7. Quantization of the Harmonic Oscillator – Ariadne's Thread in Quantization

> Whoever understands the quantization of the harmonic oscillator can understand everything in quantum physics.
>
> Folklore

> Almost all of physics now relies upon quantum physics. This theory was discovered around the beginning of this century. Since then, it has known a progress with no analogue in the history of science, finally reaching a status of universal applicability.
> The radical novelty of quantum mechanics almost immediately brought a conflict with the previously admitted corpus of classical physics, and this went as far as rejecting the age-old representation of physical reality by visual intuition and common sense. The abstract formalism of the theory had almost no direct counterpart in the ordinary features around us, as, for instance, nobody will ever see a wave function when looking at a car or a chair. An ever-present randomness also came to contradict classical determinism.[1]
>
> Roland Omnès, 1994

> Quantum mechanics deserves the interest of mathematicians not only because it is a very important physical theory, which governs all microphysics, that is, the physical phenomena at the microscopic scale of 10^{-10}m, but also because it turned out to be at the root of important developments of modern mathematics.[2]
>
> Franco Strocchi, 2005

In this chapter, we will study the following quantization methods:

- Heisenberg quantization (matrix mechanics; creation and annihilation operators),
- Schrödinger quantization (wave mechanics; the Schrödinger partial differential equation),
- Feynman quantization (integral representation of the wave function by means of the propagator kernel, the formal Feynman path integral, the rigorous infinite-dimensional Gaussian integral, and the rigorous Wiener path integral),
- Weyl quantization (deformation of Poisson structures),

[1] From the Preface to R. Omnès, The Interpretation of Quantum Mechanics, Princeton University Press, Princeton, New Jersey, 1994. Reprinted by permission of Princeton University Press. We recommend this monograph as an introduction to the philosophical interpretation of quantum mechanics.

[2] F. Strocchi, An Introduction to the Mathematical Structure of Quantum Mechanics: A Short Course for Mathematicians, Lecture Notes, Scuola Normale, Pisa (Italy). Reprinted by permission of World Scientific Publishing Co. Pte. Ltd. Singapore, 2005.

- Weyl quantization functor from symplectic linear spaces to C^*-algebras,
- Bargmann quantization (holomorphic quantization),
- supersymmetric quantization (fermions and bosons).

We will choose the presentation of the material in such a way that the reader is well prepared for the generalizations to quantum field theory to be considered later on.

Formally self-adjoint operators. The operator $A : D(A) \to X$ on the complex Hilbert space X is called formally self-adjoint iff the operator is linear, the domain of definition $D(A)$ is a linear dense subspace of the Hilbert space X, and we have the symmetry condition

$$\langle \chi | A\varphi \rangle = \langle A\chi | \varphi \rangle \qquad \text{for all} \quad \chi, \psi \in D(A).$$

Formally self-adjoint operators are also called symmetric operators. The following two observations are crucial for quantum mechanics:

- If the complex number λ is an eigenvalue of A, that is, there exists a nonzero element $\varphi \in D(A)$ such that $A\varphi = \lambda\varphi$, then λ is a real number. This follows from $\lambda = \langle \varphi | A\varphi \rangle = \langle A\varphi | \varphi \rangle = \lambda^\dagger$.
- If λ_1 and λ_2 are two different eigenvalues of the operator A with eigenvectors φ_1 and φ_2, then φ_1 is orthogonal to φ_2. This follows from

$$(\lambda_1 - \lambda_2)\langle \varphi_1 | \varphi_2 \rangle = \langle A\varphi_1 | \varphi_2 \rangle - \langle \varphi_1 | A\varphi_2 \rangle = 0.$$

In quantum mechanics, formally self-adjoint operators represent formal observables.

For a deeper mathematical analysis, we need self-adjoint operators, which are called observables in quantum mechanics.

Each self-adjoint operator is formally self-adjoint. But, the converse is not true. For the convenience of the reader, on page 683 we summarize basic material from functional analysis which will be frequently encountered in this chapter. This concerns the following notions: formally adjoint operator, adjoint operator, self-adjoint operator, essentially self-adjoint operator, closed operator, and the closure of a formally self-adjoint operator. The reader, who is not familiar with this material, should have a look at page 683. Observe that, as a rule, in the physics literature one does not distinguish between formally self-adjoint operators and self-adjoint operators. Peter Lax writes:[3]

> The theory of self-adjoint operators was created by John von Neumann to fashion a framework for quantum mechanics. The operators in Schrödinger's theory from 1926 that are associated with atoms and molecules are partial differential operators whose coefficients are singular at certain points; these singularities correspond to the unbounded growth of the force between two electrons that approach each other... I recall in the summer of 1951 the excitement and elation of von Neumann when he learned that Kato (born 1917) has proved the self-adjointness of the Schrödinger operator associated with the helium atom.[4]

[3] P. Lax, Functional Analysis, Wiley, New York, 2003 (reprinted with permission). This is the best modern textbook on functional analysis, written by a master of this field who works at the Courant Institute in New York City. For his fundamental contributions to the theory of partial differential equations in mathematical physics (e.g., scattering theory, solitons, and shock waves), Peter Lax (born 1926) was awarded the Abel prize in 2005.

[4] J. von Neumann, General spectral theory of Hermitean operators, Math. Ann. **102** (1929), 49–131 (in German).

> And what do the physicists think of these matters? In the 1960s Friedrichs[5] met Heisenberg and used the occasion to express to him the deep gratitude of the community of mathematicians for having created quantum mechanics, which gave birth to the beautiful theory of operators in Hilbert space. Heisenberg allowed that this was so; Friedrichs then added that the mathematicians have, in some measure, returned the favor. Heisenberg looked noncommittal, so Friedrichs pointed out that it was a mathematician, von Neumann, who clarified the difference between a self-adjoint operator and one that is merely symmetric. "What's the difference," said Heisenberg.

As a rule of thumb, a formally self-adjoint (also called symmetric) differential operator can be extended to a self-adjoint operator if we add appropriate boundary conditions. The situation is not dramatic for physicists, since physics dictates the 'right' boundary conditions in regular situations. However, one has to be careful. In Problem 7.19, we will consider a formally self-adjoint differential operator which cannot be extended to a self-adjoint operator.

> *The point is that self-adjoint operators possess a spectral family which allows us to construct both the probability measure for physical observables and the functions of observables (e.g., the propagator for the quantum dynamics).*

In general terms, this is not possible for merely formally self-adjoint operators. The following proposition displays the difference between formally self-adjoint and self-adjoint operators.

Proposition 7.1 *The linear, densely defined operator $A : D(A) \to X$ on the complex Hilbert space X is self-adjoint iff it is formally self-adjoint and it always follows from*

$$\langle \psi | A\varphi \rangle = \langle \chi | \varphi \rangle$$

for fixed $\psi, \chi \in X$ and all $\varphi \in D(A)$ that $\psi \in D(A)$.

Therefore, the domain of definition $D(A)$ of the operator A plays a critical role. The proof will be given in Problem 7.7.

Unitary operators. As we will see later on, for the quantum dynamics, unitary operators play the decisive role. Recall that the operator $U : X \to X$ is called unitary iff it is linear, bijective, and it preserves the inner product, that is,

$$\langle U\chi | U\varphi \rangle = \langle \chi | \varphi \rangle \qquad \text{for all} \quad \chi, \varphi \in X.$$

This implies $||U\varphi|| = ||\varphi||$ for all $\varphi \in X$. Hence

$$||U|| := \sup_{||\varphi|| \leq 1} ||U\varphi|| = 1$$

if we exclude the trivial case $X = \{0\}$.

The shortcoming of the language of matrices noticed by von Neumann. Let $A : D(A) \to X$ and $B : D(B) \to X$ be linear, densely defined, formally

J. von Neumann, Mathematical Foundations of Quantum Mechanics (in German), Springer, Berlin, 1932. English edition: Princeton University Press, 1955.
T. Kato, Fundamental properties of the Hamiltonian operators of Schrödinger type, Trans. Amer. Math. Soc. **70** (1951), 195–211.

[5] Schrödinger (1887–1961), Heisenberg (1901–1976), Friedrichs (1902–1982), von Neumann (1903–1957), Kato (born 1917).

self-adjoint operators on the infinite-dimensional Hilbert space X. Let $\varphi_0, \varphi_1, \varphi_2, \ldots$ be a complete orthonormal system in X with $\varphi_k \in D(A)$ for all k. Set

$$a_{jk} := \langle \varphi_j | A\varphi_k \rangle \qquad j, k = 0, 1, 2, \ldots$$

The way, we assign to the operator A the infinite matrix (a_{jk}). Similarly, for the operator B, we define

$$b_{jk} := \langle \varphi_j | B\varphi_k \rangle \qquad j, k = 0, 1, 2, \ldots$$

Suppose that the operator B is a proper extension of the operator A. Then

$$a_{jk} = b_{jk} \qquad \text{for all} \quad j, k = 0, 1, 2, \ldots,$$

but $A \neq B$. Thus, the matrix (a_{jk}) does not completely reflect the properties of the operator A. In particular, the matrix (a_{jk}) does not see the crucial domain of definition $D(A)$ of the operator A. Jean Dieudonné writes:[6]

> Von Neumann took pains, in a special paper, to investigate how Hermitean (i.e., formally self-adjoint) operators might be represented by infinite matrices (to which many mathematicians and even more physicists were sentimentally attached) ... Von Neumann showed in great detail how the lack of "one-to-oneness" in the correspondence of matrices and operators led to their weirdest pathology, convincing once for all the analysts that matrices were a totally inadequate tool in spectral theory.

7.1 Complete Orthonormal Systems

> A complete orthonormal system of eigenstates of an observable (e.g., the energy operator) cannot be extended to a larger orthonormal system of eigenstates.
>
> Folklore

Basic question. Let $H : D(H) \to X$ be a formally self-adjoint operator on the infinite-dimensional separable complex Hilbert space X. Physicists have invented algebraic methods for computing eigensolutions of the form

$$H\varphi_n = E_n\varphi_n, \qquad n = 0, 1, 2, \ldots \tag{7.1}$$

The idea is to apply so-called ladder operators which are based on the use of commutation relations (related to Lie algebras or super Lie algebras). We will encounter this method several times. In terms of physics, the operator H describes the energy of the quantum system under consideration. Here, the real numbers $E_0, E_1, E_2, \ldots$ are the energy values, and $\varphi_0, \varphi_1, \varphi_2, \ldots$ are the corresponding energy eigenstates. Suppose that $\varphi_0, \varphi_1, \varphi_2, \ldots$ is an orthonormal system, that is,

$$\langle \varphi_k | \varphi_n \rangle = \delta_{kn}, \qquad k, n = 0, 1, 2, \ldots$$

There arises the following crucial question.

[6] J. Dieudonné, History of Functional Analysis, 1900–1975, North-Holland, Amsterdam, 1983 (reprinted with permission).
J. von Neumann, On the theory of unbounded matrices, J. reine und angew. Mathematik **161** (1929), 208–236 (in German).

Is the system of the computed energy eigenvalues $E_0, E_1, E_2 \ldots$ complete?

The following theorem gives us the answer in terms of analysis.

Theorem 7.2 *If the orthonormal system $\varphi_0, \varphi_1, \ldots$ is complete in the Hilbert space X, then there are no other energy eigenvalues than $E_0, E_1, E_2, \ldots$, and the system $\varphi_0, \varphi_1, \varphi_2, \ldots$ cannot be extended to a larger orthonormal system of eigenstates.*

Before giving the proof, we need some analytical tools.

Completeness. By definition, the orthonormal system $\varphi_0, \varphi_1, \varphi_2 \ldots$ is complete iff, for any $\varphi \in X$, the Fourier series

$$\boxed{\varphi = \sum_{n=0}^{\infty} \langle \varphi_n | \varphi \rangle \varphi_n}$$

is convergent in X, that is, $\lim_{N\to\infty} ||\varphi - \sum_{n=0}^{N} \langle \varphi_n | \varphi \rangle \varphi_n|| = 0$. The proof of the following proposition can be found in Zeidler (1995a), Chap. 3 (see the references on page 1049).

Proposition 7.3 *Let $\varphi_0, \varphi_1, \varphi_2 \ldots$ be an orthonormal system in the infinite-dimensional separable complex Hilbert space X. Then the following statements are equivalent.*

(i) *The system $\varphi_0, \varphi_1, \varphi_2, \ldots$ is complete.*

(ii) *For all $\varphi, \psi \in X$, we have the convergent series*

$$\langle \psi | \varphi \rangle = \sum_{n=0}^{\infty} \langle \psi | \varphi_n \rangle \langle \varphi_n | \varphi \rangle, \tag{7.2}$$

which is called the Parseval equation.

(iii) $I = \sum_{n=0}^{\infty} \varphi_n \otimes \varphi_n$ *(completeness relation).*[7]

(iv) *For all $\varphi \in X$, we have the convergent series $||\varphi||^2 = \sum_{n=0}^{\infty} |\langle \varphi_n | \varphi \rangle|^2$.*

(v) *Let $\varphi \in X$. If all the Fourier coefficients of φ vanish, that is, we have $\langle \varphi_n | \varphi \rangle = 0$ for all n, then $\varphi = 0$.*

(vi) *The linear hull of the set $\{\varphi_0, \varphi_1, \varphi_2, \ldots\}$ is dense in the Hilbert space X. Explicitly, for any $\varphi \in X$ and any number $\varepsilon > 0$, there exist complex numbers $a_0, \ldots, a_n$ such that $||\varphi - (a_1\varphi_1 + \ldots + a_n\varphi_n)|| < \varepsilon$.*

Proof of Theorem 7.2. Suppose that $H\varphi = E\varphi$ with $\varphi \neq 0$ and that the eigenvalue E is different from $E_0, E_1, E_2, \ldots$. Since the eigenvectors for different eigenvalues are orthogonal to each other, we get $\langle \varphi_n | \varphi \rangle = 0$ for all indices n. By Prop. 7.3(v), $\varphi = 0$. This is a contradiction. □

The Dirac calculus. According to Dirac, we write equation (7.1) as

$$H|E_n\rangle = E_n|E_n\rangle, \qquad n = 0, 1, 2, \ldots$$

Moreover, the completeness relation from Prop. 7.3(iii) reads as

$$\boxed{I = \sum_{n=0}^{\infty} |\varphi_n\rangle\langle\varphi_n|.} \tag{7.3}$$

[7] This means that $\varphi = \lim_{N\to\infty} \sum_{n=0}^{N} (\varphi_n \otimes \varphi_n)\varphi$ for all $\varphi \in X$. Here, we use the convention $(\varphi_n \otimes \varphi_n)\varphi := \varphi_n \langle \varphi_n | \varphi \rangle$.

Mnemonically, from (7.3) we obtain $|\varphi\rangle = \sum_{n=0}^{\infty} |\varphi_n\rangle\langle\varphi_n|\varphi\rangle$ and

$$\langle\psi|\varphi\rangle = \langle\psi| \cdot |\varphi\rangle = \langle\psi| \cdot I|\varphi\rangle = \sum_{n=0}^{\infty} \langle\psi|\varphi_n\rangle\langle\varphi_n|\varphi\rangle.$$

This coincides with the Fourier series expansion $\varphi = \sum_{n=0}^{\infty} \langle\varphi_n|\varphi\rangle\varphi_n$ and the Parseval equation (7.2).

The following investigations serve as a preparation for the quantization of the harmonic oscillator in the sections to follow.

7.2 Bosonic Creation and Annihilation Operators

> Whoever understands creation and annihilation operators can understand everything in quantum physics.
>
> Folklore

The Hilbert space $L_2(\mathbb{R})$. We consider the space $L_2(\mathbb{R})$ of complex-valued (measurable) functions $\psi : \mathbb{R} \to \mathbb{C}$ with $\int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty$. This becomes a complex Hilbert space equipped with the inner product

$$\langle\varphi|\psi\rangle := \int_{-\infty}^{\infty} \varphi(x)^\dagger \psi(x) dx \qquad \text{for all} \quad \varphi, \psi \in L_2(\mathbb{R}).$$

Moreover, $||\psi|| := \sqrt{\langle\psi|\psi\rangle}$. The precise definition of $L_2(\mathbb{R})$ can be found in Vol. I, Sect. 10.2.4. Recall that the Hilbert space $L_2(\mathbb{R})$ is infinite-dimensional and separable. For example, the complex-valued function ψ on the real line is contained in $L_2(\mathbb{R})$ if we have the growth restriction at infinity,

$$|\psi(x)| \leq \frac{\text{const}}{1 + |x|} \qquad \text{for all} \quad x \in \mathbb{R},$$

and ψ is either continuous or discontinuous in a reasonable way (e.g., ψ is continuous up to a finite or a countable subset of the real line). Furthermore, we will use the space $\mathcal{S}(\mathbb{R})$ of smooth functions $\psi : \mathbb{R} \to \mathbb{C}$ which rapidly decrease at infinity (e.g., $\psi(x) := \mathrm{e}^{-x^2}$). The space $\mathcal{S}(\mathbb{R})$ is a linear subspace of the Hilbert space $L_2(\mathbb{R})$. Moreover, $\mathcal{S}(\mathbb{R})$ is dense in $L_2(\mathbb{R})$. The precise definition of $\mathcal{S}(\mathbb{R})$ can be found in Vol. I, Sect. 2.7.4.

The operators a and $a^\dagger$. Fix the positive number x_0. Let us study the operator

$$\boxed{a := \frac{1}{\sqrt{2}} \left(\frac{x}{x_0} + x_0 \frac{d}{dx} \right).}$$

More precisely, for each function $\psi \in \mathcal{S}(\mathbb{R})$, we define

$$(a\psi)(x) := \frac{1}{\sqrt{2}} \left(\frac{x\psi(x)}{x_0} + x_0 \frac{d\psi(x)}{dx} \right) \qquad \text{for all} \quad x \in \mathbb{R}. \tag{7.4}$$

This way, we get the operator $a : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$. We also define the operator $a^\dagger : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ by setting

$$\boxed{a^\dagger := \frac{1}{\sqrt{2}} \left(\frac{x}{x_0} - x_0 \frac{d}{dx} \right).} \tag{7.5}$$

Explicitly, for each function $\psi \in \mathcal{S}(\mathbb{R})$, we set[8]

$$(a^\dagger \psi)(x) := \frac{1}{\sqrt{2}} \left(\frac{x\psi(x)}{x_0} - x_0 \frac{d\psi(x)}{dx} \right) \qquad \text{for all} \quad x \in \mathbb{R}.$$

The operators a and $a^\dagger$ have the following properties:

(i) The operator $a^\dagger : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is the formally adjoint operator to the operator $a : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ on the Hilbert space $L_2(\mathbb{R})$.[9] This means that

$$\langle \varphi | a\psi \rangle = \langle a^\dagger \varphi | \psi \rangle \qquad \text{for all} \quad \varphi, \psi \in \mathcal{S}(\mathbb{R}).$$

(ii) We have the commutation relation

$$\boxed{[a, a^\dagger]_- = I}$$

where I denotes the identity operator on the Hilbert space $L_2(\mathbb{R})$. Recall that $[A, B]_- := AB - BA$.

(iii) Set $\varphi_0(x) := c_0 \mathrm{e}^{-x^2/2x_0^2}$ with the normalization constant $c_0 := \frac{1}{\sqrt{x_0 \sqrt{\pi}}}$. Then $a\varphi_0 = 0$.

(iv) The operator $N : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ given by $N := a^\dagger a$ is formally self-adjoint, and it has the eigensolutions

$$\boxed{N\varphi_n = n\varphi_n, \qquad n = 0, 1, 2, \ldots}$$

where we set

$$\boxed{\varphi_n := \frac{(a^\dagger)^n}{\sqrt{n!}}\, \varphi_0.} \tag{7.6}$$

(v) For $n = 0, 1, 2, \ldots$, we have

$$a^\dagger \varphi_n = \sqrt{n+1}\ \varphi_{n+1}, \qquad a\varphi_{n+1} = \sqrt{n+1}\ \varphi_n.$$

Because of these relations, the operators a and $a^\dagger$ are called ladder operators.[10]

(vi) The functions $\varphi_0, \varphi_1, \ldots$ form a complete orthonormal system of the complex Hilbert space $L_2(\mathbb{R})$. This means that

$$\langle \varphi_n | \varphi_m \rangle = \int_{-\infty}^{\infty} \varphi_n(x)^\dagger \varphi_m(x)\, dx = \delta_{nm}, \qquad n, m = 0, 1, 2, \ldots$$

[8] In applications to the harmonic oscillator later on, the quantity x has the physical dimension of length. We introduce the typical length scale x_0 in order to guarantee that the operators a and $a^\dagger$ are dimensionless.

[9] In functional analysis, one has to distinguish between the formally adjoint operator $a^\dagger : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ and the adjoint operator $a^* : D(a^*) \to L_2(\mathbb{R})$ which is an extension of $a^\dagger$, that is, $\mathcal{S}(\mathbb{R}) \subseteq D(a^*) \subseteq L_2(\mathbb{R})$ and $a^*\varphi = a^\dagger \varphi$ for all $\varphi \in \mathcal{S}(\mathbb{R})$ (see Problem 7.4).

[10] Ladder operators are frequently used in the theory of Lie algebras and in quantum physics in order to compute eigenvectors and eigenvalues. Many examples can be found in H. Green, Matrix Mechanics, Noordhoff, Groningen, 1965, and in Shi-Hai Dong, Factorization Method in Quantum Mechanics, Springer, Dordrecht, 2007 (including supersymmetry). We will encounter this several times later on.

Moreover, for each function ψ in the complex Hilbert space $L_2(\mathbb{R})$, the Fourier series

$$\psi = \sum_{n=0}^{\infty} \langle \varphi_n | \psi \rangle \varphi_n$$

is convergent in $L_2(\mathbb{R})$. Explicitly,

$$\lim_{k \to \infty} ||\psi - \sum_{n=0}^{k} \langle \varphi_n | \psi \rangle \varphi_n|| = 0.$$

Recall that $||f||^2 = \langle f | f \rangle = \int_{-\infty}^{\infty} |f(x)|^2 \, dx$.

(vii) The matrix elements a_{mn} of the operator a with respect to the basis $\varphi_0, \varphi_1, \ldots$ are defined by

$$a_{mn} := \langle \varphi_m | a \varphi_n \rangle, \qquad m, n = 0, 1, 2, \ldots$$

Explicitly, $a_{mn} = \sqrt{n} \;\; \delta_{m,n-1}$. Therefore,

$$(a_{mn}) = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 \ldots \\ 0 & 0 & \sqrt{2} & 0 & 0 \ldots \\ 0 & 0 & 0 & \sqrt{3} & 0 \ldots \\ \vdots & & & & \end{pmatrix}.$$

Similarly, we introduce the matrix elements $(a^\dagger)_{mn}$ of the operator $a^\dagger$ by setting

$$(a^\dagger)_{mn} := \langle \varphi_m | a^\dagger \varphi_n \rangle, \qquad m, n = 0, 1, 2, \ldots$$

Then $(a^\dagger)_{mn} = a^\dagger_{nm}$. Thus, the matrix to the operator $a^\dagger$ is the adjoint matrix to the matrix (a_{mn}).

Let us prove these statements. To simplify notation, we set $x_0 := 1$.

Ad (i). For all functions $\varphi, \psi \in \mathcal{S}(\mathbb{R})$, integration by parts yields

$$\int_{-\infty}^{\infty} \varphi(x)^\dagger \left(x + \frac{d}{dx} \right) \psi(x) dx = \int_{-\infty}^{\infty} \left(x - \frac{d}{dx} \right) \varphi(x)^\dagger \cdot \psi(x) dx.$$

Hence $\langle \varphi | a \psi \rangle = \langle a^\dagger \varphi | \psi \rangle$.

Ad (ii). Obviously, $2aa^\dagger \psi = (x + \frac{d}{dx})(x - \frac{d}{dx})\psi = x^2 \psi + \psi - \psi''$. Similarly,

$$2a^\dagger a \psi = \left(x - \frac{d}{dx} \right) \left(x + \frac{d}{dx} \right) \psi = x^2 \psi - \psi - \psi''.$$

Hence $(aa^\dagger - a^\dagger a)\psi = \psi$.

Ad (iii). Note that $\sqrt{2} \, a \mathrm{e}^{-x^2/2} = (x + \frac{d}{dx}) \mathrm{e}^{-x^2/2} = 0$.

Ad (iv). For all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$,

$$\langle \varphi | a^\dagger a \psi \rangle = \langle a \varphi | a \psi \rangle = \langle a^\dagger a \varphi | \psi \rangle.$$

Hence $\langle \varphi | N \psi \rangle = \langle N \varphi | \psi \rangle$. Thus, the operator N is formally self-adjoint. We now proceed by induction. Obviously, $N \varphi_0 = a^\dagger (a \varphi_0) = 0$. Suppose that $N \varphi_n = n \varphi_n$. Then, by (ii),

$$N(a^\dagger \varphi_n) = a^\dagger a a^\dagger \varphi_n = a^\dagger (a^\dagger a + I) \varphi_n.$$

This implies

$$N(a^\dagger\varphi_n) = a^\dagger(N+I)\varphi_n = (n+1)a^\dagger\varphi_n.$$

Thus, $N\varphi_{n+1} = (n+1)\varphi_{n+1}$.

Ad (v). By definition of the state φ_n,

$$a^\dagger\varphi_n = \frac{(a^\dagger)^{n+1}}{\sqrt{n!}}\,\varphi_0 = \sqrt{n+1}\,\frac{(a^\dagger)^{n+1}}{\sqrt{(n+1)!}}\,\varphi_0 = \sqrt{n+1}\,\varphi_{n+1}.$$

Moreover, by (ii) and (iv),

$$\sqrt{n+1}\,a\varphi_{n+1} = aa^\dagger\varphi_n = (a^\dagger a + I)\varphi_n = (n+1)\varphi_n.$$

Ad (vi). We first show that the functions $\varphi_0, \varphi_1, ...$ form an orthonormal system. In fact, by the Gaussian integral,

$$\langle\varphi_0|\varphi_0\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-x^2}}{\sqrt{\pi}}\,dx = 1.$$

We now proceed by induction. Suppose that $\langle\varphi_n|\varphi_n\rangle = 1$. Then

$$(n+1)\langle\varphi_{n+1}|\varphi_{n+1}\rangle = \langle a^\dagger\varphi_n|a^\dagger\varphi_n\rangle = \langle\varphi_n|aa^\dagger\varphi_n\rangle = \langle\varphi_n|(N+I)\varphi_n\rangle.$$

By (iv), this is equal to $(n+1)\langle\varphi_n|\varphi_n\rangle$. Hence $\langle\varphi_{n+1}|\varphi_{n+1}\rangle = 1$.

Since the operator N is formally self-adjoint, eigenvectors of N to different eigenvalues are orthogonal to each other. Explicitly, it follows from

$$n\langle\varphi_n|\varphi_m\rangle = \langle N\varphi_n|\varphi_m\rangle = \langle\varphi_n|N\varphi_m\rangle = m\langle\varphi_n|\varphi_m\rangle$$

that $\langle\varphi_n|\varphi_m\rangle = 0$ if $n \neq m$. Finally, we will show below that the functions $\varphi_0, \varphi_1, ...$ coincide with the Hermite functions which form a complete orthonormal system in $L_2(\mathbb{R})$.

Ad (vii). By (v),

$$\langle\varphi_m|a\varphi_n\rangle = \sqrt{n}\langle\varphi_m|\varphi_{n-1}\rangle = \sqrt{n}\,\delta_{m,n-1}.$$

Moreover, $(a^\dagger)_{mn} = \langle\varphi_m|a^\dagger\varphi_n\rangle = \langle a\varphi_m|\varphi_n\rangle = (a_{nm})^\dagger$. □

Physical interpretation. In quantum field theory, the results above allow the following physical interpretation.

- The function φ_n represents a normalized n-particle state.
- Since $N\varphi_n = n\varphi_n$ and the state φ_n consists of n particles, the operator N is called the particle number operator.
- Since $N\varphi_0 = 0$, the state φ_0 is called the (normalized) vacuum state; there are no particles in the state φ_0.
- By (v) above, the operator $a^\dagger$ sends the n-particle state φ_n to the $(n+1)$-particle state φ_{n+1}. Naturally enough, the operator $a^\dagger$ is called the particle creation operator. In particular, the n-particle state

$$\varphi_n = \frac{(a^\dagger)^n}{\sqrt{n!}}\,\varphi_0$$

is obtained from the vacuum state φ_0 by an n-fold application of the particle creation operator a.[11]

[11] For the vacuum state φ_0, physicists also use the notation $|0\rangle$.

- Similarly, by (v) above, the operator a sends the $(n+1)$-particle state φ_{n+1} to the n-particle state φ_n. Therefore, the operator a is called the particle annihilation operator.

The position operator Q and the momentum operator P. We set

$$Q := \frac{x_0}{\sqrt{2}}(a^\dagger + a), \qquad P := \frac{\mathrm{i}\hbar}{x_0\sqrt{2}}(a^\dagger - a).$$

This way, we obtain the two linear operators $Q, P : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ along with the commutation relation

$$\boxed{[Q, P]_- = \mathrm{i}\hbar I.}$$

This follows from $[a, a^\dagger]_- = I$. In fact,

$$[Q, P]_- = \tfrac{1}{2}[a^\dagger + a, \mathrm{i}\hbar(a^\dagger - a)]_-.$$

Hence $2[Q, P]_- = \mathrm{i}\hbar[a, a^\dagger]_- - \mathrm{i}\hbar[a^\dagger, a]_- = 2\mathrm{i}\hbar[a, a^\dagger]_- = 2\mathrm{i}\hbar I$. Explicitly, for all functions $\psi \in \mathcal{S}(\mathbb{R})$ and all $x \in \mathbb{R}$,

$$(Q\psi)(x) = x\psi(x), \qquad (P\psi)(x) = -\mathrm{i}\hbar\, \frac{d\psi(x)}{dx}.$$

Hence $P = -\mathrm{i}\hbar\frac{d}{dx}$. The operators Q, P are formally self-adjoint, that is,

$$\langle\varphi|Q\psi\rangle = \langle Q\varphi|\psi\rangle, \qquad \langle\varphi|P\psi\rangle = \langle P\varphi|\psi\rangle$$

for all functions $\varphi, \psi \in \mathcal{S}(\mathbb{R})$. In fact,

$$\langle\varphi|Q\psi\rangle = \int_{-\infty}^{\infty} \varphi(x)^\dagger x\psi(x)\, dx = \int_{-\infty}^{\infty} (x\varphi(x))^\dagger \psi(x)\, dx = \langle Q\varphi|\psi\rangle.$$

Furthermore, noting that $(\mathrm{i}\varphi(x))^\dagger = -\mathrm{i}\varphi(x)^\dagger$, integration by parts yields

$$\langle\varphi|P\psi\rangle = \int_{-\infty}^{\infty} \varphi(x)^\dagger(-\mathrm{i}\hbar\psi'(x))dx = \int_{-\infty}^{\infty} (-\mathrm{i}\hbar\varphi'(x))^\dagger \psi(x)\, dx = \langle P\varphi|\psi\rangle.$$

The Hermite functions. To simplify notation, we set $x_0 := 1$. We will show that the functions $\varphi_0, \varphi_1, \ldots$ introduced above coincide with the classical Hermite functions.[12] To this end, for $n = 0, 1, 2, \ldots$, we introduce the Hermite polynomials

$$H_n(x) := (-1)^n \mathrm{e}^{x^2}\, \frac{d^n \mathrm{e}^{-x^2}}{dx^n} \tag{7.7}$$

along with the Hermite functions

$$\psi_n(x) := \frac{\mathrm{e}^{-x^2/2} H_n(x)}{\sqrt{2^n n! \sqrt{\pi}}}, \qquad x \in \mathbb{R}. \tag{7.8}$$

Explicitly, $H_0(x) = 1, H_1(x) = 2x$, and $H_2(x) = 4x^2 - 2$. For $n = 0, 1, 2, \ldots$, the following hold:

[12] Hermite (1822–1901).

(a) For all complex numbers t and x,

$$\mathrm{e}^{-t^2+2xt} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}.$$

Therefore, the function $(t,x) \mapsto \mathrm{e}^{-t^2+2xt}$ is called the generating function of the Hermite polynomials.

(b) The polynomial H_n of nth degree has precisely n real zeros. These zeros are simple.

(c) First recursive formula:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \qquad x \in \mathbb{R}.$$

(d) $H_{2n+1}(0) = 0$, and $H_{2n}(0) = (-1)^n \cdot 2^n \cdot 1 \cdot 3 \cdot 5 \cdots (2n-1)$.

(e) $H_n(x) = 2^n x^n + a_{n-1}x^{n-1} + \ldots + a_1 x + 1$ for all $x \in \mathbb{R}$.

(f) Second recursive formula:

$$H_n(x) = H_n(0) + 2n\int_0^x H_{n-1}(y)dy, \qquad x \in \mathbb{R}.$$

(g) The Hermite functions $\psi_0, \psi_1, \ldots$ form a complete orthonormal system in the complex Hilbert space $L_2(\mathbb{R})$.

(h) $a^\dagger \psi_n = \sqrt{n+1}\ \psi_n$ for $n = 0, 1, 2, \ldots$

(j) $\psi_n = \varphi_n$ for $n = 0, 1, 2\ldots$

(k) $x^2\psi_n(x) - \psi_n''(x) = (2n+1)\psi_n(x)$ for all $x \in \mathbb{R}$.

Let us prove this.

Ad (a). By the Cauchy formula,

$$f^{(n)}(x) = \frac{n!}{2\pi\mathrm{i}}\int_C \frac{f(z)}{(z-x)^{n+1}}\,dz, \qquad x \in \mathbb{C}.$$

Here, we assume that the function f is holomorphic on the complex plane $\mathbb{C}$. Moreover, C is a counter-clockwise oriented circle centered at the point x. Hence

$$(-1)^n \mathrm{e}^{-x^2} H_n(x) = \frac{n!}{2\pi\mathrm{i}}\int_C \frac{\mathrm{e}^{-z^2}}{(z-x)^{n+1}}\,dz.$$

Substituting $z = t + x$,

$$H_n(x) = \frac{n!}{2\pi\mathrm{i}}\int_{C_0} \frac{\mathrm{e}^{-t^2+2tx}}{t^{n+1}}\,dt.$$

Here, the circle C_0 is centered at the origin. Using again the Cauchy formula along with Taylor expansion, we get the claim (a).

Ad (b). The proof will be given in Problem 7.26.

Ad (c). Differentiate relation (a) with respect to t, and use comparison of coefficients.

Ad (d). Use an induction argument based on (c).

Ad (e). Use the definition (7.7) of H_n along with an induction argument.

Ad (f). Differentiate relation (a) by x, and use comparison of coefficients. Then, $H_n' = 2nH_{n-1}$.

Ad (g). The proof can be found in Zeidler (1995a), p. 210 (see the references on page 1049).

Ad (h). Use the definition of ψ_n and the relation $\sqrt{2}\, a^\dagger = x - \frac{d}{dx}$.

Ad (j). Obviously, $\varphi_0 = \psi_0$. By (h), both ψ_1 and φ_1 are generated from φ_0 the same way. Hence $\varphi_1 = \psi_1$. Similarly, $\varphi_2 = \psi_2$, and so on.

Ad (k). This follows from $a^\dagger a \varphi_n = n\varphi_n$ together with $\varphi_n = \psi_n$ and

$$a^\dagger a \psi_n = \frac{1}{2}\left(x - \frac{d}{dx}\right)\left(x + \frac{d}{dx}\right)\psi_n.$$

□

The normal product. Let $n = 1, 2, \ldots$. Again choose $x_0 := 1$. Consider

$$Q^n = \frac{1}{\sqrt{2^n}}\,(a + a^\dagger)^n = \frac{1}{\sqrt{2^n}}(a + a^\dagger)\cdots(a + a^\dagger).$$

This is a polynomial with respect to a and $a^\dagger$. By definition, the normal product $: Q^n :$ is obtained from Q^n by rearranging the factors in such a way that $a^\dagger$ (resp. a) stands left (resp. right). Explicitly, by the binomial formula,

$$\boxed{: Q^n := \frac{1}{\sqrt{2^n}} \sum_{k=0}^{n} \binom{n}{k} (a^\dagger)^k a^{n-k}.}$$

We get the key relation

$$\langle \varphi_0 | : Q^n : \varphi_0 \rangle = 0, \qquad n = 1, 2, \ldots,$$

telling us that the vacuum expectation value of the normal product is equal to zero. This follows from $a\varphi_0 = 0$, which implies $\langle \varphi_0 | \ldots a\varphi_0 \rangle = 0$ together with $\langle \varphi_0 | a^\dagger \ldots \rangle = \langle a\varphi_0 | \ldots \rangle = 0$. Finally, we set $: Q^0 := I$ if $n = 0$.

For example, $Q^2 = \frac{1}{2}(a + a^\dagger)(a + a^\dagger)$ is equal to $\frac{1}{2}(a^2 + aa^\dagger + a^\dagger a + (a^\dagger)^2)$. Hence

$$: Q^2 := \tfrac{1}{2}a^2 + a^\dagger a + \tfrac{1}{2}(a^\dagger)^2.$$

This implies $: Q^2 : \psi = (x^2 - \frac{1}{2})\psi$. Hence $: Q^2 := x^2 - \frac{1}{2}$. It turns out that $Q^n = x^n + \ldots$ is a polynomial of degree n. Explicitly,

$$\boxed{: Q^n := \frac{H_n(x)}{2^n}, \qquad n = 0, 1, 2, \ldots.}$$

For the proof, we refer to Problem 7.27.

Coherent states. For each complex number α, we define

$$\boxed{\varphi_\alpha := \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\, \varphi_n.} \tag{7.9}$$

By the Parseval equation,

$$||\varphi_\alpha||^2 = \mathrm{e}^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} = 1 \qquad \text{for all} \quad \alpha \in \mathbb{C}.$$

Therefore, the infinite series (7.9) is convergent in the Hilbert space $L_2(\mathbb{R})$. On page 478, we will prove that

$$a\varphi_\alpha = \alpha\varphi_\alpha \qquad \text{for all} \quad \alpha \in \mathbb{C}. \tag{7.10}$$

This tells us that the so-called coherent state φ_α is an eigenstate of the annihilation operator a. There exists a continuous family $\{\varphi_\alpha\}_{\alpha\in\mathbb{C}}$ of eigenstates of the operator a. In terms of physics, the coherent state φ_α is the superposition of states $\varphi_0, \varphi_1, \varphi_2, \ldots$ with the fixed particle number $0, 1, 2, \ldots$, respectively, and it is stable under particle annihilation, by (7.10).

Coherent states are frequently used as a nice tool for studying special physical situations in quantum optics, quantum statistics, and quantum field theory (e.g., the mathematical modelling of laser beams).

A finite family of bosonic creation and annihilation operators. The normal product and the following considerations are crucial for quantum field theory. Let $n = 1, 2, ..$ On the complex Hilbert space $L_2(\mathbb{R}^n)$ equipped with the inner product[13]

$$\langle\varphi|\psi\rangle := \int_{\mathbb{R}^n} \varphi(x)^\dagger \psi(x) dx$$

for all $\varphi, \psi \in L_2(\mathbb{R}^n)$, we define the operators

$$a_j, a_j^\dagger : \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n), \qquad j = 1, ..., n$$

given by

$$a_j := \frac{1}{\sqrt{2}} \left(x_j + \frac{\partial}{\partial x_j} \right), \qquad a_j^\dagger := \frac{1}{\sqrt{2}} \left(x_j - \frac{\partial}{\partial x_j} \right).$$

Explicitly, for all functions $\psi \in \mathcal{S}(\mathbb{R}^n)$,

$$(a_j\psi)(x) := \frac{1}{\sqrt{2}} \left(x_j \psi(x) + \frac{\partial \psi(x)}{\partial x_j} \right), \qquad x \in \mathbb{R}^n.$$

For all functions $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$, we have

$$\langle\varphi|a_j\psi\rangle = \langle a_j^\dagger \varphi|\psi\rangle, \qquad j = 1, ..., n,$$

that is, the operator $a_j^\dagger$ is the formally adjoint operator to the operator a_j on $\mathcal{S}(\mathbb{R}^n)$. For $j, k = 1, ..., n$, we have the following commutation relations

$$\boxed{[a_j, a_k^\dagger]_- = \delta_{jk} I,} \tag{7.11}$$

and

$$\boxed{[a_j, a_k]_- = [a_j^\dagger, a_k^\dagger]_- = 0.} \tag{7.12}$$

A special role is played by the state

$$\varphi_0(x) := c_0 \mathrm{e}^{-x^2}, \qquad x \in \mathbb{R}^n$$

with $x^2 := x_1^2 + ... + x_n^2$ and the normalization constant $c_0 := \pi^{-n/4}$. Then

$$\langle\varphi_0|\varphi_0\rangle = \int_{\mathbb{R}^n} \frac{\mathrm{e}^{-\frac{1}{2}x_1^2 - ... - \frac{1}{2}x_n^2}}{(\sqrt{\pi})^n} \, dx_1 \cdots dx_n = \left(\int_{\mathbb{R}} \frac{\mathrm{e}^{-\frac{1}{2}y^2}}{\sqrt{\pi}} \, dy \right)^n = 1.$$

[13] The definition of the spaces $\mathcal{S}(\mathbb{R}^n)$ and $L_2(\mathbb{R}^n)$ can be found in Vol. I, Sects. 2.7.4 and 10.2.4, respectively.

The operator $N : \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n)$ given by

$$N := \sum_{j=1}^{n} a_j^\dagger a_j$$

has the eigensolutions

$$\boxed{N|k_1 k_2 \dots k_n\rangle = (k_1 + k_2 + ... + k_n)|k_1 k_2 ... k_n\rangle} \tag{7.13}$$

with $k_1, k_2, \dots, k_n = 0, 1, 2, \dots$ Here, we set

$$|k_1 k_2 \dots k_n\rangle := \frac{(a_1^\dagger)^{k_1}}{\sqrt{k_1!}} \frac{(a^\dagger)^{k_2}}{\sqrt{k_2!}} \cdots \frac{(a^\dagger)^{k_n}}{\sqrt{k_n!}} \varphi_0.$$

The system of states $|k_1 k_2 \dots k_n\rangle$ forms a complete orthonormal system in the complex Hilbert space $L_2(\mathbb{R}^n)$. The operator N is formally self-adjoint, that is,

$$\langle \varphi | N\psi \rangle = \langle N\varphi | \psi \rangle \qquad \text{for all} \quad \varphi, \psi \in \mathcal{S}(\mathbb{R}^n).$$

The proofs for the claims above proceed analogously as for the operators a and $a^\dagger$. We use the following terminology. There are n types of elementary particles called bosons.

- The state $|k_1 k_2 \dots k_n\rangle$ corresponds to k_1 bosons of type 1, k_2 bosons of type 2,..., and k_n bosons of type n.
- The operator $a_j^\dagger$ is called the creation operator for bosons of type j.
- The operator a_j is called the annihilation operator for bosons of type j.
- The operator N is called the particle number operator.
- Since $N\varphi_0 = 0$, the state φ_0 is called the (normalized) vacuum state. Instead of φ_0, physicists also write $|0\rangle$.

7.3 Heisenberg's Quantum Mechanics

> Quantum mechanics was born on December 14, 1900, when Max Planck delivered his famous lecture before the German Physical Society in Berlin which was printed afterwards under the title "On the law of energy distribution in the normal spectrum." In this paper, Planck assumed that the emission and absorption of radiation always takes place in discrete portions of energy or *energy quanta* $h\nu$, where ν is the frequency of the emitted or absorbed radiation. Starting with this assumption, Planck arrived at his famous formula
>
> $$\varrho = \frac{\alpha \nu^3}{\mathrm{e}^{h\nu/kT} - 1}$$
>
> for the energy density ϱ of black-body radiation at temperature T.[14]
>
> Barthel Leendert van der Waerden, 1967

[14] B. van der Waerden, Sources of Quantum Mechanics, North-Holland, Amsterdam, 1967 (reprinted with permission).

> The present paper seeks to establish a basis for theoretical quantum mechanics founded exclusively upon relationships between quantities which in principle are observable.[15]
>
> Werner Heisenberg, 1925

> The recently published theoretical approach of Heisenberg is here developed into a systematic theory of quantum mechanics with the aid of mathematical *matrix theory*. After a brief survey of the latter, the mechanical equations of motions are derived from a variational principle and it is shown that using Heisenberg's quantum condition, the principle of energy conservation and Bohr's frequency condition follow from the mechanical equations. Using the anharmonic oscillator as example, the question of uniqueness of the solution and of the significance of the phases of the partial vibrations is raised. The paper concludes with an attempt to incorporate electromagnetic field laws into the new theory.[16]
>
> Max Born and Pascal Jordan, 1925

There exist three different, but equivalent approaches to quantum mechanics, namely,

(i) Heisenberg's particle quantization from the year 1925 and its refinement by Born, Dirac, and Jordan in 1926,
(ii) Schrödinger's wave quantization from 1926, and
(iii) Feynman's statistics over classical paths via path integral from 1942.

In what follows we will thoroughly discuss these three approaches in terms of the harmonic oscillator. Let us start with (i).

The classical harmonic oscillator. Recall that the differential equation

$$\ddot{q}(t) + \omega^2 q(t) = 0, \qquad t \in \mathbb{R} \tag{7.14}$$

describes the motion $q = q(t)$ of a point of mass m on the real line which oscillates with the positive angular frequency ω. We add the initial condition $q(0) = q_0$ and $\dot{q}(0) = v_0$. Let us introduce the momentum $p := m\dot{q}$ and the Hamiltonian

$$H(q,p) := \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}$$

which represents the energy of the particle. Recall that the equation of motion (7.14) is equivalent to the canonical equations $\dot{p} = -H_q, \dot{q} = H_q$. Explicitly,

$$\dot{p}(t) = -m\omega^2 q(t), \qquad m\dot{q}(t) = p(t), \qquad t \in \mathbb{R},$$

along with the initial conditions $q(0) = q_0$ and $p(0) = p_0$. Note that $p_0 = mv_0$ where v_0 is the initial velocity of the particle. Let us introduce the typical length scale

$$x_0 := \sqrt{\frac{\hbar}{m\omega}}$$

which can be formed by using the parameters m, ω and $\hbar$. Let a be an arbitrary complex number. The general solution of (7.14) is given by

[15] W. Heisenberg, Quantum-theoretical re-interpretation of kinematic and mechanical relations, Z. Physik **33** (1925), 879–893 (in German).
[16] M. Born and P. Jordan, On Quantum Mechanics, Z. Physik **34** (1925), 858–888 (in German).

$$\boxed{q(t) = \frac{x_0}{\sqrt{2}}\,(a^\dagger \mathrm{e}^{\mathrm{i}\omega t} + a\mathrm{e}^{-\mathrm{i}\omega}), \qquad t \in \mathbb{R}.} \tag{7.15}$$

For the momentum, we get

$$\boxed{p(t) = m\dot{q}(t) = \frac{\mathrm{i}\hbar}{x_0\sqrt{2}}\,(a^\dagger \mathrm{e}^{\mathrm{i}\omega t} - a\mathrm{e}^{-\mathrm{i}\omega}), \qquad t \in \mathbb{R}.}$$

Letting $t = 0$, we obtain

$$a = \frac{1}{\sqrt{2}}\left(\frac{q(0)}{x_0} + \frac{\mathrm{i}x_0 p(0)}{\hbar}\right)$$

for the relation between the Fourier coefficient a and the real initial values $q(0)$ and $p(0)$. Hence, for the conjugate complex Fourier coefficient,

$$a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{q(0)}{x_0} - \frac{\mathrm{i}x_0 p(0)}{\hbar}\right).$$

For the Hamiltonian,

$$H(q(t), p(t)) = \hbar\omega(a^\dagger a + \tfrac{1}{2}), \qquad t \in \mathbb{R}.$$

This expression does not depend on time t which reflects conservation of energy for the motion of the harmonic oscillator. Note that

$$q(t)^\dagger = q(t), \qquad p(t)^\dagger = p(t) \qquad \text{for all} \quad t \in \mathbb{R},$$

and that $a, a^\dagger$ are dimensionless. In quantum mechanics, this classical reality condition will be replaced by the formal self-adjointness of the operators $q(t)$ and $p(t)$.

The classical uncertainty relation. The motion $q = q(t)$ has the time period $T = 2\pi/\omega$. Let us now study the time means of the classical motion. For a T-periodic function $f : \mathbb{R} \to \mathbb{R}$, we define the mean value

$$\bar{f} = \frac{1}{T}\int_{-T/2}^{T/2} f(t)dt,$$

and the mean fluctuation Δf by

$$(\Delta f)^2 = \overline{(f - \bar{f})^2} = \frac{1}{T}\int_{-T/2}^{T/2} (f(t) - \bar{f})^2 dt.$$

To simplify computations, let us restrict ourselves to the special case where the initial velocity of the particle vanishes, $p_0 = 0$. Then we get the energy $E = m\omega^2 q(0)^2/2$, along with[17]

$$\bar{q} = \bar{p} = 0, \qquad \Delta p = m\omega\Delta q, \qquad \Delta q = \sqrt{\frac{E}{m\omega^2}}.$$

This implies the so-called classical uncertainty relation:

$$\boxed{\Delta q \Delta p = \frac{E}{\omega}.} \tag{7.16}$$

[17] Note that $\int_{-T/2}^{T/2} \mathrm{e}^{\mathrm{i}k\omega t}dt = \int_{-T/2}^{T/2} \mathrm{e}^{\mathrm{i}2\pi kt/T}dt = 0$ if $k = 1, 2, \ldots$

Poisson brackets. In order to quantize the classical harmonic oscillator, it is convenient to write the classical equation of motion in terms of Poisson brackets. Recall that

$$\{A(q,p), B(q,p)\} := \frac{\partial A(q,p)}{\partial q}\frac{\partial B(q,p)}{\partial p} - \frac{\partial B(q,p)}{\partial q}\frac{\partial A(q,p)}{\partial p}.$$

For example, $\{q,p\} := 1$, $\{q,H\} = H_p = p/m$, and $\{p,H\} = -H_q = -m\omega^2 q$. Thus, for all times $t \in \mathbb{R}$, the equations of motion for the harmonic oscillator read as

$$\dot{q}(t) = \{q(t), H(q(t),p(t))\}, \qquad \dot{p}(t) = \{p(t), H(q(t)), p(t)\}, \tag{7.17}$$

together with $\{q(t), p(t)\} = 1$.

7.3.1 Heisenberg's Equation of Motion

> In a recent paper, Heisenberg puts forward a new theory which suggests that it is not the equations of classical mechanics that are in any way at fault, but that the mathematical operations by which physical results are deduced from them require modification. All the information supplied by the classical theory can thus be made use of in the new theory ... We make the fundamental assumption that the difference between the Heisenberg products is equal to $\mathrm{i}\hbar$ times their Poison bracket
>
> $$xy - yx = \mathrm{i}\hbar\{x,y\}. \tag{7.18}$$
>
> It seems reasonable to take (7.18) as constituting the general quantum conditions.[18]
>
> Paul Dirac, 1925

The general quantization principle. We are looking for a simple principle which allows us to pass from classical mechanics to quantum mechanics. This principle reads as follows:

- position $q(t)$ and momentum $p(t)$ of the particle at time t become operators,
- and Poisson brackets are replaced by Lie brackets,

$$\{A(q,p), B(q,p)\} \quad \Rightarrow \quad \frac{1}{\mathrm{i}\hbar}\,[A(q,p), B(q,p)]_-.$$

Recall that $[A,B]_- := AB - BA$. Using this quantization principle, the classical equation of motion (7.17) passes over to the equation of motion for the quantum harmonic oscillator

$$\boxed{\begin{aligned} \mathrm{i}\hbar\dot{q}(t) &= [q(t), H(q(t),p(t))]_-, \\ \mathrm{i}\hbar\dot{p}(t) &= [p(t), H(q(t),p(t))]_- \end{aligned}} \tag{7.19}$$

together with

[18] P. Dirac, The fundamental equations of quantum mechanics, Proc. Royal Soc. London Ser. A **109** (1925), no. 752, 642–653.
A far-reaching generalization of Dirac's principle to the quantization of general Poisson structures was proven by Kontsevich. In 1998, he was awarded the Fields medal for this (see the papers by Kontsevich (2003) and by Cattaneo and Felder (2000) quoted on page 676).

$$\boxed{[q(t), p(t)]_- = \mathrm{i}\hbar I.} \tag{7.20}$$

The latter equation is called the Heisenberg–Born–Jordan commutation relation.

The method of Fourier quantization. In order to solve the equations of motion (7.19), (7.20), we use the classical solution formula

$$\begin{aligned} q(t) &= \frac{x_0}{\sqrt{2}}\,(a^\dagger \mathrm{e}^{\mathrm{i}\omega t} + a\mathrm{e}^{-\mathrm{i}\omega t}),\\ p(t) &= m\dot{q}(t) = \frac{\mathrm{i}\hbar}{x_0\sqrt{2}}\,(a^\dagger \mathrm{e}^{\mathrm{i}\omega t} - a\mathrm{e}^{-\mathrm{i}\omega t}) \end{aligned} \tag{7.21}$$

for all times $t \in \mathbb{R}$. But we replace the classical Fourier coefficients a and $a^\dagger$ by operators a and $a^\dagger$ which satisfy the commutation relation

$$\boxed{[a, a^\dagger]_- = I.}$$

These operators can be found in Sect. 7.2. Let us check that indeed we obtain a solution. First of all note that

$$\begin{aligned} [q(t), p(t)]_- &= \tfrac{1}{2}\mathrm{i}\hbar[a^\dagger \mathrm{e}^{\mathrm{i}\omega t} + a\mathrm{e}^{-\mathrm{i}\omega t}, a^\dagger \mathrm{e}^{\mathrm{i}\omega t} - a\mathrm{e}^{-\mathrm{i}\omega t}]_-\\ &= \tfrac{1}{2}\mathrm{i}\hbar([a, a^\dagger]_- - [a^\dagger, a]_-) = \mathrm{i}\hbar[a, a^\dagger]_- = \mathrm{i}\hbar I. \end{aligned}$$

As in the classical case, one checks easily that

$$m\dot{q}(t) = p(t), \qquad \dot{p}(t) = -m\omega^2 q(t).$$

Moreover, it follows from $[q, p]_- = \mathrm{i}\hbar$ that

$$[q, p^2]_- = ([q, p]_-)p + p[q, p]_- = 2\mathrm{i}\hbar p.$$

Similarly, for $n = 1, 2, ...,$

$$[q, p^n]_- = \mathrm{i}\hbar n p^{n-1}, \qquad [p, q^n]_- = -\mathrm{i}\hbar n q^{n-1},$$

by induction. Hence

$$2m[q(t), H(q(t), p(t))]_- = [q(t), p(t)^2]_- = 2\mathrm{i}\hbar p(t) = 2m\mathrm{i}\hbar\dot{q}(t).$$

This is the first equation of motion. Similarly, we get the second equation of motion

$$[p(t), H(q(t), p(t))]_- = \tfrac{1}{2}[p(t), m\omega^2 q^2(t)]_- = -\mathrm{i}\hbar m\omega^2 q(t) = \mathrm{i}\hbar\dot{p}(t).$$

For the Hamiltonian, it follows from $[a, a^\dagger]_- = I$ that

$$H(q(t), p(t)) = \hbar\omega(a^\dagger a + \tfrac{1}{2}). \tag{7.22}$$

Matrix elements. Let us use the results from Sect. 7.2. Recall that the states

$$\varphi_n := \frac{(a^\dagger)^n}{\sqrt{n!}}\,\varphi_0, \qquad n = 0, 1, 2, ...$$

form a complete orthonormal system of the complex Hilbert space $L_2(\mathbb{R})$. In addition, $\varphi_n \in \mathcal{S}(\mathbb{R})$ for all n. For the physical interpretation of Heisenberg's quantum

mechanics, infinite-dimensional matrices play a crucial role. Let us discuss this. We assign to each linear operator $A : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ the matrix elements

$$A_{mn} := \langle \varphi_m | A\varphi_n \rangle, \qquad m, n = 0, 1, 2, \dots$$

For two linear formally self-adjoint operators $A, B : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$, we get the product rule

$$\boxed{(AB)_{mn} = \sum_{k=0}^{\infty} A_{mk} B_{kn}, \qquad m, n = 0, 1, 2, \dots} \tag{7.23}$$

In fact, by the Parseval equation (7.2), this follows from

$$\langle \varphi_m | AB\varphi_n \rangle = \langle A\varphi_m | B\varphi_n \rangle = \sum_{k=0}^{\infty} \langle A\varphi_m | \varphi_k \rangle \langle \varphi_k | B\varphi_n \rangle$$

along with $\langle A\varphi_m | \varphi_k \rangle = \langle \varphi_m | A\varphi_k \rangle$.

Examples. Let us now compute the matrix elements of $H, q(t)$, and $p(t)$. It follows from $N\varphi_n = n\varphi_n$ that

$$H\varphi_n = \hbar\omega(N + \tfrac{1}{2}I)\varphi_n = \hbar\omega(n + \tfrac{1}{2})\varphi_n.$$

Hence $H_{mn} = \langle \varphi_m | H\varphi_n \rangle = E_n \langle \varphi_m | \varphi_n \rangle = E_n \delta_{nm}$ with $E_n = \hbar\omega(n + \frac{1}{2})$. This yields the diagonal matrix

$$(H_{mn}) = \begin{pmatrix} E_0 & 0 & 0 & 0 & \dots \\ 0 & E_1 & 0 & 0 & \dots \\ \vdots & & & & \end{pmatrix}.$$

It follows from Sect. 7.2 that $a_{kn} = \sqrt{n}\, \delta_{k,n-1}$. Thus, by (7.21),

$$q_{kn}(t) = \frac{x_0}{\sqrt{2}} \left(a_{nk} \mathrm{e}^{\mathrm{i}\omega t} + a_{kn} \mathrm{e}^{-\mathrm{i}\omega t} \right). \tag{7.24}$$

This way, we get the self-adjoint matrix

$$(q_{kn}(t)) = \frac{x_0}{\sqrt{2}} \begin{pmatrix} 0 & \sqrt{1}\, \mathrm{e}^{-\mathrm{i}\omega t} & 0 & 0 & \dots \\ \sqrt{1}\, \mathrm{e}^{\mathrm{i}\omega t} & 0 & \sqrt{2}\, \mathrm{e}^{-\mathrm{i}\omega t} & 0 & \dots \\ 0 & \sqrt{2}\, \mathrm{e}^{\mathrm{i}\omega t} & 0 & 0 & \dots \\ \vdots & & & & \end{pmatrix}$$

for all times $t \in \mathbb{R}$. Similarly,

$$p_{kn}(t) = m\dot{q}_{kn}(t), \qquad k, n = 0, 1, 2, \dots$$

By the product rule (7.23), for the square of the position matrix (q_{kn}) we get

$$(q_{kn})^2 = \frac{x_0^2}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 3 & 0 & 0 & \dots \\ 0 & 0 & 5 & 0 & \dots \\ \vdots & & & & \end{pmatrix}. \tag{7.25}$$

Similarly,

$$(p_{kn})^2 = \frac{\hbar^2}{2x_0^2} \begin{pmatrix} 1\ 0\ 0\ 0\ \dots \\ 0\ 3\ 0\ 0\ \dots \\ 0\ 0\ 5\ 0\ \dots \\ \vdots \end{pmatrix}.$$

7.3.2 Heisenberg's Uncertainty Inequality for the Harmonic Oscillator

In order to discuss the physical meaning of the matrices introduced above, we will use the following terminology:

- The elements ψ of the complex Hilbert space $L_2(\mathbb{R})$ normalized by the condition $\langle\psi|\psi\rangle = 1$ are called normalized states of the quantum harmonic oscillator,
- whereas the linear, formally self-adjoint operators $A : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ are called formal observables.

Two normalized states ψ and φ are called equivalent iff

$$\varphi = \mathrm{e}^{\mathrm{i}\alpha}\psi$$

for some real number α. We say that φ and ψ differ by phase. Consider some normalized state ψ and some formal observable A. The number

$$\bar{A} := \langle\psi|A\psi\rangle$$

is interpreted as the mean value of the observable A measured in the state ψ.[19] Moreover, the nonnegative number ΔA given by

$$(\Delta A)^2 := \langle\psi|(A - \bar{A})^2\psi\rangle$$

is interpreted as the fluctuation of the measured mean value $\bar{A}$. Let us choose $n = 0, 1, 2, \dots$ For the state φ_n of the quantum harmonic oscillator, we get the following measured values for all times $t \in \mathbb{R}$.

(i) Energy: $\bar{E} = E_n = \hbar\omega(n + \frac{1}{2})$ and $\Delta E = 0$.

(ii) Position: $\bar{q}(t) = q_{nn}(t) = 0$ and $\Delta q(t) = x_0\sqrt{n + \frac{1}{2}}$.

(iii) Momentum: $\bar{p}(t) = p_{nn}(t) = 0$ and $\Delta p(t) = \frac{\hbar}{x_0}\sqrt{n + \frac{1}{2}}$.

(iv) Heisenberg's uncertainty inequality:

$$\boxed{\Delta q(t)\Delta p(t) \geq \frac{\hbar}{2}.}$$

Let us prove this.

Ad (i). For the energy, it follows from the eigensolution $H\varphi_n = E_n\varphi_n$ that

$$\bar{E} = \langle\varphi_n|H\varphi_n\rangle = E_n\langle\varphi_n|\varphi_n\rangle = E_n,$$

and $\Delta E = ||(H - E_n I)\varphi_n|| = 0$.

[19] Since the operator A is formally self-adjoint, the number $\bar{A}$ is real. Furthermore, note that $\langle\psi|(A - \bar{A})^2\psi\rangle = \langle(A - \bar{A})\psi|(A - \bar{A})\psi\rangle = ||(A - \bar{A}I)\psi||^2 \geq 0$.

Ad (ii). Note that

$$(\Delta q)^2 = \langle \varphi_n | q(t)^2 \varphi_n \rangle.$$

Therefore, $(\Delta q)^2$ is the nth diagonal element of the product matrix $(q_{kn})^2$ which can be found in (7.25). Analogously, we get (iii). The uncertainty inequality is an immediate consequence of (ii) and (iii). □

The famous Heisenberg uncertainty inequality for the quantum harmonic oscillator tells us that the state φ_n has the sharp energy E_n, but it is impossible to measure sharply both position and momentum of the quantum particle at the same time. Thus, there exists a substantial difference between classical particles and quantum particles.

It is impossible to speak of the trajectory of a quantum particle.

7.3.3 Quantization of Energy

> I have the best of reasons for being an admirer of Werner Heisenberg. He and I were young research students at the same time, about the same age, working on the same problem. Heisenberg succeeded where I failed... Heisenberg - a graduate student of Sommerfeld - was working from the experimental basis, using the results of spectroscopy, which by 1925 had accumulated an enormous amount of data[20]...
>
> Paul Dirac, 1968

The measured spectrum of an atom or a molecule is characterized by two quantities, namely,

- the wave length λ_{nm} of the emitted spectral lines (where $n, m = 0, 1, 2, \ldots$ with $n > m$), and
- the intensity of the spectral lines.

In Bohr's and Sommerfeld's semi-classical approach to the spectra of atoms and molecules from the years 1913 and 1916, respectively, the spectral lines correspond to photons which are emitted by jumps of an electron from one orbit of the atom or molecule to another orbit. If $E_0 < E_1 < E_2 < \ldots$ are the (discrete) energies of the electron corresponding to the different orbits, then a jump of the electron from the higher energy level E_n to the lower energy level E_m produces the emission of one photon of energy $E_n - E_m$. According to Einstein's light quanta hypothesis from 1905, this yields the frequency

$$\nu_{nm} = \frac{E_n - E_m}{h}, \qquad n > m \tag{7.26}$$

of the emitted photon, and hence the wave length $\lambda_{nm} = c/\nu_{nm}$ of the corresponding spectral line is obtained. The intensity of the spectral lines depends on the transition probabilities for the jumps of the electrons. In 1925 it was Heisenberg's philosophy to base his new quantum mechanics only on quantities which can be measured in physical experiments, namely,

- the energies $E_0, E_1, \ldots$ of bound states and

[20] In: A. Salam (Ed.), From a Life of Physics. Evening Lectures at the International Center for Theoretical Physics, Trieste (Italy), with outstanding contributions by Abdus Salam, Hans Bethe, Paul Dirac, Werner Heisenberg, Eugene Wigner, Oscar Klein, and Eugen Lifshitz, International Atomic Energy Agency, Vienna, Austria, 1968.
A. Sommerfeld, Atomic Structure and Spectral Lines, Methuen, London, 1923.

- the transition probabilities for changing bound states.[21]

Explicitly, Heisenberg replaced the trajectory $q = q(t), t \in \mathbb{R}$ of a particle in classical mechanics by the following family $(q_{nm}(t))$ of functions

$$q_{nm}(t) = q_{nm}(0)\mathrm{e}^{\mathrm{i}\omega_{nm}t}, \qquad n, m = 0, 1, 2, \ldots$$

where $\omega_{nm} = 2\pi\nu_{nm}$, and the frequencies ν_{nm} are given by (7.26). It follows from (7.26) that

$$\nu_{nk} + \nu_{km} = \nu_{nm}, \qquad n < k < m.$$

In physics, this is called the Ritz combination principle for frequencies.[22] In terms of mathematics, this tells us that the family $\{\nu_{nm}\}$ of frequencies represents a cocycle generated by the family $\{E_n\}$ of energies. Thus, this approach is based on a simple variant of cohomology.[23] In order to compute the intensities of spectral lines, Heisenberg was looking for a suitable quadratic expression in the amplitudes $q_{nm}(0)$. Using physical arguments and analogies with the product formula for Fourier series expansions, Heisenberg invented the composition rule

$$(q^2(0))_{nm} := \sum_{k=0}^{\infty} q_{nk}(0)q_{km}(0) \tag{7.27}$$

for defining the square $(q_{nm}(0))^2$ of the scheme $(q_{nm}(0))$. Applying this to the harmonic oscillator (and the anharmonic oscillator as a perturbed harmonic oscillator), Heisenberg obtained the energies

$$E_n = \omega\hbar(n + \tfrac{1}{2}), \qquad n = 0, 1, 2, \ldots$$

for the quantized harmonic oscillator.

After getting Heisenberg's manuscript, Born (1882–1970) noticed that the composition rule (7.27) resembled the product for matrices $q(t) = (q_{nm}(t))$, which he learned as a student in the mathematics course. He guessed the validity of the rule

$$qp - pq = \mathrm{i}\hbar. \tag{7.28}$$

But he was only able to verify this for the diagonal elements. After a few days of joint work with his pupil Pascal Jordan (1902–1980), Born finished a joint paper with Jordan on the new quantum mechanics including the commutation rule (7.28); nowadays this is called the Heisenberg–Born–Jordan commutation rule (or briefly the Heisenberg commutation rule). At that time, Heisenberg was not in Göttingen, but on the island Helgoland (North Sea) in order to cure a severe attack of hay fever. After coming back to Göttingen, Heisenberg wrote together with Born and Jordan a fundamental paper on the principles of quantum mechanics. The English translation of the following three papers can be found in van der Waerden (1968):

[21] Heisenberg's thinking was strongly influenced by the Greek philosopher Plato (428–347 B.C.). Nowadays one uses the Latin version 'Plato'. The correct Greek name is 'Platon'. Plato's Academy in Athens had unparalleled importance for Greek thought. The greatest philosophers, mathematicians, and astronomers worked there. For example, Aristotle (384–322 B.C.) studied there. In 529 A.D., the Academy was closed by the Roman emperor Justitian.

[22] Ritz (1878–1909) worked in Göttingen.

[23] The importance of cohomology for classical and quantum physics will be studied in Vol. IV on quantum mathematics.

W. Heisenberg, Quantum-theoretical re-interpretation of kinematics and mechanical relations), Z. Physik **33** (1925), 879–893.

M. Born, P. Jordan, On quantum mechanics, Z. Physik **35** (1925), 858–888.

M. Born, W. Heisenberg, and P. Jordan, On quantum mechanics II, Z. Physik **36** (1926), 557–523.

At the same time, Dirac formulated his general approach to quantum mechanics:

P. Dirac, The fundamental equations of quantum mechanics, Proc. Royal Soc. London Ser. A **109** (1926), no. 752, 642–653.

Heisenberg, himself, pointed out the following at the *Trieste Evening Lectures* in 1968:

> It turned out that one could replace the quantum conditions of Bohr's theory by a formula which was essentially equivalent to the sum-rule in spectroscopy by Thomas and Kuhn... I was however not able to get a neat mathematical scheme out of it. Very soon afterwards both Born and Jordan in Göttingen and Dirac in Cambridge were able to invent a perfectly closed mathematical scheme: Dirac with very ingenious new methods on abstract noncommutative q-numbers (i.e., quantum-theoretical numbers), and Born and Jordan with more conventional methods of matrices.

7.3.4 The Transition Probabilities

Let us discuss the meaning of the entries q_{kn} of the position matrix on page 445. Suppose that the quantum particle is an electron of electric charge $-e$ and mass m. Let ε_0 and c be the electric field constant and the velocity of light of a vacuum, respectively. Furthermore, let h be the Planck action quantum, and set $\hbar := h/2\pi$.[24] According to Heisenberg, the real number

$$\boxed{\gamma_{kn} := \frac{\omega_{kn}^3 e^2 (t_2 - t_1)}{3\pi\varepsilon_0 \hbar c^3} \, |q_{kn}(0)|^2, \qquad n, k = 0, 1, 2, \ldots, n \neq k} \tag{7.29}$$

is the transition probability for the quantum particle to pass from the state φ_k to the state φ_n during the time interval $[t_1, t_2]$. Here, $\omega_{kn} := (E_k - E_n)/\hbar$. This will be motivated below. Note that $\gamma_{kn} = \gamma_{nk}$. Explicitly,

$$\gamma_{kn} := \frac{\omega^2 e^2 (t_2 - t_1)}{6\pi\varepsilon_0 c^3 m} \, (n\delta_{k,n-1} + k\delta_{n,k-1}).$$

This means the following.

- Forbidden spectral lines: The transition of the quantum particle from the state φ_n of energy E_n to the state φ_k of energy E_k is forbidden, i.e., $\gamma_{kn} = 0$, if the energy difference $E_n - E_k$ is equal to $\pm 2\hbar\omega, \pm 3\hbar\omega, \ldots$
- Emission of radiation: The transition probability from the energy E_{n+1} to the energy E_n during the time interval $[t_1, t_2]$ is equal to

$$\gamma_{n+1,n} = \frac{\omega^2 e^2 (t_2 - t_1)}{6\pi\varepsilon_0 c^3 m} \, (n+1), \qquad n = 0, 1, 2, \ldots \tag{7.30}$$

  In this case, a photon of energy $E = \hbar\omega$ is emitted. The meaning of transition probability is the following. Suppose that we have $\mathcal{N}$ oscillating electrons in the

[24] The numerical values can be found on page 949 of Vol. I.

state φ_n. Then the number of electrons which jump to the state φ_{n+1} during the time interval $[t_1, t-2]$ is equal to $\mathcal{N}\gamma_{n,n+1}$. Then the emitted mean energy E, which passes through a sufficiently large sphere during the time interval $[t_1, t_2]$, is equal to

$$E = \mathcal{N}\gamma_{n+1,n} \cdot \hbar\omega.$$

This quantity determines the intensity of the emitted spectral line.

- Absorption of radiation: The transition probability from the energy E_n to the energy E_{n+1} during the time interval $[t_1, t_2]$ is equal to

$$\gamma_{n,n+1} = \gamma_{n+1,n}, \qquad n = 0, 1, 2, ...$$

In this case, a photon of energy $E_{n+1} - E_n = \hbar\omega$ is absorbed.

Motivation of the transition probability. We want to motivate formula (7.29).

Step 1: Classical particle. Let $q = q(t)$ describe the motion of a classical particle of mass m and electric charge $-e$ on the real line. This particle emits the mean electromagnetic energy $\mathcal{E}$ through a sufficiently large sphere during the time interval $[t_1, t_2]$. Explicitly,

$$\mathcal{E} = \frac{e^2(t_2 - t_1)}{6\pi\varepsilon_0 c^3} \operatorname{mean}(\ddot{q}^2(t))$$

(see Landau and Lifshitz (1982), Sect. 67). We assume that the smooth motion of the particle has the time period T. Then we have the Fourier expansion

$$q(t) = \sum_{r=-\infty}^{\infty} q_r \mathrm{e}^{\mathrm{i}\omega_r t}, \qquad t \in \mathbb{R}$$

with the angular frequency $\omega := 2\pi/T$ and $\omega_r := r\omega$. Since the function $t \mapsto q(t)$ is real, we get $q_r(t)^\dagger = q_{-r}(t)$ for all $r = 0, \pm 1, \pm 2, \ldots$ Hence

$$\ddot{q}^2(t) = \sum_{r,s=-\infty}^{\infty} \omega_r^2 q_r \omega_s^2 q_s \mathrm{e}^{\mathrm{i}(\omega_r+\omega_s)t}.$$

Since $\operatorname{mean}\left(\mathrm{e}^{\mathrm{i}(\omega_r+\omega_s)t}\right) = \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}(\omega_r+\omega_s)t}dt = \delta_{0,r+s}$, we get

$$\operatorname{mean}(\ddot{q}^2(t)) = \sum_{r=-\infty}^{\infty} \omega_r^4 q_r q_{-r} = 2\sum_{r=1}^{\infty} \omega_r^4 |q_r|^2.$$

This yields $\mathcal{E} = \sum_{r=1}^{\infty} \mathcal{E}_r$ with

$$\mathcal{E}_r := \frac{e^2(t_2 - t_1)}{3\pi\varepsilon_0 c^3} \cdot \omega_r^4 |q_r|^2.$$

Step 2: Quantum particle. In 1925 Heisenberg postulated that, for the harmonic oscillator, the passage from the classical particle to the quantum particle corresponds to the two replacements

(i) $\omega_r \Rightarrow \omega_{kn} := (E_k - E_n)/\hbar$, and
(ii) $q_r \Rightarrow q_{kn}(0)$.

Let $k > n$. If the quantum particle jumps from the energy level E_k to the lower energy level E_n, then a photon of energy $E_k - E_n = \hbar\omega_{kn}$ is emitted. Using the replacements (i) and (ii) above, we get $\mathcal{E} = \sum_{k\geq 1}\sum_{n=0}^{k-1}\mathcal{E}_{kn}$ with

$$\mathcal{E}_{kn} := \frac{e^2(t_2 - t_1)}{3\pi\varepsilon_0 c^3}\cdot\omega_{kn}^4|q_{kn}(0)|^2.$$

By definition, the real number

$$\gamma_{kn} := \frac{\mathcal{E}_{kn}}{\hbar\omega_{kn}}, \qquad k > n$$

is the transition probability for a passage of the quantum particle from the energy level E_k to the lower energy level E_n during the time interval $[t_1, t_2]$. From (7.24) we get $|q_{kn}(0)|^2 = \frac{\hbar}{2m\omega}\, k\delta_{n,k-1}$. Hence $\gamma_{kn} = 0$ for the choice $k = n+2, n+3, \ldots$ Moreover,

$$\gamma_{n+1,n} = \frac{\mathcal{E}_{n+1,n}}{\hbar\omega} = \frac{e^2(t_2 - t_1)}{6\pi\varepsilon_0 c^3 m}\cdot\omega^2(n+1), \qquad n = 0, 1, 2, \ldots$$

This motivates the claim (7.30).

7.3.5 The Wightman Functions

> Both the Wightman functions and the correlation functions of the quantized harmonic oscillator are the prototypes of general constructions used in quantum field theory.
>
> Folklore

As we have shown, the motion of the quantum particle corresponding to the quantized harmonic oscillator is described by the time-depending operator function

$$q(t) = \frac{x_0}{\sqrt{2}}\,(a^\dagger \mathrm{e}^{\mathrm{i}\omega t} + a\mathrm{e}^{-\mathrm{i}\omega t}), \qquad t \in \mathbb{R} \tag{7.31}$$

with the initial condition $q(0) = Q$ and $p(0) = P$. Using this, we define the n-point Wightman function of the quantized harmonic oscillator by setting

$$\boxed{W_n(t_1, t_2, \ldots, t_n) := \langle 0|q(t_1)q(t_2)\cdots q(t_n)|0\rangle} \tag{7.32}$$

for all times $t_1, t_2, \ldots, t_n \in \mathbb{R}$. This is the vacuum expectation value of the operator product $q(t_1)q(t_2)\cdots q(t_n)$. In contrast to the operator function (7.31), the Wightman functions are classical complex-valued functions. It turns out that

The Wightman functions know all about the quantized harmonic oscillator.

Using the Wightman functions, we avoid the use of operator theory in Hilbert space. This is the main idea behind the introduction of the Wightman functions.

Proposition 7.4 (i) $W_2(t, s) = \frac{x_0^2}{2}\cdot e^{-\mathrm{i}\omega(t-s)}$ *for all* $t, s \in \mathbb{R}$.

(ii) $W_n \equiv 0$ *if* n *is odd. For example,* $W_1 \equiv 0$ *and* $W_3 \equiv 0$.

(iii) $W_4(t_1, t_2, t_3, t_4) = W_2(t_1, t_2)W_2(t_3, t_4) + 2W_2(t_1, t_3)W_2(t_2, t_4)$ *for all time points* $t_1, t_2, t_3, t_4 \in \mathbb{R}$.

(iv) $W_n(t_1, t_2, \ldots, t_n)^\dagger = W(t_n, \ldots, t_2, t_1)$ *for all times* $t_1, t_2, \ldots t_n$ *and all positive integers* n.

Proof. We will systematically use the orthonormal system $\varphi_0, \varphi_1, \ldots$ introduced on page 433 together with $a\varphi_0 = 0$, $a^\dagger\varphi_0 = \varphi_1$ and

$$a\varphi_n = \sqrt{n}\,\varphi_{n-1}, \quad a^\dagger\varphi_n = \sqrt{n+1}\,\varphi_{n+1}, \qquad n = 1, 2, \ldots$$

Recall that the vacuum state φ_0 is also denoted by $|0\rangle$. The computation of vacuum expectation values becomes extremely simple when using the intuitive meaning of the operator a (resp. $a^\dagger$) as a particle creation (resp. annihilation) operator. Let us explain this by considering a few typical examples. First let us show that most of the vacuum expectation values vanish.

- The state $a^\dagger a^\dagger\varphi_0$ contains two particles. Hence

$$\langle\varphi_0|a^\dagger a^\dagger\varphi_0\rangle = \text{const}\cdot\langle\varphi_0|\varphi_2\rangle = 0,$$

  by orthogonality.
- The state $aa^\dagger a^\dagger\varphi_0$ contains one particle. Hence

$$\langle\varphi_0|aa^\dagger a^\dagger\varphi_0\rangle = \text{const}\cdot\langle\varphi_0|\varphi_1\rangle = 0.$$

- $Aa\varphi_0 = 0$ for arbitrary expressions A, since $a\varphi_0 = 0$.
- Analogously, $aaaa^\dagger a^\dagger\varphi_0 = 0$. In fact,

$$aaaa^\dagger a^\dagger\varphi_0 = a(aaa^\dagger a^\dagger)\varphi_0 = \text{const}\cdot a\varphi_0 = 0.$$

  Formally, the state $aaaa^\dagger a^\dagger\varphi_0$ contains "2 minus 3" particles. In general, states with a 'negative' number of particles are equal to zero.

Therefore, it only remains to compute vacuum expectation values $\langle\varphi_0|A\varphi_0\rangle$ where the state $A\varphi_0$ contains no particle.

> *This means that A is a product of creation and annihilation operators where the number of creation operators equals the number of annihilation operators.*

The following examples will be used below.

- The state $aa^\dagger\varphi_0$ contains no particle. Here,

$$aa^\dagger\varphi_0 = a\varphi_1 = \varphi_0. \tag{7.33}$$

  Hence $\langle\varphi_0|aa^\dagger\varphi_0\rangle = \varphi_0|\varphi_0\rangle = 1$.
- The state $aaa^\dagger a^\dagger\varphi_0$ contains no particle. Explicitly,

$$aaa^\dagger a^\dagger\varphi_0 = aaa^\dagger\varphi_1 = \sqrt{2}\,aa\varphi_2 = 2a\varphi_1 = 2\varphi_0. \tag{7.34}$$

  Hence $\langle\varphi_0|aaa^\dagger a^\dagger\varphi_0\rangle = 2$.
- Similarly,

$$aa^\dagger aa^\dagger\varphi_0 = aa^\dagger a\varphi_1 = aa^\dagger\varphi_0 = a\varphi_1 = \varphi_0. \tag{7.35}$$

  Hence $\langle aa^\dagger aa^\dagger\varphi_0\rangle = 1$.

Ad (i). To simplify notation, set

$$a_j := \frac{x_0 \mathrm{e}^{-\mathrm{i}\omega t_j}}{\sqrt{2}}\, a, \qquad a_j^\dagger := \frac{x_0 \mathrm{e}^{\mathrm{i}\omega t_j}}{\sqrt{2}}\, a^\dagger.$$

We have $W_2(t_1, t_2) = \langle \varphi_0 | A \varphi_0 \rangle$ with the state

$$A\varphi_0 = (a_1^\dagger + a_1)(a_2^\dagger + a_2)\varphi_0.$$

Only the state $a_1 a_2^\dagger \varphi_0$ gives a non-vanishing contribution to the Wightman function W_2. By (7.33), $W_2(t_1, t_2)$ is equal to

$$\langle \varphi_0 | a_1 a_2^\dagger \varphi_0 \rangle = \frac{x_0^2}{2} \cdot \mathrm{e}^{-\mathrm{i}\omega t_1} \mathrm{e}^{\mathrm{i}\omega t_2} \langle \varphi_0 | a a^\dagger \varphi_0 \rangle = \frac{x_0^2}{2} \cdot \mathrm{e}^{-\mathrm{i}\omega(t_1 - t_2)}.$$

Ad (ii). First note that $\langle \varphi_0 | (a^\dagger + a)\varphi_0 \rangle = \langle \varphi_0 | \varphi_1 \rangle = 0$. The state

$$A\varphi_0 := (a_1^\dagger + a_1)(a_2^\dagger + a_2)(a_3^\dagger + a_3)\varphi_0$$

is the sum of particle states with an odd number of particles. Hence we obtain $\langle \varphi_0 | A \varphi_0 \rangle = 0$, by orthogonality. The same is true for an odd number of factors $(a_j^\dagger + a_j)$.

Ad (iii). We have $W_4(t_1, t_2, t_3, t_4) = \langle \varphi_0 | A \varphi_0 \rangle$ with the state

$$A\varphi_0 := (a_1^\dagger + a_1)(a_2^\dagger + a_2)(a_3^\dagger + a_3)(a_4^\dagger + a_4) = a_1 a_2 a_3^\dagger a_4^\dagger + a_1 a_2^\dagger a_3 a_4^\dagger + \ldots$$

The dots denote terms whose contribution to W_4 vanishes. By (7.34) and (7.35), $W_4(t_1, t_2, t_3, t_4)$ is equal to

$$\begin{aligned} \langle \varphi_0 | a_1 a_2 a_3^\dagger a_4^\dagger \varphi_0 \rangle + \langle \varphi_0 | a_1 a_2^\dagger a_3 a_4^\dagger \varphi_0 \rangle &= 2 W_2(t_1, t_3) W_2(t_2, t_4) \\ &\quad + W_2(t_1, t_2) W_2(t_3, t_4). \end{aligned}$$

Ad (iv). Since the operator $Q(t)$ is formally self-adjoint,

$$\langle \varphi_0 | Q(s) Q(t) \varphi_0 \rangle = \langle Q(t) Q(s) \varphi_0 | \varphi_0 \rangle = \langle \varphi_0 | Q(t) Q(s) \varphi_0 \rangle^\dagger.$$

Hence $W_2(s, t) = W_2(t, s)^\dagger$. The general case proceeds analogously. □

Similar arguments for computing vacuum expectation values via creation and annihilation operators are frequently used in quantum field theory.

Theorem 7.5 (i) *Equation of motion: For any $s \in \mathbb{R}$, the 2-point Wightman function $t \mapsto W_2(t, s)$ satisfies the classical equation of motion for the harmonic oscillator, that is,*

$$\frac{\partial^2 W_2(t, s)}{\partial t^2} + \omega^2 W_2(t, s) = 0, \qquad t \in \mathbb{R}.$$

(ii) *Reconstruction property: For all times $t, s \in \mathbb{R}$,*

$$q(t - s) = \frac{\sqrt{2}}{x_0} \left(W_2(t, s) a + W_2(s, t) a^\dagger \right). \tag{7.36}$$

Relation (7.5) tells us that the knowledge of the 2-point Wightman function W_2 allows us to reconstruct the quantum dynamics of the harmonic oscillator.
Proof. Note that $\ddot{q}(t) + \omega^2 q(t) = 0$, and hence

$$\frac{\partial^2 W(t,s)}{\partial^2 t} + \omega^2 W(t,s) = \langle \varphi_0 | (\ddot{q}(t) + \omega^2 q(t)) q(s) \varphi_0 \rangle = 0.$$

□

Perspectives. In 1956 Wightman showed that it is possible to base quantum field theory on the investigation of the vacuum expectation values of the products of quantum fields. These vacuum expectation values are called Wightman functions. The crucial point is that the Wightman functions are highly singular objects in quantum field theory. In fact, they are generalized functions.[25] However, they are also boundary values of holomorphic functions of several complex variables. This simplifies the mathematical theory. Using a similar construction as in the proof of the Gelfand–Naimark–Segal (GNS) representation theorem for C^*-algebras in Hilbert spaces, Wightman proved a reconstruction theorem which shows that the quantum field (as a Hilbert-space valued distribution) can be reconstructed from its Wightman distributions. Basic papers are:

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In recent years, Klaus Fredenhagen (Hamburg University) has written a series of important papers together with his collaborators. The idea is to combine the operator-algebra methods of axiomatic quantum field theory (due to Gårding–Wightman and Haag–Kastler) with the methods of perturbation theory, by using formal power series expansions. We refer to:

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We also recommend the lectures given by Klaus Fredenhagen at Hamburg University. These lectures are available on the Internet:

`http://unith.desy.de/research/aqft/lecture-notes`

Furthermore, we recommend the lectures on quantum field theory given by Arthur Jaffe at Harvard University:

A. Jaffe, Introduction to Quantum Field Theory. Lecture Notes, partially available at: `www.rathurjaffe.com/Assets/pdf/IntroQFT.pdf`

7.3.6 The Correlation Functions

In contrast to the Wightman functions, the correlation functions reflect causality.

Folklore

Parallel to (7.32), we now define the n-point correlation function (also called the n-point Green's function) by setting

$$\boxed{C_n(t_1, t_2, \ldots, t_n) := \langle 0 | \mathcal{T}(q(t_1)q(t_2)\cdots q(t_n))|0\rangle} \tag{7.37}$$

for all times $t_1, t_2, \ldots, t_n \in \mathbb{R}$. Here, the symbol $\mathcal{T}$ denotes the time-ordering operator, that is, we define

$$\mathcal{T}(q(t_1)q(t_2)\cdots q(t_n)) := q(t_{\pi(1)})q(t_{\pi(2)})\cdots q(t_{\pi(n)})$$

where the permutation π of the indices $1, 2, \ldots, n$ is chosen in such a way that $t_{\pi(1)} \geq t_{\pi(2)} \geq \ldots \geq t_{\pi(n)}$. For example, using the slightly modified Heaviside function θ_*, we obtain[26]

[26] We set $\theta_*(t) := 1$ if $t > 0$, $\theta_*(t) := 0$ if $t < 0$, and $\theta_*(0) := \frac{1}{2}$.

$$C_2(t,s) = \theta_*(t-s)W_2(t,s) + \theta_*(s-t)W_2(s,t)) = \frac{x_0^2}{2} \cdot \mathrm{e}^{-\mathrm{i}\omega|t-s|} \tag{7.38}$$

for all $t, s \in \mathbb{R}$. This relates the 2-point correlation function C_2 to the 2-point Wightman function W_2 by taking causality into account. In particular, we have $C_2(t,s) = W_2(t,s)$ if $t \geq s$.

Theorem 7.6 *For any $s \in \mathbb{R}$, the 2-point correlation function $t \mapsto C_2(t,s)$ satisfies the inhomogeneous classical equation of motion for the harmonic oscillator, that is,*

$$\frac{\partial^2 C_2(t,s)}{\partial t^2} + \omega^2 C_2(t,s) = \frac{\hbar}{m\mathrm{i}} \cdot \delta(t-s), \qquad t \in \mathbb{R}, \tag{7.39}$$

in the sense of tempered distributions on the real line.

This theorem tells us that the function $F(t) := \frac{m\mathrm{i}}{\hbar} \cdot C_2(t,0)$ satisfies the differential equation

$$\ddot{F}(t) + \omega^2 F(t) = \delta(t), \qquad t \in \mathbb{R}.$$

In terms of mathematics, the function F is a fundamental solution of the differential operator $\frac{d^2}{dt^2} + \omega^2$, in the sense of tempered distributions (see Sect. 11.7 of Vol. I).

The language of mathematicians. In order to prove Theorem 7.6, we will use the theory of generalized functions (distributions) introduced in Chap. 11 of Vol. I. Let $\psi \in \mathcal{S}(\mathbb{R})$. Integrating by parts twice, we get

$$\begin{aligned}\int_s^\infty \mathrm{e}^{-\mathrm{i}\omega(t-s)}\ddot{\psi}(t)dt &= -\dot{\psi}(s) + \int_s^\infty \mathrm{i}\omega\mathrm{e}^{-\mathrm{i}\omega(t-s)}\dot{\psi}(t)dt \\ &= -\dot{\psi}(s) - \mathrm{i}\omega\psi(s) - \omega^2 \int_s^\infty \mathrm{e}^{-\mathrm{i}\omega(t-s)}\psi(t)dt.\end{aligned}$$

Similarly,

$$\int_{-\infty}^s \mathrm{e}^{-\mathrm{i}\omega(s-t)}\ddot{\psi}(t)dt = \dot{\psi}(s) - \mathrm{i}\omega\psi(s) - \omega^2 \int_{-\infty}^s \mathrm{e}^{-\mathrm{i}\omega(s-t)}\psi(t)dt.$$

Hence

$$\int_{-\infty}^\infty \mathrm{e}^{-\mathrm{i}\omega|t-s|}\ \ddot{\psi}(t)dt = -2\mathrm{i}\omega\psi(s) - \omega^2 \int_{-\infty}^\infty \mathrm{e}^{-\mathrm{i}\omega|t-s|}\ \psi(t)dt.$$

In terms of distribution theory, this is equivalent to

$$\frac{\partial^2 \mathrm{e}^{-\mathrm{i}\omega|t-s|}}{\partial t^2} + \omega^2 \mathrm{e}^{-\mathrm{i}\omega|t-s|} = -2\mathrm{i}\omega\delta(t-s), \qquad t \in \mathbb{R}.$$

□

The language of physicists. We want to show how to obtain the claim of Theorem 7.6 by using Dirac's delta function in a formal setting.[27] For fixed $s \in \mathbb{R}$, consider

$$C(t) := \theta_*(t-s)W(t) + \theta_*(s-t)Z(t), \qquad t \in \mathbb{R}.$$

Differentiating this with respect to time t by means of the product rule and noting that $\dot{\theta}_*(t) = \delta(t)$, we get

$$\dot{C}(t) = \delta(t-s)W(t) - \delta(s-t)Z(t) + \theta_*(t-s)\dot{W}(t) + \theta_*(s-t)\dot{Z}(t).$$

[27] Both the formal Dirac calculus and its relations to the rigorous theory are thoroughly investigated in Sect. 11.2ff of Vol. I.

Using $\delta(t-s)=\delta(s-t)$ and $\delta(t)=0$ if $t\neq 0$, we obtain

$$\dot{C}(t)=\delta(t-s)(W(s)-Z(s))+\theta_*(t-s)\dot{W}(t)+\theta_*(s-t)\dot{Z}(t).$$

Hence

$$\begin{aligned}\ddot{C}(t)=\dot{\delta}(t-s)(W(s)-Z(s))+\delta(t-s)(\dot{W}(s)-\dot{Z}(s))\\ +\theta_*(t-s)\ddot{W}(t)+\theta_*(s-t)\ddot{Z}(t).\end{aligned}$$

Choosing $C(t):=C_2(t)$ and

$$W(t):=W_2(t,s)=\frac{x_0^2}{2}\,\mathrm{e}^{-\mathrm{i}\omega(t-s)}$$

together with $Z(t):=W_2(s,t)$, we get the differential equation (7.39) above.

The physical meaning of correlation functions for the harmonic oscillator. Let $\varphi\in L_2(\mathbb{R})$ with $\langle\varphi|\varphi\rangle=1$. We regard φ as a physical state of the quantized harmonic oscillator on the real line. The operator function $q=q(t),\ t\in\mathbb{R}$ from (7.31) on page 451 describes the motion of the quantum particle. According to the general approach introduced in Sect. 7.9 of Vol. I, we assign to the state φ the following real numbers:

(i) Mean position of the particle in the state φ at time t: $\bar{q}(t):=\langle\varphi|q(t)|\varphi\rangle$.
(ii) Mean fluctuation of the particle position at time t:

$$\Delta q(t):=\sqrt{\langle\varphi|(q(t)-\bar{q}(t))^2\varphi\rangle}.$$

(iii) Correlation coefficient: For $t,s\in\mathbb{R}$, we define

$$\gamma(t,s):=\frac{\overline{(q(t)-\bar{q}(t))(q(s)-\bar{q}(s))}}{\Delta q(t)\Delta q(s)}.$$

By the Schwarz inequality, $|\gamma(t,s)|\leq 1$. If $|\gamma(t,s)|=1$ (resp. $\gamma(t,s)=0$), then the position of the particle in the state φ at time t is strongly correlated (resp. not correlated) to the position in the state φ at time s.
(iv) Causal correlation coefficient:

$$\gamma_{\mathrm{causal}}(t,s):=\gamma(t,s)\qquad\text{if } t\geq s.$$

Furthermore, $\gamma_{\mathrm{causal}}(t,s):=\gamma(s,t)$ if $s\geq t$.
(v) Transition amplitude: Let $\varphi,\psi\in L_2(\mathbb{R})$ with $\langle\varphi|\varphi\rangle=\langle\psi|\psi\rangle=1$. The complex number $\langle\psi|q(t)\varphi\rangle$ is called the transition amplitude (for the position) from the state φ to the state ψ at time t.

To illustrate this, consider the ground state φ_0 of the harmonic oscillator. Then $W_2(t,s)=\frac{\hbar}{2m\omega}\mathrm{e}^{-\mathrm{i}\omega(t-s)}$. Thus, in the ground state, we have:

- Mean position $\bar{q}(t)=0$.
- Mean fluctuation: $\Delta q(t)=\sqrt{\langle\varphi_0|q(t)q(t)\varphi_0\rangle}=\sqrt{W_2(t,t)}=\sqrt{\frac{\hbar}{2m\omega}}$.
- Correlation coefficient:

$$\gamma(t,s)=\frac{W_2(t,s)}{\sqrt{W_2(t,t)}\sqrt{W_2(s,s)}}=\mathrm{e}^{-\mathrm{i}\omega(t-s)},\quad t\geq s,$$

and $\gamma_{\mathrm{causal}}(t,s)=\mathrm{e}^{-\mathrm{i}\omega|t-s|}$. Hence $|\gamma(t,s)|=1$. This means that, in the ground state, the position of the quantum particle at time t is strongly correlated to the position at time s.

- Transition amplitude from the state φ_0 to the state φ_n:

$$\langle\varphi_1|q(t)\varphi_0\rangle = \mathrm{e}^{\mathrm{i}\omega t}, \quad \langle\varphi_n|q(t)\varphi_0\rangle = 0, \qquad n = 2, 3, 2, \ldots$$

By (7.29), the transition probability γ_{n0} for passing from the state φ_0 to the state φ_n during the time interval $[t_1, t_2]$ is proportional to $|\langle\varphi_n|q(0)\varphi_0\rangle|^2$. Explicitly, $\gamma_{10} = \frac{\omega^2 e^2 (t_2 - t_1)}{6\pi\varepsilon_0 c^3 m}$ and $\gamma_{n0} = 0$ if $n = 2, 3, \ldots$

7.4 Schrödinger's Quantum Mechanics

> In particular, I would like to mention that I was mainly inspired by the thoughtful dissertation of Mr. Louis de Broglie (Paris, 1924). The main difference here lies in the following. De Broglie thinks of travelling waves, while, in the case of the atom, we are led to standing waves... I am most thankful to Hermann Weyl with regard to the mathematical treatment of the equation of the hydrogen atom.[28]
>
> Erwin Schrödinger, 1926

7.4.1 The Schrödinger Equation

In 1926 Schrödinger invented wave quantum mechanics based on a wave function $\psi = \psi(x, t)$. The Schrödinger equation for the motion of a quantum particle of mass m on the real line is given by

$$\boxed{\mathrm{i}\hbar\psi_t = -\frac{\hbar^2}{2m}\psi_{xx} + U\psi.} \tag{7.40}$$

Explicitly, the Schrödinger equation reads as

$$\mathrm{i}\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial^2 x} + U(x)\psi(x,t).$$

Schrödinger's quantization. The Schrödinger equation (7.40) is obtained by applying Schrödinger quantization to the classical energy equation

$$\boxed{E = \frac{p^2}{2m} + U.} \tag{7.41}$$

This means that we replace the classical momentum p and the classical energy E by differential operators. Explicitly,

$$E \Rightarrow \mathrm{i}\hbar\frac{\partial}{\partial t}, \qquad p \Rightarrow -\mathrm{i}\hbar\frac{\partial}{\partial x}.$$

From (7.41) we get

$$\boxed{\mathrm{i}\hbar\frac{\partial}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U.}$$

[28] E.Schrödinger, Quantization as an eigenvalue problem (in German), Ann. Phys. **9** (1926), 361–376. See also E. Schrödinger, Collected Papers on Wave Mechanics, Blackie, London, 1928.

Applying this to the function ψ, we obtain the one-dimensional Schrödinger equation (7.40). Schrödinger generalized this in a straightforward manner to three dimensions, and he computed the spectrum of the hydrogen atom.

The physical interpretation of the wave function ψ. If the potential U vanishes, $U \equiv 0$, then the function

$$\psi_0(x,t) := C\mathrm{e}^{-\mathrm{i}E(p)t/\hbar}\mathrm{e}^{\mathrm{i}px/\hbar}$$

is a solution of the Schrödinger equation (7.40). Here, C is a fixed complex number, p is a fixed real number, and $E(p) := \frac{p^2}{2m}$. The function ψ_0 corresponds to a stream of freely moving electrons on the real line with momentum p and energy $E(p)$. There arises the following question:

What is the physical meaning of the function $\psi = \psi(x,t)$ in the general case?

Interestingly enough, Schrödinger did not know the answer when publishing his paper in 1926. The answer was found by Born a few months later.

By applying the Schrödinger equation to scattering processes, Born discovered the random character of quantum processes.

According to Born, we have to distinguish the following two cases:

(i) Single quantum particle: Suppose that $0 < \int_{\mathbb{R}} |\psi(x)|^2 dx < \infty$. Then, the value

$$\varrho(x,t) := \frac{|\psi(x,t)|^2}{\int_{\mathbb{R}} |\psi(x,t)|^2 dx}$$

represents the particle probability density at position x at time t. That is, the value

$$\int_J \varrho(x,t)dx$$

is equal to the probability of finding the particle in the interval J at time t. Naturally enough, $\int_{\mathbb{R}} \varrho(x,t)dx = 1$. If we measure the position x of the quantum particle, then the mean position $\bar{x}$ and the fluctuation Δx of the position at time t are given by

$$\boxed{\bar{x}(t) = \int_{\mathbb{R}} x\varrho(x,t)dx}$$

and

$$\boxed{(\Delta x)^2 = \overline{(x-\bar{x})^2} = \int_{\mathbb{R}} (x-\bar{x})^2 \varrho(x,t)dx.}$$

By definition, Δx is non-negative. In the theory of probability, a fundamental inequality due to Chebyshev (1821–1894) tells us that

$$P(\bar{x} - r\Delta x \le x \le \bar{x} + r\Delta x) \ge 1 - \frac{1}{r^2}$$

for all $r > 0$. In particular, choose $r = 4$. Then this inequality tells us that the probability of measuring the position x of the quantum particle in the interval $[\bar{x} - 4\Delta x, \bar{x} + 4\Delta x]$ is larger than $1 - \frac{1}{16} = 0.93$.

(ii) Stream of quantum particles: Suppose that $\int_{\mathbb{R}} |\psi(x,t))|^2 dx = \infty$. Then, the function ψ corresponds to a stream of particles on the real line with the particle density

$$\varrho(x,t) := |\psi(x,t)|^2, \qquad x \in \mathbb{R}, \quad t \in \mathbb{R},$$

and the current density vector

$$\mathbf{J}(x,t) = \mathcal{J}(x,t)\mathbf{e}, \qquad x \in \mathbb{R}, \quad t \in \mathbb{R}$$

at the point x at time t. Here, the unit vector $\mathbf{e}$ points in direction of the positive x-axis, and we define

$$\mathcal{J} := \frac{\mathrm{i}\hbar}{2m}(\psi\psi_x^\dagger - \psi^\dagger\psi_x).$$

This definition is motivated by the fact that each smooth solution ψ of the Schrödinger equation (7.40) satisfies the following conservation law[29]

$$\boxed{\varrho_t + \operatorname{div}\mathbf{J} = 0.} \tag{7.42}$$

Explicitly, $\operatorname{div}\mathbf{J} = \mathcal{J}_x$. For $a < b$, this implies the relation

$$\int_a^b \varrho(x,t)dx = \mathcal{J}(a,t) - \mathcal{J}(b,t)$$

which describes the change of the particle number on the interval $[a,b]$ by the particle stream. For example, the function

$$\psi_0(x,t) = C\mathrm{e}^{-\mathrm{i}E(p)t/\hbar}\mathrm{e}^{\mathrm{i}px/\hbar}$$

corresponds to a stream of quantum particles with the constant particle density $\varrho(x,t) = |C|^2$, the velocity $v = p/m$, and the current density vector

$$\mathbf{J} = v\varrho\mathbf{e}.$$

There exist fascinating long-term developments in mathematics. In his books "Geometry" and "Algebra" from 1550 and 1572, respectively, Bombielli (1526–1572) systematically used the symbol $\sqrt{-1}$ in order to solve algebraic equations of third and fourth order. Almost 400 years later, the physicist Schrödinger used the number $\mathrm{i} = \sqrt{-1}$ in order to formulate the basic equations of quantum mechanics. We are going to show that the use of complex numbers is substantial for quantum physics. Freeman Dyson writes in his foreword to Odifreddi's book:[30]

> One of the most profound jokes of nature is the square root of -1 that the physicist Erwin Schrödinger put into his wave equation in 1926 ... The Schrödinger equation describes correctly everything we know about the behavior of atoms. It is the basis of all of chemistry and most of physics. And that square root of -1 means that nature works with complex numbers. This discovery came as a complete surprise, to Schrödinger as well as to everybody else. According to Schrödinger, his fourteen-year-old girlfriend Itha Junger said to him at the time: "Hey, you never even thought when

[29] In fact, $\varrho_t = (\psi\psi^\dagger)_t = \psi_t\psi^\dagger + \psi\psi_t^\dagger$. By (7.40), $\varrho_t = -\mathcal{J}_x$.

[30] P. Odifreddi, The Mathematical Century: The 30 Greatest Problems of the Last 100 Years, Princeton University Press, Princeton, New Jersey, 2004. Reprinted by permission of Princeton University Press.

you began that so much sensible stuff would come out of it." All through the nineteenth century, mathematicians from Abel to Riemann and Weierstrass had been creating a magnificent theory of functions of complex variables. They had discovered that the theory of functions became far deeper and more powerful if it was extended from real to complex numbers. But they always thought of complex numbers as an artificial construction, invented by human mathematicians as a useful and elegant abstraction from real life. It never entered their heads that they had invented was in fact the ground on which atoms move. They never imagined that nature had got there first.

In what follows, we want to show that the notion of Hilbert space is an appropriate setting for describing quantum mechanics in terms of mathematics. Originally, the special Hilbert space l^2 (as an infinite-dimensional variant of $\mathbb{R}^n$) was introduced by Hilbert in the beginning of the 20th century in order to study eigenvalue problems for integral equations.

7.4.2 States, Observables, and Measurements

The Hilbert space approach. In 1926, the young Hungarian mathematician von Neumann Janos came to Göttingen as Hilbert's assistant.[31] In Göttingen, von Neumann learned about the new quantum mechanics of physicists. It was his goal to give quantum mechanics a rigorous mathematical basis. As a mathematical framework, he used the notion of Hilbert space. For example, in the present case of the motion of a quantum particle on the real line, we choose the Hilbert space $L_2(\mathbb{R})$ with the inner product

$$\boxed{\langle\psi|\chi\rangle = \int_{\mathbb{R}} \psi(x)^\dagger \chi(x) dx \qquad \text{for all} \quad \psi, \chi \in L_2(\mathbb{R}),}$$

and the norm $||\psi|| := \sqrt{\langle\psi|\psi\rangle}$. The general terminology reads as follows.

(S) States: Each nonzero element ψ of $L_2(\mathbb{R})$ is called a state. In terms of physics, this describes a state of a single quantum particle on the real line. Two nonzero elements ψ, χ of $L_2(\mathbb{R})$ represent equivalent states iff there exists a nonzero complex number μ with

$$\psi = \mu\chi.$$

In terms of physics, equivalent states represent the same physical state of the particle. The state ψ is called normalized iff $||\psi|| = 1$.

(O) Observables: The linear, formally self-adjoint operators

$$A : D(A) \subseteq X \to X$$

are called formal observables. Explicitly, this means that the domain of definition $D(A)$ is a linear subspace of X. Moreover, for all $\psi, \chi \in D(A)$ and all complex numbers α, β, we have

[31] Von Neumann (1903–1957) was born in Budapest (Hungary). He studied mathematics and chemistry in Berlin, Budapest, and Zurich. The German (resp. English) translation of the Hungarian name 'Janos' is Johann (resp. John). Von Neumann was an extraordinarily gifted mathematician. He was known for his ability to understand mathematical subjects and to solve mathematical problems extremely fast. In 1933, von Neumann got a professorship at the newly founded Institute for Advanced Study in Princeton, New Jersey (U.S.A.).

$$A(\alpha\psi + \beta\chi) = \alpha A\psi + \beta A\chi$$

together with the symmetry condition $\langle\psi|A\chi\rangle = \langle A\psi|\chi\rangle$.[32]

(M) Measurements: If we measure the formal observable A in the normalized state ψ, then we get the mean value

$$\boxed{\bar{A} := \langle\psi|A\psi\rangle,}$$

and the mean fluctuation[33]

$$\boxed{\Delta A := ||(A - \bar{A}I)\psi||.}$$

(C) Correlation coefficient: Let $A, B : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ be two formal observables. The correlation coefficient between A and B in the state ψ is defined by

$$\gamma := \frac{\mathrm{Cov}(A, B)}{\Delta A \cdot \Delta B}$$

together with the covariance

$$\mathrm{Cov}(A, B) := \overline{(A - \bar{A}I)(B - \bar{B}I)} = \langle\psi|(A - \bar{A}I)(B - \bar{B}I)\psi\rangle.$$

Hence $\mathrm{Cov}(A, B) = \langle(A - \bar{A}I)\psi|(B - \bar{B}I)\psi\rangle$.

By the Schwarz inequality, $|\gamma| \leq 1$.

- If $\gamma = 0$, then there is no correlation between the formal observables A and B. In other words, A and B are independent formal observables.
- If $|\gamma| = 1$, then the correlation between A and B is large. That is, the formal observable A depends strongly on the formal observable B.

Proposition 7.7 *The mean value is a real number.*

This is a consequence of $\langle\psi|A\psi\rangle^\dagger = \langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle$. □

The following result underlines the importance of eigenvalue problems in quantum mechanics.

Proposition 7.8 *Suppose that the normalized state ψ is an eigenvector of the formal observable A with eigenvalue λ,*

$$A\psi = \lambda\psi.$$

Then, the measurement of A in the state ψ yields $\bar{A} = \lambda$ and $\Delta A = 0$.

[32] For a deeper mathematical analysis, von Neumann introduced the stronger notion of an observable. By definition, an observable is an essentially self-adjoint operator (see Vol. I, p. 677).

[33] Explicitly, $(\Delta A)^2 = \langle A\psi - \bar{A}\psi|A\psi - \bar{A}\psi\rangle$. If $A\psi \in D(A)$, then

$$(\Delta A)^2 = \langle\psi|(A - \bar{A}I)^2\psi\rangle = \overline{(A - \bar{A}I)^2}.$$

In this case, we say that λ is a sharp value of the formal observable A. For the proof, $\langle\psi|A\psi\rangle = \lambda\langle\psi|\psi\rangle = \lambda$, and $A\psi - \bar{A}\psi = A\psi - \lambda\psi = 0$. □

Examples. The operators $Q, P, H : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ are defined by

$$(Q\psi)(x) := x\psi(x), \quad (P\psi)(x) = -\mathrm{i}\hbar\psi'(x), \qquad x \in \mathbb{R},$$

for all functions $\psi \in \mathcal{S}(\mathbb{R})$. We call Q and P the position operator and the momentum operator, respectively. Moreover, we introduce the energy operator (Hamiltonian)

$$H := \frac{P^2}{2m} + U,$$

where we assume that $U \in \mathcal{S}(\mathbb{R})$. Then the fundamental operator equation

$$\mathrm{i}\hbar\dot{\psi} = H\psi$$

coincides with the Schrödinger equation (7.40).

Proposition 7.9 *The operators $Q, P, H : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ are formally self-adjoint on the Hilbert space $L_2(\mathbb{R})$, and there holds the commutation relation*

$$QP - PQ = \mathrm{i}\hbar I \qquad \text{on } \mathcal{S}(\mathbb{R}). \tag{7.43}$$

Proof. The formal self-adjointness of Q and P together with (7.43) are proved on page 436. Let $\psi \in \mathcal{S}(\mathbb{R})$. The formal self-adjointness of H follows from

$$\langle\psi|P^2\psi\rangle = \langle P\psi|P\psi\rangle = \langle P^2\psi|\psi\rangle.$$

Hence $\langle\psi|H\psi\rangle = \langle H\psi|\psi\rangle$. □

7.4.3 The Free Motion of a Quantum Particle

The classical motion of a particle of mass m on the real line is governed by the Hamiltonian $H := \frac{p^2}{2m}$ together with the canonical equations

$$\dot{q} = H_p = \frac{p}{m}, \qquad \dot{p} = -H_q = 0.$$

For given initial position $q(0) = q_0$ and initial velocity $\dot{q}(0) = v$, the unique solution reads as $q(t) = q_0 + vt$ for all times $t \in \mathbb{R}$ with the total energy

$$E(p) := \frac{p^2}{2m} = \frac{mv^2}{2}.$$

The free motion of a quantum particle on the real line is governed by the Hamiltonian operator

$$\boxed{H := \frac{P^2}{2m}.} \tag{7.44}$$

Recall that $P = -\mathrm{i}\hbar\frac{d}{dx}$, and hence

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}.$$

At this point, we regard the operators P and H as differential operators which act on smooth functions (or on generalized functions).[34] For the functional-analytic approach to quantum mechanics, it is important to appropriately specify the domain of definition of the operators under consideration. This will be discussed below. For fixed nonzero complex number C, define the functions

$$\varphi_p(x) := C\mathrm{e}^{\mathrm{i}px/\hbar}, \qquad \psi_p(x,t) = \varphi_p(x)\mathrm{e}^{-\mathrm{i}tE(p))/\hbar}, \qquad x,t \in \mathbb{R}.$$

Then the function ψ_p satisfies the Schrödinger equation

$$\mathrm{i}\hbar\dot{\psi}_p = H\psi_p.$$

Moreover, for all parameters $p \in \mathbb{R}$, we have

$$P\varphi_p = p\varphi_p, \qquad H\varphi_p = E(p)\varphi_p.$$

These equations remain valid if we replace φ_p by ψ_p. From the physical point of view, the function ψ_p describes a homogeneous stream of quantum particles (e.g., electrons) with particle density $\varrho = |C|^2$ and velocity v. Note that the functions φ_p and $x \mapsto \psi_p(x,t)$ do not live in the Hilbert space $L_2(\mathbb{R})$.

Let $\varphi, \chi \in \mathcal{S}(\mathbb{R})$. Normalizing the function φ_p above by $C := \frac{1}{\sqrt{2\pi\hbar}}$, we get the Fourier transform

$$\hat{\varphi}(p) = \int_{\mathbb{R}} \varphi_p(x)^\dagger \varphi(x)dx, \qquad p \in \mathbb{R}$$

together with the inverse transform

$$\varphi(x) = \int_{\mathbb{R}} \varphi_p(x)\hat{\varphi}(p)dp, \qquad x \in \mathbb{R}.$$

The operator $\mathcal{F} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is bijective (see Vol. I, p. 87). We write $\hat{\varphi} = \mathcal{F}\varphi$. This Fourier transform can be uniquely extended to a unitary operator of the form $\mathcal{F} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$,s that is, we have

$$\langle\varphi|\chi\rangle = \langle\hat{\varphi}|\hat{\chi}\rangle, \qquad \text{for all} \quad \varphi,\chi \in L_2(\mathbb{R}),$$

which is called the Parseval equation of the Fourier transform.

The quantum dynamics of a freely moving particle. Let us now study the three operators

- $P : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ (momentum operator),
- $Q : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ position operator), and
- $H : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ (Hamiltonian).

These operators are formally self-adjoint on the Hilbert space $L_2(\mathbb{R})$. In the Fourier space, the operators P and H correspond to the following multiplication operators

$$(\hat{P}\hat{\varphi})(p) = p\hat{\varphi}(p), \qquad (\hat{H}\hat{\varphi})(p) = E(p)\hat{\varphi}(p), \qquad p \in \mathbb{R}.$$

This holds for all $\varphi \in \mathcal{S}(\mathbb{R})$, and hence for all $\hat{\varphi} \in \mathcal{S}(\mathbb{R})$. For given $\varphi_0 \in \mathcal{S}(\mathbb{R})$, the quantum dynamics

$$\boxed{\psi(t) = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\varphi_0, \qquad t \in \mathbb{R}}$$

is given in the Fourier space by the equation

[34] The Schwartz $\mathcal{S}'(\mathbb{R})$ of tempered distributions and the Schwartz space $\mathcal{D}'(\mathbb{R})$ of distributions are investigated in Sect. 11.3 of Vol. I. Here, $\mathcal{S}'(\mathbb{R}) \subset \mathcal{D}'(\mathbb{R})$.

$$\hat{\psi}(p,t) = \mathrm{e}^{-\mathrm{i}E(p)t/\hbar}\hat{\varphi}_0(p), \qquad p \in \mathbb{R}$$

for each time $t \in \mathbb{R}$. Transforming this back to the original Hilbert space $L_2(\mathbb{R})$ by using the Fourier transform, we get the quantum dynamics

$$\boxed{\mathrm{e}^{-\mathrm{i}tH_0/\hbar}\varphi_0 = \mathcal{F}^{-1}\hat{\psi}(t) \qquad \text{for all} \quad t \in \mathbb{R}.} \tag{7.45}$$

We have $\psi(t) \in \mathcal{S}(\mathbb{R})$ for all times $t \in \mathbb{R}$, and this function satisfies the Schrödinger equation for all times.[35]

The full quantum dynamics. Consider equation (7.45). Observe the following peculiarity. The right-hand side of (7.45) is well-defined for initial states $\varphi_0 \in L_2(\mathbb{R})$ if we do not use the classical Fourier transform, but the extended Fourier transform $\mathcal{F} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$. In this sense, we understand the dynamics

$$\psi(t) = \mathrm{e}^{-\mathrm{i}tH/\hbar}\varphi_0, \qquad t \in \mathbb{R}$$

for all initial states $\varphi_0 \in L_2(\mathbb{R})$. In terms of functional analysis, for any fixed time t, the operator $\mathrm{e}^{-\mathrm{i}tH/\hbar} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ is unitary. Therefore, $\mathrm{e}^{-\mathrm{i}tH/\hbar}\varphi_0$ makes sense for all $\varphi_0 \in L_2(\mathbb{R})$. In this general setting, the function

$$\psi : [0, +\infty[\to L_2(\mathbb{R})$$

is continuous, but not necessarily differentiable. Therefore, it can be regarded as a generalized solution of the Schrödinger equation $\mathrm{i}\hbar\dot{\psi}(t) = H\psi(t), t \in \mathbb{R}$.

Measurement of observables. Suppose that we are given a normalized state $\varphi \in \mathcal{S}(\mathbb{R})$, that is,

$$||\varphi||^2 = \int_{\mathbb{R}} |\varphi(x)|^2 dx = 1.$$

By the Parseval equation,

$$||\hat{\varphi}||^2 = \int_{\mathbb{R}} |\hat{\varphi}(p)|^2 dp = ||\varphi||^2 = 1.$$

Let us now measure the position, the momentum, and the energy of a quantum particle on the real line where the particle is in the normalized state $\varphi \in \mathcal{S}(\mathbb{R})$.

(i) Measurement of position: For the mean value $\bar{x}$ and the mean fluctuation $\Delta x \geq 0$ of the particle position, we get

$$\bar{x} = \langle \varphi | Q\varphi \rangle = \int_{\mathbb{R}} x|\varphi(x)|^2 dx$$

and

$$(\Delta x)^2 = \langle \varphi | (Q - \bar{x}I)^2 \varphi \rangle = \int_{\mathbb{R}} (x - \bar{x})^2 |\varphi(x)|^2 dx.$$

The number $\int_J |\varphi(x)|^2 dx$ is the probability for measuring the particle position in the interval J.

[35] Fix $t \in \mathbb{R}$. The symbol $\psi(t)$ (resp. $\hat{\psi}(t)$) stands for the function $x \mapsto \psi(x,t)$ (resp. $p \mapsto \hat{\psi}(p,t)$) on $\mathbb{R}$.

(ii) Measurement of momentum: For the mean value $\bar{p}$ and the mean fluctuation Δp of the particle momentum, we get

$$\bar{p} = \langle \varphi | P\varphi \rangle = \langle \hat{\varphi} | \hat{P}\hat{\varphi} \rangle = \int_{\mathbb{R}} p \, |\hat{\varphi}(p)|^2 dp$$

and

$$\Delta p = \langle \varphi | (P - \bar{p}I)^2 \varphi \rangle = \int_{\mathbb{R}} (p - \bar{p})^2 |\hat{\varphi}(p)|^2 dp.$$

The number $\int_J |\hat{\varphi}(p)|^2 dp$ is the probability for measuring the particle momentum in the interval J.

(iii) Measurement of energy: Suppose we are given a measuring instrument which analyzes the energy of freely moving particles. The measured energy corresponds to the observable H. For the mean value $\bar{E}$ and the mean fluctuation ΔE of the energy in the normalized state $\varphi \in \mathcal{S}(\mathbb{R})$, we get

$$\bar{E} = \langle \varphi | H\varphi \rangle = \langle \hat{\varphi} | \hat{H}\hat{\varphi} \rangle = \int_{\mathbb{R}} E(p) |\hat{\varphi}(p)|^2 dp$$

and

$$\Delta E = \langle \varphi | (H - \bar{E}I)^2 \varphi \rangle = \int_{\mathbb{R}} (E(p) - \bar{E})^2 |\hat{\varphi}(p)|^2 dp.$$

The number

$$\int_{E(p) \in J} |\hat{\varphi}(p)|^2 dp$$

is the probability for measuring the particle energy in the given energy interval J. Recall that $E(p) = p^2/2m$. Fix the positive real number E. Then we have $E(p) \leq E$ iff $|p|^2 \leq 2mE$. Thus, the number

$$\int_{|p| \leq \sqrt{2mE}} |\hat{\varphi}(p)|^2 dp$$

is equal to the probability for measuring the energy $E(p)$ of the particle in the interval $[0, E]$.

The full functional-analytic approach to the free quantum particle will be studied in Sect. 7.6.4 on page 509.

7.4.4 The Harmonic Oscillator

Let us quantize the classical harmonic oscillator in the sense of Schrödinger's quantum mechanics. We will see that we obtain the same results as in Heisenberg's version of quantum mechanics. In Sect. 7.4.5, we will explain why Schrödinger's quantum mechanics is equivalent to Heisenberg's quantum mechanics. Choosing $\varphi \in \mathcal{S}(\mathbb{R})$, recall the definition of the position operator Q and the momentum operator P,

$$(Q\varphi)(x) := x\varphi(x), \qquad (P\varphi)(x) := -\mathrm{i}\hbar\varphi'(x) \qquad \text{for all} \quad x \in \mathbb{R}.$$

Quantization means that we replace the classical Hamiltonian function

$$H(q,p) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}$$

by the Hamiltonian operator

$$\boxed{H := \frac{P^2}{2m} + \frac{m\omega^2 Q^2}{2}.}$$

The Schrödinger equation for the wave function $\psi = \psi(x,t),\ x,t \in \mathbb{R}$, reads as

$$\boxed{\mathrm{i}\hbar\dot{\psi} = H\psi} \tag{7.46}$$

along with the prescribed initial condition $\psi(x,0) = \psi_0(x)$ for all $x \in \mathbb{R}$. Explicitly,

$$\mathrm{i}\hbar\psi_t(x,t) = -\frac{\hbar^2}{2m}\psi_{xx}(x,t) + \frac{m\omega^2 x^2}{2}\,\psi(x,t), \qquad x,t \in \mathbb{R}.$$

We are going to show that

The Hamiltonian operator H knows all about the quantized harmonic oscillator.

This is a typical feature for all quantum systems. Making the classic Fourier ansatz

$$\psi(x,t) := \varphi(x)\mathrm{e}^{-\mathrm{i}Et/\hbar}, \qquad x,t \in \mathbb{R},$$

we get the stationary Schrödinger equation

$$\boxed{E\varphi = H\varphi} \tag{7.47}$$

for the time-independent function φ. Explicitly,

$$E\varphi(x) = -\frac{\hbar^2}{2m}\,\varphi''(x) + \frac{m\omega^2}{2}\,x^2\varphi(x), \qquad x \in \mathbb{R}.$$

Again let us use the typical length $x_0 := \sqrt{\frac{\hbar}{\omega m}}$.

The eigensolutions of the Hamiltonian. Our mathematical investigation of the quantized harmonic oscillator will be based on the eigensolutions of the Hamiltonian. Motivated by Sect. 7.2, the basic trick is to introduce the two operators $a, a^\dagger : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ by letting

$$a := \frac{1}{\sqrt{2}}\left(\frac{Q}{x_0} + \frac{\mathrm{i}x_0 P}{\hbar}\right), \qquad a^\dagger := \frac{1}{\sqrt{2}}\left(\frac{Q}{x_0} - \frac{\mathrm{i}x_0 P}{\hbar}\right). \tag{7.48}$$

This forces the crucial factorization

$$H = \hbar\omega(a^\dagger a + \tfrac{1}{2})$$

of the Hamiltonian operator. Starting from the Gaussian probability density,

$$\varrho(x) := \frac{\mathrm{e}^{-x^2/2\sigma^2}}{\sigma\sqrt{2\pi}},$$

with the mean value $\bar{x} = 0$ and the mean fluctuation $\sigma := \frac{x_0}{\sqrt{2}}$, we define

$$\varphi_0(x) := \sqrt{\varrho(x)} \qquad \text{for all} \quad x \in \mathbb{R}.$$

The following theorem is basic for quantum physics.

Theorem 7.10 *The Hamiltonian H of the quantized harmonic oscillator has the eigensolutions $H\varphi_n = E_n\varphi_n$, $n = 0, 1, 2, , ...$ with the energy eigenvalues*

$$\boxed{E_n := \hbar\omega(n + \tfrac{1}{2})} \tag{7.49}$$

and the eigenstates

$$\varphi_n := \frac{(a^\dagger)^n}{\sqrt{n!}}\ \varphi_0.$$

The system $\varphi_0, \varphi_1, ...$ forms a complete orthonormal system in the Hilbert space $L_2(\mathbb{R})$.

Proof. To simplify notation, let $x_0 = 1$ by the rescaling $x \mapsto x/x_0$. The proof follows then from Sect. 7.2 on page 432. □

Explicitly, for all $x \in \mathbb{R}$ and $n = 0, 1, 2, ...$, we have

$$\varphi_n(x) = \frac{1}{\sqrt{2^n n! x_0 \sqrt{\pi}}}\ H_n\left(\frac{x}{x_0}\right)\ \exp\left\{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2\right\}.$$

Mnemonically, physicists write $|E_n\rangle$ instead of φ_n.

Corollary 7.11 *For $n = 0, 1, 2, ...$,*
(i) $\bar{x} = \langle\varphi_n|Q\varphi_n\rangle = 0$;
(ii) $(\Delta x)^2 = \langle\varphi_n|(Q - \bar{x}I)^2\varphi_n\rangle = x_0^2(n + \frac{1}{2})$;
(iii) $\bar{p} = \langle\varphi_n|P\varphi_n\rangle = 0$;
(iv) $(\Delta p)^2 = \langle\varphi_n|(P - \bar{p}I)^2\varphi_n\rangle = \frac{\hbar^2}{x_0^2}(n + \frac{1}{2})$.

Proof. Let $x_0 = 1$ by the rescaling $x \mapsto x/x_0$.

Ad (i), (iii). Note that the Hermite functions φ_n are odd or even by (7.8). Hence

$$\int_{\mathbb{R}} x|\varphi_n(x)|^2 dx = 0, \qquad \int_{\mathbb{R}} \varphi_n(x)^\dagger \varphi_n'(x) dx = 0.$$

Ad (ii). Let $n = 0, 1, 2, ...$ By Sect. 7.2,

$$a\varphi_{n+1} = \sqrt{n+1}\ \varphi_n, \qquad a^\dagger\varphi_n = \sqrt{n+1}\ \varphi_{n+1}, \qquad a^\dagger a\varphi_n = n\varphi_n.$$

From $2\langle\varphi_n|Q^2\varphi_n\rangle = \langle\varphi_n|(a + a^\dagger)^2\varphi_n\rangle$ we get

$$2\langle\varphi_n|Q^2\varphi_n\rangle = \langle\varphi_n|(a^2 + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)\varphi_n\rangle = 2n + 1.$$

In fact, because of $\langle\varphi_{n+1}|\varphi_{n-1}\rangle = 0$, we obtain

$$\langle\varphi_n|a^2\varphi_n\rangle = \langle a^\dagger\varphi_n|a\varphi_n\rangle = 0.$$

Moreover, $\langle\varphi_n|aa^\dagger\varphi_n\rangle = \langle a^\dagger\varphi_n|a^\dagger\varphi_n\rangle = n + 1$.

Ad (iv). Similarly, $2\langle\varphi_n|P^2\varphi_n\rangle = -\hbar^2\langle\varphi_n|(a - a^\dagger)^2\varphi_n\rangle = \hbar^2(2n + 1)$. □

Physical interpretation. Let us discuss some physical consequences.

(i) Ground state: The state

$$\psi(x,t) := \mathrm{e}^{-\mathrm{i}E_0 t/\hbar}\varphi_0(x), \qquad t,x \in \mathbb{R}$$

represents the lowest-energy state of the harmonic oscillator called ground state (or vacuum state). The sharp energy of the ground state equals $E_0 = \hbar/2$. For the mean position $\bar{x}$ and the mean fluctuation Δx of the particle position in the ground state, it follows from Corollary 7.11 that

$$\bar{x} = 0, \qquad \Delta x = \sigma = \frac{x_0}{\sqrt{2}}.$$

For the mean momentum $\bar{p}$ and the mean fluctuation Δp of the particle momentum in the ground state, we get $\bar{p} = 0$ and $\Delta x \Delta p = \frac{\hbar}{2}$.

(ii) The uncertainty inequality: In the normalized state

$$\psi(x,t) := \mathrm{e}^{-\mathrm{i}E_n t/\hbar}\varphi_n(x), \qquad n = 0,1,\ldots,$$

the particle has the sharp energy $E_n = \hbar\omega(n+\frac{1}{2})$, and

$$\bar{x} = 0, \qquad \Delta x = x_0\sqrt{n+\tfrac{1}{2}}$$

as well as

$$\bar{p} = 0, \qquad \Delta x \Delta p = \frac{E_n}{\omega} = \hbar\left(n+\tfrac{1}{2}\right).$$

From this we get

$$\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}.}$$

In 1927 Heisenberg discovered that this inequality is the special case of a fundamental law in nature called the uncertainty of position and momentum (see Sect. 7.4.6 on page 475).

(iii) Measurement of energy: The energy states $\varphi_0, \varphi_1, \ldots$ form a complete orthonormal system in the Hilbert space $L_2(\mathbb{R})$.[36] This means that we have the orthogonality relation

$$\langle\varphi_n|\varphi_m\rangle = \int_{\mathbb{R}} \varphi_n(x)^\dagger \varphi_m(x)dx = \delta_{nm}, \qquad n,m = 0,1,2,\ldots.$$

Completeness means that for each $\chi \in L_2(\mathbb{R})$, the Fourier series

$$\chi = \sum_{n=0}^{\infty} \langle\varphi_n|\chi\rangle\varphi_n$$

converges in the Hilbert space $L_2(\mathbb{R})$. In other words,

$$\lim_{N\to+\infty} \int_{\mathbb{R}} \left|\chi(x) - \sum_{n=0}^{N} \langle\varphi_n|\chi\rangle\varphi_n(x)\right|^2 dx = 0.$$

Moreover, for given complex numbers a_n, the series $\sum_{n=0}^{\infty} a_n\varphi_n$ converges in $L_2(\mathbb{R})$ iff

[36] The properties of complete orthonormal systems in Hilbert spaces are thoroughly studied in Zeidler (1995a), Sect. 3.1 (see the references on page 1049).

$$\sum_{n=0}^{\infty} |a_n|^2 < \infty. \tag{7.50}$$

In addition, for all $\chi, \varphi \in L_2(\mathbb{R})$, we have the Parseval equation

$$\langle \chi | \varphi \rangle = \sum_{n=0}^{\infty} \langle \chi | \varphi_n \rangle \langle \varphi_n | \varphi \rangle. \tag{7.51}$$

Suppose now that $\langle \chi | \chi \rangle = 1$. Then

$$\sum_{n=0}^{\infty} |\langle \chi | \varphi_n \rangle|^2 = 1.$$

This motivates the following definition. If the particle is in the normalized state χ, then the number

$$\boxed{\sum_{E_n \in J} |\langle \varphi_n | \chi \rangle|^2}$$

is equal to the probability of measuring the energy value E of the particle in the interval J. In particular, choosing the open interval $J :=]-\infty, E[$, we obtain the energy distribution function

$$\mathsf{F}(E) := \sum_{E_n < E} |\langle \varphi_n | \chi \rangle|^2. \tag{7.52}$$

In particular, in the state χ we measure the mean energy

$$\bar{E} = \int_{\mathbb{R}} E \, d\mathsf{F}(E) = \sum_{n=0}^{\infty} E_n |\langle \varphi_n | \chi \rangle|^2$$

and the mean energy fluctuation

$$(\Delta E)^2 = \int_{\mathbb{R}} (E - \bar{E})^2 d\mathsf{F}(E) = \sum_{n=0}^{\infty} (E_n - \bar{E})^2 |\langle \varphi_n | \chi \rangle|^2.$$

(iv) Self-adjoint extension of the formally self-adjoint Hamiltonian H: Let us define an operator $H : D(H) \subseteq L_2(\mathbb{R}) \to L_2(\mathbb{R})$ by setting

$$H\psi := \sum_{n=0}^{\infty} E_n \langle \varphi_n | \psi \rangle \varphi_n.$$

Naturally enough, an element $\psi \in L_2(\mathbb{R})$ belongs to the domain of definition, $D(H)$, of the operator H iff the infinite series converges. This means that $\sum_{n=0}^{\infty} E_n^2 |\langle \varphi_n | \psi \rangle|^2 < \infty$. The operator $H : D(H) \to L_2(\mathbb{R})$ is an extension of the operator $H : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$. In fact, if $\psi \in \mathcal{S}(\mathbb{R})$, then we obtain $\langle \varphi_n | H\psi \rangle = \langle H\varphi_n | \psi \rangle = E_n \langle \varphi_n | \psi \rangle$. Hence

$$H\psi = \sum_{n=0}^{\infty} \langle \varphi_n | H\psi \rangle \varphi_n = \sum_{n=0}^{\infty} E_n \langle \varphi_n | \psi \rangle \varphi_n.$$

The quantum dynamics of the harmonic oscillator. For each initial state ψ_0 in $L_2(\mathbb{R})$ and each time $t \in \mathbb{R}$, we define

$$\mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0 := \sum_{n=0}^{\infty} \mathrm{e}^{-\mathrm{i}E_n t/\hbar}\langle\varphi_n|\psi_0\rangle\varphi_n.$$

This series is convergent because of

$$\sum_{n=0}^{\infty} |\mathrm{e}^{-\mathrm{i}E_n t/\hbar}\langle\varphi_n|\psi_0\rangle|^2 = \sum_{n=0}^{\infty} |\langle\varphi_n|\psi_0\rangle|^2 = ||\psi_0||^2 < \infty.$$

By definition, the equation

$$\boxed{\psi(t) = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0 \qquad \text{for all} \quad t \in \mathbb{R}}$$

describes the dynamics of the quantum harmonic oscillator on the real line. The following theorem motivates this definition.

Theorem 7.12 *For each time $t \in \mathbb{R}$, the operator $e^{-iHt/\hbar} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ is unitary.*

For given initial value $\psi_0 \in D(H)$, the function $\psi(t) := e^{-\mathrm{i}Ht/\hbar}\psi_0$ satisfies the Schrödinger equation $\mathrm{i}\hbar\dot{\psi}(t) = H\psi(t)$ for all times $t \in \mathbb{R}$.

Proof. For each $\psi_0 \in L_2(\mathbb{R})$ and all $t, s \in \mathbb{R}$,

$$\mathrm{e}^{-\mathrm{i}Hs/\hbar}(\mathrm{e}^{-\mathrm{i}\hbar Ht/\hbar}\psi_0) = \sum_{n=0}^{\infty} \mathrm{e}^{-\mathrm{i}E_n s/\hbar}\mathrm{e}^{-\mathrm{i}E_n t/\hbar}\langle\varphi_n|\psi_0\rangle\varphi_n = \mathrm{e}^{-\mathrm{i}H(t+s)/\hbar}\psi_0.$$

Choosing $s = -t$, this implies

$$\mathrm{e}^{\mathrm{i}Ht/\hbar}(\mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0) = \psi_0.$$

Thus, the operator $\mathrm{e}^{\mathrm{i}tH/\hbar}$ is the inverse operator to the operator $\mathrm{e}^{-\mathrm{i}tH/\hbar}$ on the Hilbert space $L_2(\mathbb{R})$. Moreover, because of $|\mathrm{e}^{-\mathrm{i}E_n t/\hbar}| = 1$ it follows from the Parseval equation that

$$||\mathrm{e}^{-\mathrm{i}tH/\hbar}\psi_0||^2 = \sum_{n=0}^{\infty} |\mathrm{e}^{-\mathrm{i}tE_n/\hbar}|^2|\langle\varphi_n|\psi_0\rangle|^2 = ||\psi_0||^2.$$

Therefore, the operator $\mathrm{e}^{-\mathrm{i}Ht/\hbar} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ is bijective and norm preserving, i.e., this operator is unitary. In particular, if the initial state ψ_0 is normalized, then so is $\mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0$ for each time $t \in \mathbb{R}$.

Choose now $\psi_0 \in D(H)$. Formal differentiation with respect to time t yields

$$\mathrm{i}\hbar\dot{\psi}(t) = \sum_{n=0}^{\infty} E_n \mathrm{e}^{-\mathrm{i}E_n t/\hbar}\langle\varphi_n|\psi_0\rangle\varphi_n.$$

To justify this formal differentiation, it is sufficient to use the following majorant series[37]

[37] We refer to Zeidler (1995a), Sect. 5.8 (see the references on page 1049).

$$\sum_{n=0}^{\infty} |E_n \mathrm{e}^{-\mathrm{i}E_n t/\hbar}\langle\varphi_n|\psi_0\rangle|^2 \le \sum_{n=0}^{\infty} |E_n\langle\varphi_n|\psi_0\rangle|^2 = ||H\psi_0||^2 < \infty. \qquad \square$$

Transition probabilities. Let ψ_0 and ψ_1 be two normalized states in the Hilbert space $L_2(\mathbb{R})$. By definition, the real number

$$\boxed{\tau := |\langle\psi_1|\mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0\rangle|^2}$$

represents the transition probability from the initial state ψ_0 to the final state ψ_1 during the time interval $[0, t]$. In order to motivate this definition, observe that

- $0 \le \tau \le 1$;
- $\tau = 1$ for the final state $\psi_1 := \mathrm{e}^{-\mathrm{i}tH/\hbar}\psi_0$;
- $\sum_{n=0}^{\infty} \tau_n = 1$ if τ_n corresponds to the final energy state φ_n, i.e.,

$$\tau_n := |\langle\varphi_n|\mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0\rangle|^2.$$

In fact, it follows from the Schwarz inequality that

$$\tau \le ||\psi_1|| \cdot ||\mathrm{e}^{-\mathrm{i}tH/\hbar}\psi_0|| = ||\psi_1|| \cdot ||\psi_0|| = 1.$$

Moreover, $\langle \mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0|\mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0\rangle = \langle\psi_0|\psi_0\rangle = 1$. Finally,

$$\sum_{n=0}^{\infty} |\langle\varphi_n|\mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0\rangle|^2 = ||\mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0||^2 = ||\psi_0||^2 = 1.$$

7.4.5 The Passage to the Heisenberg Picture

Using the harmonic oscillator, we want to discuss in which sense the Heisenberg approach to quantum mechanics is equivalent to the Schrödinger approach.

Formal approach. The basic transformation from the Schrödinger picture to the Heisenberg picture reads as

$$\boxed{\psi(t) \mapsto \psi(0), \qquad A \mapsto A(t) := \mathrm{e}^{\mathrm{i}Ht/\hbar} A \mathrm{e}^{-\mathrm{i}Ht/\hbar}}$$

for all times $t \in \mathbb{R}$.

(S) Schrödinger picture: In this setting, the states $\psi(t)$ of the quantum harmonic oscillator on the real line are elements of the Hilbert space $L_2(\mathbb{R})$ which depend on time t,

$$\psi(t) = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi(0), \qquad t \in \mathbb{R}.$$

The formal observables are formally self-adjoint operators

$$A : D(A) \subseteq L_2(\mathbb{R}) \to L_2(\mathbb{R})$$

which do not depend on time t. Differentiating the state function $t \mapsto \psi(t)$ with respect to time t, we get the Schrödinger equation

$$\boxed{\mathrm{i}\hbar\dot{\psi}(t) = H\psi(t), \qquad t \in \mathbb{R}.}$$

(H) Heisenberg picture: Here, the states $\psi(0)$ of the quantum harmonic oscillator are elements of the Hilbert space $L_2(\mathbb{R})$ which do not depend on time t. The formal observables $A(t)$ are operators on the Hilbert space $L_2(\mathbb{R})$ which depend on time t. Differentiating the function $t \mapsto A(t)$ with respect to time, we get the Heisenberg equation

$$\boxed{\mathrm{i}\hbar\dot{A}(t) = A(t)H - HA(t), \qquad t \in \mathbb{R}.}$$

From the physical point of view, we are interested in measurements of quantities in physical experiments. The point is that both the Schrödinger picture and the Heisenberg picture yield the same mean values. Explicitly,

$$\boxed{\bar{A}(t) = \langle\psi(t)|A\psi(t)\rangle = \langle\psi(0)|A(t)\psi(0)\rangle.}$$

Rigorous approach. Let us start with the Schrödinger picture for the quantum harmonic oscillator on the real line. Consider the self-adjoint Hamiltonian $H : D(H) \subseteq L_2(\mathbb{R}) \to L_2(\mathbb{R})$ introduced in Sect. 7.4.4. Explicitly,

$$H\varphi = \sum_{n=0}^{\infty} E_n \langle\varphi_n|\varphi\rangle\varphi_n.$$

Here, we have $\varphi \in D(H)$ iff this series is convergent in the Hilbert space $L_2(\mathbb{R})$. Define

$$D_0(H) := \mathrm{span}\{\varphi_0, \varphi_1, \varphi_2, ...\},$$

i.e., $D_0(H)$ is the set of finite linear combinations of the eigenfunctions $\varphi_0, \varphi_1, ...$ with complex coefficients.

Theorem 7.13 *Let $A : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$ be a formally self-adjoint operator which maps $D_0(H)$ into itself. Then, for each $\varphi \in D_0(H)$ and all times $t \in \mathbb{R}$, the expression*

$$A(t)\varphi := e^{\mathrm{i}Ht/\hbar} A e^{-\mathrm{i}Ht/\hbar}\varphi$$

is well-defined, and we have the differential equation

$$i\hbar\frac{d}{dt}(A(t)\varphi) = (A(t)H - HA(t))\varphi.$$

Proof. All of the expressions are well-defined, since they refer to finite linear combinations of the eigenfunctions $\varphi_0, \varphi_1, ...$ Note that $\mathrm{e}^{-\mathrm{i}Ht/\hbar}\varphi_n$ is equal to $\mathrm{e}^{-\mathrm{i}E_n t/\hbar}\varphi_n$, and we have $A\varphi_n \in D_0(H)$ for all n. □

Example. The transformation of the formal observables

$$Q, P : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$$

from the Schrödinger picture to the Heisenberg picture yields

$$Q(t)\varphi = \frac{x_0}{\sqrt{2}}\,(a^\dagger \mathrm{e}^{\mathrm{i}\omega t} + a\mathrm{e}^{-\mathrm{i}\omega t})\varphi$$

and

$$P(t)\varphi = \frac{\mathrm{i}\hbar}{x_0\sqrt{2}}\,(a^\dagger \mathrm{e}^{\mathrm{i}\omega t} - a\mathrm{e}^{-\mathrm{i}\omega t})\varphi$$

for all $\varphi \in D_0(H)$ and all times $t \in \mathbb{R}$.

Proof. To simplify notation, let $x_0 = \hbar = 1$. It follows from the basic relations $\mathrm{e}^{\mathrm{i}Ht}\varphi_n = \mathrm{e}^{\mathrm{i}E_n t}\varphi_n$ and $a\varphi_n = \sqrt{n}\,\varphi_{n-1}$ that

$$\mathrm{e}^{\mathrm{i}Ht}a\varphi_n = \mathrm{e}^{\mathrm{i}E_{n-1}t}a\varphi_n.$$

Noting that $E_n = \omega(n + \frac{1}{2})$,

$$\mathrm{e}^{\mathrm{i}Ht}a\mathrm{e}^{-\mathrm{i}Ht}\varphi_n = \mathrm{e}^{\mathrm{i}E_{n-1}t}\mathrm{e}^{-\mathrm{i}E_n t}a\varphi_n = \mathrm{e}^{-\mathrm{i}\omega t}a\varphi_n.$$

Similarly, $a^\dagger\varphi_n = \sqrt{n+1}\,\varphi_{n+1}$ implies

$$\mathrm{e}^{\mathrm{i}Ht}a^\dagger\mathrm{e}^{-\mathrm{i}Ht}\varphi_n = \mathrm{e}^{\mathrm{i}E_{n+1}t}\mathrm{e}^{\mathrm{i}E_n t}a^\dagger\varphi_n = \mathrm{e}^{\mathrm{i}\omega t}a^\dagger\varphi_n.$$

Summarizing,

$$\mathrm{e}^{\mathrm{i}Ht}Q\mathrm{e}^{-\mathrm{i}Ht}\varphi_n = \frac{1}{\sqrt{2\omega}}\,\mathrm{e}^{\mathrm{i}Ht}(a^\dagger + a)\mathrm{e}^{-\mathrm{i}Ht}\varphi_n = Q(t)\varphi_n.$$

The proof for P proceeds similarly. □

7.4.6 Heisenberg's Uncertainty Principle

In 1927 Heisenberg discovered that there exists a deep difference between classical mechanics and quantum mechanics.[38] He derived the following fundamental result in quantum physics:

> *The classical notion of the trajectory of a particle, which has a precise position and a precise velocity at the same time, is not meaningful anymore in quantum mechanics.*

Explicitly, for the operators $Q, P : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$ called position operator Q and momentum operator P, we have the Heisenberg commutation relation

$$\boxed{(QP - PQ)\varphi = \mathrm{i}\hbar\varphi \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).} \tag{7.53}$$

Let $\varphi \in \mathcal{S}(\mathbb{R})$ be a normalized state in the Hilbert space $L_2(\mathbb{R})$. We claim that

$$\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}.} \tag{7.54}$$

This means that it is impossible to measure precisely the position and the momentum of the quantum particle in the state φ at the same time. The uncertainty inequality (7.54) follows from (7.53) as a special case of Theorem 10.4 on page 524 of Vol. I.

[38] W. Heisenberg, The intuitive meaning of kinematics in quantum mechanics, Z. Physik **43** (1927), 172–199 (in German).

7.4.7 Unstable Quantum States and the Energy-Time Uncertainty Relation

> In particle accelerators, many particles are unstable; such so-called resonances only live a very short time.
>
> Folklore

We are going to show that wave packets are unstable in quantum mechanics. There exists a fundamental inequality between the life-time of the wave packet and its mean energy fluctuation which is called the energy–time uncertainty relation.

Wave packets and the Fourier transformation. Let $E(p) := p^2/2m$ denote the energy of a freely moving classical particle on the real line with mass m, momentum $p \in \mathbb{R}$, and velocity $v = p/m$. For each nonzero complex number C, the standing plane wave

$$\psi(x,t) := Ce^{-\mathrm{i}tE(p)/\hbar}\, e^{\mathrm{i}px/\hbar}, \qquad x,t \in \mathbb{R}$$

describes a stream of particles with mass m, momentum p, velocity $v = p/m$, energy $E(p)$, and particle density $\varrho = |C|^2$. Since $|\psi(x,t)|^2 = |C|^2$, the wave function ψ does not live in the Hilbert space $L_2(\mathbb{R})$. However, using the superposition

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A(p) e^{-itE(p)/\hbar}\, e^{\mathrm{i}px/\hbar} dp \tag{7.55}$$

of standing plane waves with different momenta, we can construct so-called wave packets which live in the Hilbert space $L_2(\mathbb{R})$ if the amplitude function $A = A(p)$ lives in the space $\mathcal{S}(\mathbb{R})$. The Fourier transformation yields

$$A(p)e^{-iE(p)t/\hbar} = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x,t) \mathrm{e}^{-\mathrm{i}xp/\hbar} dx.$$

Let us consider a typical example. Choose the Gauss distribution

$$A(p) = \frac{1}{\sqrt{\Delta p \sqrt{2\pi}}}\ \exp\left(-\frac{(p-\bar{p})^2}{4(\Delta p)^2}\right), \tag{7.56}$$

where the real numbers $\bar{p}$ and $\Delta p > 0$ are given. In order to understand the physics of wave packets, let us introduce the following quantities

$$\Delta x_0 := \frac{\hbar}{2\Delta p}, \qquad \Delta E := \frac{(\Delta p)^2}{2m}, \qquad \Delta t := \frac{\hbar}{2\Delta E},$$

and $\bar{v} := \bar{p}/m$, $\bar{x} := \bar{v}t$, , $\bar{E} := \bar{p}^2/2m$, as well as

$$\Delta x = \Delta x_0 \sqrt{1 + \left(\frac{t}{\Delta t}\right)^2}. \tag{7.57}$$

The following proposition summarizes the properties of the wave packet.

Proposition 7.14 *The absolute value of the wave function ψ from (7.55), (7.56) is a Gauss function,*

$$|\psi(x,t)|^2 = \frac{1}{\Delta x\sqrt{2\pi}} \exp\left(-\frac{(x-\bar{x})^2}{2(\Delta x)^2}\right).$$

The mean values and mean fluctuations of the position operator Q and the momentum operator P in the state ψ at time t are $\bar{x}, \Delta x, \bar{p}, \Delta p$, respectively.

This follows by using classical formulas for Gauss–Fresnel integrals. □

This result allows the following physical interpretation. The wave function ψ lives in the Hilbert space $L_2(\mathbb{R})$. It represents a particle with mean momentum $\bar{p}$, mean energy $\bar{E}$, mean fluctuation of momentum Δp and mean fluctuation of energy ΔE. Moreover, the mean position $\bar{x} = \bar{v}t$ of the particle moves with the velocity $\bar{v} = \bar{p}/m$ called the group velocity of the wave packet. It is quite remarkable that

The wave packet is unstable.

In fact, by (7.57), the mean fluctuations Δx of the position of the particle go to infinity as time goes to infinity, that is, the particle is spread over the whole real line after a sufficiently long time. The lifetime of the particle can be measured by the quantity Δt. According to (7.57), the position fluctuations Δx increase in the time interval $[0, \Delta t]$ by the factor $\sqrt{2}$.

The energy-time uncertainty principle. The equation

$$\Delta p \Delta x = \frac{\hbar}{2}$$

for the ground state of a harmonic oscillator represents a special case of the general momentum-position uncertainty inequality $\Delta p \Delta x \geq \frac{\hbar}{2}$. It shows that the Heisenberg uncertainty inequality cannot be improved. Furthermore, we have the equation

$$\Delta E \Delta t = \frac{\hbar}{2}$$

for the Gaussian wave packet. In general, physicists assume that for all unstable particles, there holds the energy-time uncertainty inequality

$$\boxed{\Delta E \Delta t \geq \frac{\hbar}{2}} \tag{7.58}$$

for the lifetime Δt of the particle and its energy fluctuation ΔE. In high-energy particle accelerators, physicists observe frequently so-called resonances. These are unstable particles of mass Δm which decay after the time Δt. By Einstein's mass-energy equivalence, we have

$$\Delta E = c^2 \Delta m$$

where c denotes the speed of light in a vacuum. From (7.58) we get the following fundamental inequality in particle physics

$$\boxed{\Delta m \Delta t \geq \frac{\hbar}{2c^2}}$$

between the mass Δm of a resonance and its lifetime Δt.

The energy-time uncertainty principle is motivated by Einstein's theory of special relativity. Let us explain this. In special relativity, an event corresponds to a four-vector

$$(x, y, z, ct)$$

in Minkowski space. This is a combination of space and time. Similarly, there exists a combination of momentum (p_x, p_y, p_z) and energy E described by the four-vector

$$(p_x, p_y, p_z, \frac{E}{c}).$$

The momentum-energy uncertainty principle yields

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}, \quad \Delta p_y \Delta y \geq \frac{\hbar}{2}, \quad \Delta p_z \Delta z \geq \frac{\hbar}{2}.$$

Postulating complete relativistic symmetry in nature, we can replace p_x and x by E/c and ct, respectively. This yields (7.58).

The energy-time uncertainty inequality represents one of the basic principles of modern physics. Physicists call the ground state of our world the vacuum. This ground state cannot be observed in a straight-forward way. However, there exist quantum fluctuations of the vacuum which can be observed as physical effects; for example, this concerns the fine structure of the energy spectrum of the hydrogen atom, the anomalous magnetic moment of the electron, and the vaporization of black holes in the universe. To understand this, one needs the methods of quantum field theory.

7.4.8 Schrödinger's Coherent States

There arises the following question: Is it possible to construct a stable time-dependent wave packet by the superposition of time-dependent eigenstates of the quantum harmonic oscillator? The positive answer was found by Schrödinger in 1926.[39] For each complex number $\alpha = |\alpha| e^{i\delta}$, we define the coherent state

$$\boxed{\psi_\alpha(x,t) := e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} e^{-iE_n t/\hbar} \varphi_n(x) \frac{\alpha^n}{\sqrt{n!}}, \qquad x, t \in \mathbb{R}}$$

where the pair $\varphi_n, E_n = \hbar\omega(n + \frac{1}{2})$ is the nth eigensolution of the Hamiltonian for the quantum harmonic oscillator. For each $\alpha \in \mathbb{C}$, the function ψ_α possesses the following properties:

(i) Schrödinger equation: ψ_α is a solution of the time-dependent Schrödinger equation for the harmonic oscillator.

(ii) Normalization: $x \mapsto \psi_\alpha(x,t)$ is a normalized state in the Hilbert space $L_2(\mathbb{R})$ for each time $t \in \mathbb{R}$.

(iii) Mean position: $\bar{x}(t) = \langle \psi_\alpha(t) | Q \psi_\alpha \rangle = \sqrt{2}\, x_0 |\alpha| \cos(\omega t - \delta)$ for all times $t \in \mathbb{R}$. Recall that $x_0 := \sqrt{\hbar/m\omega}$.

(iv) Probability density: For all $x, t \in \mathbb{R}$,

$$|\psi_\alpha(x,t)|^2 = \frac{1}{\sigma\sqrt{2\pi}}\, e^{-(x-\bar{x}(t))^2/2\sigma^2}.$$

This is a Gaussian distribution where the mean value $\bar{x}(t)$ oscillates with the angular frequency ω, and the time-independent mean fluctuation is given by $\sigma = x_0/\sqrt{2}$.

(v) Eigenvectors of the annihilation operator: $a\psi_\alpha(x,0) = \alpha\psi_\alpha(x,0)$ for all $x \in \mathbb{R}$.

Let us prove this. Explicitly, for all $x, t \in \mathbb{R}$,

$$\psi_\alpha(x,t) = \frac{1}{\sqrt{x_0 2^n \sqrt{\pi}}}\, e^{-|\alpha|^2/2}\, e^{-x^2/2x_0^2}\, e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{\alpha^n e^{-in\omega t}}{n!}\, H_n\left(\frac{x}{x_0}\right).$$

The generating function for the Hermite polynomials reads as

[39] E. Schrödinger, The continuous passage from micromechanics to macromechanics, Naturwissenschaften **44** (1926), 664–666 (in German).

$$A\mathrm{e}^{-\xi^2+2\xi\eta} = A\sum_{n=0}^{\infty} \frac{\xi^n}{n!}\, H_n(\eta).$$

Choosing the quantities

$$\xi := \frac{\alpha \mathrm{e}^{-\mathrm{i}\omega t}}{\sqrt{2}}, \quad \eta := \frac{x}{x_0}, \quad A := \frac{1}{\sqrt{x_0\sqrt{\pi}}}\, \mathrm{e}^{-|\alpha|^2/2}\, \mathrm{e}^{-x^2/2x_0^2}\, \mathrm{e}^{-\mathrm{i}\omega t/2},$$

we get $\psi_\alpha(x,t) = A\mathrm{e}^{-\xi^2+2\xi\eta}$. The claims follow now easily by using standard calculus formulas along with $\mathrm{e}^{\mathrm{i}z} = \cos z + \mathrm{i}\sin z$. For (v), note that $a\varphi_0 = 0$ and $a\varphi_n = \sqrt{n}\,\varphi_{n-1}$ if $n = 1, 2, \ldots$ □

In the 1960s, coherent states were used in laser optics for the representation of coherent light waves. As a standard textbook on coherent states and laser optics, we recommend the monograph by L. Mandel and E. Wolf, Optical Coherence and Quantum Optics, Cambridge University Press, 1995.

7.5 Feynman's Quantum Mechanics

> It is a curious historical fact that quantum mechanics began with two quite different mathematical formulations: the differential equation of Schrödinger, and the matrix algebra of Heisenberg. The two, apparently dissimilar approaches, were proved to be mathematically equivalent. These two points of view were destined to complement one another and to be ultimately synthesized in Dirac's transformation theory.
>
> This paper will describe what is essentially a third formulation of nonrelativistic quantum theory. This formulation was suggested by some of Dirac's remarks concerning the relation of classical action to quantum mechanics. A probability amplitude is associated with an entire motion of a particle as a function of time, rather than simply with a position of the particle at a particular time.
>
> The formulation is mathematically equivalent to the more usual formulations. There are, therefore, no fundamentally new results. However, there is a pleasure in recognizing old things from a new point of view. Also, there are problems for which the new point of view offers a distinct advantage.[40]
>
> Richard Feynman, 1948

> The calculations that I did for Hans Bethe, using the Schrödinger equation, took me several months of work and several hundred sheets of paper. Dick Feynman (1918–1988) could get the same answer, calculating on a blackboard, in half an hour.[41]
>
> Freeman Dyson, 1979

Convention. Let z be a nonzero complex number with

$$z = |z|\mathrm{e}^{\mathrm{i}\varphi}, \qquad -\pi < \varphi < \pi,$$

that is, we exclude the non-positive real values, $z \le 0$. In the following sections, $\sqrt{z}$ denotes the principal value of the square root defined by

[40] R. Feynman, Space-time approach to nonrelativistic quantum mechanics, Phys. Rev. **20** (1948), 367–387.

[41] F. Dyson, Disturbing the Universe, Harper & Row, New York, 1979.

$$\sqrt{z} := \sqrt{|z|}\, \mathrm{e}^{\mathrm{i}\varphi/2}. \tag{7.59}$$

For example, $\sqrt{\mathrm{i}} = \mathrm{e}^{\mathrm{i}\pi/4}$. If we use the principal values, then the function

$$z \mapsto \sqrt{z} \tag{7.60}$$

is holomorphic on the set $\mathbb{C}\backslash]-\infty, 0]$ (the complex plane cut along the negative real axis). Thus, analytic continuation of the function $f(x) := \sqrt{x}, x > 0$ yields the function (7.60). This fact will be frequently used in what follows. The idea is to pass from time t to imaginary time $\mathrm{i}t$ and to use analytic continuation in order to translate well-known results from diffusion processes to quantum processes. This is called the Euclidean strategy in quantum physics. The following golden rule holds:

> *Apply analytic continuation only to such quantities that you can measure in physical experiments.*

Analytic continuation of functions depending on energy plays a crucial role in studying the following subjects:

- scattering processes,
- the energies energies of bound states, and
- the energies of unstable particles having finite lifetime (called resonances).

For this, we refer to Sect. 8.3.5 on page 713. In terms of the double-sheeted Riemann surface $\mathcal{R}$ of the multi-valued square-root function (used by physicists in quantum physics), the principal value of $\sqrt{z}$ in the open upper (resp. lower) half-plane corresponds to the first (resp. second sheet) of $\mathcal{R}$ (see Fig. 8.6 on page 714).

Similarly, as for the square root, the value $\ln z := \ln|z| + \mathrm{i}\varphi$ is called the principal value of the logarithm, where the argument φ of the square root is uniquely defined as above by the condition $-\pi < \varphi < \pi$. The function $z \mapsto \ln z$ is holomorphic on $\mathbb{C}\backslash]-\infty, 0]$.

7.5.1 Main Ideas

The basic idea of Feynman's approach to quantum mechanics is

- to describe the time-evolution of a quantum system by an integral formula, which is equivalent to the Schrödinger differential equation,
- and to represent the kernel $\mathcal{K}(x, t; y, t_0)$ of the integral formula by a path integral.

From the physical point of view, Feynman emphasized that

> *The description of quantum particles becomes easier if we use probability amplitudes as basic quantities, but not transition probabilities.*

The reason is that, in contrast to transition probabilities, probability amplitudes satisfy a simple composition rule (also called product rule) which is at the heart of Feynman's approach to quantum theory. In terms of finite-dimensional Hilbert spaces, the following hold:

- Feynman's probability amplitudes are precisely the complex-valued Fourier coefficients $c_1, c_2, \ldots, c_n$ of a state vector.
- Feynman's composition rule for probability amplitudes coincides with the Parseval equation (7.81) for Fourier coefficients in mathematics.[42]

[42] Parseval des Chénes (1755–1836), Fourier (1768–1830), Dirac (1902–1984), von Neumann (1903–1957), Laurent Schwartz (1915–2004), Feynman (1918–1988), Gelfand (born 1913).

- The transition probabilities correspond to the quadratic quantities

$$|c_1|^2, |c_2|^2, \ldots, |c_n|^2,$$

which do *not* linearly depend on the corresponding state vector, in contrast to the Fourier coefficients $c_1, c_2, \ldots, c_n$.

In infinite-dimensional Hilbert spaces, one has to replace Fourier series by Fourier integrals and their generalizations (e.g., Fourier–Stieltjes integrals). In physics, this corresponds to the formal Dirac calculus. In terms of mathematics, one has to use von Neumann's spectral theory for self-adjoint operators and the more general Gelfand theory of generalized eigenfunctions based on Laurent Schwartz's language of distributions (generalized functions).

Feynman's integral formula. According to Schrödinger, the motion of a quantum particle of mass $m > 0$ on the real line is described by the differential equation

$$\mathrm{i}\hbar\psi_t(x,t) = -\frac{\hbar^2}{2m}\psi_{xx}(x,t) + U(x)\psi(x,t), \quad \psi(x,t_0) = \psi_0(x), \tag{7.61}$$

for all positions $x \in \mathbb{R}$ and all times $t > t_0$. Feynman used the fact that the solution of this initial-value problem can be represented by the integral formula

$$\boxed{\psi(x,t) = \int_{\mathbb{R}} \mathcal{K}(x,t;x_0,t_0)\psi_0(x_0)dx_0, \qquad x \in \mathbb{R},\ t > t_0.} \tag{7.62}$$

The main task is to compute the kernel $\mathcal{K}$, which is called the (retarded) Feynman propagator kernel. There exist two different methods.[43]

(i) The Fourier method: Following Fourier's approach to the heat conduction equation, one can use eigenfunction expansions (e.g., Fourier series or Fourier integrals) in order to get the kernel $\mathcal{K}$. For the heat kernel, we will discuss this in (7.77) below.[44]

(ii) The path integral method: In his 1942 Princeton dissertation, Feynman (1918–1988) invented the path integral representation

$$\boxed{\mathcal{K}(x,t;x_0,t_0) = \int_{C\{t_0,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\ \mathcal{D}q.} \tag{7.63}$$

Here, we sum over all possible classical paths $q : [t_0, t] \to \mathbb{R}$ on the real line with fixed endpoints: $q(t_0) = x_0$ and $q(t) = x$. The symbol $S[q]$ denotes the classical action of the path $q = q(\tau), t_0 < \tau < t$.

According to Feynman, the passage from classical mechanics to quantum mechanics corresponds to a statistics over all possible classical paths where the statistical weight $e^{\mathrm{i}S[q]/\hbar}$ depends on the classical action.

[43] In terms of finite-dimensional Hilbert spaces, the two methods are thoroughly investigated in Volume I. For the Fourier method (resp. the Feynman path integral method), see formula (7.82) on page 421 of Vol. I (resp. formula (7.78) on page 417 of Vol. I).

[44] J. Fourier, La théorie de la chaleur (heat theory), Paris, 1822. Interestingly enough, Fourier (1768–1830) was obsessed with heat, keeping his rooms extremely hot.

This is a highly intuitive interpretation of the quantization of classical processes. Let us discuss the intuitive background.

Causality and the product rule for the Feynman propagator. The Feynman propagator kernel satisfies the following product rule:

$$\mathcal{K}(x,t;x_0,t_0) = \int_{\mathbb{R}} \mathcal{K}(x,t;y,\tau)\mathcal{K}(y,\tau;x_0,t_0)\, dy, \qquad t > \tau > t_0. \tag{7.64}$$

It follows from (7.62) that this relation reflects causality. To explain this, choose $t_0 < \tau < t$. We start with a wave function $\psi = \psi(x_0, t_0)$ at the initial time t_0. For the wave function at the intermediate time τ and at the final time t, we get

$$\psi(y,\tau) = \int_{\mathbb{R}} \mathcal{K}(y,\tau;x_0,t_0)\psi(x_0,t_0)dx_0 \tag{7.65}$$

and

$$\psi(x,t) = \int_{\mathbb{R}} \mathcal{K}(x,t;y,\tau)\psi(y,\tau)dy, \tag{7.66}$$

respectively. By causality, we expect that $\psi(x,t)$ at the final time t can also be generated by the wave function at the initial time t_0, that is,

$$\psi(x,t) = \int_{\mathbb{R}} \mathcal{K}(x,t;x_0,t_0)\psi(x_0,t_0)dx_0. \tag{7.67}$$

Now the product formula (7.64) tells us that indeed the composition of the two formulas (7.65) and (7.66) yields (7.67).

The infinitesimal Feynman propagator kernel. In order to obtain his path integral, Feynman used the causality condition (7.64) and the following magic approximation formula:

$$\boxed{\mathcal{K}(x+\Delta x, t+\Delta t; x, t) = \mathrm{e}^{\mathrm{i}\Delta S/\hbar} \cdot \mathcal{K}_{\mathrm{fluct}}(t+\Delta t; t).} \tag{7.68}$$

This is an approximation formula for small position differences Δx and small time differences Δt. Explicitly, we use

- the classical action difference

$$\Delta S := \left(\frac{m}{2}\left(\frac{\Delta x}{\Delta t}\right)^2 - U(x)\right)\Delta t$$

  with the discrete velocity $\frac{\Delta x}{\Delta t}$ and the discrete energy $\Delta E := \Delta S/\Delta t$, and
- the infinitesimal quantum fluctuation term

$$\mathcal{K}_{\mathrm{fluct}}(t+\Delta t; t) := \sqrt{\frac{m}{2\pi\hbar \mathrm{i}\Delta t}}.$$

Here, ΔS is an approximation of the classical action

$$S[q] := \int_t^{t+\Delta t} \left\{\frac{m}{2}\,\dot{q}(\tau)^2 - U(q(\tau))\right\}\, d\tau$$

for a classical trajectory $q = q(\tau)$ which connects the two points x and $x+\Delta x$, that is, $q(t) = x$ and $q(t+\Delta t) = x + \Delta x$. Here, the symbol m denotes the mass of the particle on the real line. The magic formula (7.68) tells us that

The passage from classical mechanics to quantum mechanics is obtained by adding quantum fluctuations.

The magic formula (7.68) combines the infinitesimal strategy due to Newton (1643–1727) and Leibniz (1646–1616) with the principle of least action due to Leibniz, Maupertuis (1698–1759) and Euler (1707–1783). Introducing the (complex) characteristic length[45]

$$l := \frac{1}{\mathcal{K}_{\text{fluct}}(t+\Delta t;t)} = \sqrt{\frac{2\pi\hbar \mathrm{i}\Delta t}{m}},$$

the magic Feynman formula (7.68) reads as

$$\boxed{\mathcal{K}(x+\Delta x, t+\Delta t; x, t) = \frac{\mathrm{e}^{\mathrm{i}\Delta S/\hbar}}{l}.}$$

This reflects the fact that the Feynman propagator kernel $\mathcal{K}$ has the physical dimension $(\text{length})^{-1}$ for the motion of a quantum particle on the real line.

The global Feynman propagator kernel. Combining the causality principle (7.64) with the magic formula (7.68) for the infinitesimal propagator kernel, Feynman arrived at the following global kernel formula:

$$\boxed{\mathcal{K}(x,t;x_0,t_0) = \lim_{N\to\infty} \frac{1}{l} \int_{\mathbb{R}^{N-1}} \mathrm{e}^{\mathrm{i}\sum \Delta S/\hbar} \ \frac{dq_1}{l} \cdots \frac{dq_{N-1}}{l}} \tag{7.69}$$

with the discretized action

$$\sum \Delta S := \sum_{n=0}^{N-1} \left\{ \frac{m}{2} \left(\frac{q_{n+1}-q_n}{\Delta t} \right)^2 - U(q_n) \right\} \Delta t.$$

Here, we add the boundary conditions: $q_0 := x_0$ and $q_N := x$. The crucial Feynman formula (7.69) tells us that the global Feynman propagator kernel $\mathcal{K}(x,t;x_0,t_0)$ is obtained by summing over all possible time-ordered products of infinitesimal Feynman propagator kernels. This is a special case of the following general principle in natural philosophy:

In nature, interactions are obtained by the superposition of all possible infinitesimal interactions taking causality into account.

Introducing the path-integral notation, we briefly write

$$\int_{C\{t_0,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar} \mathcal{D}q := \lim_{N\to\infty} \frac{1}{l} \int_{\mathbb{R}^{N-1}} \mathrm{e}^{\mathrm{i}\sum \Delta S/\hbar} \ \frac{dq_1}{l} \cdots \frac{dq_{N-1}}{l}. \tag{7.70}$$

Physicists use the following two methods for computing path integrals:

(i) the limit formula (7.70) and
(ii) infinite-dimensional Gaussian integrals.

Method (i) corresponds to an approximation of continuous paths by polygons. Method (ii) generalizes the finite-dimensional formula

$$\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \ \mathrm{e}^{\langle b|x\rangle} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} = \frac{\mathrm{e}^{\langle b|A^{-1}b\rangle}}{\sqrt{\det A}}$$

[45] The square root is to be understood as principal value: $l = \mathrm{e}^{\mathrm{i}\pi/4}\sqrt{\frac{2\pi\hbar\Delta t}{m}}$.

to infinite dimensions. In this context, one has to define the determinant $\det A$ of an infinite-dimensional operator A by generalizing the finite-dimensional formula

$$\det A = \prod_{n=1}^{N} \lambda_n$$

for the eigenvalues $\lambda_1, \ldots, \lambda_N$ of the operator A. Here, we will use the analytic continuation of the Riemann zeta function and its generalization to elliptic differential operators on Riemannian manifolds (see Sect. 7.9). Summarizing, we will get the following key formula:

$$\boxed{\mathcal{K}(x,t;x_0,t_0) = \int_{C\{t_0,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar} \mathcal{D}q = \mathcal{N} \int_{C\{t_0,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}_G q} \tag{7.71}$$

which is basic for modern physics. This formuula tells us that the Feynman path integral differs from the normalized infinite-dimensional Gaussian integral by a normalization factor $\mathcal{N}$. Fortunately enough, the explicit knowledge of the normalization factor $\mathcal{N}$ is not necessary in many applications to quantum field theory. In terms of mathematics, formula (7.71) connects different subjects of mathematics with each other: spectral theory of elliptic differential operators on Riemannian manifolds, harmonic analysis, analytic number theory, distributions and pseudo-differential operators, Fourier integral operators, random walks and stochastic processes (Brownian motion), topological quantum field theory (topological invariants of knots, manifolds and algebraic varieties). This concerns the following mathematical branches: analysis, differential geometry, algebraic topology, algebraic geometry, and theory of probability.

The innocently looking formula (7.71) *emphasizes the unity of mathematics.*

The WKB (Wentzel, Kramers, Brioullin) method. The passage from Maxwell's wave optics to geometric optics corresponds to the limit $\lambda \to 0$ (i.e., the wavelength λ goes to zero). Similarly, the passage from quantum mechanics to classical mechanics corresponds to the limit

$$\hbar \to 0$$

called the classical limit. More precisely, this means that quantum effects occur if the quotient $\hbar/S_{\mathrm{daily}}$ is sufficiently small. Here, S_{daily} is the action of processes in daily life. Explicitly, $\hbar \sim 10^{-34}$Js and $S_{\mathrm{daily}} \sim 1$Js. Shortly after Schrödinger's publication of his wave mechanics in 1926, Wentzel, Kramers, and Brioullin independently investigated the limit $\hbar \to 0$ parallel to geometric optics.[46] In terms of the Feynman path integral, the refined WKB method yields the following elegant key formula

$$\boxed{\mathcal{K}(x,t;x_0,t_0) = \mathrm{e}^{\mathrm{i}S[q_{\mathrm{class}}]/\hbar}\, \mathcal{K}_{\mathrm{fluct}}(x,t;x_0,t_0)} \tag{7.72}$$

[46] G. Wentzel, A generalization of the quantum condition in wave mechanics, Z. Physik **38** (1926), 518–529 (in German).
H. Kramers, Wave mechanics and half-integer quantization, Z. Physik **39** (1927), 828–840 (in German).
M. Brioullin, La méchanique ondulatoire de Schrödinger; une méthode générale de résolution par approximations successives, Comptes Rendus Acad. Sci. (Paris) **183** (1926), 24–44 (in French).

where $S[q_{\text{class}}]$ is the action along the classical path with the boundary condition $q_{\text{class}}(t_0) = x_0$ and $q_{\text{class}}(t) = x$. The factor $\mathcal{K}_{\text{fluct}}$ describes quantum fluctuations (see Sect. 7.10 on page 580).

Diffusion processes and the Euclidean strategy in quantum mechanics. The diffusion equation

$$\frac{\partial \psi(x,t)}{\partial t} = \kappa \psi_{xx} - V(x), \quad \psi(x,t_0) = \psi_0(x) \tag{7.73}$$

for all $x \in \mathbb{R}$ and all $t > t_0$ describes the diffusion of particles on the real line, where $\psi(x,t)$ denotes the particle density at the position x at time t, and $\kappa > 0$ is the diffusion constant. Using the replacement

$$t \Rightarrow \mathrm{i}t, \tag{7.74}$$

and setting $\kappa := \hbar/2m$, $U(x) := -\hbar V(x)$, the diffusion equation (7.73) passes over to the Schrödinger equation (7.61).[47] We expect that, by the replacement (7.74), each result on the classical diffusion equation (7.73) generates a result in quantum mechanics. This is called the Euclidean strategy. For example, let $V(x) \equiv 0$. We will show below that the classical diffusion kernel

$$\mathcal{P}(x,t;x_0,t_0) = \sqrt{\frac{m}{2\pi\hbar(t-t_0)}} \cdot \mathrm{e}^{-m(x-x_0)^2/2\hbar(t-t_0)} \tag{7.75}$$

passes over to the Feynman propagator kernel $\mathcal{K}(x,t;x_0,t_0) := \mathcal{P}(x,\mathrm{i}t;x_0,\mathrm{i}t_0)$. Explicitly,

$$\mathcal{K}(x,t;x_0,t_0) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar(t-t_0)}} \cdot \mathrm{e}^{\mathrm{i}m(x-x_0)^2/2\hbar(t-t_0)} \tag{7.76}$$

for all positions $x, x_0 \in \mathbb{R}$ and all times $t > t_0$.

Brownian motion. In 1905 Einstein studied the Brownian motion of tiny particles suspended in a liquid. This was the beginning of the theory of stochastic processes, which was developed as a mathematical theory by Wiener and Kolmogorov in the early 1920s and in the early 1930s, respectively.[48] Comparing the Schrödinger equation (7.61) with the diffusion equation (7.73), we arrive at the following intuitive interpretation of quantum mechanics emphasized by Feynman:

> *The motion of a quantum particle on the real line can be regarded as Brownian motion (i.e., a random walk) in imaginary time.*

This formal analogy motivated Mark Kac in 1949 to prove the famous Feynman–Kac formula[49] which represents the diffusion kernel (7.75) as a path integral, in rigorous mathematical terms see Sect. 7.11.5 on page 588.

Historical remarks on Feynman's discovery. The following quotation is taken from the comprehensive handbook on Feynman path integrals in quantum mechanics written by Christian Grosche and Frank Steiner:[50]

[47] Alternatively, if we regard $\psi(x,t)$ as the temperature at the point x at time t, then the equation (7.73) describes the heat conduction on the real line.

[48] Robert Brown (1773–1858), Einstein (1879–1955), Schrödinger (1887–1961), Wiener (1894–1964), Kolmogorov (1903–1987), Mark Kac (1914–1984), Feynman (1918–1988).

[49] M. Kac, On distributions of certain Wiener functionals, Trans. Amer. Math. Soc. **65** (1949), 1–13.

[50] C. Grosche and F. Steiner, Handbook of Feynman Path Integrals, Springer, Berlin, 1998 (reprinted with permission).

Feynman was working as a research assistant at Princeton during 1940–41. In the course of his graduate studies he discovered with Wheeler an action principle using half advanced and half retarded potentials.[51] The problem was the infinite self-energy of the electron, and it turned out that the new "action principle" could deal successfully with the infinity arising in the application of classical electrodynamics.

The problem then became one of applying this action principle to quantum mechanics in such a way that classical mechanics could arise naturally as a special case of quantum mechanics when the Planck quantum of action h was allowed to go to zero.

Feynman searched for any ideas which might have been previously worked out in connecting quantum-mechanical behavior with such classical ideas as the Lagrangian and Hamilton's action integral ... At a Princeton beer party Richard Feynman learned from Herbert Jehle, a former student of Schrödinger in Berlin, who had newly arrived from Europe, of Dirac's paper.[52] Dirac showed that

$$\langle q(t)|q(t_0)\rangle \qquad \text{corresponds to} \qquad \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathcal{L}dt},$$

where $\mathcal{L}$ is the Lagrangian. The natural question that then arose was what Dirac had meant by the phrase "corresponds to." Feynman found that Dirac's statement actually means "proportionally to", that is,

$$\mathcal{K}(x+\Delta x, t+\Delta t; x, t) = \text{const}(\Delta t)\cdot \mathrm{e}^{\mathrm{i}\Delta S/\hbar}.$$

Based on this result and the causality composition law (7.64) in the limit $N \to \infty$, Feynman interpreted the multiple-integral construction (7.70) as an "integral over all paths" and wrote this down in his Ph. D. thesis presented to the Faculty of Princeton University on May 4, 1942.[53] During the war Feynman worked at Los Alamos (New Mexico), and after the war his primary direction of work was towards quantum electrodynamics. So it happened that a complete theory of the *path integral approach to quantum mechanics* was worked out only in 1947. Feynman submitted his paper to the *Physical Review*, but the editors rejected it! Thus he rewrote it and sent it to *Reviews of Modern Physics*, where it finally appeared in spring 1948 under the title "Space-time approach to non-relativistic quantum mechanics."[54] Feynman's paper is one of the most beautiful and most influential papers in physics written during the last fifty years.[55]

[51] J. Wheeler and R. Feynman, Interaction with the absorber as the mechanism of radiation, Rev. Mod. Phys. **17** (1945), 157–181.

[52] P. Dirac, The Lagrangian in quantum mechanics, Soviet Union Journal of Physics (in German). Reprinted in J. Schwinger (Ed.) (1958), pp. 312–320.

[53] R. Feynman, The principle of least action in quantum mechanics, Ph.D. thesis, Princeton, New Jersey, 1942.

[54] Rev. Mod. Phys. **20** (1948), 367–387.

[55] Feynman's approach to quantum mechanics has a forerunner. In 1924 Wentzel published a paper where one can find the basic formulae and their interpretation as they were adopted twenty years later by Feynman. In fact, Wentzel's paper was published before the fundamental papers by Heisenberg (1925) and Schrödinger (1926). See G. Wentzel, Zur Quantenoptik (On quantum optics), Z. Physik **22** (1924), 193–199. This is discussed in: S. Antoci and D. Liebscher, The third way to quantum mechanics is the forgotten first, Annales de Fondation Louis de Broglie **21** (1996), 349–368 (see also S. Antoci and D. Liebscher, Wentzel's path integrals, Int. J. Math. Phys. **37** (1998), 531–535).

7.5.2 The Diffusion Kernel and the Euclidean Strategy in Quantum Physics

Formal motivation of the diffusion kernel. In order to discuss the basic idea of the Euclidean strategy in quantum mechanics, let us start with considering the classical diffusion equation

$$\psi_t(x,t) = \kappa\psi_{xx}(x,t), \qquad x \in \mathbb{R}, t > t_0, \quad \psi(x,t_0) = \psi(x) \tag{7.77}$$

where $\kappa := \hbar/2m$. We want to obtain the kernel $\mathcal{P}$ from (7.75), by using the Fourier method in a formal way. We start with the following two conditions

(C1) $P_t(x,t) = \kappa P_{xx}(x,t), x \in \mathbb{R}, t > 0$, and
(C2) $\lim_{t\to+0} P(x,t) = \delta(x)$, $x \in \mathbb{R}$.

Taking the existence of P for granted, set $\mathcal{P}(x,t;x_0,t_0) := P(x-x_0;t-t_0)$. We want to show that the function

$$\psi(x,t) := \int_{\mathbb{R}} \mathcal{P}(x,t;x_0,t_0)\psi_0(x_0)dx_0, \quad x \in \mathbb{R}, t > t_0$$

is a solution of (7.77). In fact, it follows from (C1) that

$$\psi_t(x,t) - \kappa\psi_{xx}(x,t) = \int_{\mathbb{R}} (\mathcal{P}_t - \mathcal{P}_{xx})\psi_0(x_0)dx_0 = 0, \quad x \in \mathbb{R}, t > 0.$$

By (C2), $\lim_{t\to t_0+0} \psi(x,t) = \int_{\mathbb{R}} \lim_{t\to t_0+0} \mathcal{P}(x,t;x_0,t_0)\psi_0(x_0)dx_0$, and hence

$$\lim_{t\to t_0+0} \psi(x,t) = \int_{\mathbb{R}} \delta(x-x_0)\psi_0(x_0)dx_0 = \psi_0(x).$$

It remains to determine the function P. Let $p \mapsto \hat{P}(p,t)$ be the Fourier transform of $x \mapsto P(x,t)$. By (C1) and (C2),

$$\hat{P}_t(p,t) = -\kappa p^2 \hat{P}(p,t), \quad t > 0, \qquad \hat{P}(p,0) = \frac{1}{\sqrt{2\pi}}.$$

Hence $\hat{P}(p,t) = \frac{1}{\sqrt{2\pi}}\, \mathrm{e}^{-\kappa p^2 t}$. By Fourier transform,

$$P(x,t) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}px}\, \mathrm{e}^{-\kappa p^2 t}\, dp, \qquad x \in \mathbb{R}, t > 0.$$

Hence $P(x,t) = \frac{1}{\sqrt{4\pi\kappa t}}\, \mathrm{e}^{-x^2/4\kappa t}$ (see the Gaussian integral (7.182) on page 560). This finishes the classical motivation for the diffusion kernel (7.75).

The classical existence theorem for the diffusion equation. The proof of the following standard result in the theory of partial differential equations can be found in H. Triebel, Higher Analysis, Sect. 42, Barth, Leipzig, 1989.

Theorem 7.15 *We are given the initial function $\psi_0 \in \mathcal{D}(\mathbb{R})$. Choose the kernel $\mathcal{P}$ as in (7.75). Then the function*

$$\psi(x,t) := \int_{\mathbb{R}} \mathcal{P}(x,t;x_0,t_0)\psi_0(x_0)\, dx_0, \quad x \in \mathbb{R}, t > t_0 \tag{7.78}$$

is a classical solution of the diffusion equation (7.77). In addition, we have the initial condition $\lim_{t\to t_0+0} \psi(x,t) = \psi_0(x)$ for all $x \in \mathbb{R}$.

The classical existence theorem for the free quantum particle on the real line. Consider the Schrödinger equation

$$\mathrm{i}\hbar\psi_t(x,t) = -\frac{\hbar^2}{2m}\psi_{xx}(x,t), \quad x \in \mathbb{R}, t > t_0, \quad \psi(x,t_0) = \psi_0(x) \tag{7.79}$$

for the motion of a free quantum particle of mass m on the real line. Let D denote the set of all Gaussian functions $\mathrm{e}^{-\beta(x-\alpha)^2}$, $x \in \mathbb{R}$ with real parameter α and positive parameter β. The complex linear hull, span D, is a dense subset of the Hilbert space $L_2(\mathbb{R})$.

Theorem 7.16 *We are given the initial function $\psi_0 \in \operatorname{span} D$. Choose the kernel $\mathcal{K}$ as in (7.75). Then the function*

$$\psi(x,t) := \int_{\mathbb{R}} \mathcal{K}(x,t;x_0,t_0)\psi_0(x_0)\, dx_0, \qquad x \in \mathbb{R}, t > t_0 \tag{7.80}$$

is a classical solution of the Schrödinger equation (7.79). In addition, we have the initial condition $\lim_{t\to t_0+0} \psi(x,t) = \psi_0(x)$, in the sense of the convergence on the Hilbert space $L_2(\mathbb{R})$.

The proof can be found in Zeidler (1995a), Sect. 5.22.2 (see the references on page 1049).

Formal perspectives. In the next sections, we will study the following topics in a formal manner:

- Propagator theory via the formal Dirac calculus (Sect. 7.5.3).
- Formal motivation of the definition of the Feynman path integral (Sect. 7.7.6).

Rigorous perspectives. Furthermore, we will rigorously investigate the following mathematical topics:

- Von Neumann's operator calculus and the functional-analytic approach to both the Feynman propagator and the Euclidean Feynman propagator (Sect. 7.6.3).
- Functional-analytic theory of the motion of a free quantum particle on the real line (Sect. 7.6.4).
- Functional-analytic theory of the motion of a harmonic oscillator on the real line and the Maslov index (Sect. 7.6.7).
- The Euclidean Feynman propagator and von Neumann's density matrix in quantum statistics (Sect. 7.6.8).
- Computation of the Feynman path integral for both the free quantum particle and the quantized harmonic oscillator (Sects. 7.7.3 and 7.7.4).
- The relation between infinite-dimensional Gaussian integrals and the Feynman propagator kernel including applications to the free quantum particle and the quantized harmonic oscillator (Sect. 7.9).
- The semi-classical WKB method (Sect. 7.10).
- Brownian motion, the Wiener integral, and the Feynman–Kac formula for diffusion processes (Sect. 7.11).

7.5.3 Probability Amplitudes and the Formal Propagator Theory

> Feynman's approach to quantum theory can be understood best by using Dirac's formal calculus; this can be generalized straightforward to quantum field theory.
>
> Folklore

The Parseval equation. Let $\varphi_1, \dots, \varphi_N$ be an orthonormal basis of the complex N-dimensional Hilbert space Y. This means that the orthonormality condition

$$\langle \varphi_k | \varphi_l \rangle = \delta_{kl}, \qquad k, l = 1, \dots, N$$

is satisfied. The basis property tells us that, for all $\varphi, \psi \in Y$, we have

(F) the Fourier expansion $|\psi\rangle = \sum_{k=1}^{N} |\varphi_k\rangle\langle\varphi_k|\psi\rangle$,
(C) the completeness relation $I = \sum_{k=1}^{N} |\varphi_k\rangle\langle\varphi_k|$, and[56]
(P) the Parseval equation

$$\langle \psi | \varphi \rangle = \sum_{k=1}^{n} \langle \psi | \varphi_k \rangle \langle \varphi_k | \varphi \rangle. \tag{7.81}$$

These classical properties of Fourier expansions are discussed in Sect. 7.10 of Vol. I. The complex numbers $c_1 := \langle \psi | \varphi_1 \rangle, \dots, c_N := \langle \psi | \varphi_N \rangle$ are called the Fourier coefficients. Suppose that $||\psi|| = 1$. By the Parseval equation,

$$||\psi||^2 = \sum_{k=1}^{N} |c_k|^2 = 1.$$

If ψ is the state of a quantum particle, then $|c_k|^2$ is the probability for observing the particle in the state φ_k; the Fourier coefficients $c_1, \dots, c_N$ are called the probability amplitudes of the particle state ψ.

The Schrödinger equation. Consider again the Schrödinger equation

$$\mathrm{i}\hbar\psi_t = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + U\psi \tag{7.82}$$

for the motion of a quantum particle on the real line. Here, $m > 0$ is the mass of the particle. We assume that the smooth potential function $U : \mathbb{R} \to \mathbb{R}$ has compact support, that is, $U \in \mathcal{D}(\mathbb{R})$. In terms of physics, the potential U describes the force acting on the quantum particle. If $U \equiv 0$, then the quantum particle is called free. Set

$$H_0\varphi := -\frac{\hbar^2}{2m}\frac{\partial^2 \varphi}{\partial x^2} + U\varphi \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).$$

Then the operator $H_0 : \mathcal{D}(\mathbb{R}) \to L_2(\mathbb{R})$ is essentially self-adjoint on the Hilbert space $L_2(\mathbb{R})$. Let $H : W_2^2(\mathbb{R}) \to L_2(\mathbb{R})$ be the self-adjoint extension of H_0. Then the Schrödinger equation reads as

$$\mathrm{i}\hbar\dot{\psi}(t) = H\psi(t), \qquad t > t_0, \qquad \psi(t_0) = \psi_0$$

with the unique solution $\psi(t) = \mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar}\psi_0$ (see Theorem 7.25 on page 507).

The formal Dirac calculus. It is our goal to study the Schrödinger equation (7.82) by means of the formal Dirac calculus on the real line.[57] In particular, we will use

- the orthonormality condition $\langle x | x_0 \rangle = \delta(x - x_0)$ for all $x, x_0 \in \mathbb{R}$, and

[56] In mathematics, one also writes $\psi = \sum_{k=1}^{N} \langle \varphi_k | \psi \rangle \varphi_k$ and $I = \sum_{k=1}^{N} \varphi_k \otimes \varphi_k$.
[57] This formal calculus is thoroughly discussed in Sect. 11.2.5 of Vol. I. The rigorous justification of the Dirac calculus can be found in Sect. 12.2 of Vol. I.

- the completeness relation

$$\boxed{I = \int_{\mathbb{R}} |x\rangle\langle x| \, dx,} \tag{7.83}$$

where I denotes the unit operator. Using the trivial identity $\langle\psi|\varphi\rangle = \langle\psi|I\varphi\rangle$ and the completeness relation (7.83), we formally get the Parseval equation

$$\langle\psi|\varphi\rangle = \int_{\mathbb{R}} \langle\psi|x\rangle\langle x|\varphi\rangle dx. \tag{7.84}$$

This elegant formal argument is called Dirac's substitution trick.[58]

Formal operator kernel. The operator equation $\varphi = A\psi$ is equivalent to the integral relation

$$\langle x|\varphi\rangle = \int_{\mathbb{R}} \langle x|A|x_0\rangle\langle x_0|\psi\rangle \, dx_0, \qquad x \in \mathbb{R},$$

by using the completeness relation. Setting $\mathcal{A}(x, x_0) := \langle x|A|x_0\rangle$ for all positions $x, x_0 \in \mathbb{R}$, we get

$$\varphi(x) = \int_{\mathbb{R}} \mathcal{A}(x, x_0)\psi(x_0)dx_0, \qquad x, x_0 \in \mathbb{R}.$$

The function $(x, x_0) \mapsto \mathcal{A}(x, x_0)$ is called the kernel of the operator $\mathcal{A}$. In rigorous terms, this is not always a classical function. For example, the identical operator $A = I$ has the kernel

$$\mathcal{A}(x, x_0) = \langle x|x_0\rangle = \delta(x - x_0).$$

If we choose the Hamiltonian H, then the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi''(x) + U(x)\psi(x) = \varphi(x), \qquad x \in \mathbb{R} \tag{7.85}$$

means that $\varphi = H\psi$. Formally, this is equivalent to the integral relation

$$\langle x|\varphi\rangle = \int_{\mathbb{R}} \langle x|H|x_0\rangle\langle x_0|\psi\rangle dx_0, \qquad x \in \mathbb{R}, \tag{7.86}$$

by using the completeness relation (7.83). Now we want to study the kernels $\mathcal{K}$ and $\mathcal{G}$ to the Feynman propagator $\mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}$ and the negative resolvent operator $(H - \mathcal{E}I)^{-1}$, respectively. Here, $\mathcal{K}$ and $\mathcal{G}$ is called the Feynman propagator kernel and the energetic Green's function, respectively.

> *In terms of modern mathematics, the Dirac calculus is a forerunner of the theory of pseudo-differential operators, where differential operators and integral operators are treated on equal footing.*

[58] Writing $\langle x|\varphi\rangle = \varphi(x)$ and $\langle\psi|x\rangle = \langle x|\psi\rangle^\dagger = \psi(x)^\dagger$, equation (7.84) reads as

$$\langle\psi|\varphi\rangle = \int_{\mathbb{R}} \psi(x)^\dagger\varphi(x)dx.$$

This is the inner product on the Hilbert space $L_2(\mathbb{R})$.

We refer to the treatise by L. Hörmander, The Analysis of Linear Partial Differential Operators, Vols. 1–4, Springer, New York, 1983.

The key formulas. The Feynman approach to quantum physics is based on the following formal arguments.

(i) The Feynman propagator kernel $\mathcal{K}$: For all positions $x, x_0 \in \mathbb{R}$ and all times $t > t_0$, we define the Feynman propagator kernel

$$\boxed{\mathcal{K}(x,t;x_0,t_0) := \langle x|\mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar}|x_0\rangle.} \tag{7.87}$$

- Integral representation for the dynamics of the quantum particle: For the solution $\psi(t) = \mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar}\psi_0$ of the Schrödinger equation (7.82), we have

$$\boxed{\psi(x,t) = \int_{\mathbb{R}} \mathcal{K}(x,t;x_0,t_0)\psi(x_0,t_0)dx_0, \quad x \in \mathbb{R},\ t > t_0.} \tag{7.88}$$

- Schrödinger equation for the Feynman propagator kernel: For all positions $x, x_0 \in \mathbb{R}$ and all times $t > t_0$,

$$\mathrm{i}\hbar\mathcal{K}_t(x,t;x_0,t_0) = -\frac{\hbar^2}{2m}\mathcal{K}_{xx}(x,t;x_0,t_0) + U(x)\mathcal{K}(x,t;x_0,t_0).$$

- Singularity at the initial time t_0 :

$$\lim_{t\to t_0+0} \mathcal{K}(x,t;x_0,t_0) = \delta(x-x_0), \qquad x, x_0 \in \mathbb{R}. \tag{7.89}$$

- Causality relation: For all positions $x, x_0 \in \mathbb{R}$ and all times $t > \tau > t_0$,

$$\mathcal{K}(x,t;x_0,t_0) = \int_{\mathbb{R}} \mathcal{K}(x,t;y,\tau)\mathcal{K}(y,\tau;x_0,t_0)\ dy. \tag{7.90}$$

This is the product rule for the Feynman propagator kernel.

Formal proof. By the completeness relation $\int_{\mathbb{R}} |x_0\rangle\langle x_0|\ dx_0 = I$,

$$\langle x|\psi\rangle = \langle x|\mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar}|\psi_0\rangle = \int_{\mathbb{R}} \langle x|\mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar}|x_0\rangle\langle x_0|\psi_0\rangle dx_0.$$

This is (7.88). The differential equation for $\mathcal{K}$ follows from the fact that the two expressions

$$\mathrm{i}\hbar\psi_t(x,t) = \int_{\mathbb{R}} \mathrm{i}\hbar\mathcal{K}_t(x,t;x_0,t_0)\psi_0(x_0)\ dx_0,$$
$$H\psi(x,t) = \int_{\mathbb{R}} H\mathcal{K}(x,t;x_0,t_0)\psi_0(x_0)\ dx_0$$

are equal to each other for all initial functions ψ_0. Hence $\mathrm{i}\hbar\mathcal{K}_t = H\mathcal{K}$. Furthermore,

$$\lim_{t\to t_0+0}\langle x|\mathrm{e}^{-\mathrm{i}H(t-t_0)}|x_0\rangle = \langle x|x_0\rangle = \delta(x-x_0).$$

From the group property $\mathrm{e}^{u+v} = \mathrm{e}^u\mathrm{e}^v,\ u, v \in \mathbb{C}$ of the exponential function, we get

$$e^{-iH(t-t_0)/\hbar} = e^{-iH(t-\tau)\hbar} e^{-iH(\tau-t_0)/\hbar}, \qquad t_0 < \tau < t.$$

This implies

$$\langle x|e^{-iH(t-t_0)/\hbar}|x_0\rangle = \int_{\mathbb{R}} \langle x|e^{-iH(t-\tau)/\hbar}|y\rangle\langle y|e^{-iH(\tau-t_0)/\hbar}|x_0\rangle\, dy, \quad (7.91)$$

which is the causality relation (7.90). □

(ii) The resolvent kernel $\mathcal{R}$: Let $\varrho(H)$ be the resolvent set of the Hamiltonian H on the Hilbert space $L_2(\mathbb{R})$. By definition, the complex number $\mathcal{E}$ is contained in $\varrho(H)$ iff the inverse operator

$$(\mathcal{E}I - H)^{-1} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$$

exists, and it is continuous. This operator is called the resolvent[59] of the Hamiltonian H at the point $\mathcal{E}$. We briefly write $R_\mathcal{E} := (\mathcal{E}I - H)^{-1}$. The complement $\sigma(E) := \mathbb{C} \setminus \varrho(H)$ is called the spectrum of H.

The spectrum $\sigma(H)$ is a closed subset of the real line; the complementary resolvent set $\varrho(H)$ is an open subset of the complex plane.

The points E in the spectrum $\sigma(H)$ are the energy values of the quantum particle described by the Hamiltonian H. For all positions $x, x_0 \in \mathbb{R}$ and all complex numbers $\mathcal{E} \in \varrho(H)$, we define the resolvent kernel

$$\boxed{\mathcal{R}(x, x_0; \mathcal{E}) := \langle x|(\mathcal{E}I - H)^{-1}|x_0\rangle.}$$

This kernel has the following properties.

- Integral representation of the resolvent: For each given complex number $\mathcal{E} \in \varrho(H)$, the equation

$$(\mathcal{E}I - H)\psi = \chi$$

has the unique solution $\psi = (\mathcal{E}I - H)^{-1}\chi$. This is equivalent to the integral relation

$$\psi(x) = \int_{\mathbb{R}} \mathcal{R}(x, x_0; \mathcal{E})\chi(x_0)dx_0, \qquad x \in \mathbb{R}. \quad (7.92)$$

This follows from

$$\langle x|\psi\rangle = \langle x|(\mathcal{E}I - H)^{-1}\varphi\rangle = \int_{\mathbb{R}} \langle x|(\mathcal{E}I - H)^{-1}|x_0\rangle\langle x_0|\varphi\rangle\, dx_0.$$

- The resolvent equation: For all $\mathcal{E}, \mathcal{E}' \in \varrho(H)$, we have Hilbert's resolvent equation $R_\mathcal{E} - R_{\mathcal{E}'} = (\mathcal{E}' - \mathcal{E})R_{\mathcal{E}'}R_\mathcal{E}$. This implies

$$\mathcal{R}(x, x_0; \mathcal{E}) - \mathcal{R}(x, x_0; \mathcal{E}') = (\mathcal{E}' - \mathcal{E}) \int_{\mathbb{R}} \mathcal{R}(x, y; \mathcal{E}')\mathcal{R}(y, x_0; \mathcal{E})\, dy.$$

In fact, Hilbert's resolvent equation implies

$$\langle x|R_\mathcal{E} x_0\rangle - \langle x|R_{\mathcal{E}'} x_0\rangle = (\mathcal{E}' - \mathcal{E}) \int_{\mathbb{R}} \langle x|R_{\mathcal{E}'} y\rangle\langle y|R_\mathcal{E} x_0\rangle\, dy.$$

[59] Physicists frequently use the negative resolvent operator $-(\mathcal{E}I - H)^{-1}$ which is equal to $(H - \mathcal{E}I)^{-1}$.

(iii) The energetic Green's function $\mathcal{G}$: For all positions $x, x_0 \in \mathbb{R}$ and all complex numbers $\mathcal{E} \in \varrho(H)$, we define

$$\boxed{\mathcal{G}(x, x_0; \mathcal{E}) := -\mathcal{R}(x, x_0; \mathcal{E}).}$$

For each complex number $\mathcal{E} \in \varrho(H)$, the inhomogeneous stationary equation $(H - \mathcal{E}I)\psi = \varphi$, that is,

$$-\frac{\hbar^2}{2m}\psi''(x) + (U(x) - \mathcal{E})\psi(x) = \varphi(x), \qquad x \in \mathbb{R},$$

has the solution $\psi = -(\mathcal{E}I - H)^{-1}\varphi$. By (7.92),

$$\psi(x) = \int_{\mathbb{R}} \mathcal{G}(x, y; \mathcal{E})\varphi(y)dy, \qquad x \in \mathbb{R}.$$

Choosing $\varphi(x) := \delta(x - x_0)$, we obtain $\psi(x) = \mathcal{G}(x, x_0; \mathcal{E})$. This implies that, for all $\mathcal{E} \in \varrho(H)$, we get

$$-\frac{\hbar^2}{2m}\mathcal{G}_{xx}(x, x_0; \mathcal{E}) + (U(x) - \mathcal{E})\mathcal{G}(x, x_0; \mathcal{E}) = \delta(x - x_0), \qquad x, x_0 \in \mathbb{R}.$$

Therefore, the function $(x, x_0) \mapsto \mathcal{G}(x, x_0; \mathcal{E})$ is called the energetic Green's function (or the energetic 2-point function) with respect to the complex number $\mathcal{E} \notin \sigma(H)$. Now let us show that the energetic Green's function has singularities at the spectral points $\mathcal{E} \in \sigma(H)$, which correspond to the physical energy values of the quantum particle described by the Hamiltonian H.

(iv) The energetic Fourier transform: Let $\{|E_k\rangle\}_{k\in\mathcal{N}}$ be the complete orthonormal system of (generalized) eigenstates of the Hamiltonian H with the index set $\mathcal{N}$. That is, we have

- the (generalized) eigenvalue equation $H|E_k\rangle = E_k|E_k\rangle$,
- the completeness relation $\int_{\mathcal{N}} |E_k\rangle\langle E_k|\, d\mu(k) = I$, and
- the orthonormality relation $\langle E_k|E_l\rangle = \delta_\mu(k - l)$ for all $k, l \in \mathcal{N}$.

Here, μ is a measure on the set $\mathcal{N}$. This measure is called the energy measure of the Hamiltonian H. The Dirac delta function δ_μ with respect to the measure μ has the characteristic property that[60]

$$\int_{\mathcal{N}} \delta_\mu(k - k_0) f(k)\, d\mu(k) = f(k_0).$$

Thus, the Dirac delta function δ_μ generalizes the Kronecker symbol. Now let us assign to each energy state $|E_k\rangle$ the so-called energy function $\chi_k(x) := \langle x|E_k\rangle$ for all $x \in \mathbb{R}$.

- The Fourier–Stieltjes transform:

$$\boxed{\hat{\psi}(k) = \int_{\mathbb{R}} \chi_k(x)^\dagger \psi(x)dx, \qquad k \in \mathcal{N}.} \tag{7.93}$$

- The inverse Fourier–Stieltjes transform:

$$\boxed{\psi(x) = \int_{\mathcal{N}} \chi_k(x)\hat{\psi}(k)d\mu(k), \qquad x \in \mathbb{R}.} \tag{7.94}$$

[60] Mnemonically, this follows from $\int_{\mathcal{N}} \langle E_{k_0}|E_k\rangle\langle E_k|f\rangle d\mu(k) = \langle E_{k_0}|f\rangle$, by using the completeness relation.

- The stationary Schrödinger equation: For all indices $k \in \mathcal{N}$,

$$-\frac{\hbar^2}{2m}\chi_k''(x) + U(x)\chi_k(x) = E_k\chi_k(x), \qquad x \in \mathbb{R}. \tag{7.95}$$

  This tells us that the function χ_k is an eigenfunction corresponding to the energy eigenvalue E_k.
- The function $\psi_k(x,t) := \mathrm{e}^{-\mathrm{i}E_k t/\hbar}\chi_k(x)$ satisfies the instationary Schrödinger equation:

$$\mathrm{i}\hbar\frac{\partial\psi_k(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi_k(x,t)}{\partial x^2} + U(x)\psi_k(x,t) = E_k\psi(x,t), \quad x,t \in \mathbb{R}.$$

Formal proof. Ad (7.93). By the completeness relation,

$$\langle E_k|\psi\rangle = \int_R \langle E_k|x\rangle\langle x|\psi\rangle\, dx.$$

Ad (7.94). Similarly, $\langle x|\psi\rangle = \int_{\mathcal{N}}\langle x|E_k\rangle\langle E_k|\psi\rangle d\mu(k)$.
Ad (7.95). From $H|E_k\rangle = E_k|E_k\rangle$, we get

$$\langle x|E_k\rangle = \langle x|H|E_k\rangle = \int_{\mathbb{R}}\langle x|H|x_0\rangle\langle x_0|E_k\rangle dx_0.$$

Now use the formal equivalence between (7.85) and (7.86). □

(v) The energetic representation of the Feynman propagator kernel: For all positions $x, x_0 \in \mathbb{R}$ and all times $t > t_0$, we have

$$\boxed{\mathcal{K}(x,t;x_0,t_0) = \int_{\mathcal{N}} \mathrm{e}^{-\mathrm{i}E_k(t-t_0)/\hbar}\chi_k(x)\chi_k(x_0)^\dagger d\mu(k)} \tag{7.96}$$

and

$$\boxed{\mathcal{G}(x,x_0;E+\mathrm{i}\varepsilon) = \int_{\mathcal{N}} \frac{\chi_k(x)\chi_k(x_0)^\dagger}{E_k - E - \mathrm{i}\varepsilon}\, d\mu(k).} \tag{7.97}$$

Formal proof. Ad (7.96). To simplify notation, we set $\hbar := 1$ and $t_0 := 0$. By the completeness relation,

$$\langle x|\mathrm{e}^{-\mathrm{i}tH}|x_0\rangle = \int_{\mathcal{N}}\langle x|E_k\rangle\langle E_k|\mathrm{e}^{-\mathrm{i}tH}|x_0\rangle d\mu(k).$$

Moreover, $\mathrm{e}^{-\mathrm{i}tH}|E_k\rangle = \mathrm{e}^{-\mathrm{i}tE_k}|E_k\rangle$. Hence

$$\langle E_k|\mathrm{e}^{-\mathrm{i}tH}|x_0\rangle = \langle x_0|\mathrm{e}^{\mathrm{i}tH}|E_k\rangle^\dagger = \mathrm{e}^{-\mathrm{i}tE_k t}\langle x_0|E_k\rangle^\dagger = \mathrm{e}^{-\mathrm{i}tE_k t}\chi_k(x_0)^\dagger.$$

Ad (7.97). Replace $\mathrm{e}^{-\mathrm{i}tH}$ by $(H - (E+\mathrm{i}\varepsilon)I)^{-1}$. □

(vi) The passage from time to energy: For all positions $x, x_0 \in \mathbb{R}$, all times $t > t_0$, all energies $E \in \mathbb{R}$, and all energy damping parameters $\varepsilon > 0$, the following transformation formulas are valid.

- The Fourier–Laplace transform of the Feynman propagator kernel:

$$\boxed{\mathcal{G}(x,x_0;E+\mathrm{i}\varepsilon) = \frac{\mathrm{i}}{\hbar}\int_{t_0}^{\infty} \mathrm{e}^{\mathrm{i}(E+\mathrm{i}\varepsilon)(t-t_0)/\hbar}\, \mathcal{K}(x,t;x_0,t_0)dt.}$$

- The Fourier–Laplace transform of the energetic Green's function:

$$\boxed{\mathcal{K}(x,t;x_0,t_0) = \frac{1}{2\pi \mathrm{i}} \cdot PV \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}(E+\mathrm{i}\varepsilon)(t-t_0)/\hbar}\, \mathcal{G}(x,x_0;E+\mathrm{i}\varepsilon)\, dE.}$$

Recall that the symbol $PV \int_{-\infty}^{\infty} \ldots$ stands for the limit $\lim_{R\to+\infty} \int_{-R}^{R} \ldots$ (principal value of the integral).

Formal proof. This follows immediately from (7.96) and (7.97) combined with the two classical formulas

$$\frac{\mathrm{i}}{\hbar} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(E+\mathrm{i}\varepsilon)(t-t_0)/\hbar} \mathrm{e}^{-\mathrm{i}E_k(t-t_0)/\hbar} \theta(t-t_0) dt = \frac{1}{E_k - E - \mathrm{i}\varepsilon}$$

and

$$\theta(t-t_0)\mathrm{e}^{-\mathrm{i}E_k(t-t_0)/\hbar} = \frac{1}{2\pi\mathrm{i}} \cdot PV \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}(E+\mathrm{i}\varepsilon)(t-t_0)/\hbar}}{E_k - E - \mathrm{i}\varepsilon}\, dE,$$

which are valid for the following quantities: all energies $E, E_k \in \mathbb{R}$, all times $t, t_0 \in \mathbb{R}$ with $t \neq t_0$, and all damping parameters $\varepsilon > 0$. The proof of the latter two formulas can be found in Problem 7.35. □

The preceding formal propagator theory is very convenient from the mnemonical point of view. Our next goal is to show how this formal approach can be translated into a rigorous approach. To this end, we will use

- the von Neumann operator calculus in Hilbert spaces,
- tempered distributions, Gelfand triplets, and the theory of generalized eigenfunctions, and
- tempered distributions and the Schwartz kernel theorem.

We will apply this to:

- the free quantum particle (Sect. 7.6.4),
- the harmonic oscillator (Sect. 7.6.7), and
- ideal gases (Sect. 7.6.8).

7.6 Von Neumann's Rigorous Approach

> Rigorous propagator theory is based on von Neumann's operator calculus for functions of self-adjoint operators.
>
> Folklore

As a preparation for the rigorous propagator theory to be considered in the next section, let us summarize von Neumann's operator calculus. In this section, we consider an arbitrary complex separable Hilbert space X of finite or infinite dimension. The inner product on X is denoted by $\langle\psi|\varphi\rangle$ for all $\varphi, \psi \in X$. For fixed initial time t_0, the given function $\psi : [t_0, \infty[\to X$ with values in the Hilbert space X is called continuously differentiable iff the following is met:

- For all $t > t_0$, the derivative $\dot{\psi}(t) := \lim_{h\to 0} h^{-1}(\psi(t+h) - \psi(t))$ exists (in the sense of the convergence on the Hilbert space X).
- The function $t \mapsto \psi(t)$ is continuous on the closed interval $[0, \infty[$.
- The function $t \mapsto \dot{\psi}(t)$ is continuous on the open interval $]t_0, \infty[$, and the limit $\lim_{t\to t_0+0} \dot{\psi}(t)$ exists.

It is our goal to construct continuously differentiable solutions of the Schrödinger equation $\mathrm{i}\hbar\dot{\psi} = H\psi$ in the form $\psi(t) = \mathrm{e}^{-\mathrm{i}tH/\hbar}\psi_0$. To this end, we need the construction of the operator $\mathrm{e}^{-\mathrm{i}tH/\hbar}$.

7.6.1 The Prototype of the Operator Calculus

The basic idea is to use a complete orthonormal system $\varphi_0, \varphi_1, \ldots$ in the infinite-dimensional Hilbert space X.[61] The two key formulas are given by the series expansions

$$\boxed{H\varphi = \sum_{k=0}^{\infty} E_k \cdot \langle \varphi_k | \varphi \rangle \varphi_k \qquad \text{for all} \quad \varphi \in D(H)} \tag{7.98}$$

and

$$\boxed{\mathsf{F}(H)\varphi = \sum_{k=0}^{\infty} F(E_k) \cdot \langle \varphi_k | \varphi \rangle \varphi_k \qquad \text{for all} \quad \varphi \in D.} \tag{7.99}$$

To discuss this, observe first that

- the infinite series $\sum_{k=0}^{\infty} a_k \varphi_k$ with complex numbers $a_0, a_1, a_2, \ldots$ is convergent iff
- $\sum_{k=0}^{\infty} |a_k|^2 < \infty$.

In particular, the completeness of $\varphi_0, \varphi_1, \ldots$ guarantees that

$$\varphi = \sum_{k=0}^{\infty} \langle \varphi | \varphi_k \rangle \, \varphi_k \qquad \text{for all} \quad \varphi \in X.$$

(i) The operator H: We are given the real numbers $E_0, E_1, \ldots$ We define

$$H\varphi_k := E_k \varphi_k, \qquad k = 0, 1, \ldots$$

In a natural way, we want to extend the operator H to a linear subspace $D(H)$ of X. To this end, we define

$$D(H) := \{\varphi \in X : \sum_{k=0}^{\infty} |E_k|^2 |\langle \varphi | \varphi_k \rangle|^2 < \infty\}.$$

In other words, we have $\varphi \in D(H)$ iff the infinite series from (7.98) is convergent in X. Now, for all $\varphi \in D(H)$, we define $H\varphi$ by the convergent series (7.98). In particular, $\varphi_k \in D(H)$ for all k.

The operator $H : D(H) \to X$ is self-adjoint.

The spectrum $\sigma(H)$ of H is the closure of the set $\{E_0, E_1, \ldots\}$. The resolvent set $\varrho(H)$ of the operator H is the largest open subset of the complex plane which does not contain the energy values $E_0, E_1, \ldots$

(ii) The operator $\mathsf{F}(H) : D \to X$: We are given the function $F : \mathbb{R} \to \mathbb{C}$. Let D be the set of all elements φ of X such that the series (7.99) is convergent. Explicitly,

$$D := \{\varphi \in X : \sum_{k=0}^{\infty} |F(E_k)|^2 |\langle \varphi_k | \varphi \rangle|^2 < \infty\}.$$

Finally, for any $\varphi \in D$, define $\mathsf{F}(H)\varphi$ by the convergent series (7.99). The operator $\mathsf{F}(H) : D \to X$ is self-adjoint if the function F is real-valued.

[61] If the Hilbert space X is finite-dimensional with dimension $N = 1, 2, \ldots$, then all of the following formulas remain valid if we replace the symbol $\sum_{k=0}^{\infty}$ by $\sum_{k=0}^{N-1}$.

(iii) The spectral family $\{\mathsf{E}_\lambda(H)\}_{\lambda\in\mathbb{R}}$ of the self-adjoint operator H. Fix the real number λ and consider the function

$$e_\lambda(E) := \begin{cases} 1 & \text{if} \quad E < \lambda, \\ 0 & \text{if} \quad E \geq \lambda. \end{cases} \tag{7.100}$$

In other words, e_λ is the characteristic function of the open interval $]-\infty, \lambda[$. Define

$$\mathsf{E}_\lambda(H)\varphi := \sum_{k=1}^{\infty} e_\lambda(E_k)\langle\varphi_k|\varphi\rangle\varphi_k.$$

This series is convergent for all $\varphi \in X$. The operator $\mathsf{E}_\lambda(H) : X \to X$ is the orthogonal projection onto the closed linear subspace spanned by all the eigenvectors φ_k with $E_k \in]-\infty, \lambda[$.

(iv) The propagator $\mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}$: Let $t, t_0 \in \mathbb{R}$. Since $|\mathrm{e}^{-\mathrm{i}(t-t_0)/\hbar}| \leq 1$, the operator

$$\mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}\varphi := \sum_{k=0}^{\infty} \mathrm{e}^{-\mathrm{i}(t-t_0)E_k/\hbar}\langle\varphi_k|\varphi\rangle\varphi_k$$

is defined for all $\varphi \in X$. In addition, the operator $\mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar} : X \to X$ is unitary. For given $\psi_0 \in D(H)$, set

$$\psi(t) := \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}\psi_0 \qquad \text{for all} \quad t \in \mathbb{R}.$$

Then the function $\psi : \mathbb{R} \to X$ is continuously differentiable, and it is a solution of the Schrödinger equation.

$$\mathrm{i}\hbar\dot{\psi}(t) = H\psi(t), \qquad t \in \mathbb{R}, \qquad \psi(t_0) = \psi_0.$$

Proof. First use formal differentiation. This yields

$$\mathrm{i}\hbar\dot{\psi}(t) = \sum_{k=0}^{\infty} E_k \mathrm{e}^{-\mathrm{i}(t-t_0)E_k/\hbar}\langle\varphi_k|\varphi\rangle\varphi_k = H\psi(t).$$

Since we have the convergent majorant series

$$\sum_{k=0}^{\infty} |E_k \mathrm{e}^{-\mathrm{i}(t-t_0)E_k/\hbar}\langle\varphi_k|\varphi\rangle|^2 \leq \sum_{k=0}^{\infty} |E_k|^2 |\langle\varphi_k|\varphi\rangle|^2 < \infty,$$

the formal differentiation can be rigorously justified in the same way as for classical infinite series (see Sect. 5.8, Zeidler (1995a), quoted on page 1049). □

(v) The Euclidean propagator $\mathrm{e}^{-(t-t_0)H/\hbar}$: Suppose that $E_k \geq 0$ for all k. Fix the real number t_0. Let $t \geq t_0$. Since $0 \leq \mathrm{e}^{-(t-t_0)E_k/\hbar} \leq 1$, the operator

$$\mathrm{e}^{-(t-t_0)H/\hbar}\varphi := \sum_{k=0}^{\infty} \mathrm{e}^{-(t-t_0)E_k/\hbar}\langle\varphi_k|\varphi\rangle\varphi_k$$

is defined for all $\varphi \in X$. We have $||\mathrm{e}^{-(t-t_0)H/\hbar}\varphi|| \leq ||\varphi||$ for all $\varphi \in X$, that is, the operator $\mathrm{e}^{-(t-t_0)H/\hbar} : X \to X$ is non-expansive.[62] For given $\psi_0 \in D(H)$, set

[62] Note that $||\mathrm{e}^{-(t-t_0)H/\hbar}\varphi||^2 = \sum_{k=0}^{\infty} |\mathrm{e}^{-(t-t_0)E_k/\hbar}\langle\varphi_k|\varphi\rangle|^2$. Thus, for all $t \geq t_0$,

$$||\mathrm{e}^{-(t-t_0)H/\hbar}\varphi||^2 \leq \sum_{k=0}^{\infty} |\langle\varphi_k|\varphi\rangle|^2 = ||\varphi||^2.$$

$$\psi(t) := \mathrm{e}^{-(t-t_0)H/\hbar}\psi_0 \qquad \text{for all} \quad t \geq t_0.$$

Then the function $\psi : \mathbb{R} \to X$ is continuously differentiable on $[t_0, \infty[$, and it is a solution of the Euclidean Schrödinger equation

$$\hbar\dot{\psi}(t) = -H\psi(t), \qquad t \geq t_0, \qquad \psi(t_0) = \psi_0.$$

(vi) The resolvent $(\mathcal{E}I - H)^{-1}$: Let $\mathcal{E}$ be a non-real complex number. The series

$$R_\mathcal{E}\varphi := \sum_{k=0}^{\infty} \frac{\langle\varphi_k|\varphi\rangle}{\mathcal{E} - E_k}\,\varphi_k$$

is convergent for all $\varphi \in X$. This follows from

$$\left|\frac{1}{\mathcal{E} - E_k}\right|^2 = \frac{1}{(\Im\mathcal{E})^2 + (E_k - \Re\mathcal{E})^2} \leq \frac{1}{(\Im\mathcal{E})^2}.$$

Hence $||R_\mathcal{E}||^2 \leq \mathrm{const}(\mathcal{E})\cdot||\varphi||^2$. Thus, the operator $R_\mathcal{E}$ is linear and continuous. In addition, it can be easily shown that $R_\mathcal{E} = (\mathcal{E}I - H)^{-1}$.

(vii) The Fourier–Laplace transform of the propagator from time to energy: The integral

$$\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\mathcal{E}t} f(t)dt$$

does not exist (in the classical sense) if $\mathcal{E}$ is a real number and $f(t) \equiv 1$. However, if we choose both the complex energy $\mathcal{E} := E + \mathrm{i}\varepsilon$ (with $\varepsilon > 0$) and the truncation function $f(t) := \theta(t - t_0)$, then the integral[63]

$$\int_{t_0}^{\infty} \mathrm{e}^{\mathrm{i}Et}\mathrm{e}^{-\varepsilon t}dt$$

exists because of the damping factor $\mathrm{e}^{-\varepsilon t}$. This is the basic idea behind the use of both truncated propagators and complex energies in quantum physics. In order to explain this, choose the linear self-adjoint operator $H : D(H) \to X$ as in (i) above. Let t, t_0 be arbitrary real time parameters, and let $\mathcal{E}$ be a non-real complex parameter called energy. It is convenient to introduce the following operators, which we will frequently encounter in this treatise:

- $P(t, t_0) := \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}$ (propagator),
- $P^+(t, t_0) := \theta(t - t_0)P(t, t_0)$ (retarded propagator or Feynman propagator),
- $P^-(t, t_0) := -\theta(t_0 - t)P(t, t_0)$ (advanced propagator),
- $G(\mathcal{E}) := (H - \mathcal{E}I)^{-1}$ (Green's operator),[64]
- $G^+(\mathcal{E}) := G(\mathcal{E})$ if $\Im(\mathcal{E}) > 0$ (retarded!Green's operator),
- $G^-(\mathcal{E}) := G(\mathcal{E})$ if $\Im(\mathcal{E}) < 0$ (advanced!Green's operator).

Proposition 7.17 *Let $t, t_0 \in \mathbb{R}$ and $\varphi, \chi \in X$. Then:*
(i) *For all energies $\mathcal{E}$ in the open upper half-plane (i.e., $\Im(\mathcal{E}) > 0$), we have the Fourier–Laplace transformation*

[63] Recall that $\theta(t - t_0) = 1$ if $t \geq t_0$ and $\theta(t - t_0) = 0$ if $t < t_0$ (Heaviside function).
[64] Since the operator $G(\mathcal{E})$ depends on the choice of the complex energy $\mathcal{E}$, we also call it the energetic Green's operator.

$$\langle \chi | G^+(\mathcal{E})\varphi \rangle = \frac{\mathrm{i}}{\hbar} \int_{\mathbb{R}} e^{\mathrm{i}\mathcal{E}(t-t_0)/\hbar} \langle \chi | P^+(t,t_0)\varphi \rangle \, dt \tag{7.101}$$

together with the inverse transformation

$$\langle \chi | P^+(t,t_0)\varphi \rangle = \frac{1}{2\pi \mathrm{i}} \cdot PV \int_{\mathbb{R}} e^{-\mathrm{i}\mathcal{E}(t-t_0)/\hbar} \langle \chi | G^+(\mathcal{E})\varphi \rangle \, d\Re(\mathcal{E})$$

where we assume that $t \neq t_0$.
(ii) *For all energies* $\mathcal{E}$ *in the open lower half-plane (i.e.,* $\Im(\mathcal{E}) < 0$*), we have the Fourier–Laplace transformation*

$$\langle \chi | G^-(\mathcal{E})\varphi \rangle = \frac{\mathrm{i}}{\hbar} \int_{\mathbb{R}} e^{\mathrm{i}\mathcal{E}(t-t_0)/\hbar} \langle \chi | P^-(t,t_0)\varphi \rangle \, dt \tag{7.102}$$

together with the inverse transformation

$$\langle \chi | P^-(t,t_0)\varphi \rangle = \frac{1}{2\pi \mathrm{i}} \cdot PV \int_{\mathbb{R}} e^{-\mathrm{i}\mathcal{E}(t-t_0)/\hbar} \langle \chi | G^-(\mathcal{E})\varphi \rangle \, d\Re(\mathcal{E})$$

where we assume that $t \neq t_0$.

Complete proofs for this prototype of operator calculus including the statements above can be found in Zeidler (1995a), Chap. 5 (see the references on page 1049). For the proof of Prop. 7.17 above, we refer to Problem 7.36. The Fourier–Laplace transform is also briefly called the Laplace transform.[65]

Interestingly enough, both retarded (i.e., causal) propagators and advanced (i.e., non-causal) propagators play a crucial role in quantum field theory.

From the mathematical point of view, the reason is that the relevant perturbation theory depends on quantities which are constructed by using both retarded and advanced propagators. Physicists interpret this by saying that

- the interaction between elementary particles is governed by virtual particles (which are graphically represented by the internal lines of the Feynman diagrams), and
- the virtual particles violate basic laws of physics (e.g., the relation between energy and momentum or causality).

7.6.2 The General Operator Calculus

> The observation which comes closest to an explanation of the mathematical concepts cropping up in physics which I know is Einstein's statement that the only physical theories which we are willing to accept are the beautiful ones. It stands to argue that the concepts of mathematics, which invite the exercise of much a wit, have the quality of beauty.[66]
>
> Eugene Wigner, 1959

[65] Laplace (1749–1827), Fourier (1768–1830).

[66] E. Wigner, The unreasonable effectiveness of mathematics in the natural sciences, Richard Courant Lecture in Mathematical Sciences delivered at New York University, May 11, 1959. In: E. Wigner, Philosophical Reflections and Syntheses. Annotated by G. Emch. Edited by J. Mehra and A. Wightman, Springer, New York, 1995, pp. 534–549.

Let X be a complex separable finite-dimensional or infinite-dimensional Hilbert space. We make the following assumption:

(A) *The linear operator $H : D(H) \to X$ is self-adjoint.*

This includes tacitly that the domain of definition $D(H)$ is a linear dense subspace of X. Von Neumann's famous spectral theorem tells us the following.

Theorem 7.18 *For each pair $\varphi \in D(H), \chi \in X$, there exists a (complex-valued) measure $\mu_{\chi,\varphi}$ on the real line such that*

$$\langle \chi | H\varphi \rangle = \int_{\mathbb{R}} E \cdot d\mu_{\chi,\varphi}(E).$$

We have $\varphi \in D(H)$ iff $\int_{\mathbb{R}} |E|^2 d\mu_{\varphi,\varphi}(E) < \infty$.

Furthermore, if $||\varphi|| = 1$, then $\mu_{\varphi,\varphi}$ is a classical probability measure, that is, $\int_{\mathbb{R}} d\mu_{\varphi,\varphi} = 1$. In order to get a physical interpretation, assume that the operator H is the Hamiltonian of a quantum system. Let φ be a unit vector in the Hilbert space X, that is, $||\varphi|| = 1$, and let Ω be an interval on the real line. Then the real number

$$\int_{\Omega} d\mu_{\varphi,\varphi}(E)$$

is the probability of finding the quantum system in the state φ. Moreover,

$$\bar{E} := \int_{\mathbb{R}} E \cdot d\mu_{\varphi,\varphi}(E)$$

is the mean energy value measured in the state φ of the quantum system. Note that this spectral theorem depends on the self-adjointness of the operator H, but it fails for formally self-adjoint operators which are not self-adjoint. Therefore, as it was discovered by von Neumann in 1929, the full probabilistic interpretation of observables in quantum mechanics is only valid for self-adjoint operators.

Let $F : \mathbb{R} \to \mathbb{C}$ be a continuous function (or, more generally, a piecewise continuous and bounded function like the Heaviside function). Let D be the set of all elements φ in X with $\int_{\mathbb{R}} |F(E)|^2 d\mu_{\varphi,\varphi}(E) < \infty$. The von Neumann operator calculus is based on the following fact.

Theorem 7.19 *There exists a uniquely determined self-adjoint operator denoted by $\mathsf{F}(H) : D \to X$ such that, for all $\varphi \in D$, $\chi \in X$, there holds the key relation $\langle \chi | \mathsf{F}(H)\varphi \rangle = \int_{\mathbb{R}} F(E) \cdot d\mu_{\chi,\varphi}(E)$.*

For example, if $F(E) \equiv 1$, then $\mathsf{F}(H) = I$ (unit operator), and for all χ, φ in X we get $\langle \chi | \varphi \rangle = \int_{\mathbb{R}} d\mu_{\chi,\varphi}$.

Sketch of the proof. An elegant short proof of Theorems 7.18 and 7.19 can be found in I. Sigal, Scattering Theory for Many-Body Quantum Mechanical Systems: Rigorous Results, Springer, New York, 1983. In the spirit of the Dirac calculus, the idea of Sigal's proof is to use the regularized (rescaled) resolvent

$$\delta_\varepsilon(EI - H) := \frac{1}{2\pi} \cdot (H - (E + \mathrm{i}\varepsilon)I)^{-1}, \qquad E \in \mathbb{R},\ \varepsilon > 0$$

with the typical property

$$w - \lim_{E_0 \to +\infty} \int_{-E_0}^{E_0} \delta_\varepsilon(EI - H) dE = I, \qquad \varepsilon > 0. \tag{7.103}$$

This justifies the designation as a (regularized) operator delta function. Note that we use the weak limit in (7.103).[67]

Step 1: The operator $\mathsf{F}(H)$ in the regular case: Let $F \to \mathbb{C}$ be a smooth function with compact support, that is, $F \in \mathcal{D}(\mathbb{R})$. We use the key formula

$$\mathsf{F}_\varepsilon(H) := w - \lim_{E_0 \to +\infty} \int_{-E_0}^{E_0} \delta_\varepsilon(EI - H) F(E) dE$$

and the limit formula

$$\mathsf{F}(H) := w - \lim_{\varepsilon \to +0} \mathsf{F}_\varepsilon(H)$$

in order to introduce the operator $\mathsf{F}(H)$ on the Hilbert space X. It can be shown that the limits exist.

Step 2: The spectral family $\{\mathsf{E}_\lambda\}_{\lambda \in \mathbb{R}}$ of the operator H: We extend the definition of the operator $\mathsf{F}(H)$ to more general (discontinuous) bounded functions $F : \mathbb{R} \to \mathbb{C}$ which are the pointwise limit

$$F(E) = \lim_{n \to \infty} F_n(E), \qquad E \in \mathbb{R}$$

of an increasing sequence (F_n) of nonnegative functions $F_n \in \mathcal{D}(\mathbb{R})$. In particular, choosing the characteristic function e_λ of the open interval $]-\infty, \lambda[$, we get the operator $\mathsf{E}_\lambda(H)$.

Step 3: The spectral measure μ: For given $\varphi \in X$ with $||\varphi|| = 1$, we define the probability measure $\mu_{\varphi,\varphi}$ on the real line by setting

$$\int_{]-\infty,\lambda[} d\mu_{\varphi,\varphi}(E) := \langle \varphi | \mathsf{E}_\lambda \varphi \rangle.$$

This is the measure of the open interval $]-\infty, \lambda[$; the function $\lambda \mapsto \langle \varphi | \mathsf{E}_\lambda \varphi \rangle$ represents the distribution function of the measure $\mu_{\varphi,\varphi}$, in terms of the theory of probability. More generally, for given $\varphi, \chi \in X$, we construct the (complex-valued) measure $\mu_{\chi,\varphi}$ on the real line by setting

$$\int_{]-\infty,\lambda[} d\mu_{\chi,\varphi}(E) = \langle \chi | \mathsf{E}_\lambda \varphi \rangle. \tag{7.105}$$

The spectral family of H has the following properties for all real numbers λ, λ_0 and all $\varphi \in X$:

(S1) The operator $\mathsf{E}_\lambda : X \to X$ is an orthogonal projection (i.e., the operator E_λ is linear, continuous, self-adjoint, and $\mathsf{E}_\lambda^2 = \mathsf{E}_\lambda$).
(S2) The function $\lambda \mapsto \langle \varphi | \mathsf{E}_\lambda \varphi \rangle$ is nondecreasing on the real line.
(S3) $\lim_{\lambda \to -\infty} \mathsf{E}_\lambda \varphi = 0$ and $\lim_{\lambda \to \infty} \mathsf{E}_\lambda \varphi = \varphi$.
(S4) $\lim_{\lambda \to \lambda_0 - 0} \mathsf{E}_\lambda \varphi = \mathsf{E}_{\lambda_0} \varphi$. □

[67] Recall that, by definition, the weak limit

$$w - \lim_{n \to \infty} \psi_n = \psi \tag{7.104}$$

exists on the Hilbert space X iff $\lim_{n \to \infty} \langle \varphi | \psi_n \rangle = \langle \varphi | \psi \rangle$ for all $\varphi \in X$. In particular, let $\varphi_1, \varphi_2, \ldots$ be a complete orthonormal system in X. Then the weak convergence (7.104) is equivalent to the boundedness of the sequence (ψ_n) and the convergence of all the Fourier coefficients, that is, $\lim_{n \to \infty} \langle \varphi_k | \psi_n \rangle = \langle \varphi_k | \psi \rangle$ for all k.

The spectral family $\{\mathsf{E}_\lambda\}$ of H is also called the spectral resolution of H.

Corollary 7.20 *For any self-adjoint operator $H : D(H) \to X$, there exists precisely one spectral family $\{E_\lambda\}$ with the properties* (S1)–(S4) *such that Theorem* 7.18 *holds with* (7.105)*. Explictly, the spectral family is given by the limit*

$$\langle\psi|\mathsf{E}_\lambda\varphi\rangle = \lim_{\delta\to+0}\lim_{\varepsilon\to+0}\int_{-\infty}^{\lambda+\delta}\langle\psi|(R_{s-\mathrm{i}\varepsilon} - R_{s+\mathrm{i}\varepsilon})\varphi\rangle ds$$

for all $\psi, \varphi \in X$. Here, $R_\mu := (\mu I - H)^{-1}$ is the resolvent of H.

In terms of physics, the spectral family of the observable H uniquely determines the probability measure of H. The proof of the Corollary can be found in K. Jörgens and F. Rellich, Eigenvalue Problems for Ordinary Differential Equations, p. 113, Springer, Berlin, 1976 (in German). For other proofs of the crucial spectral theorem, we refer to the following monographs:

E. Nelson, Topics in Dynamics: Flows, Princeton University Press, 1969.

K. Maurin, Methods of Hilbert Spaces, Polish Scientific Publishers, Warsaw, 1972.

M. Reed and B. Simon, Methods of Modern Mathematical Physics I: Functional Analysis, Academic Press, New York, 1972.

F. Riesz and B. Nagy, Functional Analysis, Frederyck Ungar, New York, 1978.

F. Berezin and M. Shubin, The Schrödinger Equation, Kluwer, Dordrecht, 1991.

K. Yosida, Functional Analysis, Springer, New York, 1995.

P. Lax, Functional Analysis, Wiley, New York, 2002.

Von Neumann's generalized Fourier transform. Alternatively, von Neumann's spectral theorem above can be obtained from von Neumann's diagonalization theorem:

> *Each linear self-adjoint operator is unitarily equivalent to a multiplication operator $\hat{f}(\lambda) \mapsto \lambda\hat{f}(\lambda)$ on an appropriate function space.*

This represents a far-reaching generalization of the classical Fourier transformation $f \mapsto \hat{f}$. The precise formulation can be found in Sect. 12.2.3 of Vol. I in the setting of the rigorous justification of the Dirac calculus.

Gelfand's theory of C^*-algebras. It was discovered by Gelfand in the 1940s that one can use the theory of C^* algebras in order to construct von Neumann's operator calculus (see the monographs Maurin (1972) and Yosida (1995) quoted above). Note that C^*-algebras play a fundamental role in quantum mechanics, quantum field theory, statistical physics, the Standard Model in particle physics, quantum gravity, and quantum information. The point is that C^*-algebras allow us to describe states and observables in a general setting. We will thoroughly study this in Vol. IV on quantum mathematics (see also Sect. 7.16.3ff for the definition of C^*-algebras together with the construction of the Weyl quantization functor).

The Rellich–Kato perturbation theorem. The operator

$$H + C : D(H) \to X$$

is self-adjoint if the following conditions are satisfied:

- The operator $H : D(H) \to X$ is self-adjoint.

- The perturbation $C : D(C) \to X$ is linear and symmetric, and the domain of definition $D(C)$ contains the set $D(H)$.
- There are fixed real numbers $0 \le a < 1$ and $b \ge 0$ such that

$$||C\varphi|| \le a||H\varphi|| + b||\varphi|| \qquad \text{for all} \quad \varphi \in D(H).$$

In particular, the assumptions are satisfied if the operator $C : X \to X$ is linear, symmetric, and continuous. The proof can be found in Zeidler (1995a), p. 417 (see the references on page 1049). In 1951, this criterion was used by Kato in order to prove that the Hamiltonian operators of molecules are essentially self-adjoint.

Classification of the spectrum. As we will discuss below, every self-adjoint operator $H : D(H) \to X$ generates a unique decomposition

$$\boxed{X = X_{\text{bound}} \oplus X_{\text{scatt}} \oplus X_{\text{sing}}} \tag{7.106}$$

of the Hilbert space X into pairwise orthogonal closed linear subspaces. It turns out that, in terms of quantum mechanics,

- the elements of X_{bound} correspond to bound states of the quantum system,
- and the elements of X_{scatt} correspond to scattering states.

The elements of X_{sing} are called singular states. In regular situations, the singular space X_{sing} is trivial, that is, it only consists of the zero element.[68]

(i) Bound states: The element φ of X is called an eigenstate of the Hamiltonian H iff there exists a real number E such that

$$\boxed{H\varphi = E\varphi, \qquad \varphi \neq 0.}$$

The number E is called the eigenvalue to the eigenstate φ.[69] By definition, the space X_{bound} is the closed linear hull of the eigenstates of H. The eigenstates of H form a complete orthonormal system of X_{bound}.

(ii) Classification of states by means of the spectral measure: Let the nonzero state $\varphi \in X$ be given. Consider the spectral measure μ_φ on the real line.[70] Then:

- $\varphi \in X_{\text{bound}}$ iff μ_φ is a point measure, that is, there exists a finite or countable set $\Omega = \{x_1, x_2, \ldots\}$ such that $\mu_\varphi(\{x_k\}) > 0$ for all k and $\mu_\varphi(\mathbb{R} \setminus \Omega) = 0$.
- $\varphi \in X_{\text{scatt}}$ iff the measure μ_φ has a density, that is, there exists a nonnegative integrable function $\varrho : \mathbb{R} \to \mathbb{R}$ such that $\mu_\varphi(\Omega) = \int_\Omega \varrho(x)dx$ for all intervals Ω.[71]
- $\varphi \in X_{\text{sing}}$ iff the measure μ_φ is singular, that is, there exists a set Ω of Lebesgue measure zero such that $\mu_\varphi(\Omega) > 0$ and $\mu_\varphi(\mathbb{R} \setminus \Omega) = 0$.

The operator H maps each of the three Hilbert spaces X_{bound}, X_{scatt} and X_{sing} into itself.

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[68] The importance of both the absolutely continuous spectrum and the subspace X_{scatt} for the functional-analytic scattering theory will be discussed in Sect. 9 on page 747.

[69] On page 526 we will introduce eigencostates (or generalized eigenfunctions). Such costates do not always live in the infinite-dimensional Hilbert space X, but in an extension of X. Observe that each eigenstate is an eigencostate, but the converse is not always true. The eigenvalues of eigencostates are called generalized eigenvalues.

[70] To simplify notation, we write μ_φ instead of $\mu_{\varphi,\varphi}$.

[71] Equivalently, the monotone function $\lambda \mapsto \langle\varphi|\mathsf{E}_\lambda\varphi\rangle$ is differentiable almost everywhere on $\mathbb{R}$, and the first derivative is integrable over $\mathbb{R}$.

- The spectrum of the restriction $H : D(H) \cap X_{\rm bound} \to X_{\rm bound}$ is called the pure point spectrum $\sigma_{pp}(H)$.
- The spectrum of the restriction $H : D(H) \cap X_{\rm scatt} \to X_{\rm scatt}$ is called the absolutely continuous spectrum $\sigma_{\rm ac}(H)$.
- The spectrum of the restriction $H : D(H) \cap X_{\rm sing} \to X_{\rm sing}$ is called the singular spectrum $\sigma_{\rm sing}(H)$.

We have the following representation of the spectrum of the operator H:

$$\boxed{\sigma(H) = \sigma_{pp}(H) \cup \sigma_{ac}(H) \cup \sigma_{\rm sing}(H).}$$

The union $\sigma_{\rm c}(H) := \sigma_{\rm ac}(H) \cup \sigma_{\rm sing}(H)$ of the disjoint sets $\sigma_{ac}(H)$ and $\sigma_{\rm sing}(H)$ is called the continuous spectrum of H.

Recall that $\sigma(H)$ is a closed subset of the real line, and the open complement $\varrho(H) := \mathbb{C} \setminus \sigma(H)$ is the resolvent set of H. We have $E \in \varrho(H)$ iff the inverse operator $(EI - H)^{-1} : X \to X$ (i.e., the resolvent) exists as a linear continuous operator. We say that $\sigma_{pp}(H)$ is empty iff $X_{\rm bound} = \{0\}$. An analogous terminology will be used for $\sigma_{\rm ac}(H)$ and $\sigma_{\rm sing}(H)$.

The discrete spectrum. By definition, the discrete spectrum $\sigma_{\rm disc}$ of the operator H is the set of all eigenvalues of finite multiplicity which are isolated points of the spectrum $\sigma(H)$.

The Weyl stability theorem for the essential spectrum. By definition, the essential spectrum $\sigma_{\rm ess}(H)$ of the operator H is the complement to the discrete spectrum. That is, we have the disjoint decomposition

$$\sigma(H) = \sigma_{\rm disc}(H) \cup \sigma_{\rm ess}(H).$$

Explicitly, the essential spectrum contains precisely the following points:

- the eigenvalues of infinite multiplicity,
- the accumulation points of the set of eigenvalues,
- the points of the continuous spectrum.

Weyl proved that we have $E \in \sigma_{\rm ess}(H)$ iff there exists a sequence (φ_n) in the domain of definition $D(H)$ with

- $\lim_{n\to\infty} ||H\varphi_n - E\varphi_n|| = 0$;
- $||\varphi_n|| = 1$ for all n and $w - \lim_{n\to\infty} \varphi_n = 0$;
- the sequence (φ_n) has no convergent subsequence.

Such sequences are called Weyl sequences. The following theorem tells us that the essential spectrum of the self-adjoint operator H is invariant under compact perturbations. The linear operator $C : X \to X$ is called compact iff it is continuous and each sequence $(C\varphi_n)$ contains a convergent subsequence provided (φ_n) is bounded.

Theorem 7.21 *Let $H : D(H) \to X$ be a self-adjoint operator, and let C be a linear compact self-adjoint operator. Then the operator $H + C$ is self-adjoint and $\sigma_{\rm ess}(H + C) = \sigma_{\rm ess}(H)$.*

A variant of this theorem was proven by Weyl in 1909.[72]

Characterization of the spectrum by means of the spectral family. Let $H : D(H) \to X$ be a linear self-adjoint operator on the complex Hilbert space X. Set $P_{\lambda_0}\psi := \lim_{\lambda\to\lambda_0+0}(\mathsf{E}_\lambda - \mathsf{E}_{\lambda_0})\psi$ for all $\psi \in X$.

[72] H. Weyl, On the completely continuous difference of two bounded quadratic forms, Rend. Circ. Mat. Palermo **27** (1909), 373–392 (in German).

Theorem 7.22 (i) *The real number λ_0 is not contained in the spectrum $\sigma(H)$ of the operator H iff the spectral family $\{\mathsf{E}_\lambda\}_{\lambda\in\mathbb{R}}$ is constant in some open neighborhood of the point λ_0.*

(ii) *The real number λ_0 is an eigenvalue of H iff the spectral family jumps at the point λ_0. That is, $P_{\lambda_0} \neq 0$. The operator $P_{\lambda_0} : X \to X$ is the orthogonal projection operator onto the eigenspace of H to the eigenvector λ_0.*

(iii) *The real number λ_0 is contained in the essential spectrum $\sigma_{\rm ess}(H)$ iff* $\dim(\mathsf{E}_{\lambda_0+\varepsilon} - \mathsf{E}_{\lambda_0-\varepsilon})(X) = \infty$ *for all $\varepsilon > 0$.*

A comprehensive summary of spectral theory, measure theory, and other tools of modern analysis together with applications can be found in the Appendix to Zeidler, Nonlinear Functional Analysis and its Applications, Vol. IIB, Springer, New York, 1986. We also refer to Reed and Simon, Methods of Modern Mathematical Physics, Vols. 1–4, Academic Press, New York, 1972–1979.

7.6.3 Rigorous Propagator Theory

> The function $\psi(t) = \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}\psi(t_0)$, for all times $t \in \mathbb{R}$, describes the dynamics of a quantum system corresponding to the self-adjoint Hamiltonian H.
>
> Folklore

It is our goal to translate the formal propagator theory from Sect. 7.5.3 into a rigorous mathematical setting.

Quantum Dynamics

The abstract Schrödinger equation. Consider the initial-value problem

$$\mathrm{i}\hbar\dot{\psi}(t) = H\psi(t), \quad t > t_0, \quad \psi(t_0) = \psi_0. \tag{7.107}$$

This is the basic equation in quantum mechanics.

Theorem 7.23 *Let $H : D(H) \to X$ be a linear self-adjoint operator on the complex separable Hilbert space X. For given initial state $\psi_0 \in D(H)$, the Schrödinger equation (7.107) has a unique, continuously differentiable solution $\psi : [t_0, \infty[\to \mathbb{R}$. Explicitly,*

$$\psi(t) := \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}\psi_0, \qquad t \geq t_0. \tag{7.108}$$

The operator $e^{-\mathrm{i}(t-t_0)H/\hbar} : X \to X$ is unitary for all times $t \in X$.

The proof can be found in H. Triebel, Higher Analysis, Sect. 22, Barth, Leipzig, 1989.

Generalized solution. For given initial value $\psi_0 \in X$, the function $\psi = \psi(t)$ is well-defined by (7.108). This function is continuous on $[0, \infty[$. In contrast to this, if $\psi_0 \notin D(H)$, then as a rule, it is not true that the derivative $\dot{\psi}(t)$ exists. Therefore, we call $\psi(t) = \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}\psi_0$ with $\psi_0 \in X$ a generalized solution of the Schrödinger equation (7.107). This solution is defined for all times $t \in \mathbb{R}$.

One-parameter unitary groups. By definition, a one-parameter unitary group on the Hilbert space X is a family $\{U(t)\}_{t\in\mathbb{R}}$ of operators with the following properties:

- $U(t) : X \to X$ is unitary for all times $t \in \mathbb{R}$.
- $U(t+s) = U(t)U(s)$ for all $t, s \in \mathbb{R}$, and $U(0) = I$.

Such a group is called strongly continuous iff the function $t \mapsto U(t)\varphi_0$ is continuous on the real line for all $\varphi_0 \in X$. The following classical result was proven by Stone (1903–1989) in 1932. [73]

Theorem 7.24 *Let X be a complex separable Hilbert space.*

(i) *If $\{U(t)\}_{t\in\mathbb{R}}$ is a strongly continuous, one-parameter unitary group on X, then there exists a unique self-adjoint operator $H : D(H) \to X$ such that*

$$U(t) = e^{-\mathrm{i}tH/\hbar}\varphi_0 \qquad \text{for all} \quad t \in \mathbb{R}. \tag{7.109}$$

We have $H\varphi_0 = \lim_{t\to 0} \frac{U(t)\varphi_0 - \varphi_0}{t}$. This limit exists precisely iff $\varphi_0 \in D(H)$. The operator H is called the generator of the one-parameter unitary group.

(ii) *Conversely, if $H : D(H) \to X$ is a self-adjoint operator, then formula (7.109) defines a strongly continuous, one-parameter unitary group on X.*

The proof can be found in Zeidler, Nonlinear Functional Analysis and its Applications, Vol. II/A, Sect. 19.21, Springer, New York, 1986.

The Feynman propagator. Let $t, t_0 \in \mathbb{R}$. In terms of Theorem 7.23, the unitary operator

$$P(t, t_0) := \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}$$

on the Hilbert space X is called the propagator at time t (generated by the Hamiltonian H with respect to the initial time t_0). The truncated operator[74]

$$P^+(t, t_0) := P(t, t_0)\theta(t - t_0), \qquad t \in \mathbb{R}$$

is called the retarded propagator (or the Feynman propagator) at time t (with respect to the initial time t_0.) Obviously, $P(t_0, t_0) = I$. We get

$$\boxed{P(t, t_0) = P(t, \tau)P(\tau, t_0) \qquad \text{for all} \quad t, \tau, t_0 \in \mathbb{R}.}$$

This so-called reversible propagator equation (or group equation) follows from

$$U(t - \tau)U(\tau - t_0) = U(t - \tau + \tau - t_0) = U(t - t_0),$$

which is the consequence of the fact that $\{U(t)\}_{t\in\mathbb{R}}$ forms a group.

Euclidean Quantum Dynamics

The Euclidean Schrödinger equation. Consider the initial-value problem

$$\dot{\psi}(t) = -H\psi(t), \quad t > t_0, \quad \psi(t_0) = \psi_0. \tag{7.110}$$

We assume that the linear self-adjoint operator $H : D(H) \to X$ is nonnegative, that is, $\langle\varphi|H\varphi\rangle \geq 0$ for all $\varphi \in D(H)$. Observe that both the diffusion equation and the heat conduction equation are of this type. Since diffusion is an irreversible process, we expect that the initial condition ψ_0 does not uniquely determine the state $\psi(t)$ in the past $t < t_0$. Mathematically, this is reflected by the fact that the solution (7.111) below is not defined for $t < t_0$.

[73] M. Stone, On one-parameter unitary groups in Hilbert space, Ann. Math. **33** (1932), 643–648.

[74] Recall that $\theta(t-t_0) := 1$ if $t \geq t_0$, and $\theta(t-t_0) := 0$ if $t < t_0$ (Heaviside function).

Theorem 7.25 *For given $\psi_0 \in D(H)$, the Euclidean Schrödinger equation (7.110) has a unique, continuously differentiable solution $\psi : [t_0, \infty[\to \mathbb{R}$. This solution is given by*

$$\psi(t) = e^{-(t-t_0)H}\psi_0, \qquad t \geq t_0. \tag{7.111}$$

The operator family $\{e^{-tH}\}_{t\geq 0}$ forms a non-expansive semigroup, that is, the linear self-adjoint operators $e^{-tH} : X \to X$ satisfy

$$e^{-tH}e^{-sH} = e^{-(t+s)H} \qquad \text{for all} \quad t, s \geq 0,$$

as well as $e^{-tH}{}_{|t=0} = I$, and $\sup_{t\geq 0} ||e^{-tH}|| \leq 1$.

The proof can be found in H. Triebel, Higher Analysis, Sect. 22, Barth, Leipzig, 1989. In order to understand the specifics of the Euclidean quantum dynamics, suppose that the nonnegative self-adjoint operator $H : D(H) \to X$ has a complete orthonormal system $\varphi_0, \varphi_1, \varphi_2, \ldots$ of eigenvectors with $H\varphi_k = E_k\varphi_k$ for all k. Then $E_k = E_k\langle\varphi_k|\varphi_k\rangle = \langle\varphi_k|H\varphi_k\rangle \geq 0$ for all k. For $\psi_0 \in X$, the Parseval equation tells us that $||\psi_0||^2 = \sum_{k=1}^{\infty} |\langle\varphi_k|\psi\rangle|^2$. The series

$$\mathrm{e}^{-tH}\psi_0 = \sum_{k=1}^{\infty} \mathrm{e}^{-E_k t}\langle\varphi_k|\psi\rangle\varphi_k \tag{7.112}$$

is convergent iff $\sum_{k=0}^{\infty} \mathrm{e}^{-2tE_k}|\langle\varphi_k|\psi\rangle|^2 < \infty$. This is true if $t \geq 0$ because of $0 \leq \mathrm{e}^{-E_k t} \leq 1$. However, if $t < 0$, then the convergence of (7.112) can be violated. This reflects the irreversibility of diffusion and heat conduction processes.

The Euclidean propagator. Let $t \geq t_0$. The operator

$$P(t, t_0) := \mathrm{e}^{-(t-t_0)H}$$

is non-expansive on the Hilbert space X, that is $\sup_{t\geq t_0} ||\mathrm{e}^{-(t-t_0)H}|| \leq 1$. This operator is called the Euclidean propagator at time t (generated by the Hamiltonian H with respect to the initial time t_0). Obviously, $P(t_0, t_0) = I$. Furthermore, we have

$$\boxed{P(t, t_0) = P(t, \tau)P(\tau, t_0) \qquad \text{for all} \quad t \geq \tau \geq t_0.}$$

This so-called irreversible propagator equation (or semi-group equation) follows from $\mathrm{e}^{-(t-\tau)H}\mathrm{e}^{-(\tau-t_0)H} = \mathrm{e}^{-(t-\tau+\tau-t_0)H} = \mathrm{e}^{-(t-t_0)H}$, by Theorem 7.25.

Historical remarks. In the 19th century, mathematicians and physicists (e.g., Gauss, Green, Fourier, Riemann and Maxwell) discovered that one can use integral formulas of the type

$$u(x) = \int G(x, y)f(y)dy$$

in order to represent the solutions u of partial differential equations of the form $Lu = f$ which appear in hydrodynamics, gas-dynamics, elasticity, heat conduction, diffusion, and electrodynamics. The integral kernel G is called the Green's function.

Functional analysis was founded by Hilbert in the early 1910s in order to generalize Fredholm's theory of integral equations. At this time, differential equations were reduced to integral equations with Green's functions as integral kernels. In von Neumann's approach to quantum mechanics in the late 1920s, differential operators were regarded as independent mathematical objects, namely, as self-adjoint operators in a Hilbert space. In contrast to this, in his monograph

Principles of Quantum Mechanics,

Clarendon Press, Oxford, 1930, Dirac used his calculus in order to construct (generalized) integral kernels like the Dirac delta function. In the preface to his monograph

Mathematical Foundations of Quantum Mechanics,

Springer, Berlin 1932, von Neumann pointed out that he did not use Dirac's method because of lack of mathematical rigor.

In the 1940s, Feynman was strongly influenced by Dirac's approach. The Feynman propagators are nothing other than special Green's functions. In the 1950s, the two approaches due to Dirac and von Neumann were combined with each other by Gelfand; he used Laurent Schwartz's theory of generalized functions founded in the 1940s and Grothendieck's theory of nuclear spaces. As a typical example, we will consider the free quantum particle in Sect. 7.6.4. In the 1960s, the theory of pseudo-differential operators was created by Kohn and Nirenberg; this approach represents a further generalization of the theory of operator kernels. In quantum mechanics, this is related to the Weyl calculus introduced in the late 1920s by Hermann Weyl (see Sect. 7.12 on Weyl quantization).

Rigorous Operator Kernel

The operator kernel knows all about the operator.
Folklore

Let $N = 1, 2, \ldots$, and let D be a dense subset of $L_2(\mathbb{R}^N)$. The linear continuous operator $A : L_2(\mathbb{R}^N) \to L_2(\mathbb{R}^N)$ is said to have a continuous kernel iff there exists a continuous function $\mathcal{A} : \mathbb{R}^{2N} \to \mathbb{C}$ such that[75]

$$\langle \chi | A\varphi \rangle = \int_{\mathbb{R}^{2N}} \chi(x)^\dagger \mathcal{A}(x,y)\varphi(y) dx^N dy^N \tag{7.113}$$

for all $\varphi, \chi \in D$. This kernel is unique. In fact, if $\mathcal{A}$ and $\mathcal{B}$ are two continuous kernels corresponding to the operator A, then

$$\int_{\mathbb{R}^{2N}} (\chi(x)\varphi(y)^\dagger)^\dagger (\mathcal{A}(x,y) - \mathcal{B}(x,y)) dx^N dy^N = 0$$

for all $\varphi, \chi \in D$. Since the set of functions $(x,y) \mapsto \chi(x)\varphi(y)^\dagger$ with $\varphi, \chi \in D$ is dense in the complex Hilbert space $L_2(\mathbb{R}^{2N})$, we obtain the desired result $\mathcal{A}(x,y) = \mathcal{B}(x,y)$ on $\mathbb{R}^{2N}$.

More generally, if relation (7.113) is true for a function $\mathcal{A} \in L_2(\mathbb{R}^{2N})$, then this function is uniquely determined (as an element of the Hilbert space $L_2(\mathbb{R}^{2N})$ by the operator A. The function $\mathcal{A}$ is called the L_2-kernel of the operator A. Equation (7.113) generalizes the matrix equation

$$\chi^\dagger A\varphi = \sum_{j,k=1}^{n} \chi_j^\dagger A_{jk} \varphi_k.$$

[75] In classical mathematics, one uses $(A\varphi)(x) = \int_{\mathbb{R}^N} \mathcal{A}(x,y)\varphi(y)dy^N$. This is equivalent to (7.113). However, the bilinear formulation (7.113) is crucial for defining the notion of kernel for generalized functions.

Therefore, the kernel $(x, y) \mapsto \mathcal{A}(x, y)$ can be regarded as a continuous version of the complex $(n \times n)$-matrix (A_{jk}). The kernel $\mathcal{A}$ is called self-adjoint iff

$$\boxed{\mathcal{A}(x, y)^\dagger = \mathcal{A}(y, x) \qquad \text{for all} \quad x, y \in \mathbb{R}^N.}$$

This generalizes self-adjoint matrices. In 1904 Hilbert discovered the importance of self-adjoint integral kernels for both

- the spectral theory of integral operators and
- the Fourier expansions to regular boundary-value problems for second-order ordinary differential equations (i.e., the regular Sturm–Liouville problems).

In 1910, Weyl generalized this to singular Sturm–Liouville problems which are typical for computing the spectra of atoms and molecules in quantum mechanics.[76]

7.6.4 The Free Quantum Particle as a Paradigm of Functional Analysis

> Extend the pre-Hamiltonian to a self-adjoint operator on an appropriate Hilbert space X of quantum states, and use costates related to a Gelfand triplet with respect to X.
>
> The golden rule

The modern theory of differential and integral equations is based on functional analysis, which was created by Hilbert (1862–1943) in the beginning of the 20th century.[77] The development of functional analysis was strongly influenced by the questions arising in quantum mechanics and quantum field theory. In this section, we want to study thoroughly how the motion of a free quantum particle on the real line is related to fundamental notions in functional analysis.

This is Ariadne's thread in functional analysis.

This way, the formal considerations from Sect. 7.5.3 will obtain a sound basis for the free quantum particle.

The main idea of the modern strategy in mathematics and physics consists in describing differential operators and integral operators by abstract operators related to generalized integral kernels.

(i) In the language used by physicists, this concerns the Dirac calculus based on Dirac's delta function and Green's functions (also called Feynman propagators).

(ii) In the language used by mathematicians this is closely related to:
- Lebesgue's passage from the Riemann integral to the Lebesgue integral based on measure theory in about 1900;
- von Neumann's passage from formally self-adjoint operators to self-adjoint operators and his generalization of the classical Fourier transform via spectral theory in the late 1920s;
- Laurent Schwartz's theory of generalized functions including the kernel theorem in the 1940s;

[76] Weyl used methods on singular integral equations. These methods were developed in Weyl's Ph.D. thesis advised by Hilbert in Göttingen in 1908.

[77] As an introduction, we recommend P. Lax, Functional Analysis, Wiley, New York, 2002, and E. Zeidler, Applied Functional Analysis, Vols. 1, 2, Springer, New York, 1995.

- the generalization of von Neumann's spectral theory by Gelfand and Kostyuchenko in 1955 (based on quantum costates as generalized functions and the corresponding Gelfand triplets);
- the extension of the Gelfand–Kostyuchenko approach to general nuclear spaces by Maurin in 1959.[78]

Tempered Distributions

> In order to translate the very elegant, but formal Dirac calculus into mathematics, one has to leave the Hilbert space of states used by von Neumann in about 1930. Folklore

In what follows, we will use

- the space $\mathcal{S}(\mathbb{R})$ of smooth test functions $\varphi : \mathbb{R} \to \mathbb{C}$ which decrease rapidly at infinity,
- and the space $\mathcal{S}'(\mathbb{R})$ of tempered distributions introduced on page 615 of Vol. I.

Our basic tools will be

- the Fourier transform and
- the language of tempered distributions, and Gelfand triplets.

The main idea of our functional-analytic approach to the free quantum particle on the real line is to study the three energy operators

$$H_{\text{pre}} \subseteq H_{\text{free}} \subseteq H_{\text{pre}}^d.$$

Here, we start with $H_{\text{pre}}\varphi := -\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2}$ for all $\varphi \in \mathcal{S}(\mathbb{R})$. This is the one-dimensional Laplacian. We first extend the (self-dual and formally self-adjoint) pre-Hamiltonian $H_{\text{pre}} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ on the space of test functions $\mathcal{S}(\mathbb{R})$ to the dual Hamiltonian

$$H_{\text{pre}}^d : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$$

on the space of tempered distributions. The restriction of the operator H_{pre}^d to the Hilbert space $L_2(\mathbb{R})$ yields the self-adjoint Hamiltonian

$$H_{\text{free}} : D(H_{\text{free}}) \to L_2(\mathbb{R})$$

used by von Neumann. Here, $\mathcal{S}(\mathbb{R}) \subseteq D(H_{\text{free}}) \subseteq L_2(\mathbb{R})$ where the domain $D(H_{\text{free}})$ of the free Hamiltonian H_{free} is the Sobolev space $W_2^2(\mathbb{R})$. In general, Sobolev spaces play a crucial role in the modern theory of linear and nonlinear partial differential equations. We recommend:

> L. Evans, Partial Differential Equations, Amer. Math. Soc., Providence, Rhode Island, 1998.
>
> Yu. Egorov and M. Shubin, Foundations of the Classical Theory of Partial Differential Equations, Springer, New York, 1998.

[78] I. Gelfand and A. Kostyuchenkov, On the expansion in eigenfunctions of differential operators and other operators, Doklady Akad. Nauk **103** (1955), 349–352 (in Russian).
K. Maurin, General eigenfunction expansion and the spectral representation of general kernels: a generalization of distribution theory to Lie groups, Bull. Acad. Sci. Polon. Sér. math. astr. et phys. **7** (1959), 471–479 (in German).

Yu. Egorov, A. Komech, and M. Shubin, Elements of the Modern Theory of Partial Differential Equations, Springer, New York, 1999.

P. Lax, Hyperbolic Partial Differential Equations, Courant Institute, New York, 2007.

R. Dautray and J. Lions, Mathematical Analysis and Numerical Methods for Science and Technology, Vols. 1–6, Springer, New York, 1988.

H. Triebel, Theory of Function Spaces, Birkhäuser, Basel, 1992.

We also refer to the author's monographs: Zeidler (1986), Vols. 1–4, and Zeidler (1995a), (1995b) (see the references on page 1049).

The Schrödinger Equation

The instationary Schrödinger equation. The motion of a free quantum particle of mass $m > 0$ on the real line is governed by the following initial-value problem

$$\boxed{\mathrm{i}\hbar\psi_t(x,t) = -\frac{\hbar^2}{2m}\psi_{xx}(x,t), \quad x,t \in \mathbb{R}, \quad \psi(0,x) = \psi_0(x).} \tag{7.114}$$

Here, the wave function ψ_0 is given at the initial time $t = 0$.

The stationary Schrödinger equation. Using the classical Fourier ansatz $\psi(x,t) := \mathrm{e}^{-\mathrm{i}tE/\hbar}\varphi(x)$, equation (7.114) implies the eigenvalue problem

$$\boxed{-\frac{\hbar^2}{2m}\,\varphi''(x) = E\varphi(x), \qquad x \in \mathbb{R}.} \tag{7.115}$$

We are looking for a nonzero function φ and a complex number E.

The Weyl lemma tells us that each solution of (7.115), in the sense of distributions, is a classical smooth function.[79]

Explicitly, all the solutions of (7.115) are given by

$$\varphi_p(x) := \frac{\mathrm{e}^{\mathrm{i}px/\hbar}}{\sqrt{2\pi\hbar}}, \qquad x \in \mathbb{R}$$

with the energy $E(p) := \frac{p^2}{2m}$. Here, p is an arbitrary real number. For any $p \in \mathbb{R}$, we have

$$-\mathrm{i}\hbar\frac{d\varphi_p}{dx} = p\varphi_p.$$

The normalization factor of φ_p is chosen in such a way that we obtain the Parseval equation (7.118) below.

The wave number. To simplify notation, physicists introduce the wave number $k := p/\hbar$, which has the physical dimension of inverse length. Furthermore, for fixed $k \in \mathbb{R}$, let

$$\chi_k(x) := \frac{\mathrm{e}^{\mathrm{i}kx}}{\sqrt{2\pi}} \qquad \text{for all} \quad x \in \mathbb{R}.$$

[79] H. Weyl, The method of orthogonal projection in potential theory, Duke Math. J. **7** (1940), 414–444. An elementary proof of the Weyl lemma for the Laplacian can be found in Zeidler (1986), Vol. IIA, p. 78 (see the references on page 1049). This is the origin of Hörmander's theory of hypoelliptic differential operators (see Sect. 8.6.3).

Then $-\frac{\hbar^2}{2m}\chi_k'' = E_k\chi_k$ for all $k \in \mathbb{R}$ with the energy

$$E_k = \frac{\hbar^2 k^2}{2m}.$$

Hence $|k| = \frac{\sqrt{2mE_k}}{\hbar}$.

Particle stream. If $k > 0$ (resp. $k < 0$), then the function

$$\psi(x,t) := \mathrm{e}^{-\mathrm{i}tE_k/\hbar}\chi_k(x), \qquad x, t \in \mathbb{R}$$

describes a homogeneous stream of free particles which moves from left to right (resp. right to left). The particles of the stream have the momentum $p = \hbar k$, the velocity

$$v = \frac{\hbar k}{m},$$

and the particle density $\varrho = |\chi_k|^2 = \frac{1}{2\pi}$ (see Sect. 7.4.1 on page 459).

The main trouble. The plane-wave functions χ_k possess a well-defined physical meaning, but they do not live in the Hilbert space $L_2(\mathbb{R})$, since $|\chi_k(x)| = \text{const}$ and hence $\int_{\mathbb{R}} |\chi_k(x)|^2 dx = \infty$.

Thus, the Hilbert space setting is not enough for studying quantum mechanics.

In order to overcome this difficulty, one has to introduce the concept of costates and eigencostates (generalized eigenfunctions). This will be done below. Before studying the Schrödinger equation (7.114) and its Hamiltonian H_{free}, we will investigate Gelfand triplets, the extended Fourier transform, Sobolev spaces, the position operator, and the momentum operator.

The Extended Fourier Transform

We want to study the operators $\mathcal{F}_{\text{pre}} \subseteq \mathcal{F} \subseteq \mathcal{F}_{\text{pre}}^d$, where $\mathcal{F} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ is unitary (i.e., $\mathcal{F}$ is a Hilbert space isomorphism). This is the key property of the Fourier transform. As we will show below, in terms of physics the Fourier transform describes the duality between position and momentum.

The classical Fourier transform. Recall that $\chi_k(x) := \frac{\mathrm{e}^{\mathrm{i}kx}}{\sqrt{2\pi}}$ for all $x \in \mathbb{R}$ and all wave numbers $k \in \mathbb{R}$. In terms of the function χ_k, the Fourier transform $\hat{\varphi}$ of the test function $\varphi \in \mathcal{S}(\mathbb{R})$ reads as

$$\boxed{\hat{\varphi}(k) = \int_{\mathbb{R}} \chi_k(x)^\dagger \varphi(x)\, dx, \qquad \text{for all} \quad k \in \mathbb{R}.} \tag{7.116}$$

The inverse Fourier transform is given by

$$\boxed{\varphi(x) := \int_{\mathbb{R}} \chi_k(x)\hat{\varphi}(k)\, dk \qquad \text{for all} \quad x \in \mathbb{R}.} \tag{7.117}$$

Here, the function φ is represented as a superposition of plane waves χ_k. For all test functions $\psi, \varphi \in \mathcal{S}(\mathbb{R})$, we have the crucial Parseval equation

$$\int_{\mathbb{R}} \psi(x)^\dagger \varphi(x)\, dx = \int_{\mathbb{R}} \hat{\psi}(k)^\dagger \hat{\varphi}(k)\, dk, \tag{7.118}$$

which shows that the Fourier transform respects the inner product on the Hilbert space $L_2(\mathbb{R})$. Setting $(\mathcal{F}_{\rm pre}\varphi)(k) := \hat{\varphi}(k)$ for all $k \in \mathbb{R}$, we obtain the operator

$$\mathcal{F}_{\rm pre} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$$

called the classical Fourier transform (or the pre-Fourier transform). This operator is linear, bijective, and sequentially continuous (see Vol. I, p. 614). Moreover, for all $\varphi, \psi \in \mathbb{R}$, we have the following two relations:

(U) $\langle\psi|\varphi\rangle = \langle\mathcal{F}_{\rm pre}\psi|\mathcal{F}_{\rm pre}\varphi\rangle$ (pre-unitary), and

(S) $\int_{\mathbb{R}} \psi(x) \cdot (\mathcal{F}_{\rm pre}\varphi)(x)\, dx = \int_{\mathbb{R}} (\mathcal{F}_{\rm pre}\psi)(x) \cdot \varphi(x)\, dx$ (self-duality).

Relation (U) coincides with the Parseval equation (7.118), whereas relation (S) follows from interchanging integration. Explicitly,

$$\int_{\mathbb{R}} \psi(x) \left(\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}kx} \varphi(k) dk \right) dx = \int_{\mathbb{R}} \varphi(k) \left(\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}kx} \psi(x) dx \right) dk.$$

Finally, use the replacement $k \Leftrightarrow x$.

The Gelfand triplet. It is crucial to leave the Hilbert space $L_2(\mathbb{R})$ and to use the extension $\mathcal{S}'(\mathbb{R})$ of $L_2(\mathbb{R})$ by considering the functions in $L_2(\mathbb{R})$ as tempered distributions. To this end, we introduce the Gelfand triplet (also called the rigged Hilbert space $L_2(\mathbb{R})$):

$$\boxed{\mathcal{S}(\mathbb{R}) \subseteq L_2(\mathbb{R}) \subseteq \mathcal{S}'(\mathbb{R}).}$$

The elements of $L_2(\mathbb{R})$ (resp. $\mathcal{S}'(\mathbb{R})$) are called states (resp. costates). Recall that the inner product on the complex separable Hilbert space $L_2(\mathbb{R})$ is given by

$$\langle\psi|\varphi\rangle = \int_{\mathbb{R}} \psi(x)^\dagger \varphi(x) dx \qquad \text{for all} \quad \varphi, \psi \in L_2(\mathbb{R}).$$

The linear space $\mathcal{S}(\mathbb{R})$ of test functions is dense in $L_2(\mathbb{R})$. For any given function $\psi \in L_2(\mathbb{R})$, we define

$$T_\psi(\varphi) := \int_{\mathbb{R}} \psi(x)\varphi(x) dx \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).$$

Then, T_ψ is a tempered distribution. The map $\psi \mapsto T_\psi$ is an injective map from $L_2(\mathbb{R})$ into $\mathcal{S}'(\mathbb{R})$. Therefore, we may identify ψ with T_ψ. This will frequently be done in the future, by using the symbol ψ instead of T_ψ. In addition, if $\psi \in L_2(\mathbb{R})$, then we define the costate $\langle\psi|$ by setting

$$\langle\psi|(\varphi) := \int_{\mathbb{R}} \psi(x)^\dagger \varphi(x) dx \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).$$

Here, the costate $\langle\psi|$ is a tempered distribution. Obviously, $\langle\psi|(\varphi) = \langle\psi|\varphi\rangle$. Finally, for $k \in \mathbb{R}$, let us define the costate $\langle k|$ by setting

$$\langle k|(\varphi) := \int_{\mathbb{R}} \chi_k^\dagger(x) \varphi(x) dx \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).$$

Motivated by the Dirac calculus, we will write $\langle k|\varphi\rangle$ instead of $\langle k|(\varphi)$. Let $\varphi \in \mathcal{S}(\mathbb{R})$. The relation to the Fourier transform is given by

$$\langle k|\varphi\rangle = \hat{\varphi}(k) \qquad \text{for all} \quad k \in \mathbb{R}.$$

The extended Fourier transform. Recall that $\mathcal{F}_{\rm pre}\varphi := \hat{\varphi}$ for all test functions $\varphi \in \mathcal{S}(\mathbb{R})$. For any tempered distribution $T \in \mathcal{S}'(\mathbb{R})$, define

$$(\mathcal{F}^d_{\rm pre}T)(\varphi) := T(\mathcal{F}_{\rm pre}\varphi) \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).$$

The operator $\mathcal{F}^d_{\rm pre} : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$ is linear and bijective. Next we want to show that

$$\mathcal{F}^d_{\rm pre}\psi = \mathcal{F}_{\rm pre}\psi \qquad \text{for all} \quad \psi \in \mathcal{S}(\mathbb{R}). \tag{7.119}$$

Hence $\mathcal{F}_{\rm pre} \subseteq \mathcal{F}^d_{\rm pre}$. For the proof, fix $\psi \in \mathcal{S}(\mathbb{R})$. By the self-duality of the Fourier transform considered on page 513,

$$\mathcal{F}^d_{\rm pre}T_\psi = T_{\mathcal{F}_{\rm pre}\psi}.$$

Thus, identifying ψ with T_ψ, we get the claim (7.119). Our key definition reads as

$$\mathcal{F}\psi := \mathcal{F}^d_{\rm pre}\psi \qquad \text{for all} \quad \psi \in L_2(\mathbb{R}).$$

In other words, the operator $\mathcal{F}$ is the restriction of the operator $\mathcal{F}^d_{\rm rm}$ to the Hilbert space $L_2(\mathbb{R})$. The Plancherel theorem tells us that the operator

$$\mathcal{F} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$$

is unitary. That is, we have the Parseval equation $\langle \mathcal{F}\psi | \mathcal{F}\varphi \rangle = \langle \psi | \varphi \rangle$ for all functions $\psi, \varphi \in L_2(\mathbb{R})$. Explicitly,

$$\boxed{(\mathcal{F}\psi)(k) = \lim_{R\to+\infty} \frac{1}{\sqrt{2\pi}} \int_{-R}^{R} \mathrm{e}^{-\mathrm{i}kx}\psi(x)dx \qquad \text{for all} \quad k \in \mathbb{R}.}$$

The convergence is to be understood in the sense of the Hilbert space $L_2(\mathbb{R})$.

Simplifying notation. Motivated by $\mathcal{F}_{\rm pre} \subseteq \mathcal{F} \subseteq \mathcal{F}^d_{\rm pre}$, we write $\mathcal{F}$ instead of $\mathcal{F}^d_{\rm pre}$ (and $\mathcal{F}_{\rm pre}$). This way, we get the extended Fourier transform

$$\mathcal{F} : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$$

with $(\mathcal{F}T)(\varphi) = T(\mathcal{F}\varphi)$ for all $T \in \mathcal{S}'(\mathbb{R})$ and all $\varphi \in \mathcal{S}(\mathbb{R})$.

The Sobolev space $W^m_2(\mathbb{R})$. Let $m = 1, 2, \ldots$ By definition,

$$W^m_2(\mathbb{R}) := \{\varphi \in L_2(\mathbb{R}) : \varphi^{(j)} \in L_2(\mathbb{R}), j = 1, \ldots, m\}. \tag{7.120}$$

Here, the function φ and its jth derivatives $\varphi^{(j)}$, $j = 1, 2, \ldots$, are to be understood in the sense of tempered distributions (see (7.121)). Thus, $W^m_2(\mathbb{R}) \subseteq \mathcal{S}'(\mathbb{R})$. The space $W^m_2(\mathbb{R})$ becomes a complex separable Hilbert space equipped with the inner product

$$\boxed{\langle \psi | \varphi \rangle := \sum_{j=0}^{m} \int_{\mathbb{R}} \psi^{(j)}(x)^\dagger \varphi^{(j)}(x)dx.}$$

In 1936, spaces of this type were introduced by Sobolev (1885–1967) in order to study singular solutions of wave equations. The Fourier transform allows the following useful characterization of Sobolev spaces. Let $m = 1, 2, \ldots$

Proposition 7.26 *$\psi \in W^m_2(\mathbb{R})$ iff $\psi \in L_2(\mathbb{R})$ and $\int_{\mathbb{R}} |k|^{2m}|\hat{\psi}(k)|^2 dp < \infty$.*

Costates and Dual Operators

The theory of distributions is based on duality. Costates are dual states.
Folklore

Our goal is to construct eigencostates for the following observables: position, momentum, and energy of a free particle. The following investigations serve as preparation for this. Fix the state $\psi \in L_2(\mathbb{R})$. There are two possibilities for assigning a costate to ψ, namely,

- T_ψ (i.e., $T_\psi(\varphi) := \int_{\mathbb{R}} \psi(x)\varphi(x)dx$) for all $\varphi \in \mathcal{S}(\mathbb{R})$) , and
- $T_{\psi^\dagger}$ (i.e., $T_{\psi^\dagger}(\varphi) := \int_{\mathbb{R}} \psi(x)^\dagger \varphi(x)dx$ for all $\varphi \in \mathcal{S}(\mathbb{R})$).

The map $\psi \mapsto T_\psi$ (resp. $\psi \mapsto T_{\psi^\dagger}$) is injective and linear (resp. antilinear). According to Dirac, we set

$$\boxed{\langle\psi| := T_{\psi^\dagger}.}$$

Moreover, we write $|\psi\rangle$ instead of ψ. In particular, for all $\varphi \in \mathcal{S}(\mathbb{R})$,

$$\langle\psi|(\varphi) = T_{\psi^\dagger}(\varphi) = \int_{\mathbb{R}} \psi(x)^\dagger \varphi(x)dx = \langle\psi|\varphi\rangle.$$

Dual operators. In what follows, duality plays the crucial role. Let us assume that

(H) *The linear operator $A : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is sequentially continuous.*

This means that $\lim_{n\to\infty} \varphi_n = \varphi$ in $\mathcal{S}(\mathbb{R})$ implies $\lim_{n\to\infty} A\varphi_n = A\varphi$ in $\mathcal{S}(\mathbb{R})$ (see Vol. I, p. 537). We want to construct the dual operator

$$A^d : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R}).$$

To this end, choose $T \in \mathcal{S}'(\mathbb{R})$, and define

$$\boxed{(A^dT)(\varphi) := T(A\varphi) \qquad \text{for all} \quad \varphi \in \mathbb{R}.}$$

Then $A^dT \in \mathcal{S}'(\mathbb{R})$. In fact, $\lim_{n\to\infty} \varphi_n = \varphi$ in $\mathcal{S}(\mathbb{R})$ implies

$$\lim_{n\to\infty} (A^dT)(\varphi_n) = \lim_{n\to\infty} T(A\varphi_n) = T(\lim_{n\to\infty} A\varphi_n) = T(A\varphi) = (A^dT)(\varphi).$$

Obviously, the operator A^d is linear.

Formally self-adjoint operators and pre-observables. Suppose that there exists a formally adjoint operator $A^\dagger : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ to the operator A from (H) above (see Problem 7.4). Then

$$\boxed{A^d\langle\psi| = \langle A^\dagger\psi| \qquad \text{for all} \quad \psi \in \mathcal{S}(\mathbb{R}).}$$

Indeed, for all $\varphi \in \mathcal{S}(\mathbb{R})$, we obtain

$$(A^d\langle\psi|)(\varphi) = \langle\psi|(A\varphi) = \langle\psi|A\varphi\rangle = \langle A^\dagger\psi|\varphi\rangle = \langle A^\dagger\psi|(\varphi).$$

In particular, if the operator A is formally self-adjoint (i.e., $A = A^\dagger$), then we obtain $A^d\langle\psi| = \langle A\psi|$ for all $\psi \in \mathcal{S}(\mathbb{R})$.

Self-dual operators and the Fourier transform. The operator A from (H) above is called self-dual iff

$$\int_{\mathbb{R}} \psi(x) \cdot (A\varphi)(x)dx = \int_{\mathbb{R}} (A\psi)(x) \cdot \varphi(x)dx \qquad \text{for all} \quad \varphi, \psi \in \mathcal{S}(\mathbb{R}).$$

Then $(A^d T_\psi) = T_{A\psi}$ for all $\psi \in \mathcal{S}(\mathbb{R})$. Identifying ψ with $T\psi$, we obtain

$$A^d \psi = A\psi \qquad \text{for all} \quad \psi \in \mathcal{S}(\mathbb{R}).$$

Hence $A \subseteq A^d$. To simplify notation, we frequently denote the dual operator A^d by the symbol

$$A : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R}),$$

and we regard this as an extension of the operator $A : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$. A typical example is the Fourier transform considered on page 512.

Antiself-dual operators and the derivative operator. The operator A from (H) above is called antiself-dual iff

$$\int_{\mathbb{R}} \psi(x) \cdot (A\varphi)(x)dx = -\int_{\mathbb{R}} (A\psi)(x) \cdot \varphi(x)dx \qquad \text{for all} \quad \varphi, \psi \in \mathcal{S}(\mathbb{R}).$$

Then $-A^d T_\psi = T_{A\psi}$ for all $\psi \in \mathcal{S}(\mathbb{R})$. Identifying ψ with $T\psi$, we obtain

$$-A^d \psi = A\psi \qquad \text{for all} \quad \psi \in \mathcal{S}(\mathbb{R}).$$

Hence $A \subseteq (-A^d)$. To simplify notation, we frequently denote the operator $-A^d$ by the symbol

$$A : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R}),$$

and we regard this as an extension of $A : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$. As a typical example, let us consider the derivative operator $A := \frac{d}{dx}$. Integration by parts shows that this operator is antiself-dual.[80] This way, we obtain the extension

$$\frac{d}{dx} : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R}).$$

Let $T \in \mathcal{S}'(\mathbb{R})$. Then $(\frac{d}{dx}T)(\varphi) = T(-\frac{d\varphi}{dx})$ for all $\varphi \in \mathcal{S}(\mathbb{R})$. This is the usual definition of the derivative of a tempered distribution. More generally, let $T \in \mathcal{S}'(\mathbb{R})$. The nth derivative of T is defined by

$$\boxed{\left(\frac{d^n T}{dx^n}\right)(\varphi) := (-1)^n T\left(\frac{d^n \varphi}{dx^n}\right), \quad n = 1, 2, \dots} \tag{7.121}$$

for all test functions $\varphi \in \mathcal{S}(\mathbb{R})$. This definition is based on the fact that the operator $\frac{d^n}{dx^n} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is self-dual (resp. antiself-dual) if n is even (resp odd).

Each tempered distribution has derivatives of arbitrary order, which are again tempered distributions.

[80] For $n = 1, 2, \dots$ and all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$, integration by parts yields

$$\int_{\mathbb{R}} \frac{d^n \psi(x)}{dx^n}\, \varphi(x)\, dx = (-1)^n \int_{\mathbb{R}} \psi(x)\, \frac{d^n \varphi(x)}{dx^n}\, dx.$$

Eigencostates

> For quantum mechanics, it is crucial to replace eigenvectors by eigencostates.
>
> Folklore

Let $A : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ be a linear operator, and let $\{T_\gamma\}_{\gamma\in\Gamma}$ be a system of nonzero tempered distributions $T_\gamma \in \mathcal{S}'(\mathbb{R})$ with

$$A^d T_\gamma = \lambda_\gamma T_\gamma \qquad \text{for all} \quad \gamma \in \Gamma, \tag{7.122}$$

where $\lambda_\gamma \in \mathbb{C}$ for all $\gamma \in \Gamma$. Explicitly, this means that

$$\boxed{T_\gamma(A\varphi) = \lambda_\gamma T(\varphi) \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}),\ \gamma \in \Gamma.}$$

Then all the distributions T_γ are called eigencostates (or generalized eigenfunctions) of the operator A. The system $\{T_\gamma\}$ is called complete iff, for any given test function $\varphi \in \mathcal{S}(\mathbb{R})$,

$$T_\gamma(\varphi) = 0 \ \text{ for all}\, \gamma \in \Gamma \qquad \text{implies} \qquad \varphi = 0.$$

In addition, if there exists a measure μ on the index set Γ with the generalized Parseval equation

$$\boxed{\int_{\mathbb{R}} \psi(x)^\dagger \varphi(x) dx = \int_\Gamma T_\gamma(\psi)^\dagger T_\gamma(\varphi)\, d\mu(\gamma)} \tag{7.123}$$

for all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$, then the system $\{T_\gamma\}_{\gamma\in\Gamma}$ is called a complete orthonormal system of eigencostates of the operator A. Obviously, the latter property is stronger than completeness. In fact, if $T_\gamma(\varphi) = 0$ for all γ, then $\langle\varphi|\varphi\rangle = 0$, and hence $\varphi = 0$. The complex numbers $T_\gamma(\varphi)$ are called the generalized Fourier coefficients of the test function $\varphi \in \mathcal{S}(\mathbb{R})$. The function

$$\gamma \mapsto T_\gamma(\varphi)$$

is called the generalized Fourier transform of the function $\varphi \in \mathcal{S}(\mathbb{R})$ with respect to the operator A.

The Dirac calculus. It turns out that the Dirac calculus represents a very elegant method in order to formulate quantum mechanics and quantum field theory in a very elegant way. For $\varphi \in \mathcal{S}(\mathbb{R})$, we use the following notation:

- $T_\gamma \Rightarrow \langle\gamma|$,
- $T_\gamma(\varphi) \Rightarrow \langle\gamma|\varphi\rangle$, and
- $\langle\varphi|\gamma\rangle := \langle\gamma|\varphi\rangle^\dagger$.

Then, the generalized Parseval equation (7.123) reads as

$$\langle\psi|\varphi\rangle = \int_\Gamma \langle\psi|\gamma\rangle\langle\gamma|\varphi\rangle\, d\mu(\gamma) \qquad \text{for all} \quad \varphi, \psi \in \mathcal{S}(\mathbb{R}). \tag{7.124}$$

Mnemonically, in order to obtain (7.124) we write $\langle\psi|\varphi\rangle = \langle\psi| \cdot I \cdot |\varphi\rangle$ together with

$$\boxed{I = \int_\Gamma |\gamma\rangle\langle\gamma|\, d\mu(\gamma).}$$

This is Dirac's formal completeness relation.

The Position Operator

We want to study the following three operators $Q_{\rm pre} \subseteq Q \subseteq Q^d_{\rm pre}$.

- Let $\varphi \in \mathcal{S}(\mathbb{R})$. The pre-position operator $Q_{\rm pre} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is defined by $(Q_{\rm pre}\varphi)(x) := x\varphi(x)$ for all $x \in \mathbb{R}$. The operator $Q_{\rm pre}$ is formally self-adjoint and self-dual. [81]
- Let $T \in \mathcal{S}'(\mathbb{R})$. The dual position operator $Q^d_{\rm pre} : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$ is defined by $(Q^d_{\rm pre}T)(\varphi) := T(Q_{\rm pre}\varphi)$ for all $\varphi \in \mathcal{S}(\mathbb{R})$. This means that

$$(Q^d_{\rm pre}T)(\varphi) := T(Q_{\rm pre}\varphi) \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).$$

- The operator $Q : D(Q) \to L_2(\mathbb{R})$ is the restriction of $Q^d_{\rm pre}$ to $L_2(\mathbb{R})$. Explicitly, we set

$$D(Q) := \{\varphi \in L_2(\mathbb{R}) : \int_{\mathbb{R}} |x\varphi(x)|^2 dx < \infty\},$$

and $(Q\varphi)(x) := x\varphi(x)$ for all $x \in \mathbb{R}$ and all $\varphi \in D(Q)$.

The spectral family of the position operator. Fix $\lambda \in \mathbb{R}$, and choose $\varphi \in L_2(\mathbb{R})$. Define the operator $\mathsf{E}_\lambda : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ by setting

$$\boxed{(\mathsf{E}_\lambda\varphi)(x) := e_\lambda(x)\varphi(x) \qquad \text{for all} \quad x \in \mathbb{R},} \tag{7.125}$$

where e_λ is the characteristic function of the open interval $]-\infty, \lambda[$ (see (7.100) on page 497).

Proposition 7.27 *The operator family $\{\mathsf{E}_\lambda\}_{\lambda\in\mathbb{R}}$ is the spectral family of the self-adjoint position operator $Q : D(Q) \to L_2(\mathbb{R})$.*

Proof. The self-adjointness of Q will be proved in Problem 7.15. For all functions $\varphi, \psi \in L_2(\mathbb{R})$,

$$\langle\psi|\mathsf{E}_\lambda\varphi\rangle = \int_{-\infty}^{\infty} \psi(x)^\dagger e_\lambda(x)\varphi(x)dx = \int_{-\infty}^{\lambda} \psi(x)^\dagger\varphi(x)dx.$$

Hence $\frac{d}{d\lambda}\langle\psi|\mathsf{E}_\lambda\varphi\rangle = \psi(\lambda)^\dagger\varphi(\lambda)$. This implies $d\langle\psi|\mathsf{E}_\lambda\varphi\rangle = \psi(\lambda)^\dagger\varphi(\lambda)d\lambda$. Therefore,

$$\langle\psi|Q\varphi\rangle = \int_{-\infty}^{\infty} \psi(x)^\dagger x\varphi(x) = \int_{-\infty}^{\infty} \lambda \cdot d\langle\psi|\mathsf{E}_\lambda\varphi\rangle.$$

Finally, one checks easily that the conditions (S1)–(S4) for a spectral family (formulated on page 502) are satisfied. By the uniqueness statement from Corollary 7.20 on page 502, $\{\mathsf{E}_\lambda\}_{\lambda\in\mathbb{R}}$ is the spectral family of Q. □

Let the function $f : \mathbb{R} \to \mathbb{C}$ be measurable (e.g., piecewise continuous) and bounded on all compact intervals. Define

$$D(f(Q)) := \{\varphi \in L_2(\mathbb{R}) : \int_{\mathbb{R}} |f(x)|^2|\varphi(x)|^2 dx < \infty\}.$$

[81] In fact, for all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$, we have $\int_{\mathbb{R}} \psi(x)^\dagger \cdot x\varphi(x)dx = \int_{\mathbb{R}} (x\psi(x))^\dagger\varphi(x)dx$ and

$$\int_{\mathbb{R}} \psi(x) \cdot x\varphi(x)\, dx = \int_{\mathbb{R}} x\psi(x) \cdot \varphi(x)\, dx.$$

For all $\varphi \in D(f(Q))$ and all $\psi \in L_2(\mathbb{R})$, set

$$\langle \psi | f(Q)\varphi \rangle := \int_{\mathbb{R}} f(\lambda) \cdot d\langle \psi | \mathsf{E}_\lambda \varphi \rangle = \int_{\mathbb{R}} \psi(x)^\dagger f(x)\varphi(x)dx.$$

This way, we uniquely obtain the linear operator $f(Q) : D(f(Q)) \to L_2(\mathbb{R})$. This operator is self-adjoint (resp. continuous on $L_2(\mathbb{R})$) if the function f is real-valued (resp. bounded on $\mathbb{R}$).

Measurement of position. Let $\psi \in L_2(\mathbb{R})$ with $\int_{\mathbb{R}} |\psi(x)|^2 dx = 1$. According to the general approach, the spectral family of the observable Q uniquely determines the measurements of Q in the normalized state ψ.

- Distribution function F: The probability of measuring the observable Q in the open interval $]-\infty, \lambda[$ is given by

$$\mathsf{F}(\lambda) := \langle \psi | \mathsf{E}_\lambda \psi \rangle = \int_{-\infty}^{\lambda} |\psi(x)|^2 dx.$$

  This is the probability of measuring the position of the particle in the interval $]-\infty, \lambda[$.
- The probability for measuring the position of the particle in the interval $[x_0, x_1]$ is equal to $\int_{[x_0,x_1]} d\mathsf{F}(\lambda) = \int_{x_0}^{x_1} |\psi(x)|^2 dx$.
- Mean position of the particle: $\bar{x} = \int_{\mathbb{R}} x \, d\mathsf{F}(x) = \int_{\mathbb{R}} x|\psi(x)|^2 dx$.
- Square of the position fluctuation:

$$(\Delta x)^2 = \int_{\mathbb{R}} (x - \bar{x})^2 \, d\mathsf{F}(x) = \int_{\mathbb{R}} (x - \bar{x})^2 |\psi(x)|^2 dx.$$

The complete orthonormal system of eigencostates of the position operator.

Proposition 7.28 (i) *The operator $Q : D(Q) \to L_2(\mathbb{R})$ has no eigenvectors in the Hilbert space $L_2(\mathbb{R})$.*
(ii) *For the spectrum, $\sigma(Q) = \sigma_{\text{ess}}(Q) =]-\infty, \infty[$.*
(iii) *$X_{\text{scatt}} = L_2(\mathbb{R})$, and $\sigma_{\text{ac}}(Q) = \sigma(Q)$.*

Proof. Ad (i). Suppose that $Q\psi = \lambda\psi$, where $\psi \in L_2(\mathbb{R})$ and $\lambda \in \mathbb{R}$. Then we obtain $(x - \lambda)\psi(x) = 0$ for almost all $x \in \mathbb{R}$. Hence $\psi(x) = 0$ for almost all $x \in \mathbb{R}$. Thus, $\psi = 0$ in $L_2(\mathbb{R})$.

Ad (ii). Use Theorem 7.22 on page 505 and (7.125).

Ad (iii). For any $\varphi \in L_2(\mathbb{R})$, the function $\lambda \mapsto \langle \varphi | \mathsf{E}_\lambda \varphi \rangle$ is differentiable almost everywhere on $\mathbb{R}$, and the first derivative is integrable over $\mathbb{R}$. Thus, $\varphi \in X_{\text{scatt}}$ (see page 503). □

Fix $x \in \mathbb{R}$. Let us consider the Dirac delta distribution $\delta_x \in \mathcal{S}'(\mathbb{R})$ defined by $\delta_x(\varphi) := \varphi(x)$ for all $\varphi \in \mathcal{S}(\mathbb{R})$.

Proposition 7.29 *The system $\{\delta_x\}_{x\in\mathbb{R}}$ represents a complete orthonormal system of eigencostates of the position operator Q_{pre}.*

Proof. Let $\varphi, \psi \in \mathcal{S}(\mathbb{R})$. For any parameter $x \in \mathbb{R}$,

$$\boxed{Q_{\text{pre}}^d \delta_x = x\delta_x.}$$

In fact, $\delta_x(Q_{\text{pre}}\varphi) = x\varphi(x) = x\delta_x(\varphi)$. Furthermore, we have the generalized Parseval equation $\langle \psi | \varphi \rangle = \int_{\mathbb{R}} \psi(x)^\dagger \varphi(x)dx = \int_{\mathbb{R}} \delta_x(\psi)^\dagger \delta_x(\varphi)dx$. □

In the setting of the Dirac calculus, physicists write $\langle x|$ instead of δ_x. Then

$$\langle\psi|\varphi\rangle = \int_{\mathbb{R}} \langle\psi|x\rangle\langle x|\varphi\rangle \, dx \qquad \text{for all} \quad \varphi, \psi \in \mathcal{S}(\mathbb{R}).$$

Mnemonically, this remains true for all $\psi, \varphi \in L_2(\mathbb{R})$. Dirac's formal completeness relation reads as

$$\boxed{I = \int_{\mathbb{R}} |x\rangle\langle x| \, dx.}$$

The relation between eigencostates and the spectral family. Set

$$\psi_0(x) := \mathrm{e}^{-x^2/2} \qquad \text{for all} \quad x \in \mathbb{R}.$$

Then $\psi_0 \in \mathcal{S}(\mathbb{R})$. This function generates the (not normalized) Gaussian measure

$$\mu(J) := \int_J |\psi_0(x)|^2 dx = \int_J \mathrm{e}^{-x^2} \, dx$$

for all intervals J on the real line. Fix $\lambda \in \mathbb{R}$. For all test functions $\varphi \in \mathcal{S}(\mathbb{R})$, define

$$\boxed{T_\lambda(\varphi) := \frac{d\langle\psi_0|\mathsf{E}_\lambda\varphi\rangle}{d\langle\psi_0|\mathsf{E}_\lambda\psi_0\rangle}.}$$

Proposition 7.30 *The family $\{T_x\}_{x\in\mathbb{R}}$ of tempered distributions with*

$$T_x = \frac{\delta_x}{\psi_0(x)}$$

represents a complete orthonormal system of eigencostates of the position operator Q_{pre}. Using the Gaussian measure $d\mu(x) = \psi_0(x)^2 dx$, we have the generalized Parseval equation

$$\int_{\mathbb{R}} \psi(x)^\dagger \varphi(x) dx = \int_{\mathbb{R}} T_x(\psi)^\dagger T_x(\varphi) \, d\mu(x) \qquad \textit{for all} \quad \varphi, \psi \in \mathcal{S}(\mathbb{R}).$$

Proof. By the proof of Prop. 7.27, $d\langle\psi_0|\mathsf{E}_\lambda\varphi\rangle = \psi_0(\lambda)\varphi(\lambda)d\lambda$. Hence

$$T_\lambda(\varphi) = \frac{\psi_0(\lambda)\varphi(\lambda)}{\psi_0(\lambda)^2} = \frac{\varphi(\lambda)}{\psi_0(\lambda)}.$$

Finally, use $\delta_x(\varphi) = \varphi(x)$. □

The square Q^2 of the position operator. By von Neumann's functional calculus, the self-adjoint operator $Q^2 : D(Q^2) \to L_2(\mathbb{R})$ has the domain of definition

$$D(Q^2) = \{\psi \in L_2(\mathbb{R}) : \int_{\mathbb{R}} x^4 |\psi(x)|^2 dx < \infty\}.$$

For $\lambda \in \mathbb{R}$, we get $(\lambda I - Q^2)\psi(x) = f(x)$. If $\lambda < 0$ and $f \in L_2(\mathbb{R})$ then the function

$$(\lambda I - Q^2)^{-1} f(x) = \frac{f(x)}{\lambda - x^2}, \qquad x \in \mathbb{R}$$

is contained in $L_2(\mathbb{R})$. If $\lambda \geq 0$, this is not the case for special choice of f. Hence the spectrum of Q^2 is equal to $[0, \infty[$. Let us compute the spectral family of Q^2. For all $\varphi, \psi \in L_2(\mathbb{R})$,

$$\langle\psi|Q^2\varphi\rangle = \int_{-\infty}^{\infty} \psi(x)^\dagger x^2 \varphi(x) dx.$$

Setting $\lambda = x^2$, we get $\langle\psi|Q^2\varphi\rangle = \int_0^\infty \lambda \varrho_{\psi,\varphi}(\lambda) d\lambda$ with the spectral density

$$\varrho_{\psi,\varphi}(\lambda) := \frac{1}{2\sqrt{\lambda}} \Big(\psi(\sqrt{\lambda})^\dagger \varphi(\sqrt{\lambda}) + \psi(-\sqrt{\lambda})^\dagger \varphi(-\sqrt{\lambda})\Big).$$

Thus, we get $\langle\psi|\mathsf{E}_{\lambda_0}(Q^2)\varphi\rangle = \int_0^\infty e_{\lambda_0}(E)\varrho_{\psi,\varphi}(\lambda)d\lambda$ for all $\lambda_0 \in \mathbb{R}$. The definition of the function e_λ can be found in (7.100) on page 497. In particular, $\mathsf{E}_{\lambda_0} = 0$ if $\lambda_0 \le 0$.

Proposition 7.31 (i) *The operator Q^2 has no eigenvectors in the Hilbert space $L_2(\mathbb{R})$.*

(ii) *For the spectrum $\sigma(Q^2) = \sigma_{\rm ess}(Q^2) = \sigma_{\rm ac}(Q^2) = [0, \infty[$.*

Proof. Ad (i). Use the same argument as for the operator Q above.

Ad (ii). Use the spectral family together with Theorem 7.22 on page 505. □

The Momentum Operator

We want to study the following three operators $P_{\rm pre} \subseteq P \subseteq (-P^d_{\rm pre})$.

- Let $\varphi \in \mathcal{S}(\mathbb{R})$. The pre-momentum operator $P_{\rm pre} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is defined by $(P_{\rm pre}\varphi)(x) := -\mathrm{i}\hbar \frac{d}{dx}\varphi(x)$ for all $x \in \mathbb{R}$. The operator $P_{\rm pre}$ is formally self-adjoint and antiself-dual.[82]
- Let $T \in \mathcal{S}'(\mathbb{R})$. The dual momentum operator $P^d_{\rm pre} : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$ is defined by $(P^d_{\rm pre}T)(\varphi) := T(P_{\rm pre}\varphi)$ for all $\varphi \in \mathcal{S}(\mathbb{R})$. In the sense of tempered distributions, we have
$$P^d_{\rm pre} = \mathrm{i}\hbar \frac{d}{dx}.$$
This follows from $\mathrm{i}\hbar\frac{dT}{dx}(\varphi) = -\mathrm{i}\hbar T(\varphi') = T(P_{\rm pre}\varphi)$ for all $\varphi \in \mathcal{S}(\mathbb{R})$.
- The operator $P : D(P) \to L_2(\mathbb{R})$ is the natural extension of the operator $P_{\rm pre}$. Explicitly, we set $D(P) := \{\varphi \in L_2(\mathbb{R}) : \varphi' \in L_2(\mathbb{R})\}$, and
$$P\varphi := -\mathrm{i}\hbar\frac{d\varphi}{dx} \qquad \text{for all} \quad \varphi \in D(P).$$
Here, the derivative is to be understood in the sense of tempered distributions. In other words, $D(P) = W^1_2(\mathbb{R})$.

The Fourier transform, and the duality between position and momentum. Choose $\chi := P_{\rm pre}\varphi$ where $\varphi \in \mathcal{S}(\mathbb{R})$. For the Fourier transform, we get $\hat\chi(k) = \hbar k \hat\varphi(k)$ for all $k \in \mathbb{R}$. Thus, the operator $\hbar^{-1}P_{\rm pre}$ corresponds to the multiplication operator $Q_{\rm pre}$ in the Fourier space. This means that the following diagram is commutative:

[82] In fact, for all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$, we have $\int_{\mathbb{R}} \psi^\dagger(x)(-\mathrm{i}\varphi'(x))dx = \int_{\mathbb{R}}(-\mathrm{i}\psi'(x))^\dagger\varphi(x)dx$ and
$$\int_{\mathbb{R}} \psi(x)(-\mathrm{i}\varphi'(x))dx = -\int_{\mathbb{R}}(-\mathrm{i}\psi'(x))\varphi(x)dx.$$

$$\begin{array}{ccc} \mathcal{S}(\mathbb{R}) & \xrightarrow{\hbar^{-1}P_{\mathrm{pre}}} & \mathcal{S}(\mathbb{R}) \\ \mathcal{F}\downarrow & & \downarrow\mathcal{F} \\ \mathcal{S}(\mathbb{R}) & \xrightarrow{Q_{\mathrm{pre}}} & \mathcal{S}(\mathbb{R}). \end{array}$$

Passing to the extended unitary Fourier transform $\mathcal{F} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$, we obtain the following commutative diagram:

$$\begin{array}{ccc} D(P) & \xrightarrow{\hbar^{-1}P} & L_2(\mathbb{R}) \\ \mathcal{F}\downarrow & & \downarrow\mathcal{F} \\ D(Q) & \xrightarrow{Q} & L_2(\mathbb{R}). \end{array}$$

Since the operator $Q : D(Q) \to L_2(\mathbb{R})$ is self-adjoint and the property of self-adjointness is invariant under unitary transformations, the position operator $P : D(P) \to L_2(\mathbb{R})$ is self-adjoint (see Problem 7.14).

The spectral family of the wave number operator. Recall that the momentum p corresponds to the wave number $k = \hbar^{-1}p$. Therefore, the operator $K := \hbar^{-1}P$ is called the wave number operator. Since the spectral family of a self-adjoint operator is invariant under unitary transformations, we obtain the spectral family $\{\mathsf{E}_\lambda\}_{\lambda\in\mathbb{R}}$ of the wave number operator K from the spectral family $\{\mathsf{E}_\lambda(Q)\}_{\lambda\in\mathbb{R}}$ of the position operator Q in the Fourier space. Explicitly, $\mathsf{E}_\lambda = \mathcal{F}^{-1}\mathsf{E}_\lambda(Q)\mathcal{F}$ for all $\lambda \in \mathbb{R}$. This means that, for all functions $\varphi, \psi \in L_2(\mathbb{R})$ and all real numbers λ, we get

$$\boxed{\langle\psi|\mathsf{E}_\lambda\varphi\rangle = \int_{-\infty}^{\lambda} \hat{\psi}(k)^\dagger\hat{\varphi}(k)dk.}$$

Proposition 7.32 *The operator family $\{\mathsf{E}_\lambda\}_{\lambda\in\mathbb{R}}$ is the spectral family of the self-adjoint wave number operator $\hbar^{-1}P : D(P) \to L_2(\mathbb{R})$.*

Let the function $f : \mathbb{R} \to \mathbb{C}$ be measurable (e.g., piecewise continuous) and bounded on all compact intervals. Define

$$D(f(K)) := \{\varphi \in L_2(\mathbb{R}) : \int_{\mathbb{R}} |f(k)|^2|\hat{\varphi}(k)|^2dk < \infty\}.$$

For all $\varphi \in D(f(K))$ and all $\psi \in L_2(\mathbb{R})$, set

$$\langle\psi|f(K)\varphi\rangle := \int_{\mathbb{R}} f(\lambda)\cdot d\langle\psi|\mathsf{E}_\lambda\varphi\rangle = \int_{\mathbb{R}} f(k)\hat{\psi}(k)^\dagger\hat{\varphi}(k)dk.$$

This way, we obtain the linear operator $f(K) : D(f(K)) \to L_2(\mathbb{R})$. This operator is self-adjoint (resp. continuous on $L_2(\mathbb{R})$) if the function f is real-valued (resp. bounded on $\mathbb{R}$).

Measurement of the wave number. Let $\psi \in L_2(\mathbb{R})$ with the normalization condition $\int_{\mathbb{R}} |\psi(x)|^2dx = 1$. According to the general approach, the spectral family of the observable $K = \hbar^{-1}P$ uniquely determines the measurements of the wave number $k = \hbar^{-1}p$ in the normalized state ψ.

- Distribution function F: The probability of measuring the wave number observable K in the open interval $]-\infty, \lambda[$ is given by

$$\mathsf{F}(\lambda) := \langle\psi|\mathsf{E}_\lambda\psi\rangle = \int_{-\infty}^{\lambda} |\hat{\psi}(k)|^2 dk.$$

  This is the probability of measuring the wave number $k = \hbar^{-1}p$ of the particle in the open interval $]-\infty, \lambda[$.
- The probability of measuring the wave number of the particle in the interval $[k_0, k_1]$ is equal to

$$\int_{[k_0,k_1]} d\mathsf{F}(k) = \int_{k_0}^{k_1} |\hat{\psi}(k)|^2 dk.$$

- Mean wave number of the particle: $\bar{k} = \int_{\mathbb{R}} k \, d\mathsf{F}(k) = \int_{\mathbb{R}} k|\hat{\psi}(k)|^2 dk$.
- Square of the wave number fluctuation:

$$(\Delta k)^2 = \int_{\mathbb{R}} (k-\bar{k})^2 \, d\mathsf{F}(k) = \int_{\mathbb{R}} (k-\bar{k})^2 |\hat{\psi}(k)|^2 dk.$$

Moreover, we get the mean momentum $\bar{p} = \hbar\bar{k}$ and the mean momentum fluctuation $\Delta p = \hbar\Delta k$.

The complete orthonormal system of eigencostates of the momentum operator.

Proposition 7.33 (i) *The operator $P : D(P) \to L_2(\mathbb{R})$ has no eigenvectors in the Hilbert space $L_2(\mathbb{R})$.*
(ii) *For the spectrum, $\sigma(P) = \sigma_{\rm ess}(P) =]-\infty, \infty[$.*
(iii) *$X_{\rm scatt} = L_2(\mathbb{R})$, and $\sigma_{\rm ac}(P) = \sigma(P)$.*

This follows from Prop. 7.28 on page 519 and from the fact that the wave number operator $\hbar^{-1}P$ is unitarily equivalent to the position operator Q.

Proposition 7.34 *The system $\{\langle k|\}_{k\in\mathbb{R}}$ represents a complete orthonormal system of eigencostates of the momentum operator $P_{\rm pre}$.*

Proof. Let $\varphi, \psi \in \mathcal{S}(\mathbb{R})$. For any parameter $k \in \mathbb{R}$,

$$\boxed{P^d_{\rm pre}\langle k| = \hbar k \, \langle k|.}$$

In fact, using $P_{\rm pre}\chi_k = \hbar k \chi_k$, we get

$$\langle k|P_{\rm pre}\varphi\rangle = \int_{\mathbb{R}} \chi_k^\dagger P_{\rm pre}\varphi \, dx = \int_{\mathbb{R}} (P_{\rm pre}\chi_k)^\dagger \varphi dx = \hbar k \int_{\mathbb{R}} \chi_k^\dagger \varphi dx = \hbar k \, \langle k|\varphi\rangle.$$

Furthermore, we have the generalized Parseval equation

$$\langle\psi|\varphi\rangle = \int_{\mathbb{R}} \hat{\psi}(k)^\dagger \hat{\varphi}(k) dk = \int_{\mathbb{R}} \langle\psi|k\rangle\langle k|\varphi\rangle \, dk.$$

Thus, $\langle k|\varphi\rangle = 0$ for all $k \in \mathbb{R}$ implies $\langle\varphi|\varphi\rangle = 0$, and hence $\varphi = 0$. □

Dirac's formal completeness relation reads as

$$\boxed{I = \int_{\mathbb{R}} |k\rangle\langle k| \, dk.}$$

The relation between eigencostates and the spectral family. Set

$$\psi_0(x) := \sqrt{\hbar}\, \mathrm{e}^{-x^2\hbar^2/2} \qquad \text{for all} \quad x \in \mathbb{R}.$$

Then $\psi_0 \in \mathcal{S}(\mathbb{R})$, and $\hat{\psi}_0(k) = \mathrm{e}^{-k^2/2}$. This function generates the (not normalized) Gaussian measure

$$\mu(J) := \int_J \hat{\psi}_0(k)^2 dk = \int_J \mathrm{e}^{-k^2}\, dk$$

for all intervals J on the real line. Fix $\lambda \in \mathbb{R}$. For all test functions $\varphi \in \mathcal{S}(\mathbb{R})$, define

$$\boxed{T_\lambda(\varphi) := \frac{d\langle\psi_0|\mathsf{E}_\lambda\varphi\rangle}{d\langle\psi_0|\mathsf{E}_\lambda\psi_0\rangle}.}$$

Proposition 7.35 *The family $\{T_k\}_{k\in\mathbb{R}}$ of tempered distributions with*

$$T_k = \frac{\langle k|}{\hat{\psi}_0(k)}$$

represents a complete orthonormal system of eigencostates of the wave number operator $\hbar^{-1}P_{\mathrm{pre}}$. Using the Gaussian measure $d\mu(k) = |\psi_0(k)|^2 dk$, we have the generalized Parseval equation

$$\int_{\mathbb{R}} \psi(x)^\dagger \varphi(x) dx = \int_{\mathbb{R}} T_k(\psi)^\dagger T_k(\varphi)\, d\mu(k) \qquad \textit{for all} \quad \varphi, \psi \in \mathcal{S}(\mathbb{R}).$$

Proof. By the proof of Prop. 7.34, $d\langle\psi_0|\mathsf{E}_\lambda\varphi\rangle = \hat{\psi}_0(\lambda)\hat{\varphi}(\lambda)d\lambda$. Hence

$$T_\lambda(\varphi) = \frac{\hat{\psi}_0(\lambda)\hat{\varphi}(\lambda)}{\hat{\psi}_0(\lambda)^2} = \frac{\hat{\varphi}(\lambda)}{\hat{\psi}_0(\lambda)}.$$

Finally, use the Parseval equation for the Fourier transform. □

7.6.5 The Free Hamiltonian

> The free Hamiltonian is a paradigm for general Hamiltonians in quantum mechanics and quantum field theory.
>
> Folklore

The functional-analytic approach to quantum dynamics is based on the study of the energy operator (also called the Hamiltonian). In this section, we want to investigate thoroughly the Hamiltonian H_{free} of the free quantum particle on the real line, which is called the free Hamiltonian. The two key operator equations are the instationary Schrödinger equation

$$\boxed{\mathrm{i}\hbar\dot{\psi}(t) = H_{\mathrm{free}}\psi(t), \quad t > t_0, \quad \psi(t_0) = \psi_0} \tag{7.126}$$

with the solution $\psi(t) = \mathrm{e}^{-\mathrm{i}(t-t_0)H_{\mathrm{free}}/\hbar}\psi_0$ (the Feynman propagator) and the inhomogeneous stationary Schrödinger equation

$$\boxed{H_{\mathrm{free}}\varphi = \mathcal{E}\varphi + f} \tag{7.127}$$

with the solution $\varphi = (H_{\mathrm{free}} - \mathcal{E}I)^{-1}f$ (the energetic Green's operator). Here, we have to assume that the complex energy $\mathcal{E}$ is not contained in the spectrum $\sigma(H_{\mathrm{free}})$ of the free Hamiltonian. We will show that:

- The Feynman propagator kernel $\mathcal{K}$ describes the solution of the initial-value problem for the instationary Schrödinger equation (7.126),

$$\mathrm{i}\hbar\psi_t(x,t) = -\frac{\hbar^2}{2m}\psi_{xx}(x,t), \qquad \psi(t_0,x) = \psi_0(x),$$

by means of the integral formula

$$\psi(x,t) = \int_{\mathbb{R}} \mathcal{K}(x,t;x_0,t_0)\psi_0(x_0)dx_0, \quad t > t_0, x \in \mathbb{R}.$$

- The energetic Green's function $\mathcal{G}$ describes the solution of the inhomogeneous stationary Schrödinger equation (7.126),

$$-\frac{\hbar^2}{2m}\varphi''(x) = \mathcal{E}\varphi(x) + f(x), \qquad x \in \mathbb{R},\ \mathcal{E} \in \mathbb{C},$$

by means of the integral formula

$$\varphi(x) = \int_{\mathbb{R}} \mathcal{G}(x,x_0;\mathcal{E})f(x_0)dx_0, \qquad x \in \mathbb{R},\ \mathcal{E} \in \mathbb{C} \setminus \sigma(H_{\text{free}})$$

where $\sigma(H_{\text{free}}) = [0,\infty[$.

The energetic Green's function carries the information on the energy spectrum of the particle.

The Feynman propagator kernel $\mathcal{K}$ and the energetic Green's function $\mathcal{G}$ are related to each other by the Laplace transform.

This corresponds to

- the duality between energy and time, and
- the duality between causality and analyticity,

which is crucial for both quantum mechanics and quantum field theory.

Using the results on the momentum operators $P_{\text{pre}} \subseteq P \subseteq P^d_{\text{pre}}$ obtained on page 521, we want to study the energy operators $H_{\text{pre}} \subseteq H_{\text{free}} \subseteq H^d_{\text{pre}}$.

- The pre-Hamiltonian $H_{\text{pre}} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is defined by

$$H_{\text{pre}} := \frac{P^2_{\text{pre}}}{2m}.$$

Explicitly, $H_{\text{pre}}\varphi = -\frac{\hbar^2}{2m}\,\varphi''$ for all $\varphi \in \mathcal{S}(\mathbb{R})$. The operator H_{pre} is formally self-adjoint and self-dual.

- The operator $H^d_{\text{pre}} : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$ is defined by $H^d_{\text{pre}} := \frac{(P^d_{\text{pre}})^2}{2m}$. For any tempered distribution $T \in \mathcal{S}'(\mathbb{R})$,

$$H^d_{\text{pre}}T = -\frac{\hbar}{2m}\,\frac{d^2T}{dx^2}.$$

- By von Neumann's functional calculus, the operator $P^2 : D(P^2) \to L_2(\mathbb{R})$ is self-adjoint, and $D(P^2) = \{\psi \in L_2(\mathbb{R}) : \int_{\mathbb{R}} |k^2\hat{\psi}(k)|^2 dk < \infty\}$. By Prop. 7.26, $D(P^2) = W^2_2(\mathbb{R})$.
- We define the self-adjoint free Hamiltonian $H_{\text{free}} : D(H_{\text{free}}) \to L_2(\mathbb{R})$ by setting $H_{\text{free}} := \frac{P^2}{2m}$. Hence $D(H_{\text{free}}) = W^2_2(\mathbb{R})$.

Eigencostates. Recall that $\langle k|\varphi\rangle = \hat{\varphi}(k)$ for all $\varphi \in \mathcal{S}(\mathbb{R})$, where $\hat{\varphi}$ is the Fourier transform of φ. Moreover, following Dirac, we set $\langle \varphi|k\rangle := \langle k|\varphi\rangle^\dagger$. Recall that $E_k := \frac{\hbar^2 k^2}{2m}$ is the energy of a classical free particle on the real line which has the momentum $p = \hbar k$.

Proposition 7.36 *The system $\{\langle k|\}_{k\in\mathbb{R}}$ is a complete orthonormal system of eigencostates of the energy operator H_{pre}. Explicitly,*

(a) $H^d_{\mathrm{pre}}\langle k| = E_k\langle k|$ *for all wave numbers* $k \in \mathbb{R}$.

(b) $\langle\psi|\varphi\rangle = \int_{\mathbb{R}} \langle\psi|k\rangle\langle k|\varphi\rangle\, dk$ *for all* $\psi, \varphi \in L_2(\mathbb{R})$.

Proof. Since $P^d_{\mathrm{pre}}\langle k| = \hbar k\langle k|$, we get $H^d_{\mathrm{pre}}\langle k| = \frac{(P^d_{\mathrm{pre}})^2}{2m}\langle k| = \frac{(\hbar k)^2}{2m}\langle k|$. This is (a). Claim (b) coincides with the Parseval equation for the Fourier transform. □

In terms of distribution theory, the costate $\langle k|$ corresponds to the function $\chi_k^\dagger(x) = \frac{\mathrm{e}^{-\mathrm{i}kx}}{\sqrt{2\pi}}$ for all $x \in \mathbb{R}$. Passing from k to $-k$, claim (a) is equivalent to

$$-\frac{\hbar^2}{2m}\frac{d^2\chi_k}{dx^2} = \frac{\hbar^2 k^2}{2m}\cdot\chi_k \qquad \text{for all} \quad k \in \mathbb{R}.$$

The elements of the Hilbert space $L_2(\mathbb{R})$ correspond to states of a single particle. The function χ_k is not a state, but it describes a particle stream, as discussed on page 512.

The spectrum of the free Hamiltonian H_{free} acting in the Hilbert space X of states. We have $X_{\mathrm{scatt}} = L_2(\mathbb{R})$ and

$$\boxed{\sigma(H_{\mathrm{free}}) = \sigma_{\mathrm{ac}}(H_{\mathrm{free}}) = \sigma_{\mathrm{ess}}(H_{\mathrm{free}}) = [0, +\infty[.}$$

That is, the spectrum of the free Hamiltonian H_{free} contains all the energy values $E \geq 0$. The spectrum coincides with both the absolutely continuous spectrum and the essential spectrum. The pure point spectrum is empty, that is, there is no state of the free quantum particle on the real line which has a sharp energy. In other words, there are no bound states. In addition, the singular spectrum is empty. The resolvent set of the operator H_{free} is given by $\varrho(H_{\mathrm{free}}) = \mathbb{C} \setminus [0, +\infty[$.

The proof follows from the corresponding properties of the operator Q^2 and the fact that the operator $\hbar^{-2}P^2$ is unitarily equivalent to Q^2, by Fourier transform (see page 520).

The quantum dynamics: We will use Theorem 7.23 together with the Stone theorem on page 505ff. Set $P(t, t_0) := \mathrm{e}^{-\mathrm{i}(t-t_0)H_{\mathrm{free}}/\hbar}$. For all times $t, t_0 \in \mathbb{R}$, the operator

$$P(t, t_0) : L_2(\mathbb{R}) \to L_2(\mathbb{R})$$

is unitary. For each given initial state $\psi_0 \in L_2(\mathbb{R})$ at time t_0, we set

$$\boxed{\psi(t) := P(t, t_0)\psi_0, \qquad t \in \mathbb{R}.}$$

The function $t \mapsto \psi(t)$ describes the motion of the free quantum particle on the real line with the initial condition $\psi(t_0) = \psi_0$. If $\psi_0 \in D(H_{\mathrm{free}})$ (e.g., we choose $\psi_0 \in \mathcal{S}(\mathbb{R})$), then the function $\psi : [0, \infty[\to L_2(\mathbb{R})$ is continuously differentiable, and we have the Schrödinger equation

$$\mathrm{i}\hbar\dot{\psi}(t) = H_{\mathrm{free}}\psi(t), \quad t \in \mathbb{R}, \quad \psi(t_0) = \psi_0.$$

The operator $P(t,t_0)$ is called the propagator of the free quantum particle at time t (with respect to the initial time t_0). In terms of the unitary Fourier transform $\mathcal{F} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$, the propagator $P(t,t_0)$ corresponds to the multiplication with the function $k \mapsto \mathrm{e}^{-\mathrm{i}(t-t_0)E_k/\hbar}$ in the Fourier space. This means that, for all $\psi_0 \in L_2(\mathbb{R})$, we get

$$P(t,t_0)\psi_0 = \mathcal{F}^{-1} M \mathcal{F} \psi_0, \qquad t, t_0 \in \mathbb{R}$$

with the multiplication operator $(M\hat{\psi}_0)(k) := \mathrm{e}^{-\mathrm{i}(t-t_0)E_k/\hbar}\hat{\psi}_0(k)$ for all wave numbers $k \in \mathbb{R}$.

The spectral measure of the free Hamiltonian H_{free}. Let the function $F : [0,\infty[\to \mathbb{C}$ be continuous (or piecewise continuous) and bounded. Then, for all $\chi, \varphi \in \mathcal{S}(\mathbb{R})$,

$$\boxed{\langle \chi | \mathsf{F}(H_{\mathrm{free}})\varphi \rangle = \int_0^\infty F(E)\, \varrho_{\chi,\varphi}(E)dE} \tag{7.128}$$

with the smooth density function

$$\varrho_{\chi,\varphi}(E) := \sqrt{\frac{m}{2\hbar^2 E}}\Big(\hat{\chi}(k)^\dagger \hat{\varphi}(k) + \hat{\chi}(-k)^\dagger \hat{\varphi}(-k)\Big), \quad E > 0.$$

Here, $k := \sqrt{2mE}/\hbar$. Moreover, $\hat{\chi}$ (resp. $\hat{\varphi}$) is the Fourier transform of χ (resp. φ) from (7.116). Formula (7.128) can be uniquely extended to all $\chi, \varphi \in L_2(\mathbb{R})$. The operator $\mathsf{F}(H_{\mathrm{free}}) : X \to X$ is linear and continuous. Formula (7.128) remains valid if we replace the function F by its complex-conjugate function $F^\dagger$ and the operator $\mathsf{F}(H_{\mathrm{free}})$ by its adjoint operator $\mathsf{F}(H_{\mathrm{free}})^\dagger$, respectively. If the function F is real-valued, then the operator $\mathsf{F}(H_{\mathrm{free}})$ is self-adjoint. Furthermore,

$$\langle \chi | H_{\mathrm{free}} \varphi \rangle = \int_0^\infty E \varrho_{\chi,\varphi}(E)dE \qquad \text{for all} \quad \chi, \varphi \in \mathcal{S}(\mathbb{R}).$$

Proof. We have $\langle \chi | \mathsf{F}(H)\varphi \rangle = \int_{-\infty}^\infty F\left(\frac{\hbar^2 k^2}{2m}\right) \hat{\chi}^\dagger(k)\hat{\varphi}(k)dk$. This is equal to

$$\int_0^\infty F\left(\frac{\hbar^2 k^2}{2m}\right)\Big(\hat{\chi}^\dagger(k)\hat{\varphi}(k) + \hat{\chi}^\dagger(-k)\hat{\varphi}(-k)\Big)\, dk = \int_0^\infty F(E)\varrho_{\chi,\varphi}(E)dE.$$

□

The spectral family of the free Hamiltonian H_{free}. Let $\lambda \in \mathbb{R}$. Choosing the characteristic function e_λ of the interval $]-\infty, \lambda[$ (see (7.100) on page 497), we get

$$\langle \chi | \mathsf{E}_\lambda(H_{\mathrm{free}})\varphi \rangle = \int_0^\infty e_\lambda(E)\varrho_{\chi,\varphi}(E)dE \qquad \text{for all} \quad \chi, \varphi \in \mathcal{S}(\mathbb{R}).$$

In particular, if $\lambda \le 0$, then $\mathsf{E}_\lambda(H_{\mathrm{free}}) = 0$.

Measurements of the energy. Let $\varphi \in \mathcal{S}(\mathbb{R})$ be a normalized state in the Hilbert space $L_2(\mathbb{R})$ (i.e., $\int_{\mathbb{R}} |\varphi(x)|^2 dx = 1$). This state describes a free quantum particle on the real line. Let $0 \le E_0 < E_1 \le \infty$. Then:

- Probability of measuring the energy of the particle in the interval$[E_0, E_1]$:

$$\int_{E_0}^{E_1} \varrho_{\varphi,\varphi}(E)dE.$$

- Mean energy of the particle: $\bar{E} = \int_0^\infty E\varrho_{\varphi,\varphi}(E)dE$.
- Square of the energy fluctuation: $(\Delta E)^2 = \int_0^\infty (E-\bar{E})^2 \varrho_{\varphi,\varphi}(E)dE$.

The Feynman Propagator Kernel

For all positions $x, x_0 \in \mathbb{R}$ and times $t > t_0$, define

$$\mathcal{K}(x,t;x_0,t_0) := \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}} \cdot \mathrm{e}^{im(x-x_0)^2/2\hbar(t-t_0)}.$$

Let $\psi_0 \in \mathcal{S}(\mathbb{R})$. Then we have the following integral representation of the quantum dynamics:

$$\boxed{\big(P(t,t_0)\psi_0\big)(x) = \int_{\mathbb{R}} \mathcal{K}(x,t;x_0,t_0)\psi_0(x_0)dx_0, \qquad x \in \mathbb{R},\ \ t > t_0.}$$

This is the *key formula* for solving the initial-value problem for the instationary Schrödinger equation (7.126) on page 524. For all $\chi, \varphi \in \mathcal{S}(\mathbb{R})$, we obtain the kernel formula

$$\langle \chi | P(t-t_0)\varphi\rangle = \int_{\mathbb{R}^2} \chi(x)^\dagger \mathcal{K}(x,t;x_0,t_0)\varphi(x_0)dxdx_0, \qquad t > t_0.$$

For $t > t_0$, the function $(x,y) \mapsto \mathcal{K}(x,t;y,t_0)$ is called the Feynman propagator kernel of the free quantum particle.

The Euclidean Propagator Kernel

Set $P_{\mathrm{Euclid}}(t,t_0) := \mathrm{e}^{-(t-t_0)H_{\mathrm{free}}/\hbar}$. The operator

$$P_{\mathrm{Euclid}}(t,t_0) : L_2(\mathbb{R}) \to L_2(\mathbb{R}), \qquad t \geq t_0$$

is linear, continuous, and nonexpansive, that is, $||P_{\mathrm{Euclid}}(t,t_0)|| \leq 1$ for all $t \geq t_0$. For each given initial state $\psi_0 \in L_2(\mathbb{R})$ at time t_0, we set

$$\psi(t) := P_{\mathrm{Euclid}}(t,t_0)\psi_0, \qquad t \geq t_0.$$

If $\psi_0 \in \mathcal{S}(\mathbb{R})$, then the function $\psi : [0,\infty[\to L_2(\mathbb{R})$ is continuously differentiable, and we have the Euclidean Schrödinger equation

$$\hbar\dot{\psi}(t) = -H_{\mathrm{free}}\psi(t), \quad t > t_0, \quad \psi(t_0) = \psi_0. \tag{7.129}$$

The operator $P_{\mathrm{Euclid}}(t,t_0)$ is called the Euclidean propagator of the free quantum particle at time t (with respect to the initial time t_0). In terms of the unitary Fourier transform $\mathcal{F} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$, the Euclidean propagator $P(t,t_0)$ corresponds to the multiplication with the function $k \mapsto \mathrm{e}^{-(t-t_0)E_k/\hbar}$ in the Fourier space. This means that, for all initial states $\psi_0 \in L_2(\mathbb{R})$, we get

$$P_{\mathrm{Euclid}}(t,t_0)\psi_0 = \mathcal{F}^{-1}M\mathcal{F}\psi_0, \qquad t \geq t_0$$

with the multiplication operator $(M\hat{\psi}_0)(k) := \mathrm{e}^{-(t-t_0)E_k/\hbar}\hat{\psi}_0(k)$ for all $k \in \mathbb{R}$. For all positions $x, x_0 \in \mathbb{R}$ and all times $t > t_0$, define

$$\mathcal{P}(x,t;x_0,t_0) = \sqrt{\frac{m}{2\pi\hbar(t-t_0)}} \cdot \mathrm{e}^{-m(x-x_0)^2/2\hbar(t-t_0)}.$$

Then we have the following integral representation:

$$\boxed{\big(P_{\text{Euclid}}(t,t_0)\psi_0\big)(x) = \int_{\mathbb{R}} \mathcal{P}(x,t;x_0,t_0)\psi_0(x_0)dx_0, \qquad x\in\mathbb{R},\ \ t>t_0.}$$

This is the key formula for solving the initial-value problem for the Euclidean Schrödinger equation (7.129). For all $\chi,\varphi\in L_2(\mathbb{R})$, we obtain the kernel formula

$$\langle\chi|P_{\text{Euclid}}(t,t_0)\varphi\rangle = \int_{\mathbb{R}^2} \chi(x)^\dagger \mathcal{P}(x,t;x_0,t_0)\varphi(x_0)dxdx_0, \qquad t>t_0.$$

For $t>t_0$, the function $(x,x_0)\mapsto \mathcal{P}(x,t;x_0,t_0)$ is called the Euclidean propagator kernel of the free quantum particle.

The Energetic Green's Function

The inhomogeneous stationary Schrödinger equation. Consider the inhomogeneous equation.

$$\boxed{-\frac{\hbar^2}{2m}\varphi''(x) = \mathcal{E}\varphi(x) + f(x), \qquad x\in\mathbb{R},} \tag{7.130}$$

which passes over to the stationary Schrödinger equation (7.115) if $f(x)\equiv 0$. Equation (7.130) corresponds to the operator equation

$$H_{\text{free}}\varphi - \mathcal{E}\varphi = f, \qquad \varphi\in D(H_{\text{free}}). \tag{7.131}$$

We want to solve this equation. Let $\mathcal{E}\in\varrho(H_{\text{free}})$ (i.e., $\mathcal{E}\in\mathbb{C}\setminus[0,\infty[$). Then the resolvent

$$(\mathcal{E}I - H_{\text{free}})^{-1} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$$

exists as a linear continuous operator. For given $f\in L_2(\mathbb{R})$, the equation (7.131) has the unique solution

$$\varphi = (H_{\text{free}} - \mathcal{E}I)^{-1} f.$$

Von Neumann's operator calculus tells us that for all $\chi, f\in L_2(\mathbb{R})$, we have

$$\langle\chi|(H_{\text{free}} - \mathcal{E}I)^{-1}f\rangle = \int_0^\infty \frac{\varrho_{\chi,f}(E)}{E-\mathcal{E}}\,dE.$$

The retarded Green's function. Our goal is to represent the solution of the inhomogeneous Schrödinger equation (7.130) by an integral formula. To this end, we introduce the function

$$\mathcal{G}^+(x,y;\mathcal{E}) := \frac{\mathrm{i}m\cdot \mathrm{e}^{\mathrm{i}k|x-y|}}{\hbar^2 k}, \qquad x,y\in\mathbb{R}. \tag{7.132}$$

Here, $k := \sqrt{2m\mathcal{E}}/\hbar$. We assume that $\Im(\mathcal{E})>0$. The square root is to be understood as principal value. This choice of the complex energy $\mathcal{E}$ guarantees that the function $\mathcal{G}^+$ decays exponentially as $|x-y|\to\infty$.

Proposition 7.37 *Let $\Im(\mathcal{E})>0$. For given $f\in\mathcal{S}(\mathbb{R})$, the unique solution of the inhomogeneous Schrödinger equation (7.130) reads as*

$$\varphi(x) = \int_{\mathbb{R}} \mathcal{G}^+(x,y;\mathcal{E})f(y)dy, \qquad x\in\mathbb{R}. \tag{7.133}$$

The proof will be given in Sect. 8.5.2 on page 731. By Prop. 7.37, we get

$$\langle\chi|(H_{\text{free}}-\mathcal{E}I)^{-1}\varphi\rangle=\int_{\mathbb{R}^2}\chi(x)^\dagger\mathcal{G}^+(x,y;\mathcal{E})\varphi(y)dxdy,\qquad \Im(\mathcal{E})>0$$

for all $\chi,\varphi\in\mathcal{S}(\mathbb{R})$. Therefore the function $(x,y)\mapsto\mathcal{G}^+(x,y;\mathcal{E})$ is the kernel of the (negative) resolvent $(H_{\text{free}}-\mathcal{E}I)^{-1}$; this kernel is called the retarded (energetic) Green's function of the Hamiltonian H_{free}. Note that, for fixed $y\in\mathbb{R}$, the retarded Green's function behaves like

- $\mathrm{e}^{\mathrm{i}kx}$ as $x\to+\infty$, and
- $\mathrm{e}^{-\mathrm{i}kx}$ as $x\to-\infty$ where $k>0$.

This corresponds to outgoing waves at infinity, $x=\pm\infty$.

The advanced Green's function. Now we pass from the positive wave number k to the negative wave number $-k$, that is, we change outgoing waves into ingoing waves at infinity. To this end, define

$$\mathcal{G}^-(x,y;\mathcal{E}):=-\frac{\mathrm{i}m\cdot\mathrm{e}^{-\mathrm{i}k|x-y|}}{\hbar^2k},\qquad x,y\in\mathbb{R}.\tag{7.134}$$

Here, $k:=-\sqrt{2m\mathcal{E}}/\hbar$. We assume that $\Im(\mathcal{E})<0$. The square root is to be understood as principal value. This choice of the complex energy $\mathcal{E}$ guarantees that the function $\mathcal{G}^-$ decays exponentially as $|x-y|\to\infty$.

Proposition 7.38 *Let $\Im(\mathcal{E})<0$. For given $f\in\mathcal{S}(\mathbb{R})$, the unique solution of the inhomogeneous Schrödinger equation (7.130) reads as*

$$\varphi(x)=\int_{\mathbb{R}}\mathcal{G}^-(x,y;\mathcal{E})f(y)dy,\qquad x\in\mathbb{R}.$$

Thus, for all $\chi,\varphi\in\mathcal{S}(\mathbb{R})$ we obtain

$$\langle\chi|(H_{\text{free}}-\mathcal{E}I)^{-1}\varphi\rangle=\int_{\mathbb{R}^2}\chi(x)^\dagger\mathcal{G}^-(x,y;\mathcal{E})\varphi(y)dxdy.$$

This means that the function $(x,y)\mapsto\mathcal{G}^-(x,y;\mathcal{E})$ is the kernel of the (negative) resolvent $(H_{\text{free}}-\mathcal{E}I)^{-1}$; this kernel is called the advanced (energetic) Green's function of the Hamiltonian H_{free}. Note that, for fixed $y\in\mathbb{R}$, the advanced Green's function behaves like

- $\mathrm{e}^{-\mathrm{i}kx}$ as $x\to+\infty$ and
- $\mathrm{e}^{\mathrm{i}kx}$ as $x\to-\infty$ where $k>0$.

This corresponds to incoming waves at infinity, $x=\pm\infty$.

The Fourier–Laplace transform of the Feynman propagator kernel. Fix the initial-time t_0. Then, for all times $t>t_0$, all positions $x,y\in\mathbb{R}$, and all complex energies $\mathcal{E}$ in the open upper half-pane (i.e., $\Im(\mathcal{E})>0$), we have

$$\mathcal{G}^+(x,y;\mathcal{E}):=\frac{\mathrm{i}}{\hbar}\int_{t_0}^{\infty}\mathrm{e}^{\mathrm{i}\mathcal{E}(t-t_0)/\hbar}\,\mathcal{K}(x,t;y,t_0)\,dt$$

together with the inverse formula

$$\mathcal{K}(x,t;y,t_0)=\frac{1}{2\pi\mathrm{i}}\cdot PV\int_{-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}\mathcal{E}(t-t_0)/\hbar}\,\mathcal{G}^+(x,y;\mathcal{E})\,d\Re(\mathcal{E}).$$

The global energetic Green's function. The retarded Green's function is holomorphic in the open upper half-plane. This function can be analytically continued to a global analytic function on a double-sheeted Riemann surface. This global Green's function is given by

$$\mathcal{G}_{\text{global}}(x,y;\mathcal{E}) = \frac{\mathrm{i}m \cdot \mathrm{e}^{\mathrm{i}k(\mathcal{E})|x-y|}}{\hbar^2 k(\mathcal{E})}$$

where $k(\mathcal{E}) := \frac{\sqrt{2m}}{\hbar} \cdot \sqrt{\mathcal{E}}$. Here, the function $\mathcal{E} \mapsto k(\mathcal{E})$ has to be regarded as a global analytic function defined on the Riemann surface $\mathcal{R}$ of the square-root function $\sqrt{\ } : \mathcal{R} \to \mathbb{C}$. This Riemann surface will be studied in Sect. 8.3.5 on page 713. In terms of $\mathcal{R}$, the retarded (resp. advanced) Green's function is defined on the open upper (resp. lower) half-plane of the first sheet of the Riemann surface $\mathcal{R}$. The two functions jump along the positive real axis (see Fig. 8.6 on page 714).

Perturbation of the Free Quantum Dynamics

If the motion of the free particle on the real line is perturbed by the potential U, then we get the perturbed Schrödinger equation

$$\boxed{\mathrm{i}\hbar\psi_t(x,t) = -\frac{\hbar^2}{2m}\psi_{xx}(x,t) + U(x)\psi(x,t), \quad x \in \mathbb{R},\ t > t_0,\ \ \psi(x,t_0) = \psi_0.} \tag{7.135}$$

This is the prototype of a quantum system under interaction. Let us introduce the Hamiltonian

$$H\varphi := -\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + U\varphi \qquad \text{for all} \quad \varphi \in W_2^2(\mathbb{R}).$$

In other words, $H = H_{\text{free}} + U$.

Theorem 7.39 *If the function $U : \mathbb{R} \to \mathbb{R}$ is smooth and has compact support, then the Hamiltonian $H : W_2^2(\mathbb{R}) \to L_2(\mathbb{R})$ is self-adjoint.*

Proof. Let $x \in \mathbb{R}$. Define the operator $C : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ by setting

$$(C\varphi)(x) := U(x)\varphi(x) \qquad \text{for all} \quad \varphi \in L_2(\mathbb{R}).$$

Then $||C\varphi|| \le \text{const} \cdot ||\varphi||$ for all $\varphi \in L_2(\mathbb{R})$. In fact,

$$\langle U\varphi | U\varphi \rangle = \int_{\mathbb{R}} \varphi(x)^\dagger U(x)^2 \varphi(x) dx \le \text{const} \int_{\mathbb{R}} |\varphi(x)|^2 dx.$$

Since the operator $H_{\text{free}} : W_2^2(\mathbb{R}) \to L_2(\mathbb{R})$ is self-adjoint, it follows from the Rellich–Kato perturbation theorem on page 502, that the perturbed operator $H = H_{\text{free}} + C$ is also self-adjoint on $W_2^2(\mathbb{R})$. □

A detailed study of equation (7.135) can be found in Chap. 8. This concerns the relation between scattering processes and bound states.

The Beauty of Harmonic Analysis

The motion of a free quantum particle is governed by the Fourier transform. Let us explain the relation to the translation group on the real line. For each $a \in \mathbb{R}$, the transformation

$$T_a x := x + a \qquad \text{for all} \quad x \in \mathbb{R}$$

represents a translation of the real line. For each smooth function $\psi : \mathbb{R} \to \mathbb{C}$, we define the operator

$$(\mathcal{T}_a \psi)(x) := \psi(T_a^{-1} x).$$

Explicitly, $\mathcal{T}_a \psi(x) = \psi(x - a)$. The operator D defined by

$$D\psi(x) := \lim_{a \to 0} \frac{\mathcal{T}_a \psi(x) - \psi(x)}{a} = -\psi'(x) \qquad \text{for all} \quad x \in \mathbb{R}$$

is called the infinitesimal translation. By Taylor expansion,

$$\mathcal{T}_a \psi(x) = \psi(x) + D\psi(x) + \tfrac{1}{2} D^2 \psi(x) + \tfrac{1}{3!} D^3 \psi(x) + \dots$$

The Fourier transform is related to the eigenfunctions $\chi_k(x) := \frac{\mathrm{e}^{\mathrm{i}kx}}{\sqrt{2\pi}}$ of the infinitesimal operator D. Explicitly,

$$\mathrm{i}\hbar D \chi_k = \hbar k \chi_k, \qquad k \in \mathbb{R}.$$

Note that $\mathrm{i}\hbar D$ corresponds to the momentum operator on the real line. If we replace the translation group by another Lie group, then we get a generalization of the preceding situation which leads to

- more general infinitesimal transformations (differential operators),
- more general eigenfunctions (special functions of mathematical physics),
- and a generalization of the Fourier transform.

This is the subject of a beautiful branch in mathematics called harmonic analysis, which will be encountered quite often in this treatise. In the 20th century, the protagonist of harmonic analysis was Hermann Weyl (1885–1955). We recommend:

> G. Mackey, The Scope and History of Commutative and Noncommutative Harmonic Analysis, Amer. Math. Soc., Providence, Rhode Island, 1992.
>
> G. Mackey, Induced Representations of Groups and Quantum Mechanics, Benjamin, New York, 1968.
>
> G. Mackey, Unitary Group Representations in Physics, Probability, and Number Theory, Benjamin, Reading, Massachusetts, 1978.

7.6.6 The Rescaled Fourier Transform

> The rescaled Fourier transform fits best the duality between position and momentum of quantum particles in the setting of the Dirac calculus.
>
> Folklore

Introducing the function $\varphi_p(x) := \frac{\mathrm{e}^{\mathrm{i}px/\hbar}}{\sqrt{2\pi\hbar}}$ for all $x \in \mathbb{R}$, we obtain the key relation

$$-\mathrm{i}\hbar \frac{d\varphi_p}{dx} = p\varphi_p \qquad \text{for all} \quad p \in \mathbb{R}.$$

That is, the function φ_p is a generalized eigenfunction of the momentum operator with the momentum p as eigenvalue. The normalization is dictated by the Parseval

equation (7.138) below. Let $\varphi, \psi \in \mathcal{S}(\mathbb{R})$. The rescaled Fourier transform is given by the following two formulas

$$\tilde{\varphi}(p) = \int_{\mathbb{R}} \varphi_p^\dagger(x)\varphi(x)dx \qquad \text{for all} \quad p \in \mathbb{R} \tag{7.136}$$

and

$$\varphi(x) = \int_{\mathbb{R}} \varphi_p(x)\tilde{\varphi}(p)dp \qquad \text{for all} \quad x \in \mathbb{R} \tag{7.137}$$

together with the Parseval equation

$$\int_{\mathbb{R}} \psi(x)^\dagger \varphi(x)dx = \int_{\mathbb{R}} \tilde{\psi}(p)^\dagger \tilde{\varphi}(p)\, dp. \tag{7.138}$$

The classical Fourier transform is obtained by choosing $\hbar := 1$. Setting $\mathcal{F}_\hbar \varphi := \tilde{\varphi}$, we obtain the linear, bijective, sequentially continuous operator

$$\mathcal{F}_\hbar : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$$

which is called the rescaled Fourier transform. As in Sect. 7.6.4, this operator can be extended to a linear bijective operator

$$\mathcal{F}_\hbar : \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$$

such that the restriction $\mathcal{F}_\hbar : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ is unitary. The commutative diagram

$$\begin{array}{ccc} D(P) & \xrightarrow{P} & L_2(\mathbb{R}) \\ {\scriptstyle \mathcal{F}_\hbar}\downarrow & & \downarrow{\scriptstyle \mathcal{F}_\hbar} \\ D(Q) & \xrightarrow{Q} & L_2(\mathbb{R}) \end{array}$$

tells us that the momentum operator P and the position operator Q are unitarily equivalent. According to Dirac, for fixed momentum $p \in \mathbb{R}$, we introduce the momentum costate $\langle p|$ by setting

$$\boxed{\langle p|(\varphi) := \int_{\mathbb{R}} \varphi_p^\dagger(x)\varphi(x)dx, \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).}$$

Mnemonically, we write this as $\langle p|\varphi\rangle$. Replacing the wave number costate $\langle k|$ from Sect. 7.6.4 by the momentum costate $\langle p|$, we get the following formulas of the Dirac calculus:

- $\langle p|\varphi\rangle = \tilde{\varphi}(p)$,
- $I = \int_{\mathbb{R}} |p\rangle\langle p|\, dp$,
- $P_{\text{pre}}^d \langle p| = p\, \langle p|$,
- $H_{\text{pre}}^d \langle p| = E(p)\, \langle p|$ with the energy value $E(p) := \frac{p^2}{2m}$.

The system $\{\langle p|\}_{p\in\mathbb{R}}$ forms a complete orthonormal system of costates for both the momentum operator P_{pre} and the free Hamiltonian H_{pre}. Adding the mnemonical formulas

- $\langle x|\varphi\rangle = \varphi(x)$ and $\langle x|p\rangle = \varphi_p(x)$,
- $I = \int_{\mathbb{R}} |x\rangle\langle x|\, dx$,

as well as $\langle a|b\rangle^\dagger = \langle b|a\rangle$, we automatically obtain

$$\boxed{\langle p|\varphi\rangle = \int_{\mathbb{R}} \langle p|x\rangle\langle x|\varphi\rangle \, dx, \qquad \langle x|\varphi\rangle = \int_R \langle x|p\rangle\langle p|\varphi\rangle \, dp}$$

which is the rescaled Fourier transform (7.136), (7.137) above. Similarly, the Parseval equation (7.138) above is obtained by

$$\boxed{\langle \psi|\varphi\rangle = \int_{\mathbb{R}} \langle \psi|x\rangle\langle x|\varphi\rangle \, dx = \int_{\mathbb{R}} \langle \psi|p\rangle\langle p|\varphi\rangle \, dp.}$$

This shows that the rescaled Fourier transform is nothing else than a change from the position coordinate x to the momentum coordinate p which respects "inner products."

Note that, as a rule, physicists use the wave number costates $\langle k|$ in scattering theory, and the momentum costates $\langle p|$ in the Feynman path integral approach. We will follow this convention.

7.6.7 The Quantized Harmonic Oscillator and the Maslov Index

> The global behavior of the quantized harmonic oscillator is governed by the Morse indices (also called Maslov indices) of the classical harmonic oscillator.
>
> Folklore

Let us continue the study of the quantized harmonic oscillator on the real line started in Sect. 7.4.4 on page 467. The initial-value problem for the corresponding Schrödinger equation reads as

$$\mathrm{i}\hbar\psi_t(x,t) = -\frac{\hbar^2}{2m}\psi_{xx}(x,t) + \frac{m\omega^2 x^2}{2}\,\psi(x,t), \quad \psi(x,t_0) = \psi_0(x) \tag{7.139}$$

for all position coordinates $x \in \mathbb{R}$ and all times $t > t_0$. Let us introduce the pre-Hamiltonian $H_{\mathrm{pre}} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ by setting

$$\big(H_{\mathrm{pre}}\varphi\big)(x) := -\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} + \frac{m\omega^2 x^2}{2}\,\varphi(x), \qquad x \in \mathbb{R}.$$

By Sect. 7.4.4, the equation $H_{\mathrm{pre}}\varphi = E\varphi$ has the eigensolutions (φ_n, E_n) with the energy eigenvalues $E_n = \hbar\omega(n + \frac{1}{2})$ and the eigenfunctions

$$\varphi_n(x) = \frac{1}{\sqrt{2^n n! x_0 \sqrt{\pi}}}\; H_n\left(\frac{x}{x_0}\right)\; \exp\left\{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2\right\}, \qquad n = 0, 1, 2, \ldots,$$

where $x_0 := \sqrt{\frac{\hbar}{m\omega}}$. Here, $H_0, H_1, H_2, \ldots$ are the Hermite polynomials introduced on page 436. Furthermore, $\varphi_n \in \mathcal{S}(\mathbb{R})$ for all n. We will use the Hilbert space $L_2(\mathbb{R})$ with the inner product

$$\langle \chi|\varphi\rangle := \int_{\mathbb{R}} \chi^\dagger(x)\varphi(x)dx, \qquad \chi, \varphi \in L_2(\mathbb{R}).$$

For introducing operator kernels, we will also use the Hilbert space $L_2(\mathbb{R}^2)$ equipped with the inner product

$$\langle \mathcal{A}|\mathcal{B}\rangle_{L_2(\mathbb{R}^2)} := \int_{\mathbb{R}^2} \mathcal{A}(x,y)^\dagger \mathcal{B}(x,y)dxdy, \qquad \mathcal{A}, \mathcal{B} \in L_2(\mathbb{R}^2).$$

(i) The self-adjoint Hamiltonian H: The point is that the eigenfunctions $\varphi_0, \varphi_1, \ldots$ form a complete orthonormal system in the Hilbert space. The pre-Hamiltonian H_{pre} can be extended to the self-adjoint operator $H : D(H) \to L_2(\mathbb{R})$ given by

$$H\varphi := \sum_{n=0}^{\infty} E_n \langle \varphi_n | \varphi \rangle \varphi_n .$$

Here, $\varphi \in D(H)$ iff this series is convergent in the Hilbert space $L_2(\mathbb{R})$, that is, $\sum_{n=0}^{\infty} E_n^2 |\langle \varphi_n | \varphi \rangle|^2 < \infty$. The operator H is called the Hamiltonian of the quantized harmonic oscillator.

(ii) The spectrum of the Hamiltonian H: The spectrum $\sigma(H)$ consists of the energy values $E_0, E_1, E_2, \ldots$ of the quantized harmonic oscillator. This is a pure point spectrum; the absolutely continuous spectrum, the essential spectrum, and the singular spectrum of H are empty.

(iii) The kernel theorem: Let $\lambda_0, \lambda_1, \ldots$ be complex numbers. Consider the operator $A : D(A) \to L_2(\mathbb{R})$ given by

$$A\varphi = \sum_{n=0}^{\infty} \lambda_n \langle \varphi_n | \varphi \rangle \varphi_n . \tag{7.140}$$

We assume that the domain of definition $D(A)$ consists of all the functions $\varphi \in L_2(\mathbb{R})$ for which the series on the right-hand side of (7.140) is convergent in $L_2(\mathbb{R})$, that is, $\varphi \in D(A)$ iff $\sum_{k=0}^{\infty} |\lambda_n \langle \varphi_n | \varphi \rangle|^2 < \infty$.

Theorem 7.40 (a) *Hilbert–Schmidt operator with $L_2(\mathbb{R}^2)$-kernel: If*

$$\sum_{n=0}^{\infty} |\lambda_n|^2 < \infty,$$

then the operator $A : X \to X$ defined by (7.140) is linear, continuous, and compact. The series

$$\mathcal{A}(x,y) := \sum_{n=0}^{\infty} \lambda_n \varphi_n(x) \varphi_n(y)^{\dagger}, \qquad (x,y) \in \mathbb{R}^2 \tag{7.141}$$

is convergent in the Hilbert space $L_2(\mathbb{R}^2)$, and the operator A has the $L_2(\mathbb{R}^2)$-kernel $\mathcal{A}$. That is, for all $\varphi, \chi \in L_2(\mathbb{R})$, we have

$$(A\varphi)(x) = \int_{\mathbb{R}} \mathcal{A}(x,y) \varphi(y) dy, \qquad x \in \mathbb{R},$$

together with the bilinear form

$$\langle \chi | A\varphi \rangle = \int_{\mathbb{R}^2} \chi(x)^{\dagger} \mathcal{A}(x,y) \varphi(y) dx dy. \tag{7.142}$$

If all the numbers $\lambda_0, \lambda_1, \ldots$ are real, then the operator A is self-adjoint.

(b) *Trace-class operator: If $\sum_{n=0}^{\infty} |\lambda_n| < \infty$, then* (i) *is valid. The operator $A : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ is called a trace class (or nuclear) operator; its trace is given by* $\operatorname{tr}(A) = \sum_{n=0}^{\infty} \lambda_n$.[83]

[83] The general definition of Hilbert–Schmidt operators and trace-class operators will be given in Sect. 7.16.4 on page 629.

(c) *The Schwartz kernel T: If the condition* $\sup_n |\lambda_n| < \infty$ *is satisfied, then the operator* $A : X \to X$ *is linear and continuous. There exists a uniquely determined tempered distribution* $T \in \mathcal{S}'(\mathbb{R}^2)$ *such that*

$$\langle \chi | A\varphi \rangle = T(\chi^\dagger \otimes \varphi) \qquad \text{for all} \quad \chi, \varphi \in \mathcal{S}(\mathbb{R}).$$

More precisely, there exist a continuous function $\mathcal{A} : \mathbb{R}^2 \to \mathbb{C}$ *of polynomial growth and nonnegative integers* r *and* s *such that*

$$T(\chi^\dagger \otimes \varphi) = \int_{\mathbb{R}^2} \chi^{(r)}(x)^\dagger \mathcal{A}(x,y)\varphi^{(s)}(y)dxdy \quad \text{for all} \quad \chi, \varphi \in \mathcal{S}(\mathbb{R}).$$

Proof. Ad (a). Since the functions $\varphi_0, \varphi_1, \ldots$ form a complete orthonormal system in the Hilbert space $L_2(\mathbb{R})$, the tensor products

$$(\varphi_k^\dagger \otimes \varphi_l)(x,y) := \varphi_k(x)^\dagger \varphi(y), \qquad (x,y) \in \mathbb{R}^2, \quad k,l = 0,1,\ldots$$

represent a complete orthonormal system in the Hilbert space $L_2(\mathbb{R}^2)$ (see Zeidler (1995a), p. 224). Consequently, the series (7.141) is convergent in $L_2(\mathbb{R}^2)$ iff $\sum_{n=0}^\infty |\lambda_n|^2 < \infty$. The remaining claims are standard results in functional analysis (see Zeidler (1995a), Sect. 4.4).
Ad (b). If $\sum_{n=0}^\infty |\lambda_n| < \infty$, the $\lim_{n\to\infty} \lambda_n = 0$. Consequently, there exists a natural number n_0 such that $\sum_{n=n_0}^\infty |\lambda_n|^2 \le \sum_{n=n_0}^\infty |\lambda_n|$.
Ad (c). This is the Schwartz kernel theorem. The proof can be found in I. Gelfand and N. Vilenkin, Generalized Functions, Vol. 4, Sect. I.1.3, Academic Press, New York, 1964. □

(iv) The resolvent and the energetic Green's function of the Hamiltonian H: Let the complex number $\mathcal{E}$ be different from all the eigenvalues $E_0, E_1, \ldots$ Introduce $G(\mathcal{E}) := (H - \mathcal{E}I)^{-1}$. Then the energetic Green's operator

$$G(\mathcal{E}) : L_2(\mathbb{R}) \to L_2(\mathbb{R})$$

is linear and continuous. Explicitly,

$$G(\mathcal{E})\varphi = \sum_{n=0}^\infty \frac{\langle \varphi_n | \varphi \rangle}{E_n - \mathcal{E}}\, \varphi_n, \qquad \varphi \in L_2(\mathbb{R}).$$

The operator $G(\mathcal{E})$ has an $L_2(\mathbb{R}^2)$-kernel called the energetic Green's function of the quantized harmonic oscillator. Explicitly,

$$\mathcal{G}(x,y;\mathcal{E}) = \sum_{n=0}^\infty \frac{\varphi_n(x)\varphi_n(y)^\dagger}{E_n - \mathcal{E}}, \qquad x,y \in \mathbb{R}.$$

This series is convergent in $L_2(\mathbb{R}^2)$. For all $x \in \mathbb{R}$, we have

$$(G(\mathcal{E})\varphi)(x) = \int_{\mathbb{R}} \mathcal{G}(x,y;\mathcal{E})\varphi(y)dy.$$

The operator $R(\mathcal{E}) := -G(\mathcal{E})$ is called the resolvent of H.

(v) The Euclidean propagator kernel: Let $t > t_0$. Set $\beta := (t-t_0)/\hbar$. Since the series $\sum_{n=0}^{\infty} \mathrm{e}^{-\beta E_n}$ is convergent, it follows from Theorem 7.40(ii) that the Euclidean propagator $P_{\mathrm{Euclid}}(t, t_0) := \mathrm{e}^{-\beta H}$ is a trace-class operator on $L_2(\mathbb{R})$, and it has an $L_2(\mathbb{R}^2)$-kernel given by the series

$$\mathcal{P}(x,t;y,t_0) := \sum_{n=0}^{\infty} \mathrm{e}^{-\beta E_n} \varphi_n(x) \varphi_n(y)^{\dagger},$$

which is convergent in the Hilbert space $L_2(\mathbb{R}^2)$.

Proposition 7.41 *For all positions $x, y \in \mathbb{R}$ and all times $t > 0$, the Euclidean propagator kernel reads as*

$$\mathcal{P}(x,t;y,0) = \frac{1}{x_0 \sqrt{2\pi \sinh \omega t}} \exp\left\{ -\frac{(x^2+y^2)\cosh \omega t - 2xy}{2x_0^2 \sinh \omega t} \right\}.$$

For $t > t_0$, we get $\mathcal{P}(x,t;y,t_0) = \mathcal{P}(x,t-t_0;y,0)$.

Proof. This is the classical Mehler formula for Hermite polynomials which can be found in A. Erdéley et al. (Eds.), Higher Transcendental Functions, Vol. III, McGraw-Hill, New York, 2006. Explicitly, the Mehler formula reads as

$$\begin{aligned} &\frac{1}{\sqrt{1-z^2}} \exp\left\{ -\frac{1}{2(1-z^2)} [(x^2+y^2)(1+z^2) - 4xyz] \right\} \\ &\qquad = \exp\left(-\frac{x^2}{2} - \frac{y^2}{2} \right) \sum_{n=0}^{\infty} \frac{z^n}{2^n n!} H_n(x) H_n(y) \end{aligned} \tag{7.143}$$

for all $x, y \in \mathbb{R}$ and all complex numbers z with $|z| < 1$. □

We will see in Sect. 7.6.8 that the Euclidean propagator of a single harmonic oscillator governs the thermodynamics of an ideal gas if we set $\beta := 1/kT$ where T is the temperature and k is the Boltzmann constant.

(vi) The generalized Feynman propagator kernel and the Maslov indices: We want to show that analytic continuation of the Euclidean propagator kernel yields the function

$$\boxed{\mathcal{K}(x,t;y,0) := \frac{\mathrm{e}^{-\mathrm{i}\pi/4}\, \mathrm{e}^{-\mathrm{i}\pi\mu(0,t)/2}}{x_0 \sqrt{2\pi |\sin \omega t|}} \exp\left(\mathrm{i} \frac{(x^2+y^2)\cos \omega t - 2xy}{2x_0^2 \sin \omega t} \right).} \tag{7.144}$$

This so-called Feynman–Souriau formula is valid for both

- all positions $x, y \in \mathbb{R}$ and
- all non-critical times $t \in]t_{n,\mathrm{crit}}, t_{n+1,\mathrm{crit}}[$ with $n = 0, 1, 2, ...$

Here, the critical times are given by $t_{n,\mathrm{crit}} := \frac{n\pi}{\omega}$. The Maslov index is defined by

$$\mu(0,t) := n \qquad \text{for all} \quad t \in]t_{n,\mathrm{crit}},\ t_{n+1,\mathrm{crit}}[. \tag{7.145}$$

For all $t > t_0$, we set $\mathcal{K}(x,t;y,t_0) := \mathcal{K}(x,t-t_0;y,0)$. The function $\mathcal{K}$ is called the generalized Feynman propagator kernel (or briefly the Feynman propagator kernel) of the quantized harmonic oscillator. The additional factors

$$\mathrm{e}^{-\mathrm{i}\pi/4}\, \mathrm{e}^{-\mathrm{i}\pi\mu(0,t)/2} \tag{7.146}$$

appearing in (7.144) are called the critical Maslov phase factors. In terms of mathematics, in the following proof we will show that these phase factors are obtained in a natural way by means of analytic continuation. In terms of physics, we will show below that the Maslov phase factors are closely related to causality.

Proof. To simplify notation, we set $\omega := 1$. In order to find the analytic continuation, we replace the real variable t by the complex variable z. This way, using Prop. 7.41 we get

$$\mathcal{P}(x,z;y,0) = \frac{1}{x_0\sqrt{2\pi\sinh z}}\ \exp\left\{-\frac{(x^2+y^2)\cosh z - 2xy}{2x_0^2\sinh z}\right\}.$$

Now set $z := \mathrm{i}t$. Then $\sinh z = \mathrm{i}\sin t$ and $\cosh z = \cos t$ for all $t \in \mathbb{C}$. Suppose that

$$t_{n,\mathrm{crit}} < t < t_{n+1,\mathrm{crit}}, \qquad n = 0, 1, 2, \ldots$$

Then $\sin t = (-1)^n |\sin t|$. Considering the square-root function on its Riemann surface (see Fig. 8.6 on page 714), we obtain

$$\sqrt{\mathrm{i}\sin t} = \sqrt{(-1)^n \mathrm{i}|\sin t|} = \sqrt{\mathrm{e}^{\mathrm{i}n\pi}\mathrm{e}^{\mathrm{i}\pi/2}|\sin t|} = \mathrm{e}^{\mathrm{i}n\pi/2}\mathrm{e}^{\mathrm{i}\pi/4}\sqrt{|\sin t|}.$$

This yields the claim (7.144). □

Focal points and the Morse index (Maslov index). We want to show that the singularities of the Feynman propagator kernel $\mathcal{K}(x,t;y,t_0)$ are related to the Morse indices of focal points in classical mechanics. To this end, consider a harmonic oscillator of mass $m > 0$ and angular frequency $\omega > 0$ on the real line. The classical equation of motion reads as

$$m\ddot{q}(\tau) + \omega^2 q(\tau) = 0, \qquad \tau \in \mathbb{R}, \qquad q(0) = q_0, \ \ \dot{q}(0) = q_1$$

with the characteristic length $x_0 := \sqrt{\hbar/m\omega}$. In Sect. 6.5.4, we have introduced the crucial Morse (or Maslov) index which coincides with (7.145) above. Explicitly, the critical points in time are characterized by the fact that the boundary value problem

$$\ddot{q}(t) + \omega^2 q(t) = 0, \qquad 0 < t < t_{n,\mathrm{crit}}, \qquad q(0) = q(t_{n,\mathrm{crit}}) = 0$$

has not only the trivial solution $q(t) \equiv 0$, but also a nontrivial solution, namely, $q(t) := \sin \omega t$. Observe that the function $\mathcal{P}$ has singularities precisely at the critical points in time, since $\sin \omega t_{n,\mathrm{crit}} = 0$. Moreover, the Morse index $\mu(0,t)$ jumps at the critical points in time.

The Feynman propagator kernel $\mathcal{K}(x,t;y,t_0)$ of the quantized harmonic oscillator contains information about the global behavior of the classical harmonic oscillator.

This phenomenon is typical for the quantization of classical dynamical systems.[84]

Causality and the motivation of the Maslov phase factors. Using the Dirac delta function in a formal way, we want to motivate formula (7.146) above in terms of physics. To simplify notation, let us use the convention $\omega = \hbar = m := 1$. Hence $x_0 = 1$. The starting point is the product formula (7.90) for the propagator kernel, that is,

[84] See M. Gutzwiller, Chaos in Classical and Quantum Mechanics, Springer, New York, 1990.

$$\mathcal{K}(x,t;y,0) = \int_{\mathbb{R}} \mathcal{K}(x,t-\tau;z,0)\mathcal{K}(z,\tau;y,0)\, dz \tag{7.147}$$

which is based on the causality relation $\mathrm{e}^{-\mathrm{i}tH} = \mathrm{e}^{-\mathrm{i}(t-\tau)H}\mathrm{e}^{-\mathrm{i}\tau H}$.

(I) Consider the first critical time interval $0 < t < t_{1,\mathrm{crit}}$ with $t_{1,\mathrm{crit}} = \pi$. Then , then analytic continuation of the Euclidean propagator $\mathcal{P}$ from Prop. 7.41 yields the regular Feynman propagator kernel

$$\mathcal{K}(x,t;y,0) = \frac{\mathrm{e}^{-\mathrm{i}\pi/4}}{\sqrt{2\pi\sin t}} \exp\left(\mathrm{i}\frac{(x^2+y^2)\cos t - 2xy}{2\sin t}\right), \quad 0 < t < \pi.$$

Let us now study the limit $t \to \pi - 0$. If $t = \frac{\pi}{2}$, then

$$\mathcal{K}\left(x, \frac{\pi}{2}; y, 0\right) = \frac{\mathrm{e}^{-\mathrm{i}\pi/4}\mathrm{e}^{-\mathrm{i}xy}}{\sqrt{2\pi}}.$$

By the product rule (7.147), we get

$$\begin{aligned}\lim_{t\to\pi-0} \mathcal{K}(x,t;y,0) :&= \int_{\mathbb{R}} \mathcal{K}\left(x,\frac{\pi}{2};z,0\right)\mathcal{K}\left(z,\frac{\pi}{2};y,0\right) dz \\ &= \mathrm{e}^{-\mathrm{i}\pi/2}\cdot\frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}(x+y)z} dz = \mathrm{e}^{-\mathrm{i}\pi/2}\delta(x+y).\end{aligned}$$

(II) Now consider the second critical time interval $\pi < t < 2\pi$. We want to define the propagator kernel on the interval $]\pi, 2\pi[$ in such a way that

$$\lim_{t\to\pi+0} \mathcal{K}(x,t;y,0) = \lim_{t\to\pi-0} \mathcal{K}(x,t;y,0) = \mathrm{e}^{-\mathrm{i}\pi}\delta(x+y).$$

The appropriate definition looks like

$$\mathcal{K}(x,t;y,0) := \frac{\mathrm{e}^{-\mathrm{i}\pi/4}\mathrm{e}^{-\mathrm{i}\pi/2}}{\sqrt{2\pi|\sin t|}} \exp\left(\mathrm{i}\frac{(x^2+y^2)\cos t - 2xy}{2\sin t}\right), \qquad \pi < t < 2\pi.$$

To see this, set $t := \pi + \tau$. Using $\sin(\pi+\tau) = -\sin\tau$ together with $\lim_{\tau\to 0}\frac{\sin\tau}{\tau} = 1$, we obtain

$$\lim_{\tau\to+0} \mathcal{K}(x,\pi+\tau;y,0) = \mathrm{e}^{-\mathrm{i}\pi/2}\lim_{\tau\to+0}\frac{\mathrm{e}^{-\mathrm{i}\pi/4}\mathrm{e}^{\mathrm{i}(x+y)^2/2\tau}}{\sqrt{2\pi\tau}} = \mathrm{e}^{-\mathrm{i}\pi/2}\delta(x+y).$$

The latter limit follows from

$$\lim_{\tau\to+0} \mathcal{K}_{\mathrm{free}}(z,\tau;0,0) = \delta(z)$$

for the propagator kernel $\mathcal{K}_{\mathrm{free}}(z,\tau;0,0) = \mathrm{e}^{-\mathrm{i}\pi/4}\cdot\frac{\mathrm{e}^{\mathrm{i}z^2/2\tau}}{\sqrt{2\pi\tau}}$ of a free quantum particle on the real line.

(III) Similarly, we extend the definition of the propagator kernel $\mathcal{K}$ to the other critical time intervals. □

Using the theory of distributions, the formal argument above can be reformulated in terms of rigorous mathematics.

7.6.8 Ideal Gases and von Neumann's Density Operator

> The statistical physics of the multi-particle system of N harmonic oscillators is governed by the Euclidean propagator of a single harmonic oscillator.
>
> Folklore

We want to explain the following fundamental principle in physics:

> *In order to pass from quantum mechanics to statistical physics, apply the replacement*
>
> $$\frac{\mathrm{i}t}{\hbar} \mapsto \frac{1}{kT}.$$
>
> *Here, we use the following notation: t time, T absolute temperature, h Planck's quantum of action, $\hbar = h/2\pi$, and k Boltzmann constant.*

It turns out that the computation methods in statistical physics are frequently easier to handle than the corresponding methods in quantum mechanics. The reason is that, for $T > 0$ and $t > 0$, the integral

$$\int_0^\infty \mathrm{e}^{-E/kT} dE$$

is well-defined whereas the oscillating integral

$$\int_0^\infty \mathrm{e}^{-\mathrm{i}Et/\hbar} dE$$

does not exist. The Euclidean trick in physics is to start with imaginary time $t = -\mathrm{i}\tau$. Then $\mathrm{i}t = \tau$ is real. At the end of the computation, one performs an analytic continuation to real time t, if possible. Fortunately enough, this trick works well in many cases.

A gas of quantum particles on the real line. The following situation is the prototype of quantum statistics. Consider a large fixed number of N identical quantum particles (bosons) on the real line which are harmonic oscillators of mass m and fixed angular frequency $\omega > 0$. To simplify notation, physicists introduce the quantity

$$\boxed{\beta := \frac{1}{kT}}$$

in statistical physics. Here, T is the absolute temperature of the gas, and k is the universal Boltzmann constant. The physical dimension of kT is energy. For studying the physics of the gas, the following two quantities

$$x_0 := \sqrt{\frac{\hbar}{m\omega}}, \qquad \beta\hbar\omega = \frac{\hbar\omega}{kT}$$

are important. Here, x_0 has the physical dimension of length, and $\beta\hbar\omega$ is dimensionless. It is our aim to compute the following physical quantities of the gas at the temperature $T > 0$.

(i) Total energy of the gas:

$$\boxed{E = N\bar{E} = N\hbar\omega\left(\frac{1}{2} + \frac{1}{\mathrm{e}^{\beta\hbar\omega} - 1}\right).}$$

(ii) Relative energy fluctuations:

$$\frac{\Delta E}{E} = \frac{\Delta \bar{E}}{\bar{E}\sqrt{N}} = \frac{1}{\sqrt{N}\cosh\frac{\beta\hbar\omega}{2}}.$$

For large particle number N, the relative energy fluctuations are small, as expected by experience for gases in daily life.

(iii) Mass density of the gas:

$$\mu(x,T) = Nm\varrho(x,T) = \frac{Nm}{x_0}\sqrt{\frac{\tanh\frac{\beta\omega\hbar}{2}}{\pi}}\ \exp\left\{\frac{x^2(1-\cosh\beta\hbar\omega)}{x_0^2\sinh\beta\hbar\omega}\right\}.$$

Here, the density function $\varrho(x,T) := \langle x|\varrho(T)|x\rangle$ is related to von Neumann's density operator $\varrho(T)$. The derivative of energy with respect to temperature,

$$C(T) = E_T(T,N),$$

is called the heat capacity of the gas. A small change ΔT of temperature produces the following amount of heat,

$$\Delta Q = C(T)\Delta T.$$

The heat capacity can be measured in physical experiments. We will compute below the mean energy $\bar{E}$ and the mean energy fluctuation $\Delta\bar{E}$ of one particle. For the total energy, this yields $E = N\bar{E}$. Moreover, we assume that the single particles behave independently. Then, by the theory of probability, the total energy dispersion is additive,

$$(\Delta E)^2 = (\Delta\bar{E})^2 + \ldots + (\Delta\bar{E})^2 = N(\Delta\bar{E})^2.$$

Hence $\Delta E/E = \Delta\bar{E}/\bar{E}\sqrt{N}$.

Bose–Einstein condensation. To understand the physics of our gas, let us consider the two important special cases of high temperature and low temperature.

(H) For high temperature T (i.e., β is small), we get up to terms of lower order:[85]

$$E = NkT, \qquad \frac{\Delta E}{E} = \frac{1}{\sqrt{N}}, \qquad \mu(x,T) = \frac{Nm}{\sigma\sqrt{2\pi}}\ \mathrm{e}^{-x^2/2\sigma^2}.$$

The mass density function μ is a Gaussian distribution with mean fluctuation $\sigma := x_0/\sqrt{\beta\hbar\omega}$. The energy law, $E = N\cdot kT$, is a special case of the classical Boltzmann law of energy equipartition. This law tells us that, for many-particle systems at high temperature, each degree of freedom contributes the amount of mean energy kT to the total energy of the system. For the heat capacity of the gas, we get $C = Nk$.

(L) For low temperature T, we obtain:

$$\lim_{T\to+0} E = \tfrac{1}{2}\hbar\omega N, \qquad \lim_{T\to+0}\frac{\Delta E}{E} = 0.$$

As expected, the particle energy is equal to the ground state energy of the harmonic oscillator. Physicists say that the excited energy states are frozen at low temperatures. This crucial phenomenon is called Bose-Einstein condensation.[86]

[85] Note that $\sinh\beta\hbar\omega = \beta\hbar\omega + O(\beta^2)$ and $\cosh\beta\hbar\omega = 1 + \beta^2\hbar^2\omega^2 + O(\beta^4)$ as $\beta\to 0$.

[86] In 2001, Eric Cornell, Wolfgang Ketterle, and Carl Wieman were awarded the Nobel prize in physics for the experimental achievement of Bose–Einstein condensation in dilute gases of alkali atoms, and for fundamental studies of the properties of the condensates.

Note that the behavior of the gas at low temperatures is governed by typical quantum effects.

The partition function. The possible energies of the gas particles are given by

$$E_n = \hbar\omega(n + \tfrac{1}{2}), \qquad n = 0, 1, 2, , ...$$

By statistical physics, the physical properties of this many-particle system follow from the partition function

$$Z(\beta) := \sum_{n=0}^{\infty} \mathrm{e}^{-\beta E_n}.$$

Recall that $\beta := 1/kT$. For a single particle, the probability of having the energy E_n is equal to

$$p_n := \frac{\mathrm{e}^{-\beta E_n}}{Z(\beta)}.$$

This yields the mean energy $\bar{E}$ and the mean energy fluctuation $\Delta\bar{E} \geq 0$ of a single particle, namely,

$$\bar{E} = \sum_{n=0}^{\infty} E_n p_n, \qquad (\Delta\bar{E})^2 = \sum_{n=0}^{\infty} (E_n - \bar{E})^2 p_n.$$

We claim that

$$\boxed{\bar{E} = \hbar\omega \left(\frac{1}{2} + \frac{1}{\mathrm{e}^{\beta\hbar\omega} - 1} \right), \qquad \frac{\Delta\bar{E}}{\bar{E}} = \frac{1}{\cosh \frac{\beta\hbar\omega}{2}}.} \tag{7.148}$$

Proof. By the geometric series $1 + q + q^2 + ... = \frac{1}{1-q}$ for $|q| < 1$, we get

$$Z(\beta) = \sum_{n=0}^{\infty} \mathrm{e}^{-\beta E_n} = \frac{\mathrm{e}^{-\beta\hbar\omega/2}}{1 - \mathrm{e}^{-\beta\hbar\omega}} = \frac{1}{2\sinh \frac{\beta\hbar\omega}{2}}.$$

Observe now that

$$\bar{E} = -\frac{Z'(\beta)}{Z(\beta)}, \qquad \overline{E^2} = \frac{Z''(\beta)}{Z(\beta)}, \qquad (\Delta E)^2 = \overline{E^2} - \bar{E}^2.$$

This yields the claim (7.148) after an elementary computation. □

The Wick trick (source trick). Alternatively, define the modified partition function

$$\mathcal{Z}(\beta, J) := \sum_{n=0}^{\infty} \mathrm{e}^{-E_n(\beta - J)} = \frac{1}{2\sinh \frac{(\beta - J)\omega\hbar}{2}}$$

where J is an additional small real parameter. Then $\mathcal{Z}(\beta, 0) = Z(\beta)$, and

$$\bar{E} = \frac{\mathcal{Z}_J(\beta, 0)}{\mathcal{Z}(\beta, 0)}, \qquad \overline{E^2} = \frac{\mathcal{Z}_{JJ}(\beta, 0)}{\mathcal{Z}(\beta, 0)}.$$

Tricks of this kind frequently appear while computing path integrals in quantum field theory; those tricks are also closely related to the Wick theorem in quantum field theory published in 1950. Therefore, we will briefly speak of the Wick trick. Behind this trick, there is the following general strategy in physics which was introduced by Schwinger: Add some source term to the physical system, and study

the change of the physical system under a change of the source J (see Chap. 14 of Vol. I).

Von Neumann's density operator. Let $H : D(H) \to L_2(\mathbb{R})$ be the self-adjoint Hamiltonian operator of the quantum harmonic oscillator on the real line,

$$H = \frac{P^2}{2m} + \frac{m\omega^2 Q^2}{2}.$$

Let $\varphi_0, \varphi_1, ...$ be the eigensolutions of H with

$$H\varphi_n = E_n\varphi_n, \qquad n = 0, 1, 2, ...$$

For any state $\varphi \in L_2(\mathbb{R})$ and any temperature $T > 0$, define

$$\mathrm{e}^{-\beta H}\varphi := \sum_{n=0}^{\infty} \mathrm{e}^{-\beta E_n}\langle\varphi_n|\varphi\rangle\varphi_n. \tag{7.149}$$

Note that

$$||\mathrm{e}^{-\beta H}\varphi||^2 = \sum_{n=0}^{\infty} |\mathrm{e}^{-\beta E_n}\langle\varphi_n|\varphi\rangle|^2 \leq \sum_{n=0}^{\infty} |\langle\varphi_n|\varphi\rangle|^2 = ||\varphi||^2.$$

Therefore, the operator $\mathrm{e}^{-\beta H} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ is linear and continuous. For the trace, we get

$$\mathrm{tr}\,\mathrm{e}^{-\beta H} = \sum_{n=0}^{\infty}\langle\varphi_n|\mathrm{e}^{-\beta H}\varphi_n\rangle = \sum_{n=0}^{\infty}\mathrm{e}^{-\beta E_n}.$$

This is precisely the partition function Z. Therefore, the operator $\mathrm{e}^{-\beta H}$ is of trace class. In order to pass to the language of physicists, denote the vector φ_n by $|E_n\rangle$. Mnemonically, we write

$$\mathrm{e}^{-\beta H} = \sum_{n=0}^{\infty}\mathrm{e}^{-\beta E_n}|E_n\rangle\langle E_n|.$$

In fact, this implies $\mathrm{e}^{-\beta H}|\varphi\rangle = \sum_{n=0}^{\infty}\mathrm{e}^{-\beta E_n}|E_n\rangle\langle E_n|\varphi\rangle$ which coincides with (7.149). If $\chi_0, \chi_1, ...$ is an arbitrary complete orthonormal system in the Hilbert space $L_2(\mathbb{R})$, then

$$\mathrm{tr}\,\mathrm{e}^{-\beta H} = \sum_{n=0}^{\infty}\langle\chi_n|\mathrm{e}^{-\beta H}\chi_n\rangle = \sum_{n=0}^{\infty}\mathrm{e}^{-\beta E_n}\langle\chi_n|E_n\rangle\langle E_n|\chi_n\rangle.$$

The relation between the propagator $P(t, 0) := \mathrm{e}^{-\mathrm{i}Ht/\hbar}$ and the operator $\mathrm{e}^{-\beta H}$ is given by

$$\mathrm{e}^{-\beta H} = P\left(-\mathrm{i}\beta\hbar, 0\right).$$

Now to the point. The linear bounded operator $\varrho : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ defined by

$$\boxed{\varrho := \frac{\mathrm{e}^{-\beta H}}{\mathrm{tr}\,\mathrm{e}^{-\beta H}}}$$

is called the density operator for our many-particle system of quantum harmonic oscillators on the real line. Explicitly,

$$\varrho = \sum_{n=0}^{\infty} p_n |E_n\rangle\langle E_n|$$

where $p_n = \mathrm{e}^{-\beta E_n}/Z(\beta)$. The real numbers

$$\varrho_{ij} := \langle \chi_i | \varrho \chi_j \rangle, \qquad i,j = 0,1,2,...$$

are called the entries of the density matrix with respect to the complete orthonormal system $\chi_0, \chi_1, ...$ For the mean energy value $\bar{E}$ and the mean energy fluctuation $\Delta\bar{E}$ of a particle, we get

$$\boxed{\bar{E} = \mathrm{tr}(\varrho H), \qquad (\Delta E)^2 = \mathrm{tr}(\varrho(H-\bar{E})^2).}$$

In fact, since $\varrho|E_n\rangle = p_n|E_n\rangle$ for all n,

$$\mathrm{tr}(\varrho H) = \sum_{n=0}^{\infty} \langle E_n|\varrho H|E_n\rangle = \sum_{n=0}^{\infty} p_n E_n \langle E_n|E_n\rangle = \sum_{n=0}^{\infty} p_n E_n = \bar{E}.$$

A similar argument applies to $\Delta\bar{E}$. Using the language of physicists, define[87]

$$\varrho(x,T) := \frac{\langle x|\mathrm{e}^{-\beta H}|x\rangle}{\mathrm{tr}\,\mathrm{e}^{-\beta H}}.$$

Since $\varphi_n(x) = \langle x|E_n\rangle$,

$$\varrho(x,T) = \sum_{n=0} p_n \langle x|E_n\rangle\langle E_n|x\rangle = \sum_{n=0}^{\infty} p_n |\varphi_n(x)|^2.$$

Recall that the function $x \mapsto |\varphi_n(x)|^2$ is the particle density of the nth energy state of the harmonic oscillator. Moreover,

$$\int_{\mathbb{R}} \varrho(x,T)dx = \sum_{n=0}^{\infty} p_n = 1.$$

Therefore, it is reasonable to regard $\varrho(x,T)$ as the (normalized) particle density of the gas at the point x at the temperature T.

Semiclassical quantum statistics and the Dirac calculus (formal approach). We want to explain how the Dirac calculus allows us to formally pass from the density operator ϱ to the semiclassical Gibbs statistics for high temperatures. Let $A : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ be a linear continuous operator of trace class. For a complete orthonormal system $\chi_0, \chi_1, ...$ of the complex Hilbert space $L_2(\mathbb{R})$, we get

$$\boxed{\mathrm{tr}\,A = \sum_{n=0}^{\infty} \langle \chi_n | A\chi_n\rangle.} \tag{7.150}$$

The point is that this number is finite, and it does not depend on the choice of the complete orthonormal system $\chi_0, \chi_1, ...$ The trick of the Dirac calculus is to formally extend the trace formula (7.150) to complete orthonormal systems of generalized eigenfunctions. For example, using the system $\{\langle x|\}_{x\in\mathbb{R}}$, we get

[87] See the formal Dirac calculus on page 596 of Vol. I.

$$\boxed{\operatorname{tr} A = \int_{\mathbb{R}} \langle x|A|x\rangle dx.} \tag{7.151}$$

Applying this formal approach, we are going to show that for high temperatures T, we obtain the following approximative formulas.[88]

(i) Mean value of energy:

$$\boxed{\bar{E} = \int_{\mathbb{R}^2} H(x,p)\varrho(x,p;T)\frac{dxdp}{h}.}$$

(ii) Mean energy fluctuation: $(\Delta\bar{E})^2 = \int_{\mathbb{R}^2}(H(x,p)-\bar{E})^2\varrho(x,p;T)\frac{dxdp}{h}$.

Here, $H(x,p) := \frac{p^2}{2m} + \frac{m\omega^2x^2}{2}$. For the density function in the phase space,

$$\boxed{\varrho(x,p;T) := \frac{\mathrm{e}^{-\beta H(x,p)}}{\int_{\mathbb{R}^2}\mathrm{e}^{-\beta H(x,p)}\frac{dxdp}{h}}.} \tag{7.152}$$

For a given function $A = A(x,p)$, the mean value $\bar{A}$ is defined by

$$\bar{A} = \int_{\mathbb{R}^2} A(x,p)\varrho(x,p;T)\frac{dxdp}{h}.$$

If the function $A = A(x)$ only depends on the position variable x, then

$$\bar{A} = \int_{\mathbb{R}} A(x)\varrho(x,T)dx$$

where we define

$$\varrho(x,T) := \int_{\mathbb{R}} \varrho(x,p;T)\frac{dp}{h}.$$

Let us prove (i) and (ii) above in a formal way. To begin with, observe that $\langle x|P^2|p\rangle = p^2\langle x|p\rangle$ and

$$\langle x|Q^2|p\rangle = \langle Q^2x|p\rangle = x^2\langle x|p\rangle.$$

Hence

$$\langle x|H|p\rangle = \langle x|\frac{P^2}{2m} + \frac{m\omega^2Q^2}{2}|p\rangle = H(x,p)\langle x|p\rangle.$$

Up to terms of order $O(\beta^2)$ as $\beta \to 0$, we get

$$\langle x|\mathrm{e}^{-\beta H}|p\rangle = \langle x|\,(I-\beta H)\,|p\rangle.$$

Hence

$$\langle x|\mathrm{e}^{-\beta H}|p\rangle = (1-\beta H(x,p))\,\langle x|p\rangle = \mathrm{e}^{-\beta H(x,p)}\langle x|p\rangle.$$

For the trace, we obtain $\operatorname{tr}\mathrm{e}^{-\beta H} = \int_{\mathbb{R}}\langle x|\mathrm{e}^{-\beta H}|x\rangle dx$. Using Dirac's completeness relation $\int_{\mathbb{R}}|p\rangle\langle p|\,dp = I$, we obtain

$$\operatorname{tr}\mathrm{e}^{-\beta H} = \int_{\mathbb{R}^2}\langle x|\mathrm{e}^{-\beta H}|p\rangle\langle p|x\rangle dxdp.$$

[88] Note that $dxdp/h$ and $\varrho(x,p;T)$ are dimensionless.

Since $\langle x|p\rangle = \mathrm{e}^{\mathrm{i}px}/\sqrt{h}$ and $\langle p|x\rangle = \langle x|p\rangle^{\dagger}$, we get

$$\operatorname{tr}\mathrm{e}^{-\beta H} = \int_{\mathbb{R}^2} \mathrm{e}^{-\beta H(x,p)}\,\frac{dxdp}{h}.$$

Summarizing, from $\varrho = \mathrm{e}^{-\beta H}/\operatorname{tr}\mathrm{e}^{-\beta H}$ it follows that

$$\langle x|\varrho|p\rangle = \varrho(x,p;T)\langle x|p\rangle$$

where $\varrho(x,p;T)$ is defined by (7.152). Finally,

$$\bar{E} = \operatorname{tr}(\varrho H) = \int_{\mathbb{R}} \langle x|\varrho H|x\rangle dx = \int_{\mathbb{R}^2} \langle x|\varrho|p\rangle\langle p|H|x\rangle dxdp.$$

Hence $\bar{E} = \int_{\mathbb{R}^2} \varrho(x,p;T)H(x,p)\frac{dxdp}{h}$. Similarly, we argue for $\Delta\bar{E}$.

Rigorous justification. To begin with, observe that the formal Dirac calculus tells us that

$$\langle x|\mathrm{e}^{-\beta H}|x\rangle = \sum_{n=0}^{\infty} \mathrm{e}^{-\beta E_n}\langle x|E_n\rangle\langle E_n|x\rangle = \sum_{n=0}^{\infty} \mathrm{e}^{-\beta E_n}|\langle x|E_n\rangle|^2,$$

and $\operatorname{tr}\mathrm{e}^{-\beta/kT} = \int_{\mathbb{R}}\langle x|\mathrm{e}^{-\beta H}|x\rangle dx$. In order to obtain a rigorous formulation, let us write this as

$$\boxed{\operatorname{tr}\mathrm{e}^{-\beta H} = \lim_{m\to\infty}\int_{\mathbb{R}}\sum_{n=0}^{m}\mathrm{e}^{-\beta E_n}|\varphi_n(x)|^2 dx.} \tag{7.153}$$

Proposition 7.42 *The trace formula* (7.153) *holds. Explicitly, the trace* $\operatorname{tr}\, e^{-\beta H}$ *is the partition function of the quantum harmonic oscillator.*

Proof. The trace class operator $\mathrm{e}^{-\beta H}$ has the complete orthonormal system of eigenvectors $\varphi_0, \varphi_1, \ldots$ with $\mathrm{e}^{-\beta H}\varphi_n = \mathrm{e}^{-\beta E_n}\varphi_n$ for all n. The trace is the sum of the eigenvalues. Hence

$$\operatorname{tr}\mathrm{e}^{-\beta H} = \sum_{n=0}^{\infty}\mathrm{e}^{-\beta E_n}.$$

On the other hand, it follows from $||\varphi_n||^2 = \int_{\mathbb{R}}|\varphi_n(x)|^2 dx = 1$ that

$$\lim_{m\to\infty}\int_{\mathbb{R}}\sum_{n=0}^{m}\mathrm{e}^{-\beta E_n}|\varphi_n(x)|^2 dx = \lim_{m\to\infty}\sum_{n=0}^{m}\mathrm{e}^{-\beta E_n}.$$

□

Introduce the kernel to the operator $\mathrm{e}^{-\beta H}$ by setting

$$\mathcal{P}(x,y;T) = \langle x|\mathrm{e}^{-\beta H}|y\rangle = \sum_{n=0}^{\infty}\mathrm{e}^{-\beta E_n}\langle x|E_n\rangle\langle E_n|y\rangle,$$

in the language of the Dirac calculus. This means that we define

$$\boxed{\mathcal{P}(x,y;T) := \sum_{n=0}^{\infty}\mathrm{e}^{-\beta E_n}\varphi_n(x)\varphi_n(y)^{\dagger}.}$$

Recall that $\beta := 1/kT$ and $x_0 := \sqrt{\hbar/m\omega}$. The Mehler formula (7.143) tells us the following.

Proposition 7.43 *For all positions $x, y \in \mathbb{R}$ and all temperatures $T > 0$, we get*

$$\mathcal{P}(x, y; T) = \frac{1}{x_0\sqrt{2\pi \sinh \beta\hbar\omega}} \exp\left\{-\frac{(x^2+y^2)\cosh \beta\hbar\omega - 2xy}{2x_0^2 \sinh \beta\hbar\omega}\right\}.$$

Moreover, for the partition function of the quantum harmonic oscillator, we have the trace formula

$$\int_{\mathbb{R}} \mathcal{P}(x, x; T)dx = \sum_{n=0}^{\infty} e^{-E_n/kT} = \operatorname{tr} e^{-H/kT}.$$

For the density function $\varrho(x, T) := \langle x|\varrho|x\rangle$, this implies

$$\varrho(x, T) = \frac{\mathcal{P}(x, x; T)}{Z(\beta)} = \frac{1}{x_0}\sqrt{\frac{\tanh \frac{\beta\omega\hbar}{2}}{\pi}} \exp\left\{\frac{x^2(1-\cosh \beta\hbar\omega)}{x_0^2 \sinh \beta\hbar\omega}\right\}.$$

Von Neumann's equation of motion for general density operators. We are given real numbers $p_0, p_1, ...$ with $0 \le p_n \le 1$ and $p_0 + p_1 + ... = 1$. Choose a complete orthonormal system $\langle 0|, \langle 1|, ...$ in the Hilbert space $L_2(\mathbb{R})$. Define

$$\varrho_0 := \sum_{n=0}^{\infty} p_n |n\rangle\langle n|.$$

Moreover, for each time $t \in \mathbb{R}$, we define

$$\boxed{\varrho(t) := \mathrm{e}^{\mathrm{i}Ht/\hbar}\varrho_0\mathrm{e}^{-\mathrm{i}Ht/\hbar}.}$$

This is the equation of motion for an arbitrary density operator in the Hilbert space $L_2(\mathbb{R})$. This equation corresponds to the time-dependence of observables in the Heisenberg picture. For an observable $A : D(A) \to L_2(\mathbb{R})$, we define the mean value

$$\bar{A}(t) := \operatorname{tr}(\varrho(t)A), \qquad t \in \mathbb{R}$$

if this trace exists. In the special case where $\varrho_0 = \sum_{n=0}^{\infty} p_n |E_n\rangle\langle E_n|$, we obtain $\varrho(t) = \varrho_0$ for all times $t \in \mathbb{R}$.

7.7 The Feynman Path Integral

> The history of mathematics shows that every well-working formal calculus used in physics can be rigorously justified once a day, by finding the appropriate rigorous tools.
>
> Folklore

7.7.1 The Basic Strategy

In Chap. 7 of Vol. I, we studied discrete path integrals in a rigorous setting for N degrees of freedom. In this section, we will study the limit $N \to \infty$. Our plan is the following one:

(i) We start with the definition of the Feynman path integral (7.156) below as a limit in position space, where $N \to \infty$.
(ii) We rigorously show that this limit exists (in a generalized sense) in the two special cases of
- the free quantum particle on the real line (Sect. 7.7.3) and
- the harmonic oscillator (Sect. 7.7.4).

It turns out that these limits coincide with the propagator kernel introduced in Sects. 7.6.4 and 7.6.7 by using the rigorous method of Fourier analysis combined with analytic continuation.
(iii) This brings us to the formulation of the *propagator hypothesis* saying that the Feynman path integral always represents the Feynman propagator kernel of the Schrödinger equation. We motivate this propagator hypothesis by using the Dirac calculus in a formal sense (Sect. 7.7.6).
(iv) In Sect. 7.8, we will rigorously study finite-dimensional Gaussian integrals with N degrees of freedom. Motivated by this, in Sect. 7.9 we will give the definition of normalized infinite-dimensional Gaussian integrals by using the spectral theory of quadratic forms and the determinant of infinite-dimensional operators based on the analytic continuation of the corresponding zeta function.
(v) For the free quantum particle and the harmonic oscillator, we rigorously show that the normalized infinite-dimensional Gaussian integral represents the Feynman propagator kernel, up to a normalization factor (Sects. 7.9.3 and 7.9.4).
(vi) This brings us to the *spectral hypothesis* saying that the Feynman path integral can be computed by means of infinite-dimensional Gaussian integrals, up to a normalization factor. This is the basic method successfully used by physicists in quantum field theory. Fortunately enough, the normalization factor does not play any role, as a rule, since it drops out by considering quotients of path integrals.

The following remarks are in order:

- The concrete calculations performed by physicists show that the propagator hypothesis above is right in quantum mechanics.[89] Many concrete examples can be found in the following two standard references:

  C. Grosche and F. Steiner, Handbook of Feynman Path Integrals, Springer, Berlin, 1998 (950 references).

  H. Kleinert, Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics, World Scientific, River Edge, New York, 2004.
- In Sect. 7.11, we will study the rigorous Wiener path integral for Brownian motion together with Cameron's no-go theorem for the Feynman path integral.
- In Sect. 7.12, we will investigate the relation between the Weyl calculus and the Feynman path integral (method of pseudo-differential operators).

Detailed hints to both the mathematical and physical literature concerning the Feynman path integral can be found in Sect. 7.22 on page 667.

The creation of a comprehensive rigorous mathematical theory for Feynman path integrals (also called functional integrals) in quantum field theory is a challenge for the mathematics of the future.

[89] However, observe the following peculiarity: If caustics appear in classical mechanics, then one has to handle carefully the Maslov indices in quantum mechanics, as in the case of the harmonic oscillator in Sect. 7.6.7.

7.7.2 The Basic Definition

Let us consider the Schrödinger equation

$$\mathrm{i}\hbar\psi_t(x,t) = -\frac{\hbar^2}{2m}\psi_{xx}(x,t) + U(x)\psi(x,t), \qquad x \in \mathbb{R},\ t > s \tag{7.154}$$

together with the corresponding classical action

$$S[q] := \int_s^t \left\{ \tfrac{1}{2} m\dot{q}(\tau)^2 - U\big(q(\tau)\big) \right\} d\tau. \tag{7.155}$$

We assume that the potential $U : \mathbb{R} \to \mathbb{R}$ is smooth. Choose $N = 1, 2, \ldots$, and divide the time interval $[s,t]$ into the subintervals $t_0 = s < t_1 < \ldots < t_{N-1} < t_N = t$, where

$$t_j := s + j\Delta t, \quad j = 0, 1, \ldots, N, \quad \Delta t := \frac{t-s}{N}.$$

Fix the positions $x, y \in \mathbb{R}$ on the real line. Let the symbol $C\{s,t\}$ denote the set of all continuous functions $q : [s,t] \to \mathbb{R}$ with the boundary condition

$$q(s) := x, \qquad q(t) := y.$$

For each path $q \in C\{s,t\}$, we set $q_j := q(t_j)$, where $j = 0, 1, \ldots, N$. By definition, the discrete action of this path reads as

$$\boxed{S_N := \sum_{n=0}^{N-1} \left\{ \frac{m}{2} \left(\frac{q_{n+1} - q_n}{\Delta t} \right)^2 - U(q_n) \right\} \Delta t.}$$

Finally, let us introduce the characteristic length $l := \sqrt{\frac{2\pi\hbar \mathrm{i}\Delta t}{m}}$. Here, the square root is to be understood in the sense of the principal value.

Basic definition. Our definition of the Feynman path integral reads as

$$\boxed{\int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q := \lim_{N\to\infty} \frac{1}{l} \int_{\mathbb{R}^{N-1}} \mathrm{e}^{\mathrm{i}S_N/\hbar}\, \frac{dq_1}{l} \cdots \frac{dq_{N-1}}{l}.} \tag{7.156}$$

Since the boundary values $q_0 = y$ and $q_N = x$ are fixed, the integrals on the right-hand side of (7.156) are well-defined $(N-1)$-dimensional integrals of the real variables $q_1, \ldots, q_{N-1}$. We assume that the limit $N \to \infty$ exists.

Intuitive interpretation. We regard $\int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar} \mathcal{D}q$ as an integral over the paths in the space $C\{s,t\}$. The definition (7.156) will be motivated in great detail in Sect. 7.7.6 on page 555. The path integral depends on x, t, y, s. We write

$$K(x,t;y,s) = \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q.$$

In the following two sections, we will show that, for the free quantum particle and the harmonic oscillator on the real line, the function K is nothing else than the Feynman propagator kernel $\mathcal{K}$.

7.7.3 Application to the Free Quantum Particle

Let us consider the Schrödinger equation (7.154) above with vanishing potential, $U(x) \equiv 0$. The corresponding classical action reads as

$$S[q] := \int_s^t \tfrac{1}{2} m \dot{q}(\tau)^2 d\tau.$$

In Sect. 7.5.1, we have computed the corresponding Feynman propagator kernel

$$\mathcal{K}(x,t;y,s) = \sqrt{\frac{m}{2\pi\hbar \mathrm{i}(t-s)}}\ \mathrm{e}^{\mathrm{i}m(x-y)^2/2\hbar(t-s)} \tag{7.157}$$

for a freely moving quantum particle on the real line (see Theorem 7.16 on page 488).

Proposition 7.44 *For the free quantum particle, the Feynman path integral coincides with the Feynman propagator kernel, that is, we have*

$$\mathcal{K}(x,t;y,s) = \int_{C\{s,t\}} e^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q \tag{7.158}$$

for all positions $x, y \in \mathbb{R}$ and all times $t > s$.

In the following proof, we will use a slight modification (7.160) of the original definition (7.156) of the path integral. In terms of physics, we separate the classical contribution from the quantum fluctuations. In terms of mathematics, we pass to homogeneous boundary conditions.

Proof. To simplify notation, set $\hbar := 1$ and $s := 0$.

(I) The classical trajectory. The action of a classical free particle of mass m on the real line is given by

$$S[q] := \int_0^t \tfrac{1}{2} m \dot{q}(\tau)^2\, d\tau.$$

Recall that the boundary-value problem

$$m\ddot{q}(\tau) = 0, \quad 0 < \tau < t, \quad q(0) = y,\ q(t) = x$$

corresponds to the motion of the particle with given endpoints. The unique solution is $q_{\mathrm{class}}(\tau) = y + \frac{\tau}{t}(x-y)$ with the classical action

$$S[q_{\mathrm{class}}] = \int_0^t \tfrac{1}{2} m \dot{q}_{\mathrm{class}}(\tau)^2 d\tau = \frac{m(x-y)^2}{2t}.$$

(II) Decomposition of trajectories. In order to study perturbations of the classical trajectory, we consider the trajectories

$$q(\tau) = q_{\mathrm{class}}(\tau) + r(\tau), \qquad \tau \in [0,t]$$

where $r \in C_0^2[0,t]$, that is, the function $r : [0,t] \to \mathbb{R}$ is twice continuously differentiable and satisfies the boundary condition $r(0) = r(t) = 0$. Then

$$S[q] = S[q_{\mathrm{class}}] + S[r]. \tag{7.159}$$

In fact, integration by parts yields

$$\int_0^t \dot{q}_{\text{class}}(\tau)\dot{r}(\tau)d\tau = -\int_0^t \ddot{q}_{\text{class}}(\tau)r(\tau)d\tau = 0,$$

since q_{class} satisfies the classical equation of motion, $m\ddot{q}_{\text{class}}(\tau) = 0$. Motivated by (7.159), let us slightly modify the definition (7.156) of the path integral by setting

$$\boxed{\int_{C\{0,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q := \mathrm{e}^{\mathrm{i}S[q_{\text{class}}]/\hbar} \lim_{N\to\infty} \frac{1}{l} \int_{\mathbb{R}^{N-1}} \mathrm{e}^{\mathrm{i}S_N/\hbar}\, \frac{dr_1}{l} \cdots \frac{dr_{N-1}}{l}} \tag{7.160}$$

with the discrete action

$$S_N := \sum_{n=0}^{N-1} \left\{ \frac{m}{2} \left(\frac{r_{n+1} - r_n}{\Delta t} \right)^2 \right\} \Delta t$$

and the boundary values $r_0 = r_N := 0$.

(III) The generalized Gaussian integral. Let $a > 0$ or $a < 0$ and let $\beta \in \mathbb{R}$. According to (7.183) on page 561, we have the crucial Gaussian integral formula

$$\boxed{\int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}\mathrm{i}ap^2}\, \mathrm{e}^{\mathrm{i}\beta p}\, \frac{dp}{\sqrt{2\pi}} := \frac{\mathrm{e}^{-\beta^2/2\mathrm{i}a}}{\sqrt{\mathrm{i}a}}.} \tag{7.161}$$

Here, the square root is to be understood as principal value. As we will discuss in Sect. 7.8, this definition has to be understood in the sense of analytic continuation.

(IV) Computation of the integrals from (7.160). Let us first integrate over the variable r_1. This yields the integral

$$\frac{1}{l^2} \int_{\mathbb{R}} \exp\left(\frac{\mathrm{i}m}{2\Delta t} \left((r_2 - r_1)^2 + (r_1 - r_0)^2 \right) \right) dr_1$$

which is equal to

$$\frac{1}{l^2} \exp\left(\frac{\mathrm{i}mr_2^2}{4\Delta t} \right) \int_{\mathbb{R}} \exp\left\{ \frac{\mathrm{i}m}{\Delta t} \left(r_1 - \frac{r_2}{2} \right)^2 \right\} dr_1 = \sqrt{\frac{m}{2\pi\mathrm{i}(2\Delta t)}} \exp\left(\frac{\mathrm{i}mr_2^2}{4\Delta t} \right).$$

Similarly, by induction, integrating over $r_1 \cdots r_n$ we get

$$\sqrt{\frac{m}{2\pi\mathrm{i}(n+1)\Delta t}}\, \exp\left(\frac{\mathrm{i}mr_{n+1}^2}{2(n+1)\Delta t} \right).$$

Choosing $n = N - 1$ and observing that $r_0 = r_N = 0$, we obtain

$$\sqrt{\frac{m}{2\pi\mathrm{i}N\Delta t}} = \sqrt{\frac{m}{2\pi\mathrm{i}t}}.$$

This expression does not depend on N. Thus, the limit $N \to \infty$ yields the same value. □

7.7.4 Application to the Harmonic Oscillator

> The path integral for the harmonic oscillator is closely related to the difference method for the classical harmonic oscillator in numerical analysis.
> Folklore

Consider the Schrödinger equation (7.154) above for the harmonic oscillator with mass m and angular frequency $\omega > 0$. This corresponds to the potential $U(x) = \frac{m\omega^2}{2}x^2$. The classical action is given by

$$S[q] = \int_s^t \tfrac{1}{2}m\dot{q}(\tau)^2 - \tfrac{1}{2}m\omega^2 q(\tau)^2 \, d\tau. \tag{7.162}$$

In Sect. 7.6.7 on page 537, we have computed the corresponding Feynman propagator kernel

$$\mathcal{K}(x,t;y,s) = \frac{1}{x_0\sqrt{2\pi \mathrm{i}\sin\omega(t-s)}} \exp\left(\mathrm{i}\frac{(x^2+y^2)\cos\omega(t-s) - 2xy}{2x_0^2\sin\omega(t-s)}\right)$$

for the harmonic oscillator. Here, we restrict ourselves to the first critical time interval $s < t < s + t_{1,\mathrm{crit}}$, where $t_{1,\mathrm{crit}} = \frac{\pi}{\omega}$. Furthermore, $x_0 = \sqrt{\frac{\hbar}{m\omega}}$.

Proposition 7.45 *For the quantized harmonic oscillator, the Feynman path integral coincides with the Feynman propagator kernel on the first critical time interval, that is, for all positions $x, y \in \mathbb{R}$, and all times $t \in]s, s + t_{1,\mathrm{crit}}[$, we have*

$$\mathcal{K}(x,t;y,s) = \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar} \, \mathcal{D}q. \tag{7.163}$$

This proposition is to be understood in a generalized sense which will be made precise in the following proof. First the Gaussian integrals have to be understood in a generalized sense by using analytic continuation. Secondly the limit $N \to \infty$ from (7.156) does not exist in the classical sense. Therefore, we will use a summation method.

Proof. (I) The classical trajectory. The boundary-value problem

$$\ddot{q}(\tau) + \omega^2 q(\tau) = 0, \quad s < \tau < t, \quad q(s) = y,\ q(t) = x \tag{7.164}$$

has the unique solution $q_{\mathrm{class}}(\tau) = y\cos\omega(\tau - s) + \big(x - y\cos\omega(\tau - s)\big)\,\frac{\sin\omega(\tau-s)}{\sin\omega(t-s)}$. This is a trajectory of the classical harmonic oscillator with the action

$$S[q_{\mathrm{class}}] = \hbar \cdot \frac{(x^2+y^2)\cos\omega(t-s) - 2xy}{2x_0^2\sin\omega(t-s))} \ .$$

(II) Decomposition of trajectories. Now we consider perturbations of the classical trajectory, by setting

$$q(\tau) := q_{\mathrm{class}}(\tau) + r(\tau)$$

where $r \in C_0^2[s,t]$. By definition, this notation means that the function $r : [s,t] \to \mathbb{R}$ is twice continuously differentiable and satisfies the following boundary condition $r(s) = r(t) = 0$. We have

$$S[q] = S[q_{\mathrm{class}}] + S[r] \qquad \text{for all} \quad r \in C_0^2[s,t]. \tag{7.165}$$

In fact, integration by parts yields

$$\int_0^t \dot{q}_{\text{class}}\dot{r} - \omega^2 q_{\text{class}} r \, d\tau = -\int_0^t (\ddot{q}_{\text{class}} + \omega^2 q_{\text{class}}) r \, d\tau = 0,$$

since q_{class} satisfies the classical equation of motion (7.164). Motivated by (7.165), let us slightly modify the definition (7.156) of the path integral by setting

$$\boxed{\int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q := \mathrm{e}^{\mathrm{i}S[q_{\text{class}}]/\hbar} \lim_{N\to\infty} \frac{1}{l} \int_{\mathbb{R}^{N-1}} \mathrm{e}^{\mathrm{i}S_N/\hbar}\, \frac{dr_1}{l} \cdots \frac{dr_{N-1}}{l}}$$

with the discrete action

$$S_N := \sum_{n=0}^{N-1} \left\{ \frac{m}{2} \left(\frac{r_{n+1} - r_n}{\Delta t} \right)^2 - \frac{m\omega^2}{2} r_n^2 \right\} \Delta t \tag{7.166}$$

and the boundary values $r_0 = r_N := 0$.

(III) The discrete action. To simplify notation, we set $s := 0$. The function S_N is a quadratic form. Explicitly,

$$\frac{\mathrm{i}S_N}{\hbar} = \frac{\mathrm{i}m\Delta t}{2\hbar} \cdot \langle r | A_N r \rangle. \tag{7.167}$$

Here, we set $\langle r|A_N r\rangle := r^d A_N r$ with the symmetric matrix

$$A_N := \frac{1}{(\Delta t)^2} \begin{pmatrix} a & -1 & 0 & \dots & 0 & 0 \\ -1 & a & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & a & -1 \\ 0 & 0 & 0 & \dots & -1 & a \end{pmatrix}$$

and $r^d := (r_1, \dots, r_{N-1})$. Furthermore, $a := 2 - (\omega\Delta t)^2$.

(IV) The discrete eigenvalue problem. The matrix equation $A_N r = \lambda r$ reads as

$$-\frac{r_{j+1} - 2r_j + r_{j-1}}{(\Delta t)^2} - \omega^2 r_j = \lambda_j r_j, \qquad r_0 = r_N = 0, \tag{7.168}$$

where $j = 1, \dots, N-1$. This equation has the eigensolutions

$$\lambda_n = \frac{n^2\pi^2}{t^2} \left(\frac{\sin\alpha(n)}{\alpha(n)} \right)^2 - \omega^2, \qquad n = 1, \dots, N-1,$$
$$r_n^d = \left(\sin\frac{n\pi\Delta t}{t}, \sin\frac{2n\pi\Delta t}{t}, \dots, \sin\frac{(N-1)n\pi\Delta t}{t} \right),$$

where $\alpha(n) := \frac{n\pi\Delta t}{2t}$. Using the limit $N \to +\infty$ (i.e., $\Delta t \to 0$), these eigensolutions go to the eigensolutions $\lambda_n = \frac{n^2\pi^2}{t^2} - \omega^2$ and $q(\tau) = \sin\frac{n\pi\tau}{t}$ of the boundary-eigenvalue

$$-\ddot{r}(\tau) - \omega^2 r(\tau) = \lambda r(\tau), \quad 0 < \tau < t, \quad r(0) = r(t) = 0$$

for the classical harmonic oscillator.

(IV) The Gaussian integral. By (7.167), we get

$$\int_{\mathbb{R}^{N-1}} \mathrm{e}^{\mathrm{i}S_N/\hbar} \frac{dr_1}{l} \cdots \frac{dr_{N-1}}{l} = (\sqrt{\gamma})^{N-1} \int_{\mathbb{R}^{N-1}} \mathrm{e}^{-\frac{1}{2}\gamma\langle r|A_N r\rangle} \frac{dr_1}{\sqrt{2\pi}} \cdots \frac{dr_{N-1}}{\sqrt{2\pi}},$$

where $\gamma := \frac{m\Delta t}{\hbar \mathrm{i}}$ and $l = \sqrt{\frac{2\pi \mathrm{i}\hbar\Delta t}{m}}$. By the key formula (7.190) for Gaussian integrals on page 564 (based on analytic continuation), we obtain

$$\frac{1}{l} \int_{\mathbb{R}^{N-1}} \mathrm{e}^{\mathrm{i}S_N/\hbar} \frac{dr_1}{l} \cdots \frac{dr_{N-1}}{l} = \frac{1}{l\sqrt{\det A_N}}.$$

(V) The problem of convergence. It remains to compute the limit

$$\lim_{N\to\infty} \frac{1}{l\sqrt{\det A_N}}.$$

Unfortunately, this limit does not exist in the classical sense. This follows immediately from

$$\det A_N = \lambda_1\lambda_2 \cdots \lambda_{N-1} = \prod_{n=1}^{N-1} \left\{ \frac{n^2\pi^2}{t^2} \left(\frac{\sin \alpha(n)}{\alpha(n)} \right)^2 - \omega^2 \right\}$$

and $\frac{1}{l} = \sqrt{\frac{m}{2\pi\hbar \mathrm{i}\Delta t}} = \sqrt{N} \cdot \sqrt{\frac{m}{2\pi\hbar \mathrm{i} t}}$.

(VI) Summation method (generalized limit). We set $a(n\Delta t) := \Delta t \cdot \det A_n$ for the indices $n = 1, 2, \ldots, N$. Recall that $N\Delta t = t$. In addition let $a(0) := \Delta t$. By the definition of the matrix A_N, the Laplace expansion for determinants tells us that

$$\frac{a((n+1)\Delta t) - 2a(n\Delta t) + a((n-1)\Delta t)}{(\Delta t)^2} + \omega^2 a(n\Delta t) = 0$$

for all $n = 1, 2, \ldots, N-1$. Letting $\Delta t \to 0$, we obtain the ordinary differential equation

$$\ddot{a}(\tau) + \omega^2 a(\tau) = 0, \qquad 0 < \tau < t$$

with the initial condition $a(0) = 0$ and $\dot{a}(0) = 1$.[90] This initial-value problem has the unique solution

$$a(\tau) = \frac{\sin \omega\tau}{\omega}.$$

This motivates the definition

$$\lim_{N\to\infty} \Delta t \cdot \det A_N := \frac{\sin \omega t}{\omega},$$

as generalized limit. Therefore, we get

$$\lim_{N\to\infty} \frac{1}{l\sqrt{\det A_N}} = \sqrt{\frac{m}{2\pi\hbar \mathrm{i}}} \quad \lim_{N\to\infty} \frac{1}{\sqrt{\Delta t \cdot \det A_N}} = \sqrt{\frac{m\omega}{2\pi\hbar \mathrm{i} \sin \omega t}}.$$

□

The proof of Prop. 7.45 shows that the computation of the Feynman path integral for the harmonic oscillator is closely related to the eigenvalues of the corresponding classical boundary-value problem. Indeed, this is a crucial method for computing Feynman path integrals. We will study this in Sect. 7.9 on page 570 by means of the zeta-function regularization for infinite-dimensional Gaussian integrals.

[90] In fact, $a(0) = \lim_{\Delta t\to 0} \Delta t = 0$ and

$$\dot{a}(0) = \lim_{\Delta t\to 0} \frac{a(\Delta t) - a(0)}{\Delta t} = \lim_{\Delta t\to 0} A_1 - 1 = 2 - 1 = 1.$$

7.7.5 The Propagator Hypothesis

Motivated by Props. 7.44 and 7.45, let us formulate the following so-called propagator hypothesis:

(H) *For the Schrödinger equation* (7.154) *on the real line, the Feynman propagator kernel is given by the Feynman path integral, that is,*

$$\mathcal{K}(x,t;y,s) = \int_{C\{s,t\}} e^{\mathrm{i}mS[q]/\hbar}\, \mathcal{D}q.$$

Here, $S[q]$ is the classical action given by (7.155) *on page* 549.

7.7.6 Motivation of Feynman's Path Integral

It is our goal to motivate the propagator hypothesis (H) by using the formal Dirac calculus.

The classical Liouville measure in phase space. Consider a gas on the real line at high temperature $T > 0$. Let x and p denote the position and the momentum of a gas particle, respectively. In semi-classical statistical physics, the mean value $\bar{A}$ of a physical quantity $A = A(x,p)$ is given by

$$\bar{A} = \int_{\mathbb{R}} A(x,p)\varrho(x,p;T)d\mu(x,p).$$

Here, $\varrho = \varrho(x,p;T)$ denotes the density function from (7.152) on page 545. Furthermore, $d\mu := dxdp/h$ denotes the Liouville measure. This means that the Liouville measure $\mu(\Omega)$ of a compact subset Ω of the (x,p)-phase space is given by

$$\mu(\Omega) = \int_{\Omega} d\mu = \int_{\Omega} \frac{dxdp}{h}.$$

If the function $A = A(x)$ does not depend on the momentum, then we separately integrate with respect to the variable p. This yields

$$\bar{A} = \int_{\mathbb{R}} A(x)\varrho(x;T)dx$$

with $\varrho(x,T) := \int_{\mathbb{R}} \varrho(x,p;T)\frac{dp}{h}$. Note that the appearance of the Planck constant h as denominator guarantees that the Liouville measure $dxdp/h$ is dimensionless. We now want to show that the formal Feynman path integral is nothing else than an integral with respect to a formal infinite-dimensional Liouville measure. Alternatively, the Feynman path integral can also be viewed as a modified infinite-dimensional Gaussian integral.

The path integral in the phase space. Consider the motion $x = q(t)$ of a classical particle with mass m on the real line. For the momentum, $p(t) = m\dot{q}(t)$. The Hamiltonian function reads as

$$\mathcal{H}(q,p) := \frac{p^2}{2m} + U(q), \qquad q,p \in \mathbb{R}$$

with the potential U. The action along a trajectory during the time interval $[s,t]$ is given by

$$\boxed{S[q,p] := \int_s^t \frac{p(\tau)^2}{2m} - U(q(\tau))\, d\tau.} \tag{7.169}$$

Here, $p(\tau)^2/2m$ is the kinetic energy and $U(q(\tau))$ is the potential energy of the classical particle at time τ. Equivalently,

$$S[q,p] := \int_s^t p(\tau)\dot{q}(\tau) - \mathcal{H}(q(\tau),p(\tau))\, d\tau.$$

We now pass to the Schrödinger equation for the corresponding quantum particle on the real line,

$$\mathrm{i}\hbar\psi_t(x,t) = H\psi(x,t), \tag{7.170}$$

with the Hamiltonian operator $H = \frac{P^2}{2m} + U(Q)$. Recall from (7.88) on page 491 that the initial-value problem for the Schrödinger equation (7.170) has the solution

$$\boxed{\psi(x,t) = \int_{\mathbb{R}} \mathcal{K}(x,t;y,s)\psi_0(y)dy, \qquad t > s, \quad x \in \mathbb{R}}$$

with $\psi(x,s) = \psi_0(x)$ for all positions $x \in \mathbb{R}$ at the initial time s. The kernel $\mathcal{K}$ has the physical dimension of $[\text{length}]^{-1}$. In the elegant formal language of the Dirac calculus,

$$\mathcal{K}(x,t;y,s) = \langle x|\mathrm{e}^{-\mathrm{i}H(t-s)/\hbar}|y\rangle.$$

Our goal is to motivate *Feynman's magic formula*

$$\boxed{\mathcal{K}(x,t;y,s) = \int_{\mathcal{C}\{s,t\}} \mathrm{e}^{\mathrm{i}S[q,p]/\hbar}\ \mathcal{D}q\mathcal{D}p,} \tag{7.171}$$

which tells us that the propagator kernel $\mathcal{K}$ can be represented by a path integral. Here, we integrate over the space $\mathcal{C}\{s,t\}$ of all continuous paths $q,p : [s,t] \to \mathbb{R}$ with

$$q(s) = y, \qquad q(t) = x.$$

That is, we fix the initial time s, the initial point y, the final time t, and the final point x. Note that both the initial value $p(s)$ and the final value $p(t)$ of the momentum variable are unconstrained. Moreover, we use the classical action

$$S[q,p] := \int_s^t p(\tau)\dot{q}(\tau) - \mathcal{H}(q(\tau),p(\tau))\, d\tau$$

along the path $q = q(\tau), p = p(\tau),\ s \le \tau \le t$. The symbol $\mathcal{D}[q,p]$ represents a formal infinite-dimensional Liouville measure on the space $\mathcal{C}[s,t]$ of curves in the phase space. Formally,

$$\mathcal{D}[q,p] := \frac{dp(s)}{h} \prod_{s<\tau\le t} \frac{dq(\tau)dp(\tau)}{h}.$$

Since $dq(\tau)dp(\tau)/h$ is dimensionless, both the measure $\mathcal{D}[q,p]$ and the kernel from (7.171) have the same physical dimension of $[\text{length}]^{-1}$, as expected. The motivation given below will show that the magic formula (7.171) stands for the following formal limit

$$\boxed{\mathcal{K}(x,t;y,s) = \lim_{N\to\infty} \int_{\mathbb{R}^{2N-1}} \mathrm{e}^{\mathrm{i}S_N/\hbar}\, \frac{dp_0}{h} \prod_{n=1}^{N-1} \frac{dq_n dp_n}{h}} \tag{7.172}$$

along with the discrete action

$$S_N := \sum_{n=0}^{N-1} \Big(p_n\, \frac{q_{n+1}-q_n}{\Delta t} - \mathcal{H}(q_n,p_n) \Big)\, \Delta t.$$

Here, $q_0 := y$ and $q_N := x$.

Applying the Dirac calculus. We want to motivate formula (7.172). To simplify notation, set $\hbar = 1$. Then $h = 2\pi$. Let us decompose the time interval $[s,t]$ into N pieces of equal length by setting

$$s = t_0 < t_1 < \ldots < t_{N-1} < t_N = t$$

along with $t_n := s + n\Delta t$ and $\Delta t := (t-s)/N$. Recall the propagator kernel formula: $\mathcal{K}(x,t;y,s) := \langle x|\mathrm{e}^{-\mathrm{i}NH\Delta t}|y\rangle$.

(i) Causality and the product property of the propagator kernel: For all intermediate times τ with $s \le \tau \le t$, we get the following product formula

$$\boxed{\mathcal{K}(x,t;y,s) = \int_{\mathbb{R}} \mathcal{K}(x,t;q,\tau)\mathcal{K}(q,\tau;y,s)dq.} \tag{7.173}$$

In fact, by the addition theorem for the exponential function,

$$\mathrm{e}^{-\mathrm{i}H(t-s)} = \mathrm{e}^{-\mathrm{i}H(t-\tau)}\mathrm{e}^{-\mathrm{i}H(\tau-s)}.$$

Using the completeness relation $\int_{\mathbb{R}} |q\rangle\langle q|\, dq = I$, we obtain

$$\langle x|\mathrm{e}^{-\mathrm{i}H(t-s)}|y\rangle = \int_{\mathbb{R}} \langle x|\mathrm{e}^{-\mathrm{i}H(t-\tau)}|q\rangle\langle q|\mathrm{e}^{-\mathrm{i}H(\tau-s)}|y\rangle dq$$

which proves (7.173). From the physical point of view, the product formula (7.173) reflects nothing other than causality (see page 482).

(ii) The propagator kernel for small time intervals: We want to show that the propagator kernel $\mathcal{K}$ for the small time interval $[s, s+\Delta t]$ can be approximately represented by the following simple key formula

$$\boxed{\mathcal{K}(x,s+\Delta t;y,s) = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}\mathcal{H}(y,p)\Delta t}\, \mathrm{e}^{\mathrm{i}p(x-y)}\, \frac{dp}{2\pi},} \tag{7.174}$$

up to terms of order $(\Delta t)^2$. To get this, note that the following is true, up to terms of order $(\Delta t)^2$. By Taylor expansion,

$$\mathrm{e}^{-\mathrm{i}H\Delta t} = I - \mathrm{i}H\Delta t.$$

Recall that $H = \frac{P^2}{2m} + \frac{m\omega^2 Q^2}{2}$. For the position operator, $Q|y\rangle = y|y\rangle$. Hence, by the completeness relation $\int_{\mathbb{R}} |p\rangle\langle p|\, dp = I$, we get

$$\langle x|Q^2|y\rangle = y^2\langle x|y\rangle = y^2 \int_{\mathbb{R}} \langle x|p\rangle\langle p|y\rangle dp.$$

Since $\langle x|p\rangle = \frac{\mathrm{e}^{\mathrm{i}xp}}{\sqrt{2\pi}}$, we obtain

$$\langle x|Q^2|y\rangle = \int_{\mathbb{R}} y^2 \mathrm{e}^{\mathrm{i}xp}\mathrm{e}^{-\mathrm{i}yp}\frac{dp}{2\pi}.$$

For the momentum operator, $P|p\rangle = p|p\rangle$. Therefore,

$$\langle x|P^2|y\rangle = \int \langle x|P^2 p\rangle\langle p|y\rangle dp = \int_{\mathbb{R}} p^2\langle x|p\rangle\langle p|y\rangle\frac{dp}{2\pi}.$$

Hence $\langle x|P^2|y\rangle = \int_{\mathbb{R}} p^2 \mathrm{e}^{\mathrm{i}p(x-y)}\ \frac{dp}{2\pi}$. Summarizing,

$$\langle x|H|y\rangle = \int_{\mathbb{R}}\left(\frac{p^2}{2m}+\frac{m\omega^2 y^2}{2}\right)\mathrm{e}^{\mathrm{i}p(x-y)}\ \frac{dp}{2\pi} = \int_{\mathbb{R}}\mathcal{H}(y,p)\mathrm{e}^{\mathrm{i}p(x-y)}\ \frac{dp}{2\pi}.$$

Thus

$$\langle x|I-\mathrm{i}H\Delta t|y\rangle = \int_{\mathbb{R}}(1-\mathrm{i}\mathcal{H}(y,p)\Delta t)\ \mathrm{e}^{\mathrm{i}p(x-y)}\ \frac{dp}{2\pi}.$$

Finally,

$$\langle x|\mathrm{e}^{-\mathrm{i}H\Delta t}|y\rangle = \int_{\mathbb{R}}\mathrm{e}^{-\mathrm{i}\mathcal{H}(y,p)\Delta t}\ \mathrm{e}^{\mathrm{i}p(x-y)}\ \frac{dp}{2\pi},$$

up to terms of order $(\Delta t)^2$. This finishes the formal proof of the claim.

(iii) The path integral: Consider first the case where $N = 2$. Set $q_0 := y$ and $q_2 := x$. By the product formula (7.173),

$$\mathcal{K}(q_2,t_2;q_0,t_0) = \int_{\mathbb{R}}\mathcal{K}(q_2,t_2;q_1,t_1)\mathcal{K}(q_1,t_1;q_0,t_0)dq_1.$$

Using (7.174), we get the approximative formula

$$\mathcal{K}(q_2,t_2;q_0,t_0) = \int_{\mathbb{R}^3}\mathrm{e}^{\mathrm{i}S_2}\ dq_1\cdot\frac{dp_1}{2\pi}\cdot\frac{dp_0}{2\pi} \tag{7.175}$$

with the discrete action

$$S_2 := \left(p_1\frac{q_2-q_1}{\Delta t}+p_0\frac{q_1-q_0}{\Delta t}-\mathcal{H}(q_1,p_1)-\mathcal{H}(q_0,p_0)\right)\Delta t.$$

Now let $N = 2,3,\ldots$. Similarly, the product formula (7.173) yields

$$\mathcal{K}(q_N,t_N;q_0,t_0) = \int_{\mathbb{R}^{N-1}} dq_{N-1}\cdots dq_1\prod_{n=1}^{N}\mathcal{K}(q_n,t_n;q_{n-1},t_{n-1}).$$

By (7.174), we obtain the approximative formula

$$\mathcal{K}(q_N,t_N;q_0,t_0) = \int_{\mathbb{R}^{2N-1}}\mathrm{e}^{\mathrm{i}S_N}\ \frac{dp_0}{2\pi}\prod_{n=1}^{N-1}\frac{dq_n dp_n}{2\pi} \tag{7.176}$$

with the discrete action

$$S_N := \sum_{n=0}^{N-1}\left(p_n\frac{q_{n+1}-q_n}{\Delta t}-\mathcal{H}(q_n,p_n)\right)\Delta t.$$

Finally, carry out the formal limit $N\to\infty$ which implies $\Delta t\to 0$. This way, we get Feynman's magic limit formula (7.171) which we mnemonically write as (7.172).

The path integral in the position space. Feynman's magic formula (7.171) can be simplified by integrating over the momentum variables $p_0, p_1, ...$ This yields the following modified magic formula

$$\boxed{\mathcal{K}(x,t;y,s) = \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q.} \tag{7.177}$$

Here, we integrate over all continuous paths $q = q(\tau), s \le \tau \le t$, in the position space with

$$q(s) = y, \qquad q(t) = x$$

for given initial time s, initial point y, final time t, and final point x. Along this path, we use the classical action

$$S[q] := \int_s^t \left\{ \tfrac{1}{2} m \dot{q}(\tau)^2 - U(q(\tau)) \right\} d\tau.$$

Mnemonically, the magic formula (7.177) stands for the following formal limit

$$\boxed{\mathcal{K}(x,t;y,s) = \lim_{N\to\infty} \frac{1}{l} \int_{\mathbb{R}^{N-1}} \mathrm{e}^{\mathrm{i}S_N/\hbar}\, \frac{dq_1}{l} \cdots \frac{dq_{N-1}}{l}} \tag{7.178}$$

along with the discrete action

$$S_N := \sum_{n=0}^{N-1} \left\{ \frac{m}{2} \left(\frac{q_{n+1} - q_n}{\Delta t} \right)^2 - U(q_n) \right\} \Delta t,$$

and the characteristic length $l := \sqrt{\frac{2\pi\hbar \mathrm{i} \Delta t}{m}}$. Now let us motivate formula (7.178). Set $\hbar := 1$. Proceeding as above, formula (7.178) follows from the product formula

$$\mathcal{K}(q_N, t_N; q_0, t_0) = \int_{\mathbb{R}^{N-1}} dq_{N-1} \cdots dq_1 \prod_{n=1}^{N} \mathcal{K}(q_n, t_n; q_{n-1}, t_{n-1})$$

along with the approximation

$$\boxed{\mathcal{K}(x, s+\Delta t; y, s) = l^{-1} \mathrm{e}^{\mathrm{i}m(x-y)^2/2\Delta t}\, \mathrm{e}^{-\mathrm{i}U(y)\Delta t},} \tag{7.179}$$

up to terms of order $(\Delta t)^2$. It remains to justify formula (7.179). To this end, use

$$\mathcal{K}(x, s+\Delta t; y, s) = \mathrm{e}^{-\mathrm{i}U(y)\Delta t} \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}p^2 \Delta t/2m}\, \mathrm{e}^{\mathrm{i}p(x-y)}\, \frac{dp}{2\pi}, \tag{7.180}$$

by (7.174). Applying the Gaussian integral formula (7.161) on page 551 to (7.180), we get the desired formula (7.179).

7.8 Finite-Dimensional Gaussian Integrals

The rigorous theory of finite-dimensional Gaussian integrals in classical probability theory represents the prototype of the formal theory of infinite-dimensional Gaussian integrals, which play a crucial role for describing correlations in quantum field theory.

> In order to understand the formal properties of infinite-dimensional Gaussian integrals, write the well-defined N-dimensional Gaussian integrals in such a way that the formal limit $N \to \infty$ can be easily performed.
>
> Folklore

Path integrals (or more general functional integrals) can be computed by regarding them as infinite-dimensional Gaussian integrals. To discuss this, in the present section we are going to study finite-dimensional Gaussian integrals. In the next section, we will generalize this to the infinite-dimensional case. Note that

- free systems (i.e., systems without any interaction) correspond to standard Gaussian integrals, whereas
- interacting systems are described by the perturbation of standard Gaussian integrals.

In the framework of perturbation theory, the computation of perturbed Gaussian integrals can be reduced to the computation of moments for standard Gaussian integrals. Analytically, this can be based on the Wick theorem. Graphically, this corresponds to Feynman diagrams.

7.8.1 Basic Formulas

One-dimensional Gaussian integrals. The starting point is the integral

$$\boxed{\int_{\mathbb{R}} \mathrm{e}^{-x^2} dx = \sqrt{\pi}.} \tag{7.181}$$

This formula elegantly follows from $\int_{\mathbb{R}} \mathrm{e}^{-x^2} dx \int_{\mathbb{R}} \mathrm{e}^{-y^2} dy = \int_{\mathbb{R}^2} \mathrm{e}^{-x^2-y^2} dxdy$. Passing to polar coordinates, the latter integral is equal to

$$2\pi \int_0^\infty \mathrm{e}^{-r^2}\, r dr = -\pi \mathrm{e}^{-r^2}|_0^\infty = \pi.$$

(i) Rescaling: Using translation and rescaling, for all $a > 0$ and $x_0 \in \mathbb{R}$, we get

$$\int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}a(x-x_0)^2} \frac{dx}{\sqrt{2\pi}} = \frac{1}{\sqrt{a}}.$$

(ii) Quadratic supplement: Using (i) and setting $b := ax_0$, we obtain

$$\int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}ax^2} \mathrm{e}^{bx} \frac{dx}{\sqrt{2\pi}} = \frac{\mathrm{e}^{b^2/2a}}{\sqrt{a}} \tag{7.182}$$

for all $a > 0$ and $b \in \mathbb{R}$. The reduction process from (7.182) to (i) is called the method of the quadratic supplement.

(iii) Analytic continuation: Introduce the set

$$\Omega := \{(a,b) \in \mathbb{C}^2 : a = r\mathrm{e}^{\mathrm{i}\varphi},\ \ r > 0,\ \ -\pi < \varphi < \pi\}.$$

For all $(a,b) \in \Omega$, the function

$$F(a,b) := \frac{\mathrm{e}^{b^2/2a}}{\sqrt{a}}$$

is well defined. Here, the square root is to be understood in the sense of the principal value, that is, $\sqrt{a} := \sqrt{r}\, \mathrm{e}^{\mathrm{i}\varphi/2}$. In fact, the function $F : \Omega \to \mathbb{C}$ is holomorphic. We define

$$\boxed{\int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}ax^2} \mathrm{e}^{bx}\, \frac{dx}{\sqrt{2\pi}} := F(a,b) \qquad \text{for all} \quad (a,b) \in \Omega.} \tag{7.183}$$

This definition is based on the idea of analytic continuation. For example,

$$\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}x^2}\, \frac{dx}{\sqrt{2\pi}} := \frac{1}{\sqrt{-2\mathrm{i}}} = \frac{\mathrm{e}^{\mathrm{i}\pi/4}}{\sqrt{2}} = \frac{1+\mathrm{i}}{2}. \tag{7.184}$$

This Fresnel integral exists in the classical sense.[91] In the special case where $\Re(a) > 0$ and $b \in \mathbb{C}$, relation (7.183) is always valid in the classical sense (i.e., the integral exists).[92]

(iv) Fourier transform: Let $a > 0$. Then it follows from (iii) that

$$\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{e}^{-ax^2/2}\, \mathrm{e}^{-\mathrm{i}px}\, dx = \frac{\mathrm{e}^{-p^2/2a}}{\sqrt{a}} \qquad \text{for all} \quad p \in \mathbb{R}.$$

In the special case where $a = 1$, this relation shows that the Gaussian function $x \mapsto \mathrm{e}^{-x^2/2}$ is a fixed point of the Fourier transform.

(v) The method of stationary phase: Let us introduce the so-called phase function $\Phi(x) := -\frac{1}{2}ax^2 + bx$. The equation

$$\Phi'(x) = -ax + b = 0$$

has the unique solution $x_{\mathrm{crit}} := b/a$. For this point, the phase function Φ becomes stationary. Relation (7.183) can be written as

$$\boxed{\int_{\mathbb{R}} \mathrm{e}^{\Phi(x)}\, \frac{dx}{\sqrt{2\pi}} = \frac{\mathrm{e}^{\Phi(x_{\mathrm{crit}})}}{\sqrt{a}} \qquad \text{for all} \quad (a,b) \in \Omega.}$$

This so-called method of stationary phase tells us that the integral is determined by the integrand at the stationary point x_{crit}, up to a normalization constant.

(vi) Adiabatic regularization: Let $f : \mathbb{R} \to \mathbb{C}$ be a bounded function, that is, $\sup_{x\in\mathbb{R}} |f(x)| < \infty$, which is continuous (or continuous up to a set of Lebesgue measure zero). Then the integral

$$\int_{\mathbb{R}} f(x) \mathrm{e}^{-\frac{1}{2}\varepsilon x^2}\, dx, \qquad \varepsilon > 0$$

exists, which is called the adiabatic regularization of the integral $\int_{\mathbb{R}} f(x)dx$. For example, let $\alpha \in \mathbb{R}, b \in \mathbb{C}$, and let $\varepsilon > 0$. Then the integral

[91] For the computation of this integral by using Cauchy's residue method, we refer to page 734 of Vol. I.

[92] Here, $|\mathrm{e}^{-\frac{1}{2}ax^2} \mathrm{e}^{bx}| = \mathrm{e}^{-\frac{1}{2}\Re(a)x^2} \mathrm{e}^{\Re(b)x}$ for all $x \in \mathbb{R}$. Both the existence of the integral from (7.183) and its analytic dependence on the parameters a and b follow then from the majorant criterion for integrals (see Vol. I, p. 493).

$$\int_{\mathbb{R}} \left(\mathrm{e}^{-\frac{1}{2}\alpha \mathrm{i} x^2} \mathrm{e}^{bx} \right) \mathrm{e}^{-\frac{1}{2}\varepsilon x^2} \frac{dx}{\sqrt{2\pi}} = \frac{\mathrm{e}^{b^2/2(\varepsilon+\alpha \mathrm{i})}}{\sqrt{\varepsilon + \alpha \mathrm{i}}}$$

exists. If $\alpha \neq 0$, then we have the limit relation

$$\lim_{\varepsilon \to +0} \int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}\alpha \mathrm{i} x^2} \mathrm{e}^{bx} \mathrm{e}^{-\frac{1}{2}\varepsilon x^2} \frac{dx}{\sqrt{2\pi}} = \int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}\alpha \mathrm{i} x^2} \mathrm{e}^{bx} \frac{dx}{\sqrt{2\pi}} = \frac{\mathrm{e}^{b^2/2\alpha \mathrm{i}}}{\sqrt{\alpha \mathrm{i}}}.$$

(vii) Moments and the Wick trick: Let $a > 0$. We want to compute the moments

$$\langle x^k \rangle := \frac{\int_{\mathbb{R}} x^k \mathrm{e}^{-\frac{1}{2}ax^2} \frac{dx}{\sqrt{2\pi}}}{\int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}ax^2} \frac{dx}{\sqrt{2\pi}}}, \qquad k = 0, 1, 2, \dots$$

To this end, for $J \in \mathbb{C}$, we introduce the so-called generating function

$$Z(J) := \frac{\int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}ax^2} \mathrm{e}^{Jx} \frac{dx}{\sqrt{2\pi}}}{\int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}ax^2} \frac{dx}{\sqrt{2\pi}}} = \mathrm{e}^{J^2/2a}.$$

Differentiation yields $Z'(0) = \langle x \rangle$. More generally,

$$\boxed{\langle x^k \rangle = \frac{d^k Z(0)}{dJ^k}, \qquad k = 0, 1, 2 \dots} \tag{7.185}$$

For example,

$$\langle x \rangle = Z'(0) = 0, \qquad \langle x^2 \rangle = Z''(0) = a^{-1}.$$

Note that if $\Re(a) > 0$, then the integrals $M_0, M_1, M_2, \dots$ exist, and the Wick trick formula (7.185) holds true, by the majorant criterion (see Vol. I, p. 493). The entire function $Z : \mathbb{C} \to \mathbb{C}$ has the power series expansion

$$Z(J) = M_0 + M_1 J + \frac{M_2 J^2}{2!} + \frac{M_3 J^3}{3!} + \dots$$

N-dimensional Gaussian integrals. In what follows, we choose the dimensions $N = 1, 2, \dots$ All the square roots are to be understood as principal values. Let $(\lambda_k, b_k) \in \Omega$ be given for $k = 1, \dots, N$. The prototype is the definition

$$\int_{\mathbb{R}^N} \prod_{k=1}^{N} \mathrm{e}^{-\frac{1}{2}\lambda_k x_k^2 + b_k x_k} \frac{dx_k}{\sqrt{2\pi}} := \prod_{k=1}^{N} \int_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}\lambda_k x^2 + b_k x} \frac{dx}{\sqrt{2\pi}} = \prod_{k=1}^{N} \frac{\mathrm{e}^{b_k^2/2\lambda_k}}{\sqrt{\lambda_k}}. \tag{7.186}$$

The integrals are to be understood in the generalized sense. However, if $\Re(\lambda_k) > 0$ for $k = 1, \dots, N$, then the integrals exist, and relation (7.186) is to be understood in the classical sense. We make the following assumption.

(H) *All the eigenvalues of the real symmetric $(N \times N)$-matrix $A = (a_{kl})$ are positive, that is, $\lambda_1 > 0, \dots, \lambda_N > 0$.*

Then $\det A = \lambda_1 \lambda_2 \cdots \lambda_N$. By definition, the zeta function of the matrix A reads as

$$\zeta_A(s) := \sum_{k=1}^{N} \frac{1}{\lambda_k^s} \qquad \text{for all} \quad s \in \mathbb{C}.$$

For all $x, y \in \mathbb{R}^N$ and all $b \in \mathbb{C}^N$, we set

$$\langle y|Ax\rangle := \sum_{k,l=1}^{N} y_k a_{kl} x_l, \qquad \langle b|x\rangle := \sum_{k=1}^{N} b_k x_k.$$

Since $\lambda_k^{-s} = \mathrm{e}^{-s \ln \lambda_k}$, we obtain the derivative

$$\zeta_A'(s) = -\sum_{k=1}^{N} \frac{\ln \lambda_k}{\lambda_k^s}, \qquad s \in \mathbb{C}.$$

This implies the key formula

$$\boxed{\det A = \prod_{k=1}^{N} \lambda_k = \mathrm{e}^{-\zeta_A'(0)}.} \tag{7.187}$$

The following properties of finite-dimensional Gaussian integrals are crucial for the theory of infinite-dimensional Gaussian integrals.

(i) The standard Gaussian integral: For all $y \in \mathbb{R}^N$, we have

$$\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle (x-y)|A(x-y)\rangle} \, \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} = \frac{1}{\sqrt{\det A}}.$$

Proof. After a translation, we can choose $y = 0$. By the principal axis theorem on the real Hilbert space $\mathbb{R}^N$, there exists an orthogonal transformation which sends the integral to the normal form (7.186) with $b_k = 0$ for all k. □

(ii) Quadratic supplement: For all $b \in \mathbb{R}^N$, we have

$$\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \, \mathrm{e}^{\langle b|x\rangle} \, \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} = \frac{\mathrm{e}^{\frac{1}{2}\langle b|A^{-1}b\rangle}}{\sqrt{\det A}}. \tag{7.188}$$

This can be written as

$$\boxed{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \, \mathrm{e}^{\langle b|x\rangle} \, \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} = \mathrm{e}^{\frac{1}{2}\langle b|A^{-1}b\rangle} \, \mathrm{e}^{\frac{1}{2}\zeta_A'(0)}.} \tag{7.189}$$

Proof. This is an easy consequence of (i) above. Since A is symmetric, we get

$$\begin{aligned} \langle (x-y)|A(x-y)\rangle &= \langle x|Ax\rangle - \langle y|Ax\rangle - \langle x|Ay\rangle + \langle y|Ay\rangle \\ &= \langle x|Ax\rangle - 2\langle Ay|x\rangle + \langle Ay|y\rangle. \end{aligned}$$

Finally, set $b := Ay$. By (i), the integral on the left-hand side of (7.188) is equal to

$$\frac{\mathrm{e}^{\frac{1}{2}\langle Ay|y\rangle}}{\sqrt{\det A}}.$$

Finally, observe that $y = A^{-1}b$. Hence $\langle Ay|y\rangle = \langle b|A^{-1}b\rangle$. □

(iii) Analytic continuation: Let γ be a nonzero complex number with the argument $-\pi < \arg(\gamma) < \pi$ (e.g., $\gamma = \pm \mathrm{i}$). Then, for all $b \in \mathbb{C}^N$, we define

$$\boxed{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\gamma\langle x|Ax\rangle}\, \mathrm{e}^{\langle b|x\rangle}\, \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} := \frac{\mathrm{e}^{\frac{1}{2}\langle b|(\gamma A)^{-1}b\rangle}}{\sqrt{\det(\gamma A)}}.} \tag{7.190}$$

Here, the square root is to be understood as

$$\sqrt{\det(\gamma A)} := (\sqrt{\gamma})^N \sqrt{\det A}$$

where $\sqrt{\gamma}$ is the principal value of the square root. Note that equation is valid for all $\gamma > 0$, and the integral exists in the classical sense. Then we use analytic continuation.

(iv) Adiabatic regularization: Let A and b be given as in (iii) above. Furthermore, let $\alpha \in \mathbb{R}$ and $\varepsilon > 0$. Then the integral

$$\int_{\mathbb{R}^N} \left(\mathrm{e}^{-\frac{1}{2}\alpha\mathrm{i}\langle x|Ax\rangle}\, \mathrm{e}^{\langle b|x\rangle}\right) \mathrm{e}^{-\frac{1}{2}\varepsilon\langle x|x\rangle}\, \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} := \frac{\mathrm{e}^{\frac{1}{2}\langle b|(\alpha\mathrm{i}A+\varepsilon I)^{-1}b\rangle}}{\sqrt{\det(\alpha\mathrm{i}A + \varepsilon I)}}$$

exists. If $\alpha \neq 0$, then we have the limit relation

$$\lim_{\varepsilon \to +0} \int_{\mathbb{R}^N} \left(\mathrm{e}^{-\frac{1}{2}\alpha\mathrm{i}\langle x|Ax\rangle}\, \mathrm{e}^{\langle b|x\rangle}\right) \mathrm{e}^{-\frac{1}{2}\varepsilon\langle x|x\rangle}\, \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} = \frac{\mathrm{e}^{\frac{1}{2}\langle b|(\alpha\mathrm{i}A)^{-1}b\rangle}}{\sqrt{\det(\alpha\mathrm{i}A)}}.$$

(v) The method of stationary phase: Let A and b be given as in (iii) above. Introduce the phase function $\Phi(x) := -\frac{1}{2}\gamma\langle x|Ax\rangle + \langle b|x\rangle$. The equation

$$\Phi'(x) = -\gamma Ax + b = 0$$

has the unique solution $x_{\mathrm{crit}} := (\gamma A)^{-1}b$. Then relation (7.190) can be written as

$$\boxed{\int_{\mathbb{R}^n} \mathrm{e}^{\Phi(x)}\, \frac{dx^1}{\sqrt{2\pi}} \cdots \frac{dx^N}{\sqrt{2\pi}} = \frac{\mathrm{e}^{\Phi(x_{\mathrm{crit}})}}{\sqrt{\det(\gamma A)}}.}$$

7.8.2 Free Moments, the Wick Theorem, and Feynman Diagrams

In what follows, we will use a terminology which fits best the needs of quantum field theory. Our approach can be viewed as a discrete variant of quantum field theory. The basic notions are:

- free probability distribution (also called the Gaussian distribution in mathematics),
- free moments (free n-correlation functions or, briefly, called free n-point functions),
- generating function of the free moments,
- Feynman diagrams (i.e., graphic representation of free moments).

In the next section, we will generalize this to full probability distributions and full moments.

In terms of discrete quantum field theory, full moments (resp. free moments) describe particles under interaction (resp. free particles without any interaction).

Moments are fundamental quantities. The theory of moments in probability theory tells us that, roughly speaking, a probability distribution is uniquely determined by the knowledge of its moments (see Vol. I, page 751). Our main task is to reduce the computation of full moments to the computation of free moments. This is the basic trick of perturbation theory in quantum field theory.

The free probability distribution. Assume that the matrix A has the property (H) formulated on page 562. Introduce the key quantity

$$\varrho(x) := \frac{\mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle}}{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} dx_1 \cdots dx_N}, \qquad x \in \mathbb{R}^N.$$

This is called the free probability density. The function $F : \mathbb{R}^N \to \mathbb{R}$ given by

$$F(x) := \int_{-\infty}^{x} \varrho(y) dy$$

is called the free probability distribution (or Gaussian distribution).

Free Moments. Choose the indices $k_1, k_2, \ldots, k_n = 1, 2, \ldots$, and fix the positive integer $n = 1, 2, \ldots$ Define

$$\boxed{\langle x_{k_1} x_{k_2} \cdots x_{k_n} \rangle := \int_{\mathbb{R}^N} x_{k_1} x_{k_2} \cdots x_{k_n} \cdot \varrho(x) dx_1 \cdots dx_N.}$$

These expectation values are called the moments of the probability density ϱ (or, briefly, the free moments). We also use the notation[93]

$$C_{n,\mathrm{free}}(x_{k_1}, x_{k_2}, \ldots, x_{k_n}) := \langle x_{k_1} x_{k_2} \cdots x_{k_n} \rangle,$$

and we call $C_{n,\mathrm{free}}$ a free discrete n-correlation function (or a free n-point function). Explicitly, we get[94]

$$\langle x_{k_1} x_{k_2} \cdots x_{k_n} \rangle := \frac{\int_{\mathbb{R}^N} x_{k_1} x_{k_2} \cdots x_{k_n} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}}{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}}.$$

The trick of the generating function. For all $J \in \mathbb{R}^N$, introduce the so-called generating function

$$Z_{\mathrm{free}}(J) := \int_{\mathbb{R}^N} \varrho(x) \mathrm{e}^{\langle J|x\rangle} \, dx_1 \cdots dx_N.$$

Explicitly, we get

[93] The value $C_{n,\mathrm{free}}(x_{k_1}, x_{k_2}, \ldots, x_{k_n})$ only depends on the indices $k_1, k_2, \ldots, k_n$. However, mnemonically, our notation is convenient for the passage to quantum field theory. Then we can use the same notation for the continuously varying variables $x_{k_1}, x_{k_2}, \ldots, x_{k_n}$.

[94] We introduce the rescaled differential $\frac{dx_k}{\sqrt{2\pi}}$ in order to prepare the limit $N \to \infty$ to path integrals (infinite-dimensional Gaussian integrals) later on.

$$Z_{\text{free}}(J) := \frac{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle}\, \mathrm{e}^{\langle J|x\rangle}\, \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}}{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle}\, \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}} = \mathrm{e}^{\frac{1}{2}\langle J|A^{-1}J\rangle}.$$

Differentiation with respect to J yields

$$\langle x_{k_1} x_{k_2} \cdots x_{k_n}\rangle = \frac{\partial^n}{\partial J_{k_1} \partial J_{k_2} \cdots \partial J_{k_n}}\, \mathrm{e}^{\frac{1}{2}\langle J|A^{-1}J\rangle}, \tag{7.191}$$

by setting $J = 0$ after differentiation. In particular, for the free 2-point function we get

$$\boxed{\langle x_k x_l\rangle = (A^{-1})_{kl}, \qquad k, l = 1, \ldots, N}$$

where $(A^{-1})_{kl}$ is the entry of the inverse matrix A^{-1} located in the kth row and in the lth column.

Theorem 7.46 *Let $k_1, \ldots, k_n = 1, 2, \ldots N$. If n is even, then*

$$\langle x_{k_1} x_{k_2} \cdots x_{k_n}\rangle = \sum \langle x_{i_1} x_{i_2}\rangle \langle x_{i_3} x_{i_4}\rangle \cdots \langle x_{i_{n-1}} x_{i_n}\rangle.$$

Here, we sum over all possible pairings of the indices $k_1, k_2, \ldots, k_n$. If n is odd, then $\langle x_{k_1} x_{k_2} \cdots x_{k_n}\rangle = 0$.

This so-called Wick theorem tells us that the Gaussian distribution has the following important property: the 2-point function determines all the other n-point functions.

Proof. Observe that the function $J \mapsto \langle J|A^{-1}J\rangle$ is quadratic. If n is even, then use (7.191) together with the chain rule. If n is odd, then note that the function $(x_1, x_2, x_3) \mapsto x_1 x_2 x_3$ is odd, and so on. □

Feynman diagrams. For example, the Wick theorem tells us that

$$\langle x_1 x_2 x_3 x_4\rangle = \langle \underbrace{x_1}\, x_2\, \underbrace{x_3}\, x_4\rangle + \langle \overbrace{x_1 x_2}\, \overbrace{x_3 x_4}\rangle + \langle \underbrace{x_1\, \overbrace{x_2}\, x_3}\, x_4\rangle. \tag{7.192}$$

That is, we sum over all possible fully contracted symbols. Explicitly, this means

$$\langle x_1 x_2 x_3 x_4\rangle = \langle x_1 x_2\rangle\langle x_3 x_4\rangle + \langle x_1 x_3\rangle\langle x_2 x_4\rangle + \langle x_1 x_4\rangle\langle x_2 x_3\rangle.$$

This is graphically represented in Table 7.1(c) by using so-called Feynman diagrams. Here, the contractions correspond to connections of the vertices. Similarly, we get

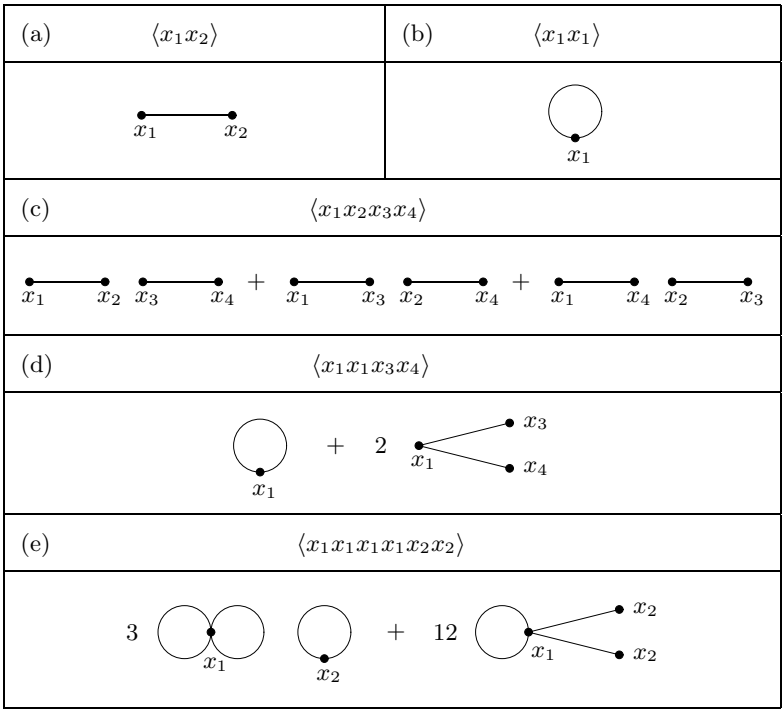
$$\langle x_1 x_1 x_3 x_4\rangle = \langle \underbrace{x_1}\, x_1\, \underbrace{x_3}\, x_4\rangle + \langle \overbrace{x_1 x_1}\, \overbrace{x_3 x_4}\rangle + \langle \underbrace{x_1\, \overbrace{x_1}\, x_3}\, x_4\rangle. \tag{7.193}$$

This is graphically represented in Table 7.1(d). Naturally enough, the diagram corresponding to $\langle x_1 x_1\rangle$ is called a loop. Analogously,

$$\langle x_1^4 x_2^2\rangle = 3\langle x_1^2\rangle^2 \langle x_2^2\rangle + 12\langle x_1^2\rangle\langle x_1 x_2\rangle^2. \tag{7.194}$$

This is computed in Problem 7.33 (see Table 7.1(e)).

Table 7.1. Feynman diagrams



7.8.3 Full Moments and Perturbation Theory

Distinguish strictly between free moments and full moments.
Folklore

Now we pass to probability distributions which are perturbations of Gaussian distributions. The strength of perturbation is measured by the coupling constant κ. This way, free moments (resp. free n-point functions) are replaced by full moments (resp. full n-point functions).

The full probability distribution under interaction. Assume that the matrix A has the property (H) formulated on page 562. Let

$$U : \mathbb{R}^N \to \mathbb{R}$$

be a polynomial with respect to the real variables $x_1, \ldots, x_N$ (e.g., we choose $U(x) := -\langle x|x\rangle^2$). We are given the real nonnegative number κ called coupling constant. Introduce

$$\boxed{\varrho_\kappa(x) := \frac{\mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle}\mathrm{e}^{\kappa U(x)}}{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle}\mathrm{e}^{\kappa U(x)} dx_1 \cdots dx_N}, \qquad x \in \mathbb{R}^N.} \tag{7.195}$$

This is called the full probability density, which depends on the coupling constant κ. The function $F_\kappa : \mathbb{R}^N \to \mathbb{R}$ given by

$$F_\kappa(x) := \int_{-\infty}^{x} \varrho_\kappa(y)dy, \qquad x \in \mathbb{R}^N$$

is called the full probability distribution (or perturbed Gaussian distribution). The function κU measures the strength of the perturbation. As a rule, we will consider the case where the coupling constant κ is small. We assume that the function ϱ_κ is well defined, that is, the denominator of ϱ_κ in (7.195) is a finite integral. Note that the free probability density corresponds to the case where the coupling constant vanishes, $\kappa = 0$. Define

$$\boxed{\langle x_{k_1} x_{k_2} \cdots x_{k_n} \rangle_{\text{full}} := \int_{\mathbb{R}^N} x_{k_1} x_{k_2} \cdots x_{k_n} \cdot \varrho_\kappa(x) dx_1 \cdots dx_N.}$$

These expectation values are called the full moments. We also use the notation

$$C_{n,\text{full}}(x_{k_1}, x_{k_2}, \ldots, x_{k_n}) := \langle x_{k_1} x_{k_2} \cdots x_{k_n} \rangle_{\text{full}},$$

and we call $C_{n,\text{full}}$ a full discrete n-correlation function (or a full n-point function). Explicitly, we get

$$\langle x_{k_1} x_{k_2} \cdots x_{k_n} \rangle_{\text{full}} := \frac{\int_{\mathbb{R}^N} x_{k_1} x_{k_2} \cdots x_{k_n} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \ \mathrm{e}^{\kappa U(x)} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}}{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \mathrm{e}^{\kappa U(x)} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}}.$$

For all $J \in \mathbb{R}^N$, introduce the full generating function

$$Z_{\text{full}}(J) := \int_{\mathbb{R}^N} \varrho_\kappa(x) \ \mathrm{e}^{\langle J|x\rangle} \ dx_1 \cdots dx_N.$$

Explicitly,

$$Z_{\text{full}}(J) = \frac{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \ \mathrm{e}^{\kappa U(x)} \ \mathrm{e}^{\langle J|x\rangle} \ \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}}{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \ \mathrm{e}^{\kappa U(x)} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}}.$$

Differentiation with respect to J yields

$$\langle x_{k_1} x_{k_2} \cdots x_{k_n} \rangle_{\text{full}} = \frac{\partial^n Z_{\text{full}}(0)}{\partial J_{k_1} \partial J_{k_2} \cdots \partial J_{k_n}}. \tag{7.196}$$

By Taylor expansion,

$$Z_{\text{full}}(J) = 1 + \sum_{n=1}^{\infty} \sum_{r_1+r_2+\ldots+r_N=n} \frac{\langle x_1^{r_1} x_2^{r_2} \cdots x_N^{r_N} \rangle_{\text{full}}}{r_1! r_2! \cdots r_N!} \ J_1^{r_1} J_2^{r_2} \cdots J_N^{r_N}.$$

Perturbation theory. We want to compute the following full moment:

$$\langle x_{k_1} x_{k_2} \cdots x_{k_n} \rangle_{\text{full}} = \frac{\int_{\mathbb{R}^N} x_{k_1} x_{k_2} \cdots x_{k_n} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \ \mathrm{e}^{\kappa U(x)} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}}{\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \mathrm{e}^{\kappa U(x)} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}}$$

where U is a polynomial.To this end, we start with the Taylor expansion

$$\mathrm{e}^{\kappa U} = 1 + \kappa U + \tfrac{1}{2}\kappa^2 U^2 + \ldots$$

Setting $a := \int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}$, we get

$$\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \mathrm{e}^{\kappa U(x)} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} = a\left(1 + \kappa\langle U(x)\rangle + \tfrac{1}{2}\kappa^2\langle U(x)^2\rangle + \ldots\right).$$

Similarly, the integral

$$\int_{\mathbb{R}^N} x_{k_1} \cdots x_{k_n} \mathrm{e}^{-\frac{1}{2}\langle x|Ax\rangle} \mathrm{e}^{\kappa U(x)} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}}$$

is equal to

$$a(\langle x_{k_1} \cdots x_{k_n}\rangle + \kappa\langle x_{k_1} \cdots x_{k_n} U(x)\rangle + \tfrac{1}{2}\kappa^2\langle x_{k_1} \cdots x_{k_n} U(x)^2\rangle + \ldots).$$

Hence

$$\boxed{\langle x_{k_1} \cdots x_{k_n}\rangle_{\mathrm{full}} = \langle x_{k_1} \cdots x_{k_n}\rangle + \kappa\big(\langle x_{k_1} \cdots x_{k_n} U(x)\rangle - \langle U(x)\rangle\big) \ldots}$$

Here, the dots stand for terms of order $O(\kappa^2)$ as $\kappa \to 0$. Since $U(x)$ is a polynomial with respect to $x_1, \ldots, x_n$, the right-hand side only contains free moments. Therefore the Wick theorem tells us that

> *The computation of full moments can be reduced to the computation of the special free moments* $\langle x_i x_j\rangle$.

This is the secret behind the success of perturbation theory in quantum field theory. For example, let $N \geq 2$. Choose $U(x) := x_1^4$. Then $\langle U(x)\rangle = 3\langle x_1^2\rangle^2$. By (7.194), we get

$$\langle x_2^2\rangle_{\mathrm{full}} = \langle x_2\rangle^2 + \kappa\big(3\langle x_1^2\rangle^2\langle x_2^2\rangle + 12\langle x_1^2\rangle\langle x_1 x_2\rangle^2 - 3\langle x_1^2\rangle^2\big) + O(\kappa^2)$$

as $\kappa \to 0$.

The reduced full moments (cumulants). In order to avoid redundant expressions, let us introduce the reduced full generating function

$$Z_{\mathrm{full,red}}(J) := \ln Z_{\mathrm{full}}(J).$$

Then

$$\boxed{Z_{\mathrm{full}}(J) = \mathrm{e}^{Z_{\mathrm{full,red}}(J)}.} \tag{7.197}$$

By definition, $Z_{\mathrm{full,red}}$ is the generating function for the so-called reduced full moments:[95]

$$\langle x_{k_1} x_{k_2} \ldots x_{k_n}\rangle_{\mathrm{full,red}} := \frac{\partial^n Z_{\mathrm{full,red}}(0)}{\partial J_{k_1} \partial J_{k_2} \cdots \partial J_{k_n}}.$$

Hence

$$Z_{\mathrm{full,red}}(J) = 1 + \sum_{n=1}^{\infty} \sum_{r_1+r_2+\ldots+r_N=n} \frac{\langle x_1^{r_1} x_2^{r_2} \cdots x_N^{r_N}\rangle_{\mathrm{full,red}}}{r_1! r_2! \cdots r_N!} J_1^{r_1} J_2^{r_2} \cdots J_N^{r_N}.$$

Using Taylor expansion with respect to κ, it follows from (7.197) that

> *The full moments can be uniquely computed by means of the reduced full moments.*

[95] In mathematics, reduced moments are also called cumulants.

In the special free case where $\kappa = 0$, we obtain

$$Z_{\text{free,red}}(J) = \ln Z_{\text{free}}(J) = \ln \mathrm{e}^{\frac{1}{2}\langle J|A^{-1}J\rangle} = \tfrac{1}{2}\langle J|A^{-1}J\rangle.$$

Hence

$$\langle x_k x_l\rangle_{\text{free red}} = \langle x_k x_l\rangle, \qquad k,l = 1,\ldots,N.$$

The remaining reduced free moments are equal to zero. This implies the following result.

The reduced full generating function satisfies the relation

$$Z_{\text{full,red}}(J) = Z_{\text{free,red}}(J) + O(\kappa) = 1 + \sum_{i,k=1}^{N} \tfrac{1}{2}\langle x_i x_k\rangle J_i J_k + O(\kappa)$$

as $\kappa \to 0$. Therefore, the function $Z_{\text{full,red}}$ describes the perturbation of the second free moments, under the influence of the coupling constant κ. In contrast to this, the formula

$$Z_{\text{full}}(J) = Z_{\text{free}}(J) + O(\kappa), \qquad \kappa \to 0$$

is full of redundance, since the function Z_{free} is redundant compared with $Z_{\text{free,red}}$. This is why physicists use reduced full correlation (or n-point) functions in quantum field theory.

7.9 Rigorous Infinite-Dimensional Gaussian Integrals

> The definition of infinite-dimensional Gaussian integrals depends on the spectrum of the linear symmetric dispersion operator.
>
> Folklore

In order to explain the basic idea, let us start with the finite-dimensional key formula

$$\int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}(\lambda_1 x_1^2 + \ldots + \lambda_N^2 x_N^2)} \mathrm{e}^{b_1 x_1 + \ldots + b_N x_N} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} = B_N$$

where

$$B_N := \frac{\mathrm{e}^{\frac{1}{2}\sum_{k=1}^N b_k^2 \lambda_k^{-1}}}{\left(\prod_{k=1}^N \lambda_k\right)^{1/2}}.$$

Here, $N = 1, 2, \ldots$. Furthermore, we assume that $\lambda_1, \lambda_2, \ldots$ are positive numbers, and $b_1, b_2 \ldots$ are real numbers. Now we want to study the limit $N \to \infty$. Obviously, we have the following result.

Proposition 7.47 *Suppose that* $\sum_{k=1}^\infty b_k^2 \lambda_k^{-1} < \infty$ *and* $0 < \prod_{k=1}^\infty \lambda_k < \infty$. *Then the following limit*

$$\lim_{N\to\infty} \int_{\mathbb{R}^N} \mathrm{e}^{-\frac{1}{2}(\lambda_1 x_1^2 + \ldots + \lambda_N^2 x_N^2)}\, \mathrm{e}^{b_1 x_1 + \ldots + b_N x_N} \frac{dx_1}{\sqrt{2\pi}} \cdots \frac{dx_N}{\sqrt{2\pi}} = \frac{\mathrm{e}^{\frac{1}{2}\sum_{k=1}^\infty b_k^2 \lambda_k^{-1}}}{\left(\prod_{k=1}^\infty \lambda_k\right)^{1/2}}$$

exists in the classical sense. We briefly write

$$\int_{\mathbb{R}^\infty} \mathrm{e}^{-\frac{1}{2}\sum_{k=1}^\infty \lambda_k x_k^2}\, e^{\sum_{k=1}^\infty b_k x_k} \prod_{k=1}^\infty \frac{dx_k}{\sqrt{2\pi}} := \frac{\mathrm{e}^{\frac{1}{2}\sum_{k=1}^\infty b_k^2 \lambda_k^{-1}}}{\left(\prod_{k=1}^\infty \lambda_k\right)^{1/2}}.$$

We call this a normalized infinite-dimensional Gaussian integral.

7.9.1 The Infinite-Dimensional Dispersion Operator

We want to generalize the preceding formulas. To this end, we are given the linear symmetric operator

$$A : D(A) \to X$$

defined on the linear dense subspace $D(A)$ of the real infinite-dimensional separable Hilbert space X. Assume that we have the eigenvector equation

$$\boxed{A\varphi_k = \lambda_k \varphi_k, \qquad k = 1, 2, \ldots}$$

where $\lambda_k > 0$ for all k, and the eigenvectors $\varphi_1, \varphi_2 \ldots$ form a complete orthonormal system of the Hilbert space X (together with $\varphi_k \in D(A)$ for all k). Then we obtain $b = \sum_{k=1}^{\infty} \langle b|\varphi_k\rangle \varphi_k$ for all $b \in X$, and

$$A\varphi = \sum_{k=1}^{\infty} \lambda_k \langle \varphi|\varphi_k\rangle \varphi_k \qquad \text{for all} \quad \varphi \in D(A).$$

This implies $\langle \varphi|A\varphi\rangle = \sum_{k=1}^{\infty} \lambda_k \langle \varphi_k|\varphi\rangle^2$. If $A\varphi = 0$, then $\varphi = 0$. Thus the operator A is injective, and the inverse operator $A^{-1} : D(A^{-1}) \to X$ exists with

$$A^{-1}\varphi_k = \lambda_k^{-1} \varphi_k, \qquad k = 1, 2, \ldots$$

In particular, we get $D(A^{-1}) \subseteq D(A)$, and

$$\langle b|A^{-1}b\rangle = \sum_{k=1}^{\infty} \lambda_k^{-1} \langle b|\varphi_k\rangle^2 \qquad \text{for all} \quad b \in D(A).$$

Furthermore, for the dispersion operator A, we define

- the trace $\operatorname{tr} A := \sum_{k=1}^{\infty} \lambda_k$,
- the determinant $\det A := \prod_{k=1}^{\infty} \lambda_k$, and
- the zeta function $\zeta_A(s) = \sum_{k=1}^{\infty} \lambda_k^{-s}$ for suitable complex numbers s.

If the trace is finite, that is $\operatorname{tr}(A) < \infty$, then

$$\det A = \mathrm{e}^{\operatorname{tr} A}.$$

In what follows, we are given $b \in D(A)$. We have to distinguish the following two cases.

(C1) Regular case: $0 < \det A < \infty$ (the determinant exists).
(C2) Singular case: $\det A = \infty$ (the determinant does not exist in the usual sense).

Regular case. Here, we define the normalized infinite-dimensional Gaussian integral by setting

$$\boxed{\int_{D(A)} \mathrm{e}^{-\frac{1}{2}\langle \varphi|A\varphi\rangle} \mathrm{e}^{\langle b|\varphi\rangle} \mathcal{D}_G\varphi := \frac{\mathrm{e}^{\frac{1}{2}\langle b|A^{-1}b\rangle}}{\sqrt{\det A}}.} \tag{7.198}$$

Observe that in concrete situations, the domain of definition $D(A)$ of the operator A describes boundary conditions. Changing the boundary conditions means changing the operator A and its eigenvalues. Since the determinant $\det A$ depends on the eigenvalues, the integral depends on the domain of definition $D(A)$. Now let us study the singular case which is typically encountered in quantum physics.

7.9.2 Zeta Function Regularization and Infinite-Dimensional Determinants

> The definition $\ln\det A := -\zeta_A'(0)$ was first used by the mathematicians Ray and Singer (1971), when they tried to give a definition of the Reidemeister–Franz torsion in analytic terms... Later zeta function regularization was used by physicists in the context of dimensional regularization when applied to quantum field theory in curved space-time.[96]
>
> Klaus Kirsten, 2002

It is our goal to use (7.198) and to redefine the determinant $\det A$ by means of the zeta function ζ_A together with analytic continuation.

Singular case. Motivated by (7.187), the key formula reads as

$$\boxed{\det A = \mathrm{e}^{-\zeta_A'(0)}.} \tag{7.199}$$

Let us assume the following:

(H) *The zeta function* $\zeta_A(s) = \sum_{n=1}^{\infty} \lambda_n^{-s}$ *converges for all sufficiently large positive real numbers* s*, and it can be analytically continued to some neighborhood of the point* $s = 0$ *in the complex plane.*

Here, we define the determinant $\det A$ of the operator A by (7.199). This generates the definition of the normalized infinite-dimensional Gaussian integral in the singular case:

$$\int_{D(A)} \mathrm{e}^{-\frac{1}{2}\langle\varphi|A\varphi\rangle} \mathrm{e}^{\langle b|\varphi\rangle} \mathcal{D}_G\varphi := \mathrm{e}^{\frac{1}{2}\langle b|A^{-1}b\rangle}\ \mathrm{e}^{\frac{1}{2}\zeta_A'(0)}. \tag{7.200}$$

The rescaling trick. Let γ be a nonzero complex number with the property $-\pi < \arg(\gamma) < \pi$, and assume (H). We define the normalized infinite-dimensional Gaussian integral by setting

$$\boxed{\int_{D(A)} \mathrm{e}^{-\frac{1}{2}\gamma\langle\varphi|A\varphi\rangle} \mathrm{e}^{\langle b|\varphi\rangle} \mathcal{D}_G\varphi := \mathrm{e}^{-\frac{1}{2}\zeta_A(0)\ln\gamma} \cdot \frac{\mathrm{e}^{\frac{1}{2}\gamma^{-1}\langle b|A^{-1}b\rangle}}{\sqrt{\det A}}} \tag{7.201}$$

with $\sqrt{\det A} := \mathrm{e}^{-\frac{1}{2}\zeta_A'(0)}$, and $\ln\gamma$ is the principal value of the logarithm. Definition (7.201) is crucial for quantum physics, as we will show in the next section. In order to motivate (7.201), observe first that the following hold.

Proposition 7.48 *Let* $\gamma > 0$*. Assume that the hypothesis* (H) *above is valid. Then*

$$\det(\gamma A) = \gamma^{\zeta_A(0)} \det A.$$

---

[96] K. Kirsten, Spectral Functions in Mathematics and Physics, Chapman, Boca Raton, Florida, 2002 (see also the hints for further reading on page 671).
D. Ray and I. Singer, Reidemeister torsion and the Laplacian on Riemann manifolds, Advances in Math. **7**, (1971) 145–210.

It was independently proven by Werner Müller and Jeff Cheeger that the original combinatorial definition of the Reidemeister–Franz torsion is equivalent to the analytic definition:
W. Müller, Analytic torsion and Reidemeister torsion of Riemannian manifolds, Advances in Math. **28** (1978), 233–305.
J. Cheeger (1979), Analytic torsion and the heat equation, Ann. Math. **109**, 259–322.

This generalizes the classical relation $\det(\gamma A) = \gamma^N \det A$ which is valid in the N-dimensional Euclidean space with $N = 1, 2, \ldots$ The proof will be given in Problem 7.34 by using Euler's gamma function. Replacing A by γA it follows from (7.200) that

$$\int_{D(A)} \mathrm{e}^{-\frac{1}{2}\langle\varphi|(\gamma A)\varphi\rangle} \mathrm{e}^{\langle b|\varphi\rangle} \mathcal{D}_G\varphi := \frac{\mathrm{e}^{\frac{1}{2}\langle b|(\gamma A)^{-1}b\rangle}}{\sqrt{\det(\gamma A)}}, \qquad \gamma > 0.$$

This yields (7.201) if $\gamma > 0$. For general complex numbers γ (outside the negative real axis), the right-hand side of (7.201) makes sense after analytic continuation.

The quotient trick. Fortunately enough, in quantum field theory one frequently encounters quotients of Gaussian integrals which dramatically simplifies the approach. To illustrate this, note that, in the regular case, it follows from (7.198) that

$$\frac{\int_{D(A)} \mathrm{e}^{-\frac{1}{2}\langle\varphi|A\varphi\rangle} \mathrm{e}^{\langle b|\varphi\rangle} \mathcal{D}_G\varphi}{\int_{D(A)} \mathrm{e}^{-\frac{1}{2}\langle\varphi|A\varphi\rangle} \mathcal{D}_G\varphi} := \mathrm{e}^{\frac{1}{2}\langle b|A^{-1}b\rangle}. \tag{7.202}$$

This expression is independent of the determinant $\det A$. Therefore, we use this as a definition for all dispersion operators A and all $b \in D(A)$. This way, the use of the critical determinant $\det A$ is completely avoided.

Example. Let $m > 0$. The following example will be used below in order to study the free quantum particle on the real line. Consider the quadratic form

$$S[r] := \tfrac{1}{2} m \langle r|Ar\rangle, \qquad r \in D(A)$$

with the linear differential operator $A : D(A) \to X$ given by

$$Ar := -\frac{d^2 r}{d\tau^2}, \qquad r \in D(A).$$

Here, X is the real Hilbert space $L_2(\mathbb{R})$, and the domain of definition $D(A)$ consists of all twice continuously differentiable functions $r : [s,t] \to \mathbb{R}$ with $r(s) = r(t) = 0$. We write $C_0^2[s,t]$ instead of $D(A)$. Integration by parts yields

$$S[r] = -\int_s^t \tfrac{1}{2} m r(\tau) \ddot{r}(\tau) d\tau = \int_s^t \tfrac{1}{2} m \dot{r}(\tau)^2 \, d\tau$$

for all $r \in C_0^2[s,t]$. This is the action of a free quantum particle on the real line with the boundary condition $r(s) = r(t) = 0$.

Proposition 7.49 *There holds* $\int_{C_0^2[s,t]} e^{\mathrm{i}S[r]/\hbar} \, \mathcal{D}_G r = \frac{1}{\sqrt{2(t-s)}} \left(\frac{m}{\hbar}\right)^{1/4} e^{-\mathrm{i}\pi/8}$.

Proof. To simplify notation, set $s := 0$. The crucial eigenvalue problem

$$A\varphi = \lambda\varphi, \qquad \varphi \in D(A)$$

corresponds to the equation $-\ddot{\varphi}(\tau) = \lambda\varphi(\tau), 0 < \tau < t$ with the boundary condition $\varphi(0) = \varphi(t) = 0$. The solutions are

$$\varphi_n(\tau) := \text{const} \cdot \sin\sqrt{\lambda_n}\tau, \qquad \lambda_n := \left(\frac{n\pi}{t}\right)^2, \qquad n = 1, 2, \ldots$$

For all complex numbers z with $\Re(z) > \frac{1}{2}$, the zeta function ζ_A of the operator A is given by the convergent series

$$\zeta_A(z) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n^z} = \left(\frac{t}{\pi}\right)^{2z} \sum_{n=1}^{\infty} \frac{1}{n^{2z}} = \left(\frac{t}{\pi}\right)^{2z} \zeta(2z).$$

Here, ζ denotes the Riemann zeta function. Note that ζ can be analytically continued to a holomorphic function on the pointed plane $\mathbb{C} \setminus \{1\}$. Here, $\zeta(0) = -\frac{1}{2}$ and $\zeta'(0) = -\frac{1}{2} \ln 2\pi$. Hence $\zeta_A(0) = -\frac{1}{2}$ and

$$\zeta_A'(0) = 2\zeta(0)(\ln t - \ln \pi) + 2\zeta'(0) = -\ln 2t.$$

This implies $\det A = \mathrm{e}^{-\zeta_A'(0)} = 2t$. Set $\gamma := \frac{m}{\hbar \mathrm{i}}$. By (7.201), the integral $\int_{C_0^2[0,t]} \mathrm{e}^{\mathrm{i}S[r]/\hbar}\, \mathcal{D}_G r$ is equal to

$$\int_{C_0^2[0,t]} \mathrm{e}^{-\frac{1}{2}\gamma\langle r|Ar\rangle} \mathcal{D}_G r = \frac{\mathrm{e}^{-\frac{1}{2}\zeta_A(0)\ln\gamma}}{\sqrt{\det A}} = \frac{1}{\sqrt{2t}} \left(\frac{m}{\hbar \mathrm{i}}\right)^{1/4}.$$

This is the desired result. □

7.9.3 Application to the Free Quantum Particle

Consider the motion of a free quantum particle on the real line. In Theorem 7.16 on page 488, we have computed the corresponding Feynman propagator kernel

$$\mathcal{K}(x,t;y,s) = \sqrt{\frac{m}{2\pi\hbar \mathrm{i}(t-s)}}\ \mathrm{e}^{\mathrm{i}m(x-y)^2/2\hbar(t-s)} \tag{7.203}$$

for all positions $x, y \in \mathbb{R}$ and all times $t > s$.[97] In addition, we have shown that the dynamics of the free quantum particle is governed by the formula

$$\boxed{\psi(x,t) := \int_{\mathbb{R}} \mathcal{K}(x,t;y,s)\psi(y,s)\, dy, \quad x \in \mathbb{R}, t > s.} \tag{7.204}$$

If we know the Schrödinger wave function ψ of the free particle at time s, then the kernel formula (7.204) tells us how to obtain the wave function at the later time t. This explains the importance of the Feynman propagator kernel. In Prop. 7.44 on page 550, we have proved that

$$\mathcal{K}(x,t;y,s) = \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q.$$

That is, the Feynman propagator kernel can be represented by a Feynman path integral. In this section, it is our goal to prove that

[97] Recall that the square root is to be understood as principal value. Explicitly,

$$\sqrt{\frac{m}{2\pi\hbar \mathrm{i}(t-s)}} = \mathrm{e}^{-\mathrm{i}\pi/4} \sqrt{\frac{m}{2\pi\hbar(t-s)}}.$$

$$\mathcal{K}(x,t;y,s) = \mathcal{N} \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}_G q.$$

This implies the key formula

$$\boxed{\mathcal{K}(x,t;y,s) = \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q = \mathcal{N} \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}_G q} \tag{7.205}$$

for all positions $x, y \in \mathbb{R}$ and all times $t > s$. This formula tells us the crucial fact that the Feynman path integral coincides with the corresponding normalized infinite-dimensional Gaussian integral, up to some normalization factor $\mathcal{N}$. Explicitly, $\mathcal{N} = \left(\frac{m}{\pi^2\hbar}\right)^{1/4} \mathrm{e}^{-\mathrm{i}\pi/8}$.

The classical trajectory. The action of a classical free particle of mass m on the real line is given by

$$S[q] := \int_s^t \tfrac{1}{2} m \dot{q}(\tau)^2 \, d\tau.$$

The boundary-value problem

$$m\ddot{q}(\tau) = 0, \quad s < \tau < t, \quad q(s) = y,\ q(t) = x$$

corresponds to the motion of the particle with given endpoints. The unique solution is $q_{\mathrm{class}}(\tau) = y + \frac{\tau - s}{t - s}(x - y)$ with the classical action

$$S[q_{\mathrm{class}}] = \int_s^t \tfrac{1}{2} m \dot{q}_{\mathrm{class}}(\tau)^2 d\tau = \frac{m(x-y)^2}{2(t-s)}.$$

Quantum fluctuations and the WKB relation. In order to study perturbations of the classical trajectory, we consider the trajectories

$$q(\tau) = q_{\mathrm{class}}(\tau) + r(\tau), \qquad \tau \in [s,t]$$

where $r \in C_0^2[s,t]$, that is, the function $r : [s,t] \to \mathbb{R}$ is twice continuously differentiable and satisfies the boundary condition $r(s) = r(t) = 0$. By (7.159) on page 550,

$$S[q] = S[q_{\mathrm{class}}] + S[r]. \tag{7.206}$$

For the Feynman propagator kernel, it follows from (7.203) that

$$\boxed{\mathcal{K}(x,t;y,s) = \mathrm{e}^{\mathrm{i}S[q_{\mathrm{class}}]/\hbar}\, \mathcal{K}_{\mathrm{fluct}}(t;s)} \tag{7.207}$$

for all positions $x, y \in \mathbb{R}$ and all times $t > s$, with the fluctuation term

$$\mathcal{K}_{\mathrm{fluct}}(t;s) := \sqrt{\frac{m}{2\pi\hbar \mathrm{i}(t-s)}}.$$

Equation (7.207) is called the WKB relation for the free quantum particle. It shows that the Feynman propagator is the product of the purely classical factor $\mathrm{e}^{\mathrm{i}S[q_{\mathrm{class}}]/\hbar}$ with a factor caused by quantum fluctuations.

The key relation. Motivated by the decomposition formula (7.206), we define

$$\int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}_G q := \mathrm{e}^{\mathrm{i}S[q_{\mathrm{class}}]/\hbar} \int_{C_0^2[s,t]} \mathrm{e}^{\mathrm{i}S[r]/\hbar}\, \mathcal{D}_G r.$$

Prop. 7.49 on page 573 tells us that

$$\int_{C_0^2[s,t]} \mathrm{e}^{\mathrm{i}S[r]/\hbar}\, \mathcal{D}_G r = \frac{\mathcal{K}_{\mathrm{fluct}}(t;s)}{\mathcal{N}}$$

with the normalization constant $\mathcal{N} = \left(\frac{m}{\pi^2\hbar}\right)^{1/4} \mathrm{e}^{-\mathrm{i}\pi/8}$. This implies the key formula (7.205).

7.9.4 Application to the Quantized Harmonic Oscillator

Parallel to the free quantum particle in the preceding section, let us now study the harmonic oscillator of mass $m > 0$ and angular frequency $\omega > 0$ on the real line. Introduce the characteristic length $x_0 := \sqrt{\frac{\hbar}{m\omega}}$. Furthermore, choose the time parameter in such a way that

$$t \;\in\;]s + t_{n,\mathrm{crit}}, s + t_{n+1,\mathrm{crit}}[, \qquad n = 0, 1, 2, \ldots \tag{7.208}$$

Here, the critical points of time are defined by $t_{n,\mathrm{crit}} := \frac{n\pi}{\omega}$. In addition, we introduce the Maslov index by $\mu(s,t) := n$. By formula (7.144) on page 537, we have computed the Feynman propagator kernel for the quantized harmonic oscillator:

$$\mathcal{K}(x,t;y,s) = \frac{\mathrm{e}^{-\mathrm{i}\pi/4}\, \mathrm{e}^{-\mathrm{i}\pi\mu(s,t)/2}}{x_0\sqrt{2\pi|\sin\omega(t-s)|}} \;\exp\left(\mathrm{i}\frac{(x^2+y^2)\cos\omega(t-s) - 2xy}{2x_0^2\sin\omega(t-s)}\right).$$

This formula is valid for all all positions $x, y \in \mathbb{R}$ and all non-critical times $t > s$ from (7.208).

The classical trajectory. The action of the classical harmonic oscillator is given by

$$S[q] := \int_s^t \tfrac{1}{2}m\dot{q}(\tau)^2 - \tfrac{1}{2}m\omega^2 q(\tau)^2 \, d\tau.$$

The boundary-value problem

$$\ddot{q}(\tau) + \omega^2 q(\tau) = 0, \quad s < \tau < t, \quad q(s) = y,\ q(t) = x \tag{7.209}$$

has the solution $q_{\mathrm{class}}(\tau) = y\cos\omega(\tau - s) + \big(x - y\cos\omega(\tau - s)\big)\, \frac{\sin\omega(\tau-s)}{\sin\omega(t-s)}$. This is a classical trajectory with the action

$$S[q_{\mathrm{class}}] = \hbar \cdot \frac{(x^2+y^2)\cos\omega(t-s) - 2xy}{2x_0^2\sin\omega(t-s)}\;.$$

Note that the trajectory q_{class} is the unique solution of (7.209) if t is a non-critical point of time. The uniqueness is violated for critical points of time. In what follows, we only consider non-critical points of time (7.208).

Quantum fluctuations and the WKB relation. Now use the perturbed trajectory

$$q(t) = q_{\mathrm{class}}(\tau) + r(\tau), \qquad \tau \in [s,t],$$

where $r \in C_0^2[s,t]$, that is, the function $r : [s,t] \to \mathbb{R}$ is twice continuously differentiable and satisfies the boundary condition $r(s) = r(t) = 0$. By (7.165) on page 552, we get

$$S[q] = S[q_{\text{class}}] + S[r]. \tag{7.210}$$

The Feynman propagator kernel for the quantized harmonic oscillator can be written as

$$\boxed{\mathcal{K}(x,t;y,s) = \mathrm{e}^{\mathrm{i}S[q_{\text{class}}]/\hbar}\, \mathcal{K}_{\text{fluct}}(t;s)} \tag{7.211}$$

with the quantum fluctuation term

$$\mathcal{K}_{\text{fluct}}(t;s) := \frac{\mathrm{e}^{-\mathrm{i}\pi/4}\, \mathrm{e}^{-\mathrm{i}\pi\mu(s,t)/2}}{x_0\sqrt{2\pi|\sin\omega(t-s)|}}.$$

This is a special case of the WKB method (see (7.216) on page 581). Observe that the fluctuation term is independent of the position coordinates x and y.

Now we restrict ourselves to the first critical time interval, that is, we assume that $t \in]s, s + t_{1,\text{crit}}[$.

Our goal is the key relation (7.214) below. Let us first compute the following normalized infinite-dimensional Gaussian integral.

Proposition 7.50 *For all times* $t \in]s, s + t_{1,\text{crit}}[$, *we have*

$$\int_{C_0^2[s,t]} \mathrm{e}^{\mathrm{i}S[r]/\hbar}\, \mathcal{D}_G r = \frac{\mathcal{K}_{\text{fluct}}(t;s)}{\mathcal{N}(\omega)}. \tag{7.212}$$

The complex non-zero constant $\mathcal{N}(\omega)$ *will be determined below.*

Proof. We will proceed as in the proof of Prop. 7.49 on page 573. To simplify notation, set $s := 0$. For $r \in C_0^2[0,t]$, integration by parts yields

$$\frac{\mathrm{i}S[r]}{\hbar} = \frac{\mathrm{i}m}{2\hbar}\int_0^t r(\tau)\left(-\ddot{r}(\tau) - \omega^2 r(\tau)\right)\, d\tau = -\tfrac{1}{2}\gamma\langle r|Br\rangle$$

with $\gamma := \frac{m}{\hbar \mathrm{i}}$. Here, we introduce the differential operator $B : D(B) \to L_2(\mathbb{R})$ with

$$Br := -\frac{d^2 r}{d\tau^2} - \omega^2 r^2$$

and the domain of definition $D(B) := C_0^2[0,t]$.

(I) The infinite-dimensional Gaussian integral. By (7.201) on page 572, we get

$$\int_{C_0^2[0,t]} \mathrm{e}^{-\frac{1}{2}\gamma\langle r|Br\rangle}\mathcal{D}_G r := \frac{\mathrm{e}^{-\frac{1}{2}\zeta_B(0)\ln\gamma}}{\sqrt{\det B}}. \tag{7.213}$$

We have to compute the determinant $\det B = \mathrm{e}^{-\zeta_B'(0)}$.

(II) The eigenvalues. The crucial eigenvalue problem

$$B\varphi = \lambda\varphi, \qquad \varphi \in D(B)$$

corresponds to the equation $-\ddot{\varphi}(\tau) - \omega^2 q(\tau) = \lambda\varphi(\tau), 0 < \tau < t$ with the boundary condition $\varphi(0) = \varphi(t) = 0$. The solutions are

$$\varphi_n(\tau) := \text{const} \cdot \sin\sqrt{\lambda_n}\tau, \qquad \lambda_n := \left(\frac{n\pi}{t}\right)^2 - \omega^2, \qquad n = 1, 2, \ldots$$

Let us also introduce $\mu_n := \left(\frac{n\pi}{t}\right)^2$ which is obtained from λ_n by setting $\omega = 0$.

(III) The zeta function: For all complex numbers z with $\Re(z) > \frac{1}{2}$, the zeta function ζ_B of the operator B is given by the convergent series

$$\zeta_B(z) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n^z} = \left(\frac{t}{\pi}\right)^{2z} \sum_{n=1}^{\infty} \frac{1}{\left(n^2 - \frac{t^2\omega^2}{\pi^2}\right)^z} \,.$$

Because of the boundary condition $r(0) = r(t) = 0$, the differential operator B can be regarded as an elliptic differential operator on a circle, which is the simplest example of a compact Riemannian manifold. There exists a general theory of elliptic operators on compact Riemannian manifolds which tells us that the corresponding zeta function can be analytically extended to a meromorphic function on the complex plane, and this extension is holomorphic at the origin $z = 0$ (see Gilkey (1995) and Kirsten (2002)). Therefore, $\zeta_B(0)$ and $\zeta_B'(0)$ are well-defined, and we can use the method of zeta-function regularization. In order to get quickly an explicit result, we will introduce a modified method which is used by physicists.

(IV) The determinant $\det B$. Formally, we get

$$\det B = \prod_{n=1}^{\infty} \lambda_n = \prod_{n=1}^{\infty} \mu_n \prod_{n=1}^{\infty} \left(1 - \frac{\omega^2}{\mu_n}\right).$$

By the classical Euler formula, we have the following convergent product

$$\sin z = z \prod_{n=1}^{\infty} \left(1 - \frac{z^2}{n^2\pi^2}\right), \qquad z \in \mathbb{C}.$$

Hence $\det B = \frac{\sin \omega t}{\omega t} \prod_{n=1}^{\infty} \mu_n$. The product $\prod_{n=1}^{\infty} \mu_n$ is divergent. In order to regularize $\det B$ it is sufficient to regularize $\prod_{n=1}^{\infty} \mu_n$. However, this product is the determinant of the operator B with $\omega = 0$ which coincides with the operator A from the proof of Prop. 7.49 on page 573. By this proof, $\det A = 2t$. Therefore, we define

$$\det B := \left(\prod_{n=1}^{\infty} \mu_n\right)_{\text{reg}} \prod_{n=1}^{\infty} \left(1 - \frac{\omega^2}{\mu_n}\right) = 2t \cdot \frac{\sin \omega t}{\omega t} = \frac{2 \sin \omega t}{\omega}.$$

(V) The constant $\mathcal{N}(\omega)$. By (7.213), the integral $\int_{C_0^2[0,t]} \mathrm{e}^{\mathrm{i}S[r]/\hbar} \mathcal{D}_G r$ is equal to

$$\frac{\mathrm{e}^{-\frac{1}{2}\zeta_B(0)\ln\gamma}\sqrt{\omega}}{\sqrt{2\sin\omega t}} = \frac{\mathcal{K}_{\text{fluct}}(t;0)}{\mathcal{N}(\omega)} = \frac{\mathrm{e}^{-\mathrm{i}\pi/4}}{\mathcal{N}(\omega) x_0 \sqrt{2\pi \sin \omega t}},$$

where $\gamma = \frac{m}{\hbar \mathrm{i}}$ and $x_0 = \sqrt{\frac{\hbar}{m\omega}}$. This yields $\mathcal{N}(\omega) = \mathrm{e}^{-\mathrm{i}\pi/4} \mathrm{e}^{\frac{1}{2}\zeta_B(0)\ln\gamma} \sqrt{\frac{m}{\pi\hbar}}$. □

The key relation. Motivated by the decomposition formula (7.210), we define

$$\int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar} \, \mathcal{D}_G q := \mathrm{e}^{\mathrm{i}S[q_{\text{class}}]/\hbar} \int_{C_0^2[s,t]} \mathrm{e}^{\mathrm{i}S[r]/\hbar} \, \mathcal{D}_G r.$$

It follows from Prop. 7.50 together with (7.211) that

$$\mathcal{K}(x,t;y,s) = \mathcal{N}(\omega) \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar} \, \mathcal{D}_G q$$

for all $x, y \in \mathbb{R}$ and all $t \in]s, s + t_{1,\mathrm{crit}}[$. By Prop. 7.45 on page 552,

$$\mathcal{K}(x,t;y,s) = \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q.$$

This implies the desired key relation

$$\boxed{\mathcal{K}(x,t;y,s) = \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q = \mathcal{N}(\omega) \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}_G q} \tag{7.214}$$

for all positions $x, y \in \mathbb{R}$ and all times $t \in]s, s + t_{1,\mathrm{crit}}[$. Observe that for $\omega = 0$, the normalization factor $\mathcal{N}(0) = \left(\frac{m}{\pi^2\hbar}\right)^{1/4} \mathrm{e}^{-\mathrm{i}\pi/8}$ is the same as for the free quantum particle.

The free quantum particle as a limit. For all times $t \in]s, s + t_{1,\mathrm{crit}}[$ and all positions $x, y \in \mathbb{R}$, we have

$$\mathcal{K}(x,t;y,s) = \frac{1}{x_0\sqrt{2\pi\mathrm{i}\sin\omega(t-s)}} \quad \exp\left(\mathrm{i}\frac{(x^2+y^2)\cos\omega(t-s) - 2xy}{2x_0^2\sin\omega(t-s)}\right).$$

Noting that $\lim_{\omega\to+0} x_0^2 \sin\omega(t-s) = \frac{\hbar(t-s)}{m} \lim_{\omega\to+0} \frac{\sin\omega(t-s)}{\omega(t-s)} = \frac{\hbar(t-s)}{m}$, we obtain the limit relation

$$\lim_{\omega\to+0} \mathcal{K}(x,t;y,s) = \mathcal{K}_{\mathrm{free}}(x,t;y,s) = \sqrt{\frac{m}{2\pi\hbar\mathrm{i}(t-s)}}\ \mathrm{e}^{\mathrm{i}m(x-y)^2/2\hbar(t-s)}.$$

This tells us the quite natural fact that the Feynman propagator kernel of the quantized harmonic oscillator passes over to the Feynman propagator kernel of the free quantum particle if the angular frequency ω goes to zero.

7.9.5 The Spectral Hypothesis

Motivated by the rigorous results above for the free quantum particle and the quantized harmonic oscillator, we formulate the following general spectral hypothesis:

$$\int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}q = \mathcal{N} \int_{C\{s,t\}} \mathrm{e}^{\mathrm{i}S[q]/\hbar}\, \mathcal{D}_G q. \tag{7.215}$$

This hypothesis tells us that the Feynman path integral coincides with the corresponding normalized infinite-dimensional Gaussian integral, up to a normalization factor $\mathcal{N}$ which depends on the action functional S. Physicists take this spectral hypothesis for granted in both quantum mechanics and quantum field theory. The experience of physicists shows that this hypothesis works well as a universal tool. In terms of mathematics, it turns out that this heuristic tool also works well for conjecturing new topological invariants in the setting of topological quantum field theory and string theory. For example, this concerns knot theory, smooth manifolds in differential geometry, and algebraic varieties (generalized manifolds including singularities) in algebraic geometry.

7.10 The Semi-Classical WKB Method

> The WKB method in physics is the prototype of singular perturbation theory in mathematics.
>
> Folklore

> To the best of our knowledge, the first paper on path integrals, apart from Feynman's, written by a physicist was submitted by Cécile Morette in 1950.[98]
> During Pauli's stay at the Institute for Advanced Study in 1949, Morette and Van Hove presented to Pauli at the occasion of an appointment with him a semiclassical formula (S) for quantum mechanics based on Morette's approach to path integrals... Pauli wrote a number of research notes ... In these notes Pauli corrected a sign factor, and he obtained the important (exact) result that for small time intervals, the semiclassical propagator kernel from (S) satisfies the Schrödinger equation up to order $\hbar^2$ ...
> Pauli was, to the best of our knowledge, the first of the older generation, having laid the foundations of quantum mechanics, who fully appreciated the new approach developed by Feynman.[99]
>
> Christian Grosche and Frank Steiner, 1998

Approximation methods play an important role in physics in order to simplify computation and to get insight. Let us study an important approximation method in quantum mechanics called the WKB method.[100] The dynamics of a particle in quantum mechanics is governed by the equation

$$\psi(t) = \mathrm{e}^{-\mathrm{i}H(t-s)/\hbar}\psi(s), \qquad t \geq s.$$

The quantum particle behaves approximately like a classical particle if Planck's quantum of action is small, $\hbar \to 0$. More precisely, we have to assume that the dimensionless quotient $S/\hbar$ is large where S is the action (energy times $t-s$). The WKB method investigates the semi-classical approximation of quantum processes with respect to the limit

$$\hbar \to 0.$$

The two key formulas for the motion of quantum particles in the 3-dimensional Euclidean space read as follows:

(K) Time evolution of Schrödinger's wave function:

$$\psi(\mathbf{x}, t) = \int_{\mathbb{R}^3} \mathcal{K}(\mathbf{x}, t; \mathbf{y}, s)\psi(\mathbf{y}, s)d^3y, \qquad \mathbf{x} \in \mathbb{R}^3, \quad t > s.$$

We assume that the function $\mathbf{y} \mapsto \psi(\mathbf{y}, s)$ is smooth with compact support (at the initial time s).

---

[98] C. Morette, On the definition and approximation of Feynman's path integral, Phys. Rev. **81** (1951), 848–852.

[99] This slightly modified quotation is taken from C. Grosche and F. Steiner, Handbook of Feynman Path Integrals, Springer, Berlin, 1998 (reprinted with permission).

[100] The three letters 'WKB' refer to the physicists 'Wentzel, Kramers, and Brioullin'. The basic papers are quoted on page 484.

Fig. 7.1. Classical trajectories

(A) Approximation of the propagator kernel as $\hbar \to 0$:

$$\boxed{\mathcal{K}(\mathbf{x},t;\mathbf{y},s) = \mathrm{e}^{\mathrm{i}S[\mathbf{q}]/\hbar}\ \frac{\mathrm{e}^{-3\mathrm{i}\pi/4}\ \mathrm{e}^{-\mathrm{i}\pi\mu(s,t)/2}}{h^{3/2}|\det J(t)|^{1/2}}\ (1+O(\hbar)).} \tag{7.216}$$

Here, $S[\mathbf{q}]$ is the action of the classical trajectory $\mathbf{q} = \mathbf{q}(\tau)$ which connects the point $\mathbf{y}$ at the initial time s with the point $\mathbf{x}$ at the final time t (Fig. 7.1(a)).[101] Furthermore, $\mu(s,t)$ denotes the Morse index (or Maslov index) of the trajectory $\mathbf{q} = \mathbf{q}(\tau)$ on the time interval $[s,t]$. Roughly speaking, the Morse index measures the number and the structure of the focal points on the trajectory. The use of the Morse index allows us to obtain a global formula for large times. As a rule, the Morse index jumps at focal points of the trajectory. Now let us discuss this more precisely.[102]

Classical particle. We start with the Newtonian equation of motion

$$m\ddot{\mathbf{q}}(\tau) = -U'(\mathbf{q}), \qquad s \le \tau \le t \tag{7.217}$$

for the trajectory

$$C : \mathbf{q} = \mathbf{q}(\tau), \qquad s \le \tau \le t$$

of a classical particle of mass m in the 3-dimensional Euclidean space. The potential $U = U(\mathbf{q})$ is assumed to be a smooth real-valued function. The action along the trajectory C is given by

$$\boxed{S[\mathbf{q}] := \int_s^t (\tfrac{1}{2}m\dot{\mathbf{q}}(\tau)^2 - U(\mathbf{q}(\tau))d\tau.}$$

For the trajectory C, we also study the corresponding Jacobi equation,

$$m\ddot{J}(\tau) + U''(\mathbf{q}(\tau))J(\tau) = 0, \qquad s \le \tau \le t,$$

along with the initial conditions $J(s) = 0$ and $\dot{J}(s) = m^{-1}I$.[103]

[101] The case where several trajectories connect the point $\mathbf{y}$ with the point $\mathbf{x}$ will be considered in (7.218) below. This corresponds to Fig. 7.1(b).

[102] The WKB method is always used in physics if a typical physical parameter goes to zero. For example, this concerns the following limits: $T \to 0$ (low temperature), $\lambda \to 0$ (short wavelength), $1/c \to 0$ (low velocity), $\nu \to 0$ (low viscosity). In terms of mathematics, the WKB method is part of singular perturbation theory.

[103] Explicitly, for the real symmetric (3×3)-matrix $J = (J_{kl})$, we get

$$m\ddot{J}_{kl}(\tau) + \sum_{r=1}^{3} \frac{\partial^2 U}{\partial x_k \partial x_r}(\mathbf{q}(\tau))J_{rl}(\tau) = 0, \qquad k,l = 1,2,3.$$

Morse index. By definition, the Morse index of the trajectory C is equal to the number of negative eigenvalues λ of the Jacobi eigenvalue problem

$$-m\ddot{\mathbf{h}}(\tau) - U''(\mathbf{q}(\tau))\mathbf{h}(\tau) = \lambda \mathbf{h}(\tau), \qquad s \le \tau \le t$$

along with the boundary condition $\mathbf{h}(s) = \mathbf{h}(t) = 0$.

Quantum particle. The Schrödinger equation for the corresponding quantum particle reads as

$$\mathrm{i}\hbar\psi_t(\mathbf{x}, t) = -\frac{\hbar^2}{2m}\,\Delta\psi(\mathbf{x}, t) + U(\mathbf{x})\psi(\mathbf{x}, t).$$

Semi-classical approximation. The approximation formula (7.216) is valid under the following assumptions.[104]

(H1) Uniqueness: There exists a unique solution $\mathbf{q} = \mathbf{q}(\tau)$, $s \le \tau \le t$, of the classical equation of motion (7.217) which satisfies the boundary condition

$$\mathbf{q}(s) = \mathbf{y}, \qquad \mathbf{q}(t) = \mathbf{x}$$

for given $\mathbf{y}, t, \mathbf{x}, s$ (Fig. 7.1(a) on page 581).

(H2) Regularity of the trajectory: At the final time t, the matrix $J(t)$ is invertible. Here, $\tau \mapsto J(\tau)$ is the solution of the Jacobi equation with respect to the trajectory from (H1).

Modifications. Replace (H1) by the assumption that the boundary value problem has not a unique solution, but at most a finite number of trajectories $\mathbf{q} = \mathbf{q}_n(\tau)$, $n = 1, \dots, N$ (Fig. 7.1(b) on page 581). In addition, assume that all of these trajectories are regular in the sense of (H2). Then, the formula (7.216) has to be replaced by the following sum formula as $\hbar \to 0$:

$$\boxed{\mathcal{K}(\mathbf{x}, t; \mathbf{y}, s) = \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}S[\mathbf{q}_n]/\hbar}\, \frac{\mathrm{e}^{-d\mathrm{i}\pi/4}\, \mathrm{e}^{-\mathrm{i}\pi\mu_n(s,t)/2}}{\hbar^{d/2}|\det J_n(t)|^{1/2}}\, (1 + O(\hbar))} \tag{7.218}$$

with $d = 3$. For motions of the particles on the real line and in the Euclidean plane, we have to choose $d = 1$ and $d = 2$, respectively. The formula (7.218) is precise (i.e., $O(\hbar) = 0$) if the potential U is a quadratic function.

Small time intervals. If the time interval $[s, t]$ is sufficiently small, then it follows from

$$J_n(t) = \frac{t - s}{m}\, I + O((t - s)^2)$$

that $\det J_n(t) \neq 1$. Moreover, $\mu_n(s, t) = 0$. This simplifies the key formula (7.218).

The quantized harmonic oscillator. To get insight, let us consider the equation of motion

$$\ddot{q}(\tau) = -\omega^2 q(\tau), \qquad 0 \le \tau \le t$$

for a classical harmonic oscillator on the real line. Here, $t > 0$. Add the boundary condition[105] $q(0) = y, q(t) = x$. This problem has the unique solution

[104] A sketch of the proof based on the path integral can be found in C. Grosche and F. Steiner, Handbook of Feynman Path Integrals, Sect. 5.2, Springer, Berlin, 1998. For the full proof embedded into a general setting, see the monograph by V. Guillemin and S. Sternberg, Geometric Asymptotics, Sect. II.7, Amer. Math. Soc., Providence, Rhode Island, 1989.

[105] To simplify notation, we set $s = 0$.

$$q(\tau) = y\cos\omega\tau + (x - y\cos\omega t)\frac{\sin\omega\tau}{\sin\omega t}$$

if the given time t is different from the critical time points $t_{n,\mathrm{crit}} := n\pi/\omega$ with $n = 1, 2, ...$ This yields the action

$$S[q] = \int_0^t (\tfrac{1}{2}m\dot{q}(\tau)^2 - \tfrac{1}{2}m\omega^2 q(\tau)^2)d\tau = \frac{(x^2+y^2)\cos\omega t - 2xy}{2x_0^2\sin\omega t}.$$

The Jacobi equation reads as

$$\ddot{J}(\tau) + \omega^2 J(\tau) = 0, \qquad 0 \le \tau \le t, \qquad J(0) = 0,\ \dot{J}(0) = \frac{1}{m}.$$

Hence

$$J(t) = \frac{\sin\omega t}{m}.$$

If $t \neq t_{n,\mathrm{crit}}$, then $J(t) \neq 0$. To compute the Morse index, consider the Jacobi eigenvalue problem

$$-\ddot{h}(\tau) - \omega^2 h(\tau) = \lambda h(\tau), \qquad 0 \le \tau \le t, \quad h(0) = h(t) = 0.$$

If $0 < t\omega < \pi$, then there is no negative eigenvalue. Hence $\mu(0,t) = 0$. However, if $n\pi < t\omega < (n+1)\pi$ with $n = 1, 2, ...$ then there are precisely n negative eigenvalues,

$$\lambda_k = \frac{k^2\pi^2}{t^2} - \omega^2, \qquad k = 1, \ldots, n$$

along with the eigenfunctions $q = \sin\tau\sqrt{\lambda_k + \omega^2}$, $k = 1, ..., n$. This way, for the harmonic oscillator, formula (7.218) reads as

$$\boxed{\mathcal{K}(x,t;y,0) = \frac{\mathrm{e}^{-\mathrm{i}\pi/4}\,\mathrm{e}^{-\mathrm{i}\pi n/2}}{x_0\sqrt{2\pi|\sin\omega t|}}\ \exp\left(\mathrm{i}\frac{(x^2+y^2)\cos\omega t - 2xy}{2x_0^2\sin\omega t}\right)} \tag{7.219}$$

for all times t with $n\pi < t\omega < (n+1)\pi$, $n = 0, 1, 2, ...$ Here, we introduce the characteristic length $x_0 := \sqrt{\hbar/m\omega}$. This is a precise formula for $\mathcal{K}$; it coincides with formula (7.144) on page 537.

The freely moving quantum particle on the real line. Let $t > 0$. We start with the classical equation of motion

$$\ddot{q}(\tau) = 0, \quad 0 \le \tau \le t.$$

Adding the boundary condition $q(0) = y, q(t) = x$, we get the unique solution $q(\tau) = y + \tau(x-y)/t$. This yields the classical action

$$S[q] = \int_0^t \tfrac{1}{2}m\dot{q}(\tau)^2 d\tau = \frac{m(x-y)^2}{2t}.$$

The Jacobi equation

$$\ddot{J}(\tau) = 0, \qquad 0 \le \tau \le t, \qquad J(0) = 0,\ \dot{J}(0) = \frac{1}{m}$$

yields $J(t) = t/m$. The Jacobi eigenvalue problem

$$-\ddot{h}(\tau) = \lambda h(\tau), \qquad 0 \le \tau \le t, \quad h(0) = h(t) = 0$$

has no negative eigenvalues. Hence $\mu(0,t) = 0$. By (7.218) with $d = 1$, we obtain

$$\mathcal{K}(x,t;y,0) = \mathrm{e}^{-\mathrm{i}\pi/4} \cdot \sqrt{\frac{m}{2\pi\hbar t}}\ \mathrm{e}^{\mathrm{i}m(x-y)^2/2\hbar t}.$$

This coincides with the Feynman propagator kernel (7.157) on page 550.

7.11 Brownian Motion

In order to understand the beauty of Feynman's approach to quantum mechanics, one has to understand the Brownian motion of immersed particles and its relation to diffusion processes.

Folklore

7.11.1 The Macroscopic Diffusion Law

We want to consider the diffusion of particles of mass $m > 0$ on the real line. Let $\varrho(x,t) > 0$ denote the mass density of the particles at the position x at time t. Then the basic diffusion equation reads as

$$\boxed{\varrho_t(x,t) = \kappa \varrho_{xx}(x,t), \qquad x \in \mathbb{R},\ t \in \mathbb{R}.} \tag{7.220}$$

Here, the positive number κ is called the diffusion coefficient. Let us motivate this.

Conservation of mass. Let $\mathbf{v}(x,t) = v(x,t)\mathbf{i}$ denote the velocity vector of the particles at the point x at time t. Here, the unit vector $\mathbf{i}$ points in direction of the positive x-axis. Furthermore, we introduce the mass current density vector

$$\mathbf{J}(x,t) := \varrho(x,t)\mathbf{v}(x,t).$$

We have $\mathbf{J}(x,t) = J(x,t)\mathbf{i}$ where

$$J(x,t) = \lim_{\Delta t \to 0} \frac{M(x;t,t+\Delta t)}{\Delta t}.$$

Here, $M(x;t,t+\Delta t)$ is the mass which flows through the point x from left to right during the time interval $[t,t+\Delta t]$. Conservation of mass tells us that the change of mass on the compact interval $[a,b]$ during the time interval $[t,t+\Delta t]$ is equal to the mass which flows through the boundary points during the time interval $[t,t+\Delta t]$. Explicitly, for small Δt, we obtain

$$\int_a^b (\varrho(x,t+\Delta t) - \varrho(x,t))dt = J(a,t)\Delta t - J(b,t)\Delta t,$$

up to terms of order $o(\Delta t)$ as $\Delta t \to 0$. Letting $\Delta t \to 0$, we get

$$\int_a^b \varrho_t(x,t)dx = J(a,t) - J(b,t) = -\int_a^b J_x(x,t)dx.$$

Contracting the interval $[a,b]$ to the point x, we obtain

$$\varrho_t(x,t) = -J_x(x,t). \tag{7.221}$$

Fick's empirical diffusion law. Motivated by physical experiments, we assume that

$$J(x,t) = -\kappa \varrho_x(x,t).$$

That is, the mass current density is proportional to the (negative) spatial derivative of the mass density. By (7.221), we get the diffusion equation (7.220).

In the three-dimensional case, the one-dimensional diffusion equation (7.220) passes over to the three-dimensional diffusion equation

$$\varrho_t(\mathbf{x},t) = -\kappa \Delta \varrho(\mathbf{x},t) \tag{7.222}$$

with the position vector $\mathbf{x}$ and time t. Furthermore, $\Delta\varrho = -\varrho_{xx} - \varrho_{yy} - \varrho_{zz}$.

7.11.2 Einstein's Key Formulas for the Brownian Motion

We are going to consider the three-dimensional motion of particles of mass $m > 0$ suspended in a resting fluid. We assume that the suspended particles have a much greater mass than the molecules of the ambient fluid. The irregular motion of the suspended particles is caused by a large number of collisions with the molecules of the ambient fluid. In 1828 the botanist Robert Brown (1773–1858) observed first such an irregular motion under the microscope, which is called Brownian motion nowadays. In his famous 1905 paper, the young Einstein (1879–1955) derived the following two key formulas for the random Brownian motion.[106]

(i) Fluctuation of the position vector $\mathbf{x}$ of a single suspended particle:

$$(\Delta \mathbf{x})^2 = 6\kappa t. \tag{7.223}$$

(ii) The Stokes–Einstein relation between the diffusion coefficient D of the suspended particles and the viscosity η of the ambient fluid:

$$\kappa = \frac{kT}{6\pi\eta r}. \tag{7.224}$$

Here, T is the absolute temperature, k is the Boltzmann constant, and r is the radius of the suspended particles.

The physical motivation of the Einstein formulas can be found in Chap. 4 of the monograph by R. Mazo, Brownian Motion: Fluctuations, Dynamics, and Applications, Oxford University Press, 2002.

7.11.3 The Random Walk of Particles

The random model. We want to investigate the random walk of a particle on the real line. To this end, we set

$$x_j := j\Delta x, \quad j = 0, \pm 1, \pm 2, \dots \quad \text{and} \quad t_k := k\Delta t, \quad k = 0, 1, 2, \dots$$

We define

$$P(x_j, t_k) := \text{probability of finding the particle at the point } x_j \text{ at time } t_k.$$

We assume the following.

(i) The initial condition: The particle is at the origin $x_0 = 0$ at the initial time $t_0 = 0$. That is, $P(0, 0) = 1$. Moreover, $P(x_j, t_k) = 0$ if $x_j \neq 0$ or $t_k > 0$.

(ii) The transition condition: Suppose that the particle is at the point x_j at time t_k. Then it will be at the point x_{j+1} (resp. x_{j-1}) at time t_{k+1} with probability $\frac{1}{2}$. Applying this to the motion from x_{j-1} to x_j and from x_{j+1} to x_j, we obtain that, for all j, k,

$$P(x_j, t_{k+1}) = \tfrac{1}{2}P(x_{j-1}, t_k) + \tfrac{1}{2}P(x_{j+1}, t_k). \tag{7.225}$$

[106] A. Einstein, Die von der molekular-kinetischen Theorie der Wärme geforderte Behandlung von in ruhenden Flüssigkeiten suspendierten Teilchen (On the motion of suspended particles in a resting fluid by using the methods of molecular kinetics), Ann. Phys. **17** (1905), 549–560 (in German). English translation: J. Stachel (Ed.), Einstein's Miraculous Year 1905: Five Papers that Changed the Universe, Princeton University Press, 1998.

The probability for the particle position. Set $p(x,t) := \frac{\mathrm{e}^{-x^2/4\kappa t}}{\sqrt{4\pi\kappa t}}$. We claim that the number

$$\int_a^b p(x,t)dx \tag{7.226}$$

equals the probability of finding the particle in the interval $[a,b]$ at time t.

Motivation. In order to motivate (7.226), let us introduce the (discrete) probability density

$$p(x_j,t_k) := \frac{P(x_j,t_k)}{\Delta x}.$$

Then the number

$$\sum_{j=0}^{j_b} p(x_j,t_k)\Delta x$$

equals the probability of finding the particle in the interval $[0,b]$ at time t_k. Here, we choose $j_b := b/\Delta x$. By (7.225),

$$P(x_j,t_{k+1}) - P(x_j,t_k) = \tfrac{1}{2}(P(x_{j+1},t_k) - 2P(x_j,t_k) + P(x_{j-1},t_k)).$$

This implies

$$p(x,t+\Delta t) - p(x,t) = \tfrac{1}{2}(p(x+\Delta x,t) - 2p(x,t) + p(x-\Delta x,t)).$$

Hence

$$\frac{p(x,t+\Delta t) - p(x,t)}{\Delta t} = \frac{p(x+\Delta x,t) - 2p(x,t) + p(x-\Delta x,t)}{(\Delta x)^2} \cdot \frac{(\Delta x)^2}{2\Delta t}.$$

Letting $\Delta x \to 0$ and $\Delta t \to 0$ such that the quotient $(\Delta x)^2/2\Delta t$ goes to the positive number κ, then

$$p_t(x,t) = \kappa p_{xx}(x,t), \quad x \in \mathbb{R},\ t > 0. \tag{7.227}$$

In addition, we obtain the formal initial condition $p(x,0) = \delta(x)$ for all points $x \in \mathbb{R}$.[107] By the study of the diffusion equation on page 487, the solution of (7.227) reads as $p(x,t) = \frac{\mathrm{e}^{-x^2/4\kappa t}}{\sqrt{4\pi\kappa t}}$.

7.11.4 The Rigorous Wiener Path Integral

Probabilities of a continuous random walk. Let us consider the random walk of a particle on the real line with diffusion coefficient $\kappa > 0$. Choose the function

$$p(x,t) := \frac{\mathrm{e}^{-x^2/4\kappa t}}{\sqrt{4\pi\kappa t}},$$

and choose the points of time $0 < t_1 < \ldots < t_N := T$. Suppose that the particle is at the point $x_0 := 0$ at time $t_0 := 0$.

- The real number $\int_{J_1} p(x_1 - x_0, t_1 - t_0)dx_1$ is the probability of finding the particle on the interval J_1 at time t_1.

[107] This follows from the discrete initial condition $p(x_j,0) = \frac{P(x_j,0)}{\Delta x} = \frac{\delta_{j0}}{\Delta x}$ by letting $\Delta x \to 0$.

- The real number $\int_{J_1}\int_{J_2} p(x_1-x_0,t_1-t_0)p(x_2-x_1,t_2-t_1)dx_1dx_2$ is the probability of finding the particle on the interval J_1 and J_2 at time t_1 and t_2, respectively.
- The real number

$$\int_{J_1}\cdots\int_{J_N}\prod_{j=1}^{N} p(x_j-x_{j-1},t_j-t_{j-1})\,dx_1\cdots dx_N \tag{7.228}$$

  is the probability of finding the particle on the interval $J_1,\ldots,J_N$ at time $t_1,\ldots,t_N$, respectively.

The Wiener measure. We want to translate the preceding probabilities into the language of measure theory. Fix the time $T>0$. By definition, the function space $\mathcal{C}_0[0,T]$ consists of all continuous functions

$$q:[0,T]\to\mathbb{R}$$

with $q(0)=0$. Intuitively, $x=q(t)$, $0\le t\le T$, describes the trajectory of a Brownian particle on the real line. We want to construct a measure W on the space $\mathcal{C}_0[0,T]$ of trajectories such that, for each measurable subset Ω of $\mathcal{C}_0[0,T]$, the real number

$$W(\Omega)$$

equals the probability of finding the trajectory $q\in\mathcal{C}_0[0,T]$ in the set Ω. We will proceed in two steps.

Step 1: Pre-measure on cylindrical subsets. Let

$$\Omega_{\text{cyl}}:=\{q\in\mathcal{C}_0[0,T]:q(t_k)\in J_k,\ k=1,\ldots,N\}$$

where $0<t_1<\ldots<t_N:=T$, $N=1,2,\ldots$, and $J_1,\ldots J_N$ are intervals on the real line. We define the number $W(\Omega_{\text{cyl}})$ by (7.228). This number is called the Wiener pre-measure of the cylindrical set Ω_{cyl}.

Step 2: Extension of the pre-measure to the Wiener measure. The Wiener pre-measure on cylindrical sets can be extended to a measure on the function space $\mathcal{C}_0[0,T]$. This measure (called the Wiener measure) is uniquely determined on the smallest σ-algebra of $\mathcal{C}_0[0,T]$ which contains all the cylindrical sets. For general measure theory and measure integrals, see Sec. 10.2.1 of Vol. I. Furthermore, we refer to:

> H. Amann and J. Escher, Analysis, Vol. 3, Birkhäuser, Basel, 2001 (in German). (English edition in preparation.)
>
> E. Stein and R. Shakarchi, Princeton Lectures in Analysis, Vol. III: Measure Theory, Princeton University Press, 2003.

A detailed summary can be found in the Appendix to Zeidler (1986), Vol. IIB (see the references on page 1049).

Example. If $\mathcal{C}_0^1[0,T]$ denotes the set of all continuously differentiable functions $q:[0,T]\to\mathbb{R}$ with $q(0)=0$, then

$$W(\mathcal{C}_0^1[0,T])=0.$$

This tells us that the trajectory of a Brownian particle is continuously differentiable with probability zero. In fact, under the microscope one observes zigzag trajectories of Brownian motion.

The Wiener path integral. General measure theory tells us that the Wiener measure W on the function space $\mathcal{C}_0[0,T]$ induces the measure integral

$$\int_{\mathcal{C}_0[0,T]} F(q)\, dW(q)$$

for appropriate functions $F : \mathcal{C}_0[0,T] \to \mathbb{R}$. This integral is called the Wiener path integral. Here, we integrate over a set of trajectories. In particular, we have

$$\int_{\mathcal{C}_0[0,T]} F(q)\, dW(q) = \sum_{n=1}^{N} F_n W(\Omega_n)$$

if $\Omega_1, \ldots, \Omega_N$ is a collection of pairwise disjoint cylindrical sets of the function space $\mathcal{C}_0[0,T]$, and the real-valued function F has the constant values $F_1, \ldots, F_N$ on $\Omega_1, \ldots, \Omega_N$, respectively, and it vanishes outside these sets. If Ω is a measurable subset of the function space $\mathcal{C}_0[0,T]$ (e.g., a cylindrical set), then the Wiener measure of Ω is given by

$$W(\Omega) = \int_{\Omega} dW = \int_{\mathcal{C}_0[0,T]} \chi(q)\, dW(q)$$

where $\chi(q) := 1$ for all $q \in \Omega$ and $\chi(q) := 0$ for all $q \notin \Omega$.

7.11.5 The Feynman–Kac Formula

In 1947, Marc Kac (1914–1984) attended a lecture given by the young Richard Feynman (1918–1988) at Cornell University. He was amazed about the fact that Feynman's formula related the quantum mechanical propagator to classical mechanics in a very elegant way. He also noticed that Feynman's idea of the path integral was close to his own ideas about stochastic processes based on the Wiener integral due to Norbert Wiener (1894–1964). A few days later Kac rigorously proved a formula which is known nowadays as the Feynman–Kac formula. In his autobiography *Enigmas of Chance*, Harper & Row, New York, 1985, Marc Kac writes:

> It is only fair to say that I had Wiener's shoulders to stand on. Feynman as in everything else he has done, stood on its own, a trick of intellectual contortion that he alone is capable of.

In order to discuss the Feynman–Kac formula, let us consider the one-dimensional diffusion equation

$$\varrho_t(x,t) = \kappa \varrho_{xx}(x,t) - U(x)\varrho(x,t), \quad x \in \mathbb{R},\ t > 0 \tag{7.229}$$

with the initial condition $\varrho(x,0) = \varrho_0(x)$ for all $x \in \mathbb{R}$. We are given the positive diffusion constant κ, the real-valued potential $U \in C_0^\infty(\mathbb{R})$, and the real-valued initial mass density $\varrho_0 \in C_0^\infty(\mathbb{R})$. Define

$$\mathcal{H}\varrho := -\kappa \varrho_{xx} + U\varrho \qquad \text{for all} \quad \varrho \in C_0^\infty(\mathbb{R}).$$

The operator $\mathcal{H} : C_0^\infty(\mathbb{R}) \to L_2(\mathbb{R})$ can be uniquely extended to a self-adjoint operator $H : D(H) \to L_2(\mathbb{R})$ on the real Hilbert space $L_2(\mathbb{R})$. In terms of functional analysis, the solution of (7.229), that is, $\varrho_t = -H\varrho$, reads as

$$\varrho(t) = \mathrm{e}^{-tH}\varrho_0, \qquad t > 0. \tag{7.230}$$

The famous Feynman–Kac formula tells us the following.

Theorem 7.51 *For all times $T > 0$ and all positions $x \in \mathbb{R}$, the solution* (7.230) *of the diffusion equation* (7.229) *is given by*

$$\varrho(x,T) = \int_{\mathcal{C}_0[0,T]} \varrho_0(x + q(t))\, \mathrm{e}^{-\int_0^T U(x+q(t))dt}\, dW(q).$$

Intuitively, this is a statistics over all possible continuous trajectories of a particle which starts at the point x at time $t = 0$. The statistical weight is related to both the Wiener measure and an exponential function which depends on the potential U. The proof can be found in:

G. Johnson and M. Lapidus, The Feynman Integral and Feynman's Operational Calculus, Chap. 12, Clarendon Press, Oxford, 2000.

We also refer to:

M. Reed and B. Simon, Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness, Academic Press, New York, 1975.

B. Simon, Functional Integration and Quantum Physics, Academic Press, New York, 1979.

In terms of the limit of classical N-dimensional integrals, the solution $\varrho(t) = \mathrm{e}^{-tH}\varrho_0$ of the diffusion equation (7.229) can be represented as

$$\varrho(x,T) = \lim_{N\to\infty} \left(\sqrt{\frac{1}{4\pi\kappa\Delta t}}\right)^N PV \int_{-\infty}^{\infty} \dots PV \int_{-\infty}^{\infty} \varrho_0(q_N)\mathrm{e}^{S_N^-} dq_1 \dots dq_N \tag{7.231}$$

with $S_N^- := \sum_{j=0}^{N-1} -\frac{m}{2}\left(\frac{q_{j+1}-q_j}{\Delta t}\right)^2 - U(q_j)$, as well as $\Delta t := T/N$, $\kappa = 1/2m$, and $q_0 := x$.

Corollary 7.52 *For all times $T > 0$ and all positions $x \in \mathbb{R}$, we have* (7.231).

Note that the principal value $PV\int_{-\infty}^{\infty}\dots$ means $\lim_{r\to\infty}\int_{-r}^{r}\dots$, and the limit $N \to \infty$ refers to the convergence on the real Hilbert space $L_2(\mathbb{R})$. The proof based on the Trotter product formula (see Sect. 8.3 of Vol. I) can be found in Reed and Simon (1975), Vol. II, Sect. X.11, quoted above.

The passage to the Schrödinger equation. We replace the diffusion equation (7.229) by the Schrödinger equation

$$\mathrm{i}\hbar\varrho_t(x,t) = \mathcal{H}\varrho(x,t), \qquad x \in \mathbb{R},\, t > 0 \tag{7.232}$$

with the initial condition $\varrho(x,0) = \varrho_0(x)$ for all $x \in \mathbb{R}$. Here, we use the differential operator $\mathcal{H}\varrho := -\kappa\varrho_{xx} + U\varrho$ with $\kappa := \frac{\hbar^2}{2m}$. In terms of the limit of classical N-dimensional integrals, the solution $\varrho(t) = \mathrm{e}^{-\mathrm{i}tH/\hbar}\varrho_0$ of the Schrödinger equation (7.232) can be represented as follows: the function $\varrho(x,T)$ at the point x at time T is equal to the limit

$$\lim_{N\to\infty} \left(\sqrt{\frac{\hbar}{4\pi\mathrm{i}\kappa\Delta t}}\right)^N PV \int_{-\infty}^{\infty} \dots PV \int_{-\infty}^{\infty} \varrho_0(q_N)\mathrm{e}^{\mathrm{i}S_N/\hbar} dq_1 \dots dq_N \tag{7.233}$$

with the discrete action

$$S_N := \sum_{j=0}^{N-1} \frac{m}{2} \left(\frac{q_{j+1} - q_j}{\Delta t} \right)^2 - U(q_j),$$

as well as $\Delta t := T/N$ and $q_0 := x$. The square root is to be understood as principal value.

Corollary 7.53 *For all times $T > 0$ and all positions $x \in \mathbb{R}$, we have* (7.233).

Here, the limits are to be understood as in Corollary 7.52. Naturally enough, formula (7.233) is obtained from (7.231) by rescaling. The proof of Corollary 7.53 can be found in Reed and Simon (1975), Vol. II, Sect. X.11, quoted on page 589.

Unfortunately, the Feynman–Kac formula from Theorem 7.51 cannot be rigorously extended to the Schrödinger equation, since the corresponding complex-valued measure does not exist. This is the statement of the famous Cameron non-existence theorem which can be found in Johnson and Lapidus (2000), Sect. 4.6, quoted on page 589.[108]

7.12 Weyl Quantization

> The use of the Moyal product for smooth functions avoids the use of Hilbert-space operators in quantum mechanics.
>
> Folklore

> We can say that quantum mechanics is a deformation of classical mechanics. The Planck constant h is the corresponding deformation parameter. This is for me the most concise formulation of the correspondence principle and explains what is meant by quantization.
> Beautiful results, which I learned from A. Lichnerowicz, M. Flato, and D. Sternheimer, allow one to say that classical mechanics is unstable and that quantum mechanics is essentially a unique deformation of it into a nonequivalent stable structure.[109]
>
> Ludwig Faddeev, 1999

[108] R. Cameron, A family of integrals serving to connect the Wiener and Feynman integrals. J. of Math. and Phys. Sci. of MIT **39** (1960), 126–140.

[109] L. Faddeev, Elementary introduction to quantum field theory, Vol. 1, pp. 513–552. In: P. Deligne, P. Etingof, D. Freed, L. Jeffrey, D. Kazhdan, J. Morgan, D. Morrison, and E. Witten (Eds.), Lectures on Quantum Field Theory: A course for mathematicians given at the Institute for Advanced Study in Princeton in 1996/97, Vols. 1, 2, Amer. Math. Soc., Providence, Rhode Island, 1999 (reprinted with permission).
We also refer to the beautiful book by L. Faddeev and A. Slavnov, Gauge Fields, Benjamin, Reading, Massachusetts, 1980. This book is based on the use of Feynman functional integrals; it represents the Faddeev–Popov approach to gauge theory which was a breakthrough in the quantization of the Standard Model in particle physics. See L. Faddeev and V. Popov, Feynman diagrams for the Yang–Mills field, Phys. Lett. **25B** (1967), 29–30.
Ludwig Faddeev made seminal contributions to mathematical physics. This is described in the book by L. Faddeev, 40 Years in Mathematical Physics, World Scientific, Singapore, 1995.
F. Bayen, M. Flato, C. Fronsdal, A. Lichnerowicz, and D. Sternheimer, Deformation theory and quantization I, II, Annals of Physics **111** (1978), 61–110; 111–151.

The elegant method of deformation quantization is based on the use of classical smooth functions equipped with the Moyal star product. This star product represents a deformation of the classical product of functions. The deformation depends on the Planck constant h. The first quantum correction of the classical product is related to the Poisson bracket in classical mechanics. The relation between deformation quantization and the operator-theoretic approach to quantum mechanics in Hilbert spaces is given by the Weyl calculus.

In the following sections, we will only sketch the basic ideas. We will start with the formal language used by physicists. From the mnemonic point of view, the language of physicists is very convenient. Unfortunately, rigorous mathematical arguments are more involved. The rigorous Weyl calculus will be considered in Sect. 7.12.6; this represents a special case of the modern theory of pseudo-differential operators, which combines differential operators with integral operators in the setting of generalized functions. We would like to encourage the reader to learn both the language of physicists and the language of mathematicians.

7.12.1 The Formal Moyal Star Product

Let $C^\infty(\mathbb{R}^2)$ be the space of smooth functions $f : \mathbb{R}^2 \to \mathbb{C}$. For $f, g \in C^\infty(\mathbb{R}^2)$, the formal Moyal star product is defined by

$$\boxed{f * g := f \mathrm{e}^{\frac{\mathrm{i}\hbar}{2}(\partial'_q \partial_p - \partial'_p \partial_q)} g.}$$

Here, the functions f and g depend on the real variables q and p, and we set $\partial_q := \partial/\partial q$ and $\partial_p := \partial/\partial p$. In addition, the prime of ∂'_q indicates that the partial derivative acts on the left factor f. Explicitly,

$$f * g = \sum_{m,n=0}^{\infty} \left(\frac{\mathrm{i}\hbar}{2}\right)^{m+n} \frac{(-1)^m}{m!n!} (\partial_p^m \partial_q^n f)(\partial_p^n \partial_q^m g). \tag{7.234}$$

This is to be understood as a formal power series with respect to the variable $\hbar$. The Moyal star product has the following properties.

(i) The correspondence principle: For all $f, g \in C^\infty(\mathbb{R}^2)$,

$$\boxed{f * g = fg + \frac{\mathrm{i}\hbar}{2}\{f, g\} + O(\hbar^2), \qquad \hbar \to 0.}$$

Here, we use the Poisson bracket $\{f, g\} := f_q g_p - g_q f_p$. Hence

$$f * g - g * f = \mathrm{i}\hbar\{f, g\} + O(\hbar^2), \qquad \hbar \to 0.$$

Therefore, the star product $f * g$ represents a deformation of the classical product fg. This deformation depends on the Planck constant $\hbar$. In terms of physics, the difference $f * g - fg$ describes quantum fluctuations which depend on $\hbar$. For example, if we choose $f(q, p) := q$ and $g(q, p) := p$, then $q*p = qp + \frac{1}{2}\mathrm{i}\hbar$ and $p * q = pq - \frac{1}{2}\mathrm{i}\hbar$. Hence

$$\boxed{q * p - p * q = \mathrm{i}\hbar.}$$

This commutation rule (for the Moyal star product of classical smooth functions) corresponds to the Born–Heisenberg–Jordan commutation relation $QP - PQ = \mathrm{i}\hbar I$ (in the operator-theoretic formulation of quantum mechanics on Hilbert spaces). As we will show below, the use of the Moyal star product avoids the use of operators.

(ii) Associativity: For all $f, g, k \in C^\infty(\mathbb{R}^2)$, we have

$$(f * g) * k = f * (g * k).$$

7.12.2 Deformation Quantization of the Harmonic Oscillator

The basic equations of deformation quantization. We want to apply the method of deformation quantization to the motion of a particle on the real line. The classical trajectory $q = q(t)$ is described by the canonical equations

$$\dot{p}(t) = -H_q(q(t), p(t)), \qquad \dot{q}(t) = H_p(q(t), p(t)), \qquad t \in \mathbb{R}.$$

We are given the Hamiltonian $H \in C^\infty(\mathbb{R}^2)$.

The corresponding quantum motion is obtained by solving the following problem. We are looking for

- a nonempty index set $\mathcal{M}$,
- a measure μ on the set $\mathcal{M}$,
- functions $\varrho_m = \varrho_m(q, p)$ on the phase space $\mathbb{R}^2$ for each index $m \in \mathcal{M}$, and
- real values E_m for each index $m \in \mathcal{M}$

such that the following equations hold.

(E) Quantized energy levels E_m:

$$\boxed{H * \varrho_m = E_m \varrho_m \qquad \text{for all} \quad m \in \mathcal{M}.}$$

(D) Distribution function ϱ_m: For all indices $m, n \in \mathcal{M}$, we have the orthogonality relation

$$\varrho_m * \varrho_n = 0, \qquad m \neq n,$$

along with the idempotent law

$$\varrho_m * \varrho_m = \varrho_m,$$

and the normalization relation on the phase space,

$$\int_{\mathbb{R}^2} \varrho_m(q, p) \frac{dqdp}{h} = 1.$$

(Q) Quantized energy decomposition of the classical Hamiltonian function:[110]

$$H(q, p) = \int_{\mathcal{M}} E_m \varrho_m(q, p) d\mu(m) \qquad \text{for all} \quad q, p \in \mathbb{R}.$$

(M) Mean value of energy: For all $m \in \mathcal{M}$,

$$\boxed{E_m = \int_{\mathbb{R}^2} H(q, p) \varrho_m(q, p) \, \frac{dqdp}{h}.}$$

In terms of physics, this means that each of the functions $\varrho_m = \varrho_m(q, p)$ is a probability distribution on the phase space which has the quantized energy level E_m as energy mean value.

[110] In the special case where $\mathcal{M} := \{0, 1, , 2 \ldots\}$, the integral $\int_{\mathcal{M}} E_m \varrho_m(q, p) d\mu(m)$ is equal to the infinite series $\sum_{m=0}^{\infty} E_m \varrho_m(q, p) \mu_m$. Here, the nonnegative number μ_m is the measure of the point $\{m\}$ for all $m = 0, 1, \ldots$

Suppose that we know a solution of the equations (E) through (M) above. Then, to a given complex-valued function $F : \mathbb{R} \to \mathbb{C}$ we can assign the star function F_* defined by

$$F_*(q,p) := \int_{\mathcal{M}} F(E_m)\varrho_m(q,p)d\mu(m) \qquad \text{for all} \quad q,p \in \mathbb{R}.$$

For example, we may formally define the exponential star function

$$\mathrm{Exp}_*(\alpha tH)(q,p) := \int_{m\in\mathcal{M}} \mathrm{e}^{\alpha tH(q,p)}\varrho_m(q,p)d\mu(m)$$

for all $q,p \in \mathbb{R}$, all times $t \in \mathbb{R}$, and fixed complex number α. Formally, it follows from (E) above that

$$\frac{d}{dt}\mathrm{Exp}_*\left(\alpha tH\right) = \alpha H * \mathrm{Exp}_*\left(\alpha tH\right).$$

This equation is called the Schrödinger equation in quantum deformation. In concrete models, one has to check that all of the equations formulated above possess a rigorous meaning, in the sense of well-defined formal expansions with respect to $\hbar$. Let us show how quantum deformation works for the harmonic oscillator. In this case, we choose $\mathcal{M} = \{0,1,2,,...\}$ and $\mu_m := 1$ for all m.

Application to the harmonic oscillator. The classical function

$$H(q,p) := \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}$$

is the Hamiltonian for a harmonic oscillator of mass m and angular frequency ω on the real line. To simplify the computation, it is useful to introduce the new dimensionless variable

$$a := \sqrt{\frac{m\omega}{2\hbar}}\left(q + \frac{\mathrm{i}p}{m\omega}\right) \tag{7.235}$$

and the conjugate complex variable

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(q - \frac{\mathrm{i}p}{m\omega}\right). \tag{7.236}$$

Hence

$$\boxed{H = \hbar\omega a a^\dagger.}$$

By the chain rule, the Moyal star product reads as

$$\boxed{f * g = f\mathrm{e}^{\frac{1}{2}(\partial'_a\partial_{a^\dagger} - \partial'_{a^\dagger}\partial_a)}g}$$

with respect to the new variables a and $a^\dagger$. Here, we set $\partial_a := \partial/\partial a$, as well as $\partial_{a^\dagger} := \partial/\partial a^\dagger$, and we regard f and g as functions of the variables a and $a^\dagger$. Explicitly, we obtain[111]

[111] If one wants to see the dependence on the parameter $\hbar$, then one has to replace a by $\sqrt{\hbar}\cdot b$. This yields $b * b^\dagger - b^\dagger * b = \hbar$, and

$$f * g = \sum_{m,n=0}^{\infty}\left(\frac{\hbar}{2}\right)^{m+n}\frac{(-1)^m}{m!n!}\,(\partial_{b^\dagger}^m\partial_b^n f)(\partial_{b^\dagger}^n\partial_b^m g).$$

$$f * g = \sum_{m,n=0}^{\infty} \frac{(-1)^m}{2^{m+n} m! n!} (\partial_{a^\dagger}^m \partial_a^n f)(\partial_{a^\dagger}^n \partial_a^m g). \tag{7.237}$$

For example, $a * a^\dagger = aa^\dagger + \frac{1}{2}$ and $a^\dagger * a = aa^\dagger - \frac{1}{2}$. This implies

$$\boxed{a * a^\dagger - a^\dagger * a = 1.} \tag{7.238}$$

For $m = 1, 2, , ..,$ define

- $E_0 := \frac{1}{2}\omega\hbar, \quad \varrho_0 := 2\mathrm{e}^{-2aa^\dagger}$;
- $E_m := \omega\hbar(m + \frac{1}{2})$;
- $\varrho_m := \frac{1}{m!}(a^\dagger)^m * \varrho_0 * a^m$.

Theorem 7.54 *For all $m, n = 0, 1, , 2, ...,$ the following hold.*
(E) *Quantized energy levels: $H * \varrho_m = E_m \varrho_m$.*
(D) *Distribution functions: $\varrho_m * \varrho_n = \delta_{nm}\varrho_m$.*
(Q) *Quantized energy decomposition of the classical Hamiltonian function:*

$$H(q,p) = \sum_{m=0}^{\infty} E_m \varrho_m(q,p) \qquad \text{for all} \quad q, p \in \mathbb{R}.$$

For the proof, see Problem 7.29.

The relation to the Laguerre polynomials. For all $w, z \in \mathbb{R}$ with $|w| < 1$, the Laguerre polynomials $L_0, L_1, ...$ are generated by the function

$$\frac{1}{1+w} \exp\left(\frac{wz}{1+w}\right) = \sum_{n=0}^{\infty} (-1)^n w^n L_n(z).$$

Explicitly, for $n = 0, 1, 2, ...,$

$$L_n(z) = \frac{\mathrm{e}^z}{n!} \frac{d^n(z^n \mathrm{e}^{-z})}{dz^n} = \sum_{m=0}^{n} \frac{(-1)^m\, n!}{(n-m)!\, m!\, n!}\, z^m.$$

The functions

$$\mathcal{L}_n(x) := \mathrm{e}^{-x/2} L_n(x) \qquad x \in \mathbb{R}, \qquad n = 0, 1, 2, ...$$

form a complete orthonormal system of the Hilbert space $L_2(0, \infty)$.

Theorem 7.55 *For all $m, n = 0, 1, , 2, ...,$ the following hold.*
(L) *Laguerre polynomials:*

$$\varrho_m = 2(-1)^m e^{-2H/\hbar\omega} L_m\left(\frac{4H}{\hbar\omega}\right)$$

with the normalization condition $\int_{\mathbb{R}^2} \varrho_m(q,p)\, \frac{dqdp}{h} = 1$.
(M) *Mean value: $E_m = \int_{\mathbb{R}^2} H(q,p)\varrho_m(q,p)\frac{dqdp}{h}$.*
(S) *The Schrödinger equation*

$$i\hbar F_t(q,p,t) = H(q,p) * F(q,p,t), \qquad q, p, t \in \mathbb{R}$$

has the solution

$$F(q,p,t) = \frac{1}{\cos\frac{\omega t}{2}} \exp\left(\frac{2H}{i\hbar\omega}\ \tan\frac{\omega t}{2}\right)$$

for all $t \in \mathbb{R}$ with $\omega t \neq 2n\pi,\ n = 0, \pm 1, \pm 2, ...$

For the proof, see Problem 7.30.

Motivation for the deformation quantization of the harmonic oscillator. We want to show how the method of deformation quantization considered above is related to Schrödinger's operator-theoretic treatment of the harmonic oscillator studied on page 534. Consider the operators

$$Q_{\mathrm{pre}}, P_{\mathrm{pre}}, H_{\mathrm{pre}} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$$

with $Q_{\mathrm{pre}}\varphi(q) := q\varphi(q)$ and $P_{\mathrm{pre}}\varphi(q) = -\mathrm{i}\hbar\varphi'(q)$ for all $q \in \mathbb{R}$, as well as

$$H_{\mathrm{pre}} := \frac{P_{\mathrm{pre}}^2}{2m} + \frac{m\omega^2 Q_{\mathrm{pre}}}{2}.$$

Using the Dirac calculus, let $|\varphi_0\rangle, |\varphi_1\rangle, \ldots$ denote the complete orthonormal system of eigenvectors of the Hamiltonian H_{pre}. That is,

$$H_{\mathrm{pre}}|\varphi_m\rangle = E_m|\varphi_m\rangle, \qquad m = 0, 1, 2, \ldots$$

with $E_m := \hbar\omega(m + \frac{1}{2})$. In addition, let us introduce the operator

$$\boldsymbol{\varrho}_m := |\varphi_m\rangle\langle\varphi_m|, \qquad m = 0, 1, \ldots$$

This is the von Neumann density operator corresponding to the eigenstate $|\varphi_m\rangle$. Then, for all indices $m, n = 0, 1, \ldots$ and all times $t \in \mathbb{R}$, the following hold:[112]

(a) $H_{\mathrm{pre}}\boldsymbol{\varrho}_m = E_m\boldsymbol{\varrho}_m$;
(b) $H_{\mathrm{pre}} = \sum_{m=0}^{\infty} E_m\boldsymbol{\varrho}_m$;
(c) $\boldsymbol{\varrho}_m\boldsymbol{\varrho}_n = \delta_{mn}\boldsymbol{\varrho}_m$;
(d) $\mathrm{i}\hbar\frac{d}{dt}\mathrm{e}^{-\mathrm{i}tH_{\mathrm{pre}}/\hbar} = H_{\mathrm{pre}}\mathrm{e}^{-\mathrm{i}tH_{\mathrm{pre}}/\hbar}$.

Relation (a) follows from

$$(H_{\mathrm{pre}}\boldsymbol{\varrho}_m)|\varphi_m\rangle = H_{\mathrm{pre}}|\varphi_m\rangle\langle\varphi_m|\varphi\rangle = E_m|\varphi_m\rangle\langle\varphi_m|\varphi\rangle = E_m\boldsymbol{\varrho}_m|\varphi\rangle.$$

Relations (b) and (d) are a consequence of

$$f(H_{\mathrm{pre}})\varphi = \sum_{m=0}^{\infty} f(E_m)|\varphi_m\rangle\langle\varphi_m|\varphi\rangle$$

for all $\varphi \in \mathcal{S}(\mathbb{R})$, where $f(x) := x$ or $f(x) := \mathrm{e}^{-\mathrm{i}xt/\hbar}$ for all $x \in \mathbb{R}$. Finally, relation (c) follows from

$$|\varphi_m\rangle\langle\varphi_m|\varphi_n\rangle\langle\varphi_m|\varphi\rangle = E_m\delta_{mn}|\varphi_m\rangle\langle\varphi_m|\varphi\rangle \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).$$

This finishes the proof of (a)–(d). In the following sections, we will introduce the Weyl calculus. Here,

[112] Explicitly, condition (b) means that $H_{\mathrm{pre}}\varphi = \sum_{m=0}^{\infty} E_m\boldsymbol{\varrho}_m\varphi$ for all $\varphi \in \mathcal{S}(\mathbb{R})$, and condition (d) is a short-hand writing for the equation

$$\mathrm{i}\hbar\frac{d}{dt}\sum_{m=0}^{\infty}\mathrm{e}^{-\mathrm{i}E_m t/\hbar}\boldsymbol{\varrho}_m\varphi = \sum_{m=0}^{\infty}E_m\mathrm{e}^{-\mathrm{i}E_m t/\hbar}\boldsymbol{\varrho}_m\varphi,$$

which is valid for all $\varphi \in \mathcal{S}(\mathbb{R})$. The limits are to be understood in the sense of the convergence on the Hilbert space $L_2(\mathbb{R})$.

- operators have to be replaced by their symbols, and
- operator products have to be replaced by the Moyal star product of the corresponding symbols.

Replacing the operators $H_{\mathrm{pre}}, \boldsymbol{\varrho}_m, \mathrm{e}^{-\mathrm{i}H_{\mathrm{pre}}/\hbar}$ by their symbols H, ϱ_m, F, the formulas (a)–(d) pass over to the following formulas:

(a*) $H * \varrho_m = E_m \varrho_m$;
(b*) $H = \sum_{m=0}^{\infty} E_m \varrho_m$;
(c*) $\varrho_m \varrho_n = \delta_{mn} \varrho_m$;
(d*) $\mathrm{i}\hbar F_t = H * F$.

This corresponds to Theorems 7.54 and 7.55 above. For the annihilation operator $\mathbf{a}$ and the creation operator $\mathbf{a}^\dagger$ given by

$$\mathbf{a} := \sqrt{\frac{m\omega}{2\hbar}} \left(Q_{\mathrm{pre}} + \frac{\mathrm{i}P_{\mathrm{pre}}}{m\omega} \right) \qquad \text{and} \qquad \mathbf{a}^\dagger := \sqrt{\frac{m\omega}{2\hbar}} \left(Q_{\mathrm{pre}} - \frac{\mathrm{i}P_{\mathrm{pre}}}{m\omega} \right),$$

the symbols a and $a^\dagger$ are given by (7.235) and (7.236), respectively. The operator commutation relation $\mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a} = I$ corresponds to the Moyal-star-product relation $a * a^\dagger - a^\dagger * a = 1$ for the symbols in the Weyl calculus. This coincides with (7.238).

7.12.3 Weyl Ordering

> The Moyal star product of classical symbols passes over to the operator product of the corresponding Weyl operators.
>
> Folklore

As a preparation for the general Weyl calculus, let us start with the rigorous theory of Weyl polynomials. In the quantum mechanics of particles on the real line, we encounter both[113]

- the position operator $Q : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ given by $(Q\psi)(q) := q\psi(q)$ and
- the momentum operator $P : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ given by $(P\psi)(q) := -\mathrm{i}\hbar\psi'(q)$

for all $\psi \in \mathcal{S}(\mathbb{R})$ and all $q \in \mathbb{R}$. These two basic operators are formally self-adjoint on the Hilbert space $L_2(\mathbb{R})$, that is,

$$\langle Q\psi|\varphi\rangle = \langle \psi|Q\varphi\rangle \quad \text{and} \quad \langle P\psi|\varphi\rangle = \langle \psi|P\varphi\rangle \qquad \text{for all} \quad \psi, \varphi \in \mathcal{S}(\mathbb{R}).$$

Here, we use the inner product $\langle \psi|\chi\rangle := \int_{\mathbb{R}} \psi^\dagger(q)\chi(q)dq$ on $L_2(\mathbb{R})$. In other words, $Q^\dagger = Q$ and $P^\dagger = P$.[114]

Weyl polynomials with respect to the operators Q and P on the linear function space $\mathcal{S}(\mathbb{R})$. Consider an arbitrary polynomial

$$\boxed{a(q,p) := \sum_{k,m=0}^{N} c_{km} q^k p^m \qquad \text{for all} \quad q, p \in \mathbb{R}} \tag{7.239}$$

with respect to the real variables q and p. Here, the coefficients c_{km} are complex numbers. It is our goal to assign to each polynomial a a linear operator

[113] To simplify notation, we write the operator symbol Q (resp. P) instead of Q_{pre} (resp. P_{pre}).

[114] In addition, the operators $Q, P : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ are essentially self-adjoint on the Hilbert space $L_2(\mathbb{R})$.

$$A(a) : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R}),$$

which is a polynomial with respect to Q and P, such that the following properties hold.

(W1) Linearity: For all polynomials a, b and all complex numbers α, β, we get

$$A(\alpha a + \beta b) = \alpha A(a) + \beta A(b).$$

In particular, if $a(q,p) := q$ and $b(q,p) := p$, then $A(a) := Q$ and $A(b) := P$. Furthermore, $A(1) = I$ (identity operator).

(W2) Weyl ordering: If $a(q,p) := qp$, then[115]

$$A(a) = \tfrac{1}{2}(QP + PQ).$$

(W3) Formal self-adjointness: If the coefficients of the polynomial a are real, then the Weyl operator $A(a)$ is formally self-adjoint. Explicitly,

$$\langle A(a)\psi|\varphi\rangle = \langle \psi|A(a)\varphi\rangle \qquad \text{for all} \quad \psi, \varphi \in \mathcal{S}(\mathbb{R}).$$

In other words, the Weyl polynomials $A(a)$ to real polynomials a are formal observables in quantum mechanics.

(W4) Composition rule: If a and b are polynomials, then[116]

$$A(a * b) = A(a)B(b).$$

This means that the Moyal star product of polynomials is translated into the operator product of Weyl polynomials on the space $\mathcal{S}(\mathbb{R})$. This is the characteristic property of the Moyal star product.

In about 1930, it was the idea of Weyl to introduce the symmetric Weyl polynomials $(q^k p^m)_W$ by setting

- $(q^k)_W := Q^k$ and $(p^m)_W := P^m$, where $m, k = 0, 1, \ldots$;
- $(qp)_W := \frac{1}{2}(QP + PQ)$;
- $(q^2 p)_W := \frac{1}{3}(Q^2 P + PQ^2 + QPQ)$;
- $(q^2 p^2)_W := \frac{1}{6}(Q^2P^2 + P^2Q^2 + QP^2Q + PQ^2P + QPQP + PQPQ)$.

In the general case, we proceed as follows. In order to obtain $(q^k p^m)_W$, we start with the symmetrized expression

$$(A_1 A_2 \cdots A_{k+m})_{\text{sym}} := \frac{1}{(k+m)!} \sum_{\pi} A_{\pi(1)} A_{\pi(2)} \cdots A_{\pi(k+m)}$$

where we sum over all possible permutations π of $1, 2, \ldots, k+m$. Finally, we set $A_1 = \ldots = A_k := Q$ and $A_{k+1} = \ldots = A_{k+m} := P$. For each polynomial a from (7.239), we now define the Weyl polynomial

[115] This expression is symmetric with respect to Q and P. Furthermore, the operator $A(a) : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is formally self-adjoint, that is,

$$A(a)^\dagger := \tfrac{1}{2}(P^\dagger Q^\dagger + Q^\dagger P^\dagger) = \tfrac{1}{2}(PQ + QP) = A(a).$$

These properties would fail if we would assign to qp the operators QP or PQ .

[116] Note that the Moyal star product $a * b$ from (7.234) on page 591 is a finite sum if $a = a(q,p)$ and $b = b(q,p)$ are polynomials.

$$\boxed{A(a) := \sum_{k,m=0}^{N} c_{km}(q^k p^m)_W.} \tag{7.240}$$

The polynomial a is called the symbol of the Weyl polynomial $A(a)$.

Proposition 7.56 *The Weyl correspondence* (7.240) *possesses the properties* (W1) *through* (W4) *formulated above.*

In particular, it follows from (W4) above that the symbol of the operator product $A(a)A(b)$ is the Moyal star product $a*b$ of the symbols a and b of the operators $A(a)$ and $B(a)$, respectively.

The proof of Prop. 7.56 is elementary. For the Moyal star product one has to use an induction argument. For example, it follows from relation (7.237) on page 594 that $q*p = qp + \frac{1}{2}\mathrm{i}\hbar$. Hence

$$A(q*p) = A(qp) + \tfrac{1}{2}\mathrm{i}\hbar A(1) = \tfrac{1}{2}(QP+PQ) + \tfrac{1}{2}\mathrm{i}\hbar I.$$

Using the commutation relation $QP - PQ = \mathrm{i}\hbar I$, we obtain

$$A(q*p) = QP = A(q)A(p).$$

Proposition 7.57 *Let $k = 0, 1, 2, \ldots$ and $r, s \in \mathbb{C}$. The operator $(rQ+sP)^k$ is the Weyl operator to the polynomial $a(q,p) := (rq+sp)^k$.*

The proof is elementary. For example, we have

$$(rq+sp)^2 = r^2q^2 + 2rsqp + s^2p^2$$

and $(rQ+sP)^2 = (rQ+sP)(rQ+sP) = r^2Q^2 + rs(QP+PQ) + s^2P^2$. Hence

$$(rQ+sP)^2 = r^2(q^2)_W + 2rs(qp)_W + s^2(p^2)_W.$$

Standard example. Let $\hat{a} \in \mathcal{S}(\mathbb{R}^2)$, and $N = 0, 1, \ldots$[117] Then the polynomial

$$a(q,p) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}^2}\sum_{k=0}^{N}\frac{\mathrm{i}^k(rq+sp)^k}{\hbar^k k!}\hat{a}(r,s)drds,$$

with respect to the real variables q and p, is well-defined. By Prop. 7.57, the Weyl operator to the symbol a reads as

$$A(a) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}^2}\sum_{k=0}^{N}\frac{\mathrm{i}^k(rQ+sP)^k}{\hbar^k k!}\hat{a}(r,s)drds.$$

Formal generalization. Now consider the well-defined integral

$$a(q,p) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}^2}\mathrm{e}^{\mathrm{i}(rq+sp)/\hbar}\hat{a}(r,s)drds.$$

Here, $a \in \mathcal{S}(\mathbb{R}^2)$. Explicitly, $\hat{a}$ is the Fourier transform of a. Using the formal limit $N \to \infty$, we get

[117] The definition of both the Schwartz function space $\mathcal{S}(\mathbb{R}^n)$ and the space of tempered distributions $\mathcal{S}'(\mathbb{R}^n)$ can be found on pages 537 and 615 of Volume I.

$$A(a) = \frac{1}{2\pi\hbar} \int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(rQ+sP)/\hbar} \hat{a}(r,s) dr ds. \tag{7.241}$$

This formal expression is frequently used by physicists.

Inductive construction of the Weyl operators. One can show that, for all polynomials a of the form (7.239), the following rigorous formulas hold:

$$\begin{aligned} QA(a) &= A(qa + \tfrac{1}{2}\mathrm{i}\hbar a_p), \quad A(a)Q = A(qa - \tfrac{1}{2}\mathrm{i}\hbar a_q), \\ PA(a) &= A(pa - \tfrac{1}{2}\mathrm{i}\hbar a_p), \quad A(a)P = A(pa + \tfrac{1}{2}\mathrm{i}\hbar a_p). \end{aligned}$$

For example, if $a(q,p) := p$, then we get $QP = QA(p) = A(qp) + \frac{1}{2}\mathrm{i}\hbar I$. In addition, we have $PQ = A(p)Q = A(qp) - \frac{1}{2}\hbar\mathrm{i}I$. Hence $QP + PQ = 2A(qp)$.

7.12.4 Operator Kernels

> Operator kernels generalize matrix elements; they relate differential operators to integral operators, in a generalized sense. The formal approach was introduced by Paul Dirac in the late 1920s (Dirac calculus). The rigorous theory is based on the kernel theorem which was proved by Laurent Schwartz in the late 1940s (theory of tempered distributions).[118]
>
> Folklore

Classical kernels. For given function $\mathcal{A} \in \mathcal{S}(\mathbb{R}^2)$, we define

$$\boxed{(A\psi)(x) := \int_{\mathbb{R}^2} \mathcal{A}(x,y)\psi(y)dy, \qquad x \in \mathbb{R}}$$

for all functions $\psi \in \mathcal{S}(\mathbb{R})$. The function $\mathcal{A}$ is called the kernel of the linear, sequentially continuous operator

$$A : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R}). \tag{7.242}$$

Each function $\varphi \in \mathcal{S}(\mathbb{R})$ corresponds to a tempered distribution $T_\varphi \in \mathcal{S}(\mathbb{R})$ given by

$$T_\varphi(\chi) := \int_{\mathbb{R}} \varphi(x)\chi(x)dx \qquad \text{for all} \quad \chi \in \mathcal{S}(\mathbb{R}).$$

The map $\varphi \mapsto T_\varphi$ is an injective, linear, sequentially continuous map from $\mathcal{S}(\mathbb{R})$ into $\mathcal{S}'(\mathbb{R})$. Identifying φ with T_φ, we get $\mathcal{S}(\mathbb{R}) \subseteq \mathcal{S}'(\mathbb{R})$. In this sense, the map $\psi \mapsto A\psi \mapsto T_{A\psi}$ yields the linear, sequentially continuous operator

$$A : \mathcal{S}(\mathbb{R}) \to \mathcal{S}'(\mathbb{R}).$$

Explicitly, we obtain

$$(A\psi)(\chi) = \int_{\mathbb{R}^2} \mathcal{A}(x,y)\chi(x)\psi(y)dxdy \qquad \text{for all} \quad \psi, \chi \in \mathcal{S}(\mathbb{R}). \tag{7.243}$$

[118] L. Schwartz, Théorie des noyaux (Theory of kernels) (in French), Proceedings of the 1950 International Congress of Mathematicians in Cambridge, Massachusetts, Vol. I, pp. 220–230, Amer. Math. Soc., Providence, Rhode Island, 1952. At this congress, Laurent Schwartz (1915–2002) was awarded the Fields medal for creating the theory of distributions in about 1945.

Here, we briefly write $(A\psi)(\chi)$ instead of $T_{A\psi}(\chi)$. Introducing the tempered distribution $\mathsf{A} \in \mathcal{S}'(\mathbb{R}^2)$ by setting

$$\mathsf{A}(\varrho) := \int_{\mathbb{R}^2} \mathcal{A}(x,y)\varrho(x,y)dxdy \qquad \text{for all} \quad \varrho \in \mathcal{S}(\mathbb{R}^2),$$

equation (7.243) tells us that

$$\boxed{(A\psi)(\chi) = \mathsf{A}(\chi \otimes \psi) \qquad \text{for all} \quad \psi, \chi \in \mathcal{S}(\mathbb{R}).} \tag{7.244}$$

The product property of kernels. If the kernels $\mathcal{A}, \mathcal{B} \in \mathcal{S}(\mathbb{R}^2)$ correspond to the operators $A, B : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$, respectively, then the product operator AB has the kernel $\mathcal{C}$ given by the product formula

$$\boxed{\mathcal{C}(x,y) := \int_{\mathbb{R}} \mathcal{A}(x,z)\mathcal{B}(z,y)dz \qquad \text{for all} \quad x, y \in \mathbb{R}.} \tag{7.245}$$

This relation generalizes the matrix product. To prove (7.245), set $\chi := A\psi$ and $\psi := B\varphi$. Then $\chi = (AB)\varphi$. Hence

$$\chi(x) = \int_{\mathbb{R}} \mathcal{A}(x,z)(B\varphi)(z)dz = \int_{\mathbb{R}} \left(\int_{\mathbb{R}} \mathcal{A}(x,z)\mathcal{B}(z,y)dz \right) \varphi(y)dy.$$

The kernel of the position operator Q. For all $\chi, \psi \in \mathcal{S}(\mathbb{R})$,

$$(Q\psi)(\chi) = \int_{\mathbb{R}^2} \chi(x)x\psi(x)dx. \tag{7.246}$$

Using the Dirac delta function, the equation $(Q\psi)(x) = x\psi(x)$ can formally be written as

$$(Q\psi)(x) = \int_{\mathbb{R}} x\delta(x-y)\psi(y)dy \qquad \text{for all} \quad x \in \mathbb{R}.$$

Thus, the function $\mathcal{Q}(x,y) := x\delta(x-y)$ is the formal kernel of the position operator Q. Using the Dirac calculus[119], the formal kernel of the position operator Q can also be obtained by

$$\mathcal{Q}(x,y) = \langle x|Q|y\rangle = y\langle x|y\rangle = y\delta(x-y) = x\delta(x-y).$$

The kernel of the momentum operator P. For all $\chi, \psi \in \mathcal{S}(\mathbb{R})$,

$$(P\psi)(\chi) = \int_{\mathbb{R}^2} (-\mathrm{i}\hbar\psi'(x))\chi(x)dx. \tag{7.247}$$

In order to get the formal kernel $\mathcal{P}$ of the operator P used by physicists, we start with the (rescaled) Fourier transformation

$$(\mathcal{F}\varphi)(p) := \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}xp/\hbar}\varphi(x)dx, \qquad \varphi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}xp/\hbar}(\mathcal{F}\varphi)(p)dp.$$

Here, the operator $\mathcal{F} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is bijective, linear, and sequentially continuous, and the inverse operator $\mathcal{F}^{-1}$ has the same properties. It follows from

[119] See page 596 of Volume I.

$$\mathcal{F}(P\psi)(p) = p(\mathcal{F}\psi)(p)$$

that we have the formal relation

$$\mathcal{F}(P\psi)(p) = \int_{\mathbb{R}} p\delta(p-r)(\mathcal{F}\psi)(r)dr \qquad \text{for all} \quad p \in \mathbb{R}.$$

This implies $(P\psi)(x) = \int_{\mathbb{R}} \mathcal{P}(x,y)\psi(y)dy$ with the formal kernel

$$\begin{aligned}\mathcal{P}(x,y) :&= \frac{1}{2\pi\hbar}\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(xp-yr)/\hbar} p\delta(p-r)dpdr \\ &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p(x-y)/\hbar} p\, dp \qquad \text{for all} \quad x,y \in \mathbb{R}. \end{aligned} \tag{7.248}$$

Using the Dirac calculus (i.e., the completeness relation $\int_{\mathbb{R}} dp\, |p\rangle\langle p| = I$), the formal kernel can also be obtained by

$$\mathcal{P}(x,y) = \langle x|P|y\rangle = \int_{\mathbb{R}} dp \int_{\mathbb{R}} dr \;\; \langle x|p\rangle\langle p|P|r\rangle\langle r|y\rangle.$$

Noting that $\langle p|P|r\rangle = r\langle p|r\rangle = r\delta(p-r) = p\delta(p-r)$ and $\langle x|p\rangle = \mathrm{e}^{\mathrm{i}xp/\hbar}/\sqrt{2\pi\hbar}$, again we get (7.248).

The Schwartz kernel theorem. *Let $A : \mathcal{S}(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$ be a linear, sequentially continuous operator (e.g., the Weyl operator $A(a)$ to the polynomial symbol a). Then there exists precisely one tempered distribution $\mathsf{A} \in \mathcal{S}'(\mathbb{R}^2)$ such that*

$$(A\psi)(\chi) = \mathsf{A}(\chi \otimes \psi) \qquad \textit{for all} \quad \psi, \chi \in \mathcal{S}(\mathbb{R}). \tag{7.249}$$

The tempered distribution A *is called the kernel of the operator A.*

This theorem generalizes (7.244). The kernels of the operators Q and P are given by (7.246) and (7.247), respectively.

Nuclear spaces. The Schwartz kernel theorem is the special case of a functional-analytic theorem about bilinear forms on nuclear spaces. A Hilbert space is nuclear iff its dimension is finite. Furthermore, the infinite-dimensional spaces $\mathcal{D}(\mathbb{R}^n)$ and $\mathcal{S}(\mathbb{R}^n)$ are nuclear for $n = 1, 2, \ldots$ For the theory of nuclear spaces and their important applications in harmonic analysis, we refer to the following monographs:

A. Pietsch, Nuclear locally convex spaces, Springer, Berlin, 1972.

A. Pietsch, Operator Ideals, Deutscher Verlag der Wissenschaften, Berlin, 1978.

A. Pietsch, History of Banach Spaces and Linear Operators, Birkhäuser, Boston, 2007.

I. Gelfand, G. Shilov, and N. Vilenkin, Generalized Functions, Vols. 1–5, Academic Press, New York, 1964.

K. Maurin, Generalized Eigenfunction Expansions and Unitary Representations of Topological Groups, Polish Scientific Publishers, Warsaw, 1968.

K. Maurin, Methods of Hilbert Spaces, Polish Scientific Publishers, Warsaw, 1972.

The theory of nuclear spaces was created by Grothendieck in the 1950s. In the 1955s, Grothendieck left analysis, and he moved to algebra and geometry. For his seminal contributions to algebraic geometry, homological algebra, and functional analysis, Alexandre Grothendieck (born 1928 in Berlin) was awarded the Fields medal in 1966. His childhood and youth was overshadowed by German fascism. His father died in the German concentration camp Auschwitz in 1942. We refer to:

A. Grothendieck, Récoltes et Semailles: réflexions et témoignage sur un passé de mathématicien, 1986 (ca. 1000 pages) (in French).(Reaping and Sowing: the life of a mathematician – reflections and bearing witness). Internet: `http://www.fermentmagazine.org/rands/recoltes1.html` Translations into English, Russian, and Spanish are ongoing.

P. Cartier, A mad day's work: from Grothendieck to Connes and Kontsevich. The evolution of concepts of space and symmetry. Bull. Amer. Math. Soc. **38**(4) (2001), 389–408.

W. Scharlau, Who is Alexander Grothendieck? Part I, 2007 (in German). Internet: `http://www.Scharlau-online.de/DOKS/ag`

7.12.5 The Formal Weyl Calculus

Our goal is to extend the relation between polynomial symbols $a = a(q,p)$ and Weyl operators $A(a)$ to more general symbols a. In order to motivate the rigorous approach to be considered in Sect. 7.12.6, let us start with purely formal arguments used by physicists. The key formulas read as follows.

(i) Superposition: For the symbol

$$a(q,p) = \frac{1}{2\pi\hbar} \int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(xq+yp)/\hbar}\, \hat{a}(x,y)dxdy, \qquad q,p \in \mathbb{R},$$

the Weyl operator is given by

$$\boxed{A(a) := \frac{1}{2\pi\hbar} \int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(xQ+yP)/\hbar}\, \hat{a}(x,y)dxdy.} \tag{7.250}$$

Here, $\hat{a} = \hat{a}(x,y)$ is the (rescaled) Fourier transform of $a = (q,p)$.

(ii) The kernel formula: We have

$$(A\psi)(x) = \int_{\mathbb{R}} \mathcal{A}(x,y)\psi(y)dy, \qquad x \in \mathbb{R}$$

with the formal kernel

$$\boxed{\mathcal{A}(x,y) = \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p(x-y)/\hbar}\, a\left(\frac{x+y}{2}, p\right) dp, \qquad x,y \in \mathbb{R}.} \tag{7.251}$$

The inverse Fourier transformation yields

$$a(q,p) = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}rp/\hbar} \mathcal{A}(q - \tfrac{1}{2}r, q + \tfrac{1}{2}r)dr, \qquad q,p \in \mathbb{R}. \tag{7.252}$$

(iii) Formal self-adjointness: For the formally adjoint operator of the Weyl operator $A(a)$ on the Hilbert space $L_2(\mathbb{R})$, we get

$$A(a)^\dagger = A(a^\dagger).$$

In particular, if the function a is real-valued, then the corresponding Weyl operator $A(a)$ is formally self-adjoint on the Hilbert space $L_2(\mathbb{R})$.

(iv) The composition formula: If the symbols $a = a(q,p)$ and $b = b(q,p)$ correspond to the Weyl operators $A(a)$ and $A(b)$, then the operator product is given by

$$\boxed{A(a)A(b) = A(a * b)}$$

with the star product

$$(a * b)(q,p) := \frac{1}{\pi^2\hbar^2} \int_{\mathbb{R}^4} \mathrm{e}^{2\varrho\,\mathrm{i}/\hbar}\; a(q_1,p_1)b(q_2,p_2)\; dq_1dp_1dq_2dp_2$$

for all $q, p \in \mathbb{R}$. Here, the function $\varrho = \varrho(q,p,q_1,p_1,q_2,p_2)$ is defined by

$$\varrho := \begin{vmatrix} q & p & 1 \\ q_1 & p_1 & 1 \\ q_2 & p_2 & 1 \end{vmatrix} = q(p_1 - p_2) + p(q_2 - q_1) + (q_1p_2 - p_1q_2).$$

If $\hat{b}$ denotes the (rescaled) Fourier transform of b, that is,

$$\hat{b}(\xi,\eta) = \frac{1}{2\pi\hbar} \int_{\mathbb{R}^2} \mathrm{e}^{-\mathrm{i}(q\xi+p\eta)/\hbar}\; b(q,p)\; dqdp, \tag{7.253}$$

then

$$\boxed{(a * b)(q,p) = \frac{1}{2\pi\hbar} \int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(q\xi+p\eta)/\hbar}\; a\left(q - \frac{\eta}{2}, p + \frac{\xi}{2}\right) \hat{b}(\xi,\eta)\; d\xi d\eta.}$$

As we will show below by using the Fourier transform together with the Taylor expansion, this implies

$$(a * b)(q,p) = a\left(q + \frac{\mathrm{i}\hbar}{2}\frac{\partial}{\partial p_2}, p - \frac{\mathrm{i}\hbar}{2}\frac{\partial}{\partial q_2}\right) b(q_2,p_2)_{|q_2=q,p_2=p}.$$

Here, we have to assume that a is a polynomial (or a formal power series expansions with respect to q and p). Finally, note that the star product $a * b$ coincides with the formal Moyal star product, that is,

$$\boxed{a * b = \sum_{m,n=0}^{\infty} \left(\frac{\mathrm{i}\hbar}{2}\right)^{m+n} \frac{(-1)^m}{m!n!}\; \frac{\partial^{m+n}a}{\partial p^m \partial q^n} \frac{\partial^{m+n}b}{\partial p^n \partial q^m}.} \tag{7.254}$$

Let us motivate this in a formal manner. To simplify notation, we set $\hbar := 1$.

Ad (i) See formula (7.241) on page 599.

Ad (ii). (I) Commutation relation. It follows from $QP - PQ = \mathrm{i}I$ that

$$Q^nP - PQ^n = \mathrm{i}nQ^{n-1}, \qquad n = 1,2,\ldots$$

by induction. If $F(Q) = a_0I + a_1Q + a_2Q^2 + \ldots$, then we formally get

$$F(Q)P - PF(Q) = \mathrm{i}F'(Q).$$

In particular, $\mathrm{e}^{-\mathrm{i}trQ}P - P\mathrm{e}^{-\mathrm{i}trQ} = tr \cdot \mathrm{e}^{-\mathrm{i}trQ}$ for all $t, r \in \mathbb{R}$.

(II) Let us prove the key relation

$$\mathrm{e}^{\mathrm{i}t(rQ+sP)} = \mathrm{e}^{\mathrm{i}t^2rs/2} \cdot \mathrm{e}^{\mathrm{i}trQ}\mathrm{e}^{\mathrm{i}tsP}, \qquad r,s \in \mathbb{R}. \tag{7.255}$$

To this end, we set $U(t) := \mathrm{e}^{-\mathrm{i}tsP}\mathrm{e}^{-\mathrm{i}trQ}\mathrm{e}^{\mathrm{i}t(rQ+sP)}$ for all $t \in \mathbb{R}$. Differentiating with respect to time t and using (I), we obtain

$$U'(t) = -\mathrm{i}s\mathrm{e}^{-\mathrm{i}tsP}\left(P\mathrm{e}^{-\mathrm{i}trQ} - \mathrm{e}^{-\mathrm{i}trQ}P\right)\mathrm{e}^{\mathrm{i}t(rQ+sP)} = \mathrm{i}trsU(t).$$

Since $U(0) = I$, we get $U(t) = \mathrm{e}^{\mathrm{i}t^2rs/2}I$. This implies (7.255).

(III) Setting $t = 1$, we obtain

$$\mathrm{e}^{\mathrm{i}(rQ+sP)} = \mathrm{e}^{\mathrm{i}rs/2}\cdot\mathrm{e}^{\mathrm{i}rQ}\mathrm{e}^{\mathrm{i}sP}, \qquad r, s \in \mathbb{R}.$$

Recall that $\mathrm{i}P\psi = \psi'$. By Taylor expansion,

$$(\mathrm{e}^{\mathrm{i}sP}\psi)(x) = \psi(x) + s\psi'(x) + \tfrac{s^2}{2!}\psi''(x) + \ldots = \psi(x+s).$$

Similarly,

$$(\mathrm{e}^{\mathrm{i}rQ}\psi)(x) = \psi(x) + \mathrm{i}rx\psi(x) + \frac{(\mathrm{i}rx)^2}{2!}\psi(x) + \ldots = \mathrm{e}^{\mathrm{i}rx}\psi(x).$$

Hence $(\mathrm{e}^{\mathrm{i}(rQ+sP)}\psi)(x) = \mathrm{e}^{\mathrm{i}rs/2}\mathrm{e}^{\mathrm{i}rx}\psi(x+s)$ for all $x \in \mathbb{R}$.

(IV) We briefly write A instead of $A(a)$. By (7.250),

$$(A\psi)(x) = \frac{1}{2\pi}\int_{\mathbb{R}^2}\mathrm{e}^{\mathrm{i}rx}\mathrm{e}^{\mathrm{i}rs/2}\psi(x+s)\,\hat{a}(r,s)drds.$$

Inserting $\hat{a}(r,s) = \frac{1}{2\pi}\int_{\mathbb{R}^2}\mathrm{e}^{-\mathrm{i}(rq+sp)}\,a(q,p)dqdp$, we get

$$(A\psi)(x) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2}\mathrm{e}^{\mathrm{i}r(x-q+\frac{1}{2}s)}\mathrm{e}^{-\mathrm{i}sp}\,a(q,p)\psi(x+s)drdsdqdp.$$

Since $\int_{\mathbb{R}}\mathrm{e}^{\mathrm{i}r(x-q+\frac{1}{2}s)}dr = 2\pi\delta(x-q+\frac{1}{2}s)$, we obtain

$$(A\psi)(x) = \frac{1}{2\pi}\int_{\mathbb{R}^2}\mathrm{e}^{-\mathrm{i}sp}\,a(x+\tfrac{1}{2}s,p)\psi(x+s)dpds.$$

Finally, the substitution $y = x + s$ yields the desired result

$$(A\psi)(x) = \frac{1}{2\pi}\int_{\mathbb{R}^2}\mathrm{e}^{\mathrm{i}(x-y)p}\,a\left(\frac{x+y}{2},p\right)\psi(y)dpdy.$$

Ad (iii). By (ii), the operator $A(a^\dagger)$ has the kernel

$$\mathcal{B}(x,y) = \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{e}^{\mathrm{i}p(x-y)/\hbar}\,a\left(\frac{x+y}{2},p\right)^\dagger dp, \qquad x, y \in \mathbb{R}.$$

Again by (ii), this is equal to $\mathcal{A}(y,x)^\dagger$. Hence $A(a^\dagger) = A(a)^\dagger$.

Ad (iv). (I) The kernel $\mathcal{C}$ of the operator product $C := A(a)A(b)$ is given by

$$\mathcal{C}(x,y) = \int_{\mathbb{R}}\mathcal{A}(x,z)\mathcal{B}(z,y)dz.$$

By (ii), we have the following relations between the symbols a, b and the kernels $\mathcal{A}, \mathcal{B}$, respectively:

$$\mathcal{A}(x,z) = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p_1(x-z)}\; a\left(\frac{x+z}{2}, p_1\right) dp_1,$$
$$\mathcal{B}(z,y) = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p_2(z-y)}\; a\left(\frac{z+y}{2}, p_2\right) dp_2.$$

Hence

$$\mathcal{C}(x,y) = \frac{1}{4\pi^2}\int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}p_1(x-z)}\mathrm{e}^{\mathrm{i}p_2(z-y)} a\left(\frac{x+z}{2}, p_1\right) b\left(\frac{z+y}{2}, p_2\right) dp_1 dp_2 dz.$$

Let c be the symbol of the operator C. Again by (ii), after the rescaling $\eta = \frac{1}{2}r$, we get

$$c(q,p) = 2\int_{\mathbb{R}} \mathrm{e}^{2\mathrm{i}p\eta}\; \mathcal{C}(q-\eta, q+\eta) d\eta.$$

Therefore,

$$c(q,p) = \frac{1}{2\pi^2}\int_{\mathbb{R}^4} \mathrm{e}^{\mathrm{i}\sigma}\; a\left(\frac{q+z-\eta}{2}, p_1\right) b\left(\frac{q+z+\eta}{2}, p_2\right) dp_1 dp_2 dz d\eta$$

with $\sigma := (q-z-\eta)p_1 + (z-q-\eta)p_2 + 2p\eta$. Using the substitution

$$q_1 = \tfrac{1}{2}(q+z-\eta), \qquad q_2 = \tfrac{1}{2}(q+z+\eta)$$

and setting $\varrho := (q-q_2)p_1 + (q_1-q)p_2 + (q_2-q_1)p$, we obtain

$$c(q,p) = \frac{1}{\pi^2}\int_{\mathbb{R}^4} \mathrm{e}^{2\mathrm{i}\varrho}\; a(q_1,p_1) b(q_2,p_2) dp_1 dp_2 dq_1 dq_2. \tag{7.256}$$

(II) Moyal product. Using the substitution $q_1 = q - \frac{1}{2}\eta, p_1 = p + \frac{1}{2}\xi$, we get

$$c(q,p) = \frac{1}{4\pi^2}\int_{\mathbb{R}^4} \mathrm{e}^{\mathrm{i}(q-q_2)\xi}\mathrm{e}^{\mathrm{i}(p-p_2)\eta}\; a\left(q-\frac{\eta}{2}, p+\frac{\xi}{2}\right) b\,(q_2,p_2)\;\, dq_2 dp_2 d\xi d\eta.$$

If $\hat{b}$ denotes the (rescaled) Fourier transform (7.253) of the function b, then

$$c(q,p) = \frac{1}{2\pi}\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(q\xi+p\eta)}\; a\left(q-\frac{\eta}{2}, p+\frac{\xi}{2}\right) \hat{b}(\xi,\eta)\; d\xi d\eta. \tag{7.257}$$

Suppose now that the symbol a is a polynomial (or a formal power series expansion). By Fourier transform, we get the formal expression

$$c(q,p) = a\left(q + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p_2}, p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial q_2}\right) b(q_2,p_2)_{|q_2=q, p_2=p}. \tag{7.258}$$

Finally, using Taylor expansion, we obtain

$$c(q,p) = \sum_{m,n=0}^{\infty} \left(\frac{\mathrm{i}}{2}\right)^{m+n} \frac{(-1)^m}{m!n!}\; \frac{\partial^{m+n}a}{\partial p^m \partial q^n}\, \frac{\partial^{m+n}b}{\partial p^n \partial q^m}. \tag{7.259}$$

(III) Motivation of (7.258). First let $a(q,p) := q$. It follows from

$$b(q_2,p_2) = \frac{1}{2\pi}\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(q_2\xi+p_2\eta)}\; \hat{b}(\xi,\eta)\; d\xi d\eta$$

that

$$\left(q + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p_2}\right) b(q_2, p_2) = \frac{1}{2\pi}\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(q_2\xi + p_2\eta)} \left(q - \frac{\eta}{2}\right) \hat{b}(\xi, \eta)\, d\xi d\eta.$$

Setting $q_2 = q$ and $p_2 = p$ and using (7.257), we obtain (7.258).

Similarly, if $a(q, p) := p$, then

$$\left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial q_2}\right) b(q_2, p_2) = \frac{1}{2\pi}\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(q_2\xi + p_2\eta)} \left(p + \frac{\xi}{2}\right) \hat{b}(\xi, \eta)\, d\xi d\eta.$$

Again this yields (7.258).

(IV) Motivation of (7.259). This follows from

$$a(q + \alpha, p + \beta) = \sum_{m,n=0}^{\infty} \frac{\partial^{m+n} a(q, p)}{\partial p^m \partial q^n} \cdot \frac{\beta^m \alpha^n}{m! n!},$$

by setting $\beta := -\frac{\mathrm{i}}{2}\frac{\partial}{\partial q}$ and $\alpha := \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}$. □

7.12.6 The Rigorous Weyl Calculus

It is possible to translate the formal Weyl calculus into a rigorous mathematical approach by using the language of generalized functions. It is our goal to assign to a general class of symbols Weyl operators in such a way that

- the theory of Weyl polynomials from Sect. 7.12.3 is generalized and
- the formal Weyl calculus from Sect. 7.12.5 gets a rigorous mathematical basis.

The proofs of the following statements can be found in the monographs by L. Hörmander, The Analysis of Linear Partial Differential Operators, Vol. 3, Springer, New York, 1983, and by M. de Gosson, Symplectic Geometry and Quantum Mechanics, Birkhäuser, Basel, 2006.

Smooth, rapidly decreasing symbols. Let $a, b \in \mathcal{S}(\mathbb{R})$. The functions a and b are called symbols. Then the following hold.

(i) Weyl operator: For given symbol a, define the Weyl operator

$$(A(a)\psi)(x) := \int_{\mathbb{R}} \mathcal{A}(x, y)\psi(y)dy, \qquad x \in \mathbb{R}$$

for all $\psi \in \mathcal{S}(\mathbb{R})$ with the kernel

$$\mathcal{A}(x, y) := \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p(x-y)/\hbar}\, a\left(\frac{x+y}{2}, p\right) dp, \qquad x, y \in \mathbb{R}.$$

Then $\mathcal{A} \in \mathcal{S}(\mathbb{R}^2)$, and the operator $A(a) : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ is linear and sequentially continuous.

(ii) Bilinear form: Let $\chi, \psi \in \mathcal{S}(\mathbb{R}^2)$. Then

$$(A(a)\psi)(\chi) = \int_{\mathbb{R}^2} \mathcal{A}(x, y)\varphi(x)\psi(y)dy, \qquad x, y \in \mathbb{R}.$$

Hence

$$(A(a)\psi)(\chi) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}p(x-y)/\hbar}\, a\left(\frac{x+y}{2}, p\right) \chi(x)\psi(y)dxdydp.$$

Using the substitution $y = 2q - x, x = x$, we get

$$(A(a)\psi)(\chi) = \frac{1}{\pi\hbar}\int_{\mathbb{R}^2} \mathrm{e}^{2\mathrm{i}p(x-q)/\hbar}\; a\,(q,p)\,\chi(x)\psi(2q-x)dxdqdp.$$

This implies

$$(A(a)\psi)(\chi) = \int_{\mathbb{R}^2} a(q,p)\varrho_{\chi,\psi}(q,p)dqdp \tag{7.260}$$

with $\varrho_{\chi,\psi}(q,p) := \frac{1}{\pi\hbar}\int_{\mathbb{R}} \mathrm{e}^{2\mathrm{i}p(x-q)/\hbar}\chi(x)\psi(2q-x)dx$.

(ii) Formal self-adjointnes: We get

$$A(a)^\dagger = A(a^\dagger).$$

This means that $\langle A(a^\dagger)\varphi|\psi\rangle = \langle\varphi|A(a)\psi\rangle$ for all $\psi,\varphi\in\mathcal{S}(\mathbb{R})$, where $\langle .|.\rangle$ is the inner product on the Hilbert space $L_2(\mathbb{R})$.

(iii) The composition formula and the rigorous Moyal star product: For the operator product, we have

$$A(a)A(b) = A(a*b)$$

together with the rigorous Moyal star product[120]

$$\boxed{(a*b)(q,p) := \frac{1}{\pi^2\hbar^2}\int_{\mathbb{R}^4} \mathrm{e}^{2\varrho\mathrm{i}/\hbar}\; a(q_1,p_1)\cdot b(q_2,p_2)\; dq_1dp_1dq_2dp_2}$$

for all $q,p\in\mathbb{R}$. Here, we use the determinant

$$\varrho := \begin{vmatrix} q & p & 1\\ q_1 & p_1 & 1\\ q_2 & p_2 & 1\end{vmatrix} = q(p_1-p_2)+p(q_2-q_1)+(q_1p_2-p_1q_2). \tag{7.261}$$

This coincides with (7.256).

(iv) Associativity of the Moyal star product: For all $a,b,c\in\mathcal{S}(\mathbb{R})$, we have

$$(a*b)*c = a*(b*c).$$

Tempered distributions as symbols. Let $a\in\mathcal{S}'(\mathbb{R}^2)$. Motivated by (7.260), define

$$\boxed{(A(a)\psi)(\chi) := a(\varrho_{\chi,\psi}) \qquad \chi,\psi\in\mathcal{S}(\mathbb{R}).}$$

Then $A(a)\psi\in\mathcal{S}'(\mathbb{R})$, and the linear operator $A(a):\mathcal{S}(\mathbb{R})\to\mathcal{S}'(\mathbb{R})$ is sequentially continuous. In particular, if $a=a(q,p)$ is a polynomial with respect to the variables q and p, then the corresponding tempered distribution is given by $a(\varrho) = \int_{\mathbb{R}^2} a(q,p)\varrho(q,p)dqdp$ for all $\varrho\in\mathcal{S}(\mathbb{R}^2)$.

[120] In the general case, the rigorous Moyal star product (7.261) differs from the formal Moyal star product (7.254). This is discussed in G. Piacitelli, Nonlocal theories: new rules for old diagrams, 2004. Internet: arXiv: hep-th/0403055

7.13 Two Magic Formulas

> According to one view, the Feynman path integral is simple a suitable hierolglyphic shorthand for an algorithm of perturbation theory. On the other hand, the traditional (Wiener) view of the path integral as an integral with respect to a measure in the function space runs into practically insurmountable difficulties here and is thus also imperfect. Our own view is that the Feynman path integral should be understood as the limit of finite-dimensional approximations. But which approximations? The path integral proves to be very sensitive to the choice of its approximations, the resulting ambiguity being of the same nature as the non-uniqueness of quantization.[121]
>
> Feliks Berezin and Mikhail Shubin, 1991

It is our goal to use the Weyl calculus in order to get the two magic formulas (7.274) on page 614 and (7.277) on page 615 for the kernel of the Feynman propagator operator and the kernel of the Heisenberg scattering operator, respectively. It turns out that the Weyl calculus relates the Feynman propagator kernel to the Feynman path integral in a quite natural manner.

Basic ideas. Consider the motion $q = q(t)$ of a classical particle on the real line with the equation of motion

$$\dot{p}(t) = -a_q(q(t), p(t)), \qquad \dot{q}(t) = a_p(q(t), p(t)), \qquad t \in \mathbb{R}.$$

Here, the given classical Hamiltonian $a : \mathbb{R}^2 \to \mathbb{R}$ is assumed to be smooth. Now we pass to the corresponding quantum particle. Then we have to study the Schrödinger equation

$$\boxed{\mathrm{i}\hbar\psi_t = H\psi, \qquad \psi(t_0) = \psi_0} \tag{7.262}$$

for the wave function $\psi = \psi(x, t)$ of the quantum particle on the Hilbert space $L_2(\mathbb{R})$.

In terms of Weyl quantization, the operator $H = A(a)$ is the Weyl operator related to the symbol $a = a(q, p)$. This operator is called the Hamiltonian (or energy operator) of the quantum particle. It is our goal to study both

- the full dynamics of the quantum particle (i.e., the Feynman propagator operator $P(t, t_0) := \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}$), and
- scattering processes for the quantum particle (i.e., the Heisenberg scattering operator $\mathsf{S}(t, t_0) := \mathrm{e}^{\mathrm{i}tH_{\mathrm{free}}/\hbar}\mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}\mathrm{e}^{-\mathrm{i}t_0H_{\mathrm{free}}/\hbar}$). Here, we assume that the Hamiltonian H is a perturbation of the free Hamiltonian H_{free}. Explicitly,

$$H = H_{\mathrm{free}} + \kappa U. \tag{7.263}$$

A scattering process is characterized by the property that the motion of the quantum particle is free in the remote past ($t_0 \to -\infty$) and in the far future ($t \to +\infty$). The free Hamiltonian $H_{\mathrm{free}} = P^2/2m$ is the Weyl operator to the symbol $a_{\mathrm{free}}(p) := p^2/2m$, and the operator U is the Weyl operator to the symbol $q \mapsto U(q)$. The real number κ is called coupling constant. Summarizing, the Hamiltonian operator H has the symbol

$$a(q, p) = \frac{p^2}{2m} + \kappa U(q).$$

[121] F. Berezin and M. Shubin, The Schrödinger Equation, Kluwer, Dordrecht, 1991 (reprinted with permission).

We will proceed in the following manner.

(a) Evolution operators: We start with time-dependent operators in the Hilbert space $L_2(\mathbb{R})$ (i.e., the Feynman propagator and the Heisenberg scattering operator).
(b) Kernels: The evolution operators can be described by kernels depending on space and time coordinates.
(c) Causality: The kernel on a finite time interval is the superposition of kernels on small time intervals.
(d) Reduction to operator symbols: The kernel of a small time interval can be computed by using the kernel formula of the Weyl calculus, which depends on the symbol of the evolution operator.
(e) Limit: If the small time interval goes to zero, then the kernel of the evolution operator can be expressed by a Feynman path integral, which depends on the symbol a of the Hamiltonian operator.

This way, we obtain an elegant relation between classical mechanics described by the classical Hamiltonian a and

- the kernel $\mathcal{K}$ of the Feynman propagator operator (called the Feynman propagator kernel), and
- the kernel $\mathcal{S}$ of the Heisenberg scattering operator (called the scattering kernel).

In what follows, we will only use formal arguments. Let us first discuss the physical meaning of both the Feynman propagator operator and the Heisenberg scattering operator.

The Feynman propagator operator. The operator

$$P(t,t_0) := \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}, \qquad t \geq t_0$$

is called the Feynman propagator. For given initial state $\psi_0 \in L_2(\mathbb{R})$, the state

$$\psi(t) = P(t,t_0)\psi_0$$

is a solution of the Schrödinger equation (7.262). From the physical point of view, the propagator $P(t,t_0)$ sends the particle state ψ_0 at the initial time t_0 to the particle state $\psi(t)$ at time t. Therefore, the propagator describes the dynamics of the quantum particle. Let

$$-\infty < t_0 < t_1 < \cdots < t_{N-1} < t_N < \infty.$$

Then the addition theorem for the exponential function tells us that we have the following operator product

$$\boxed{P(t_N,t_0) = P(t_N,t_{N-1}) \cdots P(t_2,t_1)P(t_1,t_0).} \tag{7.264}$$

This product property reflects causality. To understand this, note that it follows from $\psi(t_1) = P(t_1,t_0)\psi_0$ and $\psi(t_2) = P(t_2,t_1)\psi(t_1)$ that

$$\psi(t_2) = P(t_2,t_1)P(t_1,t_0)\psi_0 = P(t_2,t_0)\psi_0.$$

The propagator $t \mapsto P(t,t_0)$ satisfies the following equation

$$\boxed{\mathrm{i}\hbar P_t(t,t_0) = HP(t,t_0), \qquad t \geq t_0, \quad P(t_0,t_0) = I,} \tag{7.265}$$

which is called the propagator differential equation.

The Heisenberg scattering operator. Suppose that the Hamiltonian operator H is the perturbation of the free Hamiltonian H_{free} according to (7.263). Let us investigate scattering processes. The operator

$$\mathsf{S}(t,t_0) := \mathrm{e}^{\mathrm{i}tH_{\text{free}}/\hbar} P(t,t_0) \mathrm{e}^{-\mathrm{i}t_0 H_{\text{free}}/\hbar}, \qquad t \geq t_0$$

with $P(t,t_0) := \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}$ is called the Heisenberg scattering operator (or the S-matrix operator). In order to understand the physical meaning of the scattering operator, consider the free motion

$$\psi_{\text{free,in}}(t) := \mathrm{e}^{-\mathrm{i}tH_{\text{free}}/\hbar}\varphi_{\text{in}}, \qquad t \in \mathbb{R}$$

with the initial state φ_{in} at time $t = 0$, and

$$\psi_{\text{free,out}}(t) := \mathrm{e}^{-\mathrm{i}tH_{\text{free}}/\hbar}\varphi_{\text{out}}, \qquad t \in \mathbb{R}$$

with the initial state φ_{out} at time $t = 0$. The transition amplitude

$$\tau := \langle \psi_{\text{free,out}}(t) | P(t,t_0) \psi_{\text{free,in}}(t_0) \rangle, \qquad t > t_0$$

is equal to

$$\tau = \langle \varphi_{\text{out}} | \left(\mathrm{e}^{-\mathrm{i}tH_{\text{free}}/\hbar} \right)^{\dagger} P(t,t_0) \mathrm{e}^{-\mathrm{i}t_0 H_{\text{free}}/\hbar} \varphi_{\text{in}} \rangle = \langle \varphi_{\text{out}} | \mathsf{S}(t,t_0) \varphi_{\text{in}} \rangle.$$

The real number

$$\boxed{|\tau|^2 = |\langle \varphi_{\text{out}} | \mathsf{S}(t,t_0) \varphi_{\text{in}} \rangle|^2, \qquad t > t_0} \tag{7.266}$$

is the transition probability from the incoming free state $\psi_{\text{free,in}}(t_0)$ at time t_0 to the outgoing free state $\psi_{\text{free,out}}(t)$ at time t.

The transition probability (7.266)*indexscattering matrix (S-matrix)!transition probability is the key for computing cross sections of scattering processes in particle accelerators.*

We also define

$$\langle \varphi_{\text{out}} | \mathsf{S} \varphi_{\text{in}} \rangle := \lim_{t \to +\infty} \lim_{t_0 \to -\infty} = \langle \varphi_{\text{out}} | \mathsf{S}(t,t_0) \varphi_{\text{in}} \rangle$$

if this limit exists. Here, the complex number $\langle \varphi_{\text{out}} | \mathsf{S} \varphi_{\text{in}} \rangle$ is called an S-matrix element. Parallel to (7.264), we get the causal product relation

$$\boxed{\mathsf{S}(t_N,t_0) = \mathsf{S}(t_N,t_{N-1}) \cdots \mathsf{S}(t_2,t_1)\mathsf{S}(t_1,t_0).} \tag{7.267}$$

Furthermore, we have the differential equation

$$\boxed{\mathrm{i}\hbar \mathsf{S}_t(t,t_0) = \kappa \mathsf{U}(t) \mathsf{S}(t,t_0), \qquad t \geq t_0, \quad \mathsf{S}(t_0,t_0) = I} \tag{7.268}$$

for the scattering operator. Here, we introduce the transformed perturbation

$$\mathsf{U}(t) := \mathrm{e}^{\mathrm{i}tH_{\text{free}}/\hbar} U \mathrm{e}^{-\mathrm{i}t_0 H_{\text{free}}/\hbar}.$$

Let us motivate (7.268). To simplify notation, choose $\hbar := 1$. Then

$$\mathsf{i}\mathsf{S}_t(t,t_0) = -\mathrm{e}^{\mathrm{i}tH_{\mathrm{free}}}H_{\mathrm{free}}P(t,t_0)\mathrm{e}^{-\mathrm{i}t_0H_{\mathrm{free}}} + \mathrm{i}\mathrm{e}^{\mathrm{i}tH_{\mathrm{free}}}P_t(t,t_0)\mathrm{e}^{-\mathrm{i}t_0H_{\mathrm{free}}},$$

which is equal to

$$\mathrm{e}^{\mathrm{i}tH_{\mathrm{free}}}(H - H_{\mathrm{free}})P(t,t_0)\mathrm{e}^{-\mathrm{i}t_0H_{\mathrm{free}}} = \kappa\mathrm{e}^{\mathrm{i}tH_{\mathrm{free}}}U\mathrm{e}^{-\mathrm{i}t_0H_{\mathrm{free}}}\mathsf{S}(t,t_0).$$

Dyson's magic S-matrix formula. Let us pass from differential equations to integral equations. From the differential equation (7.268) for the scattering operator, we get the equivalent Volterra integral equation

$$\boxed{\mathsf{S}(t,t_0) = I - \frac{\mathsf{i}\kappa}{\hbar}\int_{t_0}^{t}\mathsf{U}(\tau)\mathsf{S}(\tau,t_0)d\tau, \qquad t \geq t_0.} \tag{7.269}$$

We have shown in Sect. 7.17.4 of Vol. I that the integral equation (7.269) has the unique solution

$$\boxed{\mathsf{S}(t,t_0) = \mathcal{T}\mathrm{e}^{-\frac{\mathsf{i}\kappa}{\hbar}\int_{t_0}^{t}\mathsf{U}(\tau)d\tau}, \qquad t \geq t_0} \tag{7.270}$$

where $\mathcal{T}$ is the chronological operator (see page 382 of Vol. I). This is Dyson's magic S-matrix formula which plays the decisive role in the operator-theoretic approach to quantum field theory. Comparing the propagator equation (7.265) with the equation (7.268) for the scattering operator, we get the following:

> *The scattering operator* $\mathsf{S}(t,t_0)$ *coincides with the Feynman propagator* $\mathsf{P}(t,t_0)$ *in the Dirac interaction picture (with respect to the transformed perturbation* $\kappa\mathsf{U}(t)$ *of the Hamiltonian operator).*[122]

This fact is of fundamental importance for understanding the S-matrix theory in quantum field theory.

The integral equation for states. For given $\varphi_{\mathrm{in}} \in L_2(\mathbb{R})$, introduce the function $\varphi(t) := \mathsf{S}(t,t_0)\varphi_{\mathrm{in}}$. By (7.269), we obtain the integral equation

$$\varphi(t) = \varphi_{\mathrm{in}} - \frac{\mathsf{i}\kappa}{\hbar}\int_{t_0}^{t}\mathsf{U}(\tau)\varphi(\tau)d\tau, \qquad t \geq t_0.$$

Let $\varphi = \varphi(t)$ be a solution of this integral equation. Set $\psi(t) := \mathrm{e}^{-\mathrm{i}tH_{\mathrm{free}}/\hbar}\varphi(t)$ for all $t \geq t_0$. Then

$$\psi(t) = P(t,t_0)\mathrm{e}^{-\mathrm{i}t_0H_{\mathrm{free}}/\hbar}\varphi_{\mathrm{in}}, \qquad t \geq t_0.$$

By the propagator equation (7.265), this is a solution of the Schrödinger equation (7.262) with the initial condition $\psi(t_0) = \psi_{\mathrm{free,in}} = \mathrm{e}^{-\mathrm{i}t_0H_{\mathrm{free}}/\hbar}\varphi_{\mathrm{in}}$.

7.13.1 The Formal Feynman Path Integral for the Propagator Kernel

> The dynamics of a quantum system is described by a time-dependent operator called the Feynman propagator. The kernel of the propagator can be formally represented by a Feynman path integral which depends on the classical Hamiltonian (i.e., the symbol of the Hamiltonian operator). This is the first magic formula in quantum physics.
>
> Folklore

[122] The Schrödinger picture, the Heisenberg picture, and the Dirac (or interaction) picture are thoroughly discussed on page 393 of Vol. I.

Euler's polygon method. Set $t_k := t_0 + k\Delta t$, $k = 1, \ldots, N$ and $t_N := t$. This way, we get the decomposition

$$t_0 < t_1 < \ldots < t_{N-1} < t_N$$

of the time interval $[t_0, t]$. Let $b : \mathbb{R} \to \mathbb{R}$ be a given smooth function. We want to solve the ordinary differential equation

$$\psi'(t) = b(t)\psi(t), \qquad t \geq t_0, \qquad \psi(t_0) = \psi_0.$$

We are looking for a smooth solution $\psi : \mathbb{R} \to \mathbb{R}$. This uniquely determined solution is denoted by $\psi(t) = P(t, t_0)\psi_0$. Then

$$P(t, t_0)\psi_0 = P(t_N, t_{N-1}) \cdots P(t_2, t_1)P(t_1, t_0)\psi_0,$$

and $P_t(t, t_0)\psi_0 = b(t)P(t, t_0)\psi_0$ for all $\psi_0 \in \mathbb{R}$. Hence $P_t(t, t) = b(t)$. By Taylor expansion, linearization of the propagator yields

$$P(t_{k+1}, t_k) = P(t_k, t_k) + \Delta t \cdot P_t(t_k, t_k) + O((\Delta t)^2), \qquad \Delta t \to 0$$

with $P(t_k, t_k) = 1$ and $P_t(t_k, t_k) = b(t_k)$. Replacing the propagator by its linearization, we obtain the approximate solution

$$\psi_{\Delta t}(t) = (1 + b(t_{N-1}\Delta t)) \cdots (1 + b(t_1)\Delta t)(1 + b(t_0)\Delta t)\psi_0.$$

A standard result in numerical analysis tells us that this approximation method is convergent, that is,

$$\lim_{\Delta t \to 0} \psi_{\Delta t}(t) = \psi(t), \qquad t \geq t_0.$$

For example, fix the real number B, and set $b(t) := B$ for all t. Then we get the well-known classical formula for Euler's exponential function:

$$\lim_{\Delta t \to 0} (1 + B\Delta t)^N \psi_0 = \mathrm{e}^{B(t-t_0)}\psi_0, \tag{7.271}$$

which is valid for all times $t \in \mathbb{R}$ and all $\psi_0 \in \mathbb{R}$.

A general approximation principle for the propagators of time-depending processes. The argument above can be generalized to fairly general time-depending processes. For example, the limit (7.271) exists on a Banach space X for all $\psi_0 \in X$ if $B : X \to X$ is a linear bounded operator. More general functional-analytic results can be found in P. Lax, Functional Analysis, Sect. 34.3, Wiley, New York, 2002.[123] The situation is more subtle if B is an unbounded operator, as in quantum mechanics. In what follows, we will only use formal arguments.

From the propagator to the kernel. Let $\mathcal{K}$ be the kernel of the Feynman propagator operator $P(t, t_0) = \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}$. Then the unique solution

$$\psi(t) = P(t, t_0)\psi_0$$

of the Schrödinger equation (7.262) on page 608 can be represented by the integral formula

$$\boxed{\psi(x, t) = \int_{\mathbb{R}} \mathcal{K}(x, t; y, t_0)\psi_0(y)dy, \qquad x \in \mathbb{R},\ t \geq t_0.}$$

It remains to compute the propagator kernel $\mathcal{K}$. Our goal is the key formula (7.274) below. The propagator possesses the linearization

[123] The proof uses the uniform boundedness theorem in functional analysis.

$$P(t_{k+1},t_k) = I - \frac{\mathrm{i}\Delta t}{\hbar}H + O((\Delta t))^2, \qquad \Delta t \to 0.$$

We set $P_{\Delta t}(t_{k+1},t_k) := I - \frac{\mathrm{i}\Delta t}{\hbar}H$. It follows from the causal product formula (7.264) on page 609 together with the approximation principle above that

$$P(t,t_0) = \lim_{\Delta t\to 0} P_{\Delta t}(t_N,t_{N-1})\cdots P_{\Delta t}(t_1,t_0).$$

Thus, we obtain

$$P(t,t_0) = \lim_{\Delta t\to 0}\left(I - \frac{\mathrm{i}\Delta t}{\hbar}H\right)^N.$$

The kernel product formula (7.245) on page 600 tells us that

$$\begin{aligned}\mathcal{K}(x,t;x_0,t_0) = \int_{\mathbb{R}^{N-1}} &\mathcal{K}(x,t;q_{N-1},t_{N-1})\times\cdots\\ &\times\mathcal{K}(q_2,t_2;q_1,t_1)\mathcal{K}(q_1,t_1;x_0,t_0)dq_{N-1}\cdots dq_2dq_1.\end{aligned} \tag{7.272}$$

From the kernel to the symbol. The Hamiltonian operator H has the symbol $a(q,p)$. Thus, the operator $P_{\Delta t}(t_{k+1},t_k)$ has the symbol $1-\frac{\mathrm{i}\Delta t}{\hbar}a(q,p)$. By the kernel formula (7.251) of the Weyl calculus on page 602, we obtain

$$\mathcal{K}_{\Delta t}(x,t_0+\Delta t;y,t_0) = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p(x-y)/\hbar}\ \left[1 - \frac{\mathrm{i}\Delta t}{\hbar}\ a\left(\frac{x+y}{2},p\right)\right]\frac{dp}{h}.$$

Up to terms of order $O(\Delta t)^2)$ as $\Delta t\to 0$, this yields

$$\mathcal{K}_{\Delta t}(x,t_0+\Delta t;y,t_0) = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p(x-y)/\hbar}\ \exp\left[-\frac{\mathrm{i}\Delta t}{\hbar}\ a\left(\frac{x+y}{2},p\right)\right]\frac{dp}{h}.$$

Since $t_{k+1} = t_k + \Delta t$, we also get the approximation $\mathcal{K}_{\Delta t}(q_{k+1},t_{k+1};q_k,t_k)$ being equal to

$$\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p_{k+1}(q_{k+1}-q_k)/\hbar}\ \exp\left[-\frac{\mathrm{i}\Delta t}{\hbar}\ a\left(\frac{q_{k+1}+q_k}{2},p_{k+1}\right)\right]\frac{dp_{k+1}}{h}$$

where $k = 0,1,\ldots,N-1$.

The Feynman path integral. Using (7.272) and replacing $\mathcal{K}$ by $\mathcal{K}_\Delta$, we obtain the approximation

$$\mathcal{K}_{\Delta t}(x,t;y,t_0) = \int_{\mathbb{R}^{2N-1}} \mathrm{e}^{\mathrm{i}S_N/\hbar}\ \frac{dp_N}{h}\prod_{k=1}^{N-1}\frac{dq_kdp_k}{h}$$

with

$$\begin{aligned}S_N := \Big[&p_N\frac{q_N-q_{N-1}}{\Delta t} + \ldots + p_1\frac{q_1-q_0}{\Delta t}\\ &-a(\tfrac{1}{2}(q_N+q_{N-1}),p_N) + \ldots + a(\tfrac{1}{2}(q_1+q_0),p_1)\Big]\cdot\Delta t.\end{aligned}$$

Since the mid-point $\frac{1}{2}(q_k+q_{k-1})$ of the interval $[q_k,q_{k-1}]$ appears, we call this the mid-point approximation.

Now we pass over to the limit $\Delta t\to 0$ (i.e., $N\to\infty$) in a formal way. Let $S[q,p]$ denote the formal limit $\lim_{N\to\infty} S_N$. Then

$$S[q,p] = \int_{t_0}^{t} [p(\tau)\dot{q}(\tau) - a(q(\tau),p(\tau))]d\tau. \tag{7.273}$$

This is the action along the classical path $q = q(\tau), p = p(\tau)$ in the phase space on the time interval $t_0 \le \tau \le t$. Furthermore, we write the limit $\lim_{\Delta t \to 0} \mathcal{K}_{\Delta t}(x,t;y,t_0)$ in the following symbolic form:[124]

$$\boxed{\mathcal{K}(x,t;y,t_0) = \int_{\mathcal{C}\{t_0,t\}} \mathrm{e}^{\mathrm{i}S[q,p]/\hbar} \cdot \frac{dp(t_0)}{h} \prod_{t_0<\tau\le t} \frac{dq(\tau)dp(\tau)}{h}} \tag{7.274}$$

for all points $x, y \in \mathbb{R}$ and all time intervals $[t_0, t]$. Here, we formally sum over all continuous paths $q = q(\tau), p = p(\tau)$, $t_0 \le \tau \le t$, which satisfy the boundary condition

$$q(t_0) = y, \qquad q(t) = x.$$

The magic formula (7.274) relates classical mechanics to quantum mechanics by means of the classical action.

The crux with differentiable paths. The reader should note that the action $S[q,p]$ from (7.273) only makes sense if the path $q = q(t), p = p(t)$ is sufficiently smooth. However, our formal argument above also takes highly irregular paths into account, which are not differentiable at all. Such irregular paths are typical for the Brownian motion of tiny particles immersed in a liquid. In fact, in Wiener's theory of Brownian motion, the probability is equal to one for the realization of continuous, but not differentiable paths (see Sect. 7.11.4). Then the action $S[q,p]$ does not make any sense, in terms of classical analysis. This indicates that our formal approach is not well defined. Fortunately enough, it turns out that the main contribution to the Feynman path integral (7.274) comes from the paths which satisfy the classical equation of motion in mechanics. This is the main idea behind the WKB approximation method (see Sect. 7.10).

The symbol of the Feynman propagator. Let $\mathrm{sym}_P(q,p\,;t,t_0)$ denote the symbol of the propagator operator $P(t,t_0)$. By the kernel formula (7.252) of the Weyl calculus on page 602, we get

$$\mathrm{sym}_P(q,p\,;t,t_0) = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}rp/\hbar}\, \mathcal{K}(q - \tfrac{1}{2}r, q + \tfrac{1}{2}r)dr \tag{7.275}$$

for all $q, p \in \mathbb{R}$ and all $t \ge t_0$. Recall that the propagator kernel $\mathcal{K}(x,t;y,t_0)$ can be represented by the Feynman path integral (7.274) above.

7.13.2 The Relation between the Scattering Kernel and the Propagator Kernel

> In perturbation theory, the scattering of free quantum particles under the action of a force is described by the Heisenberg scattering operator. The kernel of the scattering operator can be represented by the propagator kernel. This is the second magic formula in quantum physics.
>
> Folklore

Let $\mathcal{S}$ be the kernel of the propagator operator $\mathsf{S}(t,t_0)$. This means that the function $\varphi(t) := \mathsf{S}(t,t_0)\varphi_{\mathrm{in}}$ can be represented by the integral formula

[124] We also briefly write $\mathcal{K}(x,t;y,t_0) = \int_{\mathcal{C}\{t_0,t\}} \mathrm{e}^{\mathrm{i}S[q,p]/\hbar}\, \mathcal{D}q\mathcal{D}p$.

$$\varphi(x,t) = \int_{\mathbb{R}} \mathcal{S}(x,t;y,t_0)\varphi_{\rm in}(y)dy, \qquad x \in \mathbb{R},\ t \geq t_0.$$

This yields the transition amplitude

$$\boxed{\langle \varphi_{\rm out} | \mathsf{S}(t,t_0)\varphi_{\rm in}\rangle = \int_{\mathbb{R}^2} \varphi_{\rm out}(x)\mathcal{S}(x,t;y,t_0)\varphi_{\rm in}(y)dxdy,}$$

which generates the crucial transition probability $|\langle \varphi_{\rm out}|\mathsf{S}(t,t_0)\varphi_{\rm in}\rangle|^2$ from (7.266). It remains to compute the kernel $\mathcal{S}(x,t;y,t_0)$. Our goal is the key formula (7.276) below which relates the scattering kernel to the propagator kernel computed in the preceding section. The point is that there exists a simple relation between the symbol of the scattering operator and the symbol of the Feynman propagator operator. By the Weyl calculus, this implies the desired relation between the scattering kernel $\mathcal{S}(x,t;y,t_0)$ and the Feynman propagator kernel $\mathcal{K}(x,t;y,t_0)$.

The symbol of the scattering operator. Let $\mathrm{sym}_{\mathsf{S}}(q,p\,;t,t_0)$ denote the symbol of the scattering operator

$$\mathsf{S}(t,t_0) := \mathrm{e}^{\mathrm{i}tH_{\rm free}/\hbar}P(t,t_0)\mathrm{e}^{-\mathrm{i}t_0H_{\rm free}/\hbar}, \qquad t \geq t_0.$$

By the Weyl calculus, we have to replace this operator product by the Moyal star product for the corresponding symbols. Note that $\mathrm{e}^{-\mathrm{i}tp^2/2m\hbar}$ is the symbol of the free propagator $\mathrm{e}^{-\mathrm{i}tH_{\rm free}/\hbar}$. Hence

$$\mathrm{sym}_{\mathsf{S}}(q,p\,;t,t_0) = \mathrm{e}^{\mathrm{i}tp^2/2m\hbar} * \mathrm{sym}_P(q,p\,;t,t_0) * \mathrm{e}^{-\mathrm{i}t_0p^2/2m\hbar}.$$

Using formula (7.261) for the Moyal star product on page 607 together with the associativity of the Moyal star product, we obtain the key relation for the symbols:

$$\mathrm{sym}_{\mathsf{S}}(q,p\,;t,t_0) = \int_{\mathbb{R}^2} \mathcal{A}(q,p\,;t,t_0;q_1,p_1)\ \mathrm{sym}_P(q_1,p\,;t,t_0)\ dq_1dp_1. \tag{7.276}$$

Here, the kernel $\mathcal{A}(q,p\,;t,t_0;q_1,p_1)$ is given by the following formula:

$$\frac{1}{\pi\hbar}\exp\left[\frac{\mathrm{i}t(p_1-2p)^2}{2m\hbar} - \frac{\mathrm{i}t_0p_1^2}{2m\hbar} + \frac{2\mathrm{i}(q-q_1)(p-p_1)}{\hbar}\right].$$

The explicit computation of (7.276) will be performed in Problem 7.32. According to (7.275), the symbol sym_P is given by a Feynman path integral which depends on the classical action.

The kernel of the scattering operator. Finally, it follows from the kernel formula (7.251) of the Weyl calculus on page 602 that

$$\boxed{\mathcal{S}(x,t;y,t_0) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p(x-y)/\hbar}\ \mathrm{sym}_{\mathsf{S}}\left(\frac{x+y}{2},p\right)dp} \tag{7.277}$$

for all $x,y \in \mathbb{R}$ and all $t \geq t_0$. This is the magic formula for the kernel of the scattering operator.

7.14 The Poincaré–Wirtinger Calculus

The Poincaré–Wirtinger calculus reformulates real analysis in terms of the language of complex analysis. This is very useful for modern quantum theory. Folklore

Let $f : \mathbb{R}^2 \to \mathbb{C}$ be a smooth complex-valued function on the real plane $\mathbb{R}^2$. We set

$$z := x + \mathrm{i}y, \quad \bar{z} := x - \mathrm{i}y,$$

and we write $f(x, y) := u(x, y) + \mathrm{i}v(x, y)$ where $u : \mathbb{R}^2 \to \mathbb{R}$ is the real part and $v : \mathbb{R}^2 \to \mathbb{R}$ is the imaginary part of f. The main idea of the Poincaré–Wirtinger calculus is to introduce the following two differential operators:

$$\boxed{\frac{\partial}{\partial z} := \frac{1}{2}\left(\frac{\partial}{\partial x} - \mathrm{i}\frac{\partial}{\partial y}\right), \quad \frac{\partial}{\partial \bar{z}} := \frac{1}{2}\left(\frac{\partial}{\partial x} + \mathrm{i}\frac{\partial}{\partial y}\right).} \tag{7.278}$$

This yields

$$\begin{aligned}\frac{\partial f(x,y)}{\partial z} &= \frac{1}{2}(u_x(x,y) + v_y(x,y)) + \frac{\mathrm{i}}{2}(v_x(x,y) - u_y(x,y)),\\ \frac{\partial f(x,y)}{\partial \bar{z}} &= \frac{1}{2}(u_x(x,y) - v_y(x,y)) + \frac{\mathrm{i}}{2}(v_x(x,y) + u_y(x,y)).\end{aligned}$$

Therefore, the following two conditions are equivalent:

(i) $\frac{\partial f}{\partial \bar{z}} = 0$ on $\mathbb{R}^2$.

(ii) $u_x = v_y$ and $u_y = -v_x$ on $\mathbb{R}^2$ (Cauchy–Riemann differential equations).

In this case, we say that the function f is holomorphic on $\mathbb{R}^2$. In terms of complex function theory, this means that the function $z \mapsto f(x, y)$ is holomorphic on the complex plane $\mathbb{C}$, in the classical sense. Similarly, the following two conditions are equivalent:

(i) $\frac{\partial f}{\partial z} = 0$ on $\mathbb{R}^2$.

(ii) $u_x = -v_y$ and $u_y = v_x$ on $\mathbb{R}^2$ (anti-Cauchy–Riemann differential equations).

In this case, we say that the function f is anti-holomorphic on $\mathbb{R}^2$. This is equivalent to the fact that the function $z \mapsto f(x, y)^\dagger$ is holomorphic on $\mathbb{C}$.

Example. (a) For $f(x, y) := x^2 + y^2$, we get

$$\frac{\partial f(x,y)}{\partial z} = x - \mathrm{i}y, \quad \frac{\partial f(x,y)}{\partial \bar{z}} = x + \mathrm{i}y.$$

The function f is neither holomorphic nor anti-holomorphic on $\mathbb{R}^2$.

(b) For $f(x, y) := (x + \mathrm{i}y)^2$, we get

$$\frac{\partial f(x,y)}{\partial z} = 2(x + \mathrm{i}y), \quad \frac{\partial f(x,y)}{\partial \bar{z}} = 0.$$

The function f is holomorphic on $\mathbb{R}^2$.

(c) For $f(x, y) := (x - \mathrm{i}y)^2$, we get

$$\frac{\partial f(x,y)}{\partial \bar{z}} = 2(x - \mathrm{i}y), \quad \frac{\partial f(x,y)}{\partial z} = 0.$$

The function f is anti-holomorphic on $\mathbb{R}^2$.

Mnemonic elegance. The results (a)–(c) above can be reformulated as follows.
(a) For $f(x,y) = x^2 + y^2 = z\bar{z}$, we get

$$\frac{\partial f(x,y)}{\partial z} = \bar{z} = x - \mathrm{i}y, \quad \frac{\partial f(x,y)}{\partial \bar{z}} = z = x + \mathrm{i}y.$$

(b) For $f(x,y) := (x+\mathrm{i}y)^2 = z^2$, we get

$$\frac{\partial f(x,y)}{\partial z} = 2z = 2(x+\mathrm{i}y), \quad \frac{\partial f(x,y)}{\partial \bar{z}} = 0.$$

(c) For $f(x,y) := (x-\mathrm{i}y)^2 = \bar{z}^2$, we get

$$\frac{\partial f(x,y)}{\partial \bar{z}} = 2\bar{z} = 2(x-\mathrm{i}y), \quad \frac{\partial f(x,y)}{\partial z} = 0.$$

These results are formally obtained by considering f as a function of the two independent variables z and $\bar{z}$ and by using formal partial differentiation with respect to z and $\bar{z}$.

For a general smooth function $f : \mathbb{R}^2 \to \mathbb{C}$, we proceed as follows. Using the representations $x = (z+\bar{z})/2$ and $y = (z-\bar{z})/2\mathrm{i}$, we define

$$F(z,\bar{z}) := f\left(\frac{z+\bar{z}}{2}, \frac{z-\bar{z}}{2\mathrm{i}}\right). \tag{7.279}$$

Considering formally the function F as a function of the independent variables z and $\bar{z}$, the chain rule tells us that

$$\begin{aligned}\frac{\partial F(z,\bar{z})}{\partial z} &= \frac{1}{2} f_x\left(\frac{z+\bar{z}}{2}, \frac{z-\bar{z}}{2\mathrm{i}}\right) + \frac{1}{2\mathrm{i}} f_y\left(\frac{z+\bar{z}}{2}, \frac{z-\bar{z}}{2\mathrm{i}}\right) \\ &= \frac{1}{2} f_x(x,y) - \frac{\mathrm{i}}{2} f_y(x,y),\end{aligned}$$

and

$$\frac{\partial F(z,\bar{z})}{\partial \bar{z}} = \frac{1}{2} f_x(x,y) + \frac{\mathrm{i}}{2} f_y(x,y).$$

This coincides with definition (7.278). The following observation is useful.

- The function f is holomorphic on $\mathbb{R}^2$ iff F is independent of $\bar{z}$ and $z \mapsto F(z)$ is holomorphic on $\mathbb{C}^2$. Then $\frac{\partial f(x,y)}{\partial z} = F'(z)$ for all $z = x + \mathrm{i}y$ on $\mathbb{C}$.
- The function f is anti-holomorphic on $\mathbb{R}^2$ iff F is independent of z and $\zeta \mapsto F(\zeta)$ is holomorphic on $\mathbb{C}^2$. Then $\frac{\partial f(x,y)}{\partial \bar{z}} = F'(\bar{z})$ for all $\bar{z} = x - \mathrm{i}y$ on the complex plane $\mathbb{C}$.

In later volumes, the Poincaré–Wirtinger calculus will play a crucial role in studying the following subjects: Kähler geometry, conformal field theory, and string theory.

7.15 Bargmann's Holomorphic Quantization

Our goal is to realize the commutation relation

$$\boxed{a^- a^+ - a^+ a^- = I} \tag{7.280}$$

together with $(a^-)^\dagger = a^+$ by elementary operators on a Hilbert space $B(\mathbb{C})$ of holomorphic functions. The precise formulation will be given in Theorem 7.58 below.

In terms of physics, the operator a^+ (resp. a^-) is a creation (resp. annihilation) operator.[125]

The Bargmann–Fock space $B(\mathbb{C})$**.** We start with the inner product

$$\langle F|G\rangle := \frac{1}{\pi}\int_{\mathbb{R}^2} F(z)^\dagger G(z)\mathrm{e}^{-zz^\dagger}\,dxdy. \tag{7.281}$$

By definition, the space $B(\mathbb{C})$ consists of all holomorphic functions $F:\mathbb{C}\to\mathbb{C}$ with $\langle F|F\rangle < \infty$. This is a complex Hilbert space with respect to the inner product (7.281). The set of polynomials $z\mapsto F(z)$ is a dense subset of $B(\mathbb{C})$. We define the operators $a^\pm : D(a^\pm)\to B(\mathbb{C})$ by setting

$$\boxed{(a^+F)(z) := zF(z) \qquad \text{for all} \quad z\in\mathbb{C},}$$

and

$$\boxed{(a^-F)(z) := \frac{d}{dz}F(z) \qquad \text{for all} \quad z\in\mathbb{C}.}$$

More precisely, the domain of definition $D(a^\pm)$ of the operator $a^\pm$ consists of all functions $F\in B(\mathbb{C})$ with $a^\pm F\in B(\mathbb{C})$. For example, this is satisfied for all polynomials F. Setting $F_0(z):=1$ for all $z\in\mathbb{C}$, we get $\langle F_0|F_0\rangle = 1$ and

$$\boxed{a^-F_0 = 0.}$$

In terms of physics, the function F_0 is called the ground state (or the vacuum state). This state does not contain any particles.

Theorem 7.58 (i) *For all polynomials $F\in B(\mathbb{C})$, we get*

$$(a^-a^+ - a^+a^-)F = F.$$

This is the precise formulation of the commutation relation (7.280) .

(ii) *For all polynomials $F,G\in B(\mathbb{C})$, we get*

$$\langle a^-F|G\rangle = \langle F|a^+G\rangle.$$

This means that $(a^-)^\dagger = a^+$, in the sense of a formally adjoint operator.

Proof. Ad (i). Note that $(a^+a^-F)(z) = zF'(z)$ and

$$(a^-a^+F)(z) = (zF(z))' = F(z) + zF'(z).$$

Ad (ii). We will use the Poincaré–Wirtinger calculus introduced on page 616. Recall that $\bar z := z^\dagger$. Since G is holomorphic, $\frac{\partial G(z)}{\partial \bar z} = 0$. By the product rule,

$$\frac{\partial}{\partial\bar z}\left(G(z)\mathrm{e}^{-z\bar z}\right) = \frac{\partial G(z)}{\partial\bar z}\,\mathrm{e}^{-z\bar z} - G(z)z\mathrm{e}^{-z\bar z} = -G(z)z\mathrm{e}^{-z\bar z}.$$

[125] The proofs can be found in the classical paper by V. Bargmann, On a Hilbert space of analytic functions and an associated integral transform, Commun. Pure and Appl. Math. **14** (1961), 187–214. See also the last chapter of the monograph by F. Berezin and M. Shubin, The Schrödinger Equation, Kluwer, Dordrecht, 1991.
The basic idea goes back to V. Fock, Generalizing and solving Dirac's statistical equation, Z. Phys. **49** (1928), 339–357 (in German).

Hence

$$\frac{\partial}{\partial\bar z}\left(F(z)^\dagger G(z)\mathrm{e}^{-z\bar z}\right) = \left(\frac{\partial}{\partial\bar z}F(z)^\dagger\right)G(z)\mathrm{e}^{-z\bar z} - F(z)^\dagger G(z)z\mathrm{e}^{-z\bar z}$$
$$= \left(\frac{\partial}{\partial z}F(z)\right)^\dagger G(z)\mathrm{e}^{-z\bar z} - F(z)^\dagger(zG(z))\mathrm{e}^{-z\bar z}.$$

Because of the polynomial growth of F and G at infinity, we get[126]

$$\lim_{R\to\infty}\int_{x^2+y^2\le R^2}\frac{\partial}{\partial\bar z}\left(F(z)^\dagger G(z)\mathrm{e}^{-z\bar z}\right)\,dxdy = 0.$$

This yields the claim. □

Orthonormal basis. The functions

$$F_n := \frac{(a^+)^n F_0}{\sqrt{n!}}, \qquad n = 0, 1, \ldots$$

form an orthonormal basis of the Hilbert space $B(\mathbb{C})$. Explicitly, $F_n(z) = z^n/\sqrt{n!}$ for all $z \in \mathbb{C}$. In terms of physics, F_n represents a (normalized) state of n particles. Intuitively, this state is generated from the vacuum state F_0 by n-fold application of the creation operator a^+ to F_0.

Wick operators. Let α_{kn} be complex numbers for $k, n = 0, \ldots, m$, where $m = 0, 1, \ldots$. For all polynomials $z \mapsto F(z)$, define

$$AF := \sum_{k,n=0}^{m}\alpha_{kn}(a^+)^k(a^-)^n F.$$

Note that the powers of the annihilation operator a^- stand on the right. In particular, $\alpha_{kn}(a^+)^k(a^-)^n F_0 = 0$ if $n = 1, 2, \ldots$. The operators A are called Wick operators on the Hilbert space $B(\mathbb{C})$ (or normally ordered operators). The polynomial

$$\mathrm{sym}_A(z,\zeta) := \sum_{k,n=0}^{m}\alpha_{kn}z^k\zeta^n$$

with respect to the complex variables z and ζ is called the symbol of the Wick operator A. As we will show later on, Wick operators play a crucial role for describing physical quantities in quantum field theory (e.g., collision processes) and in quantum statistics (e.g., superfluidity and superconductivity).

The Bargmann–Fock space $B(\mathbb{C}^s)$. We want to apply the preceding construction to s species of particles. To this end, we define $\langle F|G\rangle$ by

$$\frac{1}{\pi^s}\int_{\mathbb{R}^{2s}}F(z_1,\ldots,z_s)^\dagger G(z_1,\ldots,z_s)\mathrm{e}^{-\sum_{k=1}^s z_k z_k^\dagger}dx_1\cdots dx_s dy_1\cdots dy_s,$$

where $z_k := x_k + \mathrm{i}y_k$, and $x_k, y_k \in \mathbb{R}$ for all $k = 1, \ldots, s$. By definition, the Fock–Bargmann space $B(\mathbb{C}^s)$ consists of all holomorphic functions[127]

[126] Note the following. Since $\frac{\partial}{\partial z} = \frac{1}{2}\left(\frac{\partial}{\partial x} - \mathrm{i}\frac{\partial}{\partial y}\right)$, the Gaussian integral theorem transforms this integral into a boundary integral (over the sphere of radius R), which goes to zero as $R \to \infty$.

[127] This means that $F : \mathbb{C}^s \to \mathbb{C}$ is a power series expansion (with complex coefficients) which is absolutely convergent for all complex numbers $z_1, \ldots, z_s$.

$$F : \mathbb{C}^s \to \mathbb{C}$$

with $\langle F|F\rangle < \infty$. The space $B(\mathbb{C}^s)$ is a complex Hilbert space equipped with the inner product $\langle F|G\rangle$. The set of polynomials $(z_1, \dots, z_s) \mapsto F(z_1, \dots, z_s)$ (with complex coefficients) is a dense subset of $B(\mathbb{C}^s)$. Let $k = 1, \dots, s$. For all polynomials F, define

$$(a_k^+ F)(z_1, \dots, z_s) := z_k F(z_1, \dots, z_s), \quad (a_k^- F)(z_1, \dots, z_s) := \frac{\partial F(z_1, \dots, z_s)}{\partial z_k},$$

where $z_1, \dots, z_s \in \mathbb{C}$. Then, for all polynomials F and all $j, k = 1, \dots, s$, we have the commutation relations

$$(a_j^- a_k^+ - a_k^+ a_j^-)F = \delta_{jk} F$$

together with $(a_j^- a_k^- - a_k^- a_j^-)F = (a_j^+ a_k^+ - a_k^+ a_j^+)F = 0$. We briefly write

$$\boxed{[a_j^-, a_k^+]_- = \delta_{jk} I, \qquad [a_j^-, a_k^-]_- = [a_j^+, a_k^+]_- = 0, \quad j, k = 1, \dots, s.}$$

Moreover, for all polynomials F, G, we have

$$\langle a_k^- F|G\rangle = \langle F|a_k^+ G\rangle, \qquad k = 1, \dots, s.$$

Hence $(a_k^-)^\dagger = a_k^+$ for $k = 1, \dots, s$ in the sense of formal adjoint operators.

In the monograph by L. Faddeev and A. Slavnov, Gauge Fields, Benjamin, Reading, Massachusetts, 1980, it is emphasized that the Feynman path integral based on Bargmann quantization is very convenient for studying the quantization of the Standard Model in particle physics (Faddev–Popov quantization of gauge theories). We will investigate this in Vol. V.

Application to the quantized harmonic oscillator. We want to show that the use of Bargmann's holomorphic quantization allows us immediately to obtain the energy spectrum of the quantized harmonic oscillator. Motivated by Sect. 7.3.1 on page 443, we use the Hamiltonian

$$H = \frac{P^2}{2m} + \frac{m\omega^2 Q^2}{2}$$

of the harmonic oscillator, and we set

$$Q := \frac{x_0}{\sqrt{2}}(a^+ + a^-), \qquad P := \frac{\mathrm{i}\hbar}{x_0\sqrt{2}}(a^+ - a^-)$$

with $x_0 := \sqrt{\frac{\hbar}{m\omega}}$. It follows from $a^- a^+ - a^+ a^- = I$ that $QP - PQ = \mathrm{i}\hbar I$ and

$$H = \hbar\omega(a^+ a^- + \tfrac{1}{2}).$$

Setting $F_n(z) := z^n$, we get $a^+ a^- F_n = z\frac{d}{dz}F_n = nF_n$. Therefore, introducing $E_n := \hbar\omega(n + \frac{1}{2})$, we obtain

$$HF_n = E_n F_n, \qquad n = 0, 1, \dots$$

7.16 The Stone–Von Neumann Uniqueness Theorem

> The name "Heisenberg commutation relation" is a bit of a misnomer; the relations were in fact first formulated in their modern form not by Heisenberg (1925), but by Born and Jordan (1925) and by Dirac (1925) in the one-dimensional case and in the "Dreimännerarbeit" (three-man work) by Born, Heisenberg and Jordan (1926) and by Dirac (1926) in the multi-dimensional case. However, it is true that they grew out of the original ground-breaking work of Heisenberg (1925), though one would have to examine Heisenberg's paper very carefully to find anything remotely suggesting the commutation relations.[128]
>
> Jonathan Rosenberg, 2004

In this chapter, we have based quantum mechanics on the Born–Heisenberg–Jordan commutation relation

$$\boxed{QP - PQ = \mathrm{i}\hbar I.} \tag{7.282}$$

We want to show that, in an appropriate sense, the construction of the theory is unique. That is, each realization of quantum mechanics is equivalent to Schrödinger's approach. This follows from the Stone–von Neumann uniqueness theorem below. Moreover, we want to show that this problem is closely related to the following mathematical topics: functional analysis (operator theory on Hilbert spaces), symplectic geometry, C^*-algebras, functors between categories (the Weyl quantization functor), Lie algebras (the Heisenberg algebra) and Lie groups (the Heisenberg group). The main trick is to replace (7.282) by the Weyl relation (7.283) below. This way, we circumvent the technical subtlety related to the fact that the operators Q and P are not defined on the total Hilbert space. The Weyl relation refers to the unitary operators $U(a) = \mathrm{e}^{\mathrm{i}aP/\hbar}$ and $V(b) = \mathrm{e}^{\mathrm{i}bQ}$ defined on the total Hilbert space. Here, a and b are real parameters. This exponentiation is an infinite-dimensional variant of the passage from Lie algebras to Lie groups.

7.16.1 The Prototype of the Weyl Relation

Prototype. Consider the motion of a quantum particle on the real line. Choose the real numbers a and b. For each wave function $\psi \in L_2(\mathbb{R})$, we define the translation operator

$$(U(a)\psi)(x) := \psi(x + a), \qquad x \in \mathbb{R},$$

and the phase operator

$$(V(b)\psi)(x) := \mathrm{e}^{\mathrm{i}bx}\psi(x), \qquad x \in \mathbb{R}.$$

Then, we have the so-called Weyl relation[129]

[128] See the references given on page 673ff. The fascinating (and surprising) discovery of the commutation relation by Born after reading Heisenberg's paper is described on page 64 of Vol. I.
J. Rosenberg, A selective history of the Stone–von Neumann Theorem. In: Operator algebras, quantization, and noncommutative geometry, Contemporary Mathematics **365**, pp. 123–158, Amer. Math. Soc., Providence, Rhode Island, 2004 (reprinted with permission).

[129] H. Weyl, Quantum mechanics and group theory, Z. Physik **46** (1928), 1–47 (in German).

$$\boxed{U(a)V(b) = \mathrm{e}^{\mathrm{i}ab}V(b)U(a) \qquad \text{for all} \quad a, b \in \mathbb{R}.} \tag{7.283}$$

In fact, $(U(a)V(b)\psi)(x) = U(a)(\mathrm{e}^{\mathrm{i}bx}\psi(x))$. This is equal to

$$\mathrm{e}^{\mathrm{i}b(x+a)}\psi(x+a) = \mathrm{e}^{\mathrm{i}ab}V(b)U(a)\psi(x).$$

Using the notion of strongly continuous one-parameter unitary group introduced on page 506, the following holds:

$\{U(a)\}_{a\in\mathbb{R}}$ and $\{V(b)\}_{b\in\mathbb{R}}$ are strongly continuous one-parameter unitary groups on the Hilbert space $L_2(\mathbb{R})$.

The Born–Heisenberg–Jordan commutation relation. Let the operators $Q : D(Q) \to L_2(\mathbb{R})$ and $P : D(P) \to L_2(\mathbb{R})$ be the self-adjoint position and momentum operator, respectively, introduced in Sect. 7.6.4 on page 518. Then, for any test function $\psi \in \mathcal{S}(\mathbb{R})$, we get

$$P\psi(x) = -\mathrm{i}\hbar\frac{d}{dx}\psi(x) = -\mathrm{i}\hbar\frac{d}{da}U(a)\psi(x)_{|a=0}$$

and

$$Q\psi(x) = x\psi(x) = -\mathrm{i}\frac{d}{db}V(b)\psi(x)_{|b=0}.$$

Differentiating successively the Weyl relation

$$(U(a)V(b) - \mathrm{e}^{\mathrm{i}ab}V(b)U(a))\psi(x) = 0$$

with respect to the parameter a at the point $a = 0$ and with respect to b at $b = 0$, we get

$$(QP - PQ)\psi = \mathrm{i}\hbar\psi. \tag{7.284}$$

Therefore, the Born–Heisenberg–Jordan commutation relation (7.284) can be regarded as the infinitesimal variant of the Weyl relation (7.283). In terms of the Stone theorem on page 506,

$$U(a) = \mathrm{e}^{\mathrm{i}aP/\hbar}, \qquad V(b) = \mathrm{e}^{\mathrm{i}bQ}, \qquad a, b \in \mathbb{R}.$$

The Heisenberg algebra $\mathcal{A}_{\mathrm{Heis}}$. Consider the linear operators

$$Q, P, \hbar\mathrm{i}I : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R}).$$

Explicitly, $(Q\psi)(x) := x\psi(x)$, $(P\psi)(x) := -\mathrm{i}\hbar\frac{d}{dx}\psi(x)$, and $\hbar\mathrm{i}I\psi(x) := \hbar\mathrm{i}\psi(x)$ for all $x \in \mathbb{R}$ and all $\psi \in \mathcal{S}(\mathbb{R})$. Set

$$\mathcal{A}_{\mathrm{Heis}} := \{aQ + bP + c\hbar\mathrm{i}I : a, b, c \in \mathbb{R}\}.$$

This is a 3-dimensional real Lie algebra with respect to the following Lie products[130]

$$[Q, P]_- = \hbar\mathrm{i}I, \quad [Q, \hbar\mathrm{i}I]_- = [P, \hbar\mathrm{i}I]_- = 0.$$

Trivially, we have $[Q, Q]_- = [P, P]_- = [\hbar\mathrm{i}I, \hbar\mathrm{i}I]_- = 0$. This Lie algebra is called the Heisenberg Lie algebra (or briefly the Heisenberg algebra).

The realization of the Heisenberg algebra as a matrix Lie algebra. Let us introduce the matrices

[130] Recall that $[A, B]_- := AB - BA$.

$$A := \begin{pmatrix} 0\ 1\ 0 \\ 0\ 0\ 0 \\ 0\ 0\ 0 \end{pmatrix}, \quad B := \begin{pmatrix} 0\ 0\ 0 \\ 0\ 0\ 1 \\ 0\ 0\ 0 \end{pmatrix}, \quad C := \begin{pmatrix} 0\ 0\ 1 \\ 0\ 0\ 0 \\ 0\ 0\ 0 \end{pmatrix}.$$

Then, we have the Lie products

$$[A, B]_- = C, \quad [A, C]_- = [B, C]_- = 0.$$

Consequently, the set of all matrices

$$aA + bB + cC = \begin{pmatrix} 0\ a\ c \\ 0\ 0\ b \\ 0\ 0\ 0 \end{pmatrix}, \qquad a, b, c \in \mathbb{R}$$

forms a real 3-dimensional Lie algebra denoted by $sut(3, \mathbb{R})$.

The Heisenberg Lie algebra $\mathcal{A}_{\text{Heis}}$ is isomorphic to the Lie algebra $sut(3)$.

This isomorphism is given by the map $aQ + bP + c\hbar iI \mapsto aA + bB + cC$. All the matrices

$$\begin{pmatrix} 1\ a\ c \\ 0\ 1\ b \\ 0\ 0\ 1 \end{pmatrix}, \qquad a, b, c \in \mathbb{R}$$

form a group (with respect to matrix multiplication). This Lie group is denoted by $SUT(3, \mathbb{R})$ (group of special upper triangular real (3×3)-matrices).

The Lie algebra of the Lie group $SUT(3, \mathbb{R})$ is equal to $sut(3, \mathbb{R})$.

For more details, we refer to both Sec. 7.6ff of Vol. I and to Baker (2002).

The universal enveloping algebra of the Heisenberg algebra. Again consider the operators $Q, P, \hbar iI : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$. Let $\mathcal{E}(\mathcal{A}_{\text{Heis}})$ denote the set of all polynomials in Q, P and $\hbar iI$ with complex coefficients. For example, the operator

$$a\hbar iI + bP^3 + cP^2Q + dQP$$

with complex coefficients a, b, c, d is an element of $\mathcal{E}(\mathcal{A}_{\text{Heis}})$.

- The set $\mathcal{E}(\mathcal{A}_{\text{Heis}})$ is a complex algebra (with respect to the sum and the product of operators).
- If $A, B \in \mathcal{A}_{\text{Heis}}$, then $A, B \in \mathcal{E}(\mathcal{A}_{\text{Heis}})$ and $[A, B]_- = AB - BA$.

That is, the Lie product $[.,.]_-$ on $\mathcal{A}_{\text{Heis}}$ can be represented by using the product on $\mathcal{E}(\mathcal{A}_{\text{Heis}})$. In terms of the general theory of Lie algebras, the algebra $\mathcal{E}(\mathcal{A}_{\text{Heis}})$ is called the universal enveloping algebra of the Heisenberg Lie algebra $\mathcal{A}_{\text{Heis}}$.

The Weyl system with respect to the symplectic form ω on the plane $\mathbb{R}^2$. For all $(a, b) \in \mathbb{R}^2$, define

$$\boxed{W(a, b) := \mathrm{e}^{-\frac{\mathrm{i}}{2}ab} U(a)V(b).} \tag{7.285}$$

Then, for all $(a, b), (c, d) \in \mathbb{R}^2$, the following hold:

(i) $W(a, b)W(b, c) = \mathrm{e}^{\frac{\mathrm{i}}{2}\omega(a,b;c,d)} W(a + c, b + d)$. Here, we set

$$\omega(a, b; c, d) := (a, b) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = ad - bc.$$

Note that ω is the symplectic form on the plane $\mathbb{R}^2$.

(ii) $W(a,b)^\dagger = W(-a,-b)$ and $W(0,0) = I$.

The operator family $\{W(a,b)\}_{(a,b)\in\mathbb{R}^2}$ is called the Weyl system of $\mathbb{R}^2$. One checks easily that (7.283), (7.285) imply (i) and (ii). For example, we have

$$\begin{aligned} W(a,b)^\dagger &= \mathrm{e}^{\frac{\mathrm{i}}{2}ab} V(b)^\dagger U(a)^\dagger = \mathrm{e}^{\frac{\mathrm{i}}{2}ab} V(-b)U(-a) \\ &= \mathrm{e}^{-\frac{\mathrm{i}}{2}ab} U(-a)V(-b) = W(-a,-b). \end{aligned}$$

Conversely, if W is given, then we set $U(a) := W(a,0)$ and $V(b) := W(0,b)$. Then (i), (ii) imply (7.283), (7.285).

The Weyl algebra of the Hilbert space $L_2(\mathbb{R})$. The linear continuous operators $A : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ form a C^*-algebra $\mathcal{A}$. The C^*-subalgebra of $\mathcal{A}$ generated by $\{W(a,b) : (a,b) \in \mathbb{R}^2\}$ is called the Weyl algebra of the Hilbert space $L_2(\mathbb{R})$ (see page 628).

The Heisenberg group $\mathcal{G}_{\mathrm{Heis}}$**.** For all $a,b,\lambda \in \mathbb{R}$, modify the Weyl system by setting

$$H(a,b,\lambda) := \mathrm{e}^{\mathrm{i}\lambda} W(a,b), \qquad a,b,\lambda \in \mathbb{R}.$$

Then, for all $a,b,c,d,\lambda,\mu \in \mathbb{R}$, we have the product formula

$$H(a,b,\lambda)H(c,d,\mu) = H\big(a+c, b+d, \lambda+\mu+\tfrac{1}{2}\omega(a,b;c,d)\big).$$

This means that the set $\{H(a,b,\lambda)\}_{a,b,\lambda\in\mathbb{R}}$ forms a group $\mathcal{H}$. The space $\mathbb{R}^3$ is a group with respect to the product

$$(a,b,\lambda)(c,d,\mu) := (a+c, b+d, \lambda+\mu)$$

for all $(a,b,\lambda),(c,d,\mu) \in \mathbb{R}^3$. If we modify this product by setting

$$(a,b,\lambda)(c,d,\mu) := \big(a+c,\ b+d,\ \lambda+\mu+\tfrac{1}{2}\omega(a,b;c,d)\big),$$

then $\mathbb{R}^3$ becomes a group which is called the Heisenberg group $\mathcal{G}_{\mathrm{Heis}}$.[131] The additional term $\frac{1}{2}\omega(a,b;c,d)$ is called a twist. There exists a group epimorphism[132]

$$\chi : \mathcal{G}_{\mathrm{Heis}} \to \mathcal{H}$$

given by the map $(a,b,\lambda) \mapsto H(a,b,\lambda)$.

The Heisenberg group $\mathcal{G}_{\mathrm{Heis}}$ is a 3-dimensional Lie group whose Lie algebra is the Heisenberg algebra $\mathcal{A}_{\mathrm{Heis}}$.

Since the Heisenberg group $\mathcal{G}_{\mathrm{Heis}}$ is arcwise connected and simply connected, it represents the universal covering Lie group of the Heisenberg Lie algebra $\mathcal{A}_{\mathrm{Heis}}$. By the general theory of Lie groups, the universal covering Lie group $\mathcal{G}_{\mathrm{universal}}$ of a given Lie algebra $\mathcal{L}$ knows everything about all of the Lie groups $\mathcal{G}$ whose Lie algebra is equal to $\mathcal{L}$.

The Heisenberg group is isomorphic to the group $SUT(3,\mathbb{R})$.

[131] The definition of the Heisenberg group is not unique in the literature. The Heisenberg group is also called the Weyl group in the physical literature. In fact, the Heisenberg group never appears in the papers written by Heisenberg; this group was introduced by Weyl.

[132] A surjective (resp. injective) group morphism is called group epimorphism (resp. group monomorphism). The same is true for rings. The general definition of epimorphisms and monomorphisms in terms of category theory will be considered in Vol. IV.

This Lie group isomorphism is given by the map

$$\begin{pmatrix} 1 & a & c \\ 0 & 1 & b \\ 0 & 0 & 1 \end{pmatrix} \mapsto (a, b, c - \tfrac{1}{2}ab).$$

Central extensions of groups. Let $\mathcal{G}$ be a group. The set of all elements A of $\mathcal{G}$ with the property that

$$AB = BA \qquad \text{for all} \quad B \in \mathcal{G}$$

is called the center $C(\mathcal{G})$ of the group $\mathcal{G}$. The center $C(\mathcal{G})$ is a normal subgroup of $\mathcal{G}$. The group $\mathcal{G}$ is said to be a central extension of the quotient group $\mathcal{G}/C(\mathcal{G})$.[133] For the Heisenberg group,

$$C(\mathcal{G}_{\text{Heis}}) := \{(0, 0, \lambda) : \lambda \in \mathbb{R}\}.$$

This center is isomorphic to the additive group $\mathbb{R}$. The map

$$(a, b, \lambda) \mapsto (a, b)$$

is a group morphism from the Heisenberg group $\mathcal{G}_{\text{Heis}}$ onto the additive group $\mathbb{R}^2$. The kernel of the unit element $(0, 0)$ of $\mathbb{R}^2$ is the center $C(\mathcal{G}_{\text{Heis}})$. Therefore, we have the group isomorphism

$$\mathcal{G}_{\text{Heis}}/C(\mathcal{G}_{\text{Heis}}) \simeq \mathbb{R}^2.$$

Consequently, the Heisenberg group $\mathcal{G}_{\text{Heis}}$ is a central extension of the additive group $\mathbb{R}^2$.

Central extensions of Lie algebras. Let X be a linear space. Introducing the Lie product $[A, B] := 0$ for all $A, B \in X$, we obtain the trivial Lie algebra X. In this sense, the linear spaces $\mathbb{R}^n$ $(n = 1, 2, \ldots)$ become trivial Lie algebras.

Let $\mathcal{L}$ be a Lie algebra. The set of all elements A of $\mathcal{L}$ with the property that

$$[A, B] = 0 \qquad \text{for all} \quad B \in \mathcal{L}$$

is called the center $C(\mathcal{L})$ of $\mathcal{L}$. The center $C(\mathcal{L})$ is an ideal of $\mathcal{L}$. The Lie algebra $\mathcal{L}$ is said to be a central extension of the quotient Lie algebra $\mathcal{L}/C(\mathcal{L})$.[134] For example, the center of the Heisenberg algebra is given by

$$C(\mathcal{A}_{\text{Heis}}) = \{c\hbar i I : c \in \mathbb{R}\}.$$

This center is isomorphic to $\mathbb{R}$. The map

$$aQ + bP + c\hbar i I \mapsto (a, b)$$

is a Lie algebra morphism from the Heisenberg algebra $\mathcal{A}_{\text{Heis}}$ onto the trivial Lie algebra $\mathbb{R}^2$. The kernel of the zero element $(0, 0)$ of $\mathbb{R}^2$ is the center $C(\mathcal{A}_{\text{Heis}})$. Therefore, we have the Lie algebra isomorphism

$$\mathcal{A}_{\text{Heis}}/C(\mathcal{A}_{\text{Heis}}) \simeq \mathbb{R}^2.$$

[133] More general, if H is a subgroup of $C(G)$, then the quotient group G/H is called a central extension of the group G by the group H.

[134] More general, if $\mathcal{J}$ is a subalgebra of $C(\mathcal{L})$, then the Lie algebra $\mathcal{L}$ is called a central extension of the Lie algebra $\mathcal{L}/\mathcal{J}$ by the Lie algebra $\mathcal{J}$.

Consequently, the Heisenberg algebra $\mathcal{A}_{\text{Heis}}$ is a central extension of the trivial Lie algebra $\mathbb{R}^2$.

Central extensions of Lie groups and Lie algebras play an important role in quantum physics (e.g., the Bargmann theorem on the lifting of projective quantum symmetries to unitary symmetries, and the Virasoro algebra in both conformal quantum field theory and string theory). As an introduction, we recommend M. Schottenloher, A Mathematical Introduction to Conformal Field Theory, Springer, Berlin, 1997.

7.16.2 The Main Theorem

Theorem 7.59 *Let $\{\mathcal{U}(a)\}_{a\in\mathbb{R}}$ and $\{\mathcal{V}(b)\}_{b\in\mathbb{R}}$ be strongly continuous one-parameter unitary groups on the complex separable non-trivial Hilbert space X.*[135] *Suppose that the Weyl relation*

$$\mathcal{U}(a)\mathcal{V}(b) = e^{\mathrm{i}ab}\mathcal{V}(b)\mathcal{U}(a) \qquad \text{for all} \quad a, b \in \mathbb{R}$$

is satisfied. Then the operators $\mathcal{U}(a)$ (resp. $\mathcal{V}(b)$) are unitarily equivalent to direct sums of translation (resp. phase) operators on $L_2(\mathbb{R})$.

More precisely, the following hold.

(i) Invariant subspaces: There exists a finite or countable family $X_1, X_2, \ldots$ of pairwise orthogonal, closed, linear subspaces of the Hilbert space X with the direct sum decomposition

$$X = \bigoplus_k X_k.$$

All of the spaces $X_1, X_2, \ldots$ are invariant under the operators $\mathcal{U}(a)$ and $\mathcal{V}(b)$.

(ii) Unitary equivalence: For all $a, b \in \mathbb{R}$, the operator $\mathcal{U}(a)$ (resp. $\mathcal{V}(b)$) is unitarily equivalent to the translation operator $U(a)$ (resp. the phase operator $V(b)$) on the Hilbert space $L_2(\mathbb{R})$ introduced on page 622. This means that there exist unitary operators $U_k : X_k \to L_2(\mathbb{R})$ such that, for all k, the following diagram is commutative:

$$\begin{array}{ccc} X_k & \xrightarrow{\mathcal{U}(a)} & X_k \\ {\scriptstyle U_k}\downarrow & & \downarrow{\scriptstyle U_k} \\ L_2(\mathbb{R}) & \xrightarrow{U(a)} & L_2(\mathbb{R}). \end{array}$$

The same is true if we replace $\mathcal{U}(a)$ and $U(a)$ by $\mathcal{V}(b)$ and $V(b)$, respectively.

The proof can be found in Putnam (1967), p. 65. Theorem 7.59 is called the Stone–von Neumann uniqueness theorem. This theorem was announced by Stone in 1930. The first proof was given by

J. von Neumann, On the uniqueness of the Schrödinger operators, Math. Ann. **104** (1931), 570–578 (in German).

[135] A Hilbert space X is called trivial iff $X = \{0\}$.

7.16.3 C^*-Algebras

> A crucial strategy in modern mathematical physics consists in using C^*-algebras.
>
> Folklore

The simplest case of a C^*-algebra is the set $\mathbb{C}$ of complex numbers equipped with the operations $z+w$, zw, $z^\dagger$, and $|z|$. Since $zw = wz$, this C^*-algebra is called commutative.

Let $n = 2, 3, \dots$ The prototype of a (noncommutative) C^*-algebra is the set of complex $(n \times n)$-matrices equipped with the operations $A+B$, AB, $A^\dagger$ (adjoint matrix), αA ($\alpha \in \mathbb{C}$), and $||A|| := \sqrt{\mathrm{tr}(AA^\dagger)}$ (norm). The unit matrix I is the unit element. Traditionally, instead of $A^\dagger$ and $z^\dagger$ we write A^* and z^*, respectively.

Definition of C^*-algebra. Let $\mathcal{A}$ be a complex associative algebra which is also a complex Banach space. In addition, suppose that there exists a map $A \mapsto A^*$ (called the $*$-map) such that the following hold for all $A, B \in \mathcal{A}$ and all complex numbers α, β:

(i) $A^* \in \mathcal{A}$ (adjoint element);
(ii) $(\alpha A + \beta B)^* = \alpha^\dagger A^* + \beta^\dagger B^*$ (the $*$-map is antilinear);
(iii) $(A^*)^* = A$ (the $*$-map is an involution);
(iv) $(AB)^* = B^* A^*$;
(iv) $||AB|| \leq ||A|| \cdot ||B||$;
(v) $||A^*|| = ||A||$ and $||A^* A|| = ||A||^2$.

Then $\mathcal{A}$ is called a C^*-algebra.

The C^*-algebra is called commutative iff $AB = BA$ for all $A, B \in \mathcal{A}$. Furthermore, the C^*-algebra is called unital iff there exists a unit element I of $\mathcal{A}$ with $||I|| = 1$.

C^*-subalgebra. A subset $\mathcal{S}$ of a C^*-algebra $\mathcal{A}$ is called a C^*-subalgebra of $\mathcal{A}$ iff it is a C^*-algebra with respect to the operations on $\mathcal{A}$.

If $\mathcal{S}$ is a subset of a C^*-algebra $\mathcal{A}$, then there exists a (uniquely determined) smallest C^*-subalgebra $\mathcal{B}$ of $\mathcal{A}$ which contains the set $\mathcal{S}$. Explicitly, $\mathcal{B}$ is the intersection of all C^*-subalgebras of $\mathcal{A}$ which contain the set $\mathcal{S}$. We say that $\mathcal{B}$ is generated by $\mathcal{S}$.

By definition, a C^*-ideal of the C^*-algebra $\mathcal{A}$ is a C^*-subalgebra $\mathcal{I}$ of $\mathcal{A}$ which has the additional property that $AB \in \mathcal{I}$ and $BA \in \mathcal{I}$ for all $A \in \mathcal{A}, B \in \mathcal{I}$.

Examples. (a) The function space $C(M)$. Let M be a nonempty compact separated topological space (e.g. $M = [0,1]$ or, more generally, M is a compact subset of $\mathbb{R}^n$, $n = 1, 2, \dots$). The space $C(M)$ of all continuous functions

$$f : M \to \mathbb{C}$$

is a unital C^*-algebra with respect to the norm

$$||f|| := \max_{x \in M} |f(x)|.$$

Moreover, we set $f^*(x) := f(x)^\dagger$ for all $x \in M$ (complex-conjugate function). The function $f(x) := 1$ for all $x \in M$ is the unit element of $C(M)$.

(b) The operator space $L(X, X)$. Let X be a complex Hilbert space. The space $L(X, X)$ of all linear continuous operators

$$A : X \to X$$

is a C^*-algebra with respect to the operator norm

$$||A|| := \sup_{||\psi||\leq 1} ||A\psi||$$

and $A^* := A^\dagger$ (adjoint operator). If $X \neq \{0\}$, then the C^*-algebra $L(X,X)$ is unital, where the unit operator I is the unit element.

(c) The Weyl algebra of the Hilbert space $L_2(\mathbb{R})$. Let $X := L_2(\mathbb{R})$. The smallest C^*-subalgebra of $L(X,X)$, which contains the Weyl operators $W(a,b)$, $a,b \in \mathbb{R}$, is called the Weyl algebra of $L_2(\mathbb{R})$. Explicitly, this is the closure of the set

$$\text{span}\{W(A,B) : a,b \in \mathbb{R}\}.$$

The closure is to be understood in the sense of the Banach space $L(X,X)$.

The Gelfand–Naimark theorem below shows that examples (a) and (b) above are typical for C^*-algebras and commutative C^*-algebras, respectively.

C^*-morphism. Let $\mathcal{A}$ and $\mathcal{B}$ be C^*-algebras. The map

$$\chi : \mathcal{A} \to \mathcal{B}$$

is called a C^*- morphism iff it respects the algebra structure, the $*$-operation, and the norm structure, that is, for all $A, B \in \mathcal{A}$ and all complex numbers α, β, we have

- $\chi(\alpha A + \beta B) = \alpha\chi(A) + \beta\chi(B)$,
- $\chi(AB) = \chi(A)\chi(B)$,
- $\chi(A)^* = \chi(A)$, and
- $||\chi(A)|| = ||A||$.

Bijective C^*-morphisms are called C^*-isomorphisms. Moreover, C^*-isomorphisms $\chi : \mathcal{A} \to \mathcal{A}$ from a C^*-algebra $\mathcal{A}$ onto itself, are called C^*-automorphisms.

The category of C^*-algebras. In order to describe the common features of mathematical structures, one uses categories in mathematics. A category consists of objects and morphisms.

- The objects of the category of C^*-algebras are the C^*-algebras,
- and the morphisms of the category of C^*-algebras are the C^*-morphisms.

The general setting of category theory will be investigated in Vol. IV on quantum mathematics.

The Gelfand–Naimark structure theorem. In 1943, Gelfand (born 1913) and Naimark (1909–1978) proved the following crucial result.

Theorem 7.60 (i) *Each C^*-algebra is C^*-isomorphic to some C^*-subalgebra of $L(X,X)$, where X is some Hilbert space.*

(ii) *Each commutative unital C^*-algebra $\mathcal{A}$ is C^*-isomorphic to a C^*-algebra $C(M)$ of continuous functions on some nonempty compact separated topological space M. Here, M is the space of maximal ideals of the algebra $\mathcal{A}$ equipped with an appropriate topology.*

The proof is based on the so-called Gelfand–Naimark–Segal (GNS) construction, which is basic for algebraic quantum field theory and quantum statistics.[136] This will be considered in Vol. IV. There, we will also show that (ii) above is crucial for the spectral theory of unitary and self-adjoint operators. For the proofs, we refer

[136] I. Gelfand, Normed rings of operators, Mat. Sbornik **9** (1941), 3–24 (in German).
I. Gelfand and M. Naimark, On the embedding of normed rings into the ring of operators in Hilbert space, Mat. Sbornik **12** (1943), 197–213.
I. Segal, Postulates for general quantum mechanics, Ann. Math. **48** (1947), 930–948.

to P. Kadison and J. Ringrose, Fundamentals of the Theory of Operator Algebras, Vols. 1, Academic Press, New York, 1983.

$*$-Algebras. Sometimes it is convenient to replace C^*-algebras by the weaker notion of $*$-algebra (star algebra). Here, all the properties of a C^*-algebra drop out which refer to the norm. For example, the complex associative algebra $\mathcal{A}$ is called a $*$-algebra iff conditions (i)–(iv) on page 627 are satisfied. Analogously, one obtains the following terms: $*$-subalgebra, $*$-morphism, $*$-isomorphism, $*$-automorphism, category of $*$-algebras.

7.16.4 Operator Ideals

In order to give the proof for special cases of Fermat's last theorem in number theory, Kummer (1810–1891) introduced so-called ideal numbers.[137] Generalizing this, Dedekind (1831–1916) created the theory of ideals in ring theory. The theory of operator ideals generalizes this to operator algebras.

Compact operators. Let $C : X \to X$ be a linear compact self-adjoint operator on the complex separable non-trivial Hilbert space X. Then the eigenvectors of C form a complete orthonormal system in X. Let $\lambda_1, \lambda_2, \ldots$ denote the eigenvalues of C. Then:

- The spectrum of C is a pure point spectrum.
- The operator C is called of trace class iff $\sum_n |\lambda_n| < \infty$. In this case, the trace $\mathrm{tr}(C) := \sum_n \lambda_n$ is finite. Operators of trace class are also called nuclear operators.
- The operator C is called a Hilbert–Schmidt operator iff $\sum_n \lambda_n^2 < \infty$.

Let us generalize this. The linear compact operator $A : X \to X$ is called a trace class (resp. Hilbert–Schmidt) operator iff $\mathrm{tr}(\sqrt{A^*A}) < \infty$ (resp. $\mathrm{tr}(A^*A) < \infty$).[138] Every trace class operator is a Hilbert–Schmidt operator. If the linear operator $A : X \to X$ is compact on the complex separable Hilbert space X, then there exist orthogonal systems $\varphi_1, \varphi_2, \ldots$ and $\psi_1, \psi_2, \ldots$ together with positive numbers $\mu_1, \mu_2, \ldots$ (called the singular values of the operator A) such that

$$A\varphi = \sum_n \mu_n \langle \varphi_n | \varphi \rangle \psi_n \qquad \text{for all} \quad \varphi_n \in X.$$

Explicitly, we choose a complete orthonormal system $\varphi_1, \varphi_2, \ldots$ of eigenvectors of the self-adjoint compact operator A^*A, that is, $A^*A\varphi_n = \lambda_n \varphi_n$. Here, $\lambda_n \geq 0$ for all n. Moreover, throw away the eigenvectors φ_m with $\lambda_m = 0$, and set $\mu_n := \sqrt{\lambda_n}$, as well as $\psi_n := \lambda_n^{-1} A\varphi_n$. Equivalently, we write

$$A = \sum_n \mu_n \psi_n \otimes \varphi_n .$$

C^*-operator ideals. Consider the C^*-algebra $L(X, X)$ of the linear continuous operators $A : X \to X$ on the complex separable Hilbert space X.

(i) The set of linear compact operators $A : X \to X$ forms a C^*-ideal of $L(X, X)$. This ideal is denoted by $\mathcal{I}_{\mathrm{compact}}$.

[137] The famous complete proof of Fermat's last theorem was given by Wiles in 1994 (see page 17 of the Prologue to Vol. I; we also refer to F. Diamond and J. Shurman, A First Course in Modular Forms, Springer, Berlin, 2005).

[138] Note that the operator A^*A is self-adjoint and compact, and its eigenvalues are nonnegative.

(ii) The trace-class operators $A : X \to X$ form a C^*-ideal of $L(X, X)$. This ideal is denoted by $\mathcal{I}_{\text{trace class}}$.
(iii) The Hilbert–Schmidt operators of $A : X \to X$ form a C^*-ideal of $L(X, X)$. This ideal is denoted by $\mathcal{I}_{\text{Hilbert}-\text{Schmidt}}$. We have the inclusions $\mathcal{I}_{\text{trace class}} \subseteq \mathcal{I}_{\text{Hilbert}-\text{Schmidt}} \subseteq \mathcal{I}_{\text{compact}} \subseteq L(X, X)$.
(iv) $A \in \mathcal{I}_{\text{trace class}}$ iff $A = BC$ with $B, C \in \mathcal{I}_{\text{Hilbert}-\text{Schmidt}}$.

For more details, we refer to M. Reed and B. Simon, Methods of Modern Mathematical Physics, Vol. I, Sects. VI.5ff, Academic Press, 1972, as well as to the monographs by R. Schatten, Norm Ideals of Completely Continuous Operators, Springer, Berlin, 1960, and by A. Pietsch (1978), (2007) quoted on page 601.

7.16.5 Symplectic Geometry and the Weyl Quantization Functor

Functors play a crucial role in modern mathematics and physics.
Folklore

Symplectic linear spaces. A symplectic linear space X is a real linear space equipped with a symplectic form

$$\omega : X \times X \to \mathbb{R}.$$

That is, for all $\mathbf{a}, \mathbf{b}, \mathbf{c} \in X$ and all real numbers α, β, the following hold:

- $\omega(\mathbf{a}, \mathbf{b}) = -\omega(\mathbf{b}, \mathbf{a})$ (antisymmetry);
- $\omega(\alpha\mathbf{a} + \beta\mathbf{b}, \mathbf{c}) = \alpha\omega(\mathbf{a}, \mathbf{c}) + \beta\omega(\mathbf{b}, \mathbf{c})$ (bilinearity);
- $\omega(\mathbf{a}, \mathbf{v}) = 0$ for all $\mathbf{v} \in X$ implies $\mathbf{a} = 0$ (non-degeneracy).

For example, the space $\mathbb{R}^2$ is a symplectic linear space with respect to the symplectic form

$$\omega((a, b), (c, d)) := \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc, \quad (a, b), (c, d) \in \mathbb{R}^2. \tag{7.286}$$

Symplectic morphism. Let X and Y be symplectic linear spaces with the symplectic forms ω and μ, respectively. The map

$$\chi : X \to Y$$

is called a symplectic morphism iff it is linear and respects the symplectic forms, that is,

$$\mu(\chi(\mathbf{a}), \chi(\mathbf{b})) = \omega(\mathbf{a}, \mathbf{b}) \qquad \text{for all} \quad \mathbf{a}, \mathbf{b} \in X.$$

Bijective symplectic morphisms are called symplectic isomorphisms. Then the inverse map is also a symplectic morphism. For example, a symplectic isomorphism of the plane $\mathbb{R}^2$ onto itself (with respect to the symplectic form (7.286)) is a linear area-preserving map from $\mathbb{R}^2$ onto itself. The category of symplectic linear spaces is defined in the following way:

- The objects are symplectic linear spaces,
- and the morphisms are symplectic morphisms.

Weyl algebras. We want to generalize the Weyl algebra of the Hilbert space $L_2(\mathbb{R})$. Let X be a linear symplectic space, and let $\mathcal{A}$ be a C^*-algebra with unit element. The map

$$W : X \to \mathcal{A}$$

is called a Weyl map iff the following hold for all $\mathbf{a}, \mathbf{b} \in X$:

(i) $W(\mathbf{a})W(\mathbf{b}) = \mathrm{e}^{\frac{\mathrm{i}}{2}\omega(\mathbf{a},\mathbf{b})}W(\mathbf{a}+\mathbf{b})$;
(ii) $W(0) = I$;
(iii) $W(\mathbf{a})^* = W(-\mathbf{a})$.

The subset $\{W(\mathbf{a}) : \mathbf{a} \in X\}$ of the C^*-algebra $\mathcal{A}$ is called a Weyl system. The smallest C^*-algebra of $\mathcal{A}$ which contains a Weyl system is called a Weyl algebra $\mathcal{W}(X)$. This algebra is also called the CCR-algebra of the linear symplectic space X with the symplectic form ω. Here, 'CCR' stands for 'canonical commutation relation'.

The existence and uniqueness theorem for Weyl algebras. The following theorem generalizes the Stone–von Neumann uniqueness theorem.

Theorem 7.61 *For each symplectic linear space X, there exists a Weyl algebra $\mathcal{W}(X)$ which is unique, up to C^*-isomorphisms.*

Proof. (I) Existence. Let $l_2(X)$ denote the space of all functions $f : X \to \mathbb{C}$ with at most countable support[139] and the property that

$$\sum_{\mathbf{a}\in X} |f(\mathbf{a})|^2 < \infty.$$

The complex linear space $l_2(X)$ becomes a complex Hilbert space equipped with the inner product $\langle f|g\rangle := \sum_{\mathbf{a}\in X} f(\mathbf{a})^\dagger g(\mathbf{a})$.

Now let us choose the C^*-algebra $\mathcal{A}$ consisting of all the linear continuous operators $A : l_2(X) \to l_2(X)$. For all $f \in l_2(X)$, we define

$$(W(\mathbf{a})f)(\mathbf{b}) := \mathrm{e}^{-\frac{\mathrm{i}}{2}\omega(\mathbf{a},\mathbf{b})} f(\mathbf{a}+\mathbf{b}), \qquad \mathbf{a},\mathbf{b} \in X.$$

One checks directly that $W(\mathbf{a}) \in \mathcal{A}$ and that $W : X \to \mathcal{A}$ is a Weyl map. To finish the argument, let $\mathcal{W}(X)$ be the C^*-subalgebra of $\mathcal{A}$ generated by the set $\{W(\mathbf{a}) : \mathbf{a} \in X\}$.

(II) Uniqueness. See Bär et al (2007), p. 121 (see the reference on page 632). □

Theorem 7.62 *If $\sigma : X \to Y$ is a symplectic morphism between the symplectic linear spaces X and Y, then there exists a uniquely determined injective C^*-morphism $\mathcal{W}(\sigma) : \mathcal{W}(X) \to \mathcal{W}(Y)$ such that the following diagram is commutative:*

$$\begin{array}{ccc} X & \xrightarrow{\ \sigma\ } & Y \\ \downarrow & & \downarrow \\ \mathcal{W}(X) & \xrightarrow{\ \mathcal{W}(\sigma)\ } & \mathcal{W}(Y). \end{array}$$

For the proof, we refer to Bär et al. (2007), p. 122.

The Weyl quantization functor. We have the following two properties:

(F1) $\mathcal{W}(\tau \circ \sigma) = \mathcal{W}(\tau) \circ \mathcal{W}(\sigma)$;
(F2) $\mathcal{W}(\mathrm{id}) = \mathrm{id}$.

[139] This means that the function f vanishes outside an at most countable subset of the linear space X.

More precisely, this means the following. If

$$X \xrightarrow{\sigma} Y \xrightarrow{\tau} Z$$

is the composition of two symplectic morphisms σ and τ, then this is transformed into the composition

$$\mathcal{W}(X) \xrightarrow{\mathcal{W}(\sigma)} \mathcal{W}(Y) \xrightarrow{\mathcal{W}(\tau)} \mathcal{W}(Z)$$

of the corresponding C^*-morphisms $\mathcal{W}(\sigma)$ and $\mathcal{W}(\tau)$. Furthermore, the identical symplectomorphism

$$X \xrightarrow{\mathrm{id}} X$$

is transformed into the identical map

$$\mathcal{W}(X) \xrightarrow{\mathrm{id}} \mathcal{W}(X)$$

of the C^*-algebra $\mathcal{W}(X)$. In terms of mathematics, the situation (F1), (F2) above describes a functor $\mathcal{W}$ between the category of symplectic linear spaces and the category of C^*-algebras. This functor is called the Weyl quantization functor.

Perspectives. In general, functors between categories map objects to objects and morphisms to morphisms such that the two properties (F1), (F2) above are satisfied. Functors play a fundamental role in the modern theory of mathematical structures. Typical examples are:

- the homology functor which sends continuous maps between topological spaces to group morphisms between homology groups,
- and the de Rham cohomology cofunctor[140] which sends smooth maps between manifolds to group morphisms between cohomology groups (i.e. linear maps between real linear spaces).

This will be studied in later volumes.

It was discovered recently, that functors are the right tool in order to generalize Einstein's principle of general relativity (also called the covariance principle) to quantum field theories on curved space-times. This principle postulates that physics does not depend on the choice of observers. Roughly speaking, the basic idea is to assign C^*-algebras to the open subsets of globally hyperbolic space-time manifolds (realization of the Haag–Kastler axioms). The point is that the change of the space-time manifolds induces a natural change of the assigned C^*-algebras. Furthermore, two different quantization functors are related to each other by a natural transformation. We refer to:

R. Brunetti, K. Fredenhagen, and R. Verch, The generally covariant locality principle – a new paradigm for local quantum field theory, Commun. Math. Phys. **237** (2003), 31–68.

C. Bär, N. Ginoux, and F. Pfäffle, Wave Equations on Lorentzian Manifolds and Quantization, European Mathematical Society 2007.

J. Baez and J. Dolan, Categorification, Contemporary Mathematics **230** (1998), 1–36.

The monograph by Bär, Ginoux, and Pfäffle contains a detailed study of the initial-value problem for normally hyperbolic differential equations on globally hyperbolic manifolds, together with applications to quantum field theory. This sophisticated global theory due to Jacques Hadamard (1865–1963), Marcel Riesz (1886–1969) and Jean Leray (1906–1998) is based on modern differential geometry (the language of bundles) and the theory of distributions on manifolds. Distributions are needed in order to handle the strong singularities of the Green's functions.

[140] In contrast to the composition rule (F2) above, a cofunctor $\mathcal{F}$ is characterized by the reverse composition rule $\mathcal{F}(\tau \circ \sigma) = \mathcal{F}(\sigma) \circ \mathcal{F}(\tau)$.

7.17 A Glance at the Algebraic Approach to Quantum Physics

In this section, we want to discuss a few basic ideas about the algebraic approach to non-relativistic quantum physics. Further material can be found in the volumes to follow. The Haag–Kastler theory, that is, the relativistic approach based on local operator algebras will be studied in Vol. IV on quantum mathematics.

7.17.1 States and Observables

> The states and the observables are basic concepts in the description of a physical system and their description has undergone a drastic fundamental change in the transition from the classical theory to the quantum theory.[141]
>
> Huzihiro Araki, 1999

The prototypes of pure states and mixed states. Consider a complex non-trivial Hilbert space X.

(a) Pure state: Fix $\psi \in X$ with $||\psi|| = 1$. Define

$$\chi(A) := \langle \psi | A\psi \rangle \qquad \text{for all} \quad A \in L(X, X).$$

Then $\chi(I) = 1$, and $\chi(A^*A) = \langle \psi | A^*A\psi \rangle = \langle A\psi | A\psi \rangle \geq 0$. Moreover, we have

$$\chi(A)^\dagger = \langle A\psi | \psi \rangle = \langle \psi | A^*\psi \rangle = \chi(A^*).$$

We call the linear continuous functional $\chi : L(X, X) \to \mathbb{C}$ a vector state (or a pure state).

(b) Mixed state: Let $\psi_0, \psi_1, \ldots$ be a complete orthonormal system of the Hilbert space X, and let $p_0, p_1, \ldots$ be real numbers contained in the unit interval $[0, 1[$ such that $\sum_k p_k = 1$. Define[142]

$$\chi(A) := \sum_k p_k \langle \psi_k | A\psi_k \rangle \qquad \text{for all} \quad A \in L(X, X).$$

Again, $\chi(I) = 1$ and $\chi(A^*A) \geq 0$ together with $\chi(A)^\dagger = \chi(A^*)$ for all operators $A \in L(X, X)$. The linear continuous functional $\chi : L(X, X) \to \mathbb{C}$ is called a mixed state. In terms of physics, the pure state ψ_k is realized with the probability p_k.

(c) Dynamics. If $H : D(H) \to X$ is a linear self-adjoint Hamiltonian operator, then the dynamics of the initial state ψ_0 is given by $\psi(t) = U(t)\psi_0$ for all times $t \in \mathbb{R}$, where we set

$$U(t) := \mathrm{e}^{-\mathrm{i}tH/\hbar}, \qquad t \in \mathbb{R}.$$

Motivated by $\langle U(t)\psi_0 | AU(t)\psi_0 \rangle = \langle \psi_0 | U(t)^{-1} AU(t)\psi_0 \rangle$, we define the operator $\mathcal{U}_t : L(X, X) \to L(X, X)$ for all $t \in \mathbb{R}$ by setting

$$\mathcal{U}_t A := U(t)^{-1} AU(t).$$

[141] H. Araki, Mathematical Theory of Quantum Fields, Oxford University Press, 1999.

[142] Since $|\langle \psi_k | A\psi_k \rangle| \leq ||\psi_k|| \cdot ||A\psi_k|| \leq ||\psi_k|| \cdot ||A|| \cdot ||\psi_k|| \leq ||A||$, the series for $\chi(A)$ is convergent.

The operator $\mathcal{U}_t$ is a C^*-isomorphism from the C^*-algebra $L(X,X)$ onto itself. As usual, such C^*-isomorphisms are also called C^*-automorphisms. Define

$$\chi_t(A) := \chi(\mathcal{U}_t A) \qquad \text{for all} \quad A \in L(X,X), \;\; t \in \mathbb{R}.$$

Then the map $t \to \chi_t$ corresponds to the map $t \mapsto U(t)\psi_0$, which describes the time evolution of the state ψ_0.

The general definition in terms of C^*-algebras. Suppose that we are given a C^*-algebra $\mathcal{A}$ with unit element I.

(i) Observables: The self-adjoint elements A of $\mathcal{A}$ (i.e., $A^* = A$) are called observables. The C^*-algebra $\mathcal{A}$ is called the extended algebra of observables.[143]

(ii) States: The linear functionals $\chi : \mathcal{A} \to \mathbb{C}$ with the normalization condition $\chi(I) = 1$ and the positivity condition

$$\chi(A^*A) \geq 0 \qquad \text{for all} \quad A \in \mathcal{A}$$

are called states.[144] A state is called mixed iff there exist two different states χ_1 and χ_2 such that

$$\chi = \lambda\chi_1 + (1-\lambda)\chi_2 \quad \text{for some number } \lambda \in]0,1[.$$

Otherwise the state is called pure.

(iii) Measurements of an observable. Let A be an observable, and let χ be a state. The real number

$$\boxed{\bar{A} := \chi(A)}$$

is called the measured mean value of the observable A in the state χ. Similarly, the nonnegative number ΔA given by

$$(\Delta A)^2 := \chi((A-\bar{A})^2)$$

is the measured fluctuation of the observable A in the state χ.[145] If A and B are two observables, then the complex number

$$\gamma := \frac{\chi\big((A-\bar{A})(B-\bar{B})\big)}{\Delta A \, \Delta B}$$

is called the correlation coefficient in the state χ.[146]

(iv) Dynamics: By definition, a dynamics on $\mathcal{A}$ is a one-parameter group $\{\mathcal{U}_t\}_{t\in\mathbb{R}}$ of C^*-automorphisms of the algebra $\mathcal{A}$. Explicitly, this means that, for all times $t, s \in \mathbb{R}$, the map $\mathcal{U}_t : \mathcal{A} \to \mathcal{A}$ is a C^*-automorphism and

$$\mathcal{U}_{t+s} = \mathcal{U}_t\mathcal{U}_s, \qquad U_0 = \mathrm{id}.$$

This yields the time evolution $t \mapsto \chi_t$ of a state χ, namely, we define

$$\chi_t(A) := \chi(\mathcal{U}_t A)) \qquad \text{for all} \quad A \in \mathcal{A}, \;\; t \in \mathbb{R}.$$

[143] Note that the algebra $\mathcal{A}$ also contains elements which are not observables, in the sense of the definition given above.

[144] It can be shown that states are always continuous. We also have $\chi(A)^\dagger = \chi(A^*)$ for all $A \in \mathcal{A}$. In particular, if A is an observable, then $\chi(A)$ is real.

[145] Since $(A-\bar{A})^* = A - \bar{A}$, we get $\chi\big((A-\bar{A})^2\big) \geq 0$, by (ii).

[146] The Schwarz inequality for C^*-algebras tells us that $|\gamma| \leq 1$.

(v) Thermodynamical equilibrium states (KMS-states): Let $\beta := 1/kT$, where k is the Boltzmann constant, and T is the absolute temperature. By definition, the state χ is called a KMS-state of temperature T with respect to the dynamics $\{\mathcal{U}_t\}_{t\in\mathbb{R}}$ iff it satisfies the β-KMS condition

$$\chi(A\mathcal{U}_t(B)) = \chi(\mathcal{U}_{t-\mathrm{i}\beta\hbar}(B)A) \qquad \text{for all} \quad A, B \in \mathcal{A}, \quad t \in \mathbb{R}.$$

One of the main problems in thermodynamics is the characterization of thermodynamic equilibrium states. The C^*-algebra approach to thermodynamics is able to do this. The three letters KMS stand for the names of the physicists Kubo, Martin, and Schwinger. For the historical background, see the discussion on page 659.

The following is crucial for distinguishing between classical physics and quantum physics.

The passage from classical physics to quantum physics corresponds to the passage from commutative algebras to noncommutative algebras.

For example, this also corresponds to the passage from classical information to quantum information, which represents the theoretical framework for the intended construction of quantum computers in the future. This will be studied in Vol. IV. We refer to N. Nielsen and M. Chuang, Quantum Computation and Quantum Information, Cambridge University Press, 2001.

Orthogonal projections as fundamental observables related to questions posed by physical experiments. The simplest observables in $L(X, X)$ are orthogonal projection operators. Let us summarize elementary properties.[147] We set

$$\mathcal{A} := L(X, X).$$

We assume that X is a complex separable non-trivial Hilbert space. We will use such a language that later on we can replace $L(X, X)$ by a von Neumann algebra $\mathcal{A}$ which is a factor (see page 657). In the language of von Neumann algebras, the following properties of orthogonal projections will tell us that $L(X, X)$ is a von Neumann algebra (more precisely, a factor) of type I.

(i) Orthogonal projections: By definition, an orthogonal projection is an element of $\mathcal{A}$ with $P^* = P$ and $P^2 = P$. Let $\mathcal{P}(\mathcal{A})$ denote the set of all orthogonal projections in $\mathcal{A}$.
Geometrically, this means the following. For any $\psi \in X$, we have the decomposition

$$\psi = P\psi + (I - P)\psi$$

where $P\psi$ is contained in the closed linear subspace $P(X)$ of X, and $(I - P)\psi$ is contained in the orthogonal complement $P(X)^\perp$.[148] By the Pythagorean theorem,

$$||\psi||^2 = ||P\psi||^2 + ||(I - P)\psi||^2.$$

Hence if $P \neq 0$, then $||P|| = 1$. Conversely, let Y be a linear closed subspace Y of X. For given $\psi \in X$, the variational problem

$$||\psi - \varphi|| = \min!, \qquad \varphi \in Y$$

has a unique solution denoted by $P\psi$. Then $P : X \to Y$ is an orthogonal projection onto the subspace Y.

[147] For the missing proofs, we refer to Zeidler (1995a) (see the references on page 1049), and to F. Riesz and B. Nagy, Functional Analysis, Frederyck Ungar, New York, 1978.

[148] Recall that, for a subset L of the Hilbert space X, the orthogonal complement is given by $L^\perp := \{\psi \in X : \ \langle\psi|\varphi\rangle = 0 \ \text{ for all } \varphi \in L\}$.

(ii) Partial ordering on $\mathcal{P}(\mathcal{A})$: Let $Q, P \in \mathcal{P}(\mathcal{A})$. We write

$$Q \leq P \qquad \text{iff} \qquad PQ = Q.$$

This is a partial ordering on $\mathcal{P}(\mathcal{A})$. Geometrically, this is equivalent to the inclusion $Q(X) \subseteq P(X)$.

(iii) Expectation values: Let $P, Q \in \mathcal{P}(\mathcal{A})$. Then,
- $0 \leq \langle\psi|P\psi\rangle \leq ||\psi||^2$ for all $\psi \in X$,[149] and
- $Q \leq P$ iff $\langle\psi|Q\psi\rangle \leq \langle\psi|P\psi\rangle$ for all $\psi \in X$.

In terms of expectation values in physics, this means

$$\boxed{0 \leq \bar{P} \leq 1 \qquad \text{and} \qquad Q \leq P \Rightarrow \bar{Q} \leq \bar{P}.}$$

Here, we exclude the trivial case $X = \{0\}$.

(iv) Eigenvalues: Let $P \in \mathcal{P}(\mathcal{A})$ with $P \neq 0$. If

$$P\psi = \lambda\psi$$

with $||\psi|| = 1$, then either $\lambda = 1$ or $\lambda = 0$. The eigenspace to the eigenvalue $\lambda = 1$ (resp. $\lambda = 0$) is $P(X)$ (resp. the orthogonal complement $P(X)^\perp$). In terms of mathematical logic, we regard the observable P as a question and the eigenvalues $\lambda = 1$ (resp. $\lambda = 0$) correspond to the answers "yes" (resp. "no").

(v) Orthogonality: Let $P, Q \in \mathcal{P}(\mathcal{A})$. We say that P is orthogonal to Q iff $PQ = 0$. Geometrically, this means that $P(X)$ is orthogonal to $Q(X)$.

(vi) Partial isometry: The linear continuous operator $U : X \to X$ is called a partial isometry iff we have

$$||U\psi|| = ||\psi|| \qquad \text{for all} \quad \psi \in \ker(U)^\perp.$$

That is, if we use the orthogonal composition, $X = Y \oplus Y^\perp$ with respect to the subspace $Y := \ker(U)$, then $U = 0$ on Y, and $U : Y^\perp \to \text{im}(U)$ is an isometry. More precisely, it follows from the Fredholm alternative that $\text{im}(U) = \ker(U^*)^\perp$, and hence the operator

$$U : \ker(U)^\perp \to \ker(U^*)^\perp$$

is a unitary operator.

(vii) The Murray–von Neumann equivalence relation: Let $Q, P \in \mathcal{P}(\mathcal{A})$. We write

$$Q \sim P$$

iff there exists an operator $U \in \mathcal{A}$ with $Q = UU^*$ and $P = U^*U$. This is a equivalence relation.

Geometrically, this means that U is a partial isometry whose restriction

$$U : P(X) \to Q(X)$$

to the space $P(X)$ is a unitary operator onto the space $Q(X)$. Similarly, U^* is a partial isometry whose restriction $U^* : Q(X) \to P(X)$ is a unitary operator.[150]

If $Q, P \in \mathcal{P}(A)$, then

$$||Q - P|| < 1 \qquad \text{implies} \quad Q \sim P.$$

[149] Note that $\langle\psi|P\psi\rangle = \langle\psi|P^2\psi\rangle = \langle P\psi|P\psi\rangle = ||P\psi||^2 \leq ||\psi||^2$.

[150] To prove this, note that $||P\psi||^2 = \langle\psi|P\psi\rangle = \langle U\psi|U\psi\rangle = ||U\psi||^2$. Thus, we obtain $\ker(U) = P(X)^\perp$. Similarly, $\ker(U^*) = Q(X)^\perp$.

(viii) The trivial center: The algebra $\mathcal{A}$ has a trivial center. This means that if $B \in \mathcal{A}$ and $AB = BA$ for all $A \in \mathcal{A}$, then B is a multiple of the unit operator (i.e., $B = \lambda I$ for some complex number λ). This is called the Schur lemma. [151]

(ix) Invariant linear subspaces of X. The linear subspace Y of X is called invariant under $\mathcal{A}$ iff $A(Y) \subseteq Y$ for all $A \in \mathcal{A}$.

(x) The dimension function: Let $P, Q \in \mathcal{P}(\mathcal{A})$. Define $d(P) := \dim P(X)$. Then:
- $d(P) = d(Q)$ iff $P \sim Q$.
- If $P(X)$ is orthogonal to $Q(X)$, then $d(P + Q) = d(P) + d(Q)$.

In what follows, we will show that orthogonal projections play a crucial role concerning

- the Gleason theorem and
- the Murray–von Neumann classification of factors of von Neumann algebras (see page 657).

7.17.2 Gleason's Extension Theorem – the Main Theorem of Quantum Logic

> Among other features, the Gleason theorem means that:
> - Probabilities provide a tool for constructing the language of physics long before they can be considered as empirically meaningful quantities.
> - The expression for the probabilities first proposed by Max Born (in 1926) is an unavoidable part of an interpretation. If any probability should ever play a part in the theory, it can be only this one.
> - The density operator (introduced by von Neumann) is the basic notion one must associate with a quantum state and not simply a pure state represented by a wave function.[152]
>
> Roland Omnès, 1994

Let X be a complex separable Hilbert space. Let $\mathcal{P}$ denote the set of all orthogonal projections $P : X \to X$. By definition, a pre-state of the C^*-algebra $L(X, X)$ is a function $s : \mathcal{P} \to [0, 1]$ with the property that we have

$$s(P_1 + \ldots + P_n) = s(P_1) + \ldots + s(P_n)$$

for each finite family of orthogonal projections $P_1, \ldots, P_n \in \mathcal{P}$ with the additional property that $P_i(X)$ is orthogonal to $P_j(X)$ if $i \neq j$. Such a pre-state is also called a finitely additive measure on $\mathcal{P}$.

Theorem 7.63 *If the dimension of the Hilbert space X is 3 or larger, then each pre-state can be uniquely extended to a state of the C^*-algebra $L(X, X)$.*

Conversely, the restriction of any state on $L(X, X)$ to the space of orthogonal projections $\mathcal{P}$ is a pre-state.

From the philosophical point of view, roughly speaking, Gleason's theorem tells us the following: [153]

[151] Schur (1875–1941).

[152] R. Omnès, The Interpretation of Quantum Mechanics, Princeton University Press, Princeton, New Jersey, 1994. Reprinted by permission of Princeton University Press.

[153] J. von Neumann and G. Birkhoff, The logic of quantum mechanics, Ann. Math. **37** (1936), 823–843.
A. Gleason, Measures on the closed subspaces of a Hilbert space, J. Math. Mech. **6** (1957), 885–893.

A quantum state is completely determined by only knowing the answers to all of the possible yes/no questions.

The Gleason theorem was generalized to von Neumann algebras by Christensen and Yeadon.[154]

7.17.3 The Finite Standard Model in Statistical Physics as a Paradigm

The partition function knows all about the thermodynamic system. The Feynman path integral can be viewed as a generalized partition function.
Folklore

The mean value. Let us consider a physical system $\mathcal{S}$ which can be in the finite number of states

$$\mathsf{S}_1, ..., \mathsf{S}_M$$

with the probabilities $p_1, \ldots, p_M$, respectively. Suppose that the physical quantity A (e.g., energy) attains the value A_m in the state S_m. By definition, if we measure the physical quantity A of the system $\mathcal{S}$, then we get the mean value

$$\boxed{\chi(A) := \sum_{m=1}^{M} p_m A_m.} \tag{7.287}$$

We also write $\bar{A}$ instead of $\chi(A)$.

Fluctuations and correlations can be described by mean values.

In fact, the fluctuation $\Delta A \geq 0$ of the physical quantity A is defined by

$$(\Delta A)^2 = \overline{(A - \bar{A})^2} = \sum_{m=1}^{M} p_m (A - \bar{A})^2.$$

Obviously, $(\Delta A)^2 = \overline{A^2} - (\bar{A})^2$. For two physical quantities A and B, the correlation coefficient is defined by

$$\mathrm{cor}(A, B) := \frac{\overline{(A - \bar{A})(B - \bar{B})}}{\Delta A \cdot \Delta B} = \frac{\sum_{k=1}^{M} p_m (A - \bar{A})(B - \bar{B})}{\Delta A \cdot \Delta B}.$$

The fundamental quantity

$$\boxed{S := -k \sum_{k=1}^{M} p_m \ln p_m}$$

is called the entropy of the physical system $\mathcal{S}$. If $0 < p_1, \ldots, p_M < 1$, then $\bar{A}$ is called the mean value of the physical quantity A with respect to the mixed state $(\mathsf{S}_1, p_1; \ldots, \mathsf{S}_M, p_M)$. If $p_{m_0} = 1$ and $p_m = 0$ for all indices $m \neq m_0$, then $\bar{A}$ is called the mean value of A with respect to the pure state S_{m_0}.

The language of C^*-algebras. The set $\{\mathsf{S}_1, \ldots, \mathsf{S}_M\}$ is called the state space S. The set of functions

[154] S. Maeda, Probability measures on projections in von Neumann algebras, Rev. Math. Phys. **1** (1989), 235–290 (survey article).

$$A : \mathsf{S} \to \mathbb{C}$$

is denoted by $\mathcal{A}$. We write $A_m := A(\mathsf{S}_m)$, and $A^*(\mathsf{S}_m) := A(\mathsf{S}_m)^\dagger$. If $A, B \in \mathcal{A}$ and $\alpha, \beta \in \mathbb{C}$, then

$$\alpha A + \beta B, \quad AB, \quad A*$$

are also contained in $\mathcal{A}$. In addition, we introduce the norm

$$||A|| := \sup_{m=1,\ldots,M} |A(\mathsf{S}_m)|.$$

The set $\mathcal{A}$ is a commutative unital C^*-algebra which is called the extended algebra of observables.

- Observables: The real-valued functions in $\mathcal{A}$ (i.e., $A^* = A$) are called observables.
- States: Let $0 \leq p_1, \ldots, p_M \leq 1$ and $p_1 + \ldots + p_M = 1$. Define the function

  $$\chi : \mathcal{A} \to \mathbb{C}$$

  by the key relation (7.287) above. Precisely all such functions are called states of the C^*-algebra $\mathcal{A}$. These functions have the following positivity property $\chi(AA^*) = \sum_{m=1}^M p_m A_m A_m^\dagger \geq 0$.
- Mean value: The value $\chi(A)$ is called the mean value of the observable A in the state χ.

The grand canonical ensemble. Now let us consider special physical systems whose states are characterized by energy and particle number. This is typical for statistical physics. More precisely, assume that the physical system $\mathcal{S}$ can be in the finite number of states $\mathsf{S}_1, \ldots, \mathsf{S}_M$; each state S_m is characterized by the energy E_m and the particle number N_m. We will motivate below that it is reasonable to assume that the number

$$\boxed{p_m = \frac{\mathrm{e}^{(\mu N_m - E_m)/kT}}{\sum_{m=1}^M \mathrm{e}^{(\mu N_m - E_m)/kT}}, \qquad m = 1, \ldots, M} \tag{7.288}$$

is the probability for finding the physical system in the state S_m. Here, the parameter $T > 0$ is called the (absolute) temperature, the real parameter μ is called the chemical potential, and k is the Boltzmann constant. The mean energy $\bar{E}$ and the energy fluctuation $\Delta E \geq 0$ are given by

$$\bar{E} = \sum_{m=1}^M p_m E_m, \qquad (\Delta E)^2 = \sum_{m=1}^M p_m (E - \bar{E})^2.$$

Similarly, the mean particle number $\bar{N}$ and the particle number fluctuation $\Delta N \geq 0$ are given by

$$\bar{N} = \sum_{m=1}^M p_m N_m, \qquad (\Delta N)^2 = \sum_{m=1}^M p_m (N - \bar{N})^2.$$

Physical interpretation. The grand canonical ensemble describes a (large) many-particle system which is able to exchange energy and particles with its environment. However, we assume that this exchange is so weak that one can attribute a mean energy and a mean particle number to the system $\mathcal{S}$. Moreover, this exchange is governed by two macroscopic parameters, namely, the absolute temperature T and the chemical potential μ. This tells us that the many-particle system does not behave wildly, but regularly. Physicists say that the system is in *thermodynamic*

equilibrium. For example, the sun radiates photons into the universe at the fixed surface temperature of about 6000 K. The change of the particle number can be caused by chemical reactions. This motivates the designation 'chemical potential' for μ.

The special case where $\mu = 0$ corresponds to a fixed particle number (i.e., there are no chemical reactions or no particle exchange with the environment). The grand canonical ensemble with $\mu = 0$ is called canonical ensemble.

The importance of the partition function. The main trick of statistical physics is to introduce the function

$$\boxed{Z(T,\mu) := \sum_{m=1}^{M} \mathrm{e}^{(\mu N_m - E_m)/kT}} \tag{7.289}$$

which is called the partition function of the grand canonical ensemble. The following proposition tells us that

> *The knowledge of the partition function allows us to compute all of the crucial thermodynamic quantities in statistical physics.*

To this end, we introduce the so-called statistical potential

$$\Omega(T,\mu) := -kT \ln Z(T,\mu). \tag{7.290}$$

This function is also called the Gibbs potential. An elementary computation shows that the following relations hold for the partial derivatives of the statistical potential.

(i) Entropy: $S = -\Omega_T$.
(ii) Mean particle number: $\bar{N} = -\Omega_\mu$.
(iii) Particle number fluctuation: $(\Delta N)^2 = kT\bar{N}_\mu$.
(iv) Free energy: By definition, $F := \Omega + \mu\bar{N}$.
(v) Mean energy: $\bar{E} = F + TS$.[155]
(vi) Energy fluctuation: If the particle number is fixed (i.e., $\mu = 0$), then we obtain $(\Delta E)^2 = kT^2\bar{E}_T$.
(vii) Pressure: Suppose that the energies $E_1, \ldots, E_M$ and the particle numbers $N_1, \ldots, N_M$ depend on the volume V of the physical system. Then the statistical potential $\Omega(T,\mu,V)$ also depends on the volume V, and the pressure of the physical system is defined by $P := -\Omega_V$.

The reader should observe that the Feynman functional integral

$$Z = \int \mathrm{e}^{\mathrm{i}S[\psi]/\hbar} \mathcal{D}\psi$$

can be regarded as a (formal) continuous variant of the partition function.

7.17.4 Information, Entropy, and the Measure of Disorder

> Many-particle systems in nature are able to store information. This is equivalent to both the measure of disorder and the notion of entropy in physics. Folklore

[155] The mean energy is also called the inner energy.

Information and words. In order to get some information in daily life, it is useful to ask L questions which have to be answered by 'yes' or 'no'. Then the typical answer looks like

$$YN \dots NN. \tag{7.291}$$

This is a word of length L with the two letters Y (yes) and N (no). Intuitively, the minimal number L of questions measures information. For example, suppose we have n balls of different weight. We want to know the heaviest ball. Using a balance, if $n = 2$, then we need one experiment (question). If $n = 3$, then we need two experiments. Generally, it follows by induction that we need $n - 1$ experiments for n balls in order to find out the heaviest ball. After knowing this, we gain the information $I = n - 1$.

Observe that in computers, we use words of the type (7.291) in order to transport information. It is our goal to generalize this simple approach to more general situations. Interestingly enough, it turns out that one has to use the methods of probability theory.

General definition of information. Let $M = 1, 2, \dots$. Consider a random experiment which has the possible M outcomes

$$O_1, O_2, \dots, O_M \tag{7.292}$$

where O_m appears with the probability p_m. Here, $0 \leq p_1, p_2, \dots, p_M \leq 1$ and $p_1 + p_2 + \dots + p_M = 1$. The nonnegative number

$$\boxed{I := -\sum_{m=1}^{M} p_m \log_2 p_m} \tag{7.293}$$

is called the information of the random experiment (7.292).[156] The unit of I is called bit. Moreover, 1 byte = 8 bits. Intuitively, we gain the information I after performing the random experiment and after knowing the outcome. For example, let us throw a coin L times. The outcome corresponds to a word of the form (7.291), where Y and N stand for head and tail, respectively. The number of words of type (7.291) is equal to 2^L. Thus, the probability for a single outcome of the random coin experiment is equal to

$$p_m = \frac{1}{2^L}, \qquad m = 1, \dots, 2^L.$$

After performing the coin experiment, we gain the information

$$I = -\sum_{m=1}^{2^L} p_m \log_2 p_m = \log_2 2^L = L.$$

This coincides with the intuitive information introduced above in terms of answering yes/no questions. The number 2^L is called the statistical weight of the event (7.291).

Suppose that we have $p_1 = 1$ and $p_2 = \dots = p_M = 0$. Then we know the outcome O_1 of our random experiment in advance. This means that we do not

[156] By convention, if $p_m := 0$ for some index m, then we set $p_m \log_2 p_m = 0$. Information theory was created by Claude Shannon (1916–2001) in his paper: A mathematical theory of communication, Bell System Techn. J. **27** (1948), 379–423; 623–656.

gain any information after knowing the outcome. In fact, by (7.293) we get $I = -\log_2 1 = 0$.

The genetic code. The DNA (desoxyribonucleic acid) encodes the genetic information. This is a double-stranded molecule held together by weak bounds between base pairs of nucleotides. The four nucleotides in DNA contain the bases: adenine (A), cytosine (C), guanine (G), and thymine (T). A single strand can be formally described by a word

$$AGCT \dots G \tag{7.294}$$

of length L with the four letters A, C, G, T. There are 4^L such words. Introducing the weight $p_m := 1/4^L$, the word (7.294) contains the information

$$I = -\sum_{m=1}^{4^L} p_m \log_2 p_m = \log_2 4^L = 2L.$$

In nature, base pairs are only formed between A and T and between C and G. Thus, the base sequence (7.294) of each single strand can be deduced from that of its partner. The crucial protein synthesis in a biological cell is encoded into the messenger RNA (ribonucleic acid). This can be formally described by a word

$$C_{m_1} C_{m_2} \dots C_{m_{\mathcal{L}}} \tag{7.295}$$

of length $\mathcal{L}$ with the twenty letters $C_1, C_2, \dots, C_{20}$. These letters are called codons. Each codon is a word of length 3 with the letters A, C, G, T. Consequently, there are $4^3 = 64$ codons. However, by redundance, only 20 codons are essential. This corresponds to the multiplicity of spectral lines in the spectroscopy of molecules. This analogy combined with supersymmetry can be used in order to model mathematically the redundance of codons.[157] The information encoded into the word (7.295) is equal to $I = \log_2 20^{\mathcal{L}} = \mathcal{L} \log_2 20$.

The properties of the information function. Let

$$\sigma_M := \{(p_1, \dots, p_M) : \ 0 \le p_1 + \dots + p_M \le 1, \ \ p_1 + \dots + p_M = 1\}$$

be an $(M-1)$-dimensional simplex in $\mathbb{R}^M$. This is the closed convex hull of the M extremal points (vertices) $(1, 0, \dots, 0), \dots, (0, \dots, 0, 1)$. The proof of the following statement will be given in Problem 7.37.

Proposition 7.64 *The function $I : \sigma_M \to \mathbb{R}$ given by (7.293) is continuous and concave.*[158] *The minimal value $I = 0$ is attained at the extremal points of σ_M. Furthermore, the maximal value $I = \log_2 M$ is attained at the point $p_k = \frac{1}{M}$ for all $k = 1, \dots, M$.*

Measure of disorder. Consider the following experiment. We are given N particles, and we want to distribute them into M boxes $\mathcal{B}_1, \dots, \mathcal{B}_M$. Each possible distribution can be described by the symbol

[157] See M. Forger and S. Sachse, Lie super-algebras and the multiplet structure of the genetic code, I. Codon representations, II. Branching rules, J. Math. Phys. **41** (2000), 5407–5422; 5423–5444.
F. Antonelli, L. Braggion, M. Forger, et al., Extending the search for symmetries in the genetic code, Intern. J. Modern Physics B **17** (2003), 3135–3204.

[158] Explicitly, $I(\lambda q + (1-\lambda)p) \ge \lambda I(q) + (1-\lambda) I(p)$ for all $q, p \in \sigma_M$ and $\lambda \in [0, 1]$.

$$N_1 N_2 \dots N_M \tag{7.296}$$

where N_m is the number of particles in the box $\mathcal{B}_m$. Then $N_1 + \dots + N_M = N$. Set $p_m := \frac{N_m}{N}$. By definition, the number

$$I := -\sum_{m=1}^{M} p_m \log_2 p_m$$

is called the measure of disorder of the distribution (7.296). In order to show that this definition is reasonable, consider the following special cases.

- By Prop. 7.64, $0 \le I \le \log_2 M$.
- If all of the particles are in the same box, say, $\mathcal{B}_1$, then we have $p_1 = 1$ and $p_2 = \dots = p_M = 0$ Hence $I = -p_1 \log_2 p_1 = 0$. This corresponds to minimal disorder.
- If each box contains the same number of particles, then $N_m = \frac{N}{M}$. Hence $p_m = \frac{1}{M}$ for $m = 1, \dots, M$. Therefore, $I = \log_2 M$. This corresponds to maximal disorder.

Entropy. For historical reasons, physicists replace the information I from (7.293) by the quantity

$$S = -k \sum_{m=1}^{M} p_m \ln p_m.$$

Here, we use the Boltzmann constant $k = 1.380 \cdot 10^{-23}$ J/K. This implies that the entropy S has the physical dimension (heat) energy per temperature (see Sect. 7.17.11 on page 654). Since $\ln p_m = \ln 2 \cdot \log_2 p_m$, the relation between entropy and information is given by

$$S = I \cdot k \ln 2.$$

Intuitively, the entropy S measures the disorder of a many-particle system in physics. We have $0 \le S \le k \ln M$. Recent astronomical observations show that our universe is expanding in an accelerated manner. This means that stars and black holes decay after a long time.[159] Hence the disorder of the universe increases, that is, the entropy increases. This was postulated by Clausius (1822–1888) in 1865. He called this the heat death of the universe.

Temperature and chemical potential as Lagrange multipliers. In order to motivate the grand canonical ensemble, let us study the following maximum problem:

$$S = -k \sum_{m=1}^{M} p_m \ln p_m = \max!, \qquad p \in C \tag{7.297}$$

with the unit cube $C := \{(p_1, \dots, p_M\} : 0 \le p_1, \dots, p_M \le 1\}$ and the constraints

$$\bar{E} = \sum_{m=1}^{M} p_m E_m, \quad \bar{N} = \sum_{m=1}^{M} p_m N_m, \quad p_1 + \dots + p_M = 1. \tag{7.298}$$

Let $M \ge 2$. We are given the positive numbers $E_1, \dots E_M, N_1, \dots, N_M$ and $\bar{E}, \bar{N}$. We are looking for a solution $(p_1, \dots, p_M)$.

[159] F. Adams and G. Laughlin, A dying universe: the long-term fate and evolution of astrophysical objects, Rev. Mod. Phys. **69** (1997), 337–372.
F. Adams and G. Laughlin, The Five Ages of the Universe: Inside the Physics of Eternity, Simon and Schuster, New York, 1999.

Theorem 7.65 *Consider* $(p_1, \ldots, p_M)$ *given by* (7.288) *on page 639. Suppose that the real parameter* μ *and the positive parameter* T *are fixed in such a way that the constraints* (7.298) *are satisfied. In addition, assume that* $0 < p_1, \ldots, p_M < 1$ *and that the matrix*

$$\begin{pmatrix} E_1 & \ldots & E_M \\ N_1 & \ldots & N_M \\ 1 & \ldots & 1 \end{pmatrix}$$

has rank three. Then $(p_1, \ldots, p_M)$ *is the unique solution of the maximum problem* (7.297), (7.298).

Proof. (I) Local existence. We will use the sufficient solvability condition for the Lagrangian multiplier rule (see Prop. 43.23 of Zeidler (1986), Vol. III (see the references on page 1049). To this end, set

$$L := S + \alpha \left(\bar{E} - \sum_m p_m E_m \right) + \beta \left(\bar{N} - \sum_m p_m N_m \right) + \gamma \left(1 - \sum_m p_m \right).$$

That is, we add the constraints (7.298) to the function S which has to be maximized. The real numbers α, β, γ (called Lagrange multipliers) will be chosen below. For the partial derivatives, we get

$$L_{p_m} = -k \ln p_m - k - \alpha E_m - \beta N_m - \gamma,$$

and

$$L_{p_j p_m} = -\frac{k \delta_{jm}}{p_m}.$$

By (7.288), we choose μ, T and $(p_1, \ldots, p_M)$ in such a way that the constraints (7.298) are satisfied. Moreover, we set

$$\alpha := \frac{1}{T}, \quad \beta := -\frac{\mu}{T}, \quad \gamma := -k + k \ln \sum_m \mathrm{e}^{(\mu N_m - E_m)/kT}.$$

Then $L_{p_m} = 0$ for all m, and the matrix $(-L_{p_j p_m})$ is positive definite. This guarantees that our choice $(p_1, \ldots, p_M)$ represents a local maximum of the entropy function S under the constraints (7.298).

(II) Global existence. Since the entropy function S is concave, each local maximum of S on a convex set is always a global maximum. (We refer to Prop. 42.3 of Zeidler (1986), Vol. III (see the references on page 1049), and note that $-S$ is convex.)

(III) Uniqueness. On the boundary of the cube C, the entropy function S vanishes. Therefore, any solution of (7.297), (7.298) lies in the interior of C. Since the matrix $(-S_{p_j p_m})$ is positive definite, the function S is strictly concave on the interior of C. This implies the uniqueness of the solution (see Theorem 38.C. of Zeidler (1986), Vol. III). □

In the special case where the particle numbers are fixed, we use the choice $N_1 = \ldots = N_M = \bar{N}$, and $\mu = 0$. Then we have merely to assume that the matrix

$$\begin{pmatrix} E_1 & \ldots & E_M \\ 1 & \ldots & 1 \end{pmatrix}$$

has rank two, that is, there exist at least two different energies.

7.17.5 Semiclassical Statistical Physics

> In semiclassical statistical physics, the extended algebra of observables is a commutative $*$-algebra of functions, and the states are generated by some probability measure.
>
> Folklore

The key relation reads as

$$\boxed{\bar{A} := \int_M A(q,p)\varrho(q,p)\frac{dqdp}{h}.}$$

Here, we use the product set $M := \mathcal{B} \times \mathbb{R}$, where $\mathcal{B}$ is a closed interval on the real line. We are given the bounded continuous function $A : M \to \mathbb{C}$ and the bounded continuous function $\varrho : M \to [0, \infty[$ with the normalization condition

$$\int_M \varrho(q,p)\frac{dqdp}{h} = 1.$$

Then the function ϱ represents a probability density on the phase space M, and $\bar{A}$ is the mean value of the function $A = A(q,p)$. Traditionally, this function is called a (physical) observable iff it is real-valued.[160] The square of the mean fluctuation is given by

$$(\Delta A)^2 = \int_M (A(q,p) - \bar{A})^2 \varrho(q,p)\frac{dqdp}{h}.$$

In terms of physics, we consider an ideal gas[161] on the interval $\mathcal{B}$, that is, the position coordinate q of a single gas particle lives on the interval $\mathcal{B}$, and the momentum coordinate p lives on the real line $\mathbb{R}$. If $H = H(q,p)$ is the Hamiltonian function of a single gas particle, then we choose the function

$$\varrho(q,p) := \frac{\mathrm{e}^{-H(q,p)/kT}}{\int_M \mathrm{e}^{-H(q,p)/kT}\frac{dqdp}{h}}.$$

This function generates the semiclassical Gibbs statistics.[162] Here, T is the absolute temperature, k is the Boltzmann constant, and h is Planck's quantum of action. For example, if the gas particles behave like harmonic oscillators, then we choose $H(q,p) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}$. We need the physical constants k and h in order to guarantee that both the quantities $\frac{H(q,p)}{kT}$ and $\frac{dqdp}{h}$ are dimensionless. This implies that the function $\mathrm{e}^{-H(q,p)/kT}$ makes sense, the probability density ϱ is dimensionless, and the mean value $\bar{A}$ has the same dimension as the physical observable $A(q,p)$. For example, if we choose $A(q,p) := H(q,p)$, then $N\bar{H}$ is the mean energy of the ideal gas at the temperature T, where N is the number of gas particles. The function

$$S(q,p) = -k\varrho(q,p)\ln\varrho(q,p)$$

[160] Note that the algebra of observables to be introduced below is not only based on real-valued functions, but on complex-valued functions in order to get a complex $*$-algebra.

[161] An ideal gas is characterized by the property that there are no interactions between the gas particles, that is, the single gas particles behave like independent random objects.

[162] Gibbs (1839–1903).

corresponds to the entropy, and $N\bar{S}$ is the entropy of the ideal gas at the temperature T. If C is a compact subset of the phase space M, then the integral

$$\int_C \varrho(q,p)\frac{dqdp}{h}$$

is the probability for finding the position-momentum coordinate (q,p) of a single gas particle in the set C. Let us translate this into the language of $*$-algebras.

The extended $*$-algebra $\mathcal{A}$ of observables. Let $\mathcal{A}$ denote the set of all bounded continuous functions $A : M \to \mathbb{C}$. With respect to the star operation $A^*(q,p) := A(q,p)^\dagger$ for all $(q,p) \in M$, the set $\mathcal{A}$ is a commutative $*$-algebra with unit element $\mathbf{1}$.[163] The $*$-algebra $\mathcal{A}$ is called the extended $*$-algebra of observables (of the gas). Precisely the real-valued functions A in $\mathcal{A}$ are called observables. In addition, equipped with the norm

$$||A|| := \sup_{(q,p)\in M} |A(q,p)|,$$

the $*$-algebra $\mathcal{A}$ becomes a normed space with

- $||A^*|| = ||A||$ and $||A^*A|| = ||A||^2$ for all $A \in \mathcal{A}$;
- $||\mathbf{1}|| = 1$.

Since the phase space M is an unbounded closed subset of $\mathbb{R}^2$ (i.e., M is not compact), the normed space $\mathcal{A}$ is not a Banach space. We call $\mathcal{A}$ an incomplete C^*-algebra (or a pre-C^*-algebra).

States. Generally, states are functionals χ which assign a real number $\chi(A)$ to each observable A. We define

$$\chi(A) := \int_M A(q,p)\varrho(q,p)\frac{dqdp}{h} \qquad \text{for all} \quad A \in \mathcal{A}.$$

Then, for all $A \in \mathcal{A}$, we have:

- $\chi(A^*A) = \int_M A(q,p)^\dagger A(q,p)\varrho(q,p)\frac{dqdp}{h} \geq 0$;
- $\chi(I) = \int_M 1 \cdot \varrho(q,p)\frac{dqdp}{h} = 1$.
- The map $\chi : \mathcal{A} \to \mathbb{C}$ is linear.
- $|\chi(A)| \leq \sup_{(q,p)\in\mathbb{R}^2} |A(q,p)| = ||A||$.

We call χ a state on the $*$-algebra $\mathcal{A}$. This state corresponds to the probability measure ν generated by the probability density ϱ (i.e., $d\nu = \varrho\frac{dqdp}{h}$).

Dynamics. To avoid technicalities, choose $J := \mathbb{R}$, that is, $M = \mathbb{R}^2$. Motivated by the classical equation of motion

$$\dot{q}(t) = H_p(q(t),p(t)), \qquad \dot{p}(t) = -H_q(q(t),p(t)), \qquad t \in \mathbb{R} \tag{7.299}$$

with the initial condition $q(0) = q_0, p(0) = p_0$, we define

$$(\mathcal{U}_t A)(q_0,p_0) := A(q(t),p(t))$$

for all times $t \in \mathbb{R}$ and all initial points $(q_0,p_0) \in \mathbb{R}^2$. We assume that, as for the harmonic oscillator, the trajectories $q = q(t), p = p(t)$ exist for all times. Then, for each time $t \in \mathbb{R}$, the map

$$\mathcal{U}_t : \mathcal{A} \to \mathcal{A}$$

[163] Here, $\mathbf{1}$ is given by the function $A(q,p) \equiv 1$.

is a $*$-automorphism. Thus, $\{\mathcal{U}_t\}_{t\in\mathbb{R}}$ is a one-parameter group of $*$-automorphisms of the $*$-algebra $\mathcal{A}$.

Our next goal is to prove that the dynamics of the gas corresponds to a family $\{U_t\}_{t\in\mathbb{R}}$ of unitary operators U_t on the Hilbert space $L_2(\mathbb{R}^2)$. To this end, let $\mathcal{A}_{\rm pre}$ denote the set of all smooth functions $A : \mathbb{R}^2 \to \mathbb{C}$ with compact support. Obviously, $\mathcal{A}_{\rm pre}$ is a $*$-subalgebra of the $*$-algebra $\mathcal{A}$ of observables. In addition, $\mathcal{A}_{\rm pre}$ is a dense subset of the Hilbert space $L_2(\mathbb{R}^2)$ equipped with the inner product $\langle A|B\rangle := \int_{\mathbb{R}^2} A(q,p)^\dagger B(q,p)dqdp$.

Proposition 7.66 *Let $A, B \in \mathcal{A}_{\rm pre}$. Then $\langle \mathcal{U}_t A|\mathcal{U}_t B\rangle = \langle A|B\rangle$ for all $t \in \mathbb{R}$.*

This tells us that the dynamics of the gas respects the inner product on the Hilbert space $L_2(\mathbb{R}^2)$. Using this result and the extension theorem from Problem 7.21, we get the following.

Corollary 7.67 *For any time $t \in \mathbb{R}$, the operator $\mathcal{U}_t : \mathcal{A}_{\rm pre} \to \mathcal{A}$ can be uniquely extended to a unitary operator $U_t : L_2(\mathbb{R}) \to L_2(\mathbb{R})$.*

It remains to prove Prop. 7.66. Using the equation (7.299) of motion, we get

$$\frac{d}{dt}(\mathcal{U}_t A)(q_0,p_0) = A_q(q(t),p(t))H_p(q(t),p(t)) - A_p(q(t),p(t))H_q(q(t),p(t)).$$

Noting that $H_{qp} = H_{pq}$, integration by parts yields

$$\int_{\mathbb{R}^2} (A_q^\dagger H_p - A_p^\dagger H_q)Bdqdp = -\int_{\mathbb{R}^2} A^\dagger(B_q H_p - B_p H_q)dqdp.$$

This implies $\frac{d}{dt}\langle \mathcal{U}_t A|\mathcal{U}_t B\rangle = \langle \frac{d}{dt}\mathcal{U}_t A|\mathcal{U}_t B\rangle + \langle \mathcal{U}_t A|\frac{d}{dt}\mathcal{U}_t B\rangle = 0$. □

Generalization. The simple special case considered above can be generalized to $2s$-dimensional phase space manifolds M by starting from the key formula

$$\bar{A} := \int_M A(q,p)d\nu(q,p)$$

with $\int_M d\nu = 1$. Here, $(q,p) = (q_1,\dots,q_s;p_1,\dots,p_s)$. As a rule, the Hamiltonian $H = H(q,p)$ describes interactions between the particles; this corresponds to so-called real gases.

For example, consider a gas consisting of N molecules in a box $\mathcal{B}$ of finite volume V in the 3-dimensional space. Then $s = 3N$, and $M = \mathcal{B}^N \times \mathbb{R}^{3N}$. Moreover,

$$d\nu := \varrho(q,p)\frac{dq^{3N}dp^{3N}}{h^{3N}N!} \qquad \text{with} \qquad \varrho(q,p) := \frac{\mathrm{e}^{-H(q,p)/kT}}{\int_M \mathrm{e}^{-H(q,p)/kT}\frac{dq^{3N}dp^{3N}}{h^{3N}N!}}.$$

We assume that the function ϱ is invariant under permutations of the particles. The factorial $N!$ takes the Pauli principle into account (principle of indistinguishable particles). If we introduce the partition function

$$Z(T,V) := \int_M \mathrm{e}^{-H(q,p)/kT}\frac{dq^{3N}dp^{3N}}{h^{3N}N!},$$

then we obtain the following thermodynamic quantities:

- Free energy: $F(T,V) := -kT\ln Z(T,V)$.
- Entropy: $S(T,V) = -F_T(T,V)$.
- Pressure: $P(T,V) = -F_V(T,V)$.
- Mean energy: $\bar{E}(T,V) = F(T,V) + TS(T,V)$.

7.17.6 The Classical Ideal Gas

Let us consider an ideal gas which consists of N freely moving molecules of mass m. The fixed particle number N is assumed to be large (of magnitude 10^{23}). We assume that the molecules move in a 3-dimensional box $\mathcal{B}$ of volume V. Then the following hold:

(i) Free energy: $F = -NkT(1 + \ln \frac{V(2\pi mkT)^{3/2}}{Nh^3})$.

(ii) Entropy: $S = Nk\left(\frac{5}{2} + \ln \frac{V(2\pi mkT)^{3/2}}{Nh^3}\right)$.

(iii) Energy: $E = \frac{3}{2}NkT$.

(iv) Energy fluctuation: $\frac{\Delta E}{E} = \sqrt{\frac{2}{3N}}$.

(v) Pressure: $P = NkT/V$.

(vi) Maxwell's velocity distribution: Fix the origin $\mathcal{O}$ and consider the velocity vector $\mathbf{v} = \overline{\mathcal{OP}}$. The probability of finding the endpoint $\mathcal{P}$ of the velocity vector $\mathbf{v}$ of a single molecule in the open subset C of $\mathbb{R}^3$ is given by the Gaussian integral

$$\left(\frac{m}{2\pi kT}\right)^{3/2} \int_C \mathrm{e}^{-m\mathbf{v}^2/2kT}\, d^3\mathbf{v}. \tag{7.300}$$

Here, $m\mathbf{v}^2/2$ is the kinetic energy of the freely moving molecule, and the normalization factor guarantees that the probability is equal to one if $C = \mathbb{R}^3$.

The experience of physicists shows that these formulas are valid if the temperature T is sufficiently high.[164] Let us compute (i) through (vi). We start with the energy function $H = \sum_{j=1}^N \frac{\mathbf{p}_j^2}{2m}$. The partition function reads as

$$\begin{aligned} Z = \int_{\mathcal{B}^N \times \mathbb{R}^{3N}} \mathrm{e}^{-H(\mathbf{P})/kT}\ \frac{d^{3N}q\, d^{3N}p}{h^{3N}N!} &= \frac{V^N}{h^{3N}N!}\left(\int_{\mathbb{R}} \mathrm{e}^{-p^2/2mkT} dp\right)^{3N} \\ &= \frac{V^N(2\pi mkT)^{3N/2}}{h^{3N}N!} \sim \left(\frac{\mathrm{e}V(2\pi mkT)^{3/2}}{Nh^3}\right)^N. \end{aligned}$$

Here, to simplify computations, we use the approximation[165] $\frac{1}{N!} \sim \left(\frac{\mathrm{e}}{N}\right)^N$. Parallel to (i)–(vii) on page 640 with $\mu = 0$, we get the following formulas

$$F = -kT \ln Z, \quad S = -F_T, \quad E = F + TS, \quad P = -F_V$$

and $(\Delta E)^2 = kT^2 E_T$. By straightforward computations, we obtain the desired formulas (i) through (v). To get (vi), we start with the Gibbs distribution

[164] More precisely, we asssume that $\frac{V(2\pi mkT)^{3/2}}{Nh^3}$ is small. This means that the de Broglie wave length $\lambda := h/(2\pi mkT)^{1/2}$ is small compared with the mean distance $(V/N)^{1/3}$ of the molecules.

[165] This can be motivated by the Stirling formula

$$\frac{1}{N!} = \left(\frac{\mathrm{e}}{N}\right)^N \cdot \frac{1}{\mathrm{e}^{\vartheta(N)/12N}\sqrt{2\pi N}}, \qquad N = 1, 2, \ldots$$

where $0 < \vartheta(N) < 1$. Hence $\frac{1}{N!} = \frac{\mathrm{e}^{N(1+o(N))}}{N^N}$ as $N \to \infty$.

$$\varrho(\mathbf{p}_1,\dots,\mathbf{p}_n)=\frac{\mathrm{e}^{-\sum_{j=1}^n \mathbf{p}_j^2/2mkT}}{\int_{\mathcal{B}^N\times\mathbb{R}^{3N}} \mathrm{e}^{-\sum_{j=1}^N \mathbf{p}_j^2/2mkT}\ \frac{d^{3N}q\,d^{3N}p}{h^{3N}N!}}=\prod_{j=1}^N \nu(\mathbf{p}_j)$$

where

$$\nu(\mathbf{p}):=\frac{\mathrm{e}^{-\mathbf{p}^2/2mkT}}{V\int_{\mathbb{R}^3}\mathrm{e}^{-\mathbf{p}^2/2mkT}\ \frac{d^3\mathbf{p}}{h^3(N!)^{1/N}}}=\frac{h^3(N!)^{1/N}\mathrm{e}^{-\mathbf{p}^2/2mkT}}{V(2\pi kT)^{3/2}}.$$

We assume that the single molecules move independently. Thus, it is reasonable to regard the function ν as the distribution function for a single molecule. For the mean momentum of a single molecule, we obtain

$$\bar{\mathbf{p}}=\int_{\mathcal{B}\times\mathbb{R}^3}\nu(\mathbf{p})\mathbf{p}\ \frac{d^3\mathbf{q}\,d^3\mathbf{p}}{h^3(N!)^{1/N}}.$$

Using $\mathbf{p}=m\mathbf{v}$, we get the mean velocity $\bar{\mathbf{v}}=\int_{\mathbb{R}^3}\mathbf{v}\mathrm{e}^{-m\mathbf{v}^2/2kT}\left(\frac{m}{2\pi kT}\right)^{3/2}d^3\mathbf{v}$ which motivates (vi).

7.17.7 Bose–Einstein Statistics

Let us consider the following situation which frequently arises in quantum statistics. Suppose that the system Γ (e.g., a gas of photons) consists of particles that may assume one of the energy values $\varepsilon_0,\dots,\varepsilon_M$. By definition, a state of Γ is characterized by

$$\varepsilon_0,\varepsilon_1,\dots,\varepsilon_J;\qquad n_0,n_1,\dots,n_J. \tag{7.301}$$

This means that precisely n_j particles of Γ have the energy ε_j, where the index j runs from 0 to J. For each such state, the particle number N and the energy E are given by

$$N=\sum_{j=0}^J n_j,\qquad E=\sum_{j=0}^J n_j\varepsilon_j.$$

Therefore, the partition function is given by

$$Z(T,\mu):=\sum_{\Gamma}\mathrm{e}^{(\mu N-E)/kT}=\prod_{j=0}^J\sum_{n_j}\mathrm{e}^{(\mu n_j-n_j\varepsilon_j)/kT}.$$

Furthermore, we introduce the statistical potential

$$\Omega(T,\mu):=-kT\ln Z(T,\mu)=-kT\sum_{j=0}^J\ln\sum_{n_j}\left(\mathrm{e}^{(\mu-\varepsilon_j)/kT}\right)^{n_j}. \tag{7.302}$$

We now make the crucial assumption that

Each occupation number n_j may assume the values $0,1,\dots,n$.

This corresponds to bosons (that is, particles with integer spin, e.g., photons). Using the geometric series, $\Omega(T,\mu)$ is equal to

$$-kT\sum_{j=0}^J\ln\sum_{n_j=0}^n\left(\mathrm{e}^{(\mu-\varepsilon_j)/kT}\right)^{n_j}=-kT\sum_{j=0}^J\ln\frac{1-\mathrm{e}^{(n+1)(\mu-\varepsilon_j)/kT}}{1-\mathrm{e}^{(\mu-\varepsilon_j)/kT}}.$$

Furthermore, assume that the maximal occupation number n is very large and $\mu - \varepsilon_j < 0$ for all j. Letting $n \to \infty$, we get the final statistical potential

$$\Omega(T,\mu) = kT \sum_{j=0}^{J} \ln\left(1 - \mathrm{e}^{(\mu-\varepsilon_j)/kT}\right).$$

By (7.290) on page 640, $N = -\Omega_\mu, S = -\Omega_T, F = \Omega + \mu N$, and $E = F + TS$. This yields the following.

(i) Mean particle number: $N = \sum_{j=0}^{J} N_j$ where $N_j := \frac{\mathrm{e}^{(\mu-\varepsilon_j)/kT}}{1-\mathrm{e}^{(\mu-\varepsilon_j)/kT}}$.
(ii) Mean energy: $E = \sum_{j=0}^{J} N_j \varepsilon_j$.
(iii) Free energy: $F = \Omega + \mu N$.
(iv) Entropy: $S = \frac{E-F}{T}$.

In particular, if each particle behaves like a quantum harmonic oscillator of angular frequency ω, then $\varepsilon_j = \hbar\omega(j + \frac{1}{2})$. We have shown in Sect. 2.3.2 of Vol. I that Planck's radiation law is a consequence of the mean energy formula (ii) for the quantum harmonic oscillator.

The Maxwell–Boltzmann statistics as a limit case for high temperature. In the special case where $\mathrm{e}^{(\mu-\varepsilon_j)/kT} \ll 1$ (e.g., $\mu - \varepsilon_j < 0$ and T is large), we approximately obtain

$$N_j = \mathrm{e}^{(\mu-\varepsilon_j)/kT}. \tag{7.303}$$

This is called the classical Maxwell–Boltzmann statistics. which generalizes the Maxwell velocity distribution (7.300) on page 648.

Bose–Einstein condensation as a limit case at low temperature. Suppose that $0 \le \varepsilon_0 < \varepsilon_1 < \varepsilon_2 < \dots$. We expect that at low temperatures most of the bosons are located in the ground state. In fact, by (i), for the particle numbers we get

$$\lim_{T\to+0} \lim_{\mu\to\varepsilon_0-0} N_j(T,\mu) = \begin{cases} +\infty & \text{if} \quad j = 0, \\ 0 & \text{if} \quad j = 1,2,\dots \end{cases}$$

This phenomenon is called Bose–Einstein condensation.

7.17.8 Fermi–Dirac Statistics

In contrast to the preceding section, we now assume that

Each occupation number n_j may only assume the values $0, 1$.

This corresponds to the Pauli exclusion principle for fermions (that is, particles with half-integer spin, e.g., electrons).[166] This yields

$$\Omega(T,\mu) = -kT \sum_{j=0}^{J} \ln(1 + \mathrm{e}^{(\mu-\varepsilon_j)/kT}).$$

As in Sect. 7.17.7, we now obtain the following:s

[166] More precisely, if s is the spin of the particles, then each energy value ε_j has to be counted with the multiplicity $2s + 1$.

(i) Mean particle number: $N = \sum_{j=0}^{J} N_j$ where $N_j := \frac{e^{(\mu-\varepsilon_j)/kT}}{1+e^{(\mu-\varepsilon_j)/kT}}$.
(ii) Mean energy: $E = \sum_{j=0}^{J} N_j \varepsilon_j$.
(iii) Free energy: $F = \Omega + \mu N$.
(iv) Entropy: $S = \frac{E-F}{T}$.

If $e^{(\mu-\varepsilon_j)/kT} \ll 1$ (e.g., $\mu - \varepsilon_j < 0$ and T is large), then we obtain the classical Maxwell–Boltzmann statistics (7.303).

The Fermi ball as a limit case at low temperature. For the particle numbers, we get

$$\lim_{T \to +0} N_j(T, \mu) = \begin{cases} 1 & \text{if} \quad \varepsilon_j < \mu, \\ 0 & \text{if} \quad \mu < \varepsilon_j. \end{cases}$$

This means that at low temperature each of the lowest energy levels is occupied by precisely one particle. In contrast to Bose–Einstein condensation, by the Pauli principle it is impossible that all of the particles are in the ground state. For example, consider a gas of N electrons in a box of volume V in the limit case of temperature $T = 0$. Since the electron has spin $s = \frac{1}{2}$, each cell of volume h^3 in the phase space contains two electrons with different spin orientations. Thus, if P denotes the maximal momentum of the electrons at $T = 0$, then the phase space volume $\frac{4}{3}\pi P^3 \cdot V$ contains N particles where

$$N = \frac{2}{h^3} \cdot \frac{4}{3}\pi P^3 V.$$

The ball of radius P is called the Fermi ball of the N-particle electron gas at zero temperature, and the surface of the Fermi ball is called the Fermi surface.

Applications of the Bose–Einstein statistics and the Fermi–Dirac statistics to interesting physical phenomena can be found in Zeidler (1986), Vol. IV, Chap. 68 (see the references on page 1049). For example, this concerns Planck's radiation law for photon gases, as well as the Fermi ball which is crucial for computing the critical Chandrasekhar mass of special stars called white dwarfs (see also N. Straumann, General Relativity with Applications to Astrophysics, Springer, New York, 2004). Using the methods of quantum field theory, the structure of Fermi surfaces for electrons in a crystal is studied in M. Salmhofer, Renormalization: An Introduction, Springer, Berlin, 1999.

7.17.9 Thermodynamic Equilibrium and KMS-States

The grand canonical example in finite quantum statistics. Let X be a finite-dimensional complex Hilbert space, $X \neq \{0\}$. Choose the density operator

$$\varrho_0 := \frac{e^{\beta(\mu N - H)}}{\operatorname{tr} e^{\beta(\mu N - H)}}.$$

Here, $H, N : X \to X$ are self-adjoint operators, and $\beta > 0$ and μ are real parameters, with the temperature T, the Boltzmann constant k, the chemical potential μ, and $\beta = 1/kT$. In the language of C^*-algebras, the following hold.

- The extended C^*-algebra $\mathcal{A} = L(X, X)$ of observables consists of all linear operators $A : X \to X$ equipped with the norm $||A|| := \sqrt{\operatorname{tr}(A^* A)}$.
- The states are defined by $\chi_0(A) := \operatorname{tr}(\varrho_0 A)$ for all $A \in \mathcal{A}$.

- The dynamics of the state χ_0 is given by

$$\chi_t(A) := \operatorname{tr}(\varrho_0 \mathcal{U}_t A)$$

for all $A \in \mathcal{A}$ and all times $t \in \mathbb{R}$. Here, $\mathcal{U}_t(A) := \mathrm{e}^{\mathrm{i}tH/\hbar} A \mathrm{e}^{-\mathrm{i}tH/\hbar}$.

Proposition 7.68 *The state χ_0 corresponding to the density operator ϱ_0 and the dynamics $\{\chi_t\}_{t\in\mathbb{R}}$ is a KMS-state of temperature T.*

Proof. Set $Z := \operatorname{tr}(\mathrm{e}^{\beta(\mu N - H)})$. To simplify notation, choose $\mu := 0$ and $\hbar := 1$. Then

$$\chi_0(A) = \operatorname{tr}(\varrho_0 A) = Z^{-1} \operatorname{tr}(\mathrm{e}^{-\beta H} A).$$

Noting the commutativity property of the trace, $\operatorname{tr}(CD) = \operatorname{tr}(DC)$, we get

$$\begin{aligned} Z\chi_0(\mathcal{U}_{t-\mathrm{i}\beta}(B)A) &= \operatorname{tr}(\mathrm{e}^{-\beta H}\mathrm{e}^{\mathrm{i}(t-\mathrm{i}\beta)H} B \mathrm{e}^{-\mathrm{i}(t-\mathrm{i}\beta)H} A) = \operatorname{tr}(\mathrm{e}^{\mathrm{i}tH} B \mathrm{e}^{-\mathrm{i}tH} \mathrm{e}^{-\beta H} A) \\ &= \operatorname{tr}(\mathrm{e}^{-\beta H} A \mathrm{e}^{\mathrm{i}tH} B \mathrm{e}^{-\mathrm{i}tH}) = Z\chi_0(A\mathcal{U}_t(B)). \end{aligned}$$

□

Example. As a typical example, choose the operators H and N in such a way that

$$H\psi_j = E_j\psi_j, \qquad N\psi_j = N_j\psi_j, \qquad j = 1, \ldots, n$$

where $\psi_1, \ldots, \psi_n$ is an orthonormal basis of X, and E_j, N_j are nonnegative numbers for all j. Then $\varrho_0\psi_j = p_j\psi_j$ with

$$p_j = \frac{\mathrm{e}^{\beta(\mu N_j - E_j)}}{\sum_{j=1}^n \mathrm{e}^{\beta(\mu N_j - E_j)}}.$$

The operator H (resp. N) is called the Hamiltonian with the energy levels $E_1, \ldots, E_n$ (resp. the particle operator with the particle numbers $N_1, \ldots, N_n$.)

7.17.10 Quasi-Stationary Thermodynamic Processes and Irreversibility

> In the huge factory of natural processes, the principle of entropy occupies the position of manager, for it dictates the manner and method of the whole business, whilst the principle of energy merely does the bookkeeping, balancing debits and credits...
> Life on the earth needs the radiation of the sun. Our conditions of existence require a determinate degree of temperature, and for the maintenance of this there is needed not addition of energy, but addition of entropy.[167]
>
> Robert Emden, 1938

Let us study the sufficiently regular time-evolution of the grand canonical ensemble. By a quasi-stationary process of the grand canonical ensemble, we understand smooth time-depending functions of temperature, chemical potential, and volume:

$$T = T(t), \quad \mu = \mu(T), \quad V = V(t), \qquad t_0 \le t \le t_1. \tag{7.304}$$

By (7.290) on page 640, this yields the following quantities:

$$E = E(t), \quad N = N(t), \quad S = S(t), \quad P = P(t), \qquad t_0 \le t \le t_1.$$

[167] R. Emden, Why do we have winter heating? Nature **14** (1938), 908–909.

Here, E is the mean energy, N is the mean particle number, S is the entropy, and P is the pressure.[168] From the physical point of view, this is an idealization. We assume that the physical system is in thermodynamic equilibrium at each time t. In reality, a certain relaxation time is needed in order to pass from a thermodynamic equilibrium state to a new one. Let $Q(t)$ be the heat added to the physical system during the time interval $[t_0, t]$. We postulate that, for all times t in the interval $[t_0, t_1]$, the process (7.304) has the following properties.

(i) The first law of thermodynamics: $\dot{E}(t) = \dot{Q}(t) - P(t)\dot{V}(t) + \mu(t)\dot{N}(t)$.

(ii) The second law of thermodynamics: $T(t)\dot{S}(t) \geq \dot{Q}(t)$.

(iii) The third law of thermodynamics. Suppose that the temperature $T(t)$ goes to zero as $t \to t_1 - 0$. Then so do the entropy $S(t)$ and its partial derivatives $S_T(t), S_\mu(t), S_V(t)$.

The first law describes conservation of energy. To discuss the second law, let us introduce the external entropy

$$S_e(t) := S(t_0) + \int_{t_0}^{t} \frac{\dot{Q}(\tau)}{T(\tau)}\, d\tau, \qquad t_0 \leq t \leq t_1,$$

which depends on the heat added to the system. In addition, we introduce the remaining internal entropy $S_i(t) := S(t) - S_e(t)$. Then

$$\dot{S}_e(t) = \frac{\dot{Q}(t)}{T(t)}, \qquad \dot{S}_i(t) \geq 0, \qquad t_0 \leq t \leq t_1.$$

Assume that $t_0 = -t_1$ where $t_1 > 0$. If the quasi-stationary process (7.304) has the property that also the time-reflected process

$$T = T(-t), \quad \mu = \mu(-T), \quad V = V(-t), \qquad t_0 \leq t \leq t_1$$

is quasi-stationary, then the process is called reversible. In this case, because of $\frac{d}{dt}S(-t) = -(\frac{d}{dt}S)(-t)$, the second law tells us that

$$-T(-t)\dot{S}(-t) \geq \dot{Q}(-t), \qquad -t_1 \leq t \leq t_1.$$

This implies

$$T(t)\dot{S}(t) \geq \dot{Q}(t), \qquad -T(t)\dot{S}(t) \geq \dot{Q}(t), \qquad -t_1 \leq t \leq t_1.$$

Hence $T(t)\dot{S}(t) = \dot{Q}(t)$ for all $t \in [-t_1, t_1]$. This means that the internal entropy S_i vanishes on the time interval $[-t_1, t_1]$. Processes are called irreversible iff they are not reversible. Typically, the time-evolution of living beings is irreversible. A more detailed discussion can be found in Zeidler (1986), Vol. IV, Chap. 67 (see the references on page 1049).

The thermodynamic limit and phase transitions. If the volume V of the physical system goes to infinity, $V \to \infty$, then this limit is called the thermodynamic limit by physicists. Then it may happen that important thermodynamic quantities become singular for appropriate parameters (e.g., temperature T). These singularities correspond to phase transitions (e.g., the transition from water to ice). Phase transitions play a fundamental role for understanding critical phenomena in nature (e.g., the inflation of the very early universe and the emergence of the three fundamental forces during the cooling process of the hot universe after the Big

[168] To simplify notation, we write E and N instead of $\bar{E}$ and $\bar{N}$, respectively.

Bang).[169] In terms of statistical physics, phase transitions correspond to a strong increase of fluctuations. We will encounter this in later volumes. As an introduction to the rigorous theory of phase transitions, we recommend the classical survey article by Griffith.[170]

7.17.11 The Photon Mill on Earth

Living objects store a lot of information related to the genetic code. There arises the following question in physics: where does this information come from? The solution of this interesting problem is given by the entropy relation

$$\Delta S_e = \frac{\Delta Q}{T_{\text{in}}} - \frac{\Delta Q}{T_{\text{out}}},$$

which is called the photon mill on earth. In fact, the sun sends photons to the earth at the temperature $T_{\text{in}} = 5800$ K, which is the high surface temperature of the sun. Most of these photons are reflected by the surface of earth, and they are sent to the universe at the lower temperature $T_{\text{out}} = 260$ K. Since $T_{\text{in}} > T_{\text{out}}$, the earth radiates the amount of entropy ΔS_e into the universe. More precisely, during one second, the surface of earth gets the heat energy $\Delta Q = 10^{17}$ J from the sun. Hence the entropy loss of earth during one second is equal to

$$\Delta S_e = -4 \cdot 10^{14} \text{ J/K}.$$

This means that one square meter of the surface of earth radiates the entropy of about 1 J/K during one second into the universe. The radiated entropy decreases the disorder on earth, that is, the earth gains order. This is mainly the information stored in living objects. Physicists describe this by saying that energy at a higher temperature has a higher quality than the same amount of energy at a lower temperature.

7.18 Von Neumann Algebras

> In order to deeply understand the mathematical structure of quantum mechanics, John von Neumann studied a special class of operator algebras. Nowadays these algebras are called von Neumann algebras.[171]
> Each von Neumann algebra is a C^*-algebra. But the converse is seldom true.
>
> Folklore

[169] See G. Börner, The Early Universe: Facts and Fiction, Springer, Berlin, 2003.
Ø. Grøn and S. Hervik, Einstein's Theory of General Relativity: with Modern Applications in Cosmology, Springer, New York, 2007.
S. Weinberg, Cosmology, Oxford University Press, 2008.

[170] R. Griffith, Rigorous results and theorems. In: C. Domb and M. Green (Eds.), Phase transitions and critical phenomena, Academic Press, New York, 1970, pp. 9–108.

[171] F. Murray and J. von Neumann, On rings of operators, Ann. Math. **37** (1936), 116–229.
J. von Neumann, On rings of operators: reduction theory, Ann. Math. **50** (1949), 401–485.

> The theory of von Neumann algebras has been growing in leaps and bounds in the last 20 years. It has always had strong connections with ergodic theory and mathematical physics. It is now beginning to make contact with other areas such as differential geometry and K-theory... The book commences with the Murray–von Neumann classification of factors, proceeds through the basic modular theory (the Tomita–Takesaki theory) to the Connes classification of von Neumann algebras of type III_λ, and concludes with a discussion of crossed-products, Krieger's ratio set, examples of factors, and Takesaki's duality theorem.[172]
>
> Viakalathur Sunder, 1987

In what follows, X is a complex separable non-trivial Hilbert space (i.e., $X \neq \{0\}$).

7.18.1 Von Neumann's Bicommutant Theorem

Commutant. Commutation relations play a crucial role in quantum mechanics. In particular, if two observables commute, then it is possible that they have common eigenvectors, that is, they can be sharply measured at the same time. This motivated John von Neumann to investigate commutants of algebras. Consider the C^*-algebra $L(X, X)$ of the linear continuous operators

$$A : X \to X.$$

Let $\mathcal{S}$ be a subset of $L(X, X)$. By definition, the operator $A \in L(X, X)$ belongs to the commutant $\mathcal{S}'$ of the set $\mathcal{S}$ iff

$$AS = SA \qquad \text{for all} \quad S \in \mathcal{S}.$$

Naturally enough, we set $\mathcal{S}'' := (\mathcal{S}')'$ and call this the bicommutant of the set $\mathcal{S}$. Obviously, $\mathcal{S} \subseteq \mathcal{S}''$. Von Neumann studied the special case where $\mathcal{S} = \mathcal{S}''$. A subset $\mathcal{A}$ of $L(X, X)$ is called a $*$-subalgebra iff $A, B \in L(X, X)$ and $\alpha, \beta \in \mathbb{C}$ imply that the operators $\alpha A + \beta B, AB, A^*$ are also contained in $L(X, X)$.

> *By definition, a von Neumann algebra is a $*$-subalgebra $\mathcal{A}$ of $L(X, X)$ with unit element and $\mathcal{A}'' = \mathcal{A}$.*

This definition is purely algebraic. Equivalently, one can characterize von Neumann algebras in topological terms by using weak convergence. Let us discuss this.

Weak operator convergence. Let (A_n) be a sequence of linear operators $A_n : X \to X$ in $L(X, X)$, $n = 1, 2, \ldots$ We write

$$w - \lim_{n\to\infty} A_n = A$$

iff $A \in L(X, X)$ and $\lim_{n\to\infty} \langle\psi|A_n\varphi\rangle = \langle\psi|A\varphi\rangle$ for all $\psi, \varphi \in X$. This is called the weak operator convergence. This corresponds to the convergence of matrix elements. In terms of physics, this guarantees the convergence of expectation values. Generalizing this, let $(A_\nu)_{\nu\in\mathcal{N}}$ be a generalized sequence in $L(X, X)$ with a directed index set $\mathcal{N}$ (see page 240). We write

$$w - \lim_{\nu\to\infty} A_\nu = A \tag{7.305}$$

iff $A \in L(X, X)$ and $\lim_{\nu\to\infty} \langle\psi|A_\nu\varphi\rangle = \langle\psi|A\varphi\rangle$ for all $\psi, \varphi \in X$, in the sense of generalized convergence. In addition, let us introduce the following two notions of convergence.

[172] V. Sunder, An Invitation to von Neumann Algebras, Springer, Berlin, 1987 (reprinted with permission).

- $s - \lim_{\nu\to\infty} A_\nu = A$ iff $\lim_{\nu\to\infty} ||(A - A_\nu)\varphi|| = 0$ for all $\varphi \in X$ (strong operator convergence);
- $u - \lim_{\nu\to\infty} A_\nu = A$ iff $\lim_{\nu\to\infty} ||A_\nu - A|| = 0$ (uniform operator convergence).

Recall that $||A_\nu - A|| = \sup_{||\varphi||\le 1} ||(A_\nu - A)\varphi||$. This justifies the notion of uniform operator convergence.

Semi-norms. A map $p : L \to \mathbb{R}$ on the complex (resp. real) linear space L is called a semi-norm iff for all $A, B \in L$ and all complex (resp. real) numbers α the following hold:

- $p(A) \ge 0$,
- $p(\alpha A) = |\alpha| p(A)$, and
- $p(A + B) \le p(A) + p(B)$.

If, in addition, $p(A) = 0$ implies $A = 0$, then p is a norm.

Topologies on $L(X, X)$. (i) Weak operator topology. For fixed $\psi, \varphi \in X$, define

$$p_{\psi,\varphi}(A) := |\langle\psi|A\varphi\rangle| \qquad \text{for all} \quad A \in L(X, X).$$

This is a semi-norm on $L(X, X)$. A subset $\mathcal{S}$ of $L(X, X)$ is called *weakly open* iff, for each operator $A_0 \in \mathcal{S}$, there exist a finite family $\psi_1, \varphi_1, \ldots, \psi_n, \varphi_n$ of elements in X and a number $\varepsilon > 0$ such that the set

$$\{A \in L(X, X) : \ \ p_{\psi_j,\varphi_j}(A - A_0) < \varepsilon, \ j = 1, \ldots, n\}$$

is contained in $\mathcal{S}$. This generates a topology on $L(X, X)$ called the weak operator topology. A subset of $L(X, X)$ is called weakly closed iff its complement in $L(X, X)$ is weakly open.

A subset $\mathcal{S}$ of $L(X, X)$ is weakly closed iff, for all generalized sequences (A_ν) in $\mathcal{S}$, it follows from $w - \lim_{\nu\to\infty} A_\nu = A$ that $A \in \mathcal{S}$.

(ii) Strong operator topology. Similarly, we obtain the strong operator topology by replacing $p_{\psi,\varphi}$ by the semi-norm $p_\varphi(A) := ||A\varphi||$. A subset $\mathcal{S}$ of $L(X, X)$ is called *strongly open* iff, for each operator $A_0 \in \mathcal{S}$, there exist a finite family $\varphi_1, \ldots, \varphi_n$ of elements in X and a number $\varepsilon > 0$ such that the set

$$\{A \in L(X, X) : \ \ p_{\varphi_j}(A - A_0)\} < \varepsilon, \ j = 1, \ldots, n\}$$

is contained in $\mathcal{S}$. This generates a topology on $L(X, X)$ called the strong operator topology. A subset of $L(X, X)$ is called strongly closed iff its complement in $L(X, X)$ is strongly open.

A subset $\mathcal{S}$ of $L(X, X)$ is strongly closed iff, for all generalized sequences (A_ν) in $\mathcal{S}$, it follows from $s - \lim_{\nu\to\infty} A_\nu = A$ that $A \in \mathcal{S}$.

(iii) Uniform operator topology. This topology is obtained by replacing p_φ by the norm $p(A) := ||A||$. A subset $\mathcal{S}$ of $L(X, X)$ is called *uniformly open* iff, for each operator $A_0 \in \mathcal{S}$, there exists a number $\varepsilon > 0$ such that the set

$$\{A \in L(X, X) : \ \ p(A - A_0) < \varepsilon\}$$

is contained in $\mathcal{S}$. This generates a topology on $L(X, X)$ called the uniform operator topology.[173] A subset of $L(X, X)$ is called uniformly closed iff its complement in $L(X, X)$ is uniformly open.

[173] This topology coincides with the topology induced by the Banach space structure on $L(X, X)$.

A subset $\mathcal{S}$ of $L(X,X)$ is uniformly closed iff, for all classical sequences $(A_n)_{n\in\mathbb{N}}$ in $\mathcal{S}$, it follows from $u-\lim_{n\to\infty} A_n = A$ that $A \in \mathcal{S}$.

The bicommutant theorem. The topological characterization of von Neumann algebras reads as follows.

Theorem 7.69 *Let X be a complex separable non-trivial Hilbert space. For a given $*$-subalgebra $\mathcal{A}$ of $L(X,X)$ with unit element, the following three statements are equivalent:*
(i) *$\mathcal{A}$ is a von Neumann algebra (i.e., $\mathcal{A}'' = \mathcal{A}$).*
(ii) *$\mathcal{A}$ is weakly closed in $L(X,X)$.*
(iii) *$\mathcal{A}$ is strongly closed in $L(X,X)$.*

More general, the following hold: If $\mathcal{A}$ is a $*$-subalgebra of $L(X,X)$ with unit element, then the closure of $\mathcal{A}$ in the weak (resp. strong) topology on $L(X,X)$ coincides with the bicommutant $\mathcal{A}''$.

Corollary 7.70 *A $*$-subalgebra algebra of $L(X,X)$ is a C^*-algebra iff it is uniformly closed in $L(X,X)$.*

Consequently, each von Neumann algebra is a C^*-algebra. But the converse is seldom true. For the proofs, we refer to P. Kadison and J. Ringrose, Fundamentals of the Theory of Operator Algebras, Vol. 1, Academic Press, New York, 1983. Many beautiful applications of von Neumann algebras to harmonic analysis can be found in

K. Maurin, Generalized Eigenfunction Expansions and Unitary Representations of Topological Groups, PWN, Warsaw, 1968.

Examples. Suppose that the operator $A \in L(X,X)$ is self-adjoint (i.e., $A^* = A$). The bicommutant $\mathcal{A}''$ of the one-point set $\mathcal{A} := \{A\}$ is the smallest von Neumann algebra in $L(X,X)$ containing the self-adjoint operator A.

Let $\mathcal{S}$ be a subset of $L(X,X)$ with the property that $A \in \mathcal{S}$ implies $A^* \in \mathcal{S}$. Then:

(i) The commutant $\mathcal{S}'$ is a von Neumann algebra.
(ii) The bicommutant $\mathcal{S}''$ is the smallest von Neumann algebra in $L(X,X)$ containing the set $\mathcal{S}$.
(iii) $\mathcal{S}' = \mathcal{S}'''$.

By induction, this implies $\mathcal{S}' = \mathcal{S}^{2n+1}$ and $\mathcal{S}'' = \mathcal{S}^{2n+2}$ for all $n = 1, 2, \ldots$ That is, all of the higher commutants are determined by $\mathcal{S}'$ and $\mathcal{S}''$.

A von Neumann algebra is called a factor iff its center $\mathcal{A} \cap \mathcal{A}'$ is trivial (i.e., it consists of the multiples of the unit operator, $\mathcal{A} \cap \mathcal{A}' = \{\alpha I : \alpha \in \mathbb{C}\}$).

The classification problem for von Neumann algebras. By von Neumann's spectral theory, a self-adjoint operator $A \in L(X,X)$ on the Hilbert space X can be represented by orthogonal projection operators E_λ ($\lambda \in \mathbb{R}$) called the spectral family of A. Now we consider the following generalization:

- self-adjoint operator $\Rightarrow$ von Neumann algebra,
- spectral family $\Rightarrow$ factors.

The building blocks of factors are orthogonal projections.

In contrast to general C^*-algebras, von Neumann algebras possess a rich structure of orthogonal projections.

Since orthogonal projections are observables corresponding to "questions," von Neumann algebras represent a nice tool for describing physical processes in quantum theory. Murray and von Neumann showed that each von Neumann algebra can be represented as a direct sum (or, more general, as a direct integral) of factors. Therefore it remains to classify the factors.[174]

7.18.2 The Murray–von Neumann Classification of Factors

Let X be a complex separable non-trivial Hilbert space, and let the subset $\mathcal{A}$ of $L(X, X)$ be a von Neumann algebra which is a factor. The factor $\mathcal{A}$ is said to be of type I, II, III iff it satisfies the following conditions, respectively:

Type I: $\mathcal{A}$ contains a minimal projection.
Type II: $\mathcal{A}$ contains no minimal projection, but does contain a non-zero projection.
Type III: $\mathcal{A}$ contains no non-zero finite projection.

Here, we use the following terminology. Let $\mathcal{P}(\mathcal{A})$ be the set of all orthogonal projections $P \in \mathcal{A}$. For $P, Q \in \mathcal{A}$, we write $Q \sim P$ iff there exists an operator $U \in \mathcal{A}$ such that $Q = UU^*$ and $P = U^*U$. This is an equivalence relation on $\mathcal{P}(\mathcal{A})$.

- The orthogonal projection P is called finite iff it follows from $Q(X) \subseteq P(X)$ and $Q \sim P$ that $Q = P$.
- The orthogonal projection P is called minimal iff the following three conditions are satisfied:
  (α) $P \neq 0$.
  (β) $P(X)$ is invariant under $\mathcal{A}'$.
  (γ) If a linear subspace Y of $P(X)$ is invariant under $\mathcal{A}'$, then Y is trivial (i.e., $Y = \{0\}$ or $Y = P(X)$).
  Minimal projections are always finite (and non-zero).

For example, if $\mathcal{A} = L(X, X)$, then P is finite iff the projection space $P(X)$ is finite-dimensional. Moreover, precisely the orthogonal projections onto one-dimensional linear subspaces are minimal.

The generalized dimension function of factors. For each factor $\mathcal{A}$, there exists a function $d : \mathcal{P}(\mathcal{A}) \to [0, \infty]$ which has the following properties:

(i) $Q \sim P$ iff $d(Q) = d(P)$.
(ii) If $P(X)$ is orthogonal to $Q(X)$, then $d(P + Q) = d(P) + d(Q)$.
(iii) P is finite iff $d(P) < \infty$, and $d(P) = 0$ iff $P = 0$.

The function d is uniquely determined, up to a positive multiplicative constant. For a suitable choice of this constant, the function d has the following range:

Type I_n : $\{0, 1, \ldots, n\}$, where $n = 1, 2, \ldots$ or $n = \infty$.
Type II_1: $[0, 1]$.
Type II_∞: $[0, \infty]$.
Type III: $\{0, \infty\}$.

A factor $\mathcal{A}$ is of type I_n iff $\mathcal{A} = L(X, X)$ where $\dim X = n$. In this simple case, $d(Q) = \dim P(X)$.

[174] Direct integrals of Hilbert spaces generalize direct sums of Hilbert spaces by summing over general index sets with respect to a measure. This will be considered in Vol. IV on quantum mathematics (see also K. Maurin, Generalized Eigenfunction Expansions and Unitary Representations of Topological Groups, PWN, Warsaw, 1968).

7.18.3 The Tomita–Takesaki Theory and KMS-States

> The Tomita–Takesaki theorem is a beautiful example of "prestabilized harmony" between physics and mathematics.[175]
> On the one hand, it is intimately related to the Kubo–Martin–Schwinger (KMS) condition. On the other hand it initiated a significant advance in the classification theory of von Neumann algebras and led to powerful computational techniques.
>
> Rudolph Haag, 1996

KMS-states in thermodynamic equilibrium. The physicists Kubo, Martin and Schwinger discovered in the late 1950s that states of thermodynamic equilibrium can be characterized by special analyticity properties of the Green's function.[176] In 1967 it was shown by Haag, Hugenholtz, and Winnink that this can be formulated in terms of von Neumann algebras. In fact, it turned out that this was closely related to the so-called Tomita–Takesaki theory for von Neumann algebras, which was created by the Japanese mathematician Tomita in the 1960s, by purely mathematical motivation.[177] Roughly speaking, the Tomita–Takesaki theory formulates conditions which guarantee the existence of a dynamics on a von Neumann algebra that can be used in order to describe the dynamics of a physical state in thermodynamic equilibrium.

The basic mathematical idea of the Tomita–Takesaki theory. Let $\mathcal{A}$ be a von Neumann algebra of operators on the complex separable non-trivial Hilbert space X. Suppose that there is a vector ψ_0 in X which has the following two properties:

- ψ_0 is cyclic, that is, the set $\{A\psi_0 : A \in \mathcal{A}\}$ is dense in X.
- ψ_0 is separating, that is, if $A, B \in \mathcal{A}$ and $A \neq B$, then $A\psi_0 \neq B\psi_0$.

Define the operator $\mathsf{S} : \mathrm{dom}(\mathsf{S}) \to X$ by setting[178]

$$\mathsf{S}(A\psi_0) := A^*\psi_0 \qquad \text{for all} \quad A \in \mathcal{A}.$$

Then, the operator S has a closure $\bar{\mathsf{S}}$. By Problem 7.24, there exists the unique polar decomposition

$$\mathsf{S} = J\Delta^{1/2}$$

with the following properties:

- The so-called modular operator $\Delta := \bar{\mathsf{S}}^*\bar{\mathsf{S}}$ is self-adjoint and $\langle\psi|\Delta\psi\rangle \geq 0$ for all $\psi \in \mathrm{dom}(\Delta)$.

---

[175] The term "prestabilized harmony" was introduced by Leibniz (1646–1716) in his philosophy of monads (which are ultimate units of being).
R. Haag, Local Quantum Physics: Fields, Particles, Algebras, Springer, Berlin, 1996 (reprinted with permission).

[176] R. Kubo, Statistical mechanical theory of irreversible processes, J. Math. Soc. Japan **12** (1957), 570–586.
P. Martin and J. Schwinger, Theory of many-particle systems. Phys. Rev. **115** (1959), 1342–1373.

[177] R. Haag, N. Hugenholtz, and M. Winnink, On the equilibrium states in quantum statistical mechanics, Commun. Math. Phys. **5** (1967), 215–236.
M. Takesaki, Tomita's Theory of Modular Hilbert Algebras and Its Applications, Springer, Berlin, 1970.

[178] Since $A^*(\alpha\varphi) = \alpha^\dagger A^*\varphi$ for all complex numbers α, the operator S is antilinear, that is, $\mathsf{A}(\alpha\varphi + \beta\psi) = \alpha^\dagger A + \beta^\dagger B$ for all $\varphi, \psi \in X$ and all $\alpha, \beta \in \mathbb{C}$.

- The so-called modular conjugation operator $J : X \to X$ is antiunitary, and it has the property $J^2 = I$.[179]

For all times $t \in \mathbb{R}$, we have

$$\boxed{\Delta^{it} \mathcal{A} \Delta^{-it} = \mathcal{A},}$$

and $J\mathcal{A}J = \mathcal{A}$.[180] Setting $\mathcal{U}_t(A) := \Delta^{it} \mathcal{A} \Delta^{-it}$ for all $A \in \mathcal{A}$, the map

$$\mathcal{U}_t : \mathcal{A} \to \mathcal{A}$$

is a C^*-automorphism of the von Neumann algebra $\mathcal{A}$, and the family $\{\mathcal{U}_t\}_{t \in \mathbb{R}}$ forms a one-parameter group of C^*-automorphisms on $\mathcal{A}$ (see page 634). These C^*-automorphisms are called modular automorphisms.

For the general mathematical theory of von Neumann algebras together with numerous applications to quantum physics, see the hints for further reading on page 677. We will come back to this in Vol. IV on quantum mathematics.

7.19 Connes' Noncommutative Geometry

> The abstract theory of commutative Banach algebras was initiated by Mazur (1905–1981) in 1936, but it blossomed in the hands of Gelfand (born 1913), who in one brilliant study gave it the final perfect shape. This was the Gelfand theory of maximal ideals, or the Gelfand spectral theory looking at it the other way... The Gelfand spectral theory soon became a powerful tool and a bonanza of new ideas. Gelfand himself, Naimark (1909–1978), and others of his co-workers found a multitude of models and applications.[181]
>
> Krysztof Maurin, 1968

> Noncommutative geometry amounts to a program of unification of mathematics under the aegis of the quantum apparatus, that is, the theory of operators and of C^*-algebras. Largely the creation of a single person, Alain Connes, noncommutative geometry is just coming of age as the new century opens.[182] The bible of the subject is, and will remain, Connes' *Noncommutative Geometry* (1994), itself the "3.8 expansion" of the French *Géométrie non commutative* from 1990. These are extraordinary books, a "tapestry" of physics and mathematics, in the words of Vaughan Jones, and the work of a "poet of modern science," according to Daniel Kastler, replete with subtle knowledge and insights apt to inspire several generations.

[179] That is, for all $\varphi, \psi \in X$ and all complex numbers, we have $\langle J\psi | J\varphi \rangle = \langle \psi | \varphi \rangle^\dagger$, and the operator J is antilinear.

[180] By definition, $B\mathcal{A}C := \{BAC : A \in \mathcal{A}.\}$.

[181] K. Maurin, Generalized Eigenfunction Expansions and Unitary Representations of Topological Groups, Polish Scientific Publishers, Warsaw, 1968 (reprinted with permission). See also the footnote on page 628.

[182] Alain Connes (born 1947) works at the *Collège de France*, Paris, and at the *l'Institut des Hautes Études Scientifiques* (IHES) (Institute of Advanced Scientific Studies), Bures-sur-Yvette (near Paris). For his contributions to the theory of von Neumann algebras of type III, Connes was awarded the Fields medal in 1983. See A. Connes, Une classification des facteurs de type III, Ann. Scient. École Norm. Sup. **6** (1973), 133–252 (in French).

> Despite an explosion of research by some of the world's leading mathematicians, and a bouquet of applications – to the reinterpretation of the phenomenological Standard Model of particle physics as a new space-time geometry, the quantum Hall effect, strings, renormalization and more in quantum field theory – the six years that have elapsed since the publication of *Noncommutative Geometry* have seen no sizeable book returning to the subject. This volume aspires to fit snugly in that gap, but does not pretend to fill it. It is rather meant to be an introduction to some of the core topics of *Noncommutative Geometry.*[183]
>
> José Gracia-Bondia, Joseph Várilly, and Héctor Figueroa, 2001

If M is a nonempty compact separated topological space (e.g., a bounded closed subset of $\mathbb{R}^n$), then the C^*-algebra $C(M)$ knows a lot about the geometry of M. For example, for a given point P, the set $\mathcal{J}_P$ of all continuous functions

$$f : M \to \mathbb{C}$$

with $f(P) = 0$ forms a maximal C^*-ideal of $C(M)$.[184] Conversely, each maximal C^*-ideal of $C(M)$ can be obtained this way. Thus,

$$P \mapsto \mathcal{J}_P$$

is a bijective map between the space M and the set of maximal ideals of the function algebra $C(M)$. Furthermore, the Gelfand–Naimark structure theorem tells us that, for each commutative C^*-algebra $\mathcal{A}$, we have the C^*-isomorphism

$$\mathcal{A} \simeq C(M)$$

where M is the set of maximal C^*-ideals of $\mathcal{A}$.

> *The basic idea of Connes' noncommutative geometry is to replace commutative C^*-algebras by noncommutative C^*-algebras.*

In this setting, properties of noncommutative geometry are identified with properties of noncommutative C^*-algebras. This identification is motivated by the corresponding identification between classical geometric properties and properties of commutative C^*-algebras. From the physical point of view, the idea is that states and observables are primary, but space and time are secondary. For example, physicists assume that space and time did not exist shortly after the Big Bang of our universe, but only physical states existed. The familiar structure of our space-time was only created later on by a stochastic process. Furthermore, below the Planck length it is assumed that space and time loose their classical properties in the setting of quantum gravity. Therefore, noncommutative geometry is one of the candidates for creating a mathematical theory of quantum gravity. Noncommutative geometry is based on so-called spectral triplets for elliptic Dirac operators. As an introduction to noncommutative geometry, we recommend:

> J. Várilly, Lectures on Noncommutative Geometry, European Mathematical Society 2006.
>
> M. Paschke, An essay on the spectral action principle and its relation to quantum gravity, pp. 127–150. In: B. Fauser, J. Tolksdorf, and E. Zeidler (Eds.), Quantum Gravity: Mathematical Models and Experimental Bounds, Birkhäuser, Basel, 2006.

[183] J. Gracia-Bondia, J. Várilly, and H. Figueroa, Elements of Noncommutative Geometry, Birkhäuser, Boston, 2001 (reprinted with permission).

[184] This means that the C^*-ideal $\mathcal{J}_P$ cannot be extended to a larger C^*-ideal of $C(M)$ which is different from the trivial ideal $C(M)$.

We also refer to the comprehensive monograph:

M. Gracia-Bondia, J. Várilly, and H. Figueroa, Elements of Noncommutative Geometry, Birkhäuser, Boston, 2001.

A detailed study of the applications of noncommutative geometry to the Standard Model in particle physics can be found in the comprehensive monograph:

A. Connes and M. Marcolli, Noncommutative Geometry, Quantum Fields, and Motives, Amer. Math. Soc., Rhode Island, 2008.
Internet: `http://www.math.fsu.edu/~marcolli/bookjune4.pdf`

In the 1930s, John von Neumann discovered that operator algebras play a fundamental role in the mathematical formulation of quantum mechanics. Noncommutative geometry stands in this tradition and allows us to approach the Standard Model in elementary particle physics.

In 2006 the first volume of the *Journal of Noncommutative Geometry* appeared. The editor-in-chief is Alain Connes. The following list of topics covered by the journal shows the scope of modern noncommutative geometry:

- operator algebras,
- Hochschild and cyclic cohomology,
- K-theory and index theory,
- measure theory and topology of noncommutative spaces,
- spectral geometry of noncommutative spaces,
- noncommutative algebraic geometry,
- Hopf algebras and quantum groups,
- foliations, gruppoids, stacks, gerbes,
- deformations and quantizations,
- noncommutative spaces in number theory and arithmetic geometry,
- noncommutative geometry in physics: quantum field theory, renormalization, gauge theory, string theory, gravity, mirror symmetry, solid state physics, statistical mechanics.

7.20 Jordan Algebras

Let $\mathcal{O}(X)$ denote the set of all observables in $L(X, X)$ (i.e., the set of all linear continuous self-adjoint operators $A : X \to X$), where X is a complex Hilbert space. If $A, B \in \mathcal{O}(X)$, then the usual operator product AB is contained in $\mathcal{O}(X)$ iff $AB = BA$. This follows from

$$(AB)^* = B^*A^* = BA.$$

Thus, as a rule, $\mathcal{O}(X)$ is not an algebra with respect to the operator product. In order to cure this defect, Pascal Jordan (1902–1980) introduced the product

$$A \circ B := \tfrac{1}{2}(AB + BA).$$

Then the set $\mathcal{O}(X)$ becomes a real algebra with respect to the real linear combinations $\alpha A + \beta B$ and the Jordan product $A \circ B$. This commutative algebra of observables is called the real Jordan algebra of the Hilbert space X. As a rule, Jordan algebras are not associative.[185] The theory of Jordan algebras is a branch

[185] P. Jordan, On the multiplication of quantum-mechanical quantities I, II, Z. Phys. **80** (1933), 285–291; **87** (1934), 505–512 (in German).
P. Jordan, J. von Neumann, and N. Wigner, On an algebraic generalization of the quantum mechanical formalism, Ann. Math. **35** (1934), 29–64.

of modern mathematics.[186] In 1994, Zelmanov was awarded the Fields medal for his contributions to Jordan algebras.

7.21 The Supersymmetric Harmonic Oscillator

> The foundations of the theory of commuting and anticommuting variables were laid by Schwinger in 1953, who presented the analysis for commuting and anticommuting variables on the physical level of strictness[187]...
> The first mathematical formalism that made it possible to operate with commuting and anticommuting coordinates was Martin's algebraic formalism proposed in 1959[188]...
> In 1974, Salam and Strathdee proposed a very apt name for a set of superpoints.[189] After this work and the work by Wess and Zumino[190] were published, the superspace became a foundation for the most important physical theories.[191]
>
> Andrei Khrennikov, 1997

> In contrast to Heisenberg's harmonic quantum oscillator, the ground state energy of the supersymmetric harmonic oscillator is equal to zero.
>
> The golden rule of supersymmetry

> Supersymmetry is a relativistic symmetry between bosons and fermions. This is the only known way available at the present to unify the four-dimensional space-time and internal symmetries of the S-matrix in relativistic particle theory. [192]
>
> Prem Srivasta, 1985

Supersymmetry describes bosons and fermions in a unified way. Recall that the bosonic harmonic oscillator has the energy values

[186] H. Upmeier, Jordan Algebras in Analysis, Operator Theory, and Quantum Mechanics, Amer. Math. Soc., Rhode Island, 1987.
T. Springer and F. Veldkamp, Octonions, Jordan Algebras, and Exceptional Groups, Springer, Berlin, 2000.
K. McCrimmon, A Taste of Jordan Algebras, Springer, New York, 2004.

[187] J. Schwinger, Note on the quantum dynamical principle, Phil. Mag. **44** (1953), 1171–1193.

[188] J. Martin, Generalized classical analysis and "classical" analogue of a Fermi oscillator, Proc. Royal Soc. **A251** (1959), 536–542; The Feynman principle for a Fermi system, Proc. Royal Soc. **A251** (1959), 543–549.

[189] A. Salam and J. Strathdee, Supergauge transformations, Nucl. Phys. **B76** (1974), 477–483; Feynman rules for superfields, Nucl. Phys. **B86** (1975), 142–152.

[190] J. Wess and B. Zumino, Supergauge transformations in four dimensions, Nucl. Phys. **B70** (1974), 39–50.

[191] A. Khrennikov, Superanalysis, Kluwer, Dordrecht, 1997 (reprinted with permission).

[192] R. Haag, J. Lopuszanski, and M. Sohnius, All possible generators of supersymmetries of the S-matrix, Nucl. Phys. **B88** (1975), 257–274.
The supersymmetric Standard Model in particle physics is studied in S. Weinberg, Quantum Field Theory, Vol. 3, Cambridge University Press, 1995.
P. Srivasta, Supersymmetry, Superfields and Supergravity, Adam Hilger, Bristol, 1985.

$$E_n = \hbar\omega(n + \tfrac{1}{2}), \qquad n = 0, 1, 2, \ldots \tag{7.306}$$

As we will show below, the energy levels of the supersymmetric harmonic oscillator are given by

$$\boxed{E_{n_b,n_f} = \hbar\omega(n_b + n_f), \qquad n_b = 0, 1, 2, \ldots,\ n_f = 0, 1.}$$

In terms of physics, this is the energy of n_b bosons and n_f fermions. The point is that an infinite number of bosonic harmonic oscillators has the ground state energy

$$\sum_{k=0}^{\infty} \tfrac{1}{2}\hbar\omega = +\infty.$$

This causes the main trouble in quantum field theory. In contrast to this pathological situation, the ground state energy of an arbitrary number of supersymmetric harmonic oscillators is equal to zero, since $E_{0,0} = 0$.

A supersymmetric harmonic oscillator is the superposition of a bosonic harmonic oscillator and a fermionic harmonic oscillator. The nonzero ground state energies of the two harmonic oscillators compensate each other.

Because of the Pauli principle, it is not possible that two fermions are in the same energy state of a harmonic oscillator. This motivates why the number n_f of fermions in an energy eigenstate only attains the values $n_f = 0, 1$.

The supersymmetric Hamiltonian. Let us introduce the following Hamiltonians:

(B) Bosonic Hamiltonian: $H_{\text{bosonic}} := \hbar\omega(a^\dagger a + \frac{1}{2})$.
(F) Fermionic Hamiltonian: $H_{\text{fermionic}} := \hbar\omega(b^\dagger b - \frac{1}{2})$.
(S) Supersymmetric Hamiltonian:

$$\boxed{H_{\text{super}} := \hbar\omega(a^\dagger a \otimes I + I \otimes b^\dagger b).} \tag{7.307}$$

As a rule, physicists briefly write $H_{\text{super}} = \hbar\omega(a^\dagger a + b^\dagger b)$.

Hilbert spaces. The bosonic Hamiltonian acts on the so-called bosonic Hilbert space $X_{\text{bosonic}} := L_2(\mathbb{R})$ with the energy eigenstates

$$H_{\text{bosonic}}|n_b\rangle = E_{n_b}|n_b\rangle, \qquad n_b = 0, 1, 2, \ldots$$

where $E_{n_b} := \hbar\omega(n_b + \frac{1}{2})$. The bosonic eigenstates

$$|n_b\rangle, \qquad n_b = 0, 1, 2, \ldots$$

form a complete orthonormal system on the Hilbert space X_{bosonic}. In terms of physics, the state $|n_b\rangle$ describes n_b bosons.

The fermionic Hamiltonian acts on the Hilbert space $X_{\text{fermionic}} := \mathbb{C}^2$ with the energy eigenstates

$$H_{\text{fermionic}}|n_f\rangle = \mathcal{E}_{n_f}|n_f\rangle, \qquad n_f = 0, 1$$

where $\mathcal{E}_{n_f} := \hbar\omega(n_f - \frac{1}{2})$. The explicit form of the states $|0\rangle$ and $|1\rangle$ will be given below. The state $|n_f\rangle$ corresponds to n_f fermions.

Bosonic-fermionic states. Let us now introduce the Hilbert space

$$X_{\text{super}} := X_{\text{bosonic}} \otimes X_{\text{fermionic}}.$$

The states

$$|n_b\rangle \otimes |n_f\rangle, \qquad n_b = 0, 1, 2, \ldots, \quad n_f = 0, 1$$

form a complete orthonormal system of X_{super}. In terms of physics, the state $|n_b\rangle \otimes |n_f\rangle$ corresponds to n_b bosons and n_f fermions.[193] For the supersymmetric Hamiltonian, we get

$$H_{\text{super}} = H_{\text{bosonic}} \otimes H_{\text{fermionic}}.$$

This operator acts on the Hilbert space X_{super}. Explicitly,

$$H_{\text{super}}(|n_b\rangle \otimes |n_f\rangle) = H_{\text{bosonic}}|n_b\rangle \otimes |n_f\rangle + |n_b\rangle \otimes H_{\text{fermionic}}|n_f\rangle.$$

Hence

$$H_{\text{super}}(|n_b\rangle \otimes |n_f\rangle) = E_{n_b,n_f}(|n_b\rangle \otimes |n_f\rangle)$$

along with the energies

$$\boxed{E_{n_b,n_f} := \hbar\omega(n_b + n_f)}$$

where $n_b = 0, 1, 2, \ldots$ and $n_f = 0, 1$. This implies that the ground state $|0\rangle \otimes |0\rangle$ of the supersymmetric harmonic oscillator has zero energy, that is,

$$H_{\text{super}}(|0\rangle \otimes |0\rangle) = 0.$$

Bosonic creation and annihilation operators. Set $a^- := a$ and $a^+ := a^\dagger$. For the bosonic annihilation operator a^- and the bosonic creation operator a^+, we have[194]

$$[a^-, a^+]_- = I, \qquad [a^-, a^-]_- = [a^+, a^+]_- = 0.$$

Furthermore, by Sect. 7.2 on page 432, for $n = 0, 1, 2, \ldots$ we have

$$a^-|n+1\rangle = \sqrt{n+1}\ |n\rangle, \qquad a^+|n\rangle = \sqrt{n+1}\ |n+1\rangle.$$

Fermionic creation and annihilation operators. For the fermionic annihilation operator b^- and the fermionic creation operator b^+, we get

$$[b^-, b^+]_+ = I, \qquad [b^-, b^-]_+ = [b^+, b^+]_+ = 0.$$

In particular, $(b^+)^2 = (b^-)^2 = 0$. Furthermore,

$$b^-|0\rangle = 0, \quad b^-|1\rangle = |0\rangle, \quad b^+|0\rangle = |1\rangle, \quad b^+|1\rangle = 0.$$

Explicitly, we set

$$|0\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The states $|0\rangle$ and $|1\rangle$ form a complete orthonormal system of the Hilbert space $X_{\text{fermionic}}$. That is, each element $\chi \in X_{\text{fermionic}}$ can be uniquely represented as

$$\chi = \alpha|0\rangle + \beta|1\rangle, \qquad \alpha, \beta \in \mathbb{C}.$$

[193] Physicists briefly write $|n_b\rangle|n_f\rangle$.
[194] Recall that $[A, B]_\pm := AB \pm BA$.

In the language of matrices, $\chi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$. Moreover, we define

$$b^- := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad b^+ := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad N := b^+ b^- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Since $N|0\rangle = 0$ and $N|1\rangle = |1\rangle$, the operator N is called the fermionic particle number operator. Obviously, b^+ is the adjoint matrix to b^-, i.e., $b^+ = (b^-)^\dagger$.

Supersymmetric creation and annihilation operators. We want to write the supersymmetric Hamiltonian in the form

$$\boxed{H_{\text{super}} = \hbar\omega(Q^+Q^- + Q^-Q^+).} \tag{7.308}$$

To this end, we introduce the operators

$$Q^+ := a^- \otimes b^+, \qquad Q^- := a^+ \otimes b^-$$

called the supersymmetric creation operator Q^+ and the supersymmetric annihilation operator Q^-. Explicitly,

$$Q^+(|n_b\rangle \otimes |n_f\rangle) = a^-|n_b\rangle \otimes b^+|n_f\rangle$$

and

$$Q^-(|n_b\rangle \otimes |n_f\rangle) = a^+|n_b\rangle \otimes b^-|n_f\rangle.$$

For example,

$$Q^+(|1\rangle \otimes |0\rangle) = |0\rangle \otimes |1\rangle, \qquad Q^-(|0\rangle \otimes |1\rangle) = |1\rangle \otimes |0\rangle.$$

Thus, the operator Q^+ sends one boson to one fermion (resp. the operator Q^- sends one fermion to one boson). We have

$$\boxed{[Q^+, Q^+]_+ = [Q^-, Q^-]_+ = 0.}$$

This is equivalent to $(Q^+)^2 = (Q^-)^2 = 0$. In fact,

$$Q^+Q^+ = (a^- \otimes b^+)(a^- \otimes b^+) = a^-a^- \otimes b^+b^+ = 0,$$

since $(b^+)^2 = 0$. Similarly, we get $(Q^-)^2 = 0$.

Let us now prove (7.308). It follows from

$$Q^+Q^- = (a^- \otimes b^+)(a^+ \otimes b^-) = a^-a^+ \otimes b^+b^-$$

together with $a^-a^+ = I + a^+a^-$ that

$$Q^+Q^- = (I + a^+a^-) \otimes b^+b^-.$$

Similarly,

$$Q^-Q^+ = (a^+ \otimes b^-)(a^- \otimes b^+) = a^+a^- \otimes b^-b^+ = a^+a^- \otimes (I - b^+b^-).$$

Therefore,

$$Q^+Q^- + Q^-Q^+ = I \otimes b^+b^- + a^+a^- \otimes I.$$

This yields (7.307), (7.308).

Supersymmetric invariance of the supersymmetric Hamiltonian. We claim that

$$\boxed{[H_{\text{super}}, Q^+]_- = [H_{\text{super}}, Q^-]_- = 0.}$$

To prove this, observe that $Q^+Q^+ = 0$. Hence

$$(Q^+Q^- + Q^-Q^+)Q^+ - Q^+(Q^+Q^- + Q^-Q^+) = Q^+Q^-Q^+ - Q^+Q^-Q^+ = 0.$$

This implies $[H_{\text{super}}, Q^+]_- = 0$. Similarly, $[H_{\text{super}}, Q^-]_- = 0$.

Perspective. Supersymmetry plays an important role in modern quantum field theory. We will come back to this in later volumes. There exists a huge amount of literature on supersymmetric models in quantum theory. Some hints for further reading can be found on page 679.

7.22 Hints for Further Reading

Textbooks on Quantum Mechanics

We refer to the following classic textbooks which use the language of physicists:

P. Dirac, The Principles of Quantum Mechanics, Clarendon Press, Oxford, 1930.

V. Fock, Fundamentals of Quantum Mechanics, Nauka, Moscow, 1931 (in Russian). (English edition: Mir, Moscow, 1978.)

R. Feynman, R. Leighton, and M. Sands, The Feynman Lectures in Physics, Addison-Wesley, Reading, Massachusetts, 1963.

L. Landau and E. Lifschitz, Course of Theoretical Physics, Vol. 3: Non-Relativistic Quantum Mechanics, Butterworth-Heinemann, Oxford, 1982.

J. Schwinger, Quantum Mechanics, Springer, New York, 2001.

F. Dyson, Advanced Quantum Mechanics, Dyson's 1951 Cornell Lecture Notes on Quantum Electrodynamics, Cornell University, Ithaca, New York. World Scientific, Singapore, 2007.

Much material can be found in the following handbooks:

G. Drake (Ed.), Springer Handbook of Atomic, Molecular, and Optical Physics, Springer, Berlin, 2005.

Encyclopedia of Mathematical Physics, Vols. 1–5. Edited by J. Françoise, G. Naber, and T. Tsun, Elsevier, Amsterdam, 2006.

Modern Encyclopedia of Mathematical Physics, Vols. 1, 2. Edited by I. Araf'eva and D. Sternheimer, Springer, Berlin, 2009 (to appear).

Furthermore, we recommend:

A. Messiah, Quantum Mechanics, Vols. 1, 2, North-Holland, Amsterdam, 1961.

J. Sakurai, Advanced Quantum Mechanics, Reading, Massachusetts, 1967.

L. Schiff, Quantum Mechanics, McGraw-Hill, New York, 1968.

M. Mizushima, Quantum Mechanics of Atomic Spectra and Atomic Structure, Benjamin, New York, 1970.

A. Galindo and P. Pascual, Quantum Mechanics, Vols. 1, 2, Springer, Berlin, 1990.

A. Bohm, Quantum Mechanics: Foundations and Applications, Springer, Berlin, 1994.

J. Sakurai and San Fu Tuan, Modern Quantum Mechanics, Benjamin and Cummings, New York, 1994.

E. Merzbacher, Quantum Mechanics, Wiley, New York, 1998.

J. Basdevant and J. Dalibard, Quantum Mechanics, Springer, Berlin, 2002.

F. Schwabl, Quantum Mechanics, Springer, Berlin, 2002.

F. Schwabl, Advanced Quantum Mechanics, Springer, Berlin, 2003.

N. Straumann, A Basic Course on Non-relativistic Quantum Mechanics, Springer, Berlin, 2002 (in German).

K. Gottfried and Tung-Mow Yan, Quantum Mechanics: Fundamentals, Springer, New York, 2003.

F. Scheck, Quantum Physics, Springer, Berlin, 2007.

Exercises can be found in:

S. Flügge, Practical Quantum Mechanics, Vols. 1, 2, Springer, Berlin, 1979.

J. Basdevant, The Quantum-Mechanics Solver: How to Apply Quantum Theory to Modern Physics, Springer, Berlin, 2000.

V. Radanovic, Problem Book in Quantum Field Theory, Springer, New York, 2006.

Visualizations of solutions in quantum mechanics are represented in:

S. Brandt and H. Dahmen, The Picture Book of Quantum Mechanics, Springer, New York, 1995.

B. Thaller, Visual Quantum Mechanics, Springer, New York, 2000.

B. Thaller, Advanced Visual Quantum Mechanics, Springer, New York, 2005.

Mathematical Methods in Quantum Mechanics

The classic monograph was written by

J. von Neumann, Mathematical Foundations of Quantum Mechanics (in German), Springer, Berlin, 1932. (English edition: Princeton University Press, 1955.)

Furthermore, we recommend:

M. Reed and B. Simon, Methods of Modern Mathematical Physics, Vols. 1–4, Academic Press, New York, 1972ff.

M. Schechter, Operator Methods in Quantum Mechanics, North-Holland, Amsterdam, 1982.

H. Triebel, Higher Analysis, Barth, Leipzig, 1989.

F. Berezin and M. Shubin, The Schrödinger Equation, Kluwer, Dordrecht, 1991.

E. Zeidler, Applied Functional Analysis: Applications to Mathematical Physics, Springer, New York, 1995.

W. Steeb, Hilbert Spaces, Wavelets, Generalized Functions and Modern Quantum Mechanics, Kluwer, Dordrecht, 1998.

W. Thirring, Quantum Mathematical Physics: Atoms, Molecules, and Large Systems, Springer, New York, 2002.

S. Gustafson and I. Sigal, Mathematical Concepts of Quantum Mechanics, Springer, Berlin, 2003.

A. Komech, Lectures on Quantum Mechanics (nonlinear PDE point of view), Lecture Notes No. 25 of the Max Planck Institute for Mathematics in the Sciences, Leipzig. Internet: `http://mis.mpg.de/preprints/ln/`

F. Strocchi, An Introduction to the Mathematical Structure of Quantum Mechanics: A Short Course for Mathematicians, Lecture Notes, Scuola Normale Superiore, Pisa (Italy), World Scientific, Singapore, 2005.

V. Varadarajan, Geometry of Quantum Theory, Springer, New York, 2007.

For the applications of Lie group theory to the spectra of atoms and molecules, we refer to the following classic monographs:

H. Weyl, The Theory of Groups and Quantum Mechanics, Springer, Berlin, 1929 (in German). (English edition: Dover, New York, 1931.)

B. van der Waerden, Group Theory and Quantum Mechanics, Springer, Berlin, 1932 (in German). (English edition: Springer, New York, 1974.)

See also the hints for further reading on axiomatic quantum field theory given on page 454. We also refer to a series of fundamental papers on the mathematical foundations of quantum mechanics and statistical physics written by

E. Lieb, The Stability of Matter: From Atoms to Stars, Selecta of Elliott Lieb. Edited by W. Thirring, Springer, New York, 2002.

E. Lieb, Inequalities: Selecta of Elliott Lieb. Edited by M. Loss, Springer, New York, 2002.

The Path Integral

It is crucial that there exist specific methods for the explicit computation of path integrals. This way, it is possible to obtain all of the explicitly known propagator kernels in quantum mechanics. We especially recommend

C. Grosche and F. Steiner, Handbook of Feynman Path Integrals, Springer, Berlin, 1998.

This comprehensive handbook contains a large list of known path integrals (200 pages), about 1000 references, and a detailed discussion of the historical background. Much material about the computation of path integrals can also be found in:

D. Khandekar, S. Lawande, and K. Bhagwat, Path-Integral Methods and their Applications, World Scientific, Singapore, 1993.

H. Kleinert, Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics, World Scientific, River Edge, New York, 2004.

W. Dittrich and M. Reutter, Classical and Quantum Dynamics, Springer, Berlin, 1999.

M. Chaichian and A. Demichev, Path Integrals in Physics. Vol. 1: Stochastic Processes and Quantum Mechanics; Vol. 2: Quantum Field Theory, Statistical Physics, and other Modern Applications, Institute of Physics Publishing, Bristol, 2001.

For the language used in physics, we recommend:

R. Feynman and R. Hibbs, Quantum Mechanics and Path Integrals, McGraw-Hill, New York, 1965.

R. Feynman, Statistical Mechanics: A Set of Lectures, 14th edn., Addison Wesley, Reading, Massachusetts, 1998.

A. Zee, Quantum Field Theory in a Nutshell, Princeton University Press, 2003.

L. Faddeev and A. Slavnov, Gauge Fields, Benjamin, Reading, Massachusetts, 1980.

L. Faddeev, Elementary Introduction to Quantum Field Theory, Vol. 1, pp. 513–552. In: P. Deligne et al. (Eds.), Lectures on Quantum Field Theory, Vols. 1, 2, Amer. Math. Soc., Providence, Rhode Island, 1999.

M. Masujima, Path Integral Quantization and Stochastic Quantization, Springer, Berlin, 2000.

M. Marinov, Path integrals in quantum theory: an outlook of basic concepts, Phys. Rep. **60** (1) (1980), 1–57.

L. Schulman, Techniques and Applications of Path Integrals, Wiley, New York, 1981.

G. Roepstorff, Path Integral Approach to Quantum Physics, Springer-Verlag, New York, 1996.

J. Zinn-Justin, Quantum Field Theory and Critical Phenomena, 4th edn., Clarendon Press, Oxford, 2003 (extensive presentation of about 1000 pages based on the path-integral technique).

K. Fujikawa and H. Suzuki, Path Integrals and Quantum Anomalies, Oxford University Press, Oxford 2004.

For the language used in mathematics, we recommend:

B. Simon, Functional Integration and Quantum Physics, Academic Press, New York, 1979.

J. Glimm and A. Jaffe, Mathematical Methods of Quantum Physics: A Functional Integral Point of View, Springer, New York, 1981.

G. Johnson and M. Lapidus, M., The Feynman Integral and Feynman's Operational Calculus, Clarendon Press, Oxford, 2000.

S. Albeverio, R. Høegh-Krohn, and S. Mazzucchi, Mathematical Theory of the Feynman Path Integral: An Introduction, Springer, Berlin, 2006.

P. Cartier and C. DeWitt-Morette, Functional Integration: Action and Symmetries, Cambridge University Press, 2006

M. Freidlin, Functional Integration and Partial Differential Equations, Princeton University Press, 1985

together with

M. Kac, Wiener and integration in function spaces, Bull. Amer. Math. Soc. **72** (1966), 52–68.

I. Daubechies and J. Klauder, Constructing measures for path integrals, J. Math. Phys. **23** (1982), 1806–1822.

I. Daubechies and J. Klauder, Quantum-mechanical path integrals with Wiener measure for all polynomial Hamiltonians, Math. Phys. **26** (1985), 2239–2256.

J. Klauder, Beyond Conventional Quantization, Cambridge University Press, 2000.

For the application of spectral methods in physics, we refer to:

K. Kirsten, Spectral Functions in Mathematics and Physics, Chapman, Boca Raton, Florida, 2002

together with

E. Elizalde, Ten Physical Applications of Spectral Zeta Functions, Springer, Berlin, 1995.

A. Bytsenko, G. Cognola, E. Elizalde, V. Moretti, and S. Zerbini, Analytic Aspects of Quantum Fields, World Scientific, Singapore, 2003.

D. Vassilievich, Heat Kernel Expansion: Users' Manual, Physics Reports **388** (2003), 279-360.

In terms of mathematics, we recommend:

H. Edwards, Riemann's Zeta Function, Academic Press, New York, 1974.

P. Gilkey, Invariance Theory, the Heat Equation, and the Atiyah–Singer Index Theorem, CRC Press, Boca Raton, Florida, 1995.

P. Gilkey, P., Asymptotic Formulae in Spectral Geometry, Chapman, CRC Press, Boca Raton, Florida, 2003.

P. Gilkey, The spectral geometry of Dirac and Laplace type, pp. 289–326. In: Handbook of Global Analysis. Edited by D. Krupka and D. Saunders, Elsevier, Amsterdam, 2008.

Brownian Motion and the Wiener Integral

As an introduction, we recommend:

M. Mazo, Brownian Motion: Fluctuations, Dynamics, and Applications, Oxford University Press, 2002.

Y. Rozanov, Introductory Probability Theory, Prentice-Hall, Englewood Cliffs, New Jersey 1969.

L. Arnold, Stochastic Differential Equations, Krieger, Malabar, Florida, 1992.

L. Evans, An Introduction to Stochastic Differential Equations, Lectures held at the University of California at Berkeley, 2005.
Internet: `http://math.berkeley.edu/∼evans/SDE.course.pdf`

Furthermore, we recommend the following books:

W. Hakenbroch and A. Thalmaier, Stochastische Analysis, Teubner, Stuttgart, 1994 (in German).

B. Øksendal, Stochastic Differential Equations, Springer, Berlin, 2003.

E. Nelson, Dynamical Theories of Brownian Motion, Princeton University Press, Princeton, New Jersey, 1967.

K. Chung and Z. Zhao, From Brownian Motion to Schrödinger's Equation, Springer, New York, 1995.

B. Hughes, Random Walks and Random Environments, Vols. 1, 2, Clarendon Press, Oxford, 1995.

A. Borodin and P. Salminen, Handbook of Brownian Motion: Facts and Formulas, Birkhäuser, Basel, 2002.

P. Del Moral, Feynman–Kac Formulae, Springer, New York, 2004.

The history of the Feynman–Kac formula is described in:

M. Kac, Enigmas of Chance: An Autobiography, Harper & Row, New York, 1985.

We also refer to the following classic survey article:

S. Chandrasekhar, Stochastic problems in physics and astronomy, Rev. Mod. Phys. **15** (1943), 1–89.

The WKB Method

As an introduction to singular perturbation theory, we recommend:

W. Eckhaus, Asymptotic Analysis of Singular Perturbation, North-Holland, Amsterdam, 1979.

J. Kevorkian and J. Cole, Perturbation Methods in Applied Mathematics, Springer, New York, 1981.

A. Nayfeh, Perturbation Methods, Wiley, New York, 1973.

A. Nayfeh and B. Balachandran, Applied Nonlinear Dynamics: Analytical, Computational, and Experimental Methods, Wiley, New York, 1995.

Simple variants of the WKB method can be found in most textbooks on quantum mechanics (see page 667). As an introduction to the relation between classical mechanics and quantum mechanics, we refer to

W. Dittrich and M. Reutter, Classical and Quantum Dynamics, Springer, Berlin, 1999.

This concerns the explicit computation of numerous physical examples related to Schwinger's action principle, the Kolmogorov–Arnold–Moser (KAM) theory, the Maslov index, the Berry phase, and the Feynman path integral. As an introduction to the mathematics of the WKB method, we recommend the monographs by

V. Guillemin and S. Sternberg, Geometric Asymptotics, Amer. Math. Soc., Providence, Rhode Island, 1989.

V. Maslov and M. Fedoryuk, Semiclassical Approximation in Quantum Mechanics, Reidel, Dordrecht, 1981.

B. Helffer, Semiclassical Analysis, World Scientific, Singapore, 2003.

V. Nazaikinskii, B. Schulze, and B. Sternin, Quantization Methods in Differential Equations, Taylor & Francis, London, 2002.

The relation between the path integral and the WKB method is studied in the following monographs:

L. Schulmann, Techniques and Applications of Path Integrals, Wiley, New York, 1981.

C. Grosche and F. Steiner, Handbook of Feynman Path Integrals, Springer, Berlin, 1998.

H. Kleinert, Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics, World Scientific, River Edge, New York, 2004.

The intellectual father of the global WKB method is Victor Maslov (born 1930). We refer to the following monographs:

V. Maslov, Théorie des perturbations et méthodes asymptotiques, Dunod, Paris, 1972 (in French).

J. Leray, Analyse Lagrangien et mécanique quantique: une structure mathématique apparantée aux développements asymtotiques et à l'indice de Maslov, Strasbourgh, France, 1978 (in French). (English edition: MIT Press, Cambridge, Massachusetts, 1981.)

Quantum chaos. Observe that the WKB method can also be applied to quantum chaos. This means that the corresponding classical dynamical system is chaotic. Here, Choquardt's expansion formula and Gutzwiller's trace formula are crucial.[195] This can be found in:

M. Gutzwiller, Chaos in Classical and Quantum Mechanics, Springer, New York, 1990.

C. Grosche and F. Steiner, Handbook of Feynman Path Integrals, Springer, New York, 1998.

Commutation Relations and the Stone–von Neumann Uniqueness Theorem

We recommend:

J. Rosenberg, A selective history of the Stone–von Neumann Theorem, Contemporary Mathematics **365** (2004), 123–158.

S. Summers, On the Stone–von Neumann uniqueness theorem and its ramifications, pp. 135–172. In: M. Rédei and M. Stöltzner (Eds.), John von Neumann and the Foundations of Quantum Physics, Kluwer, Dordrecht, 2000.

C. Putnam, Commutation Properties of Hilbert Space Operators and Related Topics, Springer, Berlin, 1967.

D. Petz, An Invitation to the Algebra of Canonical Commutation Relations, Leuven University Press, Leuven (Belgium), 1990.

V. Guillemin and S. Sternberg, Symplectic Techniques in Physics, Cambridge University Press, 1990.

N. Woodhouse, Geometric Quantization, Oxford University Press, 1997.

F. Berezin, The Method of Second Quantization, Academic Press, New York, 1966. (Second Russian edition: Nauka, Moscow, 1986.)

N. Bogoliubov et al., General Principles of Quantum Field Theory, Kluwer, Dordrecht, 1990.

Yu. Berezansky and V. Kondratiev, Spectral Methods in Infinite-Dimensional Analysis, Vols. 1, 2, Kluwer Dordrecht, 1995.

C. Bratelli and D. Robinson, Operator Algebras and Quantum Statistical Mechanics, Vols. 1, 2, Springer, New York, 2002.

The relations between classical mechanics and geometric quantization are studied in:

[195] P. Choquardt, Semi-classical approach to general forces in the setting of Feynman's path integral, Helv. Phys. Acta **28** (1955), 89–157 (in French).

R. Abraham and J. Marsden, Foundations of Mechanics, Addison-Wesley, Reading, Massachusetts, 1978.

Classical papers on commutation relations for a finite and an infinite number of operators are:

W. Heisenberg, Quantum-theoretical re-interpretation of kinematics and mechanical relations, Z. Physik **33** (1925), 879–893 (in German).[196]

M. Born and P. Jordan, On quantum mechanics, Z. Phys. **35** (1925), 858–888 (in German).

P. Dirac, The fundamental equations of quantum mechanics, Proc. Royal Soc. London Ser. A **109** (1926), no. 752, 642–653.

M. Born, P. Jordan, and W. Heisenberg, On quantum mechanics II, Z. Physik **35** (1926), 557–615 (in German).

W. Pauli, On the hydrogen spectrum from the standpoint of the new quantum mechanics, Z. Phys. **36** (1926), 336–365 (in German).

P. Jordan and E. Wigner, On the Pauli exclusion principle, Z. Phys. **47** (1928), 631–651 (in German).

H. Weyl, Quantum mechanics and group theory, Z. Phys. **46** (1928), 1–47 (in German).

M. Stone, Linear transformations in Hilbert space III, Proc. Nat. Acad. Sci. U.S.A. **16** (1930), 172–175.

J. von Neumann, The uniqueness of the Schrödinger operators, Math. Ann. **104** (1931), 570–578 (in German).

V. Fock, Configuration space and second quantization, Z. Phys. **75** (1932), 622–647 (in German).

H. Groenewold, On the principles of elementary quantum mechanics, Physica **12** (1946), 405–460.

A. Wintner, The unboundedness of quantum-mechanical matrices, Phys. Rev. **71** (2) (1947), 738–739.

H. Wielandt, On the unboundedness of the operators in quantum mechanics, Math. Ann. **121** (1949), 21–23 (in German).

G. Mackey, A theorem of Stone and von Neumann, Duke Math. J. **16** (1949), 313–326.

L. van Hove, Sur certaines representations unitaires d'un groupe infini de transformations. Mem. Acad. Royal Belgium (1951), 61–102.

J. Cook, The mathematics of second quantization, Trans. Amer. Math. Soc. **74** (1953)(2), 222–245.

K. Friedrichs, Mathematical Aspects of the Quantum Theory of Fields, Interscience Publishers, New York, 1953.

L. Gårding and A. Wightman, Representations of the anticommutation relations, Proc. Nat. Acad. Sci. U.S.A. **40** (1954), 617–621.

L. Gårding and A. Wightman, Representations of the commutation relations, Proc. Nat. Acad. Sci. U.S.A. **40** (1954), 622–625.

[196] The English translation of the classical papers by Born, Dirac, Jordan, Heisenberg, and Pauli can be found in B. van der Waerden (Ed.), Sources of Quantum Mechanics (1917–1926), Dover, New York, 1968.

I. Segal, Distributions in Hilbert space and canonical systems of operators, Trans. Amer. Math. Soc. **88** (1958), 12–42.

I. Segal, Quantization of nonlinear systems, J. Math. Phys. **1** (1960), 468–488.

I. Segal, Mathematical Problems of Relativistic Physics, Amer. Math. Soc. Providence, Rhode Island, 1963.

V. Bargmann, On a Hilbert space of analytic functions and an associated integral transform, Commun. Pure and Appl. Math. **14** (1961), 187–214.

G. Mackey, The Mathematical Foundations of Quantum Mechanics, Benjamin, New York, 1963.

A. Weil, Sur certains groupes d'opérateurs unitaires, Acta Math. **111** (1964), 143–211 (in French).

D. Kastler, The C^*-algebras of a free Boson field, Commun. Math. Phys. **1** (1965), 14–48.

G. Mackey, Induced Representations of Groups and Quantum Mechanics, Benjamin, New York, 1968.

M. Rieffel, On the uniqueness of the Heisenberg commutation relations, Duke Math. J. **39** (1972), 745–752.

G. Mackey, Unitary Group Representations in Physics, Probability, and Number Theory, Benjamin, Reading, Massachusetts, 1978.

R. Howe, On the role of the Heisenberg group in harmonic analysis, Bull. Amer. Math. Soc. (N.S.) **3**(2) (1980), 821–843.

H. Grosse and L. Pittner, A supersymmetric generalization of von Neumann's theorem, J. Math. Phys. **29**(1) (1988), 110–118.

G. Mackey, The Scope and History of Commutative and Noncommutative Harmonic Analysis, Amer. Math. Soc., Providence, Rhode Island, 1992.

A generalized version of the Stone–von Neumann uniqueness theorem plays a fundamental role in Ashtekhar's loop gravity (which represents an approach to quantum gravity). We refer to:

C. Fleischhack, Kinematical uniqueness of loop gravity, pp. 203–218. In: B. Fauser, J. Tolksdorf, and E. Zeidler (Eds.), Quantum Gravity, Birkhäuser, Basel, 2006.

Weyl Quantization

As a comprehensive introduction to deformation quantization in mathematics and physics, we recommend the following textbook which is based on the language of modern differential geometry (vector bundles, symplectic geometry, Poisson geometry, pseudo-differential operators):

S. Waldmann, Poisson Geometry and Deformation Quantization, Springer, Berlin, 2007 (in German).

For formal proofs based on the language of physicists, we refer to:

A. Hirshfeld and P. Henselder, Deformation quantization in the teaching of quantum mechanics, Am. J. Phys. **70** (2002), 537–547.

A. Hirshfeld and P. Henselder, Star products and perturbative quantum field theory, Ann. Phys. **298** (2002), 352–393.

F. Berezin and M. Shubin, The Schrödinger Equation, Kluwer, Dordrecht, 1991.

For rigorous proofs based on the language of mathematicians, we refer to:

L. Hörmander, The Weyl calculus of pseudo-differential operators, Commun. Pure Appl. Math. **32** (1979), 359–443.

M. de Gosson, Symplectic Geometry and Quantum Mechanics, Birkhäuser, Basel, 2006.

V. Nazaikinskii, B. Schulze, and B. Sternin, Quantization Methods in Differential Equations, Taylor & Francis, London, 2002.

Kontsevich proved the fundamental result that each Poisson manifold can be equipped with a formal Moyal star product. We refer to:

M. Kontsevich, Deformation quantization of Poisson manifolds, Lett. Math. Phys. **66**(3) (2003), 157–216.

A. Cattaneo and G. Felder, A path integral approach to the Kontsevich quantization formula, Commun. Math. Phys. **212** (2000), 591–611.

Concerning deformation quantization, we recommend the following books:

B. Fedosov, Deformation Quantization and Index Theory, Akademie-Verlag, Berlin, 1996.

A. Perelomov, Generalized Coherent States and Their Applications, Springer, Berlin, 1986.

M. Majid, Foundations of Quantum Group Theory, Cambridge University Press, 1995.

J. Madore, An Introduction to Noncommutative Differential Geometry and Its Applications, Cambridge University Press, 1995.

In addition, we recommend:

S. Podleś and S. Woronowicz, Quantum deformation of Lorentz group, Commun. Math. Phys. **130** (1990), 381–453.

M. Rieffel, Deformation quantization for actions of $\mathbb{R}^d$, Mem. Amer. Math. Soc. **106** (1993).

J. Wess, Gauge theories on noncommutative space-time treated by the Seiberg–Witten method, pp. 179–192. In: U. Carow-Watamura et al. (Eds.), Quantum Field Theory and Noncommutative Geometry, Springer, Berlin, 2005.

H. Grosse and R. Wulkenhaar, Renormalisation of φ^4-theory on noncommutative $\mathbb{R}^4$ in the matrix base, Commun. Math. Phys. **256** (2005), 305–374.

A survey on different quantization methods can be found in:

P. Bandyopadhyay, Geometry, Topology, and Quantization, Kluwer, Dordrecht, 1996.

S. Ali and M. Engliš, Quantization methods: a guide for physicists and analysts, 2004. Internet: `http://arxiv.org/math-ph/0405065`

N. Woodhouse, Geometric Quantization, Oxford University Press, 1997.

We also recommend:

J. Śniatycki, Geometric Quantization and Quantum Mechanics, Springer, New York, 1980.

N. Hurt, Geometric Quantization in Action, Reidel, Dordrecht, 1983.

S. Bates and A. Weinstein, Lectures on the Geometry of Quantization, Amer. Math. Soc., Providence, Rhode Island, 1997.

Furthermore, we refer to the following classic papers:

H. Weyl, The Theory of Groups and Quantum Mechanics, Dover, New York, 1931.

H. Groenewold, On the principles of elementary quantum mechanics, Physica **12** (1946), 405–460.

J. Moyal, Quantum mechanics as a statistical theory, Proc. Cambridge Phil. Soc. **45** (1949), 99–124.

M. Gerstenhaber, On the deformation of rings and algebras, Ann. Math. **79** (1964), 59–103.

F. Bayen, M. Flato, C. Fronsdal, A. Lichnerowicz, and D. Sternheimer, Deformation theory and quantization I, II, Annals of Physics **111** (1978), 61–110; 111–151.

D. Sternheimer, Deformation quantization: twenty years after, pp. 107–145. In: Particles, Fields, and Gravitation, AIP Conf. Proc. vol. 453, American Institute of Physics, Woodbury, 1998.

F. Berezin, General concept of quantization, Commun. Math. Phys. **40** (1975), 153–174.

Statistical Physics

As an introduction to the vast literature on statistical physics, we recommend:

O. Bühler, A Brief Introduction to Classical, Statistical, and Quantum Mechanics, Courant Lecture Notes, Amer. Math. Soc., Providence, Rhode Island, 2006.

K. Huang, Statistical Physics, Wiley, New York, 1987.

R. Feynman, Statistical Mechanics: A Set of Lectures, 14th edn., Addison Wesley, Reading, Massachusetts, 1998.

A. Fetter and J. Walecka, Quantum Theory of Many-Particle Systems, McGraw-Hill, New York, 1971.

G. Mahan, Many-Particle Physics, Plenum Press, New York, 1990.

P. Martin and F. Rothen, Many-Body Problems and Quantum Field Theory, Springer, Berlin, 2002.

For the second law of thermodynamics, we refer to:

E. Lieb and J. Yngvason, A guide to entropy and the second law of thermodynamics, Notices Amer. Math. Soc. **45** (1998), 571–581.

E. Lieb and J. Yngvason, The physics and mathematics of the second law of thermodynamics, Physics Reports **310**(1) (1999), 1–96.

C^*-Algebras and von Neumann Algebras

Much material can be found in:

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M. Majid, Foundations of Quantum Group Theory, Cambridge University Press, 1995.

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H. Kalka and G. Soff, Supersymmetrie, Teubner-Verlag, Stuttgart, 1997 (in German).

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Problems

In the first group of problems we want to show how to apply von Neumann's theory of self-adjoint (and essentially self-adjoint) operators to quantum mechanics. As prototypes, we will study the position operator Q, the momentum operator P, and the Hamiltonian H_{free} of a free quantum particle on the real line in Problems 7.5 and 7.15–7.17. Further typical examples can be found in Problem 7.19. Observe that in Problem 7.5, we will show that

The basic idea behind the notion of self-adjoint operator is the integration-by-parts formula and the extension of the classical derivative for functions to distributions (generalized functions).

The key observation is that the classical integration-by-parts formula for smooth functions with compact support,

$$\boxed{\int_{\mathbb{R}} \psi(x)\varphi'(x)dx = -\int_{\mathbb{R}} \psi'(x)\varphi(x)dx \qquad \text{for all} \quad \varphi, \psi \in \mathcal{D}(\mathbb{R}),} \tag{7.309}$$

remains valid if the derivatives φ', ψ' are to be understood in the sense of tempered distributions and the functions φ, ψ, as well as φ', ψ' are contained in the Hilbert space $L_2(\mathbb{R})$ of square-integrable functions (see Problem 7.3). This can be written as

$$\int_{\mathbb{R}} \psi(x)\varphi'(x)dx = -\int_{\mathbb{R}} \psi'(x)\varphi(x)dx \qquad \text{for all} \quad \varphi, \psi \in W_2^1(\mathbb{R}). \tag{7.310}$$

Let us introduce the two operators $A_{\text{pre}}\varphi := \varphi'$ for all $\varphi \in \mathcal{S}(\mathbb{R})$ and

$$A\varphi := \varphi' \qquad \text{for all} \quad \varphi \in W_2^1(\mathbb{R}).$$

Using the inner product $\langle f|g\rangle := \int_{\mathbb{R}} f(x)^\dagger g(x)dx$ on the Hilbert space $L_2(\mathbb{R})$, we get

$$\langle \psi|A_{\text{pre}}\varphi\rangle = -\langle A\psi|\varphi\rangle \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}),\ \psi \in W_2^1(\mathbb{R}). \tag{7.311}$$

Setting $P_{\text{pre}} := -\mathrm{i}\hbar A_{\text{pre}}$ and $P := -\mathrm{i}\hbar A$, formula (7.311) implies

(i) $\langle \psi|P_{\text{pre}}\varphi\rangle = \langle P_{\text{pre}}\psi|\varphi\rangle$ for all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$,
(ii) $\langle \psi|P_{\text{pre}}\varphi\rangle = \langle P\psi|\varphi\rangle$ for all $\varphi \in \mathcal{S}(\mathbb{R}), \psi \in W_2^1(\mathbb{R})$, and
(iii) $\langle \psi|P\varphi\rangle = \langle P\psi|\varphi\rangle$ for all $\varphi, \psi \in W_2^1(\mathbb{R})$.

The three formulas (i)–(iii) display the basic ideas of von Neumann's functional-analytic theory for self-adjoint operators. We will show in Problem 7.5 that the formulas (i)–(iii) imply that $P_{\text{pre}}^* = P = P^*$. In the general case, let us consider the linear operator

$$\boxed{A : D(A) \to X} \tag{7.312}$$

whose domain of definition $D(A)$ is a linear dense subspace of the complex Hilbert space X. The linearity of A means that

$$A(\alpha\varphi + \beta\psi) = \alpha A\varphi + \beta A\psi \qquad \text{for all} \quad \varphi, \psi \in D(A),\ \ \alpha, \beta \in \mathbb{C}.$$

The density of the set $D(A)$ in the Hilbert space X means that, for any element $\varphi \in X$, there exists a sequence (φ_n) in $D(A)$ such that $\lim_{n\to\infty} \varphi_n = \varphi$ in X. Suppose that we are given two operators $B : D(B) \to X$ and $C : D(C) \to X$, where $D(B)$ and $D(C)$ are subsets of the space X.

- We write $B = C$ iff $D(B) = D(C)$ and $A\varphi = B\varphi$ for all $\varphi \in D(A)$.
- We write $B \subseteq C$ iff the operator $B : D(B) \to X$ is an extension of the operator C, that is, we have $D(A) \subseteq D(B) \subseteq X$ and $A\varphi = B\varphi$ for all $\varphi \in D(A)$.

7.1 *The smoothing technique (Friedrichs' mollification).* Let $\varphi \in L_2(\mathbb{R})$. For any positive real number $\varepsilon > 0$, we define

$$\varphi_\varepsilon(x) := \frac{1}{\varepsilon} \int_{\mathbb{R}} K\left(\frac{x-y}{\varepsilon}\right) \varphi(y) dy, \qquad x \in \mathbb{R}.$$

Here, we choose $K(x) := c \cdot \mathrm{e}^{-(1-x^2)^{-1}}$ if $|x| < 1$ and $K(x) := 0$ if $|x| \geq 1$. The positive constant c is chosen in such a way that $\int_{\mathbb{R}} K(x) dx = 1$. Prove that, for all $\varepsilon > 0$, the following hold:
(i) The smooth function φ_ε is contained in the Hilbert space $L_2(\mathbb{R})$.
(ii) $\lim_{\varepsilon \to +0} \int_{\mathbb{R}} |\varphi_\varepsilon(x) - \varphi(x)|^2 dx = 0$.
Hint: We refer to Zeidler (1995a), p. 186 (see the references on page 1049).

7.2 *The Sobolev space* $W_2^1(\mathbb{R})$. By definition, the function $\varphi : \mathbb{R} \to \mathbb{C}$ is contained in the space $W_2^1(\mathbb{R})$ iff $\varphi \in L_2(\mathbb{R})$, and the derivative φ' (in the sense of distributions) is also contained in $L_2(\mathbb{R})$. This means that

$$\int_{\mathbb{R}} \varphi'(x)\chi(x) dx = -\int \varphi(x)\chi'(x) dx$$

for all test functions $\chi \in \mathcal{D}(\mathbb{R})$. Prove the following:
(i) The Sobolev space $W_2^1(\mathbb{R})$ is a Hilbert space equipped with the inner product

$$\langle \chi | \varphi \rangle_{1,2} := \langle \chi | \varphi \rangle + \langle \chi' | \varphi' \rangle = \int_R \chi(x)^\dagger \varphi(x) dx + \int_{\mathbb{R}} \chi'(x)^\dagger \varphi'(x) dx$$

for all functions $\chi, \varphi \in W_2^1(\mathbb{R})$.[197]
(ii) The sets $\mathcal{D}(\mathbb{R})$ and $\mathcal{S}(\mathbb{R})$ are dense in $W_2^1(\mathbb{R})$.
(iii) The sets $\mathcal{D}(\mathbb{R})$ and $\mathcal{S}(\mathbb{R})$ are proper linear subspaces of the Sobolev space $W_2^1(\mathbb{R})$.
(iv) The function $\varphi : \mathbb{R} \to \mathbb{C}$ is contained in $W_2^1(\mathbb{R})$ iff $\varphi \in L_2(\mathbb{R})$ and the Fourier transform $\hat{\varphi}$ satisfies the condition[198]

$$\int_{\mathbb{R}} \left(|\hat{\varphi}(p)|^2 + |p\hat{\varphi}(p)|^2 \right) dp < \infty.$$

(v) If $\varphi, \chi \in W_2^1(\mathbb{R})$, then $\langle \chi | \varphi \rangle_{1,2} = \int_{\mathbb{R}} \hat{\chi}(p)^\dagger \hat{\varphi}(p) + p^2 \hat{\chi}(p)^\dagger \hat{\varphi}(p)\, dp$.
Hint: Use Problem 7.1. Concerning (iii), note that the function $\varphi(x) := |x| \mathrm{e}^{-x^2}$ has a derivative on the pointed set $\mathbb{R} \setminus \{0\}$ which is square integrable. Hence $\varphi \in W_2^1(\mathbb{R})$, but $\varphi \notin \mathcal{S}(\mathbb{R})$. The proofs can be found in Zeidler (1986), Vol. IIA, Chap. 21 (see the references on page 1049), together with much additional material.

7.3 *Integration by parts.* Prove that the generalized integration-by-parts formula (7.310) holds true.
Solution: Let $\varphi, \psi \in W_2^1(\mathbb{R})$. Since $\mathcal{D}(\mathbb{R})$ is dense in the Hilbert space $W_2^1(\mathbb{R})$, there exist sequences (φ_n) and (ψ_n) in $\mathcal{D}(\mathbb{R})$ such that $\varphi_n \to \varphi$ and $\psi_n \to \psi$ in $W_2^1(\mathbb{R})$ as $n \to \infty$. This means that

[197] Two functions φ and ψ are considered as the same element of the Hilbert space $W_2^1(\mathbb{R})$ iff $\varphi(x) = \psi(x)$ and $\varphi'(x) = \psi'(x)$ for all $x \in \mathbb{R}$, up to a set of Lebesgue measure zero.

[198] Recall that the Fourier transform of the derivative φ' is the product function $p \mapsto \mathrm{i}p\hat{\varphi}(p)$.

$$\varphi_n \to \varphi, \quad \varphi_n' \to \varphi', \quad \psi_n \to \psi, \quad \psi_n' \to \psi' \quad \text{in } L_2(\mathbb{R}) \text{ as } n \to \infty.$$

Letting $n \to \infty$, it follows from

$$\int_{\mathbb{R}} \psi_n(x)\varphi_n'(x)dx = -\int_{\mathbb{R}} \psi_n'(x)\varphi_n(x)dx$$

that $\int_{\mathbb{R}} \psi(x)\varphi'(x)dx = -\int_{\mathbb{R}} \psi'(x)\varphi(x)dx$.

7.4 *The adjoint operator.* The linear operator $A^\dagger : D(A) \to X$ is called the formally adjoint operator to the linear operator A from (7.312) iff

$$\boxed{\langle \psi | A\varphi \rangle = \langle A^\dagger \psi | \varphi \rangle \qquad \text{for all} \quad \varphi, \psi \in D(A).}$$

The operator $A : D(A) \to X$ is called formally self-adjoint (or symmetric) iff

$$\langle \psi | A\varphi \rangle = \langle A\psi | \varphi \rangle \qquad \text{for all} \quad \varphi, \psi \in D(A).$$

The more sophisticated definition of the adjoint operator $A^* : D(A^*) \to X$ is based on the formula

$$\boxed{\langle \psi | A\varphi \rangle = \langle A^* \psi | \varphi \rangle \qquad \text{for all} \quad \varphi \in D(A), \psi \in D(A^*).} \tag{7.313}$$

More precisely, we first define the set $D(A^*)$. The element ψ is contained in $D(A^*)$ iff there exists an element χ in X such that

$$\langle \psi | A\varphi \rangle = \langle \chi | \varphi \rangle \qquad \text{for all} \quad \varphi \in D(A).$$

We then define $A^*\psi := \chi$. This yields (7.313). The following two definitions are basic for quantum mechanics. Let $A : D(A) \to X$ be a formally self-adjoint operator of the form (7.312).

- The operator A is called self-adjoint iff $A = A^*$.
- The operator A is called essentially self-adjoint iff it has precisely one self-adjoint extension.

Show that the following hold:

(i) Both the formally adjoint operator $A^\dagger$ and the adjoint operator A^* are uniquely determined by the given operator A.

(ii) The adjoint operator A^* is linear.

(iii) If the formally adjoint operator $A^\dagger$ exists, then $A^\dagger \subseteq A^*$, that is, the operator A^* is an extension of $A^\dagger$.

(iv) The operator A is formally self-adjoint iff $A \subseteq A^*$.

Hint: We refer to Zeidler (1995a), Sect. 5.2 (see the references on page 1049).

7.5 *The prototype of a self-adjoint differential operator.* Define

$$P_{\text{pre}}\varphi := -\mathrm{i}\hbar\varphi' \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}),$$

and

$$P\varphi := -\mathrm{i}\hbar\varphi' \qquad \text{for all} \quad \varphi \in W_2^1(\mathbb{R}).$$

In the latter equation, the derivative is to be understood in the sense of tempered distributions. Note that $\varphi \in W_2^1(\mathbb{R})$ implies $P\varphi \in L_2(\mathbb{R})$. Prove the following:

(i) The operator $P_{\text{pre}} : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$ is formally self-adjoint.

(ii) The adjoint operator P_{pre}^* coincides with P.

(iii) The operator $P : W_2^1(\mathbb{R}) \to L_2(\mathbb{R})$ is self-adjoint.

(iv) $P_{\text{pre}} \subseteq P_{\text{pre}}^{**} = P_{\text{pre}}^* = P$.

(v) The closure $\overline{P}_{\rm pre}$ of $P_{\rm pre}$ coincides with $P^{**}_{\rm pre}$ (see Problem 7.9).
Solution: Set $\hbar := 1$. By Problem 7.3,

$$\int_{\mathbb{R}} \psi^\dagger(-\mathrm{i}\varphi')dx = \int_{\mathbb{R}} (-\mathrm{i}\psi')^\dagger \varphi dx \qquad \text{for all} \quad \varphi, \psi \in W_2^1(\mathbb{R}). \quad (7.314)$$

Ad (i). By (7.314), $\langle\psi|P_{\rm pre}\varphi\rangle = \langle P_{\rm pre}\psi|\varphi\rangle$ for all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$.
Ad (ii). By definition of the adjoint operator $P^*_{\rm pre}$, we have $\chi = P^*_{\rm pre}\psi$ iff $\psi, \chi \in L_2(\mathbb{R})$ and

$$\langle\psi|P_{\rm pre}\varphi\rangle = \langle\chi|\varphi\rangle \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).$$

Equivalently,

$$\int_{\mathbb{R}} \psi^\dagger(-\mathrm{i}\varphi')dx = \int_{\mathbb{R}} \chi^\dagger \varphi dx \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}).$$

Passing over to conjugate complex values and setting $\varrho := -\mathrm{i}\varphi^\dagger$, we get

$$\int_{\mathbb{R}} \psi(-\varrho')dx = \int_{\mathbb{R}} (\mathrm{i}\chi)\varrho dx \qquad \text{for all} \quad \varrho \in \mathcal{S}(\mathbb{R}).$$

This means that $\frac{d}{dx}\psi = \mathrm{i}\chi$, in the sense of tempered distributions. Hence $\psi \in W_2^1(\mathbb{R})$, and $\chi = -\mathrm{i}\frac{d}{dx}\psi$. Therefore, $\chi = P\psi$.
Ad (iii). By (7.314), $\langle\psi|P\varphi\rangle = \langle P\psi|\varphi\rangle$ for all $\varphi, \psi \in W_2^1(\mathbb{R})$. Hence the operator P is formally self-adjoint. Suppose that, for fixed $\psi, \chi \in L_2(\mathbb{R})$, we have

$$\langle\psi|P\varphi\rangle = \langle\chi|\varphi\rangle \qquad \text{for all} \quad \varphi \in W_2^1(\mathbb{R}).$$

The same argument as in (ii) above shows that $P\psi = \chi$. Hence $P^*\psi = P\psi$ for all $\psi \in W_2^1(\mathbb{R})$.
Ad (iv). By definition, $P_{\rm pre} \subseteq P$. By (ii), (iii), we get $P^*_{\rm pre} = P$ and $P^* = P$.
Ad (v). Let (φ_n) be a sequence in $D(P_{\rm pre})$ with

$$\lim_{n\to\infty} \varphi_n = \varphi, \qquad \lim_{n\to\infty} P_{\rm pre}\varphi_n = \chi. \quad (7.315)$$

Then $\overline{P}_{\rm pre}\psi = \chi$. Letting $n \to \infty$, it follows from

$$\langle\varrho|P_{\rm pre}\varphi_n\rangle = \langle P\varrho|\varphi_n\rangle \qquad \text{for all} \quad \varrho \in \mathcal{S}(\mathbb{R})$$

that $\langle\varrho|\chi\rangle = \langle P\varrho|\varphi\rangle$ for all $\varrho \in \mathcal{S}(\mathbb{R})$. Hence $\chi = P\varphi$.
Conversely, if $\chi = P\varphi$, then there exists a sequence (φ_n) in $\mathcal{S}(\mathbb{R})$ with (7.315), by Problem 7.2(ii). Summarizing, $P\varphi = \overline{P}\varphi$ for all $\varphi \in W_2^1(\mathbb{R})$.

7.6 *Closed operators.* The subset

$$\mathrm{graph}(A) := \{(\varphi, A\varphi) : \varphi \in D(A)\}$$

of the product space $X \times X$ is called the graph of the operator A from (7.312). The operator A is defined to be closed iff the set $\mathrm{graph}(A)$ is closed in $X \times X$. This means that if there exists a sequence (φ_n) in $D(A)$ with the convergence property

$$\lim_{n\to\infty} \varphi_n = \varphi \quad \text{and} \quad \lim_{n\to\infty} A\varphi_n = \psi,$$

then $\varphi \in D(A)$ and $A\varphi = \psi$. This generalizes the notion of continuity.[199] Show that the adjoint operator $A^* : D(A) \to X$ from Problem 7.4 is closed.
Solution: Let $\varphi_n \in D(A^*)$ for all n, and let

$$\lim_{n\to\infty} \varphi_n = \varphi \quad \text{and} \quad \lim_{n\to\infty} A^*\varphi_n = \psi.$$

Then $\langle A^*\varphi_n|\chi\rangle = \langle\varphi_n|A\chi\rangle$. Letting $n \to \infty$, we get

$$\langle\psi|\chi\rangle = \langle\varphi|A\chi\rangle \qquad \text{for all} \quad \chi \in D(A).$$

Hence $\varphi \in D(A^*)$ and $\psi = A^*\varphi$.

7.7 *The crucial symmetry criterion for self-adjoint operators.* Prove that the linear, densely defined operator $A : D(A) \to X$ on the complex Hilbert space X is self-adjoint iff the following two conditions are satisfied:
(i) $\langle\psi|A\varphi\rangle = \langle A\psi|\varphi\rangle$ for all $\varphi, \psi \in D(A)$.
(ii) If $\langle\psi|A\varphi\rangle = \langle\chi|\varphi\rangle$ for fixed $\psi, \chi \in X$ and all $\varphi \in D(A)$, then $\psi \in D(A)$.
Solution: (I) $\Rightarrow$: Assume that A is self-adjoint. Then $A = A^*$. This implies (i). If $\langle\psi|A\varphi\rangle = \langle\chi|\varphi\rangle$ for all $\varphi \in D(A)$, then $\psi \in D(A^*)$. Hence $\psi \in D(A)$.
(II) $\Leftarrow$: Assume that (i) and (ii) hold. By (i), $A \subseteq A^*$. In order to show $A^* \subseteq A$, let $\psi \in D(A^*)$. Then

$$\langle\psi|A\varphi\rangle = \langle A^*\psi|\varphi\rangle \qquad \text{for all} \quad \varphi \in D(A).$$

By (ii), $\psi \in D(A)$. It follows from (i) that $\langle A^*\psi|\varphi\rangle = \langle A\psi|\varphi\rangle$. Hence

$$\langle A^*\psi - A\psi|\varphi\rangle = 0 \qquad \text{for all} \quad \varphi \in D(A).$$

Since $D(A)$ is dense in X, we get $A^*\psi = A\psi$. □
In the following problems we want to show that

> *The properties of self-adjointness and essential self-adjointness are closely related to natural extension properties of formally self-adjoint operators A based on the inclusions $A \subseteq \overline{A} \subseteq A^*$, where $\overline{A}$ denotes the closure of A. In addition, $\overline{A} = A^{**}$.*

7.8 *Maximal extension and the adjoint operator.* Let $A : D(A) \to X$ be a formally self-adjoint operator of the form (7.312). Show the following:
(i) There exists a maximal linear extension $B : D(B) \to X$ of A with

$$\langle\psi|A\varphi\rangle = \langle B\psi|\varphi\rangle \qquad \text{for all} \quad \varphi \in D(A), \psi \in D(B).$$

This maximal extension B is equal to the adjoint operator A^*.
(ii) The operator A is self-adjoint iff the maximal extension B coincides with A, that is, $B = A$.
Hint: Convince yourself that this is merely a reformulation of the basic definitions.

7.9 *Minimal extension and the closure.* Let $A : D(A) \to X$ be a formally self-adjoint operator of the form (7.312). Show that the operator A can be minimally extended to a linear, closed, formally self-adjoint operator. This operator is denoted by $\overline{A} : D(\overline{A}) \to X$, and it is called the closure of A.
Hint: Let D_{cl} be the set of all $\varphi \in X$ for which a sequence (φ_n) exists in $D(A)$ such that

[199] Banach's closed graph theorem tells us the crucial fact that a linear closed operator $A : X \to X$ defined on the total Hilbert space X is continuous. However, the self-adjoint Hamiltonian operators arising in quantum mechanics are not defined on the total Hilbert space; as a rule, they are not continuous, but they are closed.

- $\lim_{n\to\infty} \varphi_n = \varphi$ and
- $(A\varphi_n)$ is convergent, that is, $\lim_{n\to\infty} A\varphi_n = \psi$.

Letting $n \to \infty$, it follows from $\langle \chi | A\varphi_n \rangle = \langle A\chi | \varphi_n \rangle$ that

$$\langle \chi | \psi \rangle = \langle A\chi | \varphi \rangle \qquad \text{for all} \quad \chi \in D(A).$$

Since $D(A)$ is dense in X, the element ψ of X is uniquely determined by φ. Now we set $\overline{A}\varphi := \psi$ and $D(\overline{A}) := D_{\mathrm{cl}}$. Since

$$\langle \chi | \overline{A}\varphi \rangle = \langle A\chi | \varphi \rangle \qquad \text{for all} \quad \chi \in D(A),\ \varphi \in D(\overline{A}), \tag{7.316}$$

we get $A \subseteq \overline{A} \subseteq A^*$. Let $\varrho \in D(\overline{A})$. Then there exists a sequence (ϱ_n) in $D(A)$ such that $\lim_{n\to\infty} \chi_n = \varrho$. Considering (7.316) with $\chi := \varrho_n$ and letting $n \to \infty$, we obtain

$$\langle \varrho | \overline{A}\varphi \rangle = \langle \overline{A}\varrho | \varphi \rangle \qquad \text{for all} \quad \varrho, \varphi \in D(\overline{A}).$$

Thus, the operator $\overline{A}$ is formally self-adjoint. Finally, it remains to show that the operator $\overline{A}$ is closed (see H. Triebel, Higher Analysis, Sect. 17, Barth, Leipzig, 1989).

7.10 *Properties of the closure.* Let $A : D(A) \to X$ and $B : D(B) \to X$ be formally self-adjoint operators of the form (7.312) on page 681. Show the following:
(i) $A \subseteq B$ implies $\overline{A} \subseteq \overline{B}$ and $B^* \subseteq A^*$.
(ii) $A \subseteq \overline{A} \subseteq A^*$.
(iii) $\overline{A} = A^{**}$ and $(\overline{A})^* = A^*$.
(iii) The operator A is essentially self-adjoint iff the closure $\overline{A}$ is self-adjoint.
Hint: We refer to Zeidler (1995a), p. 415ff (see the references on page 1049).

7.11 *General properties of self-adjoint operators.* For the formally self-adjoint operator A of the form (7.312), the following statements are equivalent:
(i) The operator A is self-adjoint.
(ii) All the non-real numbers z belong to the resolvent set $\varrho(A)$.
(iv) $\mathrm{im}(\pm \mathrm{i}I - A) = X$.
(iv) The operator A is closed and $\ker(\pm \mathrm{i}I - A^*) = \{0\}$.
(v) The operator A is essentially self-adjoint and closed.
Hint: See Zeidler (1995a), p. 416.

7.12 *General properties of essentially self-adjoint operators.* For the formally self-adjoint operator operator A of the form (7.312), the following statements are equivalent:
(i) The operator A is essentially self-adjoint.
(ii) The closure $\overline{A}$ is self-adjoint.
(iv) The two sets $\mathrm{im}(\pm \mathrm{i}I - A)$ are dense in X.
(iii) $\ker(\pm \mathrm{i}I - A^*) = \{0\}$.
Hint: See Zeidler (1995a), p. 424.

7.13 *Further properties of essentially self-adjoint operators.* Let $A : D(A) \to X$ be a linear, formally self-adjoint, and densely defined operator on the complex Hilbert space X. Assume that the operator A is essentially self-adjoint, and let $B : D(B) \to X$ be the uniquely determined self-adjoint extension of A. Prove that

$$A^* = \overline{A} = A^{**} = B. \tag{7.317}$$

Solution: By Problem 7.10, $B = \overline{A}$. Moreover, $\overline{A} = A^{**}$ and $A^* = (\overline{A})^* = \overline{A}$.

7.14 *Unitary invariance.* The linear operator $A : D(A) \to X$ is said to be unitarily equivalent to the linear operator $B : D(B) \to X$ iff there exists a unitary operator $U : X \to Y$ from the complex Hilbert space X onto the complex Hilbert space Y such that the diagram

$$\begin{array}{ccc} D(A) & \xrightarrow{A} & X \\ {\scriptstyle U}\downarrow & & \downarrow{\scriptstyle U} \\ D(B) & \xrightarrow{B} & Y \end{array}$$

is commutative. This means that $D(B) = UD(A)$ and $B = UAU^{-1}$. Show that the following notions are invariant under this transformation: formally self-adjoint, self-adjoint, essentially self-adjoint, and closed.
Hint: Use the corresponding definitions.

7.15 *The position operator on the real line.* Set

$$D(Q) := \{\varphi \in L_2(\mathbb{R}) : \int_{\mathbb{R}} |x\varphi(x)|^2 dx < \infty\}.$$

Fix $x \in \mathbb{R}$. Define $(Q_{\rm pre}\varphi)(x) := x\varphi(x)$ for all $\varphi \in \mathcal{S}(\mathbb{R})$, and $(Q\varphi)(x) := x\varphi(x)$ for all $\varphi \in D(Q)$. Prove the following:
(i) The operator $Q_{\rm pre} : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$ is formally self-adjoint.
(ii) The operator $Q : D(Q) \to L_2(\mathbb{R})$ is self-adjoint.
(iii) The operator $Q_{\rm pre} : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$ is essentially self-adjoint, but not self-adjoint.
(iv) $Q^*_{\rm pre} = \overline{Q}_{\rm pre} = Q^{**}_{\rm pre} = Q$.
Solution: Ad (i). For all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$,

$$\int_{\mathbb{R}} (x\psi(x))^\dagger \varphi(x) dx = \int \psi(x)^\dagger x\varphi(x) dx.$$

Ad(ii), (iii). For given function $f \in L_2(\mathbb{R})$, the equation

$$\pm \mathrm{i}\varphi - Q\varphi = f, \qquad \varphi \in D(Q) \tag{7.318}$$

has the unique solution $\varphi(x) := \frac{f(x)}{\pm \mathrm{i} - x}$ for all $x \in \mathbb{R}$. In fact, $|\varphi(x)| \le \mathrm{const}|f(x)|$ for all $x \in \mathbb{R}$. This implies $\varphi \in L_2(\mathbb{R})$. Hence $\varphi \in D(Q)$. Thus, we get the key relation $\mathrm{im}(\pm \mathrm{i}I - Q) = L_2(\mathbb{R})$, that is, Q is self-adjoint.
In particular, if $f \in \mathcal{S}(\mathbb{R})$, then the solution of equation (7.318) is contained in $\mathcal{S}(\mathbb{R})$. Since the set $\mathcal{S}(\mathbb{R})$ is dense in $L_2(\mathbb{R})$, the sets $\mathrm{im}(\pm I - Q_{\rm pre})$ are dense in $L_2(\mathbb{R})$. Therefore, the operator $Q_{\rm pre}$ is essentially self-adjoint.
Finally, note that the set $D(Q_{\rm pre}) = \mathcal{S}(\mathbb{R})$ differs from $D(Q)$. For example, choose $\psi(x) := |x|\mathrm{e}^{-x^2}$. Then $\psi \in D(Q)$, but $\psi \notin \mathcal{S}(\mathbb{R})$.
Ad (iv). Use Problem 7.13.

7.16 *The momentum operator on the real line.* As in Problem 7.5, define

$$P_{\rm pre}\varphi := -\mathrm{i}\hbar\varphi' \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}),$$

and $P\varphi := -\mathrm{i}\hbar\varphi'$ for all $\varphi \in W_2^1(\mathbb{R})$. Use the Weyl equation

$$\boxed{\pm \mathrm{i}\varphi - P\varphi = f, \qquad \varphi \in \mathcal{S}(\mathbb{R})} \tag{7.319}$$

in order to prove the following:

(i) The operator $P_{\mathrm{pre}} : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$ is formally self-adjoint.
(ii) The operator $P : W_2^1(\mathbb{R}) \to L_2(\mathbb{R})$ is self-adjoint.
(iii) The operator $P_{\mathrm{pre}} : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$ is essentially self-adjoint, but not self-adjoint.
(iv) $P_{\mathrm{pre}}^* = \overline{P}_{\mathrm{pre}} = P_{\mathrm{pre}}^{**} = P$.
Solution: Ad (i). See Problem 7.5.
Ad (ii), (iii). For given $f \in \mathcal{S}(\mathbb{R})$, the equation (7.319) has a unique solution $\varphi \in \mathcal{S}(\mathbb{R})$. In fact, Fourier transformation yields

$$\pm \mathrm{i}\hat{\varphi}(p) - \hbar p \hat{\varphi}(p) = \hat{f}(p), \qquad p \in \mathbb{R}.$$

This yields $\hat{\varphi}(p) = \frac{\hat{f}(p)}{\pm \mathrm{i} - \hbar p}$ which is contained in $\mathcal{S}(\mathbb{R})$. Then the inverse Fourier transform yields the desired solution φ of (7.319). Since the set $\mathcal{S}(\mathbb{R})$ is dense in $L_2(\mathbb{R})$, the image set $\mathrm{im}(\pm I - P_{\mathrm{pre}})$ is dense in $L_2(\mathbb{R})$. Consequently, the operator $P_{\mathrm{pre}} : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$ is essentially self-adjoint. Thus, it has a unique self-adjoint extension.
Using the extended Fourier transform $\mathcal{F} : L_2(\mathbb{R}) \to L_2(\mathbb{R})$ together with Problem 7.2(iv), the same argument as above shows that, for given function $f \in L_2(\mathbb{R})$, the equation

$$\pm \mathrm{i}\varphi - P\varphi = f, \qquad \varphi \in W_2^1(\mathbb{R})$$

has a (unique) solution φ. Hence $\mathrm{im}(\pm \mathrm{i} I - P) = L_2(\mathbb{R})$. Consequently, the operator $P : W_2^1(\mathbb{R}) \to L_2(\mathbb{R})$ is self-adjoint. Furthermore, the operator P is the unique self-adjoint extension of the operator P_{pre}. Since $\mathcal{S}(\mathbb{R}) \neq W_2^1(\mathbb{R})$, the operator P_{pre} differs from P.
Ad (iv). Use Problem 7.13.
Historical remarks. The importance of equations of the type (7.319) for the study of the spectral properties of ordinary differential equations was discovered by Weyl in 1910 and developed by von Neumann in his 1929 theory of deficiency indices.

- H. Weyl, On ordinary differential equations with singularities, Math. Ann. **68** (1910), 220–269 (in German).
- J. von Neumann, General spectral theory of Hermitean operators, Math. Ann. **102** (1929), 49–131 (in German).
- K. Kodaira, The eigenvalue problem for ordinary differential equations of the second order and Heisenberg's theory of S-matrices. Amer. J. Math. **71** (1949), 921–945.
- K. Jörgens and F. Rellich, Eigenvalue problems for ordinary differential equations, Springer, Berlin, 1976 (in German).

The Weyl–Kodaira theory will be studied in Vol. III, together with interesting physical applications.

7.17 *The Hamiltonian of the free quantum particle on the real line.* Define

$$H_{\mathrm{pre}}\varphi := -\frac{\hbar^2}{2m}\varphi'' \qquad \text{for all} \quad \varphi \in \mathcal{S}(\mathbb{R}),$$

and

$$H_{\mathrm{free}}\varphi := -\frac{\hbar^2}{2m}\varphi'' \qquad \text{for all} \quad \varphi \in W_2^2(\mathbb{R}).$$

In the latter equation, the derivatives are to be understood in the sense of tempered distributions. If $\varphi \in W_2^2(\mathbb{R})$, then $H_{\mathrm{free}}\varphi \in L_2(\mathbb{R})$. Prove the following:
(i) The operator $H_{\mathrm{pre}} : \mathcal{S}(\mathbb{R}) \to L_2(\mathbb{R})$ is formally self-adjoint.
(ii) The operator $H_{\mathrm{free}} : W_2^2(\mathbb{R}) \to L_2(\mathbb{R})$ is self-adjoint.

(iii) $\overline{H}_{\rm pre} = H^*_{\rm pre} = H_{\rm free}$.
(iv) The operator $H_{\rm pre}$ is essentially self-adjoint, but not self-adjoint.
Hint: Apply integration by parts twice, and use analogous arguments as in Problem 7.7.

7.18 *Deficiency indices and von Neumann's extension theorem for self-adjoint operators.* Let $A : D(A) \to X$ be a linear, formally self-adjoint, densely defined, and closed operator on the complex Hilbert space X. The numbers

$$d_\pm := \dim\,(\pm \mathrm{i}I - A)^\perp$$

are called the deficiency indices of the operator A.[200] Prove the following:
(i) The operator A has a self-adjoint extension iff $d_+ = d_-$.
(ii) The operator A is self-adjoint iff $d_+ = d_- = 0$.
Hint: Use the Cayley transform in order to reduce this to the extension problem for isometric operators (see Problems 7.22 and 7.23).

7.19 *Formally self-adjoint operators which have no self-adjoint extension or infinitely many self-adjoint extensions.* Consider the operator

$$A\varphi := -\mathrm{i}\hbar \frac{d\varphi}{dx} \qquad \text{for all} \quad \varphi \in D(A)$$

where $D(A)$ is a linear dense subspace of the complex Hilbert space X. We will choose $X := L_2(0,\infty)$ or $X := L_2(0,1)$. We want to show that the properties of the operator A critically depend on the choice of the domain of definition $D(A)$. In turn, this depends on the choice of boundary conditions. Show that the following hold:
(i) Choose $D(A) := \mathcal{D}(0,\infty)$ and $X := L_2(0,\infty)$. [201] Then the operator A is formally self-adjoint, but it cannot be extended to a self-adjoint operator.
(ii) Fix the complex number α with $|\alpha| = 1$ and $\alpha \neq 1$. Choose[202]

$$D(A) := \{\varphi \in C^1[0,1] : \varphi(0) = \alpha\varphi(1)\}$$

and $X = L_2(0,1)$. Then the operator A is essentially self-adjoint.
(iii) Choose $D(A) := \{\varphi \in C^1[0,1] : \varphi(0) = \varphi(1) = 0\}$ and $X := L_2(0,1)$. Then the operator A is formally self-adjoint, but its closure $\overline{A}$ is not self-adjoint. However, the operator has an infinite number of self-adjoint extensions given by the operators from (ii).
Hint: Ad (i). Set $\hbar := 1$. Integration by parts yields

$$\langle\chi|A\varphi\rangle = \int_0^\infty \chi^\dagger(-\mathrm{i}\varphi')dx = \int_0^\infty (-\mathrm{i}\chi')^\dagger\varphi dx = \langle A\chi|\varphi\rangle$$

for all $\chi, \varphi \in \mathcal{D}(0,\infty)$. Thus, the operator A is formally self-adjoint. Now fix the non-real complex number z and study the equation $A - zI = f$, that is

$$-\mathrm{i}\varphi' - z\varphi = f, \qquad \varphi \in \mathcal{D}(0,\infty). \tag{7.320}$$

[200] If L is a linear subspace of X, then the orthogonal complement $L^\perp$ consists of all the elements φ of X which are orthogonal to L.
[201] Recall that $\varphi \in \mathcal{D}(0,\infty)$ iff the function $\varphi :]0,\infty[\to \mathbb{C}$ is smooth with compact support (i.e., it vanishes outside some interval $[a,b]$ with $0 < a < b < \infty$). Then the function φ satisfies the boundary condition $\varphi(0) = \varphi(+\infty) = 0$.
[202] The space $C^k[0,1]$, $k = 1, 2, \ldots$ consists of all continuous functions $\varphi : [0,1] \to \mathbb{C}$ which have continuous derivatives on the open interval $]0,1[$ up to order k, and all of these derivatives can be continuously extended to the closed interval $[0,1]$.

We are given $f \in L_2(0,\infty)$. If φ is a solution of (7.320), then

$$e^{-izx} f(x) = -i\frac{d}{dx}\left(\varphi(x)e^{-izx}\right).$$

Integration by parts tells us that

$$\int_0^\infty e^{-izx} f(x)dx = 0. \tag{7.321}$$

Choosing $z := -i$, we get $e^{-izx} = e^{-x}$. Then condition (7.321) is satisfied for all $f \in L_2(0,\infty)$. In contrast to this, if $z := i$, then $e^{-izx} = e^{x}$, and condition (7.321) is not valid for all $f \in L_2(0,\infty)$. Use this observation in order to show that the deficiency indices of A are given by $d_- = 0$ and $d_+ \neq 0$. By von Neumann's deficiency-index criterion (see Problem 7.18), the operator A has no self-adjoint extension.

For the complete proof of (i)–(iii), see P. Lax, Functional Analysis, Chap. 33, Wiley, New York, 2002.

7.20 *Continuity and boundedness.* Show that, for the linear operator $A : X \to X$ on the (real or complex) Hilbert space X, the following statements are equivalent:

(i) The operator A is continuous, that is, for any fixed element $\varphi_0 \in X$ and any number $\varepsilon > 0$, there exists a number $\delta(\varepsilon, \varphi_0) > 0$ such that

$$||\varphi - \varphi_0|| < \delta(\varepsilon, \varphi_0) \quad \text{implies} \quad ||A\varphi - A\varphi_0|| < \varepsilon.$$

(ii) The operator is sequentially continuous, that is, $\lim_{n\to\infty} \varphi_n = \varphi$ implies $\lim_{n\to\infty} A\varphi_n = A\varphi$.

(iii) The operator A is bounded, that is, $||A|| := \sup_{||\varphi||\leq 1} ||A\varphi|| < \infty$.

Hint: We refer to Zeidler (1995a), Sect. 1.9 (see the references on page 1049).

7.21 *Extension of a linear, densely defined, bounded operator.* Let $A : D(A) \to Y$ be a linear operator, where $D(A)$ is a linear dense subspace of the complex (resp. real) Hilbert space X, and Y is also a complex (resp. real) Hilbert space. Suppose that

$$||A\psi|| \leq \text{const } ||\psi|| \qquad \text{for all} \quad \psi \in D(A).$$

Show that the operator A can be uniquely extended to a linear bounded operator $A : X \to Y$. This statement remains true if X and Y are complex (resp. real) Banach spaces.

Hint: Let $\psi \in X$. Choose a sequence (ψ_n) in $D(A)$ with $\psi = \lim_{n\to\infty} \psi_n$. Using the Cauchy criterion, show that the sequence $(A\psi_n)$ is convergent. Set $A\psi := \lim_{n\to\infty} A\psi_n$. Finally, show that $A\psi$ is independent of the choice of the sequence (ψ_n). We refer to Zeidler (1995a), Sect. 3.6 (see the references on page 1049).

7.22 *Extension of isometric operators.* Let $A : D(A) \to X$ be a linear isometric operator on the linear subspace $D(A)$ of the complex Hilbert space X, that is, $\langle A\psi | A\varphi\rangle = \langle\psi|\varphi\rangle$ for all $\varphi, \psi \in D(A)$. Show that the operator A can be extended to a unitary operator $U : X \to X$ iff $\dim D(A)^\perp = \dim \text{im}(A)^\perp$.

Hint: (I) Assume first that $D(A)$ is a closed linear subspace of the separable Hilbert space X. Let $\dim D(A)^\perp = \dim \text{im}(A)^\perp$. Set

$$U\varphi_j := \psi_j \qquad \text{for all} \quad j,$$

where $\varphi_1, \varphi_2, \ldots$ (resp. $\psi_1, \psi_2, \ldots$) is an orthonormal basis in $D(A)^\perp$ (resp. $\text{im}(A)^\perp$).

(II) If $D(A)$ is not closed, then consider the closure $D_{\rm cl}$ of $D(A)$. This is a closed linear subspace of X. By Problem 7.21, the operator A can be uniquely extended to a linear isometric operator $B : D_{\rm cl} \to X$. Now apply argument (I) to the extension B.
(III) If the Hilbert space X is not separable, then replace $\varphi_1, \varphi_2, \dots$ (resp. $\psi_1, \psi_2, \dots$) by a generalized orthonormal basis, by using the Zorn lemma. As in Problem 7.19, see Lax (2002), Sect. 6.4.

7.23 *The Cayley transform.* The classical Möbius transformation

$$f(z) := \frac{z - \mathrm{i}}{z + \mathrm{i}}, \qquad z \in \mathbb{R}$$

generates a conformal map from the real line onto the unit circle. Generalizing this, we obtain the Cayley transformation

$$C_A := (A - \mathrm{i}I)(A + \mathrm{i}I)^{-1}$$

which was used for matrices A by Cayley.[203] In the late 1920s, von Neumann generalized this to operators in Hilbert spaces in order to solve the extension problem for self-adjoint operators (see Problem 7.18). Let $A : D(A) \to X$ be a linear, formally self-adjoint operator on the linear subspace $D(A)$ of the complex Hilbert space X. Show the following:
(i) $\mathrm{dom}(C_A) = \mathrm{im}(A + \mathrm{i}I)$ and $\mathrm{im}(C_A) = \mathrm{im}(A - \mathrm{i}I)$.
(ii) The operator C_A is isometric.
(iii) C_A is unitary on X iff A is self-adjoint.
(iv) C_A is closed iff A is closed.
(v) Let $B : D(B) \to X$ be linear and formally self-adjoint. Then, $A \subseteq B$ iff $C_A \subseteq C_B$.
(vi) If A is closed, then $\mathrm{dom}(C_A)$ and $\mathrm{im}(C_A)$ are closed linear subspaces of the Hilbert space X.
Hint: See F. Riesz and B. Nagy, Functional Analysis, Sect. 123, Frederyck Ungar, New York, 1978.

7.24 *Polar decomposition.* Each complex number z allows the polar decomposition $z = ur$ with $r := |z|$ and $u = \mathrm{e}^{\mathrm{i}\varphi}$. Here, $|u| = 1$. We want to generalize this to operators. Let $A : D(A) \to X$ be a linear (resp. antilinear), densely defined, closed operator on the complex Hilbert space X (e.g., a linear continuous operator $A : X \to X$.) Show the following:
(i) There exists a factorization

$$A = UR$$

where $R : D(R) \to X$ is a linear self-adjoint operator with $D(R) = D(A)$, and $\langle \psi | R\psi \rangle \geq 0$ for all $\psi \in D(R)$. In addition, $\ker(R) = \ker(A)$. Moreover, the operator $U : X \to X$ is linear (resp. antilinear) and the restriction

$$U : \ker(A)^{\perp} \to \mathrm{cl}(\mathrm{im}(A))$$

is unitary (resp. antiunitary), whereas $\ker(U) = \ker(A)$. Explicitly, $R = \sqrt{A^* A}$. The operator R is also called the absolute value of A (denoted by $|A|$). In particular, if the operator $A : X \to X$ is linear (resp. antilinear), continuous, and bijective, then the operator $U : X \to X$ is unitary (resp. antiunitary).
(ii) The operators R and U are uniquely determined by the properties formulated in (i).

[203] Möbius (1790–1868), Cayley (1821–1895).

(iii) If the linear operator $A : X \to X$ is continuous and normal, that is, $AA^* = A^*A$, then the operator $R : X \to X$ is linear, continuous, and self-adjoint, and the operator $U : X \to X$ is unitary. In addition, $UR = RU$.
Hint: See Reed and Simon, Methods of Modern Mathematical Physics, Vol. 1, Sect. VIII.9, Academic Press, as well as F. Riesz and B. Nagy, Functional Analysis, Sect. 110, Frederyck Ungar, New York, 1978.

7.25 *The theorem of Rolle on the zeros of functions.* Show the following for smooth functions $f : \mathbb{R} \to \mathbb{R}$:[204]

(i) If $f(a) = f(c) = 0$ with $a < c$, then there exists a number b with $a < b < c$ such that $f'(b) = 0$.
(ii) If $f(c) = 0$ and $\lim_{x\to+\infty} f(x) = 0$, then there exists a number $d > c$ such that $f'(d) = 0$.
(iii) Let $n \geq 1$. If the function f has at least n zeros on the compact interval J, then the derivative f' has at least $n-1$ zeros on J. If, in addition, the function f goes to zero as $x \to +\infty$ and $x \to -\infty$, then f' has at least $n+1$ zeros on $\mathbb{R}$.

Solution: Ad (i). By the classical mean theorem in calculus,

$$f(c) - f(a) = f'(b)(c-a) \qquad \text{for some } \ b \in]a, c[.$$

Ad (ii). Since $f(x) = \int_c^x f'(y)dy$, we get

$$\int_c^\infty f'(y)dy = \lim_{x\to+\infty} f(x) = 0.$$

Suppose that the function f' has no zeros on the interval $]c, \infty[$. Then, f' has constant sign on this interval, by the Bolzano theorem. Hence the integral of f' over $[c, \infty[$ does not vanish, a contradiction.
Ad (iii). For $n = 1$ the statement is trivial. Let $n \geq 2$. Suppose that $f(x_j) = 0$ for $j = 1, 2, ..., n$ with

$$x_1 < x_2 < ... < x_n.$$

By (ii), there exist numbers $y_1, y_2, ...$ with

$$x_1 < y_1 < x_2 < ... < x_{n-1} < y_{n-1} < x_n$$

such that $f'(y_k) = 0$ for $k = 1, ..., n-1$. In addition, if $f(x) \to 0$ as $x \to +\infty$, then there exists a number $y_n > x_n$ such that $f'(y_n) = 0$, by (ii). Similarly, it follows from $f(x) \to 0$ as $x \to -\infty$ that there exists a number $y_{-1} < x_1$ such that $f'(y_{-1}) = 0$.

7.26 *The zeros of the Hermite polynomials.* Show that, for $n = 0, 1, 2, ...$, the Hermite polynomial H_n of order n has precisely n zeros.[205]

Solution: Set $\mathcal{H}_n(x) := (-1)^n \mathrm{e}^{-x^2} H_n(x)$. By (7.7) on page 436,

$$\mathcal{H}_n(x) = \frac{d^n \mathrm{e}^{-x^2}}{dx^n}, \qquad n = 0, 1, 2, ...$$

Note that H_n is a polynomial of degree n. Thus, the maximal number of real zeros of H_n is equal to n. Moreover, $\mathcal{H}_n(x) \to 0$ as $x \to \pm\infty$ for $n = 0, 1, 2, , ...$
Using the recursive formula

[204] The French mathematician Michel Rolle (1652–1719) investigated the zeros of polynomials in his 1690 treatise *Traité d'algèbre*.
[205] This implies that the n zeros of H_n are simple.

$$\mathcal{H}_{n+1}(x) = \mathcal{H}_n'(x), \qquad n = 0, 1, 2, ...$$

and Problem 7.25, we proceed by induction. The function $H_0(x) = 1$ has no zeros. The polynomial H_1 of first order has precisely one zero. Now suppose that the polynomial H_n has n real zeros. Then, the function $\mathcal{H}_n$ has also n zeros. By Problem 7.25(iii), $\mathcal{H}_{n+1}$ has $n+1$ zeros. In turn, H_{n+1} has $n+1$ real zeros.

7.27 *The normal product* $: Q^n :$. Fix $x_0 := 1$ as on page 436. Let $m, n = 0, 1, 2, \ldots$ Define

$$P_n(x) := \sum_{k=0}^{[n/2]} (-1)^k c_{n,k} x^{n-2k}$$

where $c_{n,k} := n!/k!(n-2k)!2^k$. Here, $[n/2]$ denotes the largest integer j with $j \le n/2$. Using the normal product $: Q^n :$ introduced on page 438, prove the following:

(i) $H_n(x) = 2^{n/2} P_n(\sqrt{2}\, x)$.

(ii) $\int_{\mathbb{R}} H_n(x) H_m(x) \mathrm{e}^{-x^2} dx = 2^n n! \sqrt{\pi}\, \delta_{nm}$.

(iii) $x^n = \sum_{k=0}^{[n/2]} c_{n,k} P_{n-2k}(x)$.

(iv) $: Q^n := 2^{-n} H_n(x)$.

Hint: See J. Glimm and A. Jaffe, Mathematical Methods of Quantum Physics, Sect. 1.5, Springer, New York, 1981.

7.28 *The modified Moyal star product.* For all functions $f, g \in C^\infty(\mathbb{R}^2)$, define the modified Moyal product

$$f \star g := f \mathrm{e}^{\partial_a' \partial_{a^\dagger}} g = \sum_{m,n=0}^{\infty} \frac{1}{m!n!} \; (\partial_a^m f)(\partial_{a^\dagger}^n g).$$

Moreover, set $\pi_0 := \mathrm{e}^{-aa^\dagger}$ along with

$$\pi_n := \frac{1}{n!} \; (a^\dagger)^n \star \pi_0 \star a^n, \qquad n = 0, 1, 2, ...$$

Recall that $H := \hbar\omega a a^\dagger$ by page 593. Show that the following hold:

(i) $a^\dagger \star a = a a^\dagger, \;\; a \star a^\dagger = a a^\dagger + 1$.

(ii) $\pi_n = \pi_0 (a^\dagger)^n a^n / n!, \;\; n = 1, 2, \ldots$

(iii) $a \star \pi_0 = 0$.

(iv) $H \star \pi_n = n\hbar\omega \pi_n, \;\; n = 0, 1, 2, \ldots$

(v) The generalized Schrödinger equation

$$\mathrm{i}\hbar F_t(a, a^\dagger, t) = H \star F(a, a^\dagger, t), \qquad t \in \mathbb{R}, \;\; a \in \mathbb{C}$$

is equivalent to the equation $\mathrm{i}\hbar F_t(a, a^\dagger, t) = (H + \hbar\omega a^\dagger \partial_{a^\dagger}) F(a, a^\dagger, t)$. The solution is given by

$$F(a, a^\dagger, t) = \sum_{n=0}^{\infty} \pi_n(a, a^\dagger) \mathrm{e}^{-\mathrm{i}n\omega t}.$$

Hint: See A. Hirshfeld and P. Henselder, Deformation quantization in the teaching of quantum mechanics, Am. J. Phys. **70** (2002), 537–547.

7.29 *Proof of Theorem 7.54 on page 594.* Hint: Proceed similarly to Problem 7.28. See A. Hirshfeld and P. Henselder (2002), as above.

7.30 *Proof of Theorem 7.55 on page 594.* Hint: See A. Hirshfeld and P. Henselder (2002), as above.

7.31 *Weyl polynomials.* Prove Proposition 7.56 on page 598. Hint: Generalize the special argument given on page 598.

7.32 *The symbol of the scattering operator.* Motivate relation (7.276) on page 615, by using the Dirac delta function.
Solution: To simplify notation, we set $\hbar = m := 1$. Furthermore, choose

$$a(q,p) := \mathrm{e}^{\mathrm{i}tp^2/2}, \quad b(q,p) := \mathrm{sym}_P(q,p\,;t,t_0), \quad c(q,p) := \mathrm{e}^{-\mathrm{i}t_0p^2/2}.$$

Because of the associativity of the Moyal star product, we have to compute $(a*b)*c$.
(I) Computation of $a*b$. Set $f(q,p) := (a*b)(q,p)$. Choose the new notation $u := q_1, v := p_1, w := q_2$, and $z := p_2$. By definition of the Moyal star product (7.261) on page 607, we get

$$f(q,p) = \frac{1}{\pi^2}\int_{\mathbb{R}^4} \mathrm{e}^{2\mathrm{i}p(w-u)}\mathrm{e}^{2\mathrm{i}v(q-w)}\mathrm{e}^{2\mathrm{i}z(u-q)}\cdot\mathrm{e}^{\mathrm{i}tv^2/2}\,b(w,z)\,dudvdwdz.$$

Note that the substitution $x = 2u$ yields

$$\frac{1}{\pi}\int_{\mathbb{R}} \mathrm{e}^{2\mathrm{i}u(z-p)}du = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}x(z-p)}dx = \delta(z-p).$$

Therefore, integration over the variable u yields

$$f(q,p) = \frac{1}{\pi}\int_{\mathbb{R}^3} \delta(z-p)\mathrm{e}^{2\mathrm{i}pw}\mathrm{e}^{2\mathrm{i}v(q-w)}\mathrm{e}^{-2\mathrm{i}zq}\cdot\mathrm{e}^{\mathrm{i}tv^2/2}\,b(w,z)\,dvdwdz.$$

Using $\int_{\mathbb{R}} F(z)\delta(z-p)dz = F(p)$, we get

$$f(q,p) = \frac{1}{\pi}\int_{\mathbb{R}^2} \mathrm{e}^{2\mathrm{i}pw}\mathrm{e}^{2\mathrm{i}v(q-w)}\mathrm{e}^{-2\mathrm{i}pq}\cdot\mathrm{e}^{\mathrm{i}tv^2/2}\,b(w,p)\,dvdw.$$

Changing the integration variables, $w \mapsto \xi, v \mapsto \eta$, we obtain

$$f(q,p) = \frac{1}{\pi}\int_{\mathbb{R}^2} \mathrm{e}^{2\mathrm{i}(p-\eta)(\xi-q)}\cdot\mathrm{e}^{\mathrm{i}t\eta^2/2}\,b(\xi,p)\,d\xi d\eta. \tag{7.322}$$

(II) Computation of $f*c$. Set $g := f*c$. Again by (7.261) on page 607,

$$\begin{aligned} g(q,p) &= \frac{1}{\pi^2}\int_{\mathbb{R}^4} \mathrm{e}^{2\mathrm{i}p(w-u)}\mathrm{e}^{2\mathrm{i}v(q-w)}\mathrm{e}^{2\mathrm{i}z(u-q)}\cdot f(u,v)\mathrm{e}^{-\mathrm{i}t_0z^2/2}\,dudvdwdz \\ &= \frac{1}{\pi}\int_{\mathbb{R}^3} \delta(p-v)\mathrm{e}^{-2\mathrm{i}pu}\mathrm{e}^{2\mathrm{i}vq}\mathrm{e}^{2\mathrm{i}z(u-q)}\cdot f(u,v)\mathrm{e}^{-\mathrm{i}t_0z^2/2}\,dudvdz, \end{aligned}$$

after integrating over w. Integration over v implies

$$g(q,p) = \frac{1}{\pi}\int_{\mathbb{R}^2} \mathrm{e}^{-2\mathrm{i}pu}\mathrm{e}^{2\mathrm{i}pq}\mathrm{e}^{2\mathrm{i}z(u-q)}\,f(u,p)\mathrm{e}^{-\mathrm{i}t_0z^2/2}\,dudz.$$

(III) Inserting $f(u,p)$ from (7.322), we obtain that $g(q,p)$ is equal to the integral

$$\frac{1}{\pi^2}\int_{\mathbb{R}^4} \mathrm{e}^{2\mathrm{i}(p-z)(q-u)}\mathrm{e}^{2\mathrm{i}(p-\eta)(\xi-u)}\mathrm{e}^{\mathrm{i}t\eta^2/2}\mathrm{e}^{-\mathrm{i}t_0 z^2/2}\, b(\xi,p)\, d\xi d\eta du dz.$$

After integrating over u, we get

$$\frac{1}{\pi}\int_{\mathbb{R}^3} \delta(z+\eta-2p)\, \mathrm{e}^{2\mathrm{i}(p-z)q}\, \mathrm{e}^{2\mathrm{i}(p-\eta)\xi}\, \mathrm{e}^{\mathrm{i}t\eta^2/2}\, \mathrm{e}^{-\mathrm{i}t_0 z^2/2}\, b(\xi,p)\, d\xi d\eta dz.$$

Consequently, integrating over η, we obtain

$$g(q,p) = \frac{1}{\pi}\int_{\mathbb{R}^2} \mathrm{e}^{2\mathrm{i}(p-z)(q-\xi)}\, \mathrm{e}^{\mathrm{i}t(z-2p)^2/2}\, \mathrm{e}^{-\mathrm{i}t_0 z^2/2}\, b(\xi,p)\, d\xi dz.$$

This is the claim (7.276) on page 615.

7.33 *The Wick theorem.* Compute the moment $\langle x_1^4 x_2^2\rangle$ by using the Wick theorem.
Solution: To simplify notation, we write (ij) instead of $\langle y_i y_j\rangle$. We first compute $\langle y_1 y_2 y_3 y_4 y_5 y_6\rangle$. This is equal to

$$\begin{aligned}
&(12)(34)(56) + (12)(35)(46) + (12)(36)(45)\\
+\,&(13)(24)(56) + (13)(25)(46) + (13)(26)(45)\\
+\,&(14)(23)(56) + (14)(25)(36) + (14)(26)(35)\\
+\,&(15)(23)(46) + (15)(24)(36) + (15)(26)(34)\\
+\,&(16)(23)(45) + (16)(24)(35) + (16)(25)(34).
\end{aligned}$$

Setting $y_1 = y_2 = y_3 = y_4 := x_1$ and $y_5 = y_6 := x_2$, we get

$$\langle x_1^4 x_2^2\rangle = 3\langle x_1^2\rangle^2\langle x_2^2\rangle + 12\langle x_1^2\rangle\langle x_1 x_2\rangle^2.$$

By induction, we obtain that $\langle x_1 x_2 \cdots x_{2n}\rangle$ contains $s(2n)$ summands where $s(0) := 1$ and

$$s(2n) = (2n-1)s(2n-2), \qquad n = 1, 2, 3, \ldots$$

For example, $s(2) = 1, s(4) = 3, s(6) = 15, s(8) = 7 \cdot 15 = 105$.

7.34 *The rescaling trick.* Prove Prop. 7.48 on page 572.
Solution: Let $s \geq s_0$. By assumption, there exists a number $s_0 > 1$ such that the series $\zeta_A(s) = \sum_{n=1}^{\infty} \lambda_n^{-s}$ converges. Using Euler's gamma function

$$\Gamma(s) = \int_0^\infty t^{s-1}\mathrm{e}^{-t} dt,$$

we get

$$\Gamma(s)\zeta_A(s) = \int_0^\infty t^{s-1}\mathrm{e}^{t} \sum_{n=1}^{\infty} \lambda_n^{-s} dt.$$

Here, it is allowed to interchange summation with integration, by the majorant criterion for integrals (see page 493 of Vol. I). The substitution $t = \lambda_n u$ yields

$$\zeta_A(s) = \frac{1}{\Gamma(s)}\int_0^\infty u^{s-1} \sum_{n=1}^{\infty} \mathrm{e}^{-\lambda_n u} du.$$

Let $\gamma > 0$. Replacing $A \mapsto \gamma A$ and $\lambda_n \mapsto \gamma\lambda_n$, we obtain

$$\zeta_{\gamma A}(s) = \frac{1}{\Gamma(s)}\int_0^\infty u^{s-1} \sum_{n=1}^{\infty} \mathrm{e}^{-\gamma\lambda_n u} du.$$

The substitution $v = \gamma u$ yields

$$\zeta_{\gamma A}(s) = \frac{\gamma^{-s}}{\Gamma(s)} \int_0^\infty v^{s-1} \sum_{n=1}^\infty \mathrm{e}^{-\lambda_n v} dv = \gamma^{-s} \zeta_A(s).$$

Differentiating this with respect to s, we obtain

$$\zeta_{\gamma A}(s) = -\ln \gamma \cdot \gamma^{-s} \zeta_A(s) + \gamma^{-s} \zeta_A'(s).$$

After analytic continuation of the zeta function ζ_A, we get

$$\zeta_{\gamma A}'(0) = -\zeta_A(0) \ln \gamma + \zeta_A'(0).$$

This implies the desired result

$$\det(\gamma A) = \mathrm{e}^{-\zeta_{\gamma A}'(0)} = \gamma^{\zeta_A(0)} \mathrm{e}^{-\zeta_A'(0)} = \gamma^{\zeta_A(0)} \det A.$$

7.35 *Special Fourier–Laplace integrals.* Let $E, H \in \mathbb{R}$, and $\varepsilon > 0$. Prove the following:

(i) $\int_{-\infty}^\infty \mathrm{e}^{\mathrm{i}(E+\mathrm{i}\varepsilon)t/\hbar} \mathrm{e}^{-\mathrm{i}Ht/\hbar} \theta(t) dt = \frac{\mathrm{i}\hbar}{E+\mathrm{i}\varepsilon - H}$.

(ii) $\theta(t) \mathrm{e}^{-\mathrm{i}Ht/\hbar} = \frac{\mathrm{i}}{2\pi} PV \int_{-\infty}^\infty \frac{\mathrm{e}^{-\mathrm{i}(E+\mathrm{i}\varepsilon)t/\hbar}}{E+\mathrm{i}\varepsilon - H}\, dE$ for all $t \in \mathbb{R} \setminus \{0\}$.

Solution: To simplify notation, set $\hbar := 1$. Since $\lim_{t\to+\infty} \mathrm{e}^{-\varepsilon t} = 0$,

$$\int_0^\infty \mathrm{e}^{\mathrm{i}Et} \mathrm{e}^{-\varepsilon t} \mathrm{e}^{-\mathrm{i}Ht} dt = \lim_{N\to\infty} \frac{\mathrm{e}^{\mathrm{i}Et}\, \mathrm{e}^{-\varepsilon t} \mathrm{e}^{-\mathrm{i}Ht}}{\mathrm{i}(E+\mathrm{i}\varepsilon) - \mathrm{i}H} \Big|_0^N = \frac{\mathrm{i}}{E+\mathrm{i}\varepsilon - H}.$$

In order to get the inverse transformation, we formally apply the Fourier transform to (i). This yields

$$\theta(t) \mathrm{e}^{-\varepsilon t}\, \mathrm{e}^{-\mathrm{i}Ht} = \frac{1}{2\pi} \int_{-\infty}^\infty \mathrm{e}^{-\mathrm{i}Et} \cdot \frac{\mathrm{i}}{E+\mathrm{i}\varepsilon - H}\, dE, \qquad t \in \mathbb{R}. \tag{7.323}$$

However, the crux is that this integral does not exist because of too slow decay at infinity. Therefore, we have to argue more carefully. Observe first that the function

$$f(t) := \theta(t) \mathrm{e}^{-\varepsilon t} \mathrm{e}^{-\mathrm{i}Ht}, \qquad t \in \mathbb{R}$$

is not smooth. This is the reason for the failing of the Fourier transform, in the classical sense. However, since $|f|$ is bounded, the function f is a tempered distribution, and its Fourier transform is well defined. Thus, we may regard equation (7.323) as a short-hand notation for the Fourier transform in the sense of tempered distributions. To refine this argument, note that $\int_{\mathbb{R}} |f(t)|^2 dt < \infty$, that is, $f \in L_2(\mathbb{R})$. The Plancherel theorem tells us that the Fourier transform

$$f(t) = \lim_{R\to+\infty} \int_{-\mathbb{R}}^R \mathrm{e}^{-\mathrm{i}Et} \cdot \frac{\mathrm{i}}{E+\mathrm{i}\varepsilon - H}\, dE, \qquad t \in \mathbb{R}$$

is valid in the sense of the convergence in the Hilbert space $L_2(\mathbb{R})$ (see page 514). More precisely, applying the residue theorem, Cauchy's integration method implies that (ii) is valid for all $t \neq 0$. Argue as in Problem 12.1 of Vol. I.

7.36 *The Fourier–Laplace transform.* Prove Prop. 7.17 on page 498.
Hint: Use Problem 7.35. For interchanging limits, construct absolutely convergent majorant series. To this end, observe that the inequality $2ab \le a^2 + b^2$ (for real numbers a, b) yields

$$2|\langle\chi|\varphi_k\rangle\langle\varphi_k|\varphi\rangle| \le |\langle\chi|\varphi_k\rangle|^2 + |\langle\chi|\varphi_k\rangle|^2.$$

Finally, use the Parseval equation.

7.37 *Proof of Proposition 7.64 on page 642.* Solution: It is convenient to use the function

$$J := -\sum_{k=1}^{M} p_m \ln p_m$$

which differs from I by a positive factor. (Note that $\log_2 a = \ln a \cdot \log_2 \mathrm{e}$.) Since $\lim_{x\to+0} x \ln x = 0$, the function J is continuous on the closed simplex σ_M. For the partial derivatives of J on the interior of σ_M, we get $J_{p_m} = -\ln p_m - 1$ and

$$J_{p_m p_n} = -\frac{\delta_{mn}}{p_m}, \qquad m, n = 1, \ldots, M.$$

Thus, the symmetric matrix $(-J_{p_m p_n})$ is positive definite on the interior of σ_M, and hence the function $-J$ is convex, that is, J is concave on the interior of σ_M. By continuity, this remains true on σ_M. One checks easily that the maximal value of J is attained at an inner point of σ_M. From $J_{p_m} = 0$ for $m = 1, \ldots, M$, we get $p_1 = \ldots = p_M$.