Arno Böhm

Quantum Mechanics

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Preface

This book was written as a text, although many may consider it a monograph.

As a text it has been used several times in both the one-year graduate quantum-mechanics course and (in its shortened version) in a senior quantum mechanics course that I taught at the University of Texas at Austin. It is self-contained and does not require any prior knowledge of quantum mechanics. It also introduces the mathematical language of quantum mechanics, starting with the definitions, and attempts to teach this language by using it. Therefore, it can, in principle, be read without prior knowledge of the theory of linear operators and linear spaces, though some familiarity with linear algebra would be helpful. Prerequisites are knowledge of calculus and of vector algebra and analysis. Also used in a few places are some elementary facts of Fourier analysis and differential equations. Most physical examples are taken from the fields of atomic and molecular physics, as it is these fields that are best known to students at the stage when they learn quantum mechanics.

This book may be considered a monograph because the presentation here is different from the usual treatment in many standard textbooks on quantum mechanics. It is not that a "different kind" of quantum mechanics is presented here; this is conventional quantum mechanics ("Copenhagen interpretation"). However, in contrast to what one finds in the standard books, quantum mechanics is more than the overemphasized wave-particle dualism presented in the familiar mathematics of differential equations. "This latter dualism is only part of a more general pluralism" (Wigner) because, besides

momentum and position, there is a plurality of other observables not commuting with position and momentum. As there is no principle that brings into prominence the position and momentum operators, a general formalism of quantum mechanics, in which every observable receives the emphasis it deserves for the particular problem being considered, is not only preferable but often much more practical. The lesson that I believe can be learned from the situation in particle theory is that more is needed than just the solutions of differential equations and there exist algebraic relations other than just the canonical commutation relation. In atomic and molecular physics the use of these general algebraic methods of quantum mechanics may be merely of practical advantage but not necessary, but in particle physics they seem to be essential. It is this general form of quantum theory that is presented here.

I have attempted to present the whole range from the fundamental assumptions to the experimental numbers. To do this in the limited space available required compromises. My choice may, to a certain extent, reflect my personal taste. But it was mainly influenced by what I thought was needed for modern physics and by what I found, or did not find, in the standard textbooks. Detailed discussions of the Schrödinger differential equation for the hydrogen atom and other potentials can be found in many good books.[1] On the other hand, the description of the vibrational and rotational spectra of molecules are hardly treated in any textbooks of quantum mechanics, though they serve as simple examples for the important procedure of quantum-mechanical model building. Also, "elementary particles are much more similar to molecules than to atoms" (Heisenberg). So I have treated the former rather briefly and devoted considerable space to the latter.

Groups have not been explicitly made use of in this book. However, the reader familiar with this subject will see that group theory is behind most of the statements that have been cast here in terms of algebras of observables.

This is a physics book, and though mathematics has been used extensively, I have not endeavored to make the presentation mathematically rigorous. Most of the mathematics I believe to be rigorously justifiable within the framework of the rigged Hilbert space, which—in contrast to von Neumann's formation but in accord with Dirac's presentation[2]—is assumed to be the underlying mathematical structure. Except in the mathematical inserts, which are given in open brackets ⟦M: ⟧, the reader will not even be made aware of these mathematical details.

The mathematical inserts are of two kinds. The first kind provides the mathematics needed, and the second kind indicates the underlying mathematical justification. The whole first chapter is a mathematical insert of the first kind. As presented here, the mathematics can only be appreciated in its applications. This suggests the pedagogical advice that the reader should not attempt to read the book in a linear fashion, one fully understood page after another, but that he should be content to obtain a superficial under-

[1] It has, usually, also been adequately treated in an undergraduate course.

[2] See, for instance, Dirac (1958), Jauch (1958), Ludwig (1954), and von Neumann (1932).

standing of a subject at first reading and then return to it later for a deeper understanding.

Quantum mechanics starts with Chapter II, where the most essential basic assumptions (axioms) of quantum mechanics are made plausible from the example of the harmonic oscillator as realized by the diatomic molecule. Further basic assumptions are introduced in later chapters when the scope of the theory is extended. These basic assumptions are not to be understood as mathematical axioms from which everything can be derived without using further judgment and creativity. An axiomatic approach of this kind does not appear to be possible in physics. The basic assumptions are to be considered as a concise way of formulating the quintessence of many experimental facts.

The book consists of two clearly distinct parts, Chapters II–XI and Chapters XIV–XXI, with two intermediate chapters, Chapters XII and XIII. The first part is more elementary in presentation, though more fundamental in subject matter, and gives a more approximate description because it treats all systems as stationary. Chapter XII introduces the basic assumption of time development. Chapter XIII is just an application of previously developed concepts and attempts to illustrate the characteristic features in which quantum mechanics differs from the classical theories. The second part, which starts with Chapter XIV, treats scattering and decaying systems. The presentation there is much more advanced.

Chapter XIV gives a derivation of the cross section under very general conditions, and Section XIV.5 may be the most difficult section of the book. Section XIV.5 and Chapter XV may be omitted in first reading if the reader can accept the results without derivation. Starting with Chapter XVI, applications are restricted to rationally symmetric systems without spin. Two different points of view—one in which the Hamiltonian time development is assumed to exist, and the other making use of the S-matrix—are treated in a parallel fashion. The required analyticity of the S-matrix is deduced from causality. One of the main features of the presentation is to treat discrete and continuous spectra from the same point of view. For this the rigged Hilbert space is needed, which provides not only a mathematical simplification but also a description which is closer to physics. In the last chapter, the rigged Hilbert space is used to describe a decaying system by eigenvectors of the energy operator with complex energy. This establishes the link between the S-matrix description of a resonance at a pole and the usual description of states by vectors in a linear space, and is another example of the advantages that the rigged Hilbert space provides.

Written at the height of the atomistic point of view—this book tries to expose also the complementary way of understanding, the holistic view. [See also Heisenberg's last lecture published in Physics Today **29**, 32 (1976).] Though never mentioned explicitly except in the brief Epilogue, the duality between atomism and holism is the recurring theme throughout the book.

Austin, Texas Arno Böhm

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Contents

CHAPTER I

Mathematical Preliminaries

The mathematical language of quantum mechanics is introduced in this chapter. It does not contain much more than the basic definitions. A proper understanding of this material will come through its application in the following chapters.

I.1 The Mathematical Language of Quantum Mechanics

To formulate Newtonian mechanics, the mathematical language of differential and integral calculus was developed. Though one can get some kind of understanding of velocity, acceleration, etc., without differential calculus (in particular for special cases), the real meanings of these physical notions in their full generality become clear only after one is familiar with the idea of the derivative. On the other hand, though, the abstract mathematical definitions of calculus become familiar to us only if we visualize them in terms of their physical realizations. Nowadays, no one would attempt to understand classical mechanics without knowing calculus.

Quantum mechanics, too, has its mathematical language, whose development went parallel to the development of quantum mechanics and whose creation in its full generality was inspired by the needs of quantum physics. This is the language of linear spaces, linear operators, associative algebras, etc., which has meanwhile grown into one of the main branches of mathematics—linear algebra and functional analysis. Although one might obtain

some sort of understanding of quantum physics without knowing its mathematical language, the precise and deep meaning of the physical notions in their full generality will not reveal themselves to anyone who does not understand its mathematical language.

Therefore I shall start the quantum-mechanics course with some of the vocabulary and grammar of this language. I shall not try to be mathematically rigorous, since one can still communicate in a language that one does not speak completely correctly. I shall also not give all the mathematics that is needed at the beginning, and you need not be worried if you do not understand everything right away; one learns a language best by using it. I shall give at the beginning only as much mathematics as is necessary to make the initial statements about physics. We shall then have to learn new mathematical notions whenever they arise, while we proceed with the development of the physical ideas.

Before we start to study the mathematical structures that are employed in quantum mechanics, we should make the following observation: A mathematical structure is not something real—it only exists in our mind and is created by our mind (though often inspired by outside influences). It is obtained by taking a set of objects and equipping this set with a structure, by defining relations between these objects. Modern mathematics distinguishes three basic kinds of structures: algebraic, topological, and ordering. The mathematical structures we use are complicated combinations of these three. For example, the real numbers have an algebraic structure given by the usual laws of addition and multiplication, they have a topological structure given by the meaning of the usual limiting process for an infinite series of numbers, and they have an ordering structure given by the relations expressed by $<$.

We shall use predominantly algebraic structures, although in order to speak the mathematical language of quantum mechanics correctly, topological structures are essential. We shall start with the definition of a linear space, then introduce linear operators and give the definition of an associative algebra. That will provide us with enough vocabulary and grammar to enable us to start communicating physics, in the process of which the meaning of these mathematical structures will be filled with substance.

I.2 Linear Spaces, Scalar Product

A set R of elements $\phi, \psi, \chi, \ldots$ is called a *linear space* if the sum $\phi + \psi$ of any two elements $\phi, \psi \in R$ and the product $a\phi$ of any element $\phi \in R$ with any complex number a are defined and have the following properties:

$$\text{if } \phi, \psi \in R, \text{ then } \phi + \psi \in R. \tag{2.1a}$$

$$\phi + \psi = \psi + \phi. \tag{2.1b}$$

$$(\phi + \psi) + \chi = \phi + (\psi + \chi). \tag{2.1c}$$

There exists in R a "zero" element 0 such that $\phi + 0 = \phi$ for all $\phi \in R$. (2.1d)

$$\text{if } \phi \in R, \text{ then } a\phi \in R. \tag{2.1e}$$

$$a(b\phi) = (ab)\phi. \tag{2.1f}$$

$$1 \cdot \phi = \phi. \tag{2.1g}$$

$0 \cdot \phi = 0$ (the number zero appears on the left, the zero element on the right), (2.1h)

$$a(\phi + \psi) = a\phi + a\psi, \tag{2.1i}$$

$$(a + b)\phi = a\phi + b\phi. \tag{2.1j}$$

The element $(-1)\phi$ is then usually denoted by $-\phi$; by properties 2.1g, k, h),

$$\phi + (-\phi) = (1 + (-1))\phi = 0\phi = 0.$$

The elements ϕ, ψ, χ of the space R are called *vectors*. A set M in the linear space R is called a *subspace* of R if M is a linear space under the same definitions of the operations of addition and multiplication by a number as given for R, i.e., if it follows from $\phi, \psi \in M$ that $a\phi \in M$ and $\phi + \psi \in M$.

An expression of the form $a_1\phi_1 + a_2\phi_2 + \cdots + a_n\phi_n$ is called a *linear combination* of the vectors $\phi_1, \phi_2, \ldots, \phi_n$; the vectors $\phi_1, \phi_2, \ldots, \phi_n$ are said to be *linearly dependent* if there exist numbers $a_1, a_2, \ldots, a_n$, not all zero, for which $a_1\phi_1 + a_2\phi_2 + \cdots + a_n\phi_n = 0$. If the equation $a_1\phi_1 + a_2\phi_2 + \cdots + a_n\phi_n = 0$ holds only for $a_1 = a_2 = \cdots = a_n = 0$, then the vectors $\phi_1, \phi_2, \ldots, \phi_n$ are called *linearly independent*. A space R is said to be *finite-dimensional* and, more precisely, *n-dimensional* if there are n and not more than n linearly independent vectors in R. If the number of linearly independent vectors in R is arbitrarily great, then R is said to be *infinite-dimensional*. Every system of n linearly independent vectors in an n-dimensional space R is called a *basis* for R.

Every vector ϕ of an n-dimensional space R can be uniquely represented in the form $\phi = a_1e_1 + \cdots + a_ne_n$, where $e_1, e_2, \ldots, e_n$ is a basis for R. The numbers $a_1, \ldots, a_n$ are called the *coordinates* of the vector ϕ *relative to the basis* $e_1, \ldots, e_n$.

Evidently, when vectors are added, their corresponding coordinates relative to a fixed basis are added, and when a vector is multiplied by any number, all the coordinates are multiplied by that number.

A linear space is called a *scalar product space* (or *Euclidean space*), if in it a function (ϕ, ψ) is defined, having the following properties:

$$(\phi, \phi) \geq 0 \quad \text{and} \quad (\phi, \phi) = 0 \text{ iff } \phi = 0. \tag{2.2a}$$

$$(\psi, \phi) = \overline{(\phi, \psi)} \tag{2.2b}$$

(the bar denotes complex conjugate).

$$(\phi, a\psi) = a(\phi, \psi) \tag{2.2c}$$

($a \in C$, the set of complex numbers).

$$(\phi_1 + \phi_2, \psi) = (\phi_1, \psi) + (\phi_2, \psi). \tag{2.2d}$$

This function is called the *scalar product* of the elements ϕ and ψ. Such a scalar product can be introduced in every finite-dimensional space; for example, if $e_1, \ldots, e_n$ is a basis for R and $\phi = a_1 e_1 + \cdots + a_n e_n$, $\psi = b_1 e_1 + \cdots + b_n e_n$, then, putting

$$(\phi, \psi) = \bar{a}_1 b_1 + \cdots + \bar{a}_n b_n, \tag{2.3}$$

we get a function (ϕ, ψ) satisfying the conditions (2.2).

With the scalar product one defines the *norm* $\|\phi\|$ of a vector $\phi \in R$ by

$$\|\phi\| = \sqrt{(\phi, \phi)}. \tag{2.4}$$

A complex-valued function $h(\phi, \psi)$ of two vector arguments is a *Hermitian form* if it satisfies

$$h(\phi, \psi) = \overline{h(\psi, \phi)}, \tag{2.5b}$$

$$h(\phi, a\psi) = ah(\phi, \psi) \qquad (a \in \mathbb{C}), \tag{2.5c}$$

$$h(\phi_1 + \phi_2, \psi) = h(\phi_1, \psi) + h(\phi_2, \psi). \tag{2.5d}$$

If in addition h satisfies

$$h(\phi, \phi) \geq 0 \tag{2.5a}$$

for every vector ϕ, then h is said to be a *positive Hermitian form.* A positive Hermitian form is called *positive definite* if

$$\text{from} \quad h(\phi, \phi) = 0 \quad \text{follows} \quad \phi = 0 \text{ for every vector } \phi. \tag{2.6}$$

[Since the definition (2.5), (2.6) of a positive definite Hermitian form is the same as that of a scalar product, from now on we shall use only the term scalar product.] Positive Hermitian forms, which are not necessarily scalar products, satisfy the *Cauchy–Schwarz–Bunyakovski inequality*:

$$|h(\phi, \psi)|^2 \leq h(\phi, \phi) h(\psi, \psi). \tag{2.7}$$

If h is positive definite, equality holds iff $\varphi = a\psi$ for some $c \in \mathbb{C}$.

Keeping ψ fixed, $(\phi, \psi) = \psi(\phi)$ is a function or *functional* of $\phi \in R$, and as this functional fulfills the conditions (2.2c), (2.2d), it is called an *antilinear functional.* In general every function $F(\phi)$ that fulfills

$$F(a\phi) = \bar{a} F(\phi), \tag{2.8a}$$

$$F(\phi_1 + \phi_2) = F(\phi_1) + F(\phi_2) \qquad (\phi_1, \phi_2 \in R) \tag{2.8b}$$

is called an antilinear functional on the linear space R.

An antilinear functional is called *continuous* iff from the convergence of the infinite sequence of elements $\phi_n \in R$ $(n = 1, 2, 3, \ldots)$ to the element $\phi \in R$, i.e., from

$$\phi_n \to \phi \quad \text{as } n \to \infty, \tag{2.9}$$

it follows that

$$F(\phi_n) \to F(\phi) \quad \text{as } n \to \infty. \tag{2.10}$$