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Preface

Quantization of physical systems includes a correct definition of physical observables (such as the Hamiltonian and the momentum) as self-adjoint operators in an appropriate Hilbert space and their proper spectral analysis. A solution of this problem is not a straightforward and unambiguous procedure for nontrivial quantum systems (systems on nontrivial manifolds, in particular on manifolds with boundaries or with singular interactions). Quantum-mechanical models with singular potentials, both relativistic and nonrelativistic, and/or with boundaries, play an important role in physics. A consistent treatment of nontrivial quantum systems is beyond the scope of the mathematical apparatus in standard textbooks on quantum mechanics (QM). But a "naïve" treatment based on finite-dimensional linear algebra or even on the theory of bounded operators can result in paradoxes and incorrect results. Some paradoxes due to a "naïve" treatment demonstrate that even simple physical models can be nontrivial from the mathematical standpoint. It is well known that a rigorous pure-mathematical approach to constructing physical observables in nontrivial quantum systems leads to a result that is not unique. Additional physical arguments must eventually be used to choose a proper quantization for a given physical system. An application of the technique of self-adjoint extensions of symmetric operators makes the inherent nonuniqueness obvious and facilitates a physically proper choice.

In this book, we focus on the problem of a correct definition of quantum-mechanical observables, which is an important part of operator quantization. We show how this problem can be solved for comparatively simple but nontrivial quantum-mechanical systems. The solution of the above problem requires invoking some nontrivial notions of functional analysis concerning the theory of linear operators in Hilbert spaces, in particular, the notions of unbounded self-adjoint operators and their spectral analysis and of self-adjoint extensions of symmetric operators. The general theory is then illustrated on a number of physical examples. In particular, it is shown how the problem of a correct definition of observables is solved for a free one-dimensional particle on the whole axis, on a semiaxis, and on a finite interval. In addition, various nontrivial quantum systems are treated in accordance with the general mathematical theory of self-adjoint extensions

and a rigorous spectral theory. These are the one-dimensional particles in the Calogero potential and in the potentials localized at the origin, in particular, deltalike potentials. Additionally, a rigorous treatment of the Schrödinger operators with all the so-called exactly solvable potentials is given, and the relativistic problem for an electron in the Coulomb field of arbitrary (including supercritical) charge is considered in detail. A similar analysis is carried out for nonrelativistic and relativistic electrons in the Aharonov–Bohm field and in the so-called magnetic-solenoid field.

The book is addressed to readers who are interested in deepening their understanding of mathematical problems in QM beyond the scope of standard textbooks.

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Contents

Chapter 1
Introduction

1.1 General Remarks

Among different approaches to constructing a quantum description of physical systems and its proper interpretation, operator quantization is the oldest and most-used one. The main first-stage problem of operator quantization is the problem of a correct definition of observables as self-adjoint operators (s.a. operators in what follows) in an appropriate Hilbert space. The self-adjointness of observables is of crucial importance for quantum theory (QT). An s.a. operator possesses a real-valued spectrum and a complete orthogonal set of (generalized) eigenvectors in the corresponding Hilbert space. These properties of any observable provide a basis for the probabilistic interpretation of QT (in particular, quantum mechanics (QM), which is the principal object of our consideration). The problem of a correct definition of quantum observables is generally nontrivial in the case of physical systems with boundaries and/or with singular interactions (including QFT models). In what follows, for the sake of brevity, we call such systems *nontrivial physical systems* (or simply nontrivial systems). The interest in this problem revives periodically in connection with studies of specific nontrivial systems such as a particle on a finite interval or on a semiaxis, a particle in singular potential fields, in particular in the Aharonov–Bohm or in δ-like potential fields, and so on. The reason is that the solution of the problem, and therefore a consistent QM treatment of nontrivial systems, requires a considerable amount of preliminary information from different advanced chapters of functional analysis. However, the content of such chapters usually goes beyond the scope of the mathematical apparatus presented in standard textbooks on QM for physicists,[1] e.g., [32, 39, 44, 48, 64, 104, 109, 112, 136, 138] and even in recently published textbooks [23, 37, 63, 98].

[1] The exceptions such as [27, 57, 83, 84, 128, 144, 147, 153] are mainly intended for mathematically minded physicists and mathematicians.

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One of the aims of this book is of a pedagogical nature, namely, to convince the reader–physicist that he or she must be very careful when reading standard textbooks on QM for physicists, and particularly careful when applying the notions and prescriptions from such textbooks to nontrivial systems as regards the mathematical apparatus of QM.

The mathematical apparatus of QM is functional analysis, more specifically, the theory of linear operators in Hilbert spaces. It is a quite extensive and "subtle" science, so it takes considerable time to master it. For this reason, standard textbooks on QM for physicists present a rather simplified version of the relevant parts of functional analysis in the form of brief "rules" such that many mathematical subtleties are necessarily left aside. The simplified rules are usually based on systematic references to our experience in finite-dimensional linear algebra, which often proves to be misleading. We recall these rules below. They can be sufficient as long as we examine comparatively simple QM systems. But if we follow these rules literally in our treatment of even the simplest nontrivial systems (in what follows, we call this approach the *naïve treatment*), we encounter some paradoxes that may lead us to incorrect conclusions. In this chapter, we present a number of such paradoxes, and a resolution of them is given in subsequent chapters.

As stated above, QM generally and a consistent QM treatment of nontrivial systems particularly require the language of the theory of linear operators in Hilbert spaces and realizing subtleties associated with unbounded operators, in particular, with such basic notions as a closed operator, an adjoint operator, a symmetric operator, and an s.a. operator,[2] the spectrum of an s.a. operator and its spectral decomposition, the so-called inversion formulas for s.a. differential operators, and so on. Another aim of this book is to remind the reader–physicist of (or provide an introduction to) these notions and some related subjects.

A crucial subtlety is that an unbounded s.a. operator cannot be defined in the whole Hilbert space, i.e., on an arbitrary QM state, which is usually assumed in a preliminary "idealized" scheme of operator quantization. But there is no operator without its domain of definition: an operator is not only a rule of acting, but also a domain in a Hilbert space to which this rule is applicable. In the case of unbounded operators, the same rule for different domains generates different operators with sometimes completely different properties. Provided a rule of acting is given, it is an appropriate choice of a domain for a QM observable that makes it an s.a. operator. The main problems are related to this point. The formal rules of operator canonical quantization (see below) are of a preliminary nature and generally provide only "candidates" for unbounded QM observables, so to speak, for example in the form of the so-called s.a. differential operations,[3] because their domains are not prescribed by the canonical quantization rules. Appropriate domains even are not clear at the first stage of quantization, especially in the case of nontrivial physical systems,

[2]For unbounded operators, there is a crucial difference between the notions of symmetric (Hermitian) and s.a. operators; for bounded operators, these notions actually coincide.

[3]S.a. according to Lagrange in mathematical terminology; see Chap. 4.

although it is prescribed that observables must be s.a. operators. It should be noted that the choice of domains providing the self-adjointness of all observables involved, especially the primarily important observables such as the position, momentum, Hamiltonian, and symmetry generators, is a necessary part of quantization resulting in a specification of a QM description of a physical system in question. This is actually a physical problem. Mathematics can only help a physicist in making a choice by indicating various possibilities.

It is expected that for physical systems whose classical description includes infinite (but finite-dimensional) flat phase spaces such as $\mathbb{R}^{2n}$ and nonsingular interactions, a quantization is practically unique: the most important physical observables are defined as s.a. operators on some "natural" domains; in particular, classical symmetries can survive under quantization. The majority of textbooks for physicists begin their exposition of QM with a treatment of such physical systems. Of course, nontrivial physical systems are also examined thereafter. Nevertheless, the common belief is that no actual singularities exist in nature. They are the products of our idealization of reality, i.e., are of a model nature, which is related, for example, to our ignorance of the details of interaction at small distances. We formally extend an interaction law known for finite distances between finite objects to infinitely small distances between pointlike objects. We treat boundaries as a result of infinite potential walls that are actually always finite.[4] The consequence is that singular problems in QM are commonly solved via some regularization considered to be natural and then via a subsequent limiting process of removing the regularization. In some cases, this procedure requires the so-called infinite renormalization (of coupling constants, for example). But in some cases, no reasonable limit is known. (It should be pointed out that here, we mean conventional QM rather than quantum field theory.) It may also happen that different regularizations yield different physical results. It is precisely the case in which mathematics can help a physicist with the theory of s.a. extensions of symmetric operators. This was first recognized by Berezin and Faddeev [26] in connection with the three-dimensional δ-potential problem.

The practice of quantizing nontrivial systems shows that preliminary candidates for observables can be quite easily assigned symmetric operators defined on such domains that "avoid" problems: they do not "touch" boundaries and "escape" any singularities of interaction; this is a peculiar kind of "mathematical regularization." But such symmetric operators are commonly non-s.a. The main question then is whether these preliminary observables can be assigned s.a. operators by some extensions of the initial symmetric operators that convert the candidates to real observables. The answer is simple, positive, and unique if a symmetric operator under consideration is bounded. However, if it is unbounded, the problem is generally nontrivial.

[4] Of course, a flat infinite space is also an idealization, as is any infinity.

The theory of s.a. extensions of unbounded symmetric operators provides the main tool for solving this problem. It turns out that these extensions are generally nonunique, if they are possible at all. From the physical standpoint, this implies that when quantizing a nontrivial physical system, we are generally presented with different possibilities for its quantum description. The general theory describes all the possibilities that mathematics can offer to a physicist. Of course, a physical interpretation of available s.a. extensions is a purely physical problem. Any extension is a certain prescription for the behavior of a physical system under consideration near its boundaries and singularities. We also believe that each extension can be understood through an appropriate regularization and a subsequent limiting process, although this is generally a complicated problem in itself. But in any case, the right of a final choice belongs to the physicist.

The book is organized as follows. In the introduction, we demonstrate that an idealized scheme of operator canonical quantization applied to nontrivial systems can lead to a number of paradoxes. Chapters 2 and 5 (purely mathematical chapters in a sense) contain all the information about Hilbert spaces, linear operators in such spaces, and a strict formulation of the spectral problem for s.a. operators that physicists need and that is used in the book. This standard material is followed by the general theory of s.a. extensions of symmetric operators presented in Chap. 3. The traditional exposition (due to von Neumann) is accompanied by a nontraditional approach that is based on the notion of asymmetry forms generated by adjoint operators, see our works [156, 157]. The basic statements concerning the possibility and specification of s.a. extensions both in terms of isometries between the deficient subspaces and in terms of the sesquilinear asymmetry form are collected in the main theorem. It is followed by a comment on a direct application of the main theorem to physical problems of quantization. We outline a possible general scheme of constructing QM observables as s.a. operators starting from initial formal expressions supplied by canonical quantization rules. The subsequent Chap. 4 is devoted to the exposition of specific features and appropriate modifications of the general theory as applied to ordinary (one-dimensional) differential operators in Hilbert spaces $L^2(a, b)$ [158]. For symmetric differential operators, the isometries between deficient subspaces specifying s.a. extensions can be converted to s.a. boundary conditions, explicit or implicit, based on the fact that asymmetry forms are expressed in terms of the (asymptotic) boundary values of functions and their derivatives. We describe various ways of specifying s.a. operators by s.a. boundary conditions depending on the regularity or singularity of the ends of the interval under consideration. In particular, we propose a new method for specifying s.a. ordinary differential operators by s.a. boundary conditions based on evaluation of the quadratic asymmetry form in terms of asymptotic boundary coefficients. A comparative advantage of the method is that it makes it possible to avoid the evaluation of deficient subspaces and deficiency indices. Its effectiveness is illustrated in Chaps. 6–10 with examples of constructing QM observables for a number of nontrivial systems. In Chaps. 6–8, we consider various one-dimensional systems: a free particle on a semiaxis and on a segment of the real axis (Chap. 6), a particle in different potential fields including the Calogero potential, deltalike

potentials, and so-called exactly solvable potentials (Chaps. 7 and 8). In Chaps. 9 and 10, we study certain one-particle three-dimensional problems. In Chap. 9, we consider a Dirac particle moving in the Coulomb field of a point charge Ze. We interpret the Dirac equation with the Coulomb field as the Schrödinger equation; the corresponding quantum Hamiltonian is called the Dirac Hamiltonian. We define the Dirac Hamiltonian with the Coulomb field as an s.a. operator for any real Z and solve the corresponding spectral problem. In Chap. 10, we similarly examine the Dirac Hamiltonian with the Aharonov–Bohm field and with the so-called magnetic-solenoid field.

1.2 Idealized Scheme of Operator Canonical Quantization

For a physicist, quantization means constructing a QT for a given physical system on the basis of an initial classical theory and in accordance with the correspondence principle. The correspondence principle requires that the QT must reproduce the predictions of the initial classical theory in the classical limit (large masses, macroscopic scales, smooth potentials, and so on), which is formally the limit $\hbar \to 0$, where $\hbar$ is the Planck constant.[5] The quantization problem usually does not have a unique solution. The only criterion for whether a constructed QT is proper remains the coincidence of its predictions with experiment. The development of QT began with the quantization of the simplest systems such as a free particle, a harmonic oscillator, and a nonrelativistic particle in some potential fields. In fact, the experience in the quantization of such systems was used to formulate a consistent general scheme of operator quantization for an arbitrary system with canonical Hamiltonian equations of motion for phase-space variables. It is this scheme that was called canonical quantization. In what follows, we outline the canonical quantization rules as they are usually expounded in standard textbooks on QM for physicists. This is a "first approximation" to a proper quantization, so to speak, the naïve treatment, as was already mentioned before, or *the idealized scheme of operator canonical quantization*. In short, this scheme is as follows.

(a) It is assumed that there exists a canonical Hamiltonian formulation of the classical mechanics of a physical system under consideration. This means that a state of the system at any instant of time is specified by a point of some even-dimensional phase space; the points of this space are labeled by canonical generalized coordinates x^a and momenta p_a, $a = 1, \ldots, n$, where n is the number of degrees of freedom. The time evolution of a state of the system in the course of time t is described by the Hamiltonian (canonical) equations of motion for the canonical coordinates $x^a(t)$ and $p_a(t)$:

$$\dot{x}^a = \{x^a, H\}\,, \quad \dot{p}_a = \{p_a, H\}\,,$$

[5] For a mathematician, quantization is a quantum deformation of classical structures; the deformation parameter is the Planck constant $\hbar$.

where $H = H(x, p)$ is the Hamiltonian of the system and $\{\,,\,\}$ is the canonical Poisson bracket. The canonical Poisson bracket of two arbitrary functions f and g on the phase space is defined by

$$\{f, g\} = \sum_a \left(\frac{\partial f}{\partial x^a} \frac{\partial g}{\partial p_a} - \frac{\partial f}{\partial p_a} \frac{\partial g}{\partial x^a} \right), \tag{1.1}$$

in particular, $\{x^a, p_b\} = \delta^a_b$. All local physical quantities (classical observables) f are real functions of the phase-space variables, $f = f(x, p)$. Classical observables form a real associative commutative algebra, in particular, $[f_1, f_2] \equiv f_1 f_2 - f_2 f_1 = 0, \forall f_1, f_2$.

(b) In QM, a state of a physical system at any instant of time is specified by a vector ψ in a Hilbert space $\mathfrak{H}$, which is called the space of states. A scalar product of two vectors ψ_1 and ψ_2 is denoted by (ψ_1, ψ_2). To a first approximation, it is assumed that any state $\psi \in \mathfrak{H}$ can be realized physically; in particular, the superposition principle holds: if states ψ_1 and ψ_2 are realizable, then the state $\psi = a_1\psi_1 + a_2\psi_2$ with any $a_1, a_2 \in \mathbb{C}$ is also realizable.

(c) In QT, each classical observable $f = f(x, p)$ is assigned an s.a. operator $\hat{f}$, $f \longmapsto \hat{f}$, acting in a Hilbert space $\mathfrak{H}$. It is called a quantum observable. To a first approximation, it is assumed that any operator $\hat{f}$, including observables, is defined on any state ψ, i.e., $\hat{f}\psi \in \mathfrak{H}, \forall \psi \in \mathfrak{H}$, and is uniquely determined by its matrix elements $\left(\psi_1, \hat{f}\psi_2\right), \forall \psi_1, \psi_2 \in \mathfrak{H}$, and what is more, by its matrix $f_{mn} = (e_m, \hat{f}e_n)$ with respect to any orthonormal basis $\{e_n\}_1^\infty$, a complete orthonormalized set of vectors in $\mathfrak{H}$. Then any operator $\hat{f}$ is assigned its adjoint $\hat{f}^+$ defined by

$$\left(\psi_1, \hat{f}^+\psi_2\right) = \left(\hat{f}\psi_1, \psi_2\right), \ \forall \psi_1, \psi_2 \in \mathfrak{H},$$

and thereby the involution (conjugation) $\hat{f} \longmapsto \hat{f}^+$ is defined in the algebra of operators with the properties[6]

$$\left(\hat{f}^+\right)^+ = \hat{f}, \ \left(a\hat{f}\right)^+ = \overline{a}\hat{f}^+, \ \forall a \in \mathbb{C},$$
$$\left(\hat{f} + \hat{g}\right)^+ = \hat{f}^+ + \hat{g}^+, \ \left(\hat{f}\hat{g}\right)^+ = \hat{g}^+\hat{f}^+.$$

The self-adjointness of $\hat{f}$ means that $\hat{f} = \hat{f}^+$, or

$$\left(\psi_1, \hat{f}\psi_2\right) = \left(\hat{f}\psi_1, \psi_2\right), \ \forall \psi_1, \psi_2 \in \mathfrak{H}.$$

[6]The bar $^-$ over an expression denotes complex conjugation.

The mean value $\langle \hat{f} \rangle_\psi$ of any quantum observable $\hat{f}$ in a state ψ and the corresponding dispersion Δf are respectively defined by

$$\left\langle \hat{f} \right\rangle_\psi = \frac{\left(\psi, \hat{f}\psi\right)}{(\psi, \psi)},$$

$$\Delta f = \sqrt{\left\langle \left(\hat{f} - \langle \hat{f} \rangle_\psi\right)^2 \right\rangle_\psi} = \sqrt{\left\langle \hat{f}^2 \right\rangle_\psi - \left\langle \hat{f} \right\rangle_\psi^2}.$$

The self-adjointness of observables is assumed to imply that any observable $\hat{f}$ can be diagonalized, which means that the eigenvectors, or eigenstates, of $\hat{f}$ form an orthonormal basis in $\mathfrak{H}$; the spectrum of an observable is defined as a set of all its eigenvalues. The spectrum determines possible measurable values of the corresponding observable, while the complete orthonormalized set of the eigenstates of the observable provides a probabilistic interpretation of its measurements.

(d) According to the correspondence principle, there exists a certain relation between the Poisson bracket $\{f_1, f_2\} = f_3$ of classical observables f_1 and f_2 and the commutator $[\hat{f}_1, \hat{f}_2]$ of their quantum counterparts $\hat{f}_1$ and $\hat{f}_2$, namely, $[\hat{f}_1, \hat{f}_2] = i\hbar\hat{f}_3 + \hat{O}\left(\hbar^2\right)$; a supplementary operator $\hat{O}\left(\hbar^2\right)$ vanishes with vanishing $\hbar$ as $\hbar^2$. A more transparent form can be given to this correspondence:

$$\{f_1, f_2\} \longrightarrow \frac{1}{i\hbar}\left[\hat{f}_1, \hat{f}_2\right] + \hat{O}(\hbar).$$

That is, according to the correspondence principle, the Poisson bracket of classical observables is assigned the commutator of their quantum counterparts times the factor $(i\hbar)^{-1}$ plus, in general, a supplementary operator $\hat{O}(\hbar)$.

The position operators $\hat{x}^a$ and momentum operators $\hat{p}^a$ are postulated to be s.a. and satisfy the canonical commutation relations

$$\left[\hat{x}^a, \hat{x}^b\right] = \left[\hat{p}_a, \hat{p}_b\right] = 0, \quad \left[\hat{x}^a, \hat{p}_b\right] = i\hbar\left\{x^a, p_b\right\} = i\hbar\delta^a_b. \tag{1.2}$$

The correspondence principle requires that the quantum counterpart $\hat{f}$ of a classical observable $f(x, p)$ be of the form $\hat{f} = f(\hat{x}, \hat{p}) + \hat{O}(\hbar)$. A supplementary operator $\hat{O}(\hbar)$ is generally necessary to provide the self-adjointness of $\hat{f}$. In the general case, the correspondence principle does not allow a unique construction of the operator function $f(\hat{x}, \hat{p})$ in terms of the classical function $f(x, p)$ because of the noncommutativity of $\hat{x}$ and $\hat{p}$ (the so-called ordering problem.[7])

[7] Numerous papers have been devoted to the study of various rules of assigning operators to classical quantities. A substantial contribution to a resolution of this problem is due to Berezin [25].

To the first approximation whereby any observable can be diagonalized, it is argued that commuting observables $\hat{f}_1$ and $\hat{f}_2$ have a joint spectrum, i.e., a common set of eigenvectors, which implies the simultaneous measurability of the observables. A complete set of observables is defined as a minimum set of n commuting observables $\hat{f}_k$, $k = 1, \ldots, n$, $[\hat{f}_k, \hat{f}_l] = 0$, $\forall k, l$, whose joint spectrum is nondegenerate and whose common eigenvectors provide a unique specification of any vector in terms of the corresponding expansion with respect to these eigenvectors. For a complete set of observables, we can choose all the position operators $\hat{x}^a$. The momentum operators $\hat{p}_a$ can also be chosen for a complete set of observables. Different complete sets of observables can be considered, and their spectrum and eigenvectors specify the quantum description of a system under consideration.

(e) The time evolution of a state of the system in the course of time t is described by the Schrödinger equation for the state vector $\psi(t)$,

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi, \tag{1.3}$$

with an initial condition $\psi(t_0) = \psi_0$, where the operator $\hat{H}$, the quantum Hamiltonian, the energy observable, corresponds to the classical Hamiltonian H.

Because the initial state ψ_0 can be arbitrary, it is assumed that $\hat{H}$ is certainly applicable to any state $\psi \in \mathfrak{H}$.

A realization of the canonical commutation relations (1.2) in a specific Hilbert space (representation of canonical commutation relations) offers a practical possibility for solving the Schrödinger equation and finding probabilities of transitions from one state to another, means of physical quantities, and probabilities of measurements using the accepted rules.

It was canonical quantization that was first used to construct the QT for the simplest systems. There exist alternative formulations of QT, for example formulations in terms of Green's functions, functional integrals, and so on. Each of these formulations can either be introduced independently by a set of postulates or "derived" logically from the operator formulation based on the canonical quantization method. In the latter case, an alternative formulation of QT for a specific system is said to be obtained by the canonical quantization method. It should be noted that among all the formulations, the operator formulation based on canonical quantization is the best-developed and most consistent one. This explains the existing tendency to quantize every classical system canonically. We should note that for classical systems of general form, canonical quantization is not always possible or cannot be carried out directly as described above without an essential analysis and reformulation of the initial classical theory. The majority of modern physical theories belong to

the so-called singular theories, theories with constraints and extra nonphysical variables in the initial Hamiltonian formulation (gauge theories are a particular case of singular theories). There exist different methods for quantizing such theories; see, e.g., [49, 75, 91]. Some of these methods are based on the possibility of passing to physical variables, which allows the standard canonical quantization. Canonical quantization remains the most reliable quantization scheme.

1.3 Some Paradoxes of Naïve Implementation of an Idealized Scheme

In this section, we examine some simple QM systems obtained in the framework of the above-described idealized scheme of operator canonical quantization. We show that if we follow this scheme literally, we arrive at certain paradoxes in the form of obvious contradictions with well-known statements.

We consider an example of a very simple system: a free nonrelativistic particle of mass m moving on an interval (a, b) of the real axis. The interval can be finite or infinite, a semiaxis or the whole axis. The finite ends of an interval are considered to be included in the interval; in particular, by a finite interval, we mean a closed interval $[a, b]$.

In classical mechanics, the phase space of this system is a strip $(a, b) \times \mathbb{R}$; the ranges of the particle position x and momentum p are respectively (a, b) and $\mathbb{R}$. The Poisson bracket (1.1) of x and p is $\{x, p\} = 1$. Free motion is defined by the free Hamiltonian $\mathcal{H} = p^2/2m$. If $|a| < \infty$ and/or $|b| < \infty$, the peculiarity of the system is that its phase space is a space with boundaries. The behavior of the particle near the boundaries must be specified by some subsidiary conditions such as elastic reflection, delay, trapping, or something else.

At first glance, we may not face the problem of boundaries when quantizing this system. The canonical observables for a QM particle are the position operator $\hat{x}$ and the momentum operator $\hat{p}$ satisfying the canonical commutation relations

$$[\hat{x}, \hat{x}] = [\hat{p}, \hat{p}] = 0, \quad [\hat{x}, \hat{p}] = i\hbar\{x, p\} = i\hbar. \tag{1.4}$$

For a complete set of observables, we can take the position operator $\hat{x}$ with the prescription that its spectrum be given by $\operatorname{spec} \hat{x} = (a, b)$. It is natural to take the x-representation of canonical commutation relations (1.4) where the Hilbert space $\mathfrak{H}$ of states is the space of functions $\psi(x)$ square-integrable on the interval (a, b); $\mathfrak{H} = L^2(a, b)$; the operator $\hat{x}$ is the operator of multiplication by x, namely

$$\hat{x}\psi(x) = x\psi(x);$$

while the operator $\hat{p}$ is a multiple of the differentiation operator[8] $d_x = \mathrm{d}/\mathrm{d}x$:

$$\hat{p} = -i\hbar d_x : \ \hat{p}\psi(x) = -i\hbar\psi'(x).$$

The canonical commutation relations (1.4) seem obviously to hold.

Other observables are certain differential operators

$$\hat{f} = f(x, -i\hbar d_x) + O(\hbar).$$

In particular, the free quantum Hamiltonian is given by

$$\widehat{\mathcal{H}} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} d_x^2. \tag{1.5}$$

All this appears quite natural from the following standpoint as well. If $|a| < \infty$ and/or $|b| < \infty$, the space $L^2(a,b)$ can be considered the subspace of functions vanishing outside the interval (a,b) in the space $L^2(\mathbb{R})$ of states of a particle on the whole real axis $\mathbb{R}$, whereas all the observables defined on $L^2(a,b)$, including $\hat{x}$ and $\hat{p}$, can be considered restrictions to this subspace of well-known s.a. operators defined on $L^2(\mathbb{R})$. For the case of a finite interval $[a,b]$, the position operator $\hat{x}$ becomes a bounded s.a. operator defined everywhere. Considering $\hat{p}$ as an s.a. operator, we have a set of three s.a. operators $\hat{x}$, $\hat{p}$, and $\widehat{\mathcal{H}}$ with the commutation relations

$$[\hat{x}, \hat{p}] = i\hbar, \ \left[\hat{p}, \widehat{\mathcal{H}}\right] = 0. \tag{1.6}$$

If all the previous statements hold, then the following observations seem paradoxical and cast doubt on the consistency of the adopted quantization scheme.

1.3.1 Paradox 1

Let $\psi_p(x)$ be an eigenvector of the s.a. momentum operator, $\hat{p}\psi_p = p\psi_p$. Based on the self-adjointness of the operators $\hat{p}$ and $\hat{x}$, we have the chain of equalities

$$\begin{aligned}
\left(\psi_p, [\hat{x}, \hat{p}]\psi_p\right) &= \left(\psi_p, \hat{x}\hat{p}\psi_p\right) - \left(\psi_p, \hat{p}\hat{x}\psi_p\right) \\
&= p\left(\psi_p, \hat{x}\psi_p\right) - \left(\hat{p}\psi_p, \hat{x}\psi_p\right) \\
&= p\left[\left(\psi_p, \hat{x}\psi_p\right) - \left(\psi_p, \hat{x}\psi_p\right)\right] = 0,
\end{aligned}$$

which obviously contradicts the commutation relation (1.6).

[8] It is rather a differential operation than a differential operator; see Chap. 4. A rigorous definition of the differentiation operator $\hat{d}_x$ is given in the end of Sect. 2.3.4.

In addition, this commutation relation implies the well-known Heisenberg uncertainty relation

$$\Delta x \Delta p \geq \frac{\hbar}{2}, \tag{1.7}$$

where Δx and Δp are the respective dispersions of the position and momentum for any state ψ of a particle. But for the case of a finite interval $[a, b]$ and for $\psi = \psi_p$, we have $\Delta x \leq b - a$, $\Delta p = 0$, and therefore $\Delta x \Delta p = 0$, which contradicts (1.7).

An explanation of the above paradoxes is given in Chap. 6. It is different for different types of interval: depending on the type of interval, either an s.a. momentum operator does not exist, or it exists but has no eigenvectors, or even if such vectors exist, they do not belong to the domain of the operator $\hat{p}\hat{x}$. In addition, in the case of a semiaxis or a finite interval, the canonical commutation relations together with the uncertainty principle do not hold.

1.3.2 Paradox 2

We now consider a free particle moving on a finite interval $[0, l]$. If we treat a motion governed by the Hamiltonian (1.5) as a motion in an infinite rectangular potential well, then the eigenvalues of the Hamiltonian and the corresponding eigenfunctions are well known from any textbook:

$$\widehat{\mathcal{H}}\psi_n(x) = E_n\psi_n(x), \quad E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{l}\right)^2 n^2, \tag{1.8}$$

$$\psi_n(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{\pi n}{l}x\right), \ n \in \mathbb{N}. \tag{1.9}$$

The set $\{\psi_n(x)\}_1^\infty$ of these eigenfunctions is an orthonormal basis in $L^2(0, l)$, which confirms the self-adjointness of the Hamiltonian.

As is also well known, two commuting s.a. operators have common eigenvectors, and if the spectrum of one of the commuting s.a. operators is nondegenerate, then its eigenvectors must be eigenvectors of another s.a. operator. In our case, we have two commuting s.a. operators $\hat{p}$ and $\widehat{\mathcal{H}}$, and the spectrum (1.8) of $\widehat{\mathcal{H}}$ is nondegenerate. Therefore, eigenfunctions (1.9) must be the eigenfunctions of $\hat{p}$. But we have

$$\hat{p}\psi_n(x) = -i\hbar\sqrt{\frac{2}{l}}\frac{\pi n}{l}\cos\frac{\pi n}{l}x \neq p_n\psi_n(x)$$

for any n, which contradicts the above assertion.

As explained in Chap. 6, this paradox is a consequence of the incorrect assumption that $\hat{p}$ and $\widehat{\mathcal{H}}$ commute; in particular, it is a consequence of the naïve belief that the Hamiltonian $\widehat{\mathcal{H}}$ can be represented as $\widehat{\mathcal{H}} = \hat{p}^2/2m$.

1.3.3 Paradox 3

As mentioned above, in standard textbooks on QM for physicists, some important notions related to operators in Hilbert spaces are often introduced in terms of their matrix elements with respect to an orthonormal basis, because it is believed that the matrix elements $f_{mn} = (e_m, \hat{f} e_n)$ of an operator $\hat{f}$ with respect to an orthonormal basis $\{e_n\}_1^\infty$ completely determine the operator $\hat{f}$ according to the following chain of equalities:

$$\psi = \sum_{n=1}^{\infty} \psi_n e_n, \ \psi_n = (e_n, \psi), \ \ \hat{f} e_n = \sum_{m=1}^{\infty} f_{mn} e_m,$$

$$\hat{f}\psi = \sum_{n=1}^{\infty} \psi_n \hat{f} e_n = \sum_{m=1}^{\infty} \left(\sum_{n=1}^{\infty} f_{mn} \psi_n \right) e_m.$$

For example, the adjoint $\hat{f}^+$ of $\hat{f}$ is defined as an operator whose matrix elements are given by

$$\left(f^+\right)_{mn} = \left(e_m, \hat{f}^+ e_n\right) = \left(\hat{f} e_m, e_n\right) = \overline{\left(e_n, \hat{f} e_m\right)} = \overline{f_{nm}}.$$

Correspondingly, an s.a. operator $\hat{f} = \hat{f}^+$ is defined as an operator whose matrix is Hermitian $f_{mn} = \overline{f_{nm}}$.

But let us consider the matrix $p_{mn} = (e_m, \hat{p} e_n)$ of the momentum operator $\hat{p}$ in the Hilbert space $L^2(0, l)$ with respect to the orthonormal basis $\{e_n\}_0^\infty$,

$$e_n(x) = \sqrt{\frac{2}{l}} \cos\left(\frac{\pi n}{l} x\right), \ n \in \mathbb{R}_+. \tag{1.10}$$

A direct calculation by integrating by parts shows that

$$\overline{p_{nm}} = p_{mn} + i[e_m(l)e_n(l) - e_m(0)e_n(0)] \neq p_{mn}, \ m + n = 2k + 1, \tag{1.11}$$

i.e., the matrix p_{mn} is not Hermitian, contrary to our expectations.

As is explained in Chap. 6, the paradox is related to the fact that the orthonormal basis (1.10) does not belong to the domain of any s.a. operator $\hat{p}$ from the whole family of admissible momentum operators.

1.3.4 Paradox 4

Let us consider a free particle on a segment $[0, l]$ as a particle in an infinite rectangular potential well, and let us calculate the mean of the squared energy $\langle E^2 \rangle$ for the state given by the wave function

$$\psi(x) = Nx(x-l), \tag{1.12}$$

where N is a normalization factor. Because $\left(\widehat{\mathcal{H}}\right)^2 \psi = 0$, this mean must be zero:

$$\langle E^2 \rangle = \left(\psi, \left(\widehat{\mathcal{H}}\right)^2 \psi\right) = 0.$$

On the other hand, using the self-adjointness of $\widehat{\mathcal{H}}$, we obtain a nonzero result for the same quantity:

$$\langle E^2 \rangle = \left(\widehat{\mathcal{H}}\psi, \widehat{\mathcal{H}}\psi\right) = \frac{N^2\hbar^4 l}{m^2}.$$

As explained in Chap. 6, a solution of the paradox is related to the fact that the function $\widehat{\mathcal{H}}\psi(x)$ does not belong to the domain of a correctly defined Hamiltonian $\widehat{\mathcal{H}}$ associated with an infinite potential well, although the function $\psi(x)$ does.

1.3.5 Paradox 5

We consider the Schrödinger equation for a free particle on the segment $[0, l]$,

$$i\hbar\frac{\partial\psi(t,x)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(t,x), \; x \in [0,l]. \tag{1.13}$$

We recall that in the idealized quantization scheme, the time-evolution problem in the form (1.13) can be posed for an arbitrary initial state. Let the initial state $\psi_0(x) = \psi(t_0, x)$ at $t_0 = 0$ be

$$\psi(0,x) = C\exp\left(\frac{\mathrm{i}+1}{\sqrt{2}}\frac{kx}{\hbar}\right), \tag{1.14}$$

where k is a fixed real parameter with dimension of momentum. It is easy to verify that the solution $\psi(t, x)$ of (1.13) with initial condition (1.14) is given by

$$\psi(t,x) = \exp\left(-\frac{k^2}{2m\hbar}t\right)\psi_0(x). \tag{1.15}$$

It is surprising that the evolution of the given initial state is not unitary: the wave function $\psi(t, x)$ "vanishes" with time. This situation is evidently related to the fact that formally, we have

$$\widehat{\mathcal{H}}\psi_0(x) = -\frac{ik^2}{2m}\psi_0(x) \Longrightarrow \widehat{\mathcal{H}}\psi(t,x) = -\frac{ik^2}{2m}\psi(t,x),$$

i.e., the initial state ψ_0 and the evolving state $\psi(t)$ are the eigenstates of the s.a. Hamiltonian with a pure imaginary eigenvalue, which is impossible, as is well known.

As explained in Chap. 6, a resolution of the paradox lies in the fact that if the function $\psi_0(x)$ does not belong to the domain of any correctly defined s.a. Hamiltonian $\widehat{\mathcal{H}}$ from the whole family of admissible Hamiltonians for a free particle on the interval $[0, l]$, then $\psi(t, x)$ also does not, which is irreconcilable with the Schrödinger equation.

1.3.6 Concluding Remarks

In the foregoing, we discussed some QM paradoxes arising under a naïve treatment of simple one-dimensional systems with boundaries. The number of paradoxes can be extended (see, for example, [31, 74]), and certain of the others are examined below. In Chap. 7, we discuss possible paradoxes related to singular potentials with a simple example of a particle moving on the real axis or a semiaxis in the so-called Calogero potential field $V(x) = \alpha/x^2$. But even the above examples seem to be sufficient to convince the reader–physicist that a rigorous approach to the definition of operators and especially of observables in QM is a necessity. The point is that up to now, we were too naïve in our analysis; strictly speaking, our arguments were incorrect, and our conclusions were wrong. The reason is that all the operators involved are unbounded, and for unbounded operators, the algebraic rules and the notion of commutativity are nontrivial. In fact, the above-used rules and notions were uncritically borrowed from finite-dimensional algebra; they are valid for bounded operators, while for unbounded operators, a special treatment is necessary. The correct treatment removes all the paradoxes.

Chapter 2
Linear Operators in Hilbert Spaces

In this chapter, we remind the reader of basic notions and facts from the theory of Hilbert spaces and of linear operators in such spaces which are relevant to the subject of the present book.

2.1 Hilbert Spaces

2.1.1 Definitions and General Remarks

Definition 2.1. (A) A *Hilbert space* $\mathfrak{H}$ is a linear space over the complex numbers. As a rule, the elements of $\mathfrak{H}$ (vectors or points) are denoted by Greek letters: $\xi, \eta, \zeta, \varphi, \psi, \chi, \ldots \in \mathfrak{H}$, whereas numbers, complex or real, are denoted by italic Latin letters: $a, b, c, x, y, z, \ldots \in \mathbb{C}$ or $\mathbb{R}$. In what follows, we consider infinite-dimensional Hilbert spaces.[1]

(B) The space $\mathfrak{H}$ is endowed with a scalar product that is a positive definite sesquilinear form on $\mathfrak{H}$. This means that every pair of vectors ξ, η is assigned a complex number (ξ, η), the scalar product of ξ and η, with the properties[2]

$$(\xi, \eta) = \overline{(\eta, \xi)}\,;\ (\xi, \xi) \geq 0\,,\ \text{and}\,(\xi, \xi) = 0\ \text{iff}\ \xi = 0\,;$$

$$(\xi, a\zeta + b\eta) = a(\xi, \zeta) + b(\xi, \eta) \Longrightarrow (a\xi + b\zeta, \eta) = \overline{a}(\xi, \eta) + \overline{b}(\zeta, \eta)\,.$$

[1] Finite-dimensional Hilbert spaces (or Euclidean spaces) are also encountered in QM as spaces of states, e.g., in QM of two-level systems, finite spin systems, and so on. Finite-dimensional spaces are free from the problems that are examined in the present book.

[2] We use "iff" in its standard usage for "if and only if." For brevity, the arrow $\Longrightarrow$ stands for "implies."

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