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preface

Although there are many textbooks that deal with the formal apparatus of quantum mechanics (QM) and its application to standard problems, there are none that take into account the developments in the foundations of the subject that have taken place in the last few decades. There are specialized treatises on various aspects of the foundations of QM, but none that integrate those topics with the standard material. I hope to correct that unfortunate dichotomy, which has divorced the practical aspects of the subject from the interpretation and broader implications of the theory. This book is intended primarily as a graduate-level textbook, but it will also be of interest to physicists and philosophers who study the foundations of QM. Parts of the book could be used by senior undergraduate students. Some of the major innovations of this book are as follows.

It is generally recognized that *probability* is an essential fundamental concept needed for the interpretation and application of QM, and yet this topic has been seriously neglected in QM textbooks. In the first chapter, I briefly review probability theory and its interpretations. As the formalism of QM is developed throughout the book, it is related to the axioms of probability theory.

A great deal of care is devoted to the quantum *state* concept because it is crucial for a sound interpretation of the theory. The concept of *state* is first discussed qualitatively and related to probability in Chapter 2. This preliminary treatment is reinforced by more detailed treatments of *state preparation* and *state determination* in Chapter 8 and by the theory of *measurement* in Chapter 9. The theory of measurement is sometimes regarded as difficult or mysterious. However there are some firmly established results, which have not been taken into account in previous textbooks, but which are easy to develop and are very important in clarifying the interpretation of QM. Other chapters in which questions of interpretation come to the fore are Chapters 15 (the classical limit) and 20 (Bell's theorem). But a concern with understanding, and not merely calculation, pervades the whole book.

In addition to emphasizing the conceptual foundations and integrating the interpretation into the main body of the subject, I have introduced several innovations in the mathematical formalism. *Rigged Hilbert space* is introduced in Chapter 1 as a generalization of the more familiar Hilbert space. It allows vectors of infinite norm to be accommodated within the formalism, and eliminates the vagueness that often surrounds the question of whether the operators that represent observables possess a complete set of eigenvectors. The *space–time symmetries* of displacement, rotation, and Galilei transformations are exploited in Chapter 3 in order to derive the fundamental operators for momentum, angular momentum, and the Hamiltonian. This approach replaces the traditional heuristic, but inconclusive arguments based on analogy and wave–particle duality, which so frustrate the serious student. It also introduces *symmetry* concepts and techniques at an early stage so that they are immediately available for practical applications. This is done without requiring any prior knowledge of group theory. Indeed, a hypothetical reader who is ignorant of the mathematical meaning of the word group, and who interprets the reference to groups of transformations and operators as meaning sets of related transformations and operators, will lose none of the essential meaning.

Whenever possible I refer to real experiments that test or illustrate the fundamental aspects of quantum mechanics, such as the direct measurement of the momentum distribution in the hydrogen atom. Many of the experiments use the single-crystal neutron interferometer, which in recent years has turned thought experiments into real experiments. Others involve lasers and quantum optics.

Some other important topics, seldom included in previous QM textbooks, are the following: Landau levels of a charged particle in a magnetic field, the Aharonov–Bohm effect, and the ultrahigh-field Zeeman effect (Chapter 11); quantum beats in atomic spectroscopy (Secs. 12-4 and 19-7); quantum coherence, photon correlations (bunching and antibunching), and the limitations of classical electromagnetic theory (Chapter 19); and, finally, Bell's theorem, whose significance and implications are still being debated (Chapter 20).

The first chapter of the book consists entirely of mathematical topics (vector spaces, operators, and probability), which may be quickly skimmed by mathematically sophisticated readers who are anxious to get to the physical development that begins in Chapter 2. They have been placed at the beginning, rather than in an appendix, because one needs not only the results but also a coherent overview of the theory of these topics, since they form the mathematical language in which quantum theory is expressed. The amount of time that a student or a class spends on Chapter 1 may be expected to vary widely, depending on the degree of mathematical preparation. But, in any case, the important topics are collected together for convenient reference.

Many of the chapters are based on standard material; however I have included many novel examples and problems. Solutions to certain problems are given in Appendix D. These are not intended to be a representative selection. The solved problems are those that are particularly novel and those for which the answer or the method of solution is important for its own sake (rather than merely being an exercise).

At various places throughout the book I have segregated in double brackets, [[...]], comments of a historical, comparative, or critical nature. These remarks would not be needed by a hypothetical reader with no previous exposure to quantum mechanics. They are used to relate my approach, by way of comparison or contrast, to that of earlier writers, and sometimes to show, by means of criticism, the reason for my departure from the older approaches.

Acknowledgments

The writing of this book has drawn on a great many published sources, which are acknowledged at various places throughout the text. However I would like to give special mention to the work of Thomas F. Jordan, which forms the basis of Chapter 3. Many of the chapters and many of the problems have been field tested on classes of graduate students at Simon Fraser University. Special mention goes to my former student Bob Goldstein, who discovered a simple proof for the theorem in Sec. 8-3, and whose creative imagination was responsible for the paradox that forms the basis of Problem 9-6. In preparing Sec. 1-5 on probability theory, I benefited from discussions with Prof. C. Villegas. I would also like to thank Hans von Baeyer for the key idea in the derivation of the orbital angular momentum eigenvalues in Sec. 8-3, and W. G. Unruh for pointing out interesting features of the third example in Sec. 9-6.

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contents

chapter 1

mathematical prerequisites

Certain mathematical topics are essential for quantum mechanics, not only as computational tools, but because they form the most effective language in terms of which the theory can be formulated. These topics include the theory of linear vector spaces and linear operators and the theory of probability. The connection between quantum mechanics and linear algebra originated as an apparent by-product of the linear nature of Schrödinger's wave equation. But the theory was soon generalized beyond its simple beginnings, to include abstract "wave functions" in the $3N$-dimensional configuration space of N particles, and then to include discrete internal degrees of freedom such as spin, which have nothing to do with wave motion. The structure common to all of these diverse cases is that of linear operators on a vector space. A unified theory based on that mathematical structure was first formulated by P. A. M. Dirac, and the formulation used in this book is really a modernized version of Dirac's formalism.

That quantum mechanics does not predict a deterministic course of events, but rather the probabilities of various alternative possible events was recognized at an early stage, especially by Max Born. Modern applications seem more and more to involve correlation functions and nontrivial statistical distributions (especially in quantum optics), and therefore the relations between quantum theory and probability theory need to be expounded.

The physical development of quantum mechanics begins in Chapter 2, and the mathematically sophisticated reader may turn there at once. But since not only the results, but also the concepts and logical framework of Chapter 1 are freely used in developing the physical theory, the reader is advised to at least skim this first chapter before proceeding to Chapter 2.

1-1 LINEAR VECTOR SPACE

A *linear vector space* is a set of elements, called vectors, that is closed under addition and multiplication by scalars. That is to say, if ϕ and ψ are vectors, then so is $a\phi + b\psi$, where a and b are arbitrary scalars. If the scalars are the field of complex (real) numbers, we speak of a complex (real) linear vector space. Henceforth, the scalars will be the complex numbers unless otherwise stated.

Among the very large number of examples of linear vector spaces, there are two classes that are of common interest.

Example (i) Discrete vectors, which may be represented as columns of complex numbers,

$$\begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}$$

Example (ii) Spaces of functions of some type, for example, the space of all differentiable functions.

One can readily verify that these examples satisfy the definition of a linear vector space.

A set of vectors $\{\phi_n\}$ is said to be *linearly independent* if no nontrivial linear combination of them sums to zero, that is, if the equation $\sum_n c_n\phi_n = 0$ can hold only when $c_n = 0$ for all n. If this condition does not hold, the set of vectors is said to be *linearly dependent*, in which case it is possible to express a member of the set as a linear combination of the others.

The maximum number of linearly independent vectors in a space is called the *dimension* of the space. A maximal set of linearly independent vectors is called a *basis* for the space. Any vector in the space can be expressed as a linear combination of the basis vectors.

An *inner product* (or scalar product) for a linear vector space associates a scalar (ψ, ϕ) with every ordered pair of vectors. It must satisfy the following properties:

a. $(\psi, \phi) =$ a complex number
b. $(\phi, \psi) = (\psi, \phi)^*$
c. $(\phi, c_1\psi_1 + c_2\psi_2) = c_1(\phi, \psi_1) + c_2(\phi, \psi_2)$
d. $(\phi, \phi) \geq 0$ with equality holding if and only if $\phi = 0$

From properties b and c it follows that

$$(c_1\psi_1 + c_2\psi_2, \phi) = c_1^*(\psi_1, \phi) = c_2^*(\psi_2, \phi)$$

Therefore, we say that the inner product is *linear* in its second argument, and *antilinear* in its first argument.

Corresponding to our previous examples of vector spaces, we have the following inner products:

Example (i)

If ψ is the column vector with elements $a_1, a_2, \ldots$ and ϕ is the column vector with elements $b_1, b_2, \ldots,$ then

$$(\psi, \phi) = a_1^* b_1 + a_2^* b_2 + \cdots$$

Example (ii)

If ψ and ϕ are functions of x, then

$$(\psi, \phi) = \int \psi^*(x)\phi(x)w(x)\,dx$$

where $w(x)$ is a nonnegative weight function.

The inner product generalizes the notions of length and angle to arbitrary spaces. If the inner product of two vectors is zero, the vectors are said to be *orthogonal*.

The *norm* (or length) of a vector is defined as $\|\phi\| = (\phi, \phi)^{1/2}$. The inner product and the norm satisfy two important theorems: **Schwarz's inequality**,

$$|(\psi, \phi)|^2 \leq (\psi, \psi)(\phi, \phi) \tag{1-1}$$

and the **triangle inequality**,

$$\|(\psi + \phi)\| \leq \|\psi\| + \|\phi\| \tag{1-2}$$

In both cases, equality holds if and only if the vectors are linearly dependent.

Corresponding to any linear vector space V there exists the *dual space* of *linear functionals* on V. A linear functional F assigns a scalar $F(\phi)$ to each vector ϕ, such that

$$F(a\phi + b\psi) = aF(\phi) + bF(\psi) \tag{1-3}$$

for any vectors ϕ and ψ and any scalars a and b. The set of linear functionals may itself be regarded as forming a linear space V' if we define the sum of two functionals as

$$(F_1 + F_2)(\phi) = F_1(\phi) + F_2(\phi) \tag{1-4}$$

Riesz Theorem. There is a one-to-one correspondence between linear functionals F in V' and vectors f in V, such that all linear functionals have the form

$$F(\phi) = (f, \phi) \tag{1-5}$$

f being a fixed vector and ϕ being an arbitrary vector.

Thus the spaces V and V' are essentially isomorphic. For the present we shall only prove this theorem in a manner that ignores the convergence questions that arise when dealing rigorously with infinite dimensional spaces. (These questions are dealt with in Sec. 1-4.)

Proof. It is obvious that any given vector f in V defines a linear functional, using Eq. (1-5) as the definition. So we need only prove that for an arbitrary linear functional F we can construct a unique vector f that satisfies (1-5). Let $\{\phi_n\}$ be a system of *orthonormal* (that is, orthogonal and of unit norm) basis vectors in V, satisfying $(\phi_n, \phi_m) = \delta_{n,m}$. Let $\psi = \Sigma_n x_n \phi_n$ be an arbitrary vector in V. From (1-3), we have

$$F(\psi) = \sum_n x_n F(\phi_n)$$

Now construct the following vector:

$$f = \sum_n [F(\phi_n)]^* \phi_n$$

Its inner product with the arbitrary vector ψ is

$$\begin{aligned}(f, \psi) &= \sum_n F(\phi_n) x_n \\ &= F(\psi)\end{aligned}$$

Hence the theorem is proved.

Dirac's Bra and Ket Notation

In Dirac's notation, which is very popular in quantum mechanics, the vectors in V are called *ket* vectors and are denoted $|\phi\rangle$. The linear functionals in the dual space V' are called *bra* vectors and are denoted $\langle F|$. The numerical value of the functional is denoted as

$$F(\phi) = \langle F|\phi\rangle \tag{1-6}$$

According to the Riesz theorem, there is a one-to-one correspondence between bras and kets. Therefore we can use the same alphabetic character for the functional (a member of V') and the vector (in V) to which it corresponds, relying on the bra, $\langle F|$, or ket, $|F\rangle$, notation to determine which space is referred to. Equation (1-5) would then be written as

$$\langle F|\phi\rangle = (F, \phi) \tag{1-7}$$

with $|F\rangle$ being the vector previously denoted as f. Note, however, that the Riesz theorem establishes, by construction, an *antilinear* correspondence between bras and kets. If $\langle F| \leftrightarrow |F\rangle$, then

$$c_1^*\langle F| + c_2^*\langle F| \leftrightarrow c_1|F\rangle + c_2|F\rangle \tag{1-8}$$

Because of the relation (1-7), it is possible to regard the "braket" $\langle F|\phi\rangle$ as merely another notation for the inner product. But the reader is advised that there are situations in which it is important to remember that the primary definition of the bra vector is as a linear functional on the space of ket vectors.

[[In his original presentation, Dirac *assumed* a one-to-one correspondence between bras and kets, and it was not entirely clear whether this was a mathematical or a physical assumption. The Riesz theorem shows that there is no need, and indeed no room, for any such assumption. Moreover, we shall eventually need to consider more general spaces (rigged-Hilbert-space triplets) for which the one-to-one correspondence between bras and kets does not hold.]]

1-2 LINEAR OPERATORS

An *operator* on a vector space maps vectors onto vectors; that is, if A is an operator and ψ is a vector, then $\phi = A\psi$ is another vector. An operator is fully defined by specifying its action on every vector in the space (or in its *domain*, if that is smaller than the whole space).

A *linear operator* satisfies

$$A(c_1\psi_1 + c_2\psi_2) = c_1(A\psi_1) = c_2(A\psi_2) \tag{1-9}$$

It is sufficient to define a linear operator on a set of basis vectors, since every vector can be expressed as a linear combination of the basis vectors. We shall be treating only linear operators, and so we shall henceforth refer to them simply as operators.

To assert the equality of two operators, $A = B$, means that $A\psi = B\psi$ for *all* vectors (more precisely, for all vectors in the common domain of A and B; this qualification will usually be omitted for brevity). Thus we can define the sum and product of operators:

$$(A + B)\psi = A\psi + B\psi$$
$$AB\psi = A(B\psi)$$

Both equations must hold for all ψ. It follows from this definition that operator multiplication is necessarily *associative*: $A(BC) = (AB)C$. But it need not be commutative, AB being unequal to BA in general.

Example (i)

In a space of discrete vectors represented as columns, a linear operator is a square matrix. In fact, any operator equation in a space of N dimensions can be transformed into a matrix equation. Consider, for example, the equation

$$M|\psi\rangle = |\phi\rangle \tag{1-10}$$

Choose some orthonormal basis $\{|u_i\rangle, i = 1 \ldots N\}$ in which to expand the vectors:

$$|\psi\rangle = \sum_j a_j|u_j\rangle, \qquad |\phi\rangle = \sum_k b_k|u_k\rangle$$

Operating on (1-10) with $\langle u_i|$ yields

$$\sum_j \langle u_i|M|u_j\rangle a_j = \sum_k \langle u_i|u_k\rangle b_k$$
$$= b_i$$

which has the form of the matrix equation

$$\sum_j M_{ij} a_j = b_i \tag{1-11}$$

with $M_{ij} = \langle u_i|M|u_j\rangle$ being known as a *matrix element* of the operator M. In this way, any problem in an N-dimensional linear vector space, no matter how it arises, can be transformed into a matrix problem.

The same thing can be done formally for an infinite-dimensional vector space if it has a denumerable orthonormal basis. However, we must then deal with the problem of convergence of the infinite sums, which we postpone to a later section.