The Principles of Quantum Mechanics

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Preface

The premise of this book is that the principles of classical physics should follow from a correct and complete mathematics of quantum mechanics. The opposite approach has been taken since the origin of the "new" quantum mechanics in the 1920s, by discussing quantum mechanics as if it could be derived from classical physics. This has resulted in many issues of interpretation, and convoluted and incorrect mathematics. By applying the revised mathematics of quantum mechanics that I present in this book, it is possible to resolve some of the long standing issues in the field of quantum mechanics. As an example, the procedure of renormalization in quantum field theory can be given a precise meaning.

The ideas in this book evolved over forty years of physics education and practice, and that journey is summarized below. In college, I enjoyed a wonderfully coherent education on classical physics. The team of professors in physics, chemistry and mathematics coordinated a curriculum that aligned physics concepts with mathematical foundations and methods. This enabled me to see the beauty, elegance, and coherence of classical physics.

When I was introduced to quantum mechanics, I was disappointed by the way quantum concepts such as the probability rule, the complementarity principle, particle-wave duality, and the uncertainty principle are disconnected from the mathematics of quantum mechanics. It appeared there was a big gap in maturity, elegance, coherence and consistency between quantum mechanics and classical physics. I learned that others felt that way and that there had been an ongoing debate about this since quantum mechanics was formulated in 1926 (Jammer, 1966). That debate continues to this day (Wallace, 2008). I felt a need for a theory for quantum phenomena that achieved the same coherence and consistency as the classical theories I admired.

The existence of infinities in the theory of quantum fields was a known issue with quantum mechanics from the very beginning. Arcane computations are needed to extract finite numbers from formulas that lead to infinite results. These intricate spells and incantations first are invoked to regularize integrals, and then to "renormalize" parameters in the dynamical equations. While this has been accepted as a pragmatic solution because these manipulations do achieve miraculous agreement with experimental results, it is widely recognized that this is a problem.

In the summer of 1980, while working on my doctorate, I read "Integration in Hilbert Space" written by Skorohod (1974). It taught me the theory of measures on function spaces, not in the widely known context of probability theory and stochastic analysis, but as a basic part of functional analysis. Just as functional analysis appeared to me to be the mathematical foundation for quantum mechanics of systems with a finite number of degrees of freedom, this suggested one could formulate quantum mechanics of fields, which are infinite systems, as a natural generalization. The idea seemed so obvious that I was convinced that someone would quickly formulate an integrated theory of finite and infinite quantum systems.

As a computational scientist, much of my work was creating software that modeled

molecular reactions. I learned a method of using computers and computation as part of exploring abstract mathematical concepts, which I applied during the preparation of this book.

Over the years, I stayed informed about the developments in mathematics and in the foundations of quantum mechanics. I never saw the theoretical development that I expected from the application of functional analysis take place. This was confirmed when I sat in on a course on functional integration methods taught in the spring of 2004 by John Klauder. I decided to attempt to put together this theoretical development.

I started by gaining an understanding of functionals (functions of functions). This knowledge shed a new light for me on some of the unresolved issues in quantum field theory. I found that functionals are counterintuitive in a number of important ways. This insight provided the foundation for developing the ideas in this book, and further enabled me to carry out the required computations.

I consider what I am presenting to be a thorough revision of the principles of quantum mechanics, a revised edition as it were of the book by Dirac (1930) with the same title. There are two major areas of revision which are highlighted below.

In contrast to the traditional way of presenting quantum mechanics, I start from the premise that quantum mechanics is a theory of wave functions and of the dynamical law, the Heisenberg-Schrödinger-Dirac equation, that governs them as formulated in 1926. I do not start with quantum concepts such as the probability rule, the complementarity principle, particle-wave duality, and the uncertainty principle; instead, these are presented as derived concepts, obtained after a very lengthy and complicated mathematical journey.

Based on the work I did with functionals, I do not define interacting quantum fields by perturbation theory. Rather, quantum fields are defined as dynamical systems of quantum excitations, that have an internal structure produced by unavoidable self interaction. The methods known from and tested in nonrelativistic quantum mechanics can be generalized to apply to quantum fields. Perturbation theory can then be used to compute properties of quantum fields in ways that do not lead to Feynman diagrams with infinite integrals that must be regularized. The process of renormalization becomes a well-defined mathematical process that defines a new Hamiltonian operator, not just new parameters.

The revised principles open up new approaches to several open problems. For example, defining quantum fields with perturbation theory has obstructed a complete formulation of quantum chromodynamics and quantum gravity. The Yang-Mills quantum field theory can now be defined and used to formulate a theory of quantum chromodynamics with the property of asymptotic freedom and confinement. Similarly, a quantum theory for the dynamics of space and the effects of gravity can be formulated.

The book is organized into three parts:

1. The first part introduces the physics concepts and explains how they work together to make a consistent theory. The first chapter "Principles" gives an overview and the remaining chapters provide the details. The first part is intended primarily for physicists.
2. The second part applies the principles from the first part to give the quantum theory of electrons and photons, of quarks and gluons, and of the geometry of space.

3. The third part is for the reader who seeks precision and rigor. It provides the mathematical and computational details. This part has a number of chapters with reference material as well as derivations and proofs to provide the foundation for the results obtained in the first part. The third part is intended primarily for mathematicians, and the format reflects that.

Links and cross references between the parts should allow the reader to start with the first part, learn things from the third part as the need arises, and then read the application of the principles in the second part.

The reader may wish to leaf through the book at first, reading only the short "trail markers". They give a brief overview of what happens close to the marker and provide guidance on how the complete story hangs together. The location of every trail marker can be found in the Index under "trail marker."

I hope the reader will enjoy the exploration of the consequences that have been opened up by these updated principles of quantum mechanics as much as I did.

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Notation

In general the meaning of symbols is made clear in the immediate context of where the symbol is used, section or theorem. However, there are a number of symbols that have a consistent meaning throughout the book. These definitions are collected here for convenience.

Sets and spaces. The set of natural numbers $1, 2, 3, \dots$ is denoted $\mathbb{N}$, the set of all integers $\{0, \pm 1, \pm 2, \pm 3, \dots\}$ by $\mathbb{Z}$, and the set of rational numbers $\{n/m | n, m \in \mathbb{Z}, m \neq 0\}$ by $\mathbb{Q}$. The real numbers are $\mathbb{R}$ and the complex numbers $\mathbb{C}$.

The topological dual of a topological space X is the space of continuous linear functionals on that space and is denoted by X^*.

The physical space we live in is denoted in general by $\mathbb{R}^d$, where the dimension of space d is 3, but can be 1 or 2, or even larger than 3. The dimension of spacetime is then $d + 1$.

The convention for spacetime is to put spatial coordinates first $r = (\vec{r}, t)$ with positive signature in the metric

$$\eta = g = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$$

so that the Minkowski product is

$$a_i b^i = \eta_{ij} a^j b^i = \sum_{i,j=1}^{4} \eta_{ij} a^j b^i = a^1 b^1 + a^2 b^2 + a^3 b^3 - a^4 b^4.$$

The notation for measurable square-integrable functions on a space X with a measure μ taking values in a space Y is denoted in the literature as $L^2(X, \mu, Y)$ or as $L^2(X, Y, \mu)$. When the measure is the Lebesgue measure λ, it is often omitted, so the notation becomes $L^2(X, Y)$. When the functions are real- of complex-valued, $Y = (R)$ or $\mathbb{C}$, the Hilbert space is written simply as $L^2(X)$.

The Hilbert space of real field configurations φ on space is denoted $\mathbb{F} = L^2(\mathbb{R}^d, \lambda, \mathbb{R}) = L^2(\mathbb{R}^d)$, with the last equality as a shorter specification; λ denotes the Lebesgue measure on $\mathbb{R}^d$; the final argument denotes the target space of the functions.

The Hilbert space of complex wave functionals Φ of fields is $\mathbb{H} = L^2(\mathbb{F}, \gamma, \mathbb{C})$, where γ is a measure on $\mathbb{F}$.

The Fock space generated with a Hilbert space X is denoted by $\mathcal{F}(X)$.

The standard Lie groups are denoted with capital letters: $SO(3), SU(2), SO(3, 1)$. The universal covering group is denoted with a line over the entire name: $\overline{SO(3)}$. The Lie algebra of the group is denoted with lowercase letters: $so(3), su(2), so(3, 1)$. The infinite-dimensional Lie group that is the local gauge group obtained by allowing gauge transformations change with location in space is denoted by putting a script letter "ℓ" in front of

the name of the global gauge group: $\ell SU(3)$; The corresponding infinite-dimensional Lie algebra is denoted $\ell su(3)$.

Elements. An array of numbers is denoted with a bar over the symbol: $\bar{x} = (x_1, \ldots, x_n)$.

A possibly infinite vector $\bar{\mu} = (\mu_1, \mu_2, \ldots)$ with each entry $\mu_m = 0, 1, 2, \ldots$ an index of some kind is called a *multi-index*.

The norm of the multi-index μ is given by $|\bar{\mu}| = \sum_{m=1}^{\infty} \mu_m$.

Let $\bar{\varepsilon}_m = (0, \ldots, 0, 1, 0, \ldots)$ denote the multi-index with only the index 1 at location m. Then the multi-indices $\bar{\mu} = (\mu_1, \ldots, \mu_{m-1}, \mu_m \pm 1, \mu_{m+1}, \ldots)$ can be written as $\bar{\mu} \pm \bar{\varepsilon}_m$.

When the meaning is clear from the context, we often omit the bar over the multi-index symbol to simplify notation. The norm of a multi-index gives the total number of excitations for one type of multi-index that we will use.

The set $\mathbb{K}$ of values of the multi-index ν is not totally ordered.

We use Roman letters for position in space and time. Vectors in d-dimensional physical space are denoted with the arrow over the symbol: $\vec{x} = \sum_i x_i \vec{e}_i$.

An element of a Lie algebra with generators $T_1, \ldots, T_n$ and coefficients $\bar{\omega} = (\omega_1, \ldots, \omega_n)$ is denoted with a box superscript as $\omega^{\square} = \sum_a \omega_a T_a$. To be consistent, one should put the box superscript on the generators of the algebra; but there is no such practice in the literature, so we will not do that either.

Vectors and matrices in general linear spaces like $\mathbb{R}^N$ and $\mathbb{C}^N$ are denoted in boldface.

Fields in space in general are denoted by lowercase Greek letters $\varphi(\vec{x})$. The time evolution of a field is then a function from the real axis of time $\mathbb{R}$ into $\mathbb{F}$ and can be written as $\varphi(t)$, φ_t, or $\varphi(\vec{x}, t)$ depending on the context.

wave functions of finite systems and wave functionals of infinite systems and fields are denoted by capital Greek letters $\Psi(x)$ and $\Psi[\varphi]$, respectively. The Dirac notation for elements of the Hilbert space $\mathbb{H}$ is the bra-ket notation $|\alpha\rangle$. The wave function is then $\Psi(x) = \langle x|\Psi\rangle$.

Linear operators in $\mathbb{H}$ are in bold, those in $\mathbb{F}$ are in regular typeface, possibly with a hat.

An $\mathbb{F}$-vector-valued linear operator in $\mathbb{H}$ is denoted by a bold symbol with a bar over it, when it is desirable to clearly exhibit the vector nature of the result of the operator.

The Kronecker delta is $\delta_{kl} = 1$ for $k = l$ and zero otherwise for k and l integer.

The Levi-Civita or permutation symbol is defined as

$$\varepsilon_{ijk} = \begin{cases} 1 & (i,j,k) = \text{cyclic}(1,2,3) \\ -1 & (i,j,k) = \text{cyclic}(1,3,2) \\ 0 & \text{otherwise} \end{cases}$$

The three complex 2×2 matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are called the Pauli matrices. They are a basis for the Lie algebra of the Lie group $SU(2)$.

The 4×4 Dirac matrices (Thaller, 1992, p. 36) have a representation with real matrix elements introduced by Majorana (1937)

$$\alpha_1 = \begin{pmatrix} \sigma_1 & 0 \\ 0 & -\sigma_1 \end{pmatrix} \quad \alpha_2 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \quad \alpha_3 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix} \quad \beta' = -i\beta = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

In that representation the gamma matrices $\gamma^j = -\beta'\alpha_j, j = 1, 2, 3$ and $\gamma^4 = -\beta'$ become

$$\gamma^1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix} \quad \gamma^2 = \begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix} \quad \gamma^3 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix} \quad \gamma^4 = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}.$$

Writing the contraction of a four-vector and the gamma matrices $\sum_{\nu=1}^{4} p^\nu \gamma^\nu = \not{p}$ as 4×4 spinor matrix is known as the Feynman slash notation.

The Gell-Mann matrices λ_j are the eight complex 3×3 matrices (Burgess and Moore, 2007, p. 44) given by

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \qquad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

They are a basis for the Lie algebra of the Lie group $SU(2)$.

Operations. The composition of functions is denoted by $\circ$, which means that $(f \circ g)(x) = f(g(x))$.

The time derivative of a function or field is sometimes denoted by a dot over the symbol: $\dot{f}$.

The symbol $\circ$ is also used to denote an abstract group composition law in chapter C.

The wedge product of two one-forms is denoted $\boldsymbol{\omega} \wedge \boldsymbol{\omega}$.

Complex conjugation is denoted by the asterisk superscript: a^*.

The Fourier transform of a function f is denoted by $\mathscr{F} f = \widetilde{f}$ and is defined as

$$\widetilde{f}(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{iyx} f(x) \mathrm{d}x$$

The adjoint of an operator is denoted by the dagger superscript: $A^\dagger$.

In physics the convention is to place the complex conjugation on the first element in the scalar product, whereas the mathematical literature usually places the conjugation on the second element. We use the physics convention.

A multi-index $\bar{\alpha}$ is an array $(\alpha_1, \ldots, \alpha_m)$ of positive integers. The sum of the components is denoted $|\bar{\alpha}| = \alpha_1 + \ldots + \alpha_m$. The partial derivative of a function f of m variables can then be written as

$$D^\alpha f = D_1^{\alpha_1} \ldots D_m^{\alpha_m} f = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \ldots \partial x_1^{\alpha_1}}$$

The integral of a function f with respect to a measure μ over a measurable set $A \subset X$ is written as

$$\int_A f \mathrm{d}\mu = \int_A f(x) \mu(\mathrm{d}x)$$

where the variable x takes on values in the space X.

Use of complex numbers. Complex numbers have many uses in quantum mechanics and these uses often overlap causing some confusion. Fortunately, this rarely leads to serious errors. We will keep the uses clearly separated.

1. Quantum mechanical wave functions and wave functionals are inherently complex because the Schrödinger equation has i in it explicitly. We will use complex valued wave functionals. They are elements of the Hilbert space $\mathbb{H}$.
2. Classical fields φ, like the scalar field considered in this chapter, are assumed to be real. The Hilbert space of field configurations $\mathbb{F}$ is therefore real. When we use the Fourier transform, we use the sine-cosine form to map real functions to real functions.
3. Charged fields are often written as complex fields $\varphi = \varphi_1 + i\varphi_2$ with the gauge group $U(1)$. This would lead to loading double use on complex numbers. We will then use the two components (φ_1, φ_2) to build the Hiobert space $\mathbb{F}$ of configurations.
4. Spin one-half fields are naturally described by two-component, complex fields associated with the universal covering group $SU(2)$ of $SO(3)$. This leads to another chance for double use of the complex numbers. The four-component Dirac field itself uses complex numbers twice already: Once to create a charged field that is the sum of two Majorana fields, which themselves already use complex numbers to create spin one-half fields. As a rule we will consider real Hilbert spaces $\mathbb{F}$ with appropriate multi-component, real fields.

The complex numbers can be represented as real 2×2 matrices as follows

$$a + ib \longleftrightarrow \begin{pmatrix} a & -b \\ b & a \end{pmatrix},$$

such that matrix addition and multiplication correspond to addition and multiplication of complex numbers

$$\begin{aligned} (a+ib)(c+id) &= ac - bd + i(ad+bc) = u + iv \\ \longleftrightarrow \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \begin{pmatrix} c & -d \\ d & c \end{pmatrix} &= \begin{pmatrix} ac-bd & -ad-bc \\ bc+ad & -bd+ac \end{pmatrix} = \begin{pmatrix} u & -v \\ v & u \end{pmatrix}. \end{aligned}$$

This allows for quick transformation of any complex number into a real matrix form.

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