)^4} \frac{e^{-ip_\mu(x^\mu - y^\mu)}}{p^2 + m^2 - i\epsilon},$$

where $d^4p = dp_0 d^3p$ and $p^2 = p_\mu p^\mu = -(p_0)^2 + \mathbf{p}^2$. There are poles corresponding to the solutions of the mass shell condition, $p_0 = \sqrt{\mathbf{p}^2 + m^2}$ (positive energies) and $p_0 = -\sqrt{\mathbf{p}^2 + m^2}$ (negative energies). The Feynman $i\epsilon$ prescription sends positive energies forward in time and negative energies backward in time. It corresponds to the physical interpretation of particles and

antiparticles with positive energies and always propagating forward in time (thus propagating negative energies backward in time). Setting $E_p = \sqrt{\mathbf{p}^2 + m^2}$ one finds

$$\begin{aligned}\langle \phi(x)\phi(y) \rangle &= -iG(x-y) = -i \int \frac{d^4 p}{(2\pi)^4} \frac{e^{-ip_\mu(x^\mu-y^\mu)}}{p^2 + m^2 - i\epsilon} \\ &= i \int \frac{d^3 \mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \left[\frac{dp^0}{2\pi} \frac{e^{-ip^0(x^0-y^0)}}{(p^0 - E_p + i\epsilon')(p^0 + E_p - i\epsilon')} \right] \\ &= \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{2E_p} \left[\theta(x^0 - y^0)e^{-iE_p(x^0-y^0)} + \theta(y^0 - x^0)e^{-iE_p(y^0-x^0)} \right] \\ &= \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{2E_p} e^{-iE_p|x^0-y^0|}.\end{aligned}$$

Here again the Feynman prescription is crucial to obtain the correct time-ordering in the two-point correlation function as $\epsilon \sim \epsilon' \rightarrow 0$, and by comparing this result with the harmonic oscillator case one sees that the Klein-Gordon field theory is indeed an infinite collection of harmonic oscillators, one for each momentum mode \mathbf{p} , with frequency $\omega = E_p = \sqrt{\mathbf{p}^2 + m^2}$.

Harmonic Oscillator in Euclidean Time

The statistical partition function in the limit of vanishing temperature ($\Theta \rightarrow 0$), corresponding to an infinite euclidean propagation time ($\beta = \frac{1}{k\Theta} \rightarrow \infty$), takes a simple form

$$Z_E = \text{Tr } e^{-\beta \hat{H}} = \sum_{n=0}^{\infty} \langle n | e^{-\beta \hat{H}} | n \rangle = e^{-\beta E_0} + \text{subleading terms as } \beta \rightarrow \infty.$$

This is true even in the presence of a source J if one assumes that the source is nonvanishing for a finite interval of time only: the remaining infinite time is sufficient to project the operator $e^{-\beta \hat{H}}$ onto the ground state. This allows to rewrite the generating functional $Z[J]$ in the euclidean case in a simpler way, justifying the dropping of boundary terms in the integration by parts in the classical action. The statistical partition function is obtained by using periodic boundary conditions, and for large β one gets the projection onto the ground state

$$Z_E[J] = \int Dx e^{-S_E[x] + \int_{-\beta/2}^{\beta/2} d\tau J(\tau)x(\tau)} \xrightarrow{\beta \rightarrow \infty} \lim_{\beta \rightarrow \infty} e^{-\beta E_0(J)},$$

where the euclidean action is

$$S_E[x] = \int_{-\infty}^{\infty} d\tau \left(\frac{1}{2} \left(\frac{dx}{d\tau} \right)^2 + \frac{1}{2} \omega^2 x^2 \right).$$

where $E_0(J)$ is the ground state energy in the presence of the source J . We can now repeat the previous calculation in the present context. We integrate by parts without encountering boundary terms, as the paths are closed, and the path integral is strictly gaussian

$$\begin{aligned}Z_E[J] &= \int_{PBC} Dx e^{-\frac{1}{2} \int d\tau x(\tau) \left(-\frac{d^2}{d\tau^2} + \omega^2 \right) x(\tau) + \int d\tau J(\tau)x(\tau)} \\ &= Z_E[0] \exp \left(\frac{1}{2} \int \int d\tau d\tau' J(\tau) G_E(\tau - \tau') J(\tau') \right),\end{aligned}$$

from which we get the Green's function in euclidean time, which can be computed from the Fourier transform of the inverse kinetic operator

$$G_E(\tau - \tau') = \int_{-\infty}^{\infty} \frac{dp_E}{2\pi} \frac{e^{-ip_E(\tau-\tau')}}{p_E^2 + \omega^2} = \frac{1}{2\omega} e^{-\omega|\tau-\tau'|}. \quad (3.4.13)$$

Using it for the computation of the two-point correlation function

$$\langle x(\tau)x(\tau') \rangle = G_E(\tau - \tau') = \int \frac{dp_E}{2\pi} \frac{e^{-ip_E(\tau-\tau')}}{p_E^2 + \omega^2}$$

We now verify again the relation between quantum mechanics and statistical mechanics, realized by the analytic continuation in time, the Wick rotation. The inverse Wick rotation implies $\tau = t_E \rightarrow it_M = it$ and $p_E \rightarrow -ip_M = -ip$, with the latter arising from the requirement that the correct Fourier transform is kept during the analytic deformation. Thus the two-point correlation function becomes

$$\langle x(\tau)x(\tau') \rangle \rightarrow \langle x(t)x(t') \rangle = -iG_M(t - t') = -i \int \frac{dp_M}{2\pi} \frac{e^{-ip_M(t-t')}}{-p_M^2 + \omega^2},$$

which is the Feynman propagator of the harmonic oscillator computed previously

$$\frac{1}{2\omega} e^{-\omega|\tau-\tau'|} \rightarrow -\frac{i}{2\omega} e^{-i\omega|t-t'|}.$$

We recognize that the Feynman propagator is the unique analytical extension of the euclidean two-point function. All other Green functions, such as the retarded or advanced ones, correspond to different boundary conditions implemented with different prescriptions for performing the integration around the poles. They cannot be Wick rotated, as one would encounter poles in the analytic continuation.

This is the end for free path integrals and bosonic theories. We can now proceed to interacting theories with perturbative expansions, and later on to fermionic theories.

3.5 | Perturbative Expansion

The free theory corresponds to a gaussian path integral, which is exactly solvable. With interactions, one is often unable to compute exactly the path integral, and one must resort to some sort of approximation. The simplest one is the perturbative expansion around a free theory, which consists in expanding the solution in power series of the coupling constants that parametrize the interactions. If the couplings are small enough, the perturbative expansion might give a good approximation of the solution.

We describe the perturbative expansion taking as a guiding example the **anharmonic oscillator**

$$S[x] = \int dt \left(\frac{m}{2} \dot{x}^2 - \frac{m\omega^2}{2} x^2 - \frac{g}{3!} x^3 - \frac{\lambda}{4!} x^4 \right),$$

where if the coupling constants g and λ vanish, the theory is exactly solvable. Thus, one may try to include perturbatively the corrections that arise when g and λ are small enough. It is convenient to split the action as the sum of two terms, a free part S_0 which is exactly solvable and an interacting part S_{int}

$$\begin{aligned} S[x] &= S_0[x] + S_{int}[x], \\ S_0[x] &= \int dt \left(\frac{m}{2} \dot{x}^2 - \frac{m\omega^2}{2} x^2 \right), \\ S_{int}[x] &= \int dt \left(-\frac{g}{3!} x^3 - \frac{\lambda}{4!} x^4 \right). \end{aligned}$$

The perturbative expansion is easily generated in the path integral setup. Including a source term, one expands in a Taylor series the exponential of the interaction term

$$\begin{aligned} Z[J] &= \int Dx e^{\frac{i}{\hbar} (S[x] + \int dt Jx)} = \int Dx e^{\frac{i}{\hbar} S_{int}[x]} e^{\frac{i}{\hbar} (S_0[x] + \int dt Jx)} \\ &= \int Dx \left[\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i}{\hbar} S_{int}[x] \right)^n \right] e^{\frac{i}{\hbar} (S_0[x] + \int dt Jx)}. \end{aligned}$$

We can keep terms until we are satisfied with the resolution (depending on the entity of g and λ). Written in the last form, one proceeds in computing it term by term with the use of the Wick's theorem. It can be written also in the form

$$Z[J] = \langle e^{\frac{i}{\hbar} S_{int}[x]} \rangle_{U,0,J},$$

where the subscripts $U, 0, J$ denote unnormalized averaging (U) in the free theory (0) with an arbitrary source (J). This expression is sometimes called the "**Dyson formula**". It generates the perturbative expansion which can be depicted with *Feynman diagrams*, as we shall see.

An alternative way of writing the perturbative series is the following one

$$\begin{aligned} Z[J] &= \int Dx e^{\frac{i}{\hbar} S_{int}[x]} e^{\frac{i}{\hbar} (S_0[x] + \int dt Jx)} \\ &= \exp \left(\frac{i}{\hbar} S_{int} \left[\frac{\hbar}{i} \frac{\delta}{\delta J} \right] \right) \int Dx e^{\frac{i}{\hbar} (S_0[x] + \int dt Jx)} = \exp \left(\frac{i}{\hbar} S_{int} \left[\frac{\hbar}{i} \frac{\delta}{\delta J} \right] \right) Z_0[J], \end{aligned}$$

where $Z_0[J]$ is the generating functional of the free theory. This expression is often more convenient to work with, since it reduces the problem to computing functional derivatives of the known free generating functional. It presents the solution as a (quite complicated) differential operator acting on the functional of the free theory $Z_0[J]$. In particular, all vacuum diagrams are generated by

$$Z[0] = \int Dx e^{\frac{i}{\hbar} S[x]} = \exp \left(\frac{i}{\hbar} S_{int} \left[\frac{\hbar}{i} \frac{\delta}{\delta J} \right] \right) Z_0[J] \Big|_{J=0}.$$

The perturbative expansion can be represented using Feynman diagrams. These are constructed by expanding the interaction term in the path integral and applying Wick's theorem to compute the correlation functions within the free theory. In these diagrams, vertices, represented as dots, correspond to the interaction potentials and involve a coupling constant multiplied by quantum variables. These variables are paired in all possible combinations using free propagators, which are graphically depicted as lines.

This construction is illustrated below through the example of vacuum diagrams for the anharmonic oscillator.

3.5.1 | Vacuum Diagrams

As an example, we compute perturbatively the corrections to the ground state energy of the harmonic oscillator due to the **anharmonic potential** terms. It is often the case that one computes using the euclidean version of the theory and performs the inverse Wick rotation at the very end to obtain the final result in minkowskian time.

Thus, let us consider the euclidean generating functional and action for the **anharmonic oscillator**

$$Z_E[J] = \int Dx e^{-\frac{1}{\hbar}(S_E[x] - \int d\tau Jx)},$$

$$S_E[x] = \lim_{\beta \rightarrow \infty} \int_{-\beta/2}^{\beta/2} d\tau \left(\frac{m}{2} \dot{x}^2 + \frac{m\omega^2}{2} x^2 + \frac{g}{3!} x^3 + \frac{\lambda}{4!} x^4 \right).$$

We want to compute corrections to the ground state energy, which can be obtained from the vacuum diagrams, which correspond to $Z_E[0]$. Using the perturbative expansion, we have

$$Z_E[0] = \int Dx e^{-\frac{1}{\hbar} S_E[x]} = \langle 1 \rangle_U = \lim_{\beta \rightarrow \infty} \langle 0 | e^{-\beta \hat{H}} | 0 \rangle = \left\langle e^{-\frac{1}{\hbar} S_{E,int}[x]} \right\rangle_{U,0} = \lim_{\beta \rightarrow \infty} e^{-\beta(E_0^{(0)} + \Delta E_0)},$$

where the exact energy E_0 of the ground state $|0\rangle$ of the anharmonic oscillators differs from the ground state energy of the harmonic oscillator $E_0^{(0)}$ by the term ΔE_0 due to the anharmonic potential (here we have the contributions from interaction terms). The correction ΔE_0 can be computed perturbatively, considering the first non-vanishing corrections to exemplify the perturbative expansion with path integrals and the use of Feynman diagrams.

When we take $\beta \rightarrow \infty$, we are projecting onto the ground state, since we assume that the spectrum of the Hamiltonian is bounded from below. Thus, the euclidean time evolution operator $e^{-\beta \hat{H}}$ suppresses all contributions from excited states exponentially fast as β increases. Then we apply the perturbative expansion in the interaction term (as we did in Minkowskian time in the previous section), which gives us an unnormalized average in the free theory. Now we can recognize that this average corresponds to the vacuum amplitude of the free theory multiplied by corrections due to the interactions.

We can continue the computation for the interaction terms in the correlation function by considering separately the two terms (by setting each one to zero and effectively *turning off* one interaction at a time). Let us look first at the case with $g = 0$ and focus on the first correction in λ for the **quartic interaction**:

$$Z_E[0] = \langle 1 \rangle_U = \langle e^{-S_{E,int}[x]} \rangle_{U,0} = \left\langle \sum_{n=0}^{\infty} \frac{(-S_{E,int}[x])^n}{n!} \right\rangle_{U,0} = \langle 1 \rangle_{U,0} - \frac{\lambda}{4!} \int_{-\beta/2}^{\beta/2} d\tau \langle x^4(\tau) \rangle_{U,0} + \dots$$

$$= \langle 1 \rangle_{U,0} \left[1 - \frac{\lambda}{4!} \int_{-\beta/2}^{\beta/2} d\tau \langle x^4(\tau) \rangle_{U,0} + \dots \right] = \langle 1 \rangle_{U,0} \left[1 - \frac{\lambda}{4!} (3 \times \text{O}) + \dots \right].$$

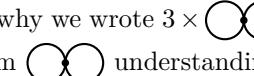
In the last line, we have used Wick contractions to calculate normalized correlation functions in the free theory, and then introduced a graphical representation in terms of **Feynman diagrams**. In this graphical representation, a line denotes a propagator that joins two points in time, while vertices arising from the interactions are denoted by dots. The term we obtained contains just one vertex where four lines can enter or exit, corresponding to the power four of the dynamical variable $x(\tau)$ associated to the interaction under consideration.

Recalling the euclidean propagator calculated in eq. (3.4.13)

$$G_E(\tau - \tau') = \langle x(\tau)x(\tau') \rangle_0 = \frac{1}{2\omega} e^{-\omega|\tau-\tau'|} = \text{---}$$

where this is the **Feynman Line** associated to the two point correlation function; we can compute the value of the previous diagram, considering that we have four fields at the same time τ . Thus, we have to consider all possible Wick contractions, which give three identical contributions (we have $x(\tau)^4$ not $x_1(\tau)x_2(\tau)\dots$ so the fields are identical), each corresponding to a pair of propagators that start and end at the same time τ . Therefore, we have

DIAGRAMS SUM

So that we understand why we wrote $3 \times \text{---}$ in the previous expression. Now, we can compute the value of the diagram  understanding it as a loop with two propagators that start and end at the same time:

$$\text{---} = \int_{-\beta/2}^{\beta/2} d\tau G_E(\tau, \tau)^2 = \int_{-\beta/2}^{\beta/2} d\tau \left(\frac{1}{2\omega} \right)^2 = \frac{\beta}{4\omega^2}.$$

Thus, up to this order (first term) in perturbation theory, we have⁵

$$Z_E[0] = \langle 1 \rangle_{U,0} \left[1 - \frac{\lambda}{4!} \left(3 \times \frac{\beta}{4\omega^2} \right) + \dots \right] = \langle 1 \rangle_{U,0} \exp \left(-\beta \frac{\lambda}{32\omega^2} + \dots \right),$$

so that we can read the correction to the ground state energy due to the quartic interaction

$$\Delta E_0 = \frac{1}{32} \frac{\lambda}{\omega^2}.$$

Similarly, one may consider the case with $g \neq 0$ and $\lambda = 0$. The first non-vanishing correction in the **cubic interaction** arises from:

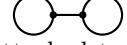
$$\begin{aligned} Z_E[0] &= \langle 1 \rangle_U = \left\langle \left(1 - S_{E,int} + \frac{1}{2} S_{E,int}^2 + \dots \right) \right\rangle_{U,0} \\ &= \langle 1 \rangle_{U,0} + \frac{g}{3!} \int_{-\beta/2}^{\beta/2} d\tau \langle x^3(\tau) \rangle_{U,0} + \frac{g^2}{2(3!)^2} \int_{-\beta/2}^{\beta/2} d\tau \int_{-\beta/2}^{\beta/2} d\tau' \langle x^3(\tau)x^3(\tau') \rangle_{U,0} + \dots \\ &= \langle 1 \rangle_{U,0} \left[1 + 0 + \frac{g^2}{2(3!)^2} \left((3!) \times \text{---} + (3^2) \times \text{---} \right) + \dots \right]. \end{aligned}$$

The first correction vanishes because there is no way to contract three fields at the same time in pairs (from Wick's theorem). The second correction is represented by a six-point correlation function, which gives two types of contributions: we have three fields at time τ and three fields at time τ' , which can be contracted in two different ways.

DIAGRAMS SUM

⁵This computation relies on the boundaries conditions we have set: with $\beta \rightarrow \infty$ we are projected on the ground state, and the propagator is computed with this precise Green function, while different boundary conditions would lead to different propagators and thus different results.

The first one has two vertices and three propagators connecting them (in $3 \times 2 \times 1$ possible permutations), while the second one has two vertices connected by a single propagator (the two vertices can be chosen from any of the present, so 3×3 possibilities), with each vertex having a loop attached to it. We can check the combinatorial factors by counting the number of Wick contractions that give rise to each diagram: $6 + 9 = 15$, which is indeed the number of ways to contract six fields in pairs.

Thus we have found two types of diagrams: one is the **sunset diagram**  where two vertices are connected by three propagators, while the other one is the **dumbbell diagram**  where two vertices are connected by a single propagator and each vertex has a loop attached to it. The combinatorial factors arise from the number of Wick contractions that give rise to each diagram. We can compute their values as follows. For the sunset diagram, we have⁶

$$\begin{aligned} \text{Diagram} &= \int_{-\beta/2}^{\beta/2} d\tau \int_{-\beta/2}^{\beta/2} d\tau' G_E(\tau, \tau')^3 = \int_{-\beta/2}^{\beta/2} d\tau \int_{-\beta/2}^{\beta/2} d\tau' \left(\frac{1}{2\omega} e^{-\omega|\tau-\tau'|} \right)^3 \\ &= \frac{1}{8\omega^3} \int_{-\beta/2}^{\beta/2} d\tau \int_{-\infty}^{\infty} d\sigma e^{-3\omega|\sigma|} = \frac{\beta}{8\omega^3} 2 \int_0^{\infty} d\sigma e^{-3\omega\sigma} \\ &= \frac{\beta}{8\omega^3} 2 \frac{e^{-3\omega\sigma}}{-3\omega} \Big|_0^\infty = \frac{\beta}{8\omega^3} \frac{2}{3\omega} = \frac{\beta}{12\omega^4}, \end{aligned}$$

while for the dumbbell diagram, we have

$$\begin{aligned} \text{Diagram} &= \int_{-\beta/2}^{\beta/2} d\tau \int_{-\beta/2}^{\beta/2} d\tau' G_E(\tau - \tau) G_E(\tau - \tau') G_E(\tau' - \tau') \\ &= \int_{-\beta/2}^{\beta/2} d\tau \int_{-\beta/2}^{\beta/2} d\tau' \left(\frac{1}{2\omega} \right)^2 \left(\frac{1}{2\omega} e^{-\omega|\tau-\tau'|} \right) \\ &= \frac{\beta}{4\omega^2} 2 \int_0^{\infty} d\sigma \frac{1}{2\omega} e^{-\omega\sigma} = \frac{\beta}{4\omega^2} 2 \frac{e^{-\omega\sigma}}{-\omega} \Big|_0^\infty \\ &= \frac{\beta}{8\omega^3} \frac{2}{\omega} = \frac{\beta}{4\omega^4}. \end{aligned}$$

Now, we can insert these results into the expression for $Z_E[0]$ to obtain

$$Z_E[0] = \langle 1 \rangle_{U,0} \left[1 + \frac{g^2}{2(3!)^2} \left((3!) \times \frac{\beta}{12\omega^4} + (3^2) \times \frac{\beta^2}{4\omega^4} \right) + \dots \right] = \langle 1 \rangle_{U,0} \exp \left(\beta \frac{11}{8(3!)^2} \frac{g^2}{\omega^4} + \dots \right),$$

finding the entity of the correction to the ground state energy due to the cubic interaction

$$\Delta E_0 = -\frac{11}{288} \frac{g^2}{\omega^4}.$$

3.5.2 | Other Correlators and Feynman Diagrams

In a similar way, one computes the perturbative expansion of other correlation functions, considering that the vacuum diagrams correspond to unnormalized 0-point function, relating to the ground state energy. We start from the vacuum, something happens during the evolution, and we return to the vacuum.

⁶We do not compute the limit for $\beta \rightarrow \infty$ yet, since we are just interested in the value of the diagram itself. We will take the limit at the very end to extract the ground state energy correction after inserting these results into the expression for $Z_E[0]$.

We can treat the two point correlation function in a similar way. We have two particles, one in the far past and one in the far future, which interacts in some way (for example the anharmonic potential seen before) during their evolution. The two point correlation function is given by

$$\begin{aligned}\langle x(t_1)x(t_2) \rangle &= \frac{1}{Z} \int Dx x(t_1)x(t_2)e^{\frac{i}{\hbar}S[x]} = \left\langle x(t_1)x(t_2)e^{\frac{i}{\hbar}S_{int}[x]} \right\rangle_0 \\ &= \left\langle x(t_1)x(t_2) \left[1 + \frac{i}{\hbar}S_{int}[x] + \frac{1}{2!} \left(\frac{i}{\hbar}S_{int}[x] \right)^2 + \dots \right] \right\rangle_0.\end{aligned}$$

We can interpret as follows: we have two external points at times t_1 and t_2 where particles are created/annihilated, and we have to consider all possible interactions that may happen during their evolution. Using Wick contractions, we can compute the perturbative expansion of this correlation function in the free theory. For the case of a cubic interaction, $S_{int} = -\frac{g}{3!} \int dt x(t)^3$, it leads to the following diagrammatic expansion up to second order in perturbation theory:

DIAGRAMS

its like studying a 8 point function but with 2 external points fixed. The first diagram corresponds to the free propagator between times t_1 and t_2 . The second diagram represents the first-order correction due to a single interaction vertex, where the two external points are connected through a loop. The third and fourth diagrams represent second-order corrections, involving two interaction vertices. The third diagram shows two vertices connected by three propagators, while the fourth diagram has two vertices connected by a single propagator with loops attached to each vertex. This exemplifies how Feynman diagrams arise naturally in the perturbative expansion of correlation functions in quantum field theory.

Let us describe graphically the corrections that must be computed for calculating perturbatively the 4-point function (in a QFT context, it is linked to the scattering of 2 incoming particles to 2 outgoing particles)

$$\langle x(t_1)x(t_2)x(t_3)x(t_4) \rangle$$

where one may keep in mind that setting $t_1, t_2 \rightarrow -\infty$ describes incoming states while $t_3, t_4 \rightarrow +\infty$ describes outgoing states. We have

$$\begin{aligned}\langle x(t_1)x(t_2)x(t_3)x(t_4) \rangle &= \frac{1}{Z} \int Dx x(t_1)x(t_2)x(t_3)x(t_4)e^{\frac{i}{\hbar}S[x]} = \left\langle x(t_1)x(t_2)x(t_3)x(t_4)e^{\frac{i}{\hbar}S_{int}[x]} \right\rangle_0 \\ &= \left\langle x(t_1)x(t_2)x(t_3)x(t_4) \left[1 + \frac{i}{\hbar}S_{int}[x] + \frac{1}{2!} \left(\frac{i}{\hbar}S_{int}[x] \right)^2 + \dots \right] \right\rangle_0.\end{aligned}$$

For the case of a cubic interaction, $S_{int} = -\frac{g}{3!} \int dt x(t)^3$, it leads to the following diagrammatic expansion which is obtained by the systematic use of Wick contractions:

TODO: Modify last diagram in first row, it needs 4 external points.

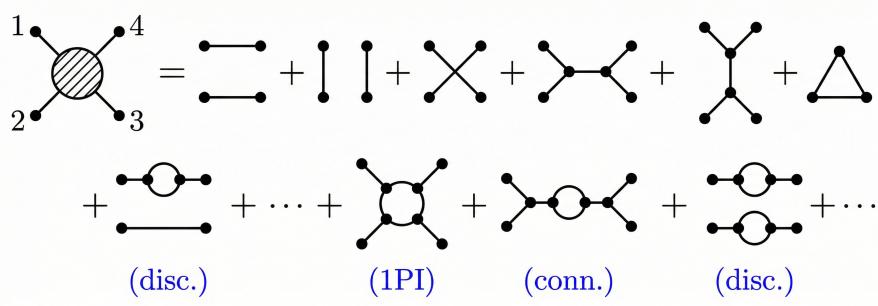


Figure 3.2: Diagrammatic expansion of the 4-point function for a cubic interaction up to second order in perturbation theory.

One notices disconnected, connected, and 1PI diagrams, which play a significant role in QFT (1PI diagrams are those diagrams that remain connected after cutting any single internal line). This exemplifies the emergence of Feynman diagrams in describing the perturbative expansion.

Nobody knows what happens during the interaction, virtually anything can happen, but we can sum over all the possibilities using the path integral formalism and Wick's theorem.

Here ends the treatment for the **bosonic path integral**: we saw that this formalism applies naturally on the KG field and scalar fields in general, and we developed the perturbative expansion with Feynman diagrams. In the next section, we extend the path integral formalism to fermionic systems.

3.6 | Path Integrals for Fermions

We now discuss how to extend the path integral method to fermionic systems. Fermions at the classical level can be described by **Grassmann variables**, also known as **anticommuting** numbers or fermionic variables. Grassmann variables allow us to define “classical” models whose quantization produces degrees of freedom that satisfy the Pauli exclusion principle.

The question is: how can we define a path integral for fermionic systems? The main difficulty arises from the anticommuting nature of fermionic variables, which makes the standard definition of the path integral inapplicable. There is no classical trajectory for fermions in the usual sense, since the fermionic nature of the particles vanishes in the classical limit $\hbar \rightarrow 0$. To overcome this issue, we introduce Grassmann variables to describe fermionic degrees of freedom at the classical level.

We need to introduce a suitable Hamiltonian theory to deal with fermionic degrees of freedom, which has **symmetric Poisson Brackets**, in order to quantize them canonically obtaining a quantum theory based on **anticommutators**. This is why we call it a **pseudoclassical model**: it is not a classical model in the usual sense, but it is a formal construction that allows us to quantize fermionic degrees of freedom, and leads to the correct quantum theory based on Grassmann variables.

$$\{\psi, \bar{\psi}\}_C \longrightarrow \{\hat{\psi}, \hat{\psi}^\dagger\} = i\hbar \dots$$

Models with Grassmann variables are often called “pseudoclassical”, as the spin at the classical level is just a formal construction (the value of any finite spin vanishes for $\hbar \rightarrow 0$, and thus cannot be measured classically). In the following, we first exemplify the use of Grassmann variables in mechanical models. The method extends to field theories as well, so that a Dirac field can be treated classically with Grassmann variables. Then, we develop canonical quantization for mechanical models containing Grassmann variables.

At last, we derive a path integral representation of the transition amplitude for fermionic systems starting from its operatorial expression and using a suitable definition of fermionic coherent states.

3.6.1 | Grassmann Algebras

A n -dimensional Grassmann algebra \mathcal{G}_n is generated by a set of generators θ_i with $i = 1, \dots, n$, which satisfy the anticommutation relations

$$\{\theta_i, \theta_j\} = \theta_i \theta_j + \theta_j \theta_i = 0, \quad \forall i, j = 1, \dots, n.$$

From these relations, it follows that

$$\theta_i^2 = 0,$$

for all i . The elements of the Grassmann algebra are linear combinations of products of the generators, with complex coefficients. This suggests already at the classical level the essence of the Pauli exclusion principle, according to which one cannot put two identical fermions in the same quantum state. Physicists often call these generators anticommuting numbers.

We will now describe some properties of Grassmann algebras that will be useful in the following: functions of Grassmann variables, derivatives with respect to Grassmann variables, integration over Grassmann variables, and reality properties, with the aim of defining a path integral for fermionic systems.

Functions. One can multiply these generators and their products by real or complex numbers and form polynomials that are used to define functions of the Grassmann variables (i.e., the elements of the Grassmann algebra). For example, for $n = 1$, there is only one Grassmann variable θ . Then, an arbitrary function is given by

$$f(\theta) = f_0 + f_1\theta,$$

where f_0 and f_1 are taken to be either real or complex numbers, and higher power of theta vanish (we can factor a $\theta^2 = 0$). Similarly, for $n = 2$ one has

$$f(\theta_1, \theta_2) = f_0 + f_1\theta_1 + f_2\theta_2 + f_3\theta_1\theta_2,$$

and so on for higher dimensions. A term with $\theta_2\theta_1$ is not written as it is not independent of $\theta_1\theta_2$: $\theta_2\theta_1 = -\theta_1\theta_2$. Terms with an even number of θ 's are called Grassmann even (or equivalently: even, commuting, bosonic). Terms with an odd number of θ 's are called *Grassmann odd* (or equivalently: odd, anticommuting, fermionic). Generic functions are always defined in terms of their Taylor expansions, which contain a finite number of terms because of the Grassmann property. For example, the exponential function e^θ means $e^\theta = 1 + \theta$ because $\theta^2 = 0$ as any other higher power.

Derivatives. Derivatives with respect to Grassmann variables are very simple. As any function can be at most linear with respect to any fixed Grassmann variable, its derivative is straightforward and one has to keep track just of signs. **Left derivatives** are defined by removing the variable from the left of its Taylor expansion: for example for the function $f(\theta_1, \theta_2)$ given above

$$\frac{\partial_L}{\partial\theta_1} f(\theta_1, \theta_2) = f_1 + f_3\theta_2,$$

since θ_1 is removed from the left. Similarly, **right derivatives** are obtained by removing the variable from the right⁷

$$\frac{\partial_R}{\partial\theta_1} f(\theta_1, \theta_2) = f_1 - f_3\theta_2,$$

where a minus sign emerges because one has first to commute θ_1 past θ_2 . One can obtain the same minus sign by left derivatives on θ_2 using the function of the last example. Equivalently, introducing Grassmann increments $\delta\theta$, one may write

$$\delta f = f(\theta + \delta\theta) - f(\theta) = \delta\theta \frac{\partial_L f}{\partial\theta} = \frac{\partial_R f}{\partial\theta} \delta\theta,$$

which helps in keeping track of signs. If not specified otherwise, we use left derivatives and omit the corresponding subscript.

Integrals. Integration can be defined, according to **Berezin**, to be identical to differentiation

$$\int d\theta = \frac{\partial_L}{\partial\theta}.$$

This definition has the virtue of producing a **translational invariant**⁸ measure:

$$\int d\theta f(\theta + \eta) = \int d(\theta + \eta) f(\theta + \eta) = \int d\tilde{\theta} f(\tilde{\theta}),$$

⁷Since before applying the derivative one has to anticommute the variables until the object of the derivation is in the last position on the right: if it is already there, no sign change occurs.

⁸Which, as we have precedently highlighted, is a property we should look for in order to define a consistent theory of integration for our path integrals (think about the previously discussed gaussian integrals).

as the measure is translational invariant, $d\theta = d\tilde{\theta}$, and $\tilde{\theta} = \theta + \eta$. This statement is easily proven by a direct calculation

$$\int d\theta f(\theta + \eta) = \frac{\partial_L}{\partial \theta} (f_0 + f_1(\theta + \eta)) = f_1 = \int d\tilde{\theta} f(\tilde{\theta}),$$

thus confirming the translational invariance of the measure, which is practically manifest and one of the main reasons for defining integration in this way.

Reality properties. Grassmann variables can be defined to be either real or complex. A real variable satisfies

$$\bar{\theta} = \theta,$$

with the bar indicating complex conjugation. For products of Grassmann variables, the complex conjugate is defined to include an exchange of their position

$$\overline{\theta_1 \theta_2} = \bar{\theta}_2 \bar{\theta}_1.$$

Thus, the complex conjugate of the product of two real variables is purely imaginary

$$\overline{\theta_1 \theta_2} = -\theta_1 \theta_2.$$

It is the combination $i\theta_1 \theta_2$ that is real, as the complex conjugate of the imaginary unit carries the additional minus sign to obtain a formally real object

$$\overline{i\theta_1 \theta_2} = -i\theta_2 \theta_1 = i\theta_1 \theta_2.$$

Complex Grassmann variables η and $\bar{\eta}$ can always be decomposed in terms of two real Grassmann variables θ_1 and θ_2 by setting

$$\eta = \frac{1}{\sqrt{2}}(\theta_1 + i\theta_2), \quad \bar{\eta} = \frac{1}{\sqrt{2}}(\theta_1 - i\theta_2).$$

These definitions on the reality properties of the Grassmann variables are the ones that are the most useful for physical applications, since one requires that *real variables become hermitian operators upon quantization*.

Gaussian integrals. These integrals are crucial in order to derive the Free theory, first step before moving to a perturbative one. Having defined integration over Grassmann variables, we consider in more detail the gaussian integration, which is at the core of fermionic path integrals. For the case of a single real Grassmann variable θ the gaussian function is trivial, $e^{-a\theta^2} = 1$, since $\theta^2 = 0$ as θ anticommutes with itself. One needs at least two real Grassmann variables θ_1 and θ_2 to have a nontrivial exponential function with an exponent quadratic in Grassmann

$$e^{-a\theta_1 \theta_2} = 1 - a\theta_1 \theta_2,$$

where a is either real or complex. With the above definitions, the corresponding “gaussian integral” is computed straightforwardly

$$\int d\theta_1 d\theta_2 e^{-a\theta_1 \theta_2} = \int d\theta_1 d\theta_2 (1 - a\theta_1 \theta_2) = \frac{\partial_L}{\partial \theta_1} \frac{\partial_L}{\partial \theta_2} (1 - a\theta_1 \theta_2) = a.$$

Note that there is a precise sign defined by the chosen measure ordering, as $\int d\theta_1 d\theta_2 = -\int d\theta_2 d\theta_1$. Defining the antisymmetric matrix

$$A = \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix}, \quad \det A = a^2,$$

one may rewrite the previous integral as

$$\int d^2\theta e^{-\frac{1}{2}\theta_i A_{ij}\theta_j} = \int d\theta_1 d\theta_2 e^{-a\theta_1\theta_2} = a = \sqrt{\det A}.$$

The square root of the determinant of an antisymmetric matrix A is called the **Pfaffian**, and often indicated by $\text{Pfaff } A$. Indeed, the determinant is always positive definite for real antisymmetric matrices, and its square root is well-defined (by analytic extensions, it is also well-defined for antisymmetric matrices with complex entries). It is easy to see that the above formula extends to an even number $n = 2m$ of real Grassmann variables, so that one may write in general

$$\int d^n\theta e^{-\frac{1}{2}\theta_i A_{ij}\theta_j} = \text{Pfaff } A = \sqrt{\det A},$$

where A is a real antisymmetric $n \times n$ matrix and $d^n\theta = d\theta_1 \cdots d\theta_n$. This formula is the fermionic counterpart of the bosonic gaussian integral seen before (where if one remember, the square root of the determinant of the matrix at the exponent was inverse: $(\det K)^{-1/2}$), and it plays a crucial role in defining fermionic path integrals. To prove this, one notices that with an orthogonal transformation it is possible to skew-diagonalize the antisymmetric matrix A_{ij} and put it in the form

$$\begin{pmatrix} 0 & a_1 & 0 & 0 & \dots & 0 & 0 \\ -a_1 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & a_2 & \dots & 0 & 0 \\ 0 & 0 & -a_2 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & a_m \\ 0 & 0 & 0 & 0 & \dots & -a_m & 0 \end{pmatrix}$$

The orthogonal transformation leaves the integration measure invariant and thus one gets the above result with $(\det A)^{1/2} = a_1 \cdots a_m$. A cautionary note: to compute correctly the jacobian under a change of variables one should recall the definition of the integration in terms of derivatives (the Berezin integration), and thus find the inverse matrix with respect to the one associated with an analogous bosonic integral.

Similarly, one finds that gaussian integration over complex Grassmann variables $(\eta_i, \bar{\eta}_i)$ produce a determinant

$$\int d^n\bar{\eta} d^n\eta e^{-\bar{\eta}_i A_{ij}\eta_j} = \det A,$$

where the measure is now defined as $d^n\bar{\eta} d^n\eta = d\eta_1 d\bar{\eta}_1 \cdots d\eta_n d\bar{\eta}_n$.

For applications to dynamical models and subsequent path integral quantization, it is useful to consider infinite dimensional Grassmann algebras ($n \rightarrow \infty$). Then, one may use Grassmann valued functions of time, i.e. $\theta_i \rightarrow \theta(t)$. For different values of t , one has different generators of the algebra, so that properties such as $\theta^2(t) = 0$ and $\theta(t)\theta(t') = -\theta(t')\theta(t)$ hold. They are used to introduce useful mechanical systems at the classical level, often named pseudoclassical models, that upon quantization produce systems satisfying the Pauli exclusion principle and the Fermi-Dirac statistic.

3.6.2 | Pseudoclassical Model and Canonical Quantization

We are going to exemplify the use of Grassmann variables in mechanical models. We will use the so called **fermionic oscillator**: if we remember the bosonic harmonic oscillator, we can define its fermionic counterpart by introducing Grassmann variables.

Classically, it is described by the function $\psi(t)$ and its complex conjugate $\bar{\psi}(t)$ that take values in a Grassmann algebra (t denotes the time). The Grassmann property implies generic relations like

$$\psi(t)^2 = 0, \quad \psi(t)\psi(t') = -\psi(t')\psi(t), \quad \dot{\psi}(t)^2 = 0, \quad \psi(t)\dot{\psi}(t) = -\dot{\psi}(t)\psi(t),$$

and so on, where dots denote time derivatives, $\dot{\psi} = \frac{d}{dt}\psi$. Note already at this stage, that $\psi(t)\dot{\psi}(t)$ is not a total derivative. These relations can be used in extremizing the action, testing the presence of symmetries, and so on.

For the bosonic harmonic oscillator, we had the action

$$S[x, p] = \int dt \left(p\dot{x} - \frac{1}{2}(p^2 + \omega^2 x^2) \right),$$

which can be rewritten with complex variables derived via linear combinations of x and p

$$a = \frac{1}{\sqrt{2\omega}}(\omega x + ip), \quad \bar{a} = \frac{1}{\sqrt{2\omega}}(\omega x - ip),$$

so that the action becomes

$$S[a, \bar{a}] = \int dt \left(\frac{i}{2}(\bar{a}\dot{a} - \dot{\bar{a}}a) - \omega\bar{a}a \right) = \int dt (i\bar{a}\dot{a} - \omega\bar{a}a),$$

up to total derivatives. Quantization of the complex variables (a, \bar{a}) gives rise to the annihilation/creation operators $(\hat{a}, \hat{a}^\dagger)$ that satisfy the algebra $[\hat{a}, \hat{a}^\dagger] = \hbar$ (however we will use mostly $\hbar = 1$). They are used in the Fock construction of the Hilbert space of the harmonic oscillator, which is reviewed later on in sec. 3.6.3 when we consider coherent states.

To define the fermionic counterpart, we introduce two complex Grassmann-valued functions $\psi(t)$ and $\bar{\psi}(t)$, and write the action

$$S[\psi, \bar{\psi}] = \int dt (i\bar{\psi}\dot{\psi} - \omega\bar{\psi}\psi). \tag{3.6.1}$$

This action is the fermionic counterpart of the bosonic harmonic oscillator action written in terms of complex variables. It is linear in time derivatives, as it must be for fermionic systems (if it were quadratic, the Grassmann property would imply that the action vanishes identically). As its bosonic counterpart, it is real.

Now if we compute the variation of the action with respect to $\bar{\psi}$ and ψ , we find the equations of motion

$$\delta S = 0 = \int dt \left[i\delta\bar{\psi} (i\dot{\psi} - \omega\psi) + (-i\dot{\bar{\psi}} - \omega\bar{\psi}) \delta\psi \right].$$

Thus, the equations of motion are

$$i\dot{\psi} - \omega\psi = 0, \quad -i\dot{\bar{\psi}} - \omega\bar{\psi} = 0, \tag{3.6.2}$$

and their solutions are easily found to be

$$\psi(t) = \psi_0 e^{-i\omega t}, \quad \bar{\psi}(t) = \bar{\psi}_0 e^{i\omega t}, \tag{3.6.3}$$

where ψ_0 and $\bar{\psi}_0$ are Grassmann constants. This equation may be called the Dirac equation in a 0+1 dimensional spacetime, as one may rewrite it as $(\gamma^0 \partial_0 + m)\psi = 0$ with $\gamma^0 = -i$, $x^0 = t$, and the frequency $\omega = m$ playing the role of the Dirac mass.

To proceed with canonical quantization, we compute the conjugate momenta

$$\pi = \frac{\partial L}{\partial \dot{\psi}} = -i\bar{\psi}, \quad \bar{\pi} = \frac{\partial L}{\partial \dot{\bar{\psi}}} = 0. \tag{3.6.4}$$

which shows that the system is already in a hamiltonian form, the conjugate momenta being $\bar{\psi}$ up to a factor. The classical Poisson bracket $\{\pi, \psi\}_{PB} = -1$ is rewritten as $\{\pi, \psi\}_{PB} = -i$, and has the property of being symmetric (this fact will be discussed in a short while).

Quantizing with anticommutators (fermionic systems must be treated this way) one obtains

$$\begin{aligned}\{\hat{\psi}, \hat{\psi}^\dagger\} &= i\hbar(-i) = \hbar, \\ \{\hat{\psi}, \hat{\psi}\} &= \{\hat{\psi}^\dagger, \hat{\psi}^\dagger\} = 0,\end{aligned}$$

that is, the classical variables ψ and $\bar{\psi}$ are promoted to linear operators $\hat{\psi}$ and $\hat{\psi}^\dagger$ satisfying anticommutation relations that are set to be equal to $i\hbar$ times the value of the classical Poisson brackets. Setting $\hbar = 1$ for simplicity, one finds the fermionic creation/annihilation algebra

$$\{\hat{\psi}, \hat{\psi}^\dagger\} = 1, \quad \{\hat{\psi}, \hat{\psi}\} = \{\hat{\psi}^\dagger, \hat{\psi}^\dagger\} = 0. \quad (3.6.5)$$

that can be realized in a two-dimensional Hilbert space and with the correct hermiticity properties. If we recall the bosonic harmonic oscillator, we had the algebra of ladder operators defined as

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad [\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}^\dagger] = 0,$$

which is similar to the fermionic one, but with commutators instead of anticommutators. The main difference is that in the bosonic case, the Hilbert space is infinite-dimensional, while in the fermionic case it is two-dimensional, due to the Pauli exclusion principle.

The Hilbert is explicitly constructed "*à la Fock*", considering $\hat{\psi}$ as destruction operator and $\hat{\psi}^\dagger$ as creation operator. One starts defining the Fock vacuum $|0\rangle$, fixed by the condition

$$\hat{\psi}|0\rangle = 0.$$

A second state is obtained by acting with $\hat{\psi}^\dagger$

$$|1\rangle = \hat{\psi}^\dagger |0\rangle.$$

No other state can be obtained acting again with the creation operator $\hat{\psi}^\dagger$, since $(\hat{\psi}^\dagger)^2 = 0$. Thus the Hilbert space is two-dimensional, spanned by the orthonormal basis $\{|0\rangle, |1\rangle\}$, encapsulating the Pauli exclusion principle at the quantum level.

Normalizing the Fock vacuum to unity, $\langle 0|0\rangle = 1$, with $\langle 0| = |0\rangle^\dagger$, one finds that these two states are orthonormal

$$\langle n|m\rangle = \delta_{nm}, \quad n, m = 0, 1,$$

and span a two-dimensional Hilbert space, $\mathcal{F}_2 = \{|0\rangle, |1\rangle\}$. In terms of matrices one computes matrix elements and finds the realization

$$\begin{aligned}\hat{\psi} &= \begin{pmatrix} \langle 0| \hat{\psi} |0\rangle & \langle 0| \hat{\psi} |1\rangle \\ \langle 1| \hat{\psi} |0\rangle & \langle 1| \hat{\psi} |1\rangle \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \\ \hat{\psi}^\dagger &= \begin{pmatrix} \langle 0| \hat{\psi}^\dagger |0\rangle & \langle 0| \hat{\psi}^\dagger |1\rangle \\ \langle 1| \hat{\psi}^\dagger |0\rangle & \langle 1| \hat{\psi}^\dagger |1\rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\end{aligned}$$

acting on the basis

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Hamiltonian Structure and Symplectic Form

The hamiltonian of the fermionic oscillator is obtained from the Legendre transform of the Lagrangian

$$H = \dot{\psi}\pi - L = \omega\bar{\psi}\psi = \frac{\omega}{2}(\bar{\psi}\psi - \psi\bar{\psi}).$$

The last form is a classically equivalent way of writing it and is the one that is quantized to resolve the ordering ambiguities

$$\hat{H} = \frac{\omega}{2}(\hat{\psi}^\dagger\hat{\psi} - \hat{\psi}\hat{\psi}^\dagger) = \omega\left(\hat{\psi}^\dagger\hat{\psi} - \frac{1}{2}\right). \quad (3.6.6)$$

Note that in the Legendre transform, the order of $\dot{\psi}$ and π matters, and we have used the one that follows from having defined the conjugate momentum in (3.6.4) with left derivatives.

Path integrals for fermions can be derived from the canonical formalism, just as in the bosonic case. To this aim, it is useful to rewrite the action in a **symplectic form**, which is the natural framework for hamiltonian systems. The hamiltonian formalism aims at producing equations of motion that are first-order differential equations in time. For a simple **bosonic model** with phase space coordinates (x, p) , the *phase space action* is usually written in the form

$$S[x, p] = \int dt (p\dot{x} - H(x, p)).$$

The first term with derivatives (the $p\dot{x}$ term) is called the symplectic term and fixes the Poisson bracket structure of phase space. Up to total derivatives, it can be written in a more symmetrical form, with the time derivatives shared equally by x and p as

$$S[x, p] = \int dt \frac{1}{2}(p\dot{x} - \dot{p}x) - H(x, p) = \int dt \frac{1}{2}z^a\Omega_{ab}\dot{z}^b - H(z),$$

where we have introduced the phase space vector for a bosonic system

$$z^a = (x, p), \quad a = 1, 2,$$

and the **symplectic matrix**

$$(\Omega^{-1})_{ab} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \Omega^{ab} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

A symmetric matrix would give terms in the action that are total derivatives and can be dropped (they would not modify the equations of motion).⁹

Symplectic structure for bosonic systems. Thus the action for a bosonic system can be written in terms of the symplectic matrix as

$$S[z] = \int dt \left[\frac{1}{2} \begin{pmatrix} x & p \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \dot{x} \\ \dot{p} \end{pmatrix} - H(x, p) \right] = \int dt \left(\frac{1}{2} z^a (\Omega^{-1})_{ab} \dot{z}^b - H(z) \right). \quad (3.6.7)$$

This action produces the correct equations of motion via Hamilton's equations, which will be of the first order in time derivatives for fermionic systems (pay attention: we are still using bosonic variables). As we have said, the first term in the action is symplectic and involves an antisymmetric matrix, which is the reason why the Poisson brackets for bosonic systems are antisymmetric (in

⁹For fermions instead, we are dealing with terms with anticommuting variables, thus a symmetric matrix would give nontrivial contributions to the action, while an antisymmetric matrix would give total derivatives.

contrast to bosonic systems, where the symplectic form is given by a symmetric matrix and the Poisson brackets are symmetric too). The Poisson brackets for generic functions $F(z)$ and $G(z)$ of the phase space variables z^a are defined as

$$\{F, G\}_{PB} = \frac{\partial F}{\partial z^a} \Omega^{ab} \frac{\partial G}{\partial z^b}, \quad (3.6.8)$$

and, for the phase space variables, one finds

$$\{z^a, z^b\}_{PB} = \Omega^{ab}.$$

This coincides with the standard definition, thus Poisson bracket satisfies the usual properties

$$\begin{aligned} \{F, G\}_{PB} &= -\{G, F\}_{PB}, \\ \{F, GH\}_{PB} &= \{F, G\}_{PB} H + G \{F, H\}_{PB}, \\ \{F, \{G, H\}_{PB}\}_{PB} + \text{c.p.} &= 0, \end{aligned} \quad (3.6.9)$$

which are *antisymmetry*, *Leibniz rule*, and *Jacobi identity* (c.p. stands for cyclic permutations), respectively. These properties make it consistent to adopt the canonical quantization rules of substituting the fundamental variables z^a by linear operators \hat{z}^a acting on a Hilbert space of physical states, with commutation relations fixed to be $i\hbar$ times the value of the classical Poisson brackets

$$[\hat{z}^a, \hat{z}^b] = i\hbar \{z^a, z^b\}_{PB} = i\hbar \Omega^{ab}. \quad (3.6.10)$$

This prescription¹⁰ is consistent as both sides satisfy the same algebraic properties, listed in (3.6.9) for the Poisson brackets. At this stage, once one has found an irreducible representation of the operator algebra (3.6.10) on a well-defined vector space (Hilbert space), the process of canonical quantization has been achieved.

Mixed bosonic and fermionic systems. We can also extend the phase space so that its vector include a generic Grassmann variable: bosonic and fermionic degrees of freedom can be treated in a unified way by introducing the extended phase space variables

$$Z^A = (x^i, p_i, \theta^\alpha) = (z^a, \theta^\alpha);$$

so that the action takes the following general form

$$S[Z^A] = \int dt \left(\frac{1}{2} Z^A (\Omega^{-1})_{AB} \dot{Z}^B - H(Z) \right).$$

Now the symplectic matrix helps into define the Poisson brackets

$$\{F, G\}_{PB} = \frac{\partial_R F}{\partial Z^A} \Omega^{AB} \frac{\partial_L G}{\partial Z^B},$$

where F and G are generic functions of the phase space variables Z^A . The Poisson brackets are symmetric when both F and G are Grassmann odd, and antisymmetric otherwise. This is the general structure of hamiltonian systems with both bosonic (z^a inside Z^A) and fermionic degrees of freedom (from the included Grassmann variables). Again, this term must be written splitting the time derivatives democratically between all variables, as in (3.6.7). The symplectic term and the hamiltonian are taken to be Grassmann even (i.e., commuting objects), so that the whole action is bosonic.

¹⁰More generally, phase space functions $F(z)$ are elevated to operators $\hat{F}(\hat{z})$ (after fixing ordering ambiguities) with commutation relations that take the form $[\hat{F}(\hat{z}), \hat{G}(\hat{z})] = i\hbar \{F, G\}_{PB} + \text{higher order terms in } \hbar$.

Then, it is seen that the matrix Ω^{AB} is antisymmetric in the sector related to the bosonic coordinates, and symmetric in the sector belonging to the Grassmann variables (other off-diagonal entries vanish as the action is taken to be commuting). Denoting the variables by $Z^A = (z^a, \theta^\alpha)$ with z^a bosonic and θ^α fermionic, the matrix Ω^{AB} (as well as its inverse) has a block diagonal form

$$\Omega^{AB} = \begin{pmatrix} \Omega^{ab} & 0 \\ 0 & \Omega^{\alpha\beta} \end{pmatrix}, \quad \begin{cases} \Omega^{ab} = -\Omega^{ba}, \\ \Omega^{\alpha\beta} = +\Omega^{\beta\alpha}, \end{cases} \quad (3.6.11)$$

where Ω^{ab} is the symplectic matrix for the bosonic sector (antisymmetric) and $\Omega^{\alpha\beta}$ is the symplectic matrix for the fermionic sector (symmetric). The Poisson brackets for the whole phase space read

$$\{F, G\}_{PB} = \frac{\partial_R F}{\partial Z^A} \Omega^{AB} \frac{\partial_L G}{\partial Z^B}, \quad (3.6.12)$$

where both left and right derivatives are used to take into account the Grassmann parity of the variables. In particular we can find

$$\{Z^A, Z^B\}_{PB} = \Omega^{AB}.$$

The Poisson brackets are thus symmetric when both F and G are Grassmann odd (fermionic), and antisymmetric otherwise.

Phase space functions are usually restricted to have a definite **Grassmann parity**. Given any such function F , we denote its Grassmann parity by $(-1)^{\epsilon_F}$, where $\epsilon_F = 0$ if F is Grassmann even (bosonic function) and $\epsilon_F = 1$ if F is Grassmann odd (fermionic function). Then, one finds that the definition (3.6.12) satisfies a graded generalization of the properties in (3.6.9), namely

$$\begin{aligned} \{F, G\}_{PB} &= (-1)^{\epsilon_F \epsilon_G + 1} \{G, F\}_{PB}, \\ \{F, GH\}_{PB} &= \{F, G\}_{PB} H + (-1)^{\epsilon_F \epsilon_G} G \{F, H\}_{PB}, \\ (-1)^{\epsilon_F (\epsilon_G + \epsilon_H)} \{F, \{G, H\}_{PB}\}_{PB} &+ \text{c.p.} = 0. \end{aligned} \quad (3.6.13)$$

The equations of motion are first order in time. They can be derived by minimizing the action and can be expressed in terms of the Poisson brackets as

$$\dot{Z}^A = \Omega^{AB} \frac{\partial_L H}{\partial Z^B} = \{Z^A, H\}_{PB},$$

which is the generalization of Hamilton's equations to systems with both bosonic and fermionic degrees of freedom.

These properties of the Poisson brackets make it consistent to adopt the canonical quantization rules, that consist in promoting the phase space coordinates Z^A to operators \hat{Z}^A with commutation/anticommutation relation fixed by their classical Poisson brackets

$$[\hat{Z}^A, \hat{Z}^B] = i\hbar \{Z^A, Z^B\} = i\hbar \Omega^{AB}, \quad (3.6.14)$$

where we have employed the compact notation

$$[\cdot, \cdot] = \begin{cases} \{\cdot, \cdot\} & \text{if both variables are fermionic,} \\ [\cdot, \cdot] & \text{otherwise.} \end{cases} \quad (3.6.15)$$

often called “**graded commutator**”. The graded commutator satisfies identities similar to those for the Poisson brackets in (3.6.13), and makes it consistent to adopt the given quantization rules. This quick exposition becomes clearer by working through simple examples.

Example (Single real Grassmann variable). If we work with a single real Grassmann variable ψ , we are practically dealing with a “single Majorana fermion in one dimension”. If we take as phase space lagrangian the following

$$L = \frac{i}{2}\psi\dot{\psi} - H(\psi),$$

which is formally real and produces equations of motion of the first order in time, one finds

$$\Omega^{-1} = i \text{ and } \Omega = -i, \quad \{\psi(t), \psi(t)\}_{PB} = -i,$$

thus we have a single Grassmann odd phase space variable with symmetric Poisson brackets at equal times. The dynamical variable $\psi(t)$ is often called a Majorana fermion in one dimension, as it satisfies the Dirac equation in one dimension plus a reality condition (akin to the Majorana condition used in four dimensions). One notices that the only possible Grassmann even hamiltonian is a constant, so that the model is rather trivial, but it can be verified that the phase space can be odd-dimensional if Grassmann variables are present.

The model is quantized by introducing the hermitian operator $\hat{\psi}$ with anticommutator

$$\{\hat{\psi}, \hat{\psi}\} = \hbar.$$

The quantum theory is also trivial, as one represents irreducibly this algebra in a one dimensional Hilbert space, with the operator $\hat{\psi}$ acting as multiplication by the constant $\sqrt{\hbar/2}$. This Hilbert space has no room for any nontrivial dynamics, as there is only the vacuum state.

Example (Several real Grassmann variables). Working with several real Grassmann variables ψ^i , which are “Majorana fermions in one dimension”, one may take as phase space lagrangian

$$L = \frac{i}{2}\psi^i\delta_{ij}\dot{\psi}^j - H(\psi), \quad i, j = 1, \dots, n,$$

which is formally real and produces equations of motion of the first order in time. One finds $(\Omega^{-1})_{ij} = i\delta_{ij}$ and $\Omega^{ij} = -i\delta^{ij}$, and Poisson brackets at equal times

$$\{\psi^i, \psi^j\}_{PB} = -i\delta^{ij}.$$

The model is quantized by introducing the hermitian operators $\hat{\psi}^i$ with anticommutators

$$\{\hat{\psi}^i, \hat{\psi}^j\} = \hbar\delta^{ij},$$

which is recognized to be proportional to the Clifford algebra of the gamma matrices, appearing in the Dirac equation in n euclidean dimensions. Indeed setting $\hat{\psi}^i = \sqrt{\hbar/2}\gamma^i$ turns the above anticommutation relations into the Clifford algebra

$$\{\gamma^i, \gamma^j\} = 2\delta^{ij}.$$

It is known that this algebra is realized on a complex vector space of dimension $2^{\lfloor n/2 \rfloor}$, where $\lfloor n/2 \rfloor$ indicates the integer part of $n/2$. For example, for $n = 2$ and $n = 3$ the gamma matrices are 2×2 , for $n = 4$ and $n = 5$ the gamma matrices are 4×4 , for $n = 6$ and $n = 7$ the gamma matrices are 8×8 , and so on. One concludes that the operators $\hat{\psi}^i$ are realised as hermitian operators in a Hilbert space of dimensions $2^{\lfloor n/2 \rfloor}$.

Example (One complex Grassmann variable). With complex Grassmann variables ψ and $\bar{\psi}$ it is possible to describe a “single Dirac fermion in one dimension”. Taking as phase space Lagrangian

$$L = i\bar{\psi}\dot{\psi} - H(\psi, \bar{\psi}),$$

one finds $\{\psi, \bar{\psi}\}_{PB} = \{\bar{\psi}, \psi\}_{PB} = -i$ as the only nontrivial Poisson brackets between the phase space coordinates $(\psi, \bar{\psi})$. It is quantized by the anticommutator $\{\hat{\psi}, \hat{\psi}^\dagger\} = \hbar$, producing a fermionic annihilation/creation algebra. It is realized in a two-dimensional Fock space, as anticipated earlier while discussing the fermionic harmonic oscillator. This model is equivalent to that with two real (Majorana) fermions, seen as the real and the imaginary part of the Dirac fermion. Also, one may straightforwardly consider the theory of a set of several Dirac fermions in one dimension.

These basic examples can be used to construct explicitly the irreducible representations of the gamma matrices in arbitrary dimensions and check their dimensionality as anticipated above.

In even dimensions $n = 2m$, one combines the $2m$ Majorana worldline fermions, corresponding to the gamma matrices, into m pairs of worldline Dirac fermions that generate a set of m copies of independent, anticommuting creation/annihilation operators. The latter act on the tensor products of m two-dimensional fermionic Fock spaces, each one realizing an independent set of fermionic creation/annihilation operators. This gives a total Hilbert space of 2^m dimensions: indeed, for each set of creation/annihilation operators, a state can only be empty or filled with the corresponding fermionic excitation. This is in accord with the assertion given above about the dimensionality of the gamma matrices.

Adding an extra Majorana fermion corresponds to a Clifford algebra in odd dimensions (i.e., $2m+1$ dimensions): the related dimension of the Hilbert space does not change as the last Majorana fermion can be realized as proportional to the chirality matrix of the $2m$ dimensional case, which always exists.

3.6.3 | Coherent States

It is useful to introduce coherent states, an overcomplete basis of vectors for the fermionic Fock space described previously, for deriving a path integral for fermionic systems. They provide ket eigenstates of the fermionic operator $\hat{\psi}$ with Grassmann-valued eigenvalues. Together with a resolution of the identity, they allow to convert the matrix elements of the quantum evolution operator (transition amplitudes) into a path integral where one sums over Grassmann valued functions.

We first review the construction of bosonic coherent states, used in the theory of the harmonic oscillator, as a guide on the construction in the fermionic case. In the theory of the harmonic oscillator, one introduces coherent states defined as eigenstates of the annihilation operator \hat{a} . Let us recall the algebra of the creation and annihilation operators \hat{a}^\dagger and \hat{a}

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad [\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}^\dagger] = 0.$$

It is realized by operators acting on an infinite dimensional Hilbert space, identified with a Fock space constructed as follows. A complete orthonormal basis of the Fock space is obtained by starting from the Fock vacuum $|0\rangle$, defined by the condition $\hat{a}|0\rangle = 0$. The other states of the basis are obtained by acting with the creation operator \hat{a}^\dagger an arbitrary number of times on the

Fock vacuum $|0\rangle$

$$\begin{aligned} |0\rangle &\text{ such that } \hat{a}|0\rangle = 0, \\ |1\rangle &= \hat{a}^\dagger|0\rangle, \\ |2\rangle &= \frac{1}{\sqrt{2!}}(\hat{a}^\dagger)^2|0\rangle, \\ &\vdots \\ |n\rangle &= \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle. \end{aligned}$$

Normalizing the Fock vacuum to the unit norm, $\langle 0|0\rangle = 1$ where $\langle 0| = |0\rangle^\dagger$, one finds that these states are orthonormal

$$\langle m|n\rangle = \delta_{mn}, \quad m, n = 0, 1, 2, \dots,$$

Now, choosing a complex number a , one builds a coherent state $|a\rangle$ as the eigenstate of the annihilation operator \hat{a} with eigenvalue a

$$e^{a\hat{a}^\dagger}, \quad \hat{a}|a\rangle = a|a\rangle.$$

A way of proving this is by expanding the exponential and viewing $|a\rangle$ as an infinite sum with suitable coefficients of the basis vectors of the Fock space

$$|a\rangle = \left(1 + a\hat{a}^\dagger + \frac{1}{2!}(a\hat{a}^\dagger)^2 + \dots\right)|0\rangle = \sum_{n=0}^{\infty} \frac{a^n}{\sqrt{n!}}|n\rangle.$$

One may verify explicitly that $\hat{a}|a\rangle = a|a\rangle$ by acting with \hat{a} on the above expansion and using the action of \hat{a} on the basis states $|n\rangle$. We can also remember the ladder operators algebra to derive

$$\hat{a}^\dagger \rightarrow \bar{a}, \quad \hat{a} \rightarrow \frac{\partial}{\partial \bar{a}},$$

acting on the coherent states viewed as functions of the complex variable \bar{a} :

$$|a\rangle \rightarrow \psi_a(\bar{a}) = \langle \bar{a}|a\rangle = e^{\bar{a}a},$$

where we have introduced the dual coherent state

$$\langle \bar{a}| = \langle 0| e^{\bar{a}\hat{a}}.$$

A set of properties can be proven by direct computation:

1. $\langle \bar{a}| = |a\rangle^\dagger = \langle 0| e^{\bar{a}\hat{a}}$ is the dual coherent state, eigenstate of the creation operator \hat{a}^\dagger with eigenvalue \bar{a}

$$\langle \bar{a}| \hat{a}^\dagger = \langle \bar{a}| \bar{a};$$

2. the **scalar product** between two coherent states is

$$\langle \bar{a}|a\rangle = e^{\bar{a}a},$$

3. the set of coherent states provides a **resolution of the identity**

$$\mathbb{I} = \int \frac{d\bar{a}da}{2\pi i} e^{-\bar{a}a} |a\rangle \langle \bar{a}|,$$

where the integration measure is defined as $d\bar{a}da = d(\text{Re } a)d(\text{Im } a)$;

4. the **trace** of an operator \hat{O} can be computed as

$$\text{Tr } \hat{O} = \int \frac{d\bar{a}da}{2\pi i} e^{-\bar{a}a} \langle \bar{a} | \hat{O} | a \rangle.$$

One should note that the set of coherent states forms an over-complete basis, in particular, they are not orthonormal, in fact $\langle \bar{b} | a \rangle = e^{\bar{b}a} \neq 0$. However, it is useful to keep this redundancy.

Coherent states may be used to rederive a form of the path integral in phase space in terms of the so-called holomorphic trajectories, corresponding to paths for the $a(t)$ and $\bar{a}(t)$ variables. We will not present it here but consider only the corresponding fermionic construction, which is, mutatis mutandis, analogous.

Fermionic Coherent States

We now turn to the construction of coherent states for fermionic systems, that is, for systems described in terms of fermionic creation/annihilation operators $\hat{\psi}^\dagger$ and $\hat{\psi}$ satisfying the algebra (3.6.5). The construction is similar to the bosonic case, thus we arrive at a description of the space given by eigenstates of the fermionic field operators, but with Grassmann-valued eigenvalues this time. One introduces two Grassmann variables ψ and $\bar{\psi}$, and defines the coherent state $|\psi\rangle$ as

$$|\psi\rangle = e^{\hat{\psi}^\dagger \psi} |0\rangle, \quad \hat{\psi} |\psi\rangle = \psi |\psi\rangle,$$

where $|0\rangle$ is the Fock vacuum defined by $\hat{\psi} |0\rangle = 0$, $\hat{\psi}^\dagger |0\rangle = |1\rangle$. We also have

$$\langle \bar{\psi} | = \langle 0 | e^{\bar{\psi}\hat{\psi}}, \quad \langle \bar{\psi} | \hat{\psi}^\dagger = \langle \bar{\psi} | \bar{\psi}.$$

The Grassmann numbers, such as ψ and its complex conjugate $\bar{\psi}$, anticommute between themselves, and we define them to anticommute also with the fermionic operators $\hat{\psi}^\dagger$ and $\hat{\psi}$. No confusion should arise between the operators $\hat{\psi}$ and $\hat{\psi}^\dagger$ that have a hat, and the complex Grassmann variables ψ and $\bar{\psi}$, eigenvalues of the eigenstates $|\psi\rangle$ and $\langle \bar{\psi} |$ respectively, that carry no hat.

The properties of fermionic coherent states can be summarized as follows:

1. the **scalar product** between two coherent states is

$$\langle \bar{\psi} | \psi \rangle = e^{\bar{\psi}\psi};$$

2. the set of coherent states provides a **resolution of the identity**

$$\mathbb{I} = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} |\psi\rangle \langle \bar{\psi}|,$$

where the integration measure is defined as $d\bar{\psi} d\psi = d\psi d\bar{\psi}$;

3. the **trace** of an operator \hat{O} can be computed as

$$\text{Tr } \hat{O} = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} \langle -\bar{\psi} | \hat{O} | \psi \rangle.$$

4. the **supertrace** of an operator \hat{O} is defined as

$$\text{Str } \hat{O} = \text{Tr} [(-1)^{\hat{F}} \hat{O}] = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} \langle \bar{\psi} | \hat{O} | \psi \rangle,$$

where $\hat{F} = \hat{\psi}^\dagger \hat{\psi}$ is the fermion number operator, defined by its action on the Fock basis states as $F |0\rangle = 0$ and $F |1\rangle = 1$.

We can now prove these properties by direct computation, using the definitions of the coherent states and the properties of Grassmann variables and fermionic operators.

(0) At first, the definitions of the coherent states imply immediately the eigenvalue equations for the annihilation and creation operators

$$\begin{aligned} |\psi\rangle &= e^{\hat{\psi}^\dagger \psi} |0\rangle = (1 + \hat{\psi}^\dagger \psi) |0\rangle \\ &= |0\rangle + \psi |1\rangle, \implies \hat{\psi} |\psi\rangle = \psi |\psi\rangle, \\ \langle \bar{\psi}| &= \langle 0| e^{\bar{\psi} \hat{\psi}} = \langle 0| (1 + \bar{\psi} \hat{\psi}) \\ &= \langle 0| + \bar{\psi} \langle 1|, \implies \langle \bar{\psi}| \hat{\psi}^\dagger = \langle \bar{\psi}| \bar{\psi}. \end{aligned}$$

Note that terms proportional to ψ^2 can be inserted or eliminated at wish, as they vanish due to the Grassmann property $\psi^2 = 0$.

(1) The scalar product between two coherent states is computed as

$$\langle \bar{\psi} | \psi \rangle = \langle 0| (1 + \bar{\psi} \hat{\psi})(1 + \hat{\psi}^\dagger \psi) |0\rangle = (\langle 0| - \langle 1| \bar{\psi}) (\langle 0| - \psi |1\rangle) = 1 + \bar{\psi} \psi = e^{\bar{\psi} \psi}.$$

We point out that the Grassmann variables are here defined to commute with the Fock vacuum $|0\rangle$, so that they commute with the coherent states, but anticommute with $|1\rangle = \hat{\psi}^\dagger |0\rangle$ (as they anticommute with $\hat{\psi}^\dagger$).

(2) The resolution of the identity is proven by direct computation. Expanding the coherent states in terms of the Fock basis states, one has

$$\mathbb{I} = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} |\psi\rangle \langle \bar{\psi}| = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} (|0\rangle + \psi |1\rangle) (\langle 0| + \bar{\psi} \langle 1|).$$

Now we can compute the Berezin integrals remembering that $\int d\psi = \frac{\partial_L}{\partial \bar{\psi}}$, with the idea to obtain the completeness relation $\mathbb{I} = |0\rangle \langle 0| + |1\rangle \langle 1|$:

$$\frac{\partial_L}{\partial \bar{\psi}} \frac{\partial_L}{\partial \psi} (1 - \bar{\psi}\psi) (|0\rangle \langle 0| + \bar{\psi} |0\rangle \langle 1| + \psi |1\rangle \langle 0| + \psi \bar{\psi} |1\rangle \langle 1|),$$

from which, since grassmann variables square to zero and the terms without both of the variables cancels out when derived, only two terms survive the differentiation:

$$\mathbb{I} = \frac{\partial_L}{\partial \psi} \frac{\partial_L}{\partial \bar{\psi}} (\psi \bar{\psi} |1\rangle \langle 1| - \bar{\psi} \psi |0\rangle \langle 0|) = |0\rangle \langle 0| + |1\rangle \langle 1|.$$

(3) The trace of a bosonic operator \hat{O} , which commutes with ψ and $\bar{\psi}$, is computed as

$$\begin{aligned} \text{Tr } \hat{O} &= \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} \langle -\bar{\psi}| \hat{O} |\psi\rangle \\ &= \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} (\langle 0| - \langle 1| \bar{\psi}) \hat{O} (|0\rangle + \psi |1\rangle) \\ &= \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} (\langle 0| \hat{O} |0\rangle + \langle 0| \hat{O} |1\rangle \psi - \bar{\psi} \langle 1| \hat{O} |0\rangle - \bar{\psi} \langle 1| \hat{O} |1\rangle \psi) \\ &= \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} (\langle 0| \hat{O} |0\rangle - \bar{\psi} \langle 1| \hat{O} |1\rangle \psi) \\ &= \langle 0| \hat{O} |0\rangle + \langle 1| \hat{O} |1\rangle = \text{Tr } \hat{O}, \end{aligned}$$

recalling the steps of the resolution of the identity proof to compute the Berezin integrals.

(4) The supertrace of an operator \hat{O} can be computed similarly as:

$$\begin{aligned} \text{STr}\hat{O} &= \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} \langle \bar{\psi} | \hat{O} | \psi \rangle \\ &= \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} (\langle 0 | + \langle 1 | \bar{\psi}) \hat{O} (| 0 \rangle + \psi | 1 \rangle) \\ &= \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} (\langle 0 | \hat{O} | 0 \rangle + \langle 0 | \hat{O} | 1 \rangle \psi + \bar{\psi} \langle 1 | \hat{O} | 0 \rangle + \bar{\psi} \langle 1 | \hat{O} | 1 \rangle \psi) \\ &= \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} (\langle 0 | \hat{O} | 0 \rangle + \bar{\psi} \langle 1 | \hat{O} | 1 \rangle \psi) \\ &= \langle 0 | \hat{O} | 0 \rangle - \langle 1 | \hat{O} | 1 \rangle = \text{STr } \hat{O}, \end{aligned}$$

The generalization to more fermionic degrees of freedom is straightforward.

3.6.4 | Fermionic Path Integrals

We now have all the tools to find a path integral representation of the transition amplitude between coherent states

$$\langle \bar{\psi}_f | e^{-i\hat{H}T} | \bar{\psi}_i \rangle,$$

where we set $\hbar = 1$ for notational simplicity. We consider an hamiltonian $\hat{H}(\hat{\psi}^\dagger, \hat{\psi})$ written in such a way that all creation operators are on the left of the annihilation operators, something that is always possible to achieve using the fundamental anticommutation relations. Note also that for a single pair of fermionic creation/annihilation operators, the most general (bosonic) hamiltonian takes the simple form $\hat{H} = \omega \hat{\psi}^\dagger \hat{\psi} + h_0$, with ω and h_0 real constants.

To turn the transition amplitude into a path integral, one divides the total propagation time T into N steps of duration $\epsilon = T/N$, so that $T = N\epsilon$. Using $N - 1$ times the decomposition of the identity in terms of coherent states, one gets the following equalities

$$\begin{aligned} \langle \bar{\psi}_f | e^{-i\hat{H}T} | \bar{\psi}_i \rangle &= \langle \bar{\psi}_f | \left(e^{-i\hat{H}\epsilon} \right)^N | \bar{\psi}_i \rangle \quad N \text{ exponentials and } N - 1 \text{ identities} \\ &= \int \prod_{k=1}^{N-1} d\bar{\psi}_k d\psi_k e^{-\bar{\psi}_k \psi_k} \prod_{k=1}^N \langle \bar{\psi}_k | e^{-i\hat{H}\epsilon} | \psi_{k-1} \rangle, \end{aligned}$$

where we have defined $\psi_0 \equiv \psi_i$ and $\bar{\psi}_N \equiv \bar{\psi}_f$. For $\epsilon \rightarrow 0$, one can approximate the elementary transition amplitudes as

$$\langle \bar{\psi}_k | e^{-i\hat{H}\epsilon} | \psi_{k-1} \rangle \approx \langle \bar{\psi}_k | (1 - i\hat{H}\epsilon) | \psi_{k-1} \rangle = \langle \bar{\psi}_k | \psi_{k-1} \rangle - i\epsilon \langle \bar{\psi}_k | \hat{H} | \psi_{k-1} \rangle.$$

The substitution $\hat{H}(\hat{\psi}^\dagger, \hat{\psi}) \rightarrow H(\bar{\psi}_k, \psi_{k-1})$ follows from the ordering of the hamiltonian specified previously ($\hat{\psi}^\dagger$ on the left and $\hat{\psi}$ on the right). This allows one to act with the creation operator on a bra eigenstate, and with the annihilation operator on a ket eigenstate, so that all operators in the hamiltonian get substituted by the respective eigenvalues, producing a function of these Grassmann numbers. This way, the hamiltonian operator $\hat{H}(\hat{\psi}^\dagger, \hat{\psi})$ gets substituted by the hamiltonian function $H(\bar{\psi}_k, \psi_{k-1})$. These approximations are valid for $N \rightarrow \infty$, i.e. $\epsilon \rightarrow 0$, so that we can write

$$\langle \psi_k | e^{-i\hat{H}\epsilon} | \psi_{k-1} \rangle \approx e^{\bar{\psi}_k \psi_{k-1}} e^{-i\epsilon H(\bar{\psi}_k, \psi_{k-1})}.$$

Thus we can reinsert this expression into the previous formula for the transition amplitude, obtaining

$$\begin{aligned}\langle \bar{\psi}_f | e^{-i\hat{H}T} | \bar{\psi}_i \rangle &= \int \prod_{k=1}^{N-1} d\bar{\psi}_k d\psi_k \exp \left\{ \sum_{k=1}^N [\bar{\psi}_k \psi_{k-1} - \bar{\psi}_k \psi_k - i\epsilon H(\bar{\psi}_k, \psi_{k-1})] \right\} \\ &= \int D\bar{\psi} D\psi \exp \left\{ \int_0^T dt \left[\bar{\psi}(t) \frac{\partial}{\partial t} \psi(t) - iH(\bar{\psi}(t), \psi(t)) \right] \right\} = \int D\bar{\psi} D\psi e^{iS[\bar{\psi}, \psi]}.\end{aligned}$$

This is the path integral for one complex fermionic degree of freedom. We recognize in the exponent the discretization of the classical action

$$S[\bar{\psi}, \psi] = \int_0^T dt \left[i\bar{\psi}(t) \frac{\partial}{\partial t} \psi(t) - H(\bar{\psi}(t), \psi(t)) \right], \rightarrow S[\psi, \bar{\psi}] = \sum_{k=1}^N \epsilon \left[i\bar{\psi}_k \frac{\psi_k - \psi_{k-1}}{\epsilon} - H(\bar{\psi}_k, \psi_{k-1}) \right] - i\bar{\psi}_N \psi_N,$$

where $T = N\epsilon$ is the total propagation time. The discrete values ψ_k and $\bar{\psi}_k$ are those corresponding to the values of the continuous functions evaluated at times $t = k\epsilon$, i.e. $\psi_k = \psi(k\epsilon)$ and $\bar{\psi}_k = \bar{\psi}(k\epsilon)$. The last way of writing the amplitude in (197) is symbolic and indicates the formal sum over all paths $\bar{\psi}(t), \psi(t)$ with boundary conditions $\psi(0) = \psi_0 \equiv \psi_i$ and $\bar{\psi}(T) = \bar{\psi}_N \equiv \bar{\psi}_f$, weighed by the exponential of i times the classical action $S[\bar{\psi}, \psi]$. Note that the action contains the boundary term $-i\bar{\psi}(T)\psi(T)$. It is essential for formulating a variational principle where the boundary data are fixed by specifying the initial value of the function $\psi(t)$ and the final value of the function $\bar{\psi}(t)$ (i.e. $\psi(0) = \psi_i$ and $\bar{\psi}(T) = \bar{\psi}_f$).

Trace. One can now produce a path integral expression for the trace of the transition amplitude $e^{-i\hat{H}T}$. Using the expression of the trace in the coherent state basis, and the path integral representation of the transition amplitude, one finds

$$\begin{aligned}\text{Tr } e^{-i\hat{H}T} &= \int d\bar{\psi}_0 d\psi_0 e^{-\bar{\psi}_0 \psi_0} \langle -\bar{\psi}_0 | e^{-i\hat{H}T} | \psi_0 \rangle \\ &= \lim_{N \rightarrow \infty} \int \left(\prod_{k=0}^{N-1} d\bar{\psi}_k d\psi_k \right) \exp \left\{ i\epsilon \sum_{k=1}^N \left[i\bar{\psi}_k \frac{\psi_k - \psi_{k-1}}{\epsilon} - H(\bar{\psi}_k, \psi_{k-1}) \right] \right\} \\ &= \int_A D\bar{\psi} D\psi e^{iS[\bar{\psi}, \psi]},\end{aligned}$$

where we have identified $\bar{\psi}_N = -\bar{\psi}_0$ and $\psi_N = -\psi_0$, and used that the exponential $e^{-\bar{\psi}_0 \psi_0}$ from the trace cancels the boundary term $e^{\bar{\psi}_N \psi_N}$. Note that with this identification, the path integral measure can also be written as a sum from 1 to N , as $\prod_{k=1}^N d\bar{\psi}_k d\psi_k$. In the continuum limit, one finds a sum on all antiperiodic paths i.e. paths with $\psi(T) = -\psi(0)$ and $\bar{\psi}(T) = -\bar{\psi}(0)$ (A on the integral stands for **antiperiodic boundary conditions**). This representation finds obvious applications in statistical mechanical problems involving fermions.

Supertrace. Similarly, the supertrace is calculated by

$$\begin{aligned}\text{STr } e^{-i\hat{H}T} &= \int d\bar{\psi}_0 d\psi_0 e^{-\bar{\psi}_0 \psi_0} \langle \bar{\psi}_0 | e^{-i\hat{H}T} | \psi_0 \rangle \\ &= \lim_{N \rightarrow \infty} \int \left(\prod_{k=0}^{N-1} d\bar{\psi}_k d\psi_k \right) \exp \left\{ i\epsilon \sum_{k=1}^N \left[i\bar{\psi}_k \frac{\psi_k - \psi_{k-1}}{\epsilon} - H(\bar{\psi}_k, \psi_{k-1}) \right] \right\} \\ &= \int_P D\bar{\psi} D\psi e^{iS[\bar{\psi}, \psi]},\end{aligned}$$

where we have now identified $\bar{\psi}_N = \bar{\psi}_0$ and $\psi_N = \psi_0$. Again the term $e^{-\bar{\psi}_0\psi_0}$ from the supertrace cancels the boundary term $e^{\bar{\psi}_N\psi_N}$. In the continuum limit, the sum is over all periodic trajectories defined by the boundary conditions $\psi(T) = \psi(0)$ and $\bar{\psi}(T) = \bar{\psi}(0)$ (P stands for **periodic boundary conditions**).

To conclude, we have derived the path integral for fermionic systems from the operatorial formulation using a time slicing of the total propagation time. Time slicing produces a discretization of the classical action and defines concretely the meaning of the path integral once written in the continuum notation (i.e., it provides a regularization). We have discussed a simple model with one complex degree of freedom $\psi(t)$ and its complex conjugate $\bar{\psi}(t)$ (it may be called a Dirac fermion in one dimension). The extension to several complex degrees of freedom is immediate.

3.6.5 | Correlation Functions

Correlation functions are defined as normalized averages of the dynamical variables. Similar to the bosonic case, a generating functional can be introduced by incorporating sources into the path integral formulation. Using a hypercondensed notation, all fermionic fields are represented by ψ^i and the corresponding sources denoted by η_i are taken to be Grassmann-valued variables as well. Then, the generating functional for correlation functions is expressed as follows:

$$Z[\eta] = \int D\psi e^{i(S[\psi] + \eta_i \psi^i)}.$$

As an example, the two-point function is given by

$$\langle \psi^i \psi^j \rangle = \frac{1}{Z[0]} \left(\frac{1}{i} \right)^2 \frac{\delta^2 Z[\eta]}{\delta \eta_i \delta \eta_j} \Big|_{\eta=0}.$$

In a free theory, identified by a quadratic action of the form

$$S[\psi] = \frac{1}{2} \psi^i K_{ij} \psi^j,$$

with K_{ij} an antisymmetric matrix, one formally computes the path integral with sources by gaussian integration (after completing squares in terms of $\psi^i + G^{ij}\eta_j$ and using the transitional invariance of the measure). The answer takes the form

$$Z[\eta] = Z[0] e^{-\frac{i}{2} \eta_i G^{ij} \eta_j} = \sqrt{\det K_{ij}} e^{-\frac{i}{2} \eta_i G^{ij} \eta_j},$$

where G^{ij} is the inverse of the kinetic operator K_{ij} , defined by the relation

$$K_{ij} G^{jk} = \delta_i^k.$$

The two-point function is then found to be

$$\langle \psi^i \psi^j \rangle = -i G^{ij},$$

which lead us to identify G^{ij} as the fermionic propagator of the theory, the Green function in quantum mechanical applications. To check the overall normalization, one must be careful with signs arising from the anticommuting character of the Grassmann variables and from the antisymmetric properties of K_{ij} and G^{ij} . Similar formulae may be written down for complex fermions (they are contained in the above formula as well, for example setting $\psi^i \equiv (\psi^a, \bar{\psi}_a)$). As they apply to the

case of a Dirac fermion, let us write down the main formulae for the variables ψ^i with complex conjugates $\bar{\psi}_i$

$$Z[\eta, \bar{\eta}] = \int D\psi D\bar{\psi} e^{i(S[\psi, \bar{\psi}] + \bar{\eta}_i \psi^i + \bar{\psi}_i \eta^i)} = \det K^i_j e^{i\bar{\eta}_i G^i_j \eta^j},$$

$$\langle \psi^i \bar{\psi}_j \rangle = \frac{1}{Z[0, 0]} \left(\frac{1}{i} \right)^2 \frac{\delta^2 Z[\eta, \bar{\eta}]}{\delta \bar{\eta}_i \delta \eta^j} \Big|_{\eta=\bar{\eta}=0} = -i G^i_j,$$

where the results are obtained for a free theory with quadratic action

$$S[\psi, \bar{\psi}] = \bar{\psi}_i K^i_j \psi^j,$$

and $Z[\eta, \bar{\eta}]$ has been computed completing the squares in the path integral (using G^i_j , the inverse of the kinetic operator K^i_j). Suitable boundary conditions are implicit in the path integral and Green functions G^i_j . The entire set of generating functionals discussed in the bosonic case can similarly be introduced here. Wick's theorem similarly goes through, and one need only keep track of the signs that emerge when commuting Grassmann numbers.

Let us consider the examples of the fermionic oscillator and Dirac field.

Example (Fermionic Oscillator). The fermionic oscillator has classical action (see eq. (3.6.1))

$$S[\psi, \bar{\psi}] = \int dt \bar{\psi}(t) \left[i \frac{\partial}{\partial t} - \omega \right] \psi(t),$$

and the path integral with sources is computed by completing squares

$$Z[\eta, \bar{\eta}] = \int D\psi D\bar{\psi} e^{i(S[\psi, \bar{\psi}] + \int dt [\bar{\eta}(t)\psi(t) + \bar{\psi}(t)\eta(t)])}$$

$$= N \exp \left\{ i \int \int dt dt' \bar{\eta}(t) G(t-t') \eta(t') \right\},$$

where $G(t-t')$ is the Green function of the operator $K = -i\partial_t + \omega$, with

$$(-i\partial_t + \omega) G(t-t') = \delta(t-t'),$$

and reads:

$$G(t-t') = \int \frac{dp}{2\pi} \frac{e^{-ip(t-t')}}{-p + \omega} = \int \frac{dp}{2\pi} e^{-ip(t-t')} \frac{p + \omega}{-p^2 + \omega^2 - i\epsilon} = i\theta(t-t') e^{-i\omega(t-t')},$$

where only a pole is present, in $p = \omega$. As usual, the $i\epsilon$ prescription has been introduced to define the propagator properly (positive frequencies forward in time). The two-point function is then found to be

$$\langle \psi(t) \bar{\psi}(t') \rangle = -iG(t-t') = \theta(t-t') e^{-i\omega(t-t')}.$$

Example (Dirac Field). Similar considerations apply to the **Dirac field**, with classical action

$$S[\psi, \bar{\psi}] = \int d^4x \bar{\psi}(x) (i\gamma^\mu \partial_\mu - m) \psi(x),$$

and path integral with sources

$$Z[\eta, \bar{\eta}] = \int D\psi D\bar{\psi} e^{i(S[\psi, \bar{\psi}] + \int d^4x [\bar{\eta}(x)\psi(x) + \bar{\psi}(x)\eta(x)])}$$

$$= N \exp \left\{ i \int \int d^4x d^4y \bar{\eta}(x) G(x-y) \eta(y) \right\},$$

TODO: compute it if you want

where $G(x - y)$ is the Green function of the operator $K = i\gamma^\mu \partial_\mu + m = \not{p} + m$, with

$$(i\gamma^\mu \partial_\mu + m) G(x - y) = \delta^{(4)}(x - y),$$

and reads:

$$G(x - y) = \int \frac{d^4 p}{(2\pi)^4} e^{ip^\mu(x^\mu - y^\mu)} \frac{(-i\not{p} + m)}{p^2 + m^2 - i\epsilon}.$$

It is often indicated also by $S(x - y)$ (S for spinor). The two-point function (propagator) then becomes

$$\langle \psi(x) \bar{\psi}(y) \rangle = -iG(x - y) = - \int \frac{d^4 p}{(2\pi)^4} e^{ip^\mu(x^\mu - y^\mu)} \frac{(\not{p} + im)}{p^2 + m^2 - i\epsilon}.$$

which is interpreted as describing a particle propagating from y^μ to x^μ if $x^0 > y^0$, or an antiparticle propagating from x^μ to y^μ if $y^0 > x^0$.

Wick's theorem and perturbation theory for fermionic systems can be developed similarly to the bosonic case, with suitable signs arising from the anticommuting nature of the Grassmann variables. To conclude, a last remark: a well-known property of perturbation theory written in terms of Feynman diagram (and related Feynman rules that translate them into equations) states that fermionic loops carry a minus sign. This is easily seen as arising for the Grassmann character of the fermionic variables. In a hypercondensed notation, the free propagator is denoted by

$$\langle \psi^i \bar{\psi}_j \rangle = j \bullet \overline{\bullet} i,$$

and considering an interaction of the form $S_{int} = \lambda \bar{\psi}_i \psi^i$, one finds in diagrams arising from the expansion of the Dyson formula $\langle e^{iS_{int}} \rangle$ terms of the form

$$\langle S_{int}^2 \rangle_c = \lambda^2 \langle \bar{\psi}_i \psi^i \bar{\psi}_j \psi^j \rangle_c = -\lambda^2 \langle \psi^j \bar{\psi}_i \rangle \langle \psi^i \bar{\psi}_j \rangle = j \bullet \overline{\bullet} i,$$

where we recognize the propagators forming the loop and the explicit minus sign. The minus sign is due to the fact that the first term ψ^i must be moved past three Grassmann variables to reach the last position. Then, we see a propagator going from the first point to the second one and the second propagator bringing back to the first point.

Appendices

A | Notation and Conventions

Upper and Lower Indices, Dotted Indices

In section 1.3, we defined Lie groups using matrices that directly identify a representation, the so-called defining (or fundamental) representation. We denote the dimension of the defining representation by N . As mentioned earlier, we can think of the $N \times N$ matrices of this representation as operators acting on a vector space V of dimension N . We denote the vectors in V by their components v^a , where the index $a = 1, 2, \dots, N$. The vectors $v^a \in V$ are transformed by the matrices $[R(g)]^a_b$ of the representation. By definition, a generic vector v^a transforms under the action of the group G as follows:

$$v^a \xrightarrow{g \in G} v'^a = [R(g)]^a_b v^b.$$

Note that the convention is used where repeated indices are automatically summed over all their possible values. Vectors that transform in the manner described above are defined to have upper indices. Vectors whose components have upper indices belong to vector spaces equivalent to V and transform the same way under the action of G , as described by the equation above.

Relativistic Framework Notation

In the relativistic framework, we use Greek letters $\mu, \nu, \rho, \sigma, \dots$ to denote spacetime indices that run from 0 to 3. The time component is indicated by the index 0, while the spatial components are indicated by Latin indices i, j, k, \dots that run from 1 to 3. The metric tensor of Minkowski spacetime is denoted by $\eta_{\mu\nu}$ and has the *mostly plus* signature $\eta^{\mu\nu} = \text{diag}(-1, +1, +1, +1)$. The Einstein summation convention is used, where repeated upper and lower indices are summed over all their possible values.

Our main conventions for special relativity are as follows:

$x^\mu = (ct, x, y, z) = (x^0, x^1, x^2, x^3)$	(spacetime coordinates)
$x'^\mu = \Lambda^\mu_\nu x^\nu$	(Lorentz transformations)
$\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$	(Minkowski metric)
$s^2 = \eta_{\mu\nu} x^\mu x^\nu = x^\mu x_\mu$	(invariant length)
$\eta^{\mu\nu} = (\eta^{-1})^{\mu\nu}$	(inverse metric)
$x_\mu = \eta_{\mu\nu} x^\nu, \quad x^\mu = \eta^{\mu\nu} x_\nu$	(lowering/raising indices)
$O(3, 1) = \{\text{real } 4 \times 4 \text{ matrices } \Lambda \mid \Lambda^T \eta \Lambda = \eta\}$	(Lorentz group)
$SO^+(3, 1) = \{\text{real } 4 \times 4 \text{ matrices } \Lambda \mid \Lambda^T \eta \Lambda = \eta, \det \Lambda = 1, \Lambda^0_0 \geq 1\}$	(restricted Lorentz group)
$x'^\mu = \Lambda^\mu_\nu x^\nu + a^\mu$	(Poincaré transformations)
$\partial_\mu = \frac{\partial}{\partial x^\mu}$	(spacetime derivative)
$\partial'_\mu = \Lambda_\mu^\nu \partial_\nu, \quad \Lambda_\mu^\nu \equiv \eta_{\mu\alpha} \Lambda^\alpha_\beta \eta^{\beta\nu} = (\eta \Lambda \eta^{-1})_\mu^\nu = (\Lambda^{T,-1})_\mu^\nu$	(Lorentz transformation of derivatives)
$F'^{\mu\nu} = \Lambda^\mu_\alpha \Lambda^\nu_\beta F^{\alpha\beta}$	(Lorentz transformation of rank 2 tensor)

B | Theoretical insights

Noether's theorem and Action formalism

Action Principle. Let us briefly review the action principle in mechanics and field theories, considering the case of a particle. The main purpose is to underline its relation to canonical quantization and to stress the relevance of symmetries. As anticipated, the action is essential for the path integral quantization.

Consider a non-relativistic particle of mass m that moves in a single dimension with coordinate q and subject to a conservative force $F = -\frac{\partial}{\partial q}V$. Newton's equations of motion reads

$$F = m\ddot{q},$$

and can be derived from an action principle. The action is a functional of the trajectory of the particle $q(t)$ (the dynamical variable of the system) and associates a real number to each function $q(t)$. In general, physical systems are described by an action of the type

$$S[q(t)] = \int dt L(q(t), \dot{q}(t)), \quad L(q(t), \dot{q}(t)) =$$

[...]

Hamiltonian formalism. The basic idea of the hamiltonian formalism is to have equations of motion that are first order in time. To review it, we follow a simple example: a non-relativistic particle of coordinates q^i and configuration space lagrangian

$$pdf$$

where indices are lowered with the metric δ_{ij} (and are thus equivalent to upper indices in our model, the distinction of upper and lower indices is, however, useful in more general contexts). Transition to the hamiltonian formalism takes place as follows:

1. The dynamical variables are doubled by introducing conjugate momentum p^i to each coordinate q_i

$$pdf$$

The set (q_i, p^i) constitutes the coordinates of phase space.

2. The hamiltonian $H(q, p)$ is defined as the Legendre transform of the lagrangian L

$$pdf$$

It is a function on phase space.

3. The **Poisson brackets** are defined as follows. For any two functions A and B of phase space, their Poisson brackets are defined by

$$pdf$$

where we have used the summation convention for repeated indices. In particular,

$$pdf$$

4. The hamiltonian equations of motion can be written as

$$pdf$$

and are of the first order in time. In our example, they become

$$pdf$$

and are evidently equivalent to the lagrangian equations [...] . The hamiltonian H is interpreted as the generator of time translations, and moves the initial conditions (a point in phase space) over time by an infinitesimal amount dt . The generator of these canonical transformations is given by Hdt , and acts through the Poisson brackets ([...]).

These equations can be obtained from an action. In phase space, the action takes the form

$$pdf$$

and minimizing it, one finds

$$pdf$$

from which one recognizes Hamilton's equations of motion. Note that in this formulation one needs $2n$ integration constants, which are given by specifying the coordinates q^i at initial and final times.

The hamiltonian structure is the starting point of canonical quantization:

$$pdf$$

where the classical dynamical variables z^a are elevated to linear operators \hat{z}^a acting on a Hilbert space. The quantum commutation relations are fixed by the values of the classical Poisson bracket. The vectors of the Hilbert space describe the possible quantum states of the system, whose evolution is governed by the Schrödinger equation.