An excerpt from the Introduction

Theoretical physics, especially quantum mechanics, has always both supplied ideas to and used the results of the theory of differential equations. As a product of the interaction between the two disciplines, there arose a new and very productive science, known as *mathematical physics*. Not only has its development led to new results in the natural sciences, but it has also given an impetus for new ideas in other mathematical fields, such as representation theory, algebraic topology, and differential geometry. Unfortunately, in the last decades the theory of differential equations has moved ever farther away from its physical origins. This is already obvious from the names of mathematical disciplines taught in high school. The traditional course of equations of mathematical physics changed its name to "partial differential equations," and apart from rather isolated derivation of the heat equation and the equation for the motion of a vibrating string, physically meaningful examples are often missed in such courses.

The present book gives a new systematic mathematically rigorous exposition of methods for studying linear partial differential equations on the basis of quantization of appropriate objects in phase space. The quantization of all three types of classical objects (states, observables, and canonical transformations) is carried out in a unified way, by means of a special integral transform. The book covers a wide variety of results, both old and new, and treats them all within a unified framework.

We also consider a number of applications. The microlocal classification of differential equations is described. Some problems of mechanics and theoretical physics are considered, e.g., the propagation of electromagnetic waves in plasma. The relationship between the quantization of contact structures and the index theory for elliptic pseudodifferential operators and Fourier integral operators is also discussed. In addition, the quantization of symplectics structures is applied to the proof of various generalizations of the Atiyah–Bott–Lefschetz fixed point theorem that are important in studying the topology of manifolds.

The exposition moves gradually from the simple to the complex. Numerous examples are included to help the reader understand the material.

The book is intended for a wide readership, including undergraduates, graduate students, and scientists specializing in differential equations, applied mathematics, mathematical and theoretical physics, and differential geometry and topology.

Chapter 1

Quantization and the Wave Packet Transform

Contents

The applications of quantization methods in the theory of differential equations are based on the following "experimental fact," known as the *correspondence principle* in quantum mechanics:

> *As Planck's constant h tends to zero, the quantum-mechanical description passes into the classical description of the same physical system.*

Of course, we have to explain what the relation $h \to 0$ means when h is supposedly Planck's *constant*. This can be understood as follows. When considering some physical system, we can use various scales (or units of measure). As we gradually pass from "micro" units, well suited to describe quantum phenomena, to "macro" units, suitable for classical phenomena, the numerical value of h expressed in the corresponding units tends to zero. At the same time, the quantum nature of the system becomes less and less apparent, and we continuously pass from the quantum to the classical description.

The power of the correspondence principle is not actually restricted to quantum mechanics; it turns out that whenever we deal with phenomena described by linear differential equations, the behavior of solutions is largely determined by an appropriately constructed "classical mechanics."

Eventually, the correspondence principle, and, accordingly, *quantization* (more precisely, *semiclassical*, or *asymptotic* quantization, which is only dealt with in this book) penetrates throughout the theory of differential equations, and in this book we show how the unified quantization-based approach helps one solve various problems related to linear differential equations.

With this objective in mind, in the first chapter we deal with asymptotic quantization in Euclidean phase space, which corresponds to the simplest physical model. Namely, here we describe an integral transform that provides a unified quantization procedure for all objects of classical mechanics: states, observables, and transformations. This transform has quite a long history. It was originally introduced in 1961 by V. Bargmann [1] as a transform relating the harmonic oscillator representation of the creation-annihilation operators to the Fock representation by operators acting on holomorphic functions. The *Bargmann*

transform enjoys numerous applications in representation theory as well as mathematical physics. Later, many authors reintroduced or rediscovered this transform in various contexts, sometimes in a slightly different or a more general form. Let us indicate some of these results. In 1978 Cordoba and Fefferman [5] defined a *wave packet transform* on smooth manifolds and used it to give an alternative construction of Fourier integral operators; their construction was closely followed in 1989 by Karasev [7] in his "global description" of Maslov's canonical operator. In 1975-6, Bros and Iagolnitzer [4] introduced what was later called the *Fourier–Bros–Iagolnitzer* (*FBI*) *transformation* and developed and generalized to general (nonquadratic) phase functions by Sjöstrand [16] (see also [3], [10], and [17]). The FBI transformation is used in the context of analytic wave front, microsupport, and related topics; some details and applications, as well as further references, can be found, e.g., in [6], [9], [12], and [11]. In the framework of a unified quantization procedure, this transform was considered by Sternin and Shatalov in [19], [18] (where it was termed the Fourier–Gauss transform), and by Nazaikinskii and Sternin in [15]. Here we develop the approach adopted in the last three papers. Of the numerous names assigned to Bargmann type transforms since 1961, we prefer "wave packet transform". Indeed, in our approach the transform arises from quantization of states, which gives wave packets as ψ-functions of minimum uncertainty.

1.1 Classical and Quantum Descriptions of a Physical System

Suppose that we intend to describe a physical system. Regardless of whether our description will be classical or quantum, it must necessarily contain certain basic elements. Indeed, at each instant of time the system resides in some *state*, and so we must explain how states are described and what the overall supply of states is—that is, we must define what is called the *state space*. Next, all our knowledge about a specific system comes from *observation*, or *measurement*. So we must explain what and how can be measured and how the measurement re-

sults can be interpreted. Thus, we arrive at the notion of an *observable*. Our system develops in time, and so we must explain how to specify the *dynamics* (the evolution law) of states and how to describe it in terms of states themselves and in terms of what can be measured, i.e. observables. Last, but not least, we must indicate admissible *transformations* of our objects, i.e., transformations that do not affect the form of the model and hence provide equivalent representations of the same physical system. (Note that the dynamic flow specified by the evolution law will then give particular cases of such transformations.)

Summarizing, we see that any description of a physical system must necessarily include the following elements:

1. States;
2. Observables;
3. Dynamics (evolution law);
4. Transformations.

Now let us see how all these elements are described in the framework of classical and quantum mechanics.

By way of example, we consider the simplest physical system S with n degrees of freedom and flat *configuration space* $\mathbf{R}^n$. If $n = 3k$, this may be a system of k particles, possibly interacting and acted upon by an external field; points $x \in \mathbf{R}^n$ represent the coordinates of particles in three-dimensional space: $x = (\vec{y}_1, \vec{y}_2, ..., \vec{y}_k)$, $\vec{y}_j \in \mathbf{R}^3$, $j = 1, ..., k$.

1.1.1 Classical mechanics

The phase space. According to the principles of classical Newtonian mechanics, the state of such a system will be uniquely determined if we specify the position vector and the momentum of each of the particles. Thus, every state s of S is depicted by some point $(q, p) \in \mathbf{R}^{2n}$, where $q = (q_1, ..., q_n)$ is the vector of coordinates of all particles[1] and

[1]Essentially, q denotes the same object as x above; however, we shall see later on that using distinct letters for the coordinate variables in the configuration space and the phase space is convenient.

$p = (p_1, ..., p_n)$ is the vector of the corresponding momenta. The space $\mathbf{R}^{2n} = \mathbf{R}^{2n}_{q,p}$ is called the *phase space* of the system S.

For a more complicated physical system, whose configuration space is some manifold M, the phase space is the cotangent bundle T^*M. This case will be discussed in the forthcoming chapters; here we only deal with the simplest situation.

Observables. Now let f be an observable in the system S. In classical mechanics, observables are functions of state: once the system is in a given state s, the measurement of f will invariably give the same value. If s is represented[2] by a point (q, p), then we denote this value by $f(q, p)$. Thus an observable is none other than a function $f : \mathbf{R}^{2n} \to \mathbf{R}$ (there is of course no law against considering, say, complex-valued or matrix observables, etc.). The simplest observables are the coordinates q and the momenta p themselves; they are represented by the functions $f(q, p) = q$ and $f(q, p) = p$, respectively.

The evolution law. One of the most important observables is the *energy* h, represented in classical mechanics by a function $H(q, p)$, also referred to as the *Hamiltonian* of the system. The system dynamics is uniquely determined by the Hamiltonian. Namely, the evolution of the phase point (q, p) is described by the *Hamilton system* of ordinary differential equations

$$\dot{q} = H_p(q, p), \qquad \dot{p} = -H_q(q, p). \tag{1.1}$$

(the dot stands for the derivative with respect to time).

Accordingly, the value of any observable evolves in time according to the equation[3]

$$\dot{f} \equiv \frac{d}{dt} f(q(t), p(t)) = \dot{p} f_p + \dot{q} f_q = H_p f_q - H_q f_p. \tag{1.2}$$

[2] In what follows we sometimes do not distinguish between objects and their representatives in a model provided this cannot lead to a misunderstanding.

[3] In expressions like those on the right-hand in (1.2), summation from 1 to n is assumed: $H_p f_q \equiv \sum_{j=1}^{n} H_{p_j} f_{q_j}$, etc.

The right-hand side of (1.2) is denoted by $\{H, f\}$ and is called the *Poisson bracket* of H and f. Thus, f satisfies the *Liouville equation*

$$\dot{f} = \{H, f\}. \tag{1.3}$$

Under appropriate assumptions on the Hamiltonian, system (1.1) determines a one-parameter group

$$g_t : \mathbf{R}^{2n} \to \mathbf{R}^{2n} \tag{1.4}$$

of diffeomorphisms of the state space. Moreover, these diffeomorphisms are canonical, that is, they prefer the *symplectic 2-form* $\omega^2 = dp \wedge dq \equiv \sum_{j=1}^{n} dp_j \wedge dq_j$:

$$g_t^* \omega^2 = \omega^2. \tag{1.5}$$

Transformations. It is also useful to consider general transformations g satisfying (1.5). They preserve the form of the Hamilton system (1.1) and the Liouville equation (1.3) (the Hamiltonian itself is, of course, transformed according to the law $H \mapsto g^* H$), and so they can be viewed just as *admissible coordinate transformations* of the state space $\mathbf{R}^{2n}$ of classical mechanics.

1.1.2 Quantum mechanics

First, let us recall some general principles of quantum mechanics without referring to the specific nature of the system S.

The state space. In quantum mechanics, the states of S are described by elements $\psi \in \mathcal{H}$ of a Hilbert space $\mathcal{H}$, called the *state space* of the system. More precisely, the elements ψ corresponding to states have unit norm, $||\psi|| = 1$, and any two elements ψ, φ differing by a unimodular complex factor, $\psi = \varphi e^{i\alpha}$, correspond to the same state. (Putting this other way round, we can say that the set of states of a system in quantum mechanics is the *projective space* $P(\mathcal{H})$.) The inner product on $\mathcal{H}$ will be denoted by $(\cdot, \cdot)$. We adopt the convention, usual in quantum mechanics, that the inner product is linear in the second argument and antilinear in the first argument.

Observables. Observables are not functions of state in quantum mechanics: the measurement of an observable in some state is not uniquely determined by the state but can produce different values obeying some probability distribution law. Specifically, any observable f is represented by a linear (in general, unbounded) operator

$$\widehat{f} : \mathcal{H} \to \mathcal{H}$$

in the state space; for physically meaningful observables, this operator is usually self-adjoint. This operator is related to measurements as follows. Any measurement of f yields some number λ belonging to the spectrum $\sigma(\widehat{f})$. For simplicity, let us consider the case in which the spectrum is discrete, $\sigma(\widehat{f}) = \{\lambda_k\}_{k=1}^{\infty}$. Let $\{\psi_k\}_{k=1}^{\infty}$ be the corresponding orthonormal basis of eigenfunctions of $\widehat{f}$. Then the probability of obtaining the value λ_k when measuring f in a state ψ is given by

$$\mathbf{P}_{\psi}(\lambda = \lambda_k) = |(\psi_k, \psi)|^2. \tag{1.6}$$

This is none other than the squared absolute value of the kth coefficient in the expansion of ψ with respect to the basis $\{\psi_k\}$. Since $\|\psi\| = 1$, we see that these probabilities sum to 1, and moreover, the *expectation* of the value produced by the measurement of f in a state ψ (also referred to as the expectation of $\widehat{f}$) is given by

$$\overline{\widehat{f}} = \sum_{k=1}^{\infty} \lambda_k \mathbf{P}_{\psi}(\lambda = \lambda_k) = \left(\psi, \sum_{k=1}^{\infty} (\psi_k, \psi)\lambda_k \psi_k\right) = (\psi, \widehat{f}\psi). \tag{1.7}$$

When the spectrum of f is not purely discrete, the above formulas undergo obvious modifications: sums are supplemented by integrals over the continuous spectrum, where instead of probabilities we have probability measures like $\mu_{\psi}(\lambda) = |(\psi_{\lambda}, \psi)|^2 \, d\lambda$, where ψ_{λ} is the "generalized eigenfunction" corresponding to a point λ of the continuous spectrum.

Since the expectations are the only entities that can be measured, this explains why vectors ψ, ψ_1 differing by a unimodular complex factor describe the same state: the factor does not affect the value of the expectation (1.7).

Mixed states and the density matrix. The above quantum-mechanical description of states of the physical system S by vectors of the Hilbert space $\mathcal{H}$ is perfectly valid if the system is closed or at least if the environment is purely classical (say, if S is a system of interacting quantum particles in a classical field). If, however, S is part of a larger system S_1 whose remaining part also displays *quantum* properties, then the situation is different. A simple analysis shows that if we wish to describe the states of S in terms of $\mathcal{H}$, then we have to admit states more complicated than those described by separate elements of $\mathcal{H}$. Indeed, let $\mathsf{S}_1 = \mathsf{S} \cup \mathsf{T}$, where T is another system, whose quantum state space will be denoted by $\mathcal{G}$. Then the quantum state space of S_1 is $\mathcal{H}_1 = \mathcal{H} \otimes \mathcal{G}$, where $\otimes$ stands for the tensor product of Hilbert spaces. Now suppose that the system S_1 is in a state $\chi \in \mathcal{H}_1$. By the definition of the tensor product, we have

$$\chi = \sum \alpha_j \, \psi_j \otimes \phi_j, \quad \alpha_j \in \mathbf{C}, \quad \psi_j \in \mathcal{H}, \quad \phi_j \in \mathcal{G}, \quad ||\psi_j|| = ||\phi_j|| = 1,$$

where the sum may be infinite. We can assume without loss of generality that the ϕ_j form an orthonormal system. Then

$$\sum \alpha_j^2 = ||\chi||^2 = 1.$$

Let $\widehat{f}$ be a quantum observable in the system S. The expectation of $\widehat{f}$ can be calculated as follows:

$$\begin{aligned} \overline{\widehat{f}} &= (\chi, \widehat{f} \otimes 1 \, \chi) = \Big(\sum \alpha_j \, \psi_j \otimes \phi_j, \widehat{f} \otimes 1 \sum \alpha_k \, \psi_k \otimes \phi_k\Big) \\ &= \sum_j \overline{\alpha}_j \, \alpha_k (\psi_j, \widehat{f}\psi_k)(\phi_j, \phi_k) = \sum |\alpha_j|^2 (\psi_j, \widehat{f}\psi_j). \end{aligned} \tag{1.8}$$

By comparing (1.8) with (1.7), we arrive at the following interpretation of the expectation (1.8): our system is in the state ψ_1 with probability $|\alpha_1|^2$, in the state ψ_2 with probability $|\alpha_2|^2$, and so on. Such complicated states are referred to as *mixed states*, in contrast with *pure states*, described by elements of $\mathcal{H}$. To describe mixed states more conveniently, note that Eq. (1.8) can be rewritten in the form

$$\overline{\widehat{f}} = \mathrm{trace}(\widehat{\rho}\widehat{f}),$$

where

$$\widehat{\rho} = \sum |\alpha_j|^2 \psi_j(\psi_j, \cdot) \tag{1.9}$$

is an operator in $\mathcal{H}$, which is called the *density matrix* corresponding to our mixed state. Density matrices are characterized by the following properties.

1. $\widehat{\rho} = \widehat{\rho}^* \geq 0$, that is, $\widehat{\rho}$ is self-adjoint and nonnegative;
2. $\operatorname{trace} \widehat{\rho} = 1$.

In the sequel we shall sometimes use the description of states via the density matrix. However, we almost invariably deal with pure states. We can readily see that the density matrix corresponding to a pure state $\psi \in \mathcal{H}$ is the rank one orthogonal projection

$$\widehat{\rho} = \widehat{P}_\psi = \psi(\psi, \cdot) \tag{1.10}$$

on the subspace generated by ψ.

The evolution law. Just as in classical mechanics, the evolution of the system in quantum mechanics is determined by a distinguished observable, the *energy* h. Here it is represented by the *energy operator* (*Hamiltonian*) $\widehat{H}$. The state $\psi = \psi_t$ evolves in time according to the *Schrödinger equation*

$$ih\dot{\psi} = \widehat{H}\psi, \tag{1.11}$$

where h is Planck's constant. The solution of (1.11) is given by

$$\psi_t = U_t \psi_0, \tag{1.12}$$

where

$$U_t = e^{-\frac{i}{h}\widehat{H}t} \tag{1.13}$$

is the one-parameter group of unitary operators generated by $\widehat{H}$.

We recall that the wave function ψ itself cannot be measured; only expectations (1.7) can be observed. Let us calculate the expectation of an observable $\widehat{f}$ in the state ψ_t. We have

$$(\psi_t, \widehat{f}\psi_t) = (U_t\psi_0, \widehat{f}U_t\psi_0) = (\psi_0, U_t^{-1}\widehat{f}U_t\psi_0) = (\psi_0, \widehat{f}_t\psi_0),$$

where

$$\widehat{f}_t = U_t^{-1} \widehat{f} U_t \tag{1.14}$$

satisfies the *Heisenberg equation*

$$ih \frac{d\widehat{f}}{dt} = -[\widehat{H}, \widehat{f}]. \tag{1.15}$$

(Here $[\widehat{H}, \widehat{f}] = \widehat{H}\widehat{f} - \widehat{f}\widehat{H}$ is the *commutator* of the operators $\widehat{H}$ and $\widehat{f}$.) Thus, without changing the expectations, we can replace the *Schrödinger picture,* in which observables are independent of time and states evolve according to (1.12), by the *Heisenberg picture*, in which states are independent of time and observables evolve according to the rule (1.14).

Let us also write out the equation that governs the evolution of the density matrix in the Schrödinger picture. We derive it for the density matrix (1.10) corresponding to a pure state ψ_0 (this is just the case in which we shall need it). We have

$$\widehat{\rho}_t = U_t \psi_0 (U_t \psi_0, \cdot) = U_t \widehat{\rho}_0 U_t^{-1};$$

by differentiating this with respect to t, we find that $\widehat{\rho}_t$ satisfies the *Wigner equation*

$$ih \frac{d\widehat{\rho}_t}{dt} = [\widehat{H}, \widehat{\rho}_t]. \tag{1.16}$$

Note the difference between the Wigner and the Heisenberg equation. Although very similar in the appearance (they differ only in the sign of the commutator), they describe two opposite points of view: the Wigner equation shows how the density matrix (i.e. the state) evolves, whereas the Heisenberg equation describes the evolution of observables in the different picture where the states are "frozen."

Transformations. Just as in classical mechanics, it is useful to consider general unitary transformations $U : \mathcal{H} \to \mathcal{H}$ that do not necessarily have the form (1.13). These transformations preserve the form of the Schrödinger equation (1.11) and the Heisenberg equation (1.15) (the Hamiltonian is transformed according to the rule $\widehat{H} \to \widehat{U}\widehat{H}\widehat{U}^{-1}$), and so they can be viewed as admissible transformations of the state space $\mathcal{H}$ of quantum mechanics.

Quantum mechanics of the simplest system. Now let us proceed to what is specific to the quantum description of our simplest physical system S.

In this system, we have the fundamental observables q and p (the coordinates and the momenta). Quantum mechanics postulates that these observables must be represented by self-adjoint operators

$$(\widehat{q},\widehat{p}) = (\widehat{q}_1,...,\widehat{q}_n,\widehat{p}_1,...,\widehat{p}_n)$$

in the Hilbert state space $\mathcal{H}$ such that the commutation relations

$$[\widehat{p}_j,\widehat{p}_k] = [\widehat{q}_j,\widehat{q}_k] = 0, \qquad [\widehat{p}_j,\widehat{q}_k] = -ih\delta_{jk}, \qquad j,k = 1,...,n, \quad (1.17)$$

are valid, where δ_{jk} is the Kronecker delta. (We shall recall the motivation for this later on in the discussion of quantization and the correspondence principle.) Moreover, this representation must be *irreducible* in the sense that there is no proper subspace of $\mathcal{H}$ invariant under all the operators $(\widehat{q},\widehat{p})$.

Technically, things are a bit more complicated. Relations (1.17) mean that the $2n+1$ self-adjoint operators $(\widehat{q}_1,...,\widehat{q}_n,\widehat{p}_1,...,\widehat{p}_n,1)$ (where 1 is the identity operator) form a representation of a specific Lie algebra, known as the Heisenberg algebra and denoted by h_n. The Heisenberg algebra is the real Lie algebra with $2n+1$ basis elements $e_1,...,e_n,f_1,...,f_n,\xi$ with the Lie brackets

$$\begin{aligned}[e_j,e_k] = [f_j,f_k] = [e_j,\xi] = [f_j,\xi] = 0, \quad [f_j,e_k] &= \delta_{jk}\xi, \quad (1.18)\\ j,k &= 1,...,n.\end{aligned}$$

The term "representation" means that there is a mapping of h_n into the set of self-adjoint operators on $\mathcal{H}$ such that

$$\begin{aligned}e_j \mapsto \widehat{q}_j, \quad f_j &\mapsto \widehat{p}_j, \quad \xi \mapsto h, \quad \text{and}\\ (\text{Lie bracket}) &\longmapsto -ih \times (\text{commutator})\end{aligned}$$

(the factor $-ih$ has been introduced for convenience, so that all operators in the representation be self-adjoint rather than skew-self-adjoint and Planck's constant h occur in convenient places in all formulas.) However, since the representation operators are unbounded, we must take extreme care with their domains. The standard way of handling this difficulty is to assume, as is customary in representation theory of Lie algebras and Lie groups, that our representation of the Lie algebra h_n

comes from an irreducible unitary representation of the corresponding Lie group H_n, which is called the Heisenberg group. Further details can be found in standard textbooks on Lie groups and representation theory.

The celebrated Stone–von Neumann theorem says that *these conditions uniquely determine the representation up to a unitary equivalence (an isometric isomorphism).* The standard *coordinate representation* is the one in which the state space $\mathcal{H}$ is just $L^2(\mathbf{R}^n_x)$, where $\mathbf{R}^n_x$ is the configuration space of the system, and the operators $\widehat{p}, \widehat{q}$ have the form

$$\widehat{q} = x \quad \text{(the operator of multiplication);} \tag{1.19}$$

$$\widehat{p} = -ih\frac{\partial}{\partial x}. \tag{1.20}$$

Thus, the states are represented by square integrable functions $\psi(x)$ on the configuration space $\mathbf{R}^n_x$. The squared absolute value $|\psi(x)|^2$ has the meaning of the *probability density* of the system at the point x. (If the system is in a state $\psi(x)$, then the probability of finding the system in a small cube $(x_1, x_1 + \Delta x_1) \times \cdots \times (x_n, x_n + \Delta x_n)$ of the configuration space is $|\psi(x)|^2 \Delta x_1 \ldots \Delta x_n$.)

We shall study a number of other representations in Section 1.2.

1.1.3 Classical vs. quantum

For convenience, let us bring together all main elements of the classical and quantum descriptions of the simplest physical system S. They are shown in Table 1.1, where the first column displays classical objects and the second contains their quantum counterparts.

1.1.4 Quantization problem and the correspondence principle

So far, we have described the main elements of the classical and quantum descriptions of a physical system. However, nothing has been said as to how the classical and the quantum descriptions are related to each other. The quantum description involves Planck's fundamental constant h, and one of the basic postulates of quantum mechanics is the *correspondence principle*, already discussed in the beginning of this chapter. Now we state it in the following form.

Main objects	Classical Mechanics	Quantum Mechanics
States	points (q,p) of the phase space $\mathbf{R}^{2n} = \mathbf{R}^n_q \oplus \mathbf{R}^n_p$	Elements $\psi \in \mathcal{H}$ of the Hilbert state space $\mathcal{H} = L^2(\mathbf{R}^n_x)$
Observables	functions $f(q,p)$ on the phase space	Linear operators $\widehat{f} : \mathcal{H} \to \mathcal{H}$ (usually self-adjoint and unbounded)
Dynamics	Hamilton system for states: $\dot{p} = -H_q$, $\dot{q} = H_p$ Liouville equation for observables $\dot{f} = \{H, f\}$ H is the *Hamiltonian*	Schrödinger equation for states: $ih\,\dot{\psi} = \widehat{H}\psi$ Heisenberg equation for observables $ih\frac{\partial \widehat{f}}{\partial t} = -[\widehat{H}, \widehat{f}]$ $\widehat{H}$ is the *energy operator*
Transformations	canonical transformations of the phase space: $g : \mathbf{R}^{2n} \to \mathbf{R}^{2n}$ $(p,q) \mapsto g(p,q)$ $f(p,q) \mapsto (g^* f)(p,q) \equiv f(g(p,q))$	Unitary transformations $U : \mathcal{H} \to \mathcal{H}$ $\psi \mapsto U\psi$ $\widehat{f} \mapsto U\widehat{f}U^{-1}$

Table 1.1: Classical and quantum objects

As Planck's constant h tends to zero, the solutions of quantum-mechanical equations result in the solutions of the corresponding equations of classical mechanics for the same physical system.

More precisely, the evolution of the mean values $\overline{\widehat{f}} = (\psi, \widehat{f}\psi)$ of quantum observables is described in the limit as $h \to 0$ by the classical equations of notion (1.3), where f and H are the classical observables corresponding to the quantum observables $\widehat{f}$ and $\widehat{H}$, respectively (of course, the latter correspondence must also be described). The passage

$$\left(\begin{array}{c}\text{quantum}\\ \text{description}\end{array}\right) \stackrel{h\to 0}{\longrightarrow} \left(\begin{array}{c}\text{classical}\\ \text{description}\end{array}\right) \tag{1.21}$$

is known as the *(semi)classical limit*.

Now we are faced with the following problem: Suppose that we know the classical description of some objects related to the system S. What can we say then about the quantum description of the same objects? The passage

$$\left(\begin{array}{c}\text{classical}\\ \text{description}\end{array}\right) \longrightarrow \left(\begin{array}{c}\text{quantum}\\ \text{description}\end{array}\right)$$

is known as *quantization*. The quantum description of a physical system is much richer than the classical one, and so quantization is by no means unique. One obvious restriction is that the quantization procedure must be the right inverse of the semiclassical limit (by passing from the classical description to a quantum description and then back we obtain the original classical description). However, this requirement alone gives us insufficient information on how to quantize. Thus we must add some extra requirements.

Suppose that we have already constructed the quantum state space $\mathcal{H}$. (This is just the first step of the quantization procedure in the wide sense. For our simplest model system, as the Stone–von Neumann theorem guarantees, this step is unique). Then we must do *quantization in the narrow sense* (which will be referred to as simply *quantization* in what follows): to each classical observable $f(q,p)$ we must assign a quantum observable $\widehat{f}$. Apparently the oldest quantization recipe

going back to the creators of quantum mechanics and incorporated by them in the correspondence principle says that we must have

$$[\widehat{f},\widehat{g}] = -ih\widehat{\{f,g\}}. \tag{1.22}$$

(On the left-hand side, $[\,\cdot\,,\,\cdot\,]$ is the commutator, and $\{\,\cdot\,,\,\cdot\,\}$ on the right-hand side is the Poisson bracket). Later Dirac indicated that (1.22) cannot be achieved exactly for arbitrary f, g, and so the actual requirement will be[4]

$$[\widehat{f},\widehat{g}] = -ih\{\widehat{f},\widehat{g}\} + O(h^2). \tag{1.23}$$

Moreover, we require that

$$\widehat{1} = 1 \quad \text{(the identity operator in } \mathcal{H}) \tag{1.24}$$

and

$$\widehat{f}\widehat{g} = \widehat{fg} + O(h). \tag{1.25}$$

There is extensive literature devoted to the quantization problem (see Bibliographic remarks in the end of the book). Here we do not consider the problem in its full generality and restrict ourselves to the simplest physical system. The phase space $\mathbf{R}^{2n}_{q,p}$ of this system is linear, and the space $C^\infty(\mathbf{R}^{2n}_{q,p})$ of classical observables contains the subspace h_n of linear functions, spanned by the functions $\{q_1,\dots,q_n,p_1,\dots,p_n,1\}$. This subspace is just the Heisenberg Lie algebra of coordinates and momenta with respect to the Poisson bracket:

$$\{p_i,q_j\} = \delta_{ij}, \quad \{p_j,1\} = \{q_j,1\} = 0.$$

By virtue of the above description of the simplest physical system, regardless of what quantization we take, the following must be satisfied:

1. quantization takes any element $l \in \mathsf{h}_n$ to a self-adjoint operator $\widehat{l}: \mathcal{H} \to \mathcal{H}$;

2. relation (1.22) is satisfied exactly if $f, g \in \mathsf{h}_n$.

[4]The exact meaning of $O(h^2)$ also needs to be further explained. This will be done in due place.

However, the quantization of observables that are not linear functions of (p,q) is not uniquely determined. Since a classical observable $f(p,q)$ is a function of the coordinates and momenta, we can try to quantize $f(p,q)$ by substituting $\widehat{p}$ and $\widehat{q}$ for p and q, that is, by considering a function $f(\widehat{p},\widehat{q})$ of the operators $\widehat{p}$, $\widehat{q}$:

$$\widehat{f} = f(\widehat{p},\widehat{q}). \tag{1.26}$$

The correct definition of functions (1.26) is the subject of noncommutative analysis (see Chapter 8). In few words, we can assign a precise meaning to the expression (1.26) by specifying the order of action of the operators $(\widehat{p},\widehat{q})$ in this expression. Various orderings are possible, say, the Feynman orderings $f(\overset{1}{\widehat{p}},\overset{2}{\widehat{q}})$ and $f(\overset{2}{\widehat{p}},\overset{1}{\widehat{q}})$, the Weyl ordering $f\left(\frac{\overset{1}{\widehat{p}}+\overset{3}{\widehat{p}}}{2},\overset{2}{\widehat{q}}\right)$, the Jordan ordering $\frac{1}{2}f\left((\overset{1}{\widehat{p}},\overset{2}{\widehat{q}})+f(\overset{2}{\widehat{p}},\overset{1}{\widehat{q}})\right)$, and so on.

Further discussion of the quantization problem will be given in the forthcoming sections and in Chapter 2.

1.2 Representations and Transforms

The Hilbert state space of a given physical system can be described in many different ways. For example, the quantum-mechanical state space $\mathcal{H}$ of the simplest system S was described in the preceding section as $L^2(\mathbf{R}^n_x)$, but this is not the only possible choice. We can pass to a different description as follows. Let $\mathcal{H}_1$ be another Hilbert space, and let

$$U : \mathcal{H} \to \mathcal{H}_1 \tag{1.27}$$

be an isometric isomorphism (a unitary operator). Then to each element $\psi \in \mathcal{H}$ we assign the element

$$\widetilde{\psi} = U\psi \in \mathcal{H}_1,$$

and to each observable

$$\widehat{A} : \mathcal{H} \to \mathcal{H}$$

we assign the operator

$$\widetilde{B} = U\widehat{A}U^{-1} : \mathcal{H}_1 \to \mathcal{H}_1.$$

This procedure takes $\widehat{A}\psi$ to $\widehat{B}\widetilde{\psi}$ and moreover preserves the mean values of observables:

$$(\psi, \widehat{A}\psi) = (\widetilde{\psi}, \widehat{B}\widetilde{\psi}),$$

so that the two descriptions are indistinguishable from the viewpoint of an experimenter. The mapping U and the space $\mathcal{H}_1$ are said to define a *representation* of the quantum-mechanical system in question.[5]

If we have two representations, $(U_1, \mathcal{H}_1)$ and $(U_2, \mathcal{H}_2)$, of the same system , then they are obviously related by a *transform*

$$U : \mathcal{H}_1 \longrightarrow \mathcal{H}_2.$$

Namely, U is the transform such that the diagram

$$\begin{array}{ccc} \mathcal{H}_1 & \stackrel{U}{\longrightarrow} & \mathcal{H}_2. \\ \uparrow U_1 & & \uparrow U_2 \\ \mathcal{H} & \Longleftrightarrow & \mathcal{H} \end{array}$$

commutes.

An instructive example of two different representations is given by the Schrödinger picture and the Heisenberg picture (see (1.12) and (1.14)). Here the operator U relating the two representations depends on time (and hence the dynamics is described differently in the two pictures!), and $\mathcal{H}_1 = \mathcal{H}$ is the same (abstract) Hilbert space.

Clearly, there are many different quantum-mechanical representations of the same physical system. In practice, the construction of a representation often does not start from the unitary operator U. One constructs $\mathcal{H}_1$ independently and then tries to find U.

In the remaining part of this section we solely deal with quantum-mechanical representations of the simplest system S and study the transforms relating these representations to each other. In this study, the following consideration will be useful for us. Suppose that we have two representations of S in Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, and moreover, we know the coordinate and momenta operators in both representations:

$$\widehat{q}_j^{(k)}, \widehat{p}_j^{(k)} : \mathcal{H}_k \longrightarrow \mathcal{H}_k, \quad k = 1, 2.$$

[5] Although this notion of a representation is in some respect close to the notion of a representation used, say, in representation theory of groups, they must not be confused.

Then by the Stone–von Neumann theorem *there is a unique unitary operator*

$$U = \mathcal{H}_1 \to \mathcal{H}_2$$

such that

$$U\widehat{p}_j^{(1)}U^{-1} = \widehat{p}_j^{(2)}, \qquad U\widehat{q}_j^{(1)}U^{-1} = \widehat{q}_j^{(2)}, \qquad j = 1, \ldots, n. \tag{1.28}$$

Thus, the operator U can be found by solving Eq. (1.28).

Let us now proceed to the description of specific representations.

1.2.1 Coordinate and momentum representations and the Fourier transform

Mixed representations. The coordinate representation. There are various methods for obtaining representations; one of these methods is to take a set of commuting observables and reduce them to a diagonal form in some basis of $\mathcal{H}$. Then each vector $\psi \in \mathcal{H}$ is naturally represented by the set of its coordinates with respect to this basis. The coordinate and momentum representations are constructed as follows. From the set of $2n$ operators

$$\widehat{q}_1, \ldots, \widehat{q}_n, \widehat{p}_1, \ldots, \widehat{p}_n,$$

we choose a maximal subset of pairwise commuting operators and reduce them to a "diagonal form." Any such subset can be constructed as follows: for each $j = 1, \ldots, n$, we take *either* $\widehat{q}_j$ *or* $\widehat{p}_j$. (Clearly, there are 2^n distinct choices.) Thus we obtain *mixed coordinate-momentum representations* in general. However, there are two basic cases in which we make the same choice for all $j = 1, \ldots, n$. Suppose that we have chosen all coordinate operators. What does it mean to reduce these operators to a diagonal form? The spectrum of each of these operators is purely continuous and fills the entire real axis. Hence there are no eigenvectors in the usual sense, but there are "generalized eigenvectors," which are numbered by points of $\mathbf{R}^n$. The corresponding diagonal form is achieved in the space of square integrable functions of $x \in \mathbf{R}^n$, where the coordinate operators become just the multiplication operators

$$\widehat{q}_j = x_j, \quad j = 1, \ldots, n.$$

The generalized eigenfunctions are the Dirac delta functions $\delta(x-q)$, where q is the parameter numbering the eigenfunctions and, at the same time, the corresponding n-tuple of eigenvalues:

$$x_j\delta(x-q) = q_j\delta(x-q)_j, \quad j = 1,\dots,n.$$

We can find the form of the momentum operators in this representation by solving the commutation relations (1.17):

$$[\widehat{p}_j,\widehat{p}_k] = [\widehat{q}_j,\widehat{q}_k] = 0, \qquad [\widehat{p}_j,\widehat{q}_k] = -ih\delta_{jk}, \qquad j,k = 1,...,n.$$

With regard to the additional requirement that the $\widehat{p}_j$ must be self-adjoint, we can show that

$$\widehat{p}_j = -ih\frac{\partial}{\partial x_j} + \Phi_j(x), \quad j = 1,\dots,n, \tag{1.29}$$

where the $\Phi_j(x)$ are real-valued functions such that

$$\frac{\partial\Phi_j(x)}{\partial x_k} = \frac{\partial\Phi_k(x)}{\partial x_j}, \qquad j,k = 1,...,n. \tag{1.30}$$

Let $S(x)$ be a real-valued function such that

$$\frac{\partial S}{\partial x_j}(x) = \Phi_j(x), \quad j = 1,\dots,n.$$

(The existence of $S(x)$ follows from condition (1.30).)Then

$$-ih\frac{\partial}{\partial x_j}\circ e^{\frac{i}{h}S(x)} = e^{\frac{i}{h}S(x)}\circ\left(-ih\frac{\partial}{\partial x_j} + \Phi_j(x)\right),$$

whence we see that the multiplication by $e^{\frac{i}{h}S(x)}$ (which is a unitary operator in $L^2(\mathbf{R}^n_x)$) reduces the momentum operators to the simplest form in which $\Phi_j(x) \equiv 0, \quad j = 1,\dots,n$.

We see that in the representation that we have just constructed, the state space is $\mathcal{H} = L^2(\mathbf{R}^n_x)$, and the coordinate and momenta operators are given by

$$\widehat{q} = x, \qquad \widehat{p} = -ih\frac{\partial}{\partial x}. \tag{1.31}$$

Thus, this is none other than the *coordinate* representation, mentioned in the preceding section.

The momentum representation and the quantum Fourier transform. Equally important is the *momentum* representation, $\mathcal{H} \cong L^2(\mathbf{R}_p^n)$, in which the momentum operators are diagonal, that is, are represented by the multiplication operators,

$$\widehat{p}_j = p_j \tag{1.32}$$

(the corresponding generalized eigenfunctions are, of course, the delta functions $\delta(p-\xi)$, where ξ is the spectral point) and the coordinate operators are represented by differentiations,

$$\widehat{x}_j \cong ih\frac{\partial}{\partial p_j}. \tag{1.33}$$

(Here we are very brief, since the argument is much the same as in the preceding case.)

Let us derive the well-known transform relating these two representations. Let an element $\psi \in \mathcal{H}$ be represented by a function $\psi(x) \in L^2(\mathbf{R}_x^n)$ and a function $\widetilde{\psi}(p) \in L^2(\mathbf{R}_p^n)$ in the coordinate and momentum representations, respectively.

Then

$$\widetilde{\psi}(p) = F[\psi(x)], \tag{1.34}$$

where

$$F:\ L^2(\mathbf{R}_x^n) \to L^2(\mathbf{R}_p^n) \tag{1.35}$$

is the desired unitary transformation. We seek F in the form of an integral operator,

$$(F\psi)(p) = \int K(x,p)\,\psi(x)\,dx, \tag{1.36}$$

where $K(x,p)$ is the Schwartz kernel of F.

According to (1.19) and (1.32), we have

$$-ih\int K(x,p)\frac{\partial\psi(x)}{\partial x}\,dx = p\int K(x,p)\,\psi(x)\,dx$$

for any $\psi(x) \in L^2(\mathbf{R}_x^n)$ and any $p \in \mathbf{R}_x^n$, or, after integration by parts,

$$ih\int \frac{\partial K}{\partial x}(x,p)\psi(x)\,dx = p\int K(x,p)\,\psi(x)\,dx. \tag{1.37}$$

Since $\psi(x)$ is arbitrary, we see that

$$ih\frac{\partial K}{\partial x}(x,p) = pK(x,p),$$

whence it follows that

$$K(x,p) = e^{-\frac{i}{h}px}a(p), \qquad px = \sum p_j x_j, \tag{1.38}$$

where $a(p)$ is so far arbitrary. (However, we must take care that our operator must be unitary. In particular, $a(p) \neq 0$ for any p.) Thus F has the form

$$[F\psi](p) = a(p)\int e^{-\frac{i}{h}px}\psi(x)\,dx. \tag{1.39}$$

Under this transform the operator $\widehat{x}_j$ is represented by

$$\widehat{x}_j \cong ih\frac{\partial}{\partial p_j} - iha^{-1}(p)\frac{\partial a(p)}{\partial p}. \tag{1.40}$$

It is only natural to choose $a(p) = \text{const}$, and then we shall have (1.33). The specific value of the constant is determined by the normalization condition; the choice $a(p) = \left(\frac{-i}{2\pi h}\right)^{n/2}$ makes F unitary. (This is obvious, since with $a(p) = \text{const}$ the mapping F is just a rescaling of the ordinary Fourier transform.) Thus

$$[F\psi](p) = \left(\frac{-i}{2\pi h}\right)^{n/2}\int e^{-\frac{i}{h}px}\psi(x)\,dx. \tag{1.41}$$

The transform defined by (1.41) will be called the *quantum Fourier transform*. The inverse F^{-1} of (1.41) is given by

$$[F^{-1}\chi](x) = \left(\frac{i}{2\pi h}\right)^{n/2}\int e^{\frac{i}{h}px}\chi(p)\,dp.$$

Again, this follows from the inversion formula for the usual Fourier transform.

1.2.2 Fock representations and Bargmann transform

Now we shall describe some other representations of the same quantum-mechanical system.

The oscillator representation. To obtain this representation, we again choose some set of commuting operators and find a basis in which they all become diagonalized. Namely, let us consider the *quantum oscillator* operators

$$\widehat{H}_j = \frac{1}{2}(\hat{p}_j^2 + \hat{q}_j^2), \quad j = 1, \ldots, n. \tag{1.42}$$

Each of these self-adjoint operators has a discrete spectrum consisting of the eigenvalues

$$\lambda_k = h\left(k + \frac{1}{2}\right), \quad k = 0, 1, 2, \ldots$$

In the coordinate representation, the orthonormal basis of joint eigenfunctions corresponding to these eigenvalues has the form

$$\begin{aligned} \psi_{k_1 \ldots k_n}(x) &= c_{k_1 \ldots k_n} H_{k_1}\left(\frac{x_1}{\sqrt{h}}\right) \cdots H_{k_n}\left(\frac{x_n}{\sqrt{h}}\right) e^{-\frac{x^2}{2h}}, \\ & k_1, \ldots, k_n = 0, 1, 2, \ldots, \end{aligned} \tag{1.43}$$

where the $H_j(y)$, $y \in \mathbf{R}^1$, are Hermite polynomials and $c_{k_1 \ldots k_n}$ are normalizing constants. The *oscillator representation* is the representation in which every ψ-function is represented by the sequence of coefficients in its generalized Fourier series expansion with respect to the basis (1.43). Thus, the space of the oscillator representation is

$$\mathcal{H}_1 = \underbrace{l^2 \otimes \cdots \otimes l^2}_{n \text{ times}} \equiv (l^2)^{\otimes n}.$$

Let us find the transform

$$\Psi : L^2(\mathbf{R}_x^n) \longrightarrow (l^2)^{\otimes n}$$

relating the coordinate representation to the oscillator representation. Since (1.43) is an orthonormal basis, the coefficients $a_{k_1 \ldots k_n}$ in the expansion

$$\psi(x) = \sum_{k_1, \ldots, k_n = 0}^{\infty} a_{k_1 \ldots k_n} \psi_{k_1 \ldots k_n}(x)$$

can be found readily:

$$a_{k_1\dots k_n} = \int_{\mathbf{R}^n} \psi_{k_1\dots k_n}(x)\psi(x)\,dx$$

(recall that the functions $\psi_{k_1\dots k_n}$ are real-valued, so we omit the complex conjugation). We conclude that Ψ is the integral transformation with kernel

$$\Psi(k,x) = \psi_{k_1\dots k_n}(x), \quad x \in \mathbf{R}^n, \quad k = k_1,\dots,k_n \in \mathbf{Z}_+^n. \tag{1.44}$$

This kernel is real-valued, and since the transformation is unitary, it follows that the inverse transformation Ψ^{-1} has the same kernel (with the roles of the arguments interchanged).

Second quantization method. The oscillator representation can also be obtained in a completely different way, by applying the so-called *second quantization* method due to V. Fock to the phase space of classical mechanics. (In this context, the oscillator representation is called the *Fock representation*.) We shall first recall this method in its usual context, as it is applied to the Schrödinger equation. Since we do this for clarity and motivation alone, we shall never treat the convergence issues there (for the mathematically rigorous treatment of second quantization in the infinite-dimensional situation, see Berezin [2]).

In fact, we deal with the simplest version of second quantization, namely, the one that deals with the "one-particle" Schrödinger equation (so that the many-particle system obtained by second quantization is a system of *noninteracting particles*).

Let $\mathcal{H}$ be the state space of an "elementary" quantum-mechanical system (for short, we refer to this system as a "particle," even though actually it can be rather complicated. The second quantization method is a construction that provides a description of the ensemble of a variable number of particles. Any state of the system of k particles is described by an element of the Hilbert tensor product $\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_k$, where $\mathcal{H}_i$ is the state space of the ith particle. This assertion pertains to the case in which all particles are distinct. If all particles are identical, then they are *indistinguishable* in quantum mechanics (no one can say

which particle is the first, which is the second, and so on). Accordingly, the state described by a vector

$$\psi \in \mathcal{H}^{\otimes k} = \underbrace{\mathcal{H} \otimes \ldots \otimes \mathcal{H}}_{k \text{ times}}$$

must be invariant under the permutation of any two particles, that is,

$$\Pi_{jl}\psi = \lambda_{jl}\psi,$$

where Π_{jl} is the operator of permutation of the jth and lth particle and $\lambda_{jl} \in \mathbf{C}$. Since $\Pi_{jl}^2 = 1$, we have $\lambda_{jl}^2 = 1$, that is,

$$\lambda_{jl} = \pm 1.$$

The case $\lambda_{jl} = +1$ corresponds to the so-called Bose statistics (which is the only one we consider here). Hence, for bosons (Bose particles) any k-particle state is described by an element of the symmetric tensor power

$$S^k(\mathcal{H}) \subset \mathcal{H}^{\otimes k}$$

of the main space $\mathcal{H}$. The state of the system with a variable number of particles is described by an element of the *Fock space*

$$\mathcal{F} \equiv \mathcal{F}(\mathcal{H}) = \bigoplus_{k=0}^{\infty} S^k(\mathcal{H}) \qquad (S^0(\mathcal{H}) = \mathbf{C}),$$

where the infinite orthogonal sum of Hilbert spaces is naturally understood as the completion of the algebraic direct sum with respect to the corresponding norm. Note that $\mathcal{H}$ itself is embedded in $\mathcal{F}(\mathcal{H})$ in a natural way as $S^1(\mathcal{H})$.

A natural orthonormal basis in $\mathcal{F}(\mathcal{H})$ can be constructed as follows. Let $\{e_1, \ldots, e_k, \ldots\}$ be an orthonormal basis in $\mathcal{H}$. We take an arbitrary tuple $(e_{l_1}, \ldots, e_{l_k})$, symmetrize the tensor product $e_{l_1} \otimes \ldots \otimes e_{l_k}$, and normalize the resulting product to 1. The set of all possible vectors provided by this procedure is an orthonormal basis in $\mathcal{F}(\mathcal{H})$; it will be called the *Fock basis*.

It is convenient to describe this procedure in terms of the so-called *occupation numbers*. Let

$$\vec{\mathbf{n}} = (n_1, \ldots, n_s, \ldots)$$

be a sequence of nonnegative integers such that

$$|\vec{\mathbf{n}}| = \sum_{j=0}^{\infty} n_j = k.$$

Next, let $(f_1, \ldots, f_k)$ be the sequence of basis vectors in $\mathcal{H}$ such that

$$(f_1, \ldots, f_k) = (\underbrace{e_1, \ldots, e_1}_{n_1 \text{ times}}, \underbrace{e_2, \ldots, e_2}_{n_2 \text{ times}}, \ldots).$$

We set

$$|\vec{\mathbf{n}}\rangle = \frac{1}{\sqrt{k!}\sqrt{n_1!n_2!\ldots}} \sum_{\pi \in \sigma^k}^{n} f_{\pi(1)} \otimes \ldots \otimes f_{\pi(k)}, \tag{1.45}$$

where the sum is taken over all permutations $\pi \in \mathsf{S}^k$ of k elements. Then the set of all vectors $|\vec{\mathbf{n}}\,\rangle$ with $|\vec{\mathbf{n}}| = k$ is an orthonormal basis in $S^k(\mathcal{H})$; the union of all these bases is an orthonormal basis in $\mathcal{F}(\mathcal{H})$. Let $\mathbf{1}_j$ be the sequence $\vec{\mathbf{n}}$ such that $n_j = 1$ and $n_k = 0$ for $k \neq j$. We introduce the creation-annihilation operators a_j^*, a_j, $j = 1, 2, \ldots$, in the Fock space $\mathcal{F}(\mathcal{H})$ by the formulas

$$\begin{aligned} a_j^*|\vec{\mathbf{n}}\,\rangle &= \sqrt{n_j + 1}\,|\vec{\mathbf{n}} + \mathbf{1}_j\rangle \\ a_j|\vec{\mathbf{n}}\,\rangle &= \begin{cases} \sqrt{n_j}\,|\vec{\mathbf{n}} - \mathbf{1}_j\rangle & \text{if } n_j > 0, \\ 0 & \text{if } n_j = 0. \end{cases} \end{aligned} \tag{1.46}$$

Obviously, the operators a_j and a_j^* satisfy the commutation relations

$$[a_j, a_j^*] = \delta_{jk};$$

furthermore, we can readily see that a_j^* is the adjoint of a_j with respect to the inner product on $\mathcal{F}(\mathcal{H})$. Indeed,

$$(|\vec{\mathbf{m}}\rangle, a_j|\vec{\mathbf{n}}\,\rangle) \neq 0$$

if and only if $|\vec{\mathbf{m}}\rangle = |\vec{\mathbf{n}} - \mathbf{1}_j\rangle$; in this case,

$$(|\vec{\mathbf{m}}\rangle, a_j|\vec{\mathbf{n}}\,\rangle) = \sqrt{n_j} = (a_j^*|\vec{\mathbf{m}}\rangle, |\vec{\mathbf{n}}\,\rangle).$$

In quantum mechanics, the common value of these expressions is usually denoted by $\langle \vec{\mathbf{m}}\,|\,a_j\,|\,\vec{\mathbf{n}}\,\rangle$ (the $\langle$bra|c|ket$\rangle$ notation due to Dirac).

Now let $\widehat{H}$ be the one-particle energy operator. We assume that the particles are noninteracting, that is, the energy operator of the k-particle system has the form

$$\begin{aligned}\widehat{H}_k &= \widehat{H}\otimes 1\otimes\ldots\otimes 1+1\otimes\widehat{H}\otimes 1\otimes\ldots\otimes 1+\ldots\\ &\qquad +1\otimes 1\otimes\ldots\otimes 1\otimes\widehat{H},\\ \widehat{H}_0 &= 1.\end{aligned}$$

Thus we have defined the Hamiltonian (the energy operator) in the Fock space:

$$\widehat{H}_{\mathcal{F}}=\operatorname{diag}(\widehat{H}_0,\widehat{H}_1,\ldots,\widehat{H}_k,\ldots,\ldots).$$

It turns out (this explains the term "second quantization") that the Schrödinger equation with Hamiltonian $\widehat{\mathcal{H}}_{\mathcal{F}}$ in the Fock space can be obtained in the following simple way. Consider the mean value of the energy of one particle:

$$<\widehat{H}>=(\psi,\widehat{H}\psi)=(z,\widetilde{H}z)=\sum_{j,k=0}^{\infty}H_{jk}z_k\overline{z}_j, \tag{1.47}$$

where $z=(z_1,z_2,\ldots)$ are the coordinates of the wave function ψ in the basis $\{e_l\}$ and $\widetilde{H}=\{H_{jk}\}$ is the matrix of the operator $\widehat{H}$ in the same basis. Here we replace all z_k by creation operators and all $\overline{z}_j$ by annihilation operators, that is, consider the operator

$$\widehat{\widehat{H}}=\sum_{j,k}H_{jk}a_k^*a_j \tag{1.48}$$

in the Fock space. The operator (1.48) is essentially obtained from the symbol (1.47) by quantization: the coordinates of the wave function are replaced by the creation–annihilation operators. Straightforward computation shows that

$$\widehat{H}_{\mathcal{F}}=\widehat{\widehat{H}}.$$

In quantum mechanics and quantum field theory, what is called "second quantization" is usually applied to infinite-dimensional systems like the Schrödinger equation (as discussed above) or the classical field

equations. However, to obtain the Fock representation, we only need to "second-quantize" a certain finite-dimensional system.

In fact, second quantization is based on the following observations.

1^o. There exists an "exact" quantization of quadratic Hamiltonians (this will be clarified below).

2^o. The Schrödinger equation can be viewed as a Hamilton system with quadratic Hamiltonian of a special form related to the complex structure (we have just seen this in the preceding).

Essentially, by 2^o, in second quantization we reinterpret the quantum system as a classical system, which is then quantized. By 1^o, it proves to be possible to embed the "classical" system thus obtained in the quantized system (more precisely, the "classical" phase space is embedded in the quantum state space as a subspace) so that the "classical" evolution is just the restriction of the quantum evolution. Thus, in the usual context of second quantization we have the following "shift" of notions:

1. The *classical system* is the original quantum system.

2. The *quantum system* is the system with variable number of particles (the second-quantized system).

Though interpreting the quantum system as classical, this technique uses both aspects of the original system. Therefore, to apply the "second quantization" technique to the classical system, we must learn how to interpret this system as a quantum system (which of course will be degenerate, i.e. finite-dimensional).

With regard to all these considerations, we start from the analysis of quadratic Hamiltonians.

Exact quantization of quadratic Hamiltonians. Dirac's famous problem on the quantization of observables (already mentioned in Subsection 1.1) can be stated as follows: for a given set of symbols $f(q,p)$ on the phase space $\mathbf{R}^{2n}_{q,p} = T^*\mathbf{R}^n_q$, find a quantization rule

$$f(q,p) \to \widehat{f} \tag{1.49}$$

taking each symbol $f(q,p)$ to an operator $\widehat{f}$ in the quantum state space $L^2(\mathbf{R}^n_x)$ so that the following conditions hold:

$$\begin{array}{ll} \text{a)} & \text{The mapping (1.49) is linear;} \\ \text{b)} & \widehat{1} \text{ is the identity operator;} \\ \text{c)} & [\widehat{f},\widehat{g}] = -ih\widehat{\{f,g\}}, \end{array} \tag{1.50}$$

where $\{\,,\,\}$ is the classical Poisson bracket.

As was already mentioned in Section 1.1, this problem is known to have no natural solutions[6] for arbitrary (and even polynomial) symbols; we can only achieve (1.50) modulo $O(h^2)$.

However, this problem *does* have a solution if we restrict ourselves to the case of quadratic Hamiltonians, i.e., symbols of the form

$$\begin{aligned} f(q,p) \;\; = \;\; & \frac{1}{2} < p, Ap > + \frac{1}{2} < q, Bq > + < p, Cq > \\ & + \;\; < a, p > + < b, q > + c, \end{aligned}$$

where $A = {}^tA$, $B = {}^tB$ and C are $n \times n$ matrices, a and b are n-vectors, and $c \in \mathbf{C}$. Specifically, the solution is given by the Weyl quantization

$$\widehat{f} = f\left(\frac{\overset{1}{\widehat{p}} + \overset{3}{\widehat{p}}}{2}, \overset{2}{\widehat{q}}\right), \tag{1.51}$$

where $\widehat{p} = -ih\frac{\partial}{\partial x}$ and $\widehat{q} = x$. For polynomial (in particular, quadratic) symbols this definition can be restated as follows: let $f(q,p)$ be a polynomial. We represent f in the form

$$f = \sum c_\alpha f_\alpha, \tag{1.52}$$

where the c_α are constants and

$$f_\alpha = (a_1 p_1 + \ldots + a_n p_n + b_1 q_1 + \ldots + b_n q_n)^k \tag{1.53}$$

where the coefficients $a_1, \ldots, a_n$, $b_1, \ldots, b_n$ and the nonnegative integer exponent k depend on α. Then

$$\widehat{f} = \sum c_\alpha \widehat{f}_\alpha, \tag{1.54}$$

[6]Natural solutions must satisfy $\widehat{f}\widehat{g} = \widehat{fg} + O(h)$; this condition excludes the nonnatural solution (used in geometric quantization) given by first-order operators on the phase space (see [8]).

where

$$\widehat{f}_\alpha = (a_1\widehat{p}_1 + \ldots + a_n\widehat{p}_n + b_1\widehat{q}_1 + \ldots + b_n\widehat{q}_n)^k. \tag{1.55}$$

We can readily verify that for the Weyl quantization

$$[\widehat{f},\widehat{g}] = \widehat{\{f,g\}} + O(h^3), \tag{1.56}$$

where the $O(h^3)$ is bilinear in the third- and higher order derivatives of f and g. It follows that for quadratic Hamiltonians Eq. (1.50) is satisfied exactly.

From now on, until the end of this section, we use the system of units in which $h = 1$, as is customary in the theory of second quantization.

The complex structure of the classical phase space. The phase space $\mathbf{R}^{2n}_{q,p} = T^*\mathbf{R}^n_q$ bears the standard symplectic structure $\omega^2 = dp \wedge dq$. Since this space is linear, it can be identified with its tangent space at an arbitrary point, and so $\omega^2(v,w)$ is well-defined for any $v, w \in \mathbf{R}^{2n}$. Next, let us consider the standard Euclidean structure

$$(v,w)_{\mathbf{R}} = \sum_{j=1}^{2n} v_j w_j. \tag{1.57}$$

Then

$$\omega^2(v,w) = (v, Iw)_{\mathbf{R}}, \tag{1.58}$$

where I is the $2n \times 2n$ matrix

$$I = \begin{pmatrix} 0 & E_n \\ -E_n & 0 \end{pmatrix} \tag{1.59}$$

and E_n is the $n \times n$ identity matrix (we assume that the coordinates in $\mathbf{R}^{2n}_{q,p}$ are ordered as follows: $(p_1, \ldots, p_n, q_1, \ldots, q_n)$.) We have $I^2 = -E_{2n}$, and hence I defines a complex structure on $\mathbf{R}^{2n}_{q,p}$. More precisely, let us define a one-to-one mapping of $\mathbf{R}^{2n}_{q,p}$ onto $\mathbf{C}^n$ by setting

$$\mathbf{R}^{2n}_{q,p} \ni w = (q,p) \mapsto jw = z = \frac{1}{\sqrt{2}}(q - ip) \in \mathbf{C}^n. \tag{1.60}$$

Then $Iw \mapsto iz$, that is, the matrix I is taken to multiplication by i. Next, let $(\cdot, \cdot)$ be the standard inner product on $\mathbf{C}^n$,

$$(z\widetilde{z}) = <\overline{z}, \widetilde{z}> = \sum_{k=1}^{n} \overline{z}_k \widetilde{z}_k \qquad \text{for any} \qquad z, \widetilde{z} \in \mathbf{C}^n. \tag{1.61}$$

Then

$$(jw, jv) = \frac{1}{2}(w, v)_{\mathbf{R}} + \frac{i}{2}\omega^2(w, v). \tag{1.62}$$

Next, we readily see that the operators $\frac{\partial}{\partial z}$ and $\frac{\partial}{\partial \overline{z}}$ are expressed in the coordinates (q, p) as follows:

$$\frac{\partial}{\partial z} = \sqrt{2}\left(\frac{\partial}{\partial q} + i\frac{\partial}{\partial p}\right), \quad \frac{\partial}{\partial \overline{z}} = \sqrt{2}\left(\frac{\partial}{\partial q} - i\frac{\partial}{\partial p}\right). \tag{1.63}$$

Conversely,

$$\frac{\partial}{\partial q} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial z} + \frac{\partial}{\partial \overline{z}}\right), \quad \frac{\partial}{\partial p} = \frac{i}{\sqrt{2}}\left(\frac{\partial}{\partial \overline{z}} - \frac{\partial}{\partial z}\right). \tag{1.64}$$

An easy computation shows that for arbitrary functions f, g on $\mathbf{R}^{2n}_{q,p} \overset{j}{\cong} \mathbf{C}^n$ the Poisson bracket is given by

$$\{f, g\} = i\left(\frac{\partial f}{\partial \overline{z}}\frac{\partial g}{\partial z} - \frac{\partial f}{\partial z}\frac{\partial g}{\partial \overline{z}}\right). \tag{1.65}$$

Accordingly, the Hamiltonian vector field of f is given by

$$V_f = i\left(\frac{\partial f}{\partial \overline{z}}\frac{\partial}{\partial z} - \frac{\partial f}{\partial z}\frac{\partial}{\partial \overline{z}}\right). \tag{1.66}$$

Let us now consider *quadratic Hamiltonians*. A general quadratic Hamiltonian has the form

$$H(z, \overline{z}) = \frac{1}{2} < z, Az > + \frac{1}{2} < \overline{z}, B\overline{z} > + < \overline{z}, Hz > + \text{linear terms}, \tag{1.67}$$

where A, B, and H are $n \times n$ matrices with complex entries and $<,>$ is the bilinear pairing

$$< z, \widetilde{z} > = \sum_{k=1}^{n} z_k \widetilde{z}_k. \tag{1.68}$$

We shall consider special Hamiltonians in which only the third term on the right-hand side in (1.67) is present, i.e.

$$H(z,\overline{z}) =< \overline{z}, Hz >\equiv (z, Hz). \tag{1.69}$$

Moreover, we require that the Hamiltonian be real-valued, that is $H = H^*$ is a self-adjoint matrix.

Let us write out the Hamilton system for the Hamiltonian (1.69). According to (1.65), (1.66), this system has the form

$$\dot{z} = iHz, \tag{1.70}$$

that is, is given by a $\mathbf{C}$-linear equation.

We see that the equation of motion (1.70) coincides with the "Schrödinger equation" corresponding to the Hamiltonian $H : \mathbf{C}^n \to \mathbf{C}^n$ of a quantum-mechanical system with finitely many degrees of freedom.

The Fock representation. Now we can construct the Fock representation of a system S. We denote the complexified phase space constructed in the preceding item by Φ and proceed in complete analogy with the infinite-dimensional case considered above.

Let

$$S^k(\Phi) \subset \Phi^{\otimes k}$$

be the subspace of completely symmetric tensors. We adopt the convention that $S^0(\Phi) = \mathbf{C}$. The Fock space is again defined as

$$\mathcal{F}(\Phi) = \bigoplus_{k=0}^{\infty} S^k(\Phi),$$

and we have the embedding

$$\Phi = S^1(\Phi) \subset \mathcal{F}(\Phi).$$

Let $e_1, \ldots, e_n$ be an orthonormal basis in Φ (say, the standard basis in the q-plane; then $z = \sum_{i=1}^n z_i e_i$). We construct the Fock basis in $\mathcal{F}(\Phi)$ corresponding to $e_1, \ldots, e_n$ along the same lines as above. The only difference is that now the sequence $\vec{\mathbf{n}} = (n_1, \ldots, n_n)$ of occupation numbers is finite. The vector $|\vec{\mathbf{n}}\,\rangle$ is defined by the same formula

(1.45), and the creation-annihilation operators a_j^*, a_j, $j = 1, \ldots, n$ in the Fock space $\mathcal{F}(\Phi)$ are given by the formulas (1.46) and satisfy the same commutation relations $[a_j, a_j^*] = \delta_{jk}$.

To make $\mathcal{F}(\Phi)$ the quantum state space of the simplest physical system S, it remains to define the action of the Heisenberg algebra h_n on $\mathcal{F}(\Phi)$. The Fock representation is specified by the condition that the Heisenberg algebra elements are quantized as follows (recall that we assume $h = 1$ in this section)

$$\begin{aligned} 1 \mapsto \widehat{1} &= id \quad \text{(the identity operator in } \mathcal{F}(\Phi)) \\ z_j &= \frac{1}{\sqrt{2}}(q_j - ip_j) \mapsto a_j^* \qquad j = 1, \ldots, n \\ \overline{z}_j &= \frac{1}{\sqrt{2}}(q_j + ip_j) \mapsto a_j. \end{aligned} \tag{1.71}$$

In particular,

$$\widehat{q}_j = \frac{1}{\sqrt{2}}(a_j + a_j^*), \qquad \widehat{p}_j = \frac{1}{\sqrt{2}i}(a_j - a_j^*) \tag{1.72}$$

are self-adjoint operators and satisfy the desired commutation relations (1.17).

The Bargmann–Fock representation. There is yet another convenient representation, which can be obtained from the Fock representation and which will be called the "Bargmann–Fock representation."[7] The introduction of it is motivated by the following simple considerations. According to (1.71), in the Fock quantization the classical variable $z_j = \frac{1}{\sqrt{2}}(q_j - ip_j)$ corresponds to the creation operator associated with the jth basis state in quantum mechanics. We seek for some analog of the coordinate representation: just as the coordinate representation can be described as a representation in which the coordinate operators are depicted as the operators of multiplication by the corresponding classical variables, so in our would-be representation the creation operators a_j^* will be depicted as the operators of multiplication

[7] This representation was discovered by Fock and later studied thoroughly by Bargmann.

by z_j. Naturally, the elements of the state space will then be treated as functions of $z_1, \ldots, z_n$ (that is, functions on Φ). More precisely, let us isomorphically map $S^k(\Phi)$ onto the space of kth-order homogeneous polynomials in $z = (z_1, \ldots, z_n)$ by letting

$$|\vec{\mathbf{n}}\rangle \longmapsto c_{\vec{\mathbf{n}}} z_1^{n_1} \cdots z_n^{n_n}. \tag{1.73}$$

Thus, each basis vector in $S^k(\Phi)$ is taken to the corresponding monomial. According to (1.46), we have

$$a_j^* |\vec{\mathbf{n}}\rangle \longmapsto \sqrt{n_j + 1} c_{\vec{\mathbf{n}}+1_j} z_1^{n_1} \cdots z_j^{n_j+1} \cdots z_n^{n_n}.$$

To ensure that this is the same as the multiplication by z_j, we require that

$$\sqrt{n_j + 1} c_{\vec{\mathbf{n}}+1_j} = c_{\vec{\mathbf{n}}}.$$

This is the case if we choose the coefficient $c_{\vec{\mathbf{n}}}$ in the form

$$c_{\vec{\mathbf{n}}} = \frac{1}{\sqrt{n_1! \ldots n_n!}}.$$

Now, after obvious modifications, we can write out the correspondence between the basic classical and quantum variables in the Bargmann–Fock representation:[8]

$$\begin{aligned} z_j &\longmapsto a_j^* = z_j \\ \overline{z}_j &\longmapsto a_j = \frac{\partial}{\partial z_j} \end{aligned} \tag{1.74}$$

The elements (1.73) by definition form an orthonormal basis in the newly defined representation space. Thus, we have mapped $\mathcal{F}(\Phi)$ onto the space $\mathcal{H}_{\mathcal{B}}$ of power series

$$f(z) = \sum_s f_{s_1 \ldots s_n} z_1^{s_1} \ldots z_n^{s_n} \tag{1.75}$$

with finite norm

$$||f||^2 = \sum_s s_1! \ldots s_n! \, |f_{s_1 \ldots s_n}|^2. \tag{1.76}$$

[8] The verification of the second formula is straightforward.

Let us represent the norm (1.76) in a somewhat different form. It is generated by the inner product

$$(f,g)=\sum_s s_1!\dots s_n!\,\bar f_{s_1\dots s_n}g_{s_1\dots s_n}.$$

First, suppose that the series (1.75) of f and g contain only one term,

$$f(z)=az^s,\quad g(z)=bz^l,$$

where $s=(s_1,\dots,s_n)$ and $l=(l_1,\dots,l_n)$ are multiindices. Then an easy computation shows that

$$(f,g)=\frac{1}{\pi^n}\int_{\mathbf{C}^n}\bar f(z)g(z)e^{-z\overline{z}}dq\,dp\qquad(z=q-ip),\tag{1.77}$$

and, accordingly,

$$||f||^2=\frac{1}{\pi^n}\int_{\mathbf{C}^n}|f(z)|^2e^{-z\overline{z}}dq\,dp.\tag{1.78}$$

Next, the finiteness of the norm (1.76) readily implies that the series (1.75) converges everywhere in $\mathbf{C}^n$ in the general case. Hence f is an analytic function, and now a standard argument shows that formula (1.78) remains valid in the general case.

Finally, the result can be stated as follows:

The Bargmann–Fock space $\mathcal{H}_{\mathcal{B}}$ is the space of entire analytic functions in $\mathbf{C}^n$ with finite norm (1.78). This is a Hilbert space with respect to the inner product (1.77).

The Bargmann transform and its properties. Let us now find the transform relating the usual Schrödinger coordinate representation to the Fock–Bargmann representation. By the Stone–von Neumann theorem, it suffices to find the unique unitary transformation

$$A_n:\mathcal{H}=L^2(\mathbf{R}^n_x)\to\mathcal{H}_{\mathcal{B}}$$

such that

$$\begin{aligned}A_n\cdot\frac{1}{\sqrt{2}}(\widehat{q}-i\widehat{p}) &= z\cdot A_n,\\ A_n\cdot\frac{1}{\sqrt{2}}(\widehat{q}+i\widehat{p}) &= \frac{\partial}{\partial z}\cdot A_n\end{aligned}\tag{1.79}$$

where $\widehat{q} = x$, $\widehat{p} = -i\partial/\partial x$ (recall that $h = 1$ in this section).

The transformation A_n is called the *Bargmann transform* [1]. Let us represent the Bargmann transform A_n as an integral operator that acts from $L^2(\mathbf{R}^n_q)$ into $\mathcal{H}_{\mathcal{B}}$ according to the formula

$$(A_n\psi)(z) = \int\limits_{\mathbf{R}^n_x} A_n(z,x)\,\psi(x)\,dx, \quad \psi \in L^2(\mathbf{R}^n_x). \tag{1.80}$$

Equations (1.79) yield linear first-order differential equations for the kernel $A_n(z,x)$. These equations have the form

$$\begin{aligned} zA_n(z,x) &= \frac{1}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right) A_n(z,x), \\ \frac{\partial}{\partial z}A_n(z,x) &= \frac{1}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right) A_n(z,x). \end{aligned}$$

The solution of these equations yields

$$A_n(z,x) = \frac{1}{\pi^{n/4}} \exp\left\{-\frac{1}{2}(z^2 + x^2) + \sqrt{2}zx\right\}. \tag{1.81}$$

(The normalization constant $\frac{1}{\pi^{n/4}}$ is chosen from the condition that A_n must be an isometry).

The main properties of the Bargmann transform are given by the following theorem.

Theorem 1 *1. The transform*

$$A_n : L^2(\mathbf{R}^n_x) \to \mathcal{H}_{\mathcal{B}}$$

is an isometric isomorphism (that is, a unitary operator).

2. The inverse transform is given by the formula

$$(A_n^{-1}f)(x) = \lim_{\lambda\to 1} \frac{1}{\pi^n} \int\limits_{\mathbf{C}^n} \overline{A}_n(z,x) f(\lambda z) e^{-\bar{z}z}\,dq\,dp, \tag{1.82}$$

where $\lambda \to 1$ from below and the limit is understood in the strong sense in $L^2(\mathbf{R}^n_x)$.

3. The intertwining formulas (1.79) hold.

The proof can be found in [1].

1.2.3 Summary on representations and transforms

So far we have defined four quantum-mechanical representations for the simplest physical system S with n degrees of freedom and flat phase space $\mathbf{R}^{2n}_{p,q}$:

1. the coordinate representation;

2. the momentum representation;

3. the Fock "occupation numbers" representation in the space $S(\Phi)$ (or, which is the same, the oscillator representation);

4. the Bargmann–Fock representation in the space $\mathcal{H}_{\mathcal{B}}$ of analytic functions on $\mathbf{C}^n$ square integrable with weight $e^{-z\overline{z}}$.

For convenience, we list these representations in Table 1.2.

Furthermore, we have unitary operators relating these representations to each other:

$$L^2(\mathbf{R}^n_p) \xleftarrow{F} L^2(\mathbf{R}^n_x) \xrightarrow{A_n} \mathcal{H}_{\mathcal{B}} \xrightarrow{j} S(\Phi),$$

where F is the Fourier transform, A_n is the Bargmann transform, and j acts according to the rule

$$j : z_1^{n_1} \dots z_n^{n_n} \longmapsto |\vec{\mathbf{n}}\rangle.$$

In the next section we shall see that there is a transform very close to the Bargmann transform and arising within a completely different approach: if here we were comparing various representations and deriving our transforms as *intertwining mappings* between these representations, in the next section we use a semiclassical argument to obtain quantization of states and, on the basis of it, a decomposition of an arbitrary quantum state in a superposition of elementary ones, hence the transform.

	Name	Hilbert space	Coordinate and momentum operators
1	coordinate representation	$L^2(\mathbf{R}^n_x)$	$\widehat{q} = x,\ \widehat{p} = -i\frac{\partial}{\partial x}$
2	momentum representation	$L^2(\mathbf{R}^n_p)$	$\widehat{q} = i\frac{\partial}{\partial p} \qquad \widehat{p} = p$
3	Fock representation	$S(\Phi)$	see (1.72) and (1.71)
4	Bargmann–Fock representation	$\mathcal{H}_{\mathcal{B}} \subset L^2(\Phi, e^{-z\overline{z}})$	$\widehat{q} = \frac{1}{\sqrt{2}}\left(z + \frac{\partial}{\partial z}\right)$ $\widehat{p} = \frac{1}{\sqrt{2}}\left(z - \frac{\partial}{\partial z}\right)$

Table 1.2: Quantum-mechanical representations

1.3 Semiclassical Quantization of States and the Wave Packet Transform

1.3.1 Semiclassical states and the quantum Sobolev spaces

The construction of the wave packet transform carried out in this section is based on the quantisation of classical one-point states. The idea of this quantization is to assign to each classical state some quantum state that "passes" into the classical state as $h \to 0$. First of all, let us introduce the important class of states that "behave well" as $h \to 0$.

Semiclassical states. What does it mean that we deal with semiclassical states of a physical system? This means that we have an entire hierarchy of scales in which we perform our measurements, from "micro" to "macro" size, and as we move along this hierarchy to its "macro" end (which corresponds to successively choosing units of measurement so that $h \to 0$), the system displays less and less of quantum and more and more of classical behavior. Mathematically, this corresponds to considering quantum states—elements ψ of the quantum state space $\mathcal{H}$—depending on the small parameter $h \in (0, 1]$ rather that defined for some fixed value of h. Moreover, the dependence on h has to be such that the expectations $(\psi, \widehat{A}\psi)$ of quantum observables (all or from some specified set) be convergent as $h \to 0$ to the corresponding classical observables A. This condition is however too subtle to define a linear space of semiclassical states in its terms. We shall actually use a weaker condition and thus define a broader space of states. Truly semiclassical states form a (nonclosed) subset of this space. The condition is stated as follows:

The expectations $(\psi, \widehat{A}\psi)$ depend on h continuously and remain bounded as $h \to 0$.

We must further specify for which class of observables this condition must be satisfied. (For example, if an observable itself is "pathological" in that it behaves singularly as $h \to 0$, then there is no point in demanding that the above condition be met for this observable). In

the simplest physical system, we already have distinguished observables, namely, the coordinate and momentum operators. We require that the above condition be satisfied for operators $\widehat{A}$ that are arbitrary nonnegative powers of the coordinates and momenta:

$$\sup_{h\in(0,1]} (|(\psi, \widehat{p}^{\alpha}\psi)| + |(\psi, \widehat{q}^{\alpha}\psi)|) \le C_{\alpha}, \quad |\alpha| = 0, 1, 2, \dots \tag{1.83}$$

Quantum Sobolev spaces. We can readily see that condition (1.83) is equivalent to the requirement that

$$\sup_{h\in(0,1]} (\psi, (1 + \widehat{q}^2 + \widehat{p}^2)^k \psi) = \sup_{h\in(0,1]} \left\| (1 + \widehat{q}^2 + \widehat{p}^2)^{k/2} \psi \right\|^2 \le c_k, \tag{1.84}$$
$$k = 0, 1, 2, \dots$$

We denote by $\mathcal{H}^k \subset C((0,1], \mathcal{H})$ the subspace of vectors $\psi = \psi(h)$ such that the kth norm (1.84) is finite. For $k < 0$ these spaces can be defined in the usual manner as the dual spaces of $\mathcal{H}^{-k}$ with respect to the pairing given by the inner product in $\mathcal{H} = \mathcal{H}^0$. By $\mathcal{H}^{\infty}$ we denote the intersection

$$\mathcal{H}^{\infty} = \bigcap_k \mathcal{H}^k.$$

This is clearly a Fréchet space whose topology is defined by the system of seminorms (1.84) for all k.

The above treatment pertains to the "abstract" Hilbert state space $\mathcal{H}$. However, in this section we shall mainly work with the coordinate representation.

In the coordinate representation, where the space $\mathcal{H}$ is isomorphically mapped onto $L^2(\mathbf{R}^n_x)$ the spaces $\mathcal{H}^k$ become the *quantum Sobolev spaces* $H^s(\mathbf{R}^n_x)$. These are the spaces of functions $f(x,h)$ for which the following norm is finite:[9]

$$||f||_s = \sup_{h\in(0,1]} ||(1 + x^2 + \widehat{p}^2)^{s/2} f||_{L_2}, \tag{1.85}$$

[9]The reader shall not mix up these spaces with the ordinary Sobolev spaces, which are sometimes denoted in the same way. Formally, the definition of the ordinary Sobolev space is obtained from our definition by setting $h = 1$ and by dropping out the term x^2 in the expression for the norm.

where $||\cdot||_{L_2}$ is the usual L_2-norm in the space $\mathbf{R}^n_x$ and

$$\widehat{p}^2 = \sum_{j=1}^n \widehat{p}_j^2 = \sum_{j=1}^n \left(-ih\frac{\partial}{\partial x_j}\right)^2.$$

Further, we denote by $H(\mathbf{R}^n_x)$ the intersection of all spaces $H^s(\mathbf{R}^n_x)$:

$$H(\mathbf{R}^n_x) = \bigcap_s H^s(\mathbf{R}^n_x).$$

Likewise, in the momentum representation the spaces $\mathcal{H}^k$ become the *quantum Sobolev spaces* $H^s(\mathbf{R}^n_p)$. These are the spaces of functions $f(p,h)$ for which the norm

$$||f||_s = \sup_{h\in(0,1]} ||(1+\widehat{q}^2+p^2)^{s/2} f||_{L_2},$$

where

$$\widehat{q}^2 = \sum_{j=1}^n \widehat{q}_j^2 = \sum_{j=1}^n \left(ih\frac{\partial}{\partial p_j}\right)^2.$$

is finite.

Let us find out how the quantum Fourier transform acts in these spaces. We have already seen in Section 1.2 that the quantum Fourier transform is just the transformation from the coordinate to the momentum representation and hence is an intertwining operator for the following pairs of operators:

$$x \leftrightarrow \widehat{q} = ih\frac{\partial}{\partial p}, \quad p \leftrightarrow \widehat{p} = -ih\frac{\partial}{\partial x}.$$

As a consequence, we obtain the following statement.

Theorem 2 *The quantum Fourier transform defines an isometric isomorphism (denoted by the same letter)*

$$F \ : \ H^s(\mathbf{R}^n_x) \to H^s(\mathbf{R}^n_p),$$

for any s.

In particular, it follows that the quantum Fourier transform is an isomorphism between the spaces

$$F \ : \ H(\mathbf{R}^n_x) \to H(\mathbf{R}^n_p).$$

Examples of semiclassical states. To give natural examples of semiclassical states, we ask how states satisfying the dynamic equations can behave as $h \to 0$. As the simplest example, consider the Schrödinger equation with translation invariant Hamiltonian $\widehat{H} = H(\widehat{p})$, independent of x:

$$-ih\frac{\partial \psi}{\partial t} + H\left(-ih\frac{\partial}{\partial x}\right)\psi = 0. \tag{1.86}$$

We can seek particular solutions of this equation in the form of exponentials (plane waves)[10]

$$\psi(x,t) = ce^{\frac{i}{h}(kx-Et)}, \tag{1.87}$$

where c is an arbitrary constant, and k and E are real constants satisfying the *eikonal equation*

$$H(k) - E = 0. \tag{1.88}$$

Suppose now that the Hamiltonian is not translation invariant, $\widehat{H} = H\left(x, -ih\frac{\partial}{\partial x}\right)$. It is known from the WKB method (e.g., see [14] and references therein), that in this case solutions are similar to (1.87); specifically, the linear phase function $kx - Et$ and the constant amplitude c are replaced, respectively, by a general (not necessarily linear) phase function $S(x,t)$ and an amplitude $a = a(x,h)$, which need not to be constant. Furthermore, the function $S(x,t)$ satisfies the Hamilton–Jacobi equation

$$\frac{\partial S}{\partial t} + H\left(x, \frac{\partial S}{\partial x}\right) = 0,$$

the amplitude $a(x,h)$ possesses a regular expansion in powers of h, and the coefficients of this expansion can be computed from a recursion chain of ordinary differential equations known as the transport equations (all these issues will be discussed in detail in the chapter devoted to asymptotic solutions of differential equations). Thus, a typical

[10] These exponentials do not belong to L^2 (in fact, they are generalized eigenfunctions of the momentum operator) and hence can only be viewed as *generalized states*.

(though by now means general) semiclassical wave function may have the form

$$\psi(x,t) = e^{\frac{i}{h}S(x,t)}a(x,t,h), \tag{1.89}$$

where $S(x,t)$ is a smooth real-valued function and the amplitude $a(x,t,h)$ is a smooth function that can be expanded in a regular asymptotic series in powers of h.

1.3.2 Oscillation front

Consider the simplest physical system in a semiclassical quantum state ψ. As $h \to 0$, the system becomes classical. However, this generally does not mean that the system will be in some uniquely determined classical state. In general, it can be in one of a set of classical states; this set is known as the *oscillation front* of ψ. After this physical preliminary, let us proceed to more rigorous mathematical treatment of the subject. First, we describe the coarser notion of *support of oscillations*. It describes the possible values of the coordinates in the limit state, whereas the oscillation front does the same for the pairs (q,p) of coordinates and momenta.

Support of oscillations. Let us first recall the notion of ordinary support. The *support* of a function $u(x)$ is the closure of the set of points where $u(x)$ does not vanish,

$$\operatorname{supp} u = \overline{\{x \in \mathbf{R}^n \mid u(x) \neq 0\}}.$$

Alternatively, we can say that $x_0 \in u$ if and only if for any smooth compactly supported function $\varphi(x)$ such that $\varphi(x)u(x) \equiv 0$ one has $\varphi(x_0) = 0$.

The notion of *support of oscillations* makes sense for functions depending on a small parameter h. Let $u(x,h)$ be a given function.We write $u = O(h^l)$ or $u(x,h) \equiv 0 \pmod{h^l}$ if $h^{-l}u \in H(\mathbf{R}^n_x)$. By definition, $u = O(h^\infty)$ if $u = O(h^l)$ for every l.

Definition 3 *A point x_0 belongs to the* support of oscillations *of a function u,*

$$x_0 \in \text{osc - supp } u$$

if and only if for any smooth compactly supported function $\varphi(x)$*such that* $\varphi u = O(h^\infty)$ *one has* $\varphi(x_0) = 0$.

We shall not use the more delicate notion of the kth-order support of oscillations, where $O(h^\infty)$ is replaced by $O(h^k)$

The notion of support of oscillations is useful because it behaves well under the action of observables. Let $\widehat{H} = H\left(\overset{2}{x}, \overset{1}{\widehat{p}}\right)$ be a quantum observable. We shall always assume that the corresponding classical observable is a function $H(q,p)$ that is infinitely differentiable and grows at infinity together with all derivatives no faster than a given power of $r = (q^2 + p^2)^{1/2}$. (The power is solely determined by H and is independent of the number of derivatives.)[11] Then the following assertion holds.

$$\text{osc - supp } H\left(\overset{2}{x}, \overset{1}{\widehat{p}}\right) u \subset \text{osc - supp } u.$$

Localization in the phase space and oscillation front. Now let us define the notion of the oscillation front. Let $u(x,h)$ be a given function. Furtermore, let (q_0, p_0) be a given point of the phase space. We wish to find out whether this point is a possible limit classical state for our semiclassical state u. To this end, we can act as follows. Let $\varphi(x)$ be a smooth function of compact support, independent of h and localized in a sufficiently small neighbourhood of q_0. If

$$\varphi(x)u(x,h) = O(h^\infty), \tag{1.90}$$

then q_0 cannot be the limit classical value of the coordinate s and (q_0, p_0) definitely cannot belong to the oscillation front. If however (1.90) fails,then we must put further effort and study what the situation is with the momentum. To this end, we apply the quantum Fourier transform to the function $\varphi(x)u(x,h)$ and investigate whether p_0 belongs to the support of oscillations of $F[\varphi(x)u(x,h)]$. If no, then (q_0, p_0) is not in the oscillation front. The above discussion justifies the following definition.

---

[11] We have taken the Maslov quantization $\overset{2}{x}, \overset{1}{\widehat{p}}$, but this does not matter, since the class of quantum observables is the same for the opposite Maslov quantization, Weyl quantization, etc.

Definition 4 *The oscillation front of u is the set $OF[u] \subset \mathbf{R}^{2n}_{q,p}$ determined by the following condition. A point (q_0, p_0) does not belong to $OF[u]$ if and only if there exist compactly supported functions $\varphi(x)$ and $\psi(p)$ such that*

$$\varphi(q_0) \neq 0, \quad \psi(p_0) \neq 0, \text{ and } \psi(p) F[\varphi(x)u(x)] = O(h^\infty),$$

where F is the quantum Fourier transform. In other words,

$$F[\varphi(x)u(x)] = O(h^\infty)$$

in a neighborhood of the point p_0.

Since the notion of oscillation front pertains to localization in the phase space, it is not surprising that it can also be defined by analogy with the support of oscillations but with cutoff functions substituted by observables with compactly supported symbols. Let us state this property, along with two other properties of oscillation fronts, in the form of a theorem.

Theorem 5 *1. A point (q_0, p_0) of the phase space belongs to $OF[u]$ if and only if for any observable $H\left(\overset{2}{x}, \overset{1}{\widehat{p}}\right)$ with compactly supported symbol $H(q,p)$ the estimate $H\left(\overset{2}{x}, \overset{1}{\widehat{p}}\right) u = O(h^\infty)$ implies $H(q_0, p_0) = 0$. Eqivalently, $(q_0, p_0) \notin OF[u]$ if for some compactly supported classical observable $H(x,p)$ such that $H(x_0, p_0) \neq 0$ we have $H\left(\overset{2}{x}, \overset{1}{\widehat{p}}\right) u = O(h^\infty)$.*

2. If $H(q,p) = 0$ in a neighborhood of the point (q_0, p_0), then $(x_0, p_0) \notin OF[H(\overset{2}{x}, \overset{1}{\widehat{p}})u]$.

3. $OF[H(\overset{2}{x}, \overset{1}{\widehat{p}})u] \subset OF[u]$.

4. $\pi(OF[u]) = \text{osc-supp } u$, where $\pi : \mathbf{R}^{2n}_{q,p} \to \mathbf{R}^n_x$, $(q,p) \mapsto q$, is the natural projection.

The proof can be found in numerous expositions.

Examples. Now let us calculate the wave front for the two examples of semiclassical states considered above. (We disregard the dependence on t, since anyway the oscillation fronts have to be calculated for fixed values of t.)

The first example is $u(x,h) = e^{\frac{i}{h}xp_0}$.We have

$$F\{\varphi(x)u(x,h)\} = \left(\frac{-i}{2\pi h}\right)^{n/2} \int e^{\frac{i}{h}x(p-p_0)}\varphi(x)\,dx = \frac{1}{h^{n/2}}\widetilde{\varphi}\left(\frac{p-p_0}{h}\right),$$

where $\widetilde{\varphi}(p)$ is the usual Fourier transform of φ. For any N we have

$$|\widetilde{\varphi}(p)| \leq \frac{C_N}{|p|^N}$$

as $p \to \infty$ provided that $\varphi(x) \in C_0^\infty$. Thus $F\{\varphi u\} = O(h^\infty)$ for $p \neq p_0$, whereas $F\{\varphi u\}(p_0) \sim h^{-n/2}$. We conclude that $OF[e^{\frac{i}{h}xp_0}]$ is the n-dimesional plane $\{p = p_0\} \subset \mathbf{R}^n \oplus \mathbf{R}^n$.

The second example is $u(x,h) = e^{\frac{i}{h}S(x)}\varphi(x)$. To calculate the oscillation front, we use the first assertion of Theorem 5. We have

$$H(x,\widehat{p})\,u(x,h) = \left(\frac{1}{2\pi h}\right)^n \int e^{\frac{i}{h}p(x-y)+S(y)}H(y,p)\varphi(y)\,dp\,dy.$$

By applying the stationary phase formula to this integral, we find that

$$OF\{e^{\frac{i}{h}S(x)}\varphi(x)\} = \left\{p = \frac{\partial S(x)}{\partial x}\right\} \cap \pi^{-1}(\mathrm{supp}\varphi),$$

where $\pi : \mathbf{R}^{2n}_{q,p} \to \mathbf{R}^n_x$, $(q,p) \mapsto q$, is the natural projection.

1.3.3 Quantization of one-point states and Gaussian wave packets

The problem that will be dealt with in this subsection is that of *quantization* of classical states. Thus, to each classical state $(q,p) \in \mathbf{R}^{2n}$ we shall assign some quantum state $\psi = \psi_{(q,p)}(x)$. For this to make sense, we must require that the quantum state be "localized" as $h \to 0$ near the point (q,p). What does that mean? According to the *uncertainly principle* (which will essentially be derived here), one cannot localize

a quantum particle (or a system of particles) in the coordinate and momentum spaces simultaneously. More precisely, in any state ψ we have

$$\Delta q_j \Delta p_j \geq h, \tag{1.91}$$

where Δq_j and Δp_j are the mean-square deviations of the corresponding variables,

$$\begin{aligned} (\Delta q_j)^2 &= (\psi, (\widehat{q}_j - \overline{q}_j)^2 \psi), \\ (\Delta p_j)^2 &= (\psi, (\widehat{p}_j - \overline{p}_j)^2 \psi), \end{aligned} \tag{1.92}$$

where $\overline{q}_j$ and $\overline{p}_j$ are the corresponding expectations.

Thus, the best localization that we can expect to achieve is as follows.

1) $OF(\psi_{(q,p)})$ consists of the single point (q,p).

2) In the state $\psi_{(q,p)}$, both Δq_j and Δp_j are of the order of $\sqrt{h}$, $j = 1, \ldots, n$.

Quantum states of minimum mean-square deviation. It turns out that these are quite a few states satisfying these two conditions. More precisely, let $f(y)$, $y \in \mathbf{R}^n$, be an arbitrary function of the Schwartz class (independent of h) such that $||f||_{L^2} = 1$. Set

$$\psi_{(q,p)}(x) = \frac{1}{h^{n/4}} e^{\frac{i}{h} p(x-q)} f\left(\frac{x-q}{\sqrt{h}}\right). \tag{1.93}$$

We claim that $\psi_{(q,p)}(x)$ has the desired properties. Indeed, since the multiplication by the exponential $e^{\frac{i}{h}px}$ and the change of variables $x \mapsto x - q$ just represent shifts in the coordinate and momentum spaces, respectively, it suffices to prove that the function

$$\psi(x) \equiv \psi_{(0,0)}(x) = \frac{1}{h^{n/4}} f\left(\frac{x}{\sqrt{h}}\right) \tag{1.94}$$

has the oscillation front $OF(\psi) = \{(0,0)\}$ and that

$$\Delta x_j = O(\sqrt{h}), \qquad \Delta p_j = O(\sqrt{h}) \tag{1.95}$$

in the state ψ.

We have

$$\begin{aligned}\widetilde{\psi}(p) &= \left(\frac{-i}{2\pi h}\right)^{n/2} \frac{1}{h^{n/4}} \int e^{-\frac{i}{h}px} f\left(\frac{x}{\sqrt{h}}\right) dx \\ &= \left(\frac{-i}{2\pi}\right)^{n/2} \frac{1}{h^{n/4}} \int e^{-i\frac{p}{\sqrt{h}}\frac{x}{\sqrt{h}}} f\left(\frac{x}{\sqrt{h}}\right) d\left(\frac{x}{\sqrt{h}}\right) \\ &= \frac{1}{h^{n/4}} \chi\left(\frac{p}{\sqrt{h}}\right),\end{aligned}$$

where

$$\chi(\xi) = \left(\frac{-i}{2\pi}\right)^{n/2} \int e^{-i\xi y} f(y)\, dy$$

is the ordinary (rather than quantum) Fourier transform of $f(y)$. Thus, $\widetilde{\psi}(p)$ has the same structure as $\psi(x)$.

Let $\varphi(x)$ be an arbitrary cutoff function such that $O \notin \operatorname{supp}\varphi$. Then

$$\begin{aligned}|\varphi(x)\psi(x)| &\le \sup|\varphi| \cdot h^{-n/4} \cdot \max_{|x|\ge\varepsilon} \left| f\left(\frac{x}{\sqrt{h}}\right)\right| \\ &\le C_N \sup|\varphi| \cdot h^{-n/4} \left(1 + \frac{\varepsilon}{\sqrt{h}}\right)^{-N} \\ &\le C \cdot h^{\frac{N}{2}-n/4}, \qquad N = 1, 2, \ldots,\end{aligned}$$

since $f(\eta)$ belongs to the Schwartz class. (Here ε is the distance between $\operatorname{supp}\varphi$ and zero.) It follows that osc-supp $\psi = \{0\}$, and hence $OF(\psi) \subset \{(q,p)\,|\,q = 0\}$. Likewise, osc-supp $\widetilde{\psi} = \{0\}$, and hence $OF(\psi) \subset \{(q,p)\,|\,p = 0\}$. By combining these two assertions, we obtain

$$OF(\psi) = \{(0,0)\},$$

as desired. Let us prove that $\Delta x_j = O(\sqrt{h})$ (for Δp_j, the proof is similar). We have

$$\overline{x}_j = \frac{1}{h^{n/2}} \int x_j |f|^2 \left(\frac{x}{\sqrt{h}}\right) dx = \sqrt{h} \int y_j |f^2|(y)\, dy = O(\sqrt{h}).$$

Next,

$$\begin{aligned}(\Delta x_j)^2 &= \frac{1}{h^{n/2}}\int (x_j-\overline{x}_j)^2|f^2|\left(\frac{x}{\sqrt{h}}\right)dx\\ &= h\int (y_j-\overline{y}_j)|f|^2(y)\,dy,\end{aligned}$$

where $\overline{y}_j=\int y_j|f|^2(y)\,dy$ is independent of h. This completes the proof.

The function (1.93) will be called the *wave packet with amplitude* $f(y)$.

Gaussian packets. In what follows we mainly deal with *Gaussian wave packets*, where the amplitude has the special form

$$f(y)=e^{\frac{i}{2}<y,Ay>} \tag{1.96}$$

and the symmetric matrix $A={}^tA$ has a positive imaginary part, Im $A>0$. The motivation for considering packets of the form (1.96) is as follows. Suppose that we intend to find a state $\psi(x,h)$ with zero expectations of coordinate and momenta and minimum mean-square deviations of these exactly. (Note that in the general wave packet we only have (1.95) but not the optimal constants in the $O(\sqrt{h})$ estimates.) To simplify the calculations, we consider the one-dimensional case $n=1$. Thus, our minimization problem is as follows:

$$(\Delta q)^2 = (\psi,\hat{q}^2\psi)\to\min,\quad (\Delta p)^2=(\psi,\hat{p}^2\psi)\to\min, \tag{1.97}$$

$$||\psi||^2 = 1. \tag{1.98}$$

(Note that on the solution of this problem the expectations of the coordinate and the momentum are necessarily zero.) Problem (1.97) with condition (1.98) is a two-criterion problem that has optimal solutions in the sense of Pareto. To single out a specific solution, we proceed to a single-criterion problem with the weighted criterion

$$\alpha(\psi,\hat{q}^2\psi)+\beta(\psi,\hat{p}^2\psi)\to\min \tag{1.99}$$

and with the same condition (1.98). Here α and β are arbitrary positive constants. For example, let us take $\alpha=\beta=\frac{1}{2}$. Then the criterion

(1.99) acquires the form

$$(\psi, \widehat{H}_{\text{osc}}\psi) \to \min, \tag{1.100}$$

where

$$\widehat{H}_{\text{osc}} = \frac{1}{2}(\hat{q}^2 + \hat{p}^2)$$

is the Hamiltonian of the quantum-mechanical oscillator. The Euler–Lagrange equations for the conditional minimization problem (1.100)–(1.98) have the form

$$\widehat{H}_{\text{osc}}\psi = \lambda\psi,$$

and the minimum is provided by the ground eigenfunction

$$\psi_0(x, h) = Ce^{-x^2/(2h)},$$

where C is a normalization constant, corresponding to the eigenvalue $\lambda_0 = h/2$. Thus we have arrived at a special Gaussian wave packet. Note that the mean-square variations of the coordinate and the momentum are equal to the same number $\sqrt{\frac{h}{2}}$. By assigning different weights, we would obtain different Gaussian packets. However, the product of the mean-square variations remains constant, and hence from the inequality relating the arithmetic and geometric means we can observe that this product is optimal. Furthermore, for the case of several variables, we can obtain various Gaussian packets (with pure imaginary matrix A) by considering various quadratic self-adjoint Hamiltonians.

Time evolution of Gaussian packages. It is a very attractive, natural idea to use wave packets as the quantizations of the corresponding classical states (p, q). However, for this idea to be fruitful, we have to verify that the quantum dynamics preserves the class of wave packets and that the corresponding classical states obey the classical dynamic law. We do this in the spirit of [13]. Let

$$\widehat{H} = H\left(\overset{2}{x}, -\overset{1}{ih}\frac{\partial}{\partial x}\right) \tag{1.101}$$

be the energy operator of the system. We consider the Schrödinger equation

$$-ih\frac{\partial\psi}{\partial t}+\widehat{H}\psi=0 \tag{1.102}$$

with the initial function in the form of a Gaussian wave packet:

$$\psi|_{t=0}=\frac{1}{h^{n/4}}e^{\frac{i}{h}p(x-q)}f\left(\frac{x-q}{\sqrt{h}}\right). \tag{1.103}$$

We seek the asymptotic solution of problem (1.102)–(1.103) in the form

$$\psi(x,t,h)=\frac{1}{h^{h/4}}e^{\frac{i}{h}(S(t)+P(t)(x-Q(t)))}f\left(t,\frac{x-Q(t)}{\sqrt{h}}\right). \tag{1.104}$$

By substituting (1.104) into (1.102), we obtain

$$\begin{aligned}
&-ih\frac{\partial\psi}{\partial t}+H\left(\overset{2}{x},-ih\overset{1}{\frac{\partial}{\partial x}}\right)\psi\\
&\quad=\frac{1}{h^{n/4}}e^{\frac{i}{h}(S(t)+P(t)(x-Q(t)))}\left[\dot{S}+\dot{P}\,(x-Q)-P\,\dot{Q}\,-ih\frac{\partial}{\partial t}\right.\\
&\quad\left.+H\left(\overset{2}{x},-ih\overset{1}{\frac{\partial}{\partial x}}+P(t)\right)\right]f\left(t,\frac{x-Q}{\sqrt{h}}\right)\\
=\;&\frac{1}{h^{n/4}}e^{\frac{i}{h}(S(t)+P(t)(x-Q(t)))}\\
&\quad\times\left\{\left[\dot{S}+\dot{P}\,(x-Q)-P\,\dot{Q}\,+H\left(\overset{2}{x},-ih\overset{1}{\frac{\partial}{\partial x}}+P(t)\right)\right]\right.\\
&\quad\left.\times f\left(t,\frac{x-Q}{\sqrt{h}}\right)+i\sqrt{h}\,\dot{Q}\,\frac{\partial f}{\partial y}\left(t,\frac{x-Q}{\sqrt{h}}\right)-ih\frac{\partial f}{\partial t}\left(t,\frac{x-Q}{\sqrt{h}}\right)\right\}.
\end{aligned}$$

Let us make the change of variables

$$\xi=\frac{x-Q(t)}{\sqrt{h}},\qquad\frac{\partial}{\partial x}=\frac{1}{\sqrt{h}}\frac{\partial}{\partial\xi}. \tag{1.105}$$

Then (1.105) is reduced to

$$-ih\frac{\partial\psi}{\partial t}+\widehat{H}\psi=\frac{1}{h^{n/4}}e^{\frac{i}{h}(S(t)+P(t)(x-Q(t)))}$$
$$\times\left\{\left[\dot{S}-P\,\dot{Q}+\sqrt{h}\,\dot{P}\,\xi+H\left(Q+\sqrt{h}\,\xi,P-i\sqrt{h}\frac{\partial}{\partial\xi}\right)\right.\right.$$
$$\left.\left.+i\sqrt{h}\,\dot{Q}\,\frac{\partial}{\partial\xi}-ih\frac{\partial}{\partial t}\right]f(\xi)\right\}\Bigg|_{\xi=\frac{x-Q(t)}{\sqrt{h}}}. \tag{1.106}$$

In the expression in braces on the right-hand side of (1.106), we can expend in powers of $\sqrt{h}$. The first three equations (for the coefficients of h^0, $h^{1/2}$, and h^1) read

$$[\dot{S}-P\,\dot{Q}+H(Q,P)]\,f(t,\xi)=0, \tag{1.107}$$

$$\left[\dot{P}+H_q\xi+i\,\dot{Q}\,\frac{\partial}{\partial\xi}-iH_p\frac{\partial}{\partial\xi}\right]f(t,\xi)=0, \tag{1.108}$$

$$\left[-i\frac{\partial}{\partial t}+\frac{1}{2}H_{qq}\xi^2-\frac{1}{2}H_{pp}\frac{\partial^2}{\partial\xi^2}-i<\xi,H_{qp}\frac{\partial}{\partial\xi}>\right]f(t,\xi)=0. \tag{1.109}$$

Equation (1.108) will be satisfied identically if $(P(t),Q(t))$ is the trajectory of the Hamilton system

$$\dot{P}=-H_q(Q,P),\quad \dot{Q}=H_p(Q,P)$$
$$Q(0)=q,\quad P(0)=p. \tag{1.110}$$

Then from (1.107) we obtain

$$S(t)=\int_0^t(P\,\dot{Q}-H)\,dt. \tag{1.111}$$

that is, $S(t)$ is just the classical *action* along the trajectory $(P(t),Q(t))$. Now let us solve Eq. (1.109). Let the initial Gaussian wave packet be given by

$$f(0,\xi)=e^{\frac{i}{2}(\xi,A_0\xi)}. \tag{1.112}$$

We seek the solution $f(t,\xi)$ of Eq. (1.109) in the form

$$f(t,\xi)=a(t)e^{\frac{i}{2}<\xi,A(t)\xi>}, \tag{1.113}$$

where $A(t) = {}^tA(t)$, $A(0) = A_0$, Im $A(t) > 0$, $a(0) = 1$, and $a(t)$ is a smooth scalar function. We have (we omit the argument t)

$$\begin{aligned}
\frac{\partial f}{\partial t} &= e^{\frac{i}{2}<\xi, A\xi>}\left(\frac{\partial a}{\partial t} + \frac{i}{2} < \xi, \frac{\partial A}{\partial t}\xi > a\right), \\
\frac{\partial f}{\partial \xi} &= iA\xi \cdot a e^{\frac{i}{2}<\xi, A\xi>}, \qquad (1.114) \\
\frac{\partial^2 f}{\partial \xi_j \partial \xi_k} &= -(A\xi)_j (A\xi)_k a e^{\frac{i}{2}<\xi, A\xi>} + iA_{jk} a e^{\frac{i}{2}<\xi, A\xi>}.
\end{aligned}$$

Let us substitute (1.114) into (1.109) and cancel the exponential factor. Then we obtain the equation

$$\begin{aligned}
-i\,\dot{a} \;\; &+\frac{1}{2} < \xi, \dot{A}\,\xi > a + \frac{1}{2} < \xi, H_{qq} > a + < \xi, H_{qp} A\xi > a \\
&+\frac{1}{2} < A\xi, H_{pp}, A\xi > a - \frac{i}{2}\mathrm{tr}(H_{pp}A)\, a = 0, \qquad (1.115)
\end{aligned}$$

whence, by separating the powers of ξ, we get

$$\dot{a} + \frac{1}{2}\mathrm{tr}(H_{pp}A)\, a = 0, \qquad (1.116)$$

$$\frac{1}{2}\,\dot{A} + \frac{1}{2}H_{qq} + \frac{1}{2}AH_{pq} + \frac{1}{2}H_{qp}A + \frac{1}{2}\,{}^tAH_{pp}A = 0. \qquad (1.117)$$

Equation (1.117) is a matrix Riccati equation. We seek the solution in the form

$$A = BC^{-1}, \qquad (1.118)$$

where B and C are some new matrices depending on t. Then

$$\dot{A} = \dot{B}\, C^{-1} - BC^{-1}\,\dot{C}\, C^{-1};$$

with regard to the fact that ${}^tA = A$, from (1.117) we obtain

$$\dot{B}C^{-1} - BC^{-1}\,\dot{C}\,C^{-1} + H_{qq} + BC^{-1}H_{pq} + H_{qp}BC^{-} + BC^{-1}H_{pp}BC^{-1} = 0. \qquad (1.119)$$

Let us multiply Eq. (1.119) by C on the right. Then we obtain

$$\dot{B} + H_{qq}C + H_{qp}B + BC^{-1}(-\dot{C} + H_{pq}C + H_{pp}B) = 0. \qquad (1.120)$$

For (1.120) to be valid, it suffices to require that

$$\begin{aligned} \dot{B} + H_{qq}C + H_{qp}B &= 0, \\ \dot{C} + H_{pq}C - H_{pp} &= 0, \end{aligned} \tag{1.121}$$

or, in the block matrix form,

$$\begin{pmatrix} \dot{B} \\ \dot{C} \end{pmatrix} = \begin{pmatrix} -H_{qp} & -H_{qq} \\ H_{pp} & H_{pq} \end{pmatrix} \begin{pmatrix} B \\ C \end{pmatrix}. \tag{1.122}$$

Note that (1.122) is just the variational system for (1.110). It remains to verify that the evolution law (1.122) preserves the symmetry of BC^{-1}. Routine computations show that

$$\begin{aligned} \frac{d}{dt}(BC^{-1} - {}^t(BC^{-1})) &= -H_{pq}(BC^{-1} - {}^t(BC^{-1})) \\ &\quad -(BC^{-1} - {}^t(BC^{-1}))H_{qp} + (BC^{-1} - {}^t(BC^{-1}))H_{pp}BC^{-1} \\ &\quad -{}^t(BC^{-1})H_{pp}(BC^{-1} - {}^t(BC^{-1})), \end{aligned} \tag{1.123}$$

whence the desired result follows by the uniqueness theorem for systems of ordinary differential equations. Now we solve Eq. (1.116) by integration:

$$a(t) = \exp\left\{-1/2 \int_0^t \operatorname{trace}(H_{pp}A)\, d\tau\right\}. \tag{1.124}$$

We have thereby proved that the class of Gaussian wave packets is preserved (modulo lower-order terms) by the quantum dynamics and that the "reference point" (P, Q) of the packet obeys the classical evolution law (1.110).

In the next subsection, we shall construct the "wave packet transform" using Gaussian wave packets. The main idea of this transform is very simple: we decompose any function $\psi(x) \in L^2(\mathbf{R}^n_x)$ into a "continuous linear combination" of wave packets $\psi_{p,q}(x)$, where the reference point p, q ranges over the entire phase space.

1.3.4 Definition and the main properties of the wave packet transform

We have seen in the preceding subsection that there are many wave packets corresponding to the same point (p, q) of the phase space. To define the wave packet transform, we first choose a single wave packet for each point (p, q). This choice is somewhat arbitrary. We take the family of functions

$$G_{(q,p)}(x,h) = \frac{1}{2^{n/2}(\pi h)^{3n/4}} \exp\left\{\frac{i}{h}\left[p(x-q) + \frac{i}{2}(x-q)^2\right]\right\} \quad (1.125)$$

of the variables (x, h) with parameters $(q, p) \in T^*\mathbf{R}^n$. (The coefficient of the exponential is just the normalization factor.) This is just the wave packet obtained (in the one-dimensional case) in the preceding subsection by considering the minimization problem with the quantum oscillator Hamiltonian.

We intend to decompose an arbitrary state into a superposition of the simplest Gaussian states (1.125). Thus, the problem is as follows. For each function $f(x, h) \in L^2(\mathbf{R}^n_x)$, find a function $\widetilde{f}(q, p, h)$ such that

$$f(x,h) = \int G_{(q,p)}(x,h)\widetilde{f}(q,p,h)\,dq\,dp.$$

Simultaneously, we have to describe the class of functions $\widetilde{f}(q, p, h)$ to be used in our expansions.

This problem can be solved as follows. First, we consider smooth compactly supported states.

Definition 6 Let $f(x, h)$ be a compactly supported smooth function on $\mathbf{R}^n_x$. The function

$$\widetilde{f}(q,p,h) = Uf(q,p,h) = \int \overline{G_{(q,p)}(x,h)} f(x,h)\,dx \quad (1.126)$$

is called the *wave packet transform* (or, briefly, *U-transform*) of the function $f(x, h)$. Here the bar means complex conjugation.

It turns out that the transformation (1.126) is invertible on the left (that is, on its range), and the inverse just solves our decomposition problem.

Specifically, consider the formal L^2-adjoint mapping U^*. It is obtained by taking the complex conjugate and by exchanging the roles of the variables (q,p) and x in the kernel. Specifically, it is given by the formula

$$U^*\widetilde{f}(x,h) = \int G_{(q,p)}(x,h)\widetilde{f}(q,p,h)\,dq\,dp. \tag{1.127}$$

The following statement is valid.

Theorem 7 *The inversion formula*

$$U^* \circ Uf = f \tag{1.128}$$

holds for any smooth compactly supported function f on $\mathbf{R}^n_x$.

Proof. A standard integration-by-parts shows that for $f \in C_0^\infty(\mathbf{R}^n_x)$, the transform Uf is rapidly decaying as $|p|+|q| \to \infty$, so that the left-hand side of (1.128) is well-defined. By (1.126) and (1.127), the left-hand side of (1.128) becomes[12]

$$U^* \circ Uf(x) = \int G_{(q,p)}(x)\left\{\int \overline{G_{(q,p)}(x'')}f(x'')\,dx''\right\}\,dq\,dp,$$

or, by definition (1.125) of the $G_{(q,p)}(x)$,

$$\begin{aligned} U^* \circ Uf(x) \;=\; & \int \exp\left\{\frac{i}{h}\left[p(x-x'') + \frac{i}{2}(x-q)^2 + \frac{i}{2}(x''-q)^2\right]\right\} \\ & \times f(x'')\,\frac{dx''\,dq\,dp}{2^n(\pi h)^{3n/2}}. \end{aligned}$$

The usual technique of oscillatory integrals permits us to change the order of integration. Then the integral over q can be computed explicitly, whence we obtain

$$U^* \circ Uf(x) = \left(\frac{1}{2\pi h}\right)^n \int e^{\frac{i}{h}p(x-x'')}\left\{e^{-\frac{1}{4h}(x-x'')^2}f(x'')\right\}\,dx''\,dp. \tag{1.129}$$

On the other hand, the inversion formula for the quantum Fourier transform yields

$$\left(\frac{1}{2\pi h}\right)^n \int e^{\frac{i}{h}p(x-x'')}\left\{e^{-\frac{1}{4h}(x_0-x'')^2}f(x'')\right\}\,dx''\,dp = e^{-\frac{1}{4h}(x_0-x'')^2}f(x)$$

[12] From now, we usually omit the explicit indication of the dependence on h.

for any $x_0 \in \mathbf{R}^n$. By substituting $x_0 = x$ there, we reduce (1.129) to the form

$$U^* \circ Uf(x) = f(x),$$

as desired. The proof is complete.

Now we intend to extend our transformation U to arbitrary states $f(x,h) \in L^2(\mathbf{R}^n_x)$. To this end, let us prove that U satisfies *the Parseval identity.*

Theorem 8 *If $f(x), g(x) \in L^2(\mathbf{R}^n_x)$, then*

$$(Uf, Ug) = (f, g),$$

where the inner products on the phase and the physical spaces are given by the usual formulas

$$\left(\widetilde{f}(q,p), \widetilde{g}(q,p)\right) = \int \widetilde{f}(q,p)\overline{\widetilde{g}(q,p)}\, dq\, dp$$

and

$$(f(x), g(x)) = \int f(x)\overline{g(x)}\, dx,$$

respectively.

Proof. The proof is by straightforward computation:

$$\begin{aligned}(Uf, Ug) &= \int \left\{ \int \overline{G_{(q,p)}(x)} f(x)\, dx \right\} \overline{Ug(q,p)}\, dq\, dp \\ &= \int f(x) \overline{\left\{ \int G_{(q,p)}(x) Ug(q,p)\, dq\, dp \right\}}\, dx \\ &= \int f(x)\overline{U^* \circ Ug(x)}\, dx = \int f(x)\overline{g(x)}\, dx = (f, g).\end{aligned}$$

We obtain the following corollary.

Corollary 9 *The mapping U extends by continuity to a partially isometric mapping (denoted by the same letter)*

$$U : L^2(\mathbf{R}^n_x) \longrightarrow L^2(\mathbf{R}^{2n}_{q,p}). \tag{1.130}$$

The left inverse of U is the adjoint operator U^*.

However, U is indeed only partially isometric, that is, the range of U (which is automatically closed) *does not coincide with the entire space* $L^2(\mathbf{R}^{2n}_{q,p})$, and, accordingly, the formula

$$U \circ U^* = \mathrm{id} \tag{1.131}$$

is *not valid*. This is not surprising, since U takes functions of n variables x to functions of $2n$ variables (q,p). Let use describe the range of U.

Theorem 10 *The range of the transformation* (1.130) *is the set* $\mathcal{F}$ *of functions* $F(q,p)$ *with the following two properties:*

1) $\int |F(q,p)|^2\,dx\,dp < \infty$;

2) the function $\exp\left[\frac{1}{2h}p^2\right] F(x,p)$ is an analytic function of the variable $z = q - ip$, that is, satisfies the Cauchy–Riemann equations

$$\left(\frac{\partial}{\partial q_j} - i\frac{\partial}{\partial p_j}\right)\left\{\exp\left[\frac{1}{2h}p^2\right] F(q,p)\right\} = 0, \quad j = 1,\dots,n.$$

Proof. The first property just means that $\mathcal{F} \subset L^2(\mathbf{R}^{2n}_{q,p})$. To prove that any function $\widetilde{f} = Uf$ possesses the second property, we note that

$$\exp\left[\frac{1}{2h}p^2\right] \widetilde{f}(q,p) = \frac{1}{2^{n/2}(\pi h)^{3n/4}} \int \exp\left[-\frac{1}{2h}(x-z)^2\right] f(x)\,dx,$$

where $z = q - ip$, which proves the required assertion.

To complete the proof, we check that formula (1.131) is valid on the set of functions possessing properties 1) and 2). The proof of this fact, based on the Bargman representation of an analytic function (see [1]) is purely technical and we omit it.

In the following, we write

$$U^{-1} = U|_{\mathcal{F}}.$$

The transformation U naturally acts in quantum Sobolev spaces with positive indices and can be extended by continuity to act in quantum Sobolev spaces with negative indices. Specifically, the following theorem holds.

Theorem 11 *The transformation U is a continuous isomorphism (but generally not an isometry) of the spaces*

$$U : H^s(\mathbf{R}^n_x) \longrightarrow \mathcal{F}H^s(\mathbf{R}^{2n}_{q,p}).$$

Here $H^s(\mathbf{R}^n_x)$ is the quantum Sobolev space over the classical configuration space and

$$\mathcal{F}H^s(\mathbf{R}^{2n}_{q,p}) = \mathcal{F} \bigcap H^s(\mathbf{R}^{2n}_{q,p}), \quad s \geq 0.$$

For negative s, the space $\mathcal{F}H^s(\mathbf{R}^{2n}_{q,p})$ is defined as the closure of $\mathcal{F}$ in $H^s(\mathbf{R}^{2n}_{q,p})$.

The proof can be found in [15].

Finally, let us carry out the comparison of the Bargmann transform with the wave packet transform. Straightforward computation shows that

$$U[f](q,p) = (2\pi\sqrt{h})^{-n/2} \exp\left(-\frac{p^2}{2h}\right) \left[\exp\left(-\frac{z^2}{2}\right) F(z)\right]\Big|_{z=\frac{q-ip}{\sqrt{2h}}}, \tag{1.132}$$

where $F(z) = \mathcal{B}[f](z)$ is the Bargmann transform of $f(x\sqrt{h})$. This is not surprising at all, since the Bargmann transform, as well as the wave packet transform, is based on the eigenfunctions of the quantum-mechanical oscillator; in the latter, they arose from the minimization problem for mean-square deviations, whereas in the former they arose as vacuum states in the Fock space.

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