MAT 561 Mathematical Physics II. Quantum Theory

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Part 1

Quantum Mechanics

CHAPTER 1

Review of classical mechanics

This is an extended content of Lectures 1-2. Details and proofs for Sections 1.1–1.2 can be found in the notes to MAT 560 class and in our forthcoming book with A. Kirillov, as well as in my QM book. For details on Section 1.3 see Section 2.8 in my QM book.

1.1. Lagrangian formulation

A mechanical system with a configuration space M is determined by the *Lagrangian* — a smooth, real-valued function L on TM (assuming no explicit dependence on time), and its motion is determined by the *principle of least action*.

Definition. For a path $\gamma\colon [t_0, t_1] \to M$, its action $S(\gamma) \in \mathbb{R}$ is defined by

$$S(\gamma) = \int_{t_0}^{t_1} L(\gamma(t), \dot{\gamma}(t), t)dt.$$

Principle of the Least Action. Classical trajectories are critical points of the action on the space of smooth paths with fixed endpoints

$$P(M)_{q_0,t_0}^{q_1,t_1} = \{\gamma\colon [t_0, t_1] \to M \mid \gamma(t_0) = q_0,\, \gamma(t_1) = q_1\},$$

usually abbreviated as $P(M)$.

A path $\gamma \in P(M)$ is a critical point of the action, if for any one-parameter family $\gamma_\varepsilon \in P(M)$ with $\gamma_0 = \gamma$, one has

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} S(\gamma_\varepsilon) = 0. \tag{1.1}$$

The critical points of the action are called *extremals*.

The equations of motion have the most simple form for the special choice of local coordinates on TM.

DEFINITION. Let (U, φ) be a coordinate chart on M with local coordinates $\boldsymbol{q} = (q^1, \dots, q^n)$. Coordinates

$$(\boldsymbol{q}, \boldsymbol{v}) = (q^1, \dots, q^n, v^1, \dots, v^n)$$

on a chart TU on TM, where $\boldsymbol{v} = (v^1, \dots, v^n)$ are coordinates in the fiber corresponding to the basis $\frac{\partial}{\partial q^1}, \dots, \frac{\partial}{\partial q^n}$ for $T_q M$, are called *standard coordinates.*

We denote standard coordinates by

$$(\boldsymbol{q}, \dot{\boldsymbol{q}}) = (q^1, \dots, q^n, \dot{q}^1, \dots, \dot{q}^n),$$

where the dot *does not* stand for the time derivative. However, when $\gamma'(t)$ is the tangential lift of a path $\gamma(t)$ in M, then in its coordinates the dot does stand for the time derivative.

THEOREM 1.1. *The equations of motion of a Lagrangian system (M, L) in standard coordinates on TM are given by the Euler-Lagrange equations*

$$\frac{\partial L}{\partial \boldsymbol{q}}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t)) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t))\right) = 0. \tag{1.2}$$

In expanded form, the Euler-Lagrange equations are given by the following system of second order ordinary differential equations:

$$\begin{aligned} \frac{\partial L}{\partial q^i}(\boldsymbol{q}, \dot{\boldsymbol{q}}) &= \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}(\boldsymbol{q}, \dot{\boldsymbol{q}})\right) \\ &= \sum_{j=1}^{n}\left(\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}(\boldsymbol{q}, \dot{\boldsymbol{q}})\, \ddot{q}^j + \frac{\partial^2 L}{\partial \dot{q}^i \partial q^j}(\boldsymbol{q}, \dot{\boldsymbol{q}})\, \dot{q}^j\right) + \frac{\partial^2 L}{\partial \dot{q}^i \partial t}(\boldsymbol{q}, \dot{\boldsymbol{q}}), \quad i = 1, \dots, n. \end{aligned} \tag{1.3}$$

In order for this system to be solvable for the highest derivatives, the symmetric $n \times n$ matrix

$$H_L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \left\{\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}(\boldsymbol{q}, \dot{\boldsymbol{q}})\right\}_{i,j=1}^{n}$$

should be invertible on TU.

DEFINITION. A Lagrangian system (M, L) is called *non-degenerate* if for every coordinate chart U on M the matrix $H_L(\boldsymbol{q}, \dot{\boldsymbol{q}})$ is invertible on TU. Otherwise the Lagrangian system is called *singular*.

Inverting the matrix H_L, we can write Euler-Lagrange equations for a non-degenerate Lagrangian in the form

$$\ddot{q}^i = F^i(\boldsymbol{q}, \dot{\boldsymbol{q}}, t), \quad i = 1, \ldots, n. \tag{1.4}$$

The Newtonian space E^3 is a 3-dimensional Riemannian manifold which is isometric to the standard Euclidean space $\mathbb{R}^3$ with the usual metric. However, a choice of an isometry between E^3 and $\mathbb{R}^3$ is not fixed, and such isometry is called a *frame* in E^3. Any two choices of a frame in E^3 are related by an affine transformation

$$\boldsymbol{r} \mapsto g \cdot \boldsymbol{r} + \boldsymbol{r}_0, \qquad g \in \mathrm{O}(3), \quad \boldsymbol{r}_0 \in \mathbb{R}^3.$$

The Newtonian *spacetime* is the direct product $E^3 \times \mathbb{R}$, and its points are called *events*. Two events $(\boldsymbol{r}, t)$ and $(\boldsymbol{r}', t')$ are called *simultaneous* if $t = t'$. The distance is defined only for simultaneous events and is the Euclidean distance $|\boldsymbol{r} - \boldsymbol{r}'|$.

An *inertial* reference frame in the Newtonian spacetime $E^3 \times \mathbb{R}$ is an isomorphism $E^3 \times \mathbb{R} \to \mathbb{R}^3 \times \mathbb{R}$ which has the following properties.

- It preserves the notion of simultaneous events and the distance between such events.
- It preserves time intervals and time direction.

Any two inertial frames are related by.the Galilean transformation

$$\begin{pmatrix} \boldsymbol{r} \\ t \end{pmatrix} \mapsto \begin{pmatrix} g \cdot \boldsymbol{r} + \boldsymbol{v}t + \boldsymbol{r}_0 \\ t + t_0 \end{pmatrix} \tag{1.5}$$

for some $g \in \mathrm{O}(3)$, $\boldsymbol{r}_0 \in \mathbb{R}^3$, $\boldsymbol{v} \in \mathbb{R}^3$, $t_0 \in \mathbb{R}$. They form the *Galilean group* $G = \mathrm{E}(3) \ltimes \mathbb{R}^4$, a semidirect product of the Euclidean group $\mathrm{E}(3)$ and the abelian group $\mathbb{R}^4$ of the uniform motions of spacetime. The Galilean group is a 10-dimensional Lie group. Its action on the spacetime can be described by the following subgroup in $\mathrm{GL}(5, \mathbb{R})$:

$$\begin{pmatrix} \boldsymbol{r} \\ t \\ 1 \end{pmatrix} \mapsto \begin{pmatrix} g & \boldsymbol{v} & \boldsymbol{r}_0 \\ 0 & 1 & t_0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{r} \\ t \\ 1 \end{pmatrix} = \begin{pmatrix} g \cdot \boldsymbol{r} + \boldsymbol{v}t + \boldsymbol{r}_0 \\ t + t_0 \\ 1 \end{pmatrix}. \tag{1.6}$$

One of the fundamental principles of Newtonian mechanics is the relativity principle, formulated by Galileo.

Galileo's Relativity Principle. The laws of motion are invariant with respect to the Galilean group.

In particular, it shows that in Newtonian mechanics, the space is *homogeneous* (laws of nature are invariant under translations) and *isotropic* (invariance under rotations) and the time is *homogeneous*. However, the time in Newtonian mechanics is absolute (up to translations).

The Galilean invariance imposes restrictions on Lagrangians of mechanical systems. In particular, the Lagrangian of a *closed system*[1] in Newtonian mechanics does not explicitly depend on time.

Physical systems are described by special Lagrangians, in agreement with the experimental facts about the motion of material bodies.

Example 1.1 (Free particle in Euclidean space). The configuration space for a free particle is $M = \mathbb{R}^3$, and the Lagrangian is given by

$$L = \tfrac{1}{2} m \dot{\boldsymbol{r}}^2.$$

Here $m > 0$ is the mass of a particle[2] and $\dot{\boldsymbol{r}}^2 = |\dot{\boldsymbol{r}}|^2$ is the square of the magnitude of the velocity vector $\dot{\boldsymbol{r}} \in T_{\boldsymbol{r}}\mathbb{R}^3 \simeq \mathbb{R}^3$.

This system is invariant under Galilean transformations. Indeed, under the Galilean transformation $\boldsymbol{r} \mapsto \boldsymbol{r} + \boldsymbol{v}t$ we have

$$L = \tfrac{1}{2} m \dot{\boldsymbol{r}}^2 \mapsto L' = \tfrac{1}{2} m (\dot{\boldsymbol{r}} + \boldsymbol{v})^2 = L + \frac{d}{dt}(m \boldsymbol{r}\boldsymbol{v} + \tfrac{1}{2}\boldsymbol{v}^2 t), \tag{1.7}$$

so that Lagrangians L and L' have the same equations of motion

Specifically, Euler-Lagrange equations give *Newton's law of inertia*,

$$\ddot{\boldsymbol{r}} = 0.$$

Also, it is not hard to show that $\ddot{\boldsymbol{r}} = 0$ is the only possible equation of motion in $\mathbb{R}^3$ which is invariant under the Galilean group.

Example 1.2 (Harmonic oscillator). Consider a particle of mass m on a line $M = \mathbb{R}$ in a potential field $V(x) = \frac{1}{2}kx^2$, i.e. with the Lagrangian

$$L(x, \dot{x}) = \tfrac{1}{2} m \dot{x}^2 - \tfrac{1}{2} k x^2. \tag{1.8}$$

The Euler–Lagrange equation of motion takes the form

$$m\ddot{x} = -kx.$$

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[1]A system is called closed if its motion is not influenced by the outside material bodies.

[2]Condition $m > 0$ is necessary for the action functional to be bounded from below.

Denoting $\omega = \sqrt{k/m}$, we can rewrite this equation in the familiar form

$$\ddot{x} + \omega^2 x = 0.$$

Solutions of this equation are

$$x = A\cos(\omega t + \alpha)$$

and describe a periodic motion with frequency ω and with period $T = 2\pi/\omega$.

This system is called the *harmonic oscillator* and is probably the simplest mechanical system after the free particle.

EXAMPLE 1.3 (Particle in an external potential field). Here $M = \mathbb{R}^3$ and

$$L = \tfrac{1}{2}m\dot{\boldsymbol{r}}^2 - V(\boldsymbol{r}),$$

with the potential energy $V(\boldsymbol{r})$. Equations of motion are Newton's equations

$$m\ddot{\boldsymbol{r}} = \boldsymbol{F} = -\frac{\partial V}{\partial \boldsymbol{r}}.$$

If $V = V(r)$ is a function only of the distance $r = |\boldsymbol{r}|$, the potential field is called *central*. In particular, when

$$V(r) = -G\frac{mM}{r},$$

where G is the gravitational constant, describes a particle in the gravitational field generated by a body of mass M (located at $\boldsymbol{r} = 0$).

1.2. Hamiltonian formulation

In this approach, a state of the system is described by a point in the cotangent bundle T^*M of an n-dimensional manifold M. As in case of the tangent bundle, a choice of local coordinates $\boldsymbol{q} = (q^1, \dots, q^n)$ on an open chart $U \subset M$ defines, for any point $x \in U$, a basis dq^i in the cotangent space T_x^*M and thus a choice of coordinates

$$(\boldsymbol{p}, \boldsymbol{q}) = (p_1, \dots, p_n, q^1, \dots, q^n)$$

on T^*U. Such coordinates will be called *standard coordinates.*

DEFINITION. Legendre transform associated with the Lagrangian L is the fiberwise mapping $\tau_L \colon TM \to T^*M$ given in the standard coordinates by

$$\tau_L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = (\boldsymbol{p}, \boldsymbol{q}), \quad \text{where} \quad \boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}, \dot{\boldsymbol{q}}).$$

The element $\boldsymbol{p} \in T_{\boldsymbol{q}}^*M$ is called the *momentum*, and the space T^*M is called the *phase space.*

The mapping τ_L is a local diffeomorphism if and only if the Lagrangian L is non-degenerate.

EXAMPLE 1.4. Let $M = \mathbb{R}^n$ and let the Lagrangian be given by

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \tfrac{1}{2} m \dot{\boldsymbol{q}}^2 - V(\boldsymbol{q}).$$

In this case, it is immediate that the Legendre transform is given by $p_i = m\dot{q}^i$, or $\boldsymbol{p} = m\dot{\boldsymbol{q}}$.

Let (M, L) be a Lagrangian system, and assume that Legendre τ_L is a diffeomorphism. Then equations of motion, rewritten in terms of the phase space T^*M, take an especially simple form.

DEFINITION. The *Hamiltonian* function $H\colon T^*M \to \mathbb{R}$, associated with the Lagrangian L, is defined by

$$H \circ \tau_L = \dot{\boldsymbol{q}}\,\frac{\partial L}{\partial \dot{\boldsymbol{q}}} - L.$$

In other words, the Hamiltonian is the energy E_L in terms of the coordinates on T^*M. system. Explicitly,

$$H(\boldsymbol{p}, \boldsymbol{q}) = \left(\boldsymbol{p}\dot{\boldsymbol{q}} - L(\boldsymbol{q}, \dot{\boldsymbol{q}})\right)\Big|_{\boldsymbol{p}=\frac{\partial L}{\partial \dot{\boldsymbol{q}}}}, \tag{1.9}$$

where $\dot{\boldsymbol{q}}$ is a function of $\boldsymbol{p}$ and $\boldsymbol{q}$ defined by the equation $\boldsymbol{p} = \dfrac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}, \dot{\boldsymbol{q}})$.

THEOREM 1.2. *Suppose that the Legendre transform $\tau_L\colon TM \to T^*M$ is a diffeomorphism. Then Euler-Lagrange equations on TM are equivalent to the following system of first order differential equations in standard coordinates on T^*M:*

$$\begin{aligned} \dot{p}_i &= -\frac{\partial H}{\partial q^i}, \\ \dot{q}^i &= \frac{\partial H}{\partial p_i}, \end{aligned} \tag{1.10}$$

where $i = 1, \dots, n$. These equations are called Hamilton's equations (or canonical equations).

EXAMPLE 1.5. Consider the particle of mass m in a potential field $V(\boldsymbol{r})$ in $\mathbb{R}^3$. In this case the configuration space is $M = \mathbb{R}^3$ and the Lagrangian is given by

$$L = \tfrac{1}{2} m \dot{\boldsymbol{r}}^2 - V(\boldsymbol{r}) = T - V, \quad \boldsymbol{r} \in \mathbb{R}^3.$$

In this case, the momenta are

$$\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{r}}} = m\dot{\boldsymbol{r}}. \tag{1.11}$$

Thus the Legendre transform $\tau_L \colon T\mathbb{R}^3 \to T^*\mathbb{R}^3$ is a global diffeomorphism, linear on the fibers, and

$$H(\boldsymbol{p}, \boldsymbol{r}) = (\boldsymbol{p}\dot{\boldsymbol{r}} - L)\big|_{\dot{\boldsymbol{r}}=\frac{\boldsymbol{p}}{m}} = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r}) = T + V.$$

In this case Hamilton's equations are equivalent to Newton's equations.

In general, consider the Lagrangian

$$L = \sum_{i,j=1}^{n} \tfrac{1}{2} a_{ij}(\boldsymbol{q})\dot{q}^i\dot{q}^j - V(\boldsymbol{q}),\ \ \boldsymbol{q} \in \mathbb{R}^n,$$

where $A(\boldsymbol{q}) = \{a_{ij}(\boldsymbol{q})\}_{i,j=1}^{n}$ is a symmetric $n \times n$ matrix. We have

$$p_i = \frac{\partial L}{\partial \dot{q}^i} = \sum_{j=1}^{n} a_{ij}(\boldsymbol{q})\dot{q}^j, \quad i = 1, \dots, n,$$

and the Legendre transform is linear on the fibers. It is a global diffeomorphism if and only if the matrix $A(\boldsymbol{q})$ is non-degenerate for all $\boldsymbol{q} \in \mathbb{R}^n$. In this case,

$$H(\boldsymbol{p}, \boldsymbol{q}) = (\boldsymbol{p}\,\dot{\boldsymbol{q}} - L(\boldsymbol{q}, \dot{\boldsymbol{q}}))\big|_{\boldsymbol{p}=\frac{\partial L}{\partial \dot{\boldsymbol{q}}}} = \sum_{i,j=1}^{n} \tfrac{1}{2} a^{ij}(\boldsymbol{q})p_i p_j + V(\boldsymbol{q}),$$

where $\{a^{ij}(\boldsymbol{q})\}_{i,j=1}^{n} = A^{-1}(\boldsymbol{q})$ is the inverse matrix.

Since T^*M is a symplectic manifold, Hamilton's equations on the phase space can be rewritten in an invariant form. Recall, that a manifold $\mathscr{M}$ is called a symplectic manifold, if it comes with a symplectic form: a closed, non-degenerate 2-form $\omega \in \Omega^2(\mathscr{M})$.

The basic example of a symplectic manifold is T^*M with the symplectic form

$$\omega = d\boldsymbol{p} \wedge d\boldsymbol{q} = \sum_{i=1}^{n} dp_i \wedge dq^i. \tag{1.12}$$

By the Darboux theorem, any symplectic manifold admits local coordinates p_i, q^i such that the symplectic form takes the form (1.12). Such coordinates are called *canonical or Darboux coordinates.*

On a symplectic manifold $\mathscr{M}$, the symplectic form ω defines an isomorphism

$$J\colon T^*\mathscr{M} \to T\mathscr{M} \tag{1.13}$$

between tangent and cotangent bundles, given by

$$\omega(u, J\vartheta) = \langle u, \vartheta\rangle, \qquad u \in T_x\mathscr{M},\ \vartheta \in T_x^*\mathscr{M},$$

or equivalently

$$\omega(u_1, u_2) = \langle u_1, J^{-1}(u_2)\rangle, \quad u_1, u_2 \in T_x\mathscr{M}.$$

The mapping J induces the isomorphism

$$\Omega^1(\mathscr{M}) \simeq \mathrm{Vect}(\mathscr{M})$$

between the infinite-dimensional vector spaces of one-forms and vector fields on $\mathscr{M}$, which is linear over the ring $C^\infty(\mathscr{M})$. Namely, if ϑ is a one-form, then the corresponding vector field $X = J(\vartheta)$ on $\mathscr{M}$ satisfies

$$\omega(Y, X) = \langle Y, \vartheta\rangle \quad \text{for all} \quad Y \in \mathrm{Vect}(\mathscr{M}), \tag{1.14}$$

and, correspondingly,

$$\vartheta = J^{-1}(X) = -\imath_X\omega. \tag{1.15}$$

As a corollary, we see that on a symplectic manifold $\mathscr{M}$ any function $H \in C^\infty(\mathscr{M})$ defines a vector field $X_H = J(dH)$, called the *Hamiltonian vector field*. This vector field satisfies

$$dH = -\imath_{X_H}\omega. \tag{1.16}$$

In canonical coordinates, this vector field is given by

$$X_H = \sum_{i=1}^n \left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i}\frac{\partial}{\partial p_i}\right) = \frac{\partial H}{\partial \boldsymbol{p}}\frac{\partial}{\partial \boldsymbol{q}} - \frac{\partial H}{\partial \boldsymbol{q}}\frac{\partial}{\partial \boldsymbol{p}}. \tag{1.17}$$

In particular,

$$X_{\boldsymbol{p}} = \frac{\partial}{\partial \boldsymbol{q}} \quad \text{and} \quad X_{\boldsymbol{q}} = -\frac{\partial}{\partial \boldsymbol{p}}.$$

Thus we see that in case $\mathscr{M} = T^*M$ and $H = \boldsymbol{p}\dot{\boldsymbol{q}} - L$, the Hamilton's equations (1.10), can be rewritten in the following simple form

$$\dot{x} = X_H, \tag{1.18}$$

where $x = (\boldsymbol{p}, \boldsymbol{q}) \in T^*M$.

DEFINITION. A *Hamiltonian system* is the pair $(\mathscr{M}, H)$, where $\mathscr{M}$ is a symplectic manifold and $H \in C^\infty(\mathscr{M})$.

If the vector field X_H on $\mathscr{M}$ is complete, then the corresponding one-parameter group $\{g_t\}_{t\in\mathbb{R}}$ of diffeomorphisms of $\mathscr{M}$ generated by X_H is called the *Hamiltonian phase flow* generated by H. It is defined by $g_t(x) = x(t)$, where $x(t)$ is a solution of Hamilton's equations satisfying $x(0) = x$.

THEOREM 1.3. *Hamiltonian phase flow on a symplectic manifold $\mathscr{M}$ preserves the symplectic form.*

The canonical symplectic form ω on a symplectic manifold $\mathscr{M}$ defines the volume form

$$\frac{\omega^n}{n!} = \frac{1}{n!}\underbrace{\omega \wedge \cdots \wedge \omega}_{n}, \quad n = \dim \mathscr{M}/2, \tag{1.19}$$

on $\mathscr{M}$, called the *Liouville's volume form.*

COROLLARY 1.4 (Liouville's theorem). *The Hamiltonian phase flow on T^*M preserves Liouville's volume form.*

With a symplectic manifold $\mathscr{M}$ one associates the algebra of *classical observables*, an algebra $\mathcal{A} = C^\infty(\mathscr{M})$ of smooth functions. It is a commutative with respect to pointwise multiplication. Since $\mathscr{M}$ is a symplectic manifold, the algebra $\mathcal{A}$ has an additional structure, called the *Poisson bracket.*

Recall that on a symplectic manifold any function f gives rise to a Hamiltonian vector field $X_f = J(df)$, defined by (1.14):

$$\omega(v, X_f) = \langle v, df\rangle = \partial_v f, \quad v \in \operatorname{Vect}\mathscr{M}.$$

DEFINITION. Let $f, g \in \mathcal{A}$. Their Poisson bracket $\{f, g\}\mathcal{A}$ is defined by

$$\{f, g\} = \partial_{X_f} g = \omega(X_f, X_g). \tag{1.20}$$

This definition immediately implies that for any observable H, we have

$$\partial_{X_H} f = \{H, f\}. \tag{1.21}$$

It follows from (1.17) that in canonical coordinates the Poisson bracket takes the form

$$\{f, g\} = \sum_{i=1}^{n}\left(\frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i} - \frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i}\right) = \frac{\partial f}{\partial \boldsymbol{p}}\frac{\partial g}{\partial \boldsymbol{q}} - \frac{\partial f}{\partial \boldsymbol{q}}\frac{\partial g}{\partial \boldsymbol{p}}. \tag{1.22}$$

In particular, we have the relations

$$\begin{aligned}\{p_i, p_j\} &= \{q^i, q^j\} = 0,\\ \{p_i, q^j\} &= \delta_i^j, \qquad i, j = 1, \dots n,\end{aligned} \tag{1.23}$$

which are called *canonical Poisson brackets.*

THEOREM 1.5. *The Poisson bracket map* $\{\ ,\ \} : \mathcal{A} \times \mathcal{A} \to \mathcal{A}$ *has the following properties.*

(1) *It satisfies the Leibniz rule:*

$$\{f, gh\} = \{f, g\}h + g\{f, h\}.$$

(2) *It is skew-symmetric:* $\{f, g\} = -\{g, f\}$.

(3) *It satisfies Jacobi identity:*

$$\{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} = 0.$$

(4)

$$X_{\{f,g\}} = [X_f, X_g],$$

where the $[\, ,\,]$ *in the right hand side is the commutator of vector fields, which is defined by*

$$\partial_{[\xi,\eta]} = \partial_\xi \partial_\eta - \partial_\eta \partial_\xi.$$

Parts (2)–(4) of the theorem can be restated as follows.

COROLLARY 1.6. *The Poisson bracket defines on the algebra of classical observables* $\mathcal{A} = C^\infty(\mathscr{M})$ *a structure of a Lie algebra, and the map* $\mathcal{A} \to \mathrm{Vect}(\mathscr{M})\colon f \mapsto X_f$ *is a morphism of Lie algebras.*

REMARK 1.1. A manifold P with a bilinear operation $\{\, ,\, \}$ on $C^\infty(P)$, satisfying properties (1)–(3) of Theorem 1.5 is called a *Poisson manifold*; thus, Theorem 1.5 can be restated by saying that any symplectic manifold is also automatically a Poisson manifold. Converse is obviously false (e.g., one can take the Poisson bracket to be identically zero).

Using Poisson bracket, one can rewrite Hamiltonian equations of motion in terms of observables as follows.

LEMMA 1.1. *Let* $(\mathscr{M}, H)$ *be a Hamiltonian system. Let* $x(t)$ *be a classical trajectory, i.e. a solution of Hamilton's equations. Then for any observable* $f \in \mathcal{A}$*, we have*

$$\frac{d}{dt} f(x(t)) = \{H, f\}(x(t)). \tag{1.24}$$

DEFINITION. A classical observable $f \in \mathcal{A}$ is an integral of motion (or conserved quantity) if it is constant on classical trajectories: $\frac{d}{dt} f(x(t)) = 0$.

COROLLARY 1.7. *An observable* $f \in C^\infty(\mathscr{M})$ *is an integral of motion of a system* $(\mathscr{M}, H)$ *if and only if* $\{H, f\} = 0$.

In particular, this implies that H itself is an integral of motion: the Poisson bracket is skew-symmetric, so $\{H, H\} = 0$.

1.3. Measurement in classical mechanics

A measurement of a classical system is the result of a physical experiment, which gives numerical values for classical observables. The experiment consists of creating certain conditions that can be repeated over and over. These conditions define a *state* of the system, if they yield probability distributions for the values of all observables of the system.

Mathematically, a state μ on the algebra $\mathcal{A} = C^\infty(\mathscr{M})$ of classical observables on the phase space $\mathscr{M}$ is the assignment

$$\mathcal{A} \ni f \mapsto \mu_f \in \mathscr{P}(\mathbb{R}),$$

where $\mathscr{P}(\mathbb{R})$ is a set of probability measures on $\mathbb{R}$ — Borel measures on $\mathbb{R}$ such that the total measure of $\mathbb{R}$ is 1. For every Borel subset $E \subseteq \mathbb{R}$ the quantity $0 \leq \mu_f(E) \leq 1$ is a probability that in the state μ an observable f takes values in E. The *expectation value* of an observable f in the state μ is given by the Lebesgue-Stieltjes integral

$$\mathsf{E}_\mu(f) = \int_{-\infty}^{\infty} \lambda d\mu_f(\lambda),$$

where $\mu_f(\lambda) = \mu_f((-\infty, \lambda))$ is a distribution function of the measure $d\mu_f$. The correspondence $f \mapsto \mu_f$ should satisfy the following natural properties.

S1. $|\mathsf{E}_\mu(f)| < \infty$ for $f \in \mathcal{A}_0$ — the subalgebra of bounded observables.

S2. $\mathsf{E}_\mu(1) = 1$, where 1 is the unit in $\mathcal{A}$.

S3. For all $a, b \in \mathbb{R}$ and $f, g \in \mathcal{A}$,

$$\mathsf{E}_\mu(af + bg) = a\mathsf{E}_\mu(f) + b\mathsf{E}_\mu(g),$$

if both $\mathsf{E}_\mu(f)$ and $\mathsf{E}_\mu(g)$ exist.

S4. If $f_1 = \varphi \circ f_2$ with smooth $\varphi : \mathbb{R} \to \mathbb{R}$, then for every Borel subset $E \subseteq \mathbb{R}$,

$$\mu_{f_1}(E) = \mu_{f_2}(\varphi^{-1}(E)).$$

It follows from property **S4** and the definition of the Lebesgue-Stieltjes integral that

$$\mathsf{E}_\mu(\varphi(f)) = \int_{-\infty}^{\infty} \varphi(\lambda) d\mu_f(\lambda). \tag{1.25}$$

In particular, $\mathsf{E}_\mu(f^2) \geq 0$ for all $f \in \mathcal{A}$, so that the states define normalized, positive, linear functionals on the subalgebra $\mathcal{A}_0$.

Assuming that the functional E_μ extends to the space of bounded, piecewise continuous functions on $\mathscr{M}$, and satisfies (1.25) for measurable functions φ, one can recover the distribution function from the expectation values by the formula

$$\mu_f(\lambda) = \mathsf{E}_\mu\left(\theta(\lambda - f)\right), \tag{1.26}$$

where $\theta(x)$ is the Heavyside step function,

$$\theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x \leq 0. \end{cases}$$

Every probability measure $d\mu$ on $\mathscr{M}$ defines the state on $\mathcal{A}$ by assigning[3] to every observable f a probability measure $\mu_f = f_*(\mu)$ on $\mathbb{R}$ — a push-forward of the measure $d\mu$ on $\mathscr{M}$ by the mapping $f : \mathscr{M} \to \mathbb{R}$. It is defined by $\mu_f(E) = \mu(f^{-1}(E))$ for every Borel subset $E \subseteq \mathbb{R}$, and has the distribution function

$$\mu_f(\lambda) = \mu(f^{-1}(-\infty, \lambda)) = \int_{\mathscr{M}_\lambda(f)} d\mu,$$

where $\mathscr{M}_\lambda(f) = \{x \in \mathscr{M} : f(x) < \lambda\}$. It follows from the Fubini theorem that

$$E_\mu(f) = \int_{-\infty}^{\infty} \lambda d\mu_f(\lambda) = \int_{\mathscr{M}} f d\mu. \tag{1.27}$$

[3]There should be no confusion in denoting the state and the measure by μ.

It turns out that probability measures on $\mathscr{M}$ are essentially the only examples of states. Namely, for a locally compact topological space $\mathscr{M}$ the Riesz-Markov theorem asserts that for every positive, continuous linear functional l on the space $C_{\mathrm{c}}(\mathscr{M})$ of continuous functions on $\mathscr{M}$ with compact support, there is a unique regular Borel measure $d\mu$ on $\mathscr{M}$ such that

$$l(f) = \int_{\mathscr{M}} f d\mu \quad \text{for all} \quad f \in C_{\mathrm{c}}(\mathscr{M}).$$

This leads to the following definition of the states in classical mechanics.

DEFINITION. The set of states $\mathcal{S}$ for a Hamiltonian system with the phase space $\mathscr{M}$ is the convex set $\mathscr{P}(\mathscr{M})$ of all probability measures on $\mathscr{M}$. The states corresponding to Dirac measures $d\mu_x$ supported at points $x \in \mathscr{M}$ are called *pure states*, and the phase space $\mathscr{M}$ is also called the *space of states*[4]. All other states are called *mixed states*. A process of measurement in classical mechanics is the correspondence

$$\mathcal{A} \times \mathcal{S} \ni (f, \mu) \mapsto \mu_f = f_*(\mu) \in \mathscr{P}(\mathbb{R}),$$

which to every observable $f \in \mathcal{A}$ and state $\mu \in \mathcal{S}$ assigns a probability measure μ_f on $\mathbb{R}$ — a push-forward of the measure $d\mu$ on $\mathscr{M}$ by f. For every Borel subset $E \subseteq \mathbb{R}$ the quantity $0 \leq \mu_f(E) \leq 1$ is the probability that for a system in the state μ the result of a measurement of the observable f is in the set E. The expectation value of an observable f in a state μ is given by (1.27).

Pure states are characterized by the property that a measurement of every observable always gives a well-defined result. Namely, let

$$\sigma_\mu^2(f) = \mathsf{E}_\mu\left((f - \mathsf{E}_\mu(f))^2\right) = \mathsf{E}_\mu(f^2) - \mathsf{E}_\mu(f)^2 \geq 0$$

be the *variance* of an observable f in the state μ. The following result is easy to prove.

LEMMA 1.2. *Pure states are the only states in which every observable has zero variance.*

In particular, a *mixture* of pure states $d\mu_x$ and $d\mu_y$, $x, y \in \mathscr{M}$, is a mixed state with

$$d\mu = \alpha\, d\mu_x + (1 - \alpha) d\mu_y, \quad 0 < \alpha < 1,$$

so that $\sigma_\mu^2(f) > 0$ for every observable f such that $f(x) \neq f(y)$.

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[4]The space of pure states, to be precise.

Pure states are used for systems consisting of few interacting particles (say, a motion of planets in celestial mechanics), when it is possible to measure all coordinates and momenta. Mixed states necessarily appear for *macroscopic* systems, when it is impossible to measure all coordinates and momenta[5].

Remark 1.2. As a topological space, the space of states $\mathscr{M}$ can be reconstructed from the commutative algebra $\mathcal{A}$ of classical observables (equipped with the $\mathbb{C}^*$-algebra structure) by Gelfand-Naimark theorem. It states that every commutative $\mathbb{C}^*$-algebra (not necessarily with a unit) is $\mathbb{C}^*$-isometrically isomorphic to the algebra of continuous functions that vanish at infinity[6] on a locally compact Hausdorff space, the so-called spectrum of $\mathcal{A}$[7].

1.4. Hamilton's and Liouville's dynamical pictures

There are two equivalent ways of describing the dynamics — the time evolution of a Hamiltonian system $((\mathscr{M}, \{\ ,\ \}), H)$ with the algebra of observables $\mathcal{A} = C^\infty(\mathscr{M})$ and the set of states $\mathcal{S} = \mathscr{P}(\mathscr{M})$. Here we assume that the Hamiltonian phase flow g_t exists for all times, and that the phase space $\mathscr{M}$ carries a volume form dx invariant under the phase flow[8].

Hamilton's Description of Dynamics. States do not depend on time, and time evolution of observables is given by Hamilton's equations of motion,

$$\frac{d\mu}{dt} = 0, \quad \mu \in \mathcal{S} \quad \text{and} \quad \frac{df}{dt} = \{H, f\}, \quad f \in \mathcal{A}.$$

The expectation value of an observable f in the state μ at time t is given by

$$\mathsf{E}_\mu(f_t) = \int_{\mathscr{M}} f \circ g_t \, d\mu = \int_{\mathscr{M}} f(g_t(x))\rho(x)dx,$$

where $\rho(x) = \dfrac{d\mu}{dx}$ is the Radon-Nikodim derivative. In particular, the expectation value of f in the pure state $d\mu_x$ corresponding to the point $x \in \mathscr{M}$

[5]Typically, a macroscopic system consists of $N \sim 10^{23}$ molecules. Macroscopic systems are studied in classical statistical mechanics.

[6]If $\mathcal{A}$ is unital, the spectrum of $\mathcal{A}$ is compact.

[7]If $\mathcal{A}$ is an algebra of all continuous complex-valued functions on a compact topological space X, then its spectrum is X. If, however, a $\mathbb{C}^*$-algebra $\mathcal{A}$ is an algebra of bounded continuous functions on a space X, then its spectrum is the Stone-Čech compactification of X.

[8]It is Liouville's volume form when the Poisson structure on $\mathscr{M}$ is non-degenerate.

is $f(g_t(x))$. Hamilton's picture is commonly used for mechanical systems describing few interacting particles.

Liouville's Description of Dynamics. The observables do not depend on time

$$\frac{df}{dt} = 0, \quad \in \mathcal{A},$$

and states $d\mu(x) = \rho(x)dx$ satisfy the Liouville's equation

$$\frac{d\rho}{dt} = -\{H, \rho\}, \quad \rho(x)dx \in \mathcal{S}.$$

Here the Radon-Nikodim derivative $\rho(x) = \dfrac{d\mu}{dx}$ and the Liouville's equation are both understood in the distributional sense. The expectation value of an observable f in the state μ at time t is given by

$$\mathsf{E}_{\mu_t}(f) = \int_{\mathscr{M}} f(x)\rho(g_{-t}(x))dx.$$

Liouville's picture, where states are described by the distribution functions $\rho(x)$ — positive distributions on $\mathscr{M}$ corresponding to probability measures $\rho(x)dx$ — is commonly used in statistical mechanics. The equality

$$\mathsf{E}_{\mu}(f_t) = \mathsf{E}_{\mu_t}(f) \quad \text{for all} \quad f \in \mathcal{A}, \;\; \mu \in \mathcal{S}$$

follows from the invariance of the volume form dx and the change of variables, and expresses the equivalence between Liouville's and Hamilton's descriptions of dynamics.

Problem 1.1. Prove all results in Section 1.3.

CHAPTER 2

Observables and states in quantum mechanics

Quantum mechanics studies the microworld — the physical laws at an atomic scale — that cannot be adequately described by classical mechanics. Thus classical mechanics and classical electrodynamics cannot explain the stability of atoms and molecules. Neither can these theories reconcile different properties of light, its wave-like behavior in interference and diffraction phenomena, and its particle-like behavior in photo-electric emission and scattering by free photons. Moreover, in classical physics it is always assumed that one can neglect the disturbances the measurement brings upon a system, whereas in the microworld every experiment results in interaction with the system and thus disturbs its properties. In particular, there exist observables which cannot be measured simultaneously.

Still, it is quite remarkable that we can formulate quantum mechanics using the general notions of states, observables, and time evolution, described in Chapter 1! Since commutativity of the algebra of observables $\mathcal{A}$ brings us to the realm of classical mechanics, in order to get a different realization of observables and states we must assume that the $\mathbb{C}^*$-algebra associated with the quantum observables is no longer commutative. A basic example of a non-commutative $\mathbb{C}^*$-algebra is the algebra of all bounded operators on a complex Hilbert space, and it turns out that it is this algebra that is used in quantum mechanics.

2.1. Dirac–von Neumann axioms

The following axioms constitute the basis of quantum mechanics.

A1. With every *quantum system* there is associated an infinite-dimensional separable complex Hilbert space $\mathscr{H}$, in physics terminology called the *space of states*[1]. The Hilbert space of a *composite quantum system* is a tensor product of Hilbert spaces of component systems.

[1]The space of pure states, to be precise.

A2. The set of *observables* $\mathscr{A}$ of a quantum system with the Hilbert space $\mathscr{H}$ consists of all self-adjoint operators on $\mathscr{H}$. The subset $\mathscr{A}_0 = \mathscr{A} \cap \mathscr{L}(\mathscr{H})$ of bounded observables is a vector space over $\mathbb{R}$.

A3. The set of *states* $\mathscr{S}$ of a quantum system with a Hilbert space $\mathscr{H}$ consists of all positive (and hence self-adjoint) trace class operators M with $\operatorname{Tr} M = 1$. *Pure states* are projection operators onto one-dimensional subspaces of $\mathscr{H}$. For $\psi \in \mathscr{H}$, $\|\psi\| = 1$, the corresponding projection onto $\mathbb{C}\psi$ is denoted by P_ψ. All other states are called *mixed states*[2].

A4. A process of measurement is the correspondence

$$\mathscr{A} \times \mathscr{S} \ni (A, M) \mapsto \mu_A \in \mathscr{P}(\mathbb{R}),$$

which to every observable $A \in \mathscr{A}$ and state $M \in \mathscr{S}$ assigns a probability measure μ_A on $\mathbb{R}$. For every Borel subset $E \subseteq \mathbb{R}$, the quantity $0 \leq \mu_A(E) \leq 1$ is the probability that for a quantum system in the state M the result of a measurement of the observable A belongs to E. The expectation value (the mean-value) of the observable $A \in \mathscr{A}$ in the state $M \in \mathscr{S}$ is

$$\langle A|M\rangle = \int_{-\infty}^{\infty} \lambda d\mu_A(\lambda),$$

where $\mu_A(\lambda) = \mu_A((-\infty, \lambda))$ is a distribution function for the probability measure μ_A.

The set of states $\mathscr{S}$ is a convex set. According to the Hilbert-Schmidt theorem on the canonical decomposition for compact self-adjoint operators, for every $M \in \mathscr{S}$ there exists an orthonormal set $\{\psi_n\}_{n=1}^N$ in $\mathscr{H}$ (finite or infinite, in the latter case $N = \infty$) such that

$$M = \sum_{n=1}^N \alpha_n P_{\psi_n} \quad \text{and} \quad \operatorname{Tr} M = \sum_{n=1}^N \alpha_n = 1, \tag{2.1}$$

where $\alpha_n > 0$ are non-zero eigenvalues of M. Thus every mixed state is a convex linear combination of pure states. The following result characterizes the pure states.

LEMMA 2.1. *A state $M \in \mathscr{S}$ is a pure state if and only if it cannot be represented as a non-trivial convex linear combination in $\mathscr{S}$.*

[2]In physics terminology, the operator M is called the *density operator*.

Explicit construction of the correspondence $\mathscr{A} \times \mathscr{S} \to \mathscr{P}(\mathbb{R})$ is based on the general spectral theorem of von Neumann, which emphasizes the fundamental role the self-adjoint operators play in quantum mechanics.

Namely, let P_A be the *projection-valued measure* on $\mathbb{R}$ associated with the self-adjoint operator A on $\mathscr{H}$ — a countably additive (in the strong operator topology) map $\mathsf{P} : \mathscr{B}(\mathbb{R}) \to \boldsymbol{P}(\mathscr{H})$ of the σ-algebra $\mathscr{B}(\mathbb{R})$ of Borel subsets of $\mathbb{R}$ into the set[3] $\boldsymbol{P}(\mathscr{H})$ of orthogonal projection operators on $\mathscr{H}$ such that

$$D(A) = \left\{ \varphi \in \mathscr{H} : \int_{-\infty}^{\infty} \lambda^2 d(\mathsf{P}(\lambda)\varphi, \varphi) < \infty \right\},$$

where $\mathsf{P}(\lambda) = \mathsf{P}((-\infty, \lambda))$, is the domain of A, and for every $\varphi \in D(A)$

$$A\varphi = \int_{-\infty}^{\infty} \lambda \, d\mathsf{P}(\lambda)\varphi,$$

defined as a limit of Riemann-Stieltjes sums in the strong topology on $\mathscr{H}$. Now the correspondence $(A, M) \mapsto \mu_A$ can be explicitly described as follows.

A5. The probability measure μ_A on $\mathbb{R}$, which defines the correspondence $\mathscr{A} \times \mathscr{S} \to \mathscr{P}(\mathbb{R})$, is given by the celebrated *Born-von Neumann formula*

$$\mu_A(E) = \operatorname{Tr} \mathsf{P}_A(E) M, \quad E \in \mathscr{B}(\mathbb{R}), \tag{2.2}$$

where P_A is a projection-valued measure on $\mathbb{R}$ associated with the self-adjoint operator A

REMARK 2.1. The probability measure μ_A on $\mathbb{R}$ can be considered as a "quantum push-forward" of the state M by the observable A.

From the Hilbert-Schmidt decomposition (2.1) we get

$$\mu_A(E) = \sum_{n=1}^{N} \alpha_n (\mathsf{P}_A(E)\psi_n, \psi_n) = \sum_{n=1}^{N} \alpha_n \|\mathsf{P}_A(E)\psi_n\|^2 \leq \sum_{n=1}^{N} \alpha_n = 1,$$

so that indeed $0 \leq \mu_A(E) \leq 1$. In particular, for $M = P_\psi$ we have

$$\mu_A(E) = (\mathsf{P}_A(E)\psi, \psi) = \|\mathsf{P}_A(E)\psi\|^2. \tag{2.3}$$

This implies that

$$\mu_A(\lambda) = (\mathsf{P}_A(\lambda)\psi, \psi),$$

[3]Actually a complete lattice.

so when $\psi \in D(A)$,

$$\langle A|M\rangle = \int_{-\infty}^{\infty} \lambda d(\mathsf{P}_A(\lambda)\psi, \psi) = (A\psi, \psi).$$

Self-adjoint operators A and B commute if the corresponding projection-valued measures P_A and P_B commute,

$$\mathsf{P}_A(E_1)\mathsf{P}_B(E_2) = \mathsf{P}_B(E_2)\mathsf{P}_A(E_1) \quad \text{for all} \quad E_1, E_2 \in \mathscr{B}(\mathbb{R}).$$

Of course, for bounded operators this condition is equivalent to

$$AB = BA.$$

Slightly abusing notation[4], we will often write $[A, B] = AB - BA = 0$ for commuting self-adjoint operators A and B.

Remark 2.2. It follows from the spectral theorem that commutativity of self-adjoint operators A and B is equivalent to the commutativity of the unitary operators e^{iuA} and e^{ivB} for all $u, v \in \mathbb{R}$, or to the commutativity of the resolvents[5]

$$R_\lambda(A) = (A - \lambda I)^{-1} \quad \text{and} \quad R_\mu(B) = (B - \mu I)^{-1}$$

for all $\lambda, \mu \in \mathbb{C}$, $\operatorname{Im}\lambda, \operatorname{Im}\mu \neq 0$. In particular, a bounded operator B commutes with A if and only if

$$[R_\mu(A), B] = 0.$$

For the simultaneous measurement of a finite set of observables $\boldsymbol{A} = \{A_1, \ldots, A_n\}$ in the state $M \in \mathscr{S}$ it seems natural to introduce the probability measure $\mu_{\boldsymbol{A}}$ on $\mathbb{R}^n$ given by the following generalization of the Born-von Neumann formula:

$$\mu_{\boldsymbol{A}}(\boldsymbol{E}) = \operatorname{Tr}(\mathsf{P}_{A_1}(E_1) \ldots \mathsf{P}_{A_n}(E_n)M), \quad \boldsymbol{E} = E_1 \times \cdots \times E_n \in \mathscr{B}(\mathbb{R}^n). \tag{2.4}$$

However, formula (2.4) defines a probability measure on $\mathbb{R}^n$ if and only if $\mathsf{P}_{A_1}(E_1) \ldots \mathsf{P}_{A_n}(E_n)$ defines a projection-valued measure on $\mathbb{R}^n$. Since a product of orthogonal projections is an orthogonal projection only when the

[4] In general, for unbounded self-adjoint operators A and B the commutator $[A, B] = AB - BA$ is not necessarily closed, i.e., it could be defined only for $\varphi = 0$.

[5] Not that for a self-adjoint operator A its resolvent $R_\lambda(A)$, defined for $\operatorname{Im}\lambda \neq 0$, is a bounded operator from $\mathscr{H}$ to $D(A)$.

projection operators commute, we conclude that the operators $A_1, \dots, A_n$ should form a commutative family. This agrees with the requirement that simultaneous measurement of several observables should be independent of the order of the measurements of individual observables. We summarize these arguments as the following axiom.

A6. A finite set of observables $\boldsymbol{A} = \{A_1, \dots, A_n\}$ can be measured simultaneously (*simultaneously measured observables*) if and only if they form a commutative family. Simultaneous measurement of the commutative family $\boldsymbol{A} \subset \mathscr{A}$ in the state $M \in \mathscr{S}$ is described by the probability measure $\mu_{\boldsymbol{A}}$ on $\mathbb{R}^n$ given by

$$\mu_{\boldsymbol{A}}(\boldsymbol{E}) = \operatorname{Tr} \mathsf{P}_{\boldsymbol{A}}(\boldsymbol{E}) M, \quad \boldsymbol{E} \in \mathscr{B}(\mathbb{R}^n),$$

where $\mathsf{P}_{\boldsymbol{A}}(\boldsymbol{E}) = \mathsf{P}_{A_1}(E_1) \dots \mathsf{P}_{A_n}(E_n)$ for $\boldsymbol{E} = E_1 \times \cdots \times E_n \in \mathscr{B}(\mathbb{R}^n)$. For every Borel subset $\boldsymbol{E} \subseteq \mathbb{R}^n$ the quantity $0 \leq \mu_{\boldsymbol{A}}(\boldsymbol{E}) \leq 1$ is the probability that for a quantum system in the state M the result of simultaneous measurement of observables $A_1, \dots, A_n$ belongs to $\boldsymbol{E}$.

The axioms **A1-A6** are known as Dirac–von Neumann axioms.

2.2. Heisenberg's uncertainty relations

The variance of the observable A in the state M measures the mean deviation of A from its expectation value and is defined by

$$\sigma_M^2(A) = \langle (A - \langle A|M\rangle I)^2 | M\rangle = \langle A^2|M\rangle - \langle A|M\rangle^2 \geq 0,$$

provided the expectation values $\langle A^2|M\rangle$ and $\langle A|M\rangle$ exist. Thus for $M = P_\psi$ and one has $\psi \in D(A)$,

$$\sigma_M^2(A) = \|(A - \langle A|M\rangle I)\psi\|^2 = \|A\psi\|^2 - (A\psi, \psi)^2.$$

Lemma 2.2. *For $A \in \mathscr{A}$ and $M \in \mathscr{S}$ the variance $\sigma_M(A) = 0$ if and only if $\operatorname{Im} M$ is an eigenspace for the operator A with the eigenvalue $a = \langle A|M\rangle$ or, equivalently, μ_A is a Dirac measure supported at a. In particular, if $M = P_\psi$ and $\sigma_M(A) = 0$, then ψ is an eigenvector of A, $A\psi = a\psi$.*

Proof. It follows from the spectral theorem that

$$\sigma_M^2(A) = \int_{-\infty}^{\infty} (\lambda - a)^2 d\mu_A(\lambda),$$

so that $\sigma_M(A) = 0$ if and only if the probability measure μ_A is supported at the point $a \in \mathbb{R}$, i.e., $\mu_A(\{a\}) = 1$. It follows from the spectral theorem that support of the projection-valued measure P_A coincides with the spectrum of A: $\lambda \in \sigma(A)$ if and only if $\mathsf{P}_A((\lambda-\varepsilon, \lambda+\varepsilon)) \neq 0$ for all $\varepsilon > 0$. Since $\mu_A(\{a\}) = \operatorname{Tr} P_A(\{a\})M$ and $\operatorname{Tr} M = 1$, we conclude that this is equivalent to $\operatorname{Im} M$ being an invariant subspace for $P_A(\{a\})$ so that $\operatorname{Im} M$ is an eigenspace for A with the eigenvalue a. □

Now we formulate generalized *Heisenberg's uncertainty relations.*

PROPOSITION 2.1 (H. Weyl). *Let $A, B \in \mathscr{A}$ and let $M = P_\psi$ be the pure state such that $\psi \in D(A) \cap D(B)$ and $A\psi, B\psi \in D(A) \cap D(B)$. Then*

$$\sigma_M^2(A)\sigma_M^2(B) \geq \tfrac{1}{4}\langle i[A, B]|M\rangle^2.$$

The same inequality holds for $M \in \mathscr{S}$.

PROOF. Let $M = P_\psi$. Since

$$[A - \langle A|M\rangle I, B - \langle B|M\rangle I] = [A, B],$$

it is sufficient to prove the inequality

$$\langle A^2|M\rangle\langle B^2|M\rangle \geq \tfrac{1}{4}\langle i[A, B]|M\rangle^2.$$

We have for all $\alpha \in \mathbb{R}$,

$$\begin{aligned}\|(A + i\alpha B)\psi\|^2 &= \alpha^2(B\psi, B\psi) - i\alpha(A\psi, B\psi) + i\alpha(B\psi, A\psi) + (A\psi, A\psi)\\ &= \alpha^2(B^2\psi, \psi) + \alpha(i[A, B]\psi, \psi) + (A^2\psi, \psi) \geq 0,\end{aligned}$$

so that necessarily $4(A^2\psi, \psi)(B^2\psi, \psi) \geq (i[A, B]\psi, \psi)^2$.

The same argument works for the mixed states. □

Heisenberg's uncertainty relations provide a quantitative expression of the fact that even in a pure state non-commuting observables cannot be measured simultaneously. This shows a fundamental difference between the process of measurement in classical mechanics and in quantum mechanics.

2.3. Dynamics

The set $\mathscr{A}$ of quantum observables does not form an algebra with respect to an operator product[6]. Nevertheless, a real vector space $\mathscr{A}_0$ of bounded observables has a Lie algebra structure with the Lie bracket

$$i[A, B] = i(AB - BA), \quad A, B \in \mathscr{A}_0.$$

[6]The product of two non-commuting self-adjoint operators is not self-adjoint.

REMARK 2.3. In fact, the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$ of bounded operators on $\mathscr{H}$ has a structure of a complex Lie algebra with the Lie bracket given by a commutator $[A, B] = AB - BA$. It satisfies the Leibniz rule

$$[AB, C] = A[B, C] + [A, C]B,$$

so that the Lie bracket is a derivation of the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$.

In analogy with classical mechanics, we postulate that the time evolution of a quantum system with the space of states $\mathscr{H}$ is completely determined by a special observable $H \in \mathscr{A}$, called a *Hamiltonian operator* (Hamiltonian for brevity). As in classical mechanics, the Lie algebra structure on $\mathscr{A}_0$ leads to corresponding *quantum equations of motion.*

Specifically, the analog of Hamilton's picture in classical mechanics is the *Heisenberg picture* in quantum mechanics, where the states do not depend on time

$$\frac{dM}{dt} = 0, \quad M \in \mathscr{S},$$

and bounded observables satisfy the *Heisenberg equation of motion*

$$\frac{dA}{dt} = \{H, A\}_\hbar, \quad A \in \mathscr{A}_0, \tag{2.5}$$

where

$$\{\ ,\ \}_\hbar = \frac{i}{\hbar}[\ ,\ ] \tag{2.6}$$

is the *quantum bracket* — the $\hbar$-dependent Lie bracket on $\mathscr{A}_0$. The positive number $\hbar$, called the *Planck constant*, is one of the fundamental constants in physics[7].

The Heisenberg equation (2.5) is well defined when $H \in \mathscr{A}_0$. Indeed, let $U(t)$ be a strongly continuous one-parameter group of unitary operators associated with a bounded self-adjoint operator $H/\hbar$,

$$U(t) = e^{-\frac{i}{\hbar}tH}, \quad t \in \mathbb{R}. \tag{2.7}$$

It satisfies the differential equation

$$i\hbar\frac{dU(t)}{dt} = HU(t) = U(t)H, \tag{2.8}$$

[7]The Planck constant has a physical dimension of the action (energy $\times$ time). Its value $\hbar = 1.054 \times 10^{-27}$ erg $\times$ sec, which is determined from the experiment, manifests that quantum mechanics is a microscopic theory.

so that the solution $A(t)$ of the Heisenberg equation of motion with the initial condition $A(0) = A \in \mathscr{A}_0$ is given by

$$A(t) = U(t)^{-1} A U(t). \tag{2.9}$$

In general, a strongly one-parameter group of unitary operators (2.7), associated with a self-adjoint operator H by the spectral theorem, satisfies differential equation (2.8) only on $D(H)$ in a strong sense, that is, applied to $\varphi \in D(H)$. The quantum dynamics is defined by the same formula (2.9), and in this sense all quantum observables satisfy the Heisenberg equation of motion (2.5). The *evolution operator* $U_t : \mathscr{A} \to \mathscr{A}$ is defined by $U_t(A) = A(t) = U(t)^{-1} A U(t)$, and is an automorphism of the Lie algebra $\mathscr{A}_0$ of bounded observables. This is a quantum analog of the statement that the evolution operator in classical mechanics is an automorphism of the Poisson algebra of classical observables.

By Stone's theorem, every strongly-continuous one-parameter group of unitary operators[8] $U(t)$ is of the form (2.7), where

$$D(H) = \left\{ \varphi \in \mathscr{H} : \lim_{t \to 0} \frac{U(t) - I}{t} \varphi \ \text{ exists} \right\} \quad \text{and} \quad H\varphi = i\hbar \lim_{t \to 0} \frac{U(t) - I}{t} \varphi.$$

The domain $D(H)$ of the self-adjoint operator H, called the *infinitesimal generator* of $U(t)$, is an invariant linear subspace for all operators $U(t)$.

We summarize these arguments as the following axiom.

A7 (Heisenberg's Picture). The dynamics of a quantum system is described by the strongly continuous one-parameter group $U(t)$ of unitary operators. Quantum states do not depend on time,

$$\mathscr{S} \ni M \mapsto M(t) = M \in \mathscr{S},$$

and time dependence of quantum observables is given by the evolution operator U_t,

$$\mathscr{A} \ni A \mapsto A(t) = U_t(A) = U(t)^{-1} A U(t) \in \mathscr{A}.$$

Infinitesimally, the evolution of quantum observables is described by the Heisenberg equation of motion (2.5), where the Hamiltonian operator H is the infinitesimal generator of $U(t)$.

The analog of Liouville's picture in classical mechanics is *Schrödinger's picture* in quantum mechanics, defined as follows.

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[8]According to a theorem of von Neumann, on a separable Hilbert space every weakly measurable one-parameter group of unitary operators is strongly continuous.

A8 (Schrödinger's Picture). The dynamics of a quantum system is described by the strongly continuous one-parameter group $U(t)$ of unitary operators. Quantum observables do not depend on time,

$$\mathscr{A} \ni A \mapsto A(t) = A \in \mathscr{A},$$

and time dependence of states is given by the inverse of the evolution operator $U_t^{-1} = U_{-t}$,

$$\mathscr{S} \ni M \mapsto M(t) = U_{-t}(M) = U(t)MU(t)^{-1} \in \mathscr{S}. \tag{2.10}$$

Infinitesimally, the evolution of quantum states is described by the Schrödinger equation of motion

$$\frac{dM}{dt} = -\{H, M\}_h, \quad M \in \mathscr{S}, \tag{2.11}$$

where the Hamiltonian operator H is the infinitesimal generator of $U(t)$.

Proposition 2.2. *Heisenberg and Schrödinger descriptions of dynamics are equivalent.*

Proof. Let $\mu_{A(t)}$ and $(\mu_t)_A$ be, respectively, probability measures on $\mathbb{R}$ associated with $(A(t), M) \in \mathscr{A} \times \mathscr{S}$ and $(A, M(t)) \in \mathscr{A} \times \mathscr{S}$ according to **A3**-**A4**, where $A(t) = U_t(A)$ and $M(t) = U_{-t}(M)$. We need to show that $\mu_{A(t)} = (\mu_t)_A$. It easily follows from the spectral theorem that $\mathsf{P}_{A(t)} = U(t)^{-1}\mathsf{P}_A U(t)$, so that using the Born-von Neumann formula (2.2) and the cyclic property of the trace, we get for $E \in \mathscr{B}(\mathbb{R})$,

$$\begin{aligned}\mu_{A(t)}(E) &= \operatorname{Tr} \mathsf{P}_{A(t)}(E)M = \operatorname{Tr}(U(t)^{-1}\mathsf{P}_A(E)U(t)M) \\ &= \operatorname{Tr}(\mathsf{P}_A(E)U(t)MU(t)^{-1}) = \operatorname{Tr} \mathsf{P}_A(E)M(t) = (\mu_t)_A(E). \quad \square\end{aligned}$$

Corollary 2.1. $\langle A(t)|M\rangle = \langle A|M(t)\rangle$.

In analogy with classical mechanics, we have the following definition.

Definition. An observable $A \in \mathscr{A}$ is a *quantum integral of motion* (or a *constant of motion*) for a quantum system with the Hamiltonian H if in Heisenberg's picture

$$\frac{dA(t)}{dt} = 0,$$

i.e., A commutes with $U(t)$. Thus $A \in \mathscr{A}$ is an integral of motion if and only if it commutes with the Hamiltonian H, so that, in agreement with (2.5),

$$\{H, A\}_\hbar = 0.$$

This is a quantum analog of the Poisson commutativity property.

It follows from (2.11) that the time evolution of a pure state $M = P_\psi$ is given by $M(t) = P_{\psi(t)}$, where $\psi(t) = U(t)\psi$. Suppose that $\psi \in D(H)$. Since $D(H)$ is invariant under $U(t)$, the vector $\psi(t) = U(t)\psi$ satisfies the *time-dependent Schrödinger equation*

$$i\hbar\frac{d\psi}{dt} = H\psi \tag{2.12}$$

with the initial condition $\psi(0) = \psi$.

DEFINITION. A state $M \in \mathscr{S}$ is called *stationary* for a quantum system with Hamiltonian H if in Schrödinger's picture

$$\frac{dM(t)}{dt} = 0.$$

The state M is stationary if and only if $[M, U(t)] = 0$ for all t, i.e.

$$\{H, M\}_\hbar = 0,$$

in agreement with (2.11). The following simple result is fundamental.

LEMMA 2.3. *The pure state $M = P_\psi$ is stationary if and only if ψ is an eigenvector for H,*

$$H\psi = \lambda\psi,$$

and in this case

$$\psi(t) = e^{-\frac{i}{\hbar}\lambda t}\psi.$$

PROOF. It follows from $U(t)P_\psi = P_\psi U(t)$ that ψ is a common eigenvector for unitary operators $U(t)$ for all t, $U(t)\psi = c(t)\psi$, $|c(t)| = 1$. Since $U(t)$ is a strongly continuous one-parameter group of unitary operators, the continuous function $c(t) = (U(t)\psi, \psi)$ satisfies the equation $c(t_1 + t_2) = c(t_1)c(t_2)$ for all $t_1, t_2 \in \mathbb{R}$, so that $c(t) = e^{-\frac{i}{\hbar}\lambda t}$ for some $\lambda \in \mathbb{R}$. Thus by Stone's theorem $\psi \in D(H)$ and $H\psi = \lambda\psi$. □

REMARK 2.4. Another simple proof uses Remark 2.2. Namely, $M = P_\psi$ commute with H if and only if $R_\mu(H)P_\psi = P_\psi R_\mu(H)$ for all μ with $\operatorname{Im}\mu \neq 0$, so

$$R_\mu(H)\psi = c(\mu)\psi,$$

and $c(\mu) \neq 0$ since $R_\mu(H)$ is injective. Thus $\psi \in D(H)$, and applying $(H - \mu I)$ to $R_\mu(H)\psi$, we obtain

$$\psi = c(\mu)(H\psi - \mu\psi),$$

or

$$H\psi = \lambda\psi,$$

where $\lambda = \dfrac{1+\mu}{c(\mu)}$ does not depend on μ and is necessarily real, so $c(\mu) = (\mu - \lambda)^{-1}$.

In physics terminology, the eigenvectors of H are called *bound states.* The corresponding eigenvalues are called *energy levels* and are usually denoted by E.

PROBLEM 2.1. Prove Lemma 2.1.

PROBLEM 2.2. Prove that the state M is a pure state if and only if $\operatorname{Tr} M^2 = 1$.

PROBLEM 2.3. Prove that the Born-von Neumann formula (2.2) defines a probability measure on $\mathbb{R}$, i.e., μ_A is a σ-additive function on $\mathscr{B}(\mathbb{R})$.

PROBLEM 2.4. Prove that if the sum P_1+P_2 of orthogonal projection operators is a projection operator, then $P_1P_2 = P_2P_1 = 0$. Using this, show that if P is a projection-valued measure, then $\mathsf{P}(E_1 \cap E_2) = \mathsf{P}(E_1)\mathsf{P}(E_2)$.

PROBLEM 2.5. Show that if an observable A is such that for every state M the expectation value $\langle A|M(t)\rangle$ does not depend on t, then A is a quantum integral of motion. (This is the definition of integrals of motion in the Schrödinger picture.)

PROBLEM 2.6. Prove Heisenberg uncertainty relation

$$\sigma_M^2(A)\sigma_M^2(B) \geq \tfrac{1}{4}\langle i[A,B]|M\rangle^2$$

for mixed states.

PROBLEM 2.7. Show that a solution of the initial value problem for the time-dependent Schrödinger equation (2.12) is given by

$$\psi(t) = \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}t\lambda} d\mathsf{P}(\lambda)\psi,$$

where P is the projection-valued measure associated with the Hamiltonian H.

PROBLEM 2.8. Let D be a linear subspace of $\mathscr{H}$, consisting of *Gårding vectors*

$$\psi_f = \int_{-\infty}^{\infty} f(s)U(s)\psi\, ds, \quad f \in \mathscr{S}(\mathbb{R}), \;\; \psi \in \mathscr{H},$$

where $\mathscr{S}(\mathbb{R})$ is the Schwartz space of rapidly decreasing functions on $\mathbb{R}$. Prove that D is dense in $\mathscr{H}$ and is invariant for $U(t)$ and for the Hamiltonian H. (*Hint:* Show that $U(t)\psi_f = \psi_{f_t} \in D$, where $f_t(s) = f(s-t)$, and deduce $H\psi_f = \frac{\hbar}{i}\psi_{f'}$.)

CHAPTER 3

Quantization

A quantum system is described by the Hilbert space $\mathscr{H}$ and the Hamiltonian H, a self-adjoint operator in $\mathscr{H}$, which determines the evolution of a system. When the system has a classical analog, the procedure of constructing the corresponding Hilbert space $\mathscr{H}$ and the Hamiltonian H is called *quantization*.

DEFINITION. Quantization of a classical system $((\mathscr{M},\{\ ,\ \}),H_{\mathrm{c}})$ with the Hamiltonian function[1] H_{c} is a one-to-one mapping $\mathrm{Q}_\hbar : \mathcal{A}\to\mathscr{A}$ from the set of classical observables $\mathcal{A} = C^\infty(\mathscr{M})$ to the set $\mathscr{A}$ of quantum observables — the set of self-adjoint operators on a Hilbert space $\mathscr{H}$. The map $\mathrm{Q}_\hbar$ depends on the parameter $\hbar > 0$, and its restriction to the subspace of bounded classical observables $\mathcal{A}_0$ is a linear mapping to the subspace $\mathscr{A}_0$ of bounded quantum observables, which satisfies the properties

$$\lim_{\hbar\to 0}\tfrac{1}{2}\mathrm{Q}_\hbar^{-1}\big(\mathrm{Q}_\hbar(f_1)\mathrm{Q}_\hbar(f_2)+\mathrm{Q}_\hbar(f_2)\mathrm{Q}_\hbar(f_1)\big) = f_1f_2$$

and

$$\lim_{\hbar\to 0}\mathrm{Q}_\hbar^{-1}\big(\{\mathrm{Q}_\hbar(f_1),\mathrm{Q}_\hbar(f_2)\}_\hbar\big) = \{f_1,f_2\}\quad\text{for all}\quad f_1,f_2\in\mathcal{A}_0.$$

The latter property is the celebrated *correspondence principle* of N. Bohr. In particular, $H_{\mathrm{c}}\mapsto \mathrm{Q}_\hbar(H_{\mathrm{c}}) = H$ — the Hamiltonian operator for a quantum system.

REMARK 3.1. In physics literature the correspondence principle is often stated in the form

$$[\ ,\ ]\simeq\frac{\hbar}{i}\{\ ,\ \}\quad\text{as}\quad\hbar\to 0.$$

Quantum mechanics is different from classical mechanics, so that the correspondence $f\mapsto \mathrm{Q}_\hbar(f)$ cannot be an isomorphism between the Lie algebras of bounded classical and quantum observables with respect to classical

[1]Notation H_{c} is used to distinguish the Hamiltonian function in classical mechanics from the Hamiltonian operator H in quantum mechanics.

and quantum brackets. It becomes an isomorphism only in the limit $\hbar \to 0$ when quantum mechanics turns into classical mechanics. Since quantum mechanics provides a more accurate and refined description than classical mechanics, quantization of a classical system may not be unique.

DEFINITION. Two quantizations $\mathrm{Q}_\hbar^{(1)}$ and $\mathrm{Q}_\hbar^{(2)}$ of a given classical system $((\mathscr{M}, \{\ ,\ \}), H_\mathrm{c})$ are said to be equivalent if there exists a linear mapping $\mathscr{U}_\hbar : \mathcal{A} \to \mathcal{A}$ such that $\mathrm{Q}_\hbar^{(2)} = \mathrm{Q}_\hbar^{(1)} \circ \mathscr{U}_\hbar$ and $\lim\limits_{\hbar \to 0} \mathscr{U}_\hbar = \mathrm{id}$.

For many "real world" quantum systems — the systems describing actual physical phenomena — the corresponding Hamiltonian H does not depend on a choice of equivalent quantization, and is uniquely determined by the classical Hamiltonian function H_c.

3.1. Heisenberg commutation relations

The simplest classical system with one degree of freedom is described by the phase space $\mathbb{R}^2$ with coordinates p, q and the Poisson bracket $\{\ ,\ \}$, associated with the canonical symplectic form $\omega = dp \wedge dq$. The Poisson bracket between classical observables p and q — momentum and coordinate of a particle — has the following simple form:

$$\{p, q\} = 1. \tag{3.1}$$

It is another postulate of quantum mechanics that under quantization classical observables p and q correspond to quantum observables P and Q — self-adjoint operators on a Hilbert space $\mathscr{H}$, satisfying the following properties.

CR1. There is a dense linear subset $D \subset \mathscr{H}$ such that $P : D \to D$ and $Q : D \to D$.

CR2. For all $\psi \in D$,

$$(PQ - QP)\psi = -i\hbar\psi.$$

CR3. Every bounded operator on $\mathscr{H}$ which commutes with P and Q is a multiple of the identity operator I.

Property **CR2** is called the *Heisenberg commutation relation* for one degree of freedom. In terms of the quantum bracket (2.6) it takes the form

$$\{P, Q\}_\hbar = I, \tag{3.2}$$

which is exactly the same as the Poisson bracket (11.16)! Property **CR3** is a quantum analog of the classical property that the Poisson manifold $(\mathbb{R}^2, \{\ ,\ \})$ is non-degenerate: every function which Poisson commutes with p and q is a constant.

The operators P and Q are called, respectively, the *momentum operator* and the *coordinate operator*. The correspondence $p \mapsto P$, $q \mapsto Q$ with P and Q satisfying **CR1-CR3** is the cornerstone for the quantization of classical systems. The validity of (3.2), as well as of quantum mechanics as a whole, is confirmed by the agreement of the theory with numerous experiments.

REMARK 3.2. It is tempting to extend the correspondence $p \mapsto P$, $q \mapsto Q$ to all observables by defining the mapping $f(p, q) \mapsto f(P, Q)$. However, this approach to quantization is rather naive: operators P and Q satisfy (3.2) and do not commute, so that one needs to understand how $f(P, Q)$ — a "function of non-commuting variables" — is actually defined. We will address this problem of the ordering of non-commuting operators P and Q later.

It follows from Heisenberg's uncertainty relations (see Proposition 2.1), that for any pure state $M = P_\psi$ with $\psi \in D$,

$$\sigma_M(P)\sigma_M(Q) \geq \frac{\hbar}{2}.$$

This is a fundamental result saying that it is impossible to measure the coordinate and the momentum of a quantum particle simultaneously: the more accurate the measurement of one quantity is, the less accurate the value of the other is. It is often said that a quantum particle has no observed path, so that "quantum motion" differs dramatically from the motion in classical mechanics.

It is straightforward to consider a classical system with n degrees of freedom, described by the phase space $\mathbb{R}^{2n}$ with coordinates $\boldsymbol{p} = (p_1, \dots, p_n)$ and $\boldsymbol{q} = (q^1, \dots, q^n)$, and the Poisson bracket $\{\ ,\ \}$, associated with the canonical symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$. The Poisson brackets between classical observables $\boldsymbol{p}$ and $\boldsymbol{q}$ — momenta and coordinates of a particle — have the form

$$\{p_k, p_l\} = 0, \quad \{q^k, q^l\} = 0, \quad \{p_k, q^l\} = \delta_k^l, \quad k, l = 1, \dots, n. \tag{3.3}$$

Corresponding momenta and coordinate operators $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ are self-adjoint operators that have a common invariant dense linear subset $D \subset \mathscr{H}$, and on D satisfy the following commutation relations:

$$\{P_k, P_l\}_\hbar = 0, \quad \{Q^k, Q^l\}_\hbar = 0, \quad \{P_k, Q^l\}_\hbar = \delta_k^l I, \quad k, l = 1, \dots, n. \tag{3.4}$$

These relations are called *Heisenberg commutation relations* for n degrees of freedom. The analog of **CR3** is the property that every bounded operator on $\mathscr{H}$ which commutes with all operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ is a multiple of the identity operator I.

The fundamental algebraic structure associated with Heisenberg commutation relations is the so-called *Heisenberg algebra*.

Definition. The Heisenberg algebra $\mathfrak{h}_n$ with n degrees of freedom is a Lie algebra with the generators $e^1, \dots, e^n, f_1, \dots, f_n, c$ and the relations

$$[e^k, c] = 0, \quad [f_k, c] = 0, \quad [e^k, f_l] = \delta_l^k c, \quad k, l = 1, \dots, n. \tag{3.5}$$

The Heisenberg algebra $\mathfrak{h}_n$ is realized as a nilpotent subalgebra of the Lie algebra $\mathfrak{gl}_{n+2}$ of $(n+2) \times (n+2)$ matrices with the elements

$$\sum_{k=1}^{n} (u^k f_k + v_k e^k) + \alpha c = \begin{pmatrix} 0 & v_1 & v_2 & \dots & v_n & \alpha \\ 0 & 0 & 0 & \cdots & 0 & u^1 \\ 0 & 0 & 0 & \cdots & 0 & u^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & u^n \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}. \tag{3.6}$$

Remark 3.3. The faithful representation $\mathfrak{h}_n \to \mathfrak{gl}_{n+2}$, given by (3.6), is clearly reducible: the subspace $V = \{\boldsymbol{x} = (x_1, \dots, x_{n+2}) \in \mathbb{R}^{n+2} : x_{n+2} = 0\}$ is an invariant subspace for $\mathfrak{h}_n$ with the central element c acting by zero. However, this representation is not decomposable: the vector space $\mathbb{R}^{n+2}$ cannot be written as a direct sum of V and a one-dimensional invariant subspace for $\mathfrak{h}_n$. This explains why the central element c is not represented by a diagonal matrix with the first $n+1$ zeros, but rather has a special form given by (3.6).

Analytically, Heisenberg commutation relations (3.5) correspond to an irreducible unitary representation of the Heisenberg algebra $\mathfrak{h}_n$. Recall that a unitary representation ρ of $\mathfrak{h}_n$ in the Hilbert space $\mathscr{H}$ is the linear mapping $\rho : \mathfrak{h}_n \to i\mathscr{A}$ — the space of skew-Hermitian operators in $\mathscr{H}$ — such that all self-adjoint operators $i\rho(x)$, $x \in \mathfrak{h}_n$, have a common invariant dense linear subset $D \subset \mathscr{H}$ and satisfy

$$\rho([x, y])\varphi = (\rho(x)\rho(y) - \rho(y)\rho(x))\varphi, \quad x, y \in \mathfrak{h}_n, \ \varphi \in D.$$

Formally applying Schur's lemma we say that the representation ρ is irreducible if every bounded operator which commutes with all operators $i\rho(x)$ is a multiple of the identity operator I. Then Heisenberg commutation relations (3.5) define an irreducible unitary representation ρ of the Heisenberg algebra $\mathfrak{h}_n$ in the Hilbert space $\mathscr{H}$ by setting

$$\rho(f_k) = -iP_k, \quad \rho(e^k) = -iQ^k, \quad k = 1, \dots, n, \quad \rho(c) = -i\hbar I. \tag{3.7}$$

Since the operators P^k and Q_k are necessarily unbounded, the condition

$$P_k P_l \varphi = P_l P_k \varphi \quad \text{for all} \quad \varphi \in D$$

does not necessarily imply that self-adjoint operators P_k and P_l commute in the sense of the definition in Section 2.1. To avoid such "pathological" representations, we will assume that ρ is an *integrable* representation, i.e., it can be integrated (in a precise sense specified below) to an irreducible unitary representation of the *Heisenberg group* $\mathbf{H}_n$ — a connected, simply-connected Lie group with the Lie algebra $\mathfrak{h}_n$.

Explicitly, the Heisenberg group is a unipotent subgroup of the Lie algebra $\mathrm{SL}(n+2, \mathbb{R})$ with the elements

$$g = \begin{pmatrix} 1 & v_1 & v_2 & \cdots & v_n & \alpha \\ 0 & 1 & 0 & \cdots & 0 & u^1 \\ 0 & 0 & 1 & \cdots & 0 & u^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & u^n \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}.$$

The exponential map $\exp : \mathfrak{h}_n \to \mathbf{H}_n$ is onto, and the Heisenberg group $\mathbf{H}_n$ is generated by two n-parameter abelian subgroups

$$\exp \boldsymbol{u}X = \exp\left(\sum_{k=1}^{n} u^k f_k\right), \quad \exp \boldsymbol{v}Y = \exp\left(\sum_{k=1}^{n} v_k e^k\right), \quad \boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n,$$

and a one-parameter center $\exp \alpha c$, which satisfy the relations

$$\exp \boldsymbol{u}X \exp \boldsymbol{v}Y = \exp(-\boldsymbol{u}\boldsymbol{v}c) \exp \boldsymbol{v}Y \exp \boldsymbol{u}X, \quad \boldsymbol{u}\boldsymbol{v} = \sum_{k=0}^{n} u^k v_k. \tag{3.8}$$

Indeed, it follows from (3.5) that

$$[\boldsymbol{u}X, \boldsymbol{v}Y] = -\boldsymbol{u}\boldsymbol{v}c$$

is a central element, so that using the Baker-Campbell-Hausdorff formula we obtain

$$\exp \boldsymbol{u}X \exp \boldsymbol{v}Y = \exp(-\tfrac{1}{2}\boldsymbol{u}\boldsymbol{v}c)\exp(\boldsymbol{u}X + \boldsymbol{v}Y),$$
$$\exp \boldsymbol{v}Y \exp \boldsymbol{u}X = \exp(\tfrac{1}{2}\boldsymbol{u}\boldsymbol{v}c)\exp(\boldsymbol{u}X + \boldsymbol{v}Y).$$

In the matrix realization, the exponential map is given by the matrix exponential and we get $e^{\boldsymbol{u}X} = I + \boldsymbol{u}X$, $e^{\boldsymbol{v}Y} = I + \boldsymbol{v}Y$, and $e^{\alpha c} = I + \alpha c$, where I is the $(n+2)\times(n+2)$ identity matrix, and the relation (3.8) is immediately verified.

Let R be an irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ in the Hilbert space $\mathscr{H}$ — a strongly continuous group homomorphism $R : \mathbf{H}_n \to \mathscr{U}(\mathscr{H})$, where $\mathscr{U}(\mathscr{H})$ is the group of unitary operators in $\mathscr{H}$. By Schur's lemma, $R(e^{\alpha c}) = e^{-i\lambda\alpha}I$, $\lambda \in \mathbb{R}$. Suppose now that $\lambda = \hbar$, and define two strongly continuous n-parameter abelian groups of unitary operators

$$U(\boldsymbol{u}) = R(\exp \boldsymbol{u}X),\ \ V(\boldsymbol{v}) = R(\exp \boldsymbol{v}Y), \quad \boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n.$$

Then it follows from (3.8) that unitary operators $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$ satisfy *Weyl commutation relations*

$$U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar \boldsymbol{u}\boldsymbol{v}}V(\boldsymbol{v})U(\boldsymbol{u}). \tag{3.9}$$

It follows from Stone theorem that

$$U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{P}} = e^{-i\sum_{k=1}^{n} u^k P_k} \quad \text{and} \quad V(\boldsymbol{v}) = e^{-i\boldsymbol{v}\boldsymbol{Q}} = e^{-i\sum_{k=1}^{n} v_k Q^k},$$

where infinitesimal generators $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ given by

$$P_k = i\,\frac{\partial U(\boldsymbol{u})}{\partial u^k}\bigg|_{\boldsymbol{u}=0} \quad \text{and} \quad Q^k = i\,\frac{\partial V(\boldsymbol{v})}{\partial v_k}\bigg|_{\boldsymbol{v}=0}, \quad k = 1, \dots, n.$$

Taking the second partial derivatives of Weyl relations (3.9) at the origin $\boldsymbol{u} = \boldsymbol{v} = 0$, we easily obtain the following result.

LEMMA 3.1. *Let $R : \mathbf{H}_n \to \mathscr{U}(\mathscr{H})$ be an irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ in $\mathscr{H}$ such that $R(e^{\alpha c}) = e^{-i\hbar\alpha}I$, and let $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ be, respectively, infinitesimal generators of the strongly continuous n-parameter abelian subgroups $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$. Then formulas* (3.7) *define an irreducible unitary representation ρ of the Heisenberg algebra $\mathfrak{h}_n$ in $\mathscr{H}$.*

The representation ρ in Lemma 3.1 is called the differential of a representation R, and is denoted by dR. The irreducible unitary representation ρ of $\mathfrak{h}_n$ is called *integrable* if $\rho = dR$ for some irreducible unitary representation R of $\mathbf{H}_n$.

REMARK 3.4. Not every irreducible unitary representation of the Heisenberg algebra is integrable, so that Weyl relations cannot be obtained from the Heisenberg commutation relations.

The celebrated Stone-von Neumann theorem asserts that all integrable irreducible unitary representations of the Heisenberg algebra $\mathfrak{h}_n$ with the same action of the central element c are unitarily equivalent. This justifies the following mathematical formulation of the Heisenberg commutation relations for n degrees of freedom.

A9 (HEISENBERG'S COMMUTATION RELATIONS). Momenta and coordinate operators $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ for a quantum particle with n degrees of freedom are defined by formulas (3.7), where ρ is an integrable irreducible unitary representation of the Heisenberg algebra $\mathfrak{h}_n$ with the property $\rho(c) = -i\hbar I$.

3.2. Coordinate and momentum representations

We start with the case of one degree of freedom and consider two natural realizations of the Heisenberg commutation relation. They are defined by the property that one of the self-adjoint operators P and Q is "diagonal" (i.e., is a multiplication by a function operator in the corresponding Hilbert space).

In the *coordinate representation*, $\mathscr{H} = L^2(\mathbb{R}, dq)$ is the L^2-space on the configuration space $\mathbb{R}$ with the coordinate q, which is a Lagrangian subspace of $\mathbb{R}^2$ defined by the equation $p = 0$. Set

$$D(Q) = \left\{\varphi \in \mathscr{H} : \int_{-\infty}^{\infty} q^2 |\varphi(q)|^2 dq < \infty\right\}$$

and for $\varphi \in D(Q)$ define the operator Q as a "multiplication by q operator",

$$(Q\varphi)(q) = q\varphi(q), \;\; q \in \mathbb{R},$$

justifying the name coordinate representation. The coordinate operator Q is obviously self-adjoint and its projection-valued measure is given by

$$(\mathsf{P}(E)\varphi)(q) = \chi_E(q)\varphi(q), \tag{3.10}$$

where χ_E is the characteristic function of a Borel subset $E \subseteq \mathbb{R}$. Therefore $\operatorname{supp} \mathsf{P} = \mathbb{R}$ and $\sigma(Q) = \mathbb{R}$.

Recall that a self-adjoint operator A has an absolutely continuous spectrum if for every $\psi \in \mathscr{H}$, $\|\psi\| = 1$, the probability measure ν_ψ,

$$\nu_\psi(E) = (\mathsf{P}_A(E)\psi, \psi), \quad E \in \mathscr{B}(\mathbb{R}),$$

is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$.

LEMMA 3.2. *The coordinate operator Q has an absolutely continuous spectrum $\mathbb{R}$, and every bounded operator B which commutes with Q is a function of Q, $B = f(Q)$ with $f \in L^\infty(\mathbb{R})$.*

PROOF. It follows from (3.10) that $\nu_\psi(E) = \int_E |\psi(q)|^2 dq$, which proves the first statement. Now a bounded operator B on $\mathscr{H}$ commutes with Q if and only if $B\mathsf{P}(E) = \mathsf{P}(E)B$ for all $E \in \mathscr{B}(\mathbb{R})$, and using (3.10) we get

$$B(\chi_E \varphi) = \chi_E B(\varphi). \tag{3.11}$$

Choosing in (3.11) $E = E_1$ and $\varphi = \chi_{E_2}$, where E_1 and E_2 have finite Lebesgue measure, we obtain

$$B(\chi_{E_1} \cdot \chi_{E_2}) = B(\chi_{E_1 \cap E_2}) = \chi_{E_1} B(\chi_{E_2}) = \chi_{E_2} B(\chi_{E_1}),$$

so that denoting $f_E = B(\chi_E)$ we get $\operatorname{supp} f_E \subseteq E$, and

$$f_{E_1}|_{E_1 \cap E_2} = f_{E_2}|_{E_1 \cap E_2}$$

for all $E_1, E_2 \in \mathscr{B}(\mathbb{R})$ with finite Lebesgue measure. Thus there exists a measurable function f on $\mathbb{R}$ such that $f|_E = f_E|_E$ for every $E \in \mathscr{B}(\mathbb{R})$ with finite Lebesgue measure. The linear subspace spanned by all $\chi_E \in L^2(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ and the operator B is continuous, so that we get

$$(B\varphi)(q) = f(q)\varphi(q) \quad \text{for all} \quad \varphi \in L^2(\mathbb{R}).$$

Since B is a bounded operator, $f \in L^\infty(\mathbb{R})$ and $\|B\| = \|f\|_\infty$. □

For a pure state $M = P_\psi$, $\|\psi\| = 1$, the corresponding probability measure μ_Q on $\mathbb{R}$ is given by

$$\mu_Q(E) = \nu_\psi(E) = \int_E |\psi(q)|^2 dq, \quad E \in \mathscr{B}(\mathbb{R}).$$

Physically, this is interpreted that in the state P_ψ with the "wave function" $\psi(q)$, the probability of finding a quantum particle between q and $q + dq$

is $|\psi(q)|^2 dq$. In other words, the modulus square of a wave function is the probability distribution for the coordinate of a quantum particle.

The corresponding momentum operator P is given by a differential operator

$$P = \frac{\hbar}{i}\frac{d}{dq}$$

with $D(P) = W^{1,2}(\mathbb{R})$ — the Sobolev space of absolutely continuous functions f on $\mathbb{R}$ such that f and its derivative f' (defined a.e.) are in $L^2(\mathbb{R})$. The operator P is self-adjoint and it is straightforward to verify that on $D = C_c^\infty(\mathbb{R})$, the space of smooth functions on $\mathbb{R}$ with compact support,

$$QP - PQ = i\hbar I.$$

PROPOSITION 3.1. *The coordinate representation defines an irreducible, unitary, integrable representation of the Heisenberg algebra.*

PROOF. To show that the coordinate representation is integrable, let $U(u) = e^{-iuP}$ and $V(v) = e^{-ivQ}$ be the corresponding one-parameter groups of unitary operators. Clearly, $(V(v)\varphi)\psi(q) = e^{-ivq}\varphi(q)$ and it easily follows from the Stone theorem (or by the definition of a derivative) that $(U(u)\varphi)(q) = \varphi(q - \hbar u)$, so that unitary operators $U(u)$ and $V(v)$ satisfy the Weyl relation (3.9). Such a realization of the Weyl relation is called the *Schrödinger representation*.

To prove that the coordinate representation is irreducible, let B be a bounded operator commuting with P and Q. By Lemma 3.2, $B = f(Q)$ for some $f \in L^\infty(\mathbb{R})$. Now commutativity between B and P implies that

$$BU(u) = U(u)B \quad \text{for all} \quad u \in \mathbb{R},$$

which is equivalent to $f(q - \hbar u) = f(q)$ for all $q, u \in \mathbb{R}$, so that $f = \text{const}$ a.e. on $\mathbb{R}$. □

To summarize, the coordinate representation is characterized by the property that the coordinate operator Q is a multiplication by q operator and the momentum operator P is a differentiation operator,

$$Q = q \quad \text{and} \quad P = \frac{\hbar}{i}\frac{d}{dq}.$$

Similarly, *momentum representation* is defined by the property that the momentum operator P is a multiplication by p operator. Namely let $\mathscr{H} = L^2(\mathbb{R}, dp)$ be the Hilbert L^2-space on the "momentum space" $\mathbb{R}$ with the coordinate p, which is a Lagrangian subspace of $\mathbb{R}^2$ defined by the equation $q = 0$. The coordinate and momentum operators are given by

$$\hat{Q} = i\hbar\frac{d}{dp} \quad \text{and} \quad \hat{P} = p,$$

and satisfy the Heisenberg commutation relation. As the coordinate representation, the momentum representation is an irreducible, unitary, integrable representation of the Heisenberg algebra. In the momentum representation, the modulus square of the wave function $\psi(p)$ of a pure state $M = P_\psi$, $\|\psi\| = 1$, is the probability distribution for the momentum of the quantum particle, i.e., the probability that a quantum particle has momentum between p and $p + dp$ is $|\psi(p)|^2 dp$.

Let $\mathscr{F}_\hbar : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the $\hbar$-dependent Fourier transform operator, defined by

$$\hat{\varphi}(p) = \mathscr{F}_\hbar(\varphi)(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}pq}\varphi(q)dq.$$

Here the integral is understood as the limit $\hat{\varphi} = \lim_{n\to\infty}\hat{\varphi}_n$ in the strong topology on $L^2(\mathbb{R})$, where

$$\hat{\varphi}_n(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-n}^{n} e^{-\frac{i}{\hbar}pq}\varphi(q)dq.$$

By Plancherel's theorem, $\mathscr{F}_\hbar$ is a unitary operator on $L^2(\mathbb{R})$,

$$\mathscr{F}_\hbar\mathscr{F}_\hbar^* = \mathscr{F}_\hbar^*\mathscr{F}_\hbar = I,$$

and

$$\hat{Q} = \mathscr{F}_\hbar Q \mathscr{F}_\hbar^{-1}, \quad \hat{P} = \mathscr{F}_\hbar P \mathscr{F}_\hbar^{-1},$$

so that coordinate and momentum representations are unitarily equivalent. In particular, since the operator $\hat{P}$ is obviously self-adjoint, this immediately shows that the operator P is self-adjoint.

For n degrees of freedom, the coordinate representation is defined by setting $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$, where $d^n\boldsymbol{q} = dq^1\cdots dq^n$ is the Lebesgue measure on $\mathbb{R}^n$, and

$$\boldsymbol{Q} = \boldsymbol{q} = (q^1, \dots, q^n), \quad \boldsymbol{P} = \frac{\hbar}{i}\frac{\partial}{\partial\boldsymbol{q}} = \left(\frac{\hbar}{i}\frac{\partial}{\partial q^1}, \dots, \frac{\hbar}{i}\frac{\partial}{\partial q^n}\right).$$

Here $\mathbb{R}^n$ is the configuration space with coordinates $\boldsymbol{q}$ — a Lagrangian subspace of $\mathbb{R}^{2n}$ defined by the equations $\boldsymbol{p} = 0$. The coordinate and momenta operators are self-adjoint and satisfy Heisenberg commutation relations. Projection-valued measures for the operators Q^k are given by

$$(\mathsf{P}_k(E)\varphi)(\boldsymbol{q}) = \chi_{\lambda_k^{-1}(E)}(\boldsymbol{q})\varphi(\boldsymbol{q}),$$

where $E \in \mathscr{B}(\mathbb{R})$ and $\lambda_k : \mathbb{R}^n \to \mathbb{R}$ is a canonical projection onto the k-th component, $k = 1, \dots, n$. Correspondingly, the projection-valued measure P for the commutative family $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ is defined on the Borel subsets $\boldsymbol{E} \subseteq \mathbb{R}^n$ by

$$(\mathsf{P}(\boldsymbol{E})\varphi)(\boldsymbol{q}) = \chi_{\boldsymbol{E}}(\boldsymbol{q})\varphi(\boldsymbol{q}).$$

The family $\boldsymbol{Q}$ has absolutely continuous joint spectrum $\mathbb{R}^n$.

Coordinate operators $Q^1, \dots, Q^n$ form a *complete system of commuting observables*. By definition this means that none of these operators is a function of the other operators, and that every bounded operator commuting with $Q^1, \dots, Q^n$ is a function of $Q^1, \dots, Q^n$, i.e., is a multiplication by $f(\boldsymbol{q})$ operator for some $f \in L^\infty(\mathbb{R}^n)$. The proof repeats verbatim the proof of Lemma 3.2. For a pure state $M = P_\psi$, $\|\psi\| = 1$, the modulus square $|\psi(\boldsymbol{q})|^2$ of the wave function is the density of a joint distribution function $\mu_{\boldsymbol{Q}}$ for the commutative family $\boldsymbol{Q}$, i.e., the probability of finding a quantum particle in a Borel subset $\boldsymbol{E} \subseteq \mathbb{R}^n$ is given by

$$\mu_{\boldsymbol{Q}}(\boldsymbol{E}) = \int_{\boldsymbol{E}} |\psi(\boldsymbol{q})|^2 d^n\boldsymbol{q}.$$

The coordinate representation defines an irreducible, unitary, integrable representation of the Heisenberg algebra $\mathfrak{h}_n$. Indeed, n-parameter groups of unitary operators $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{P}}$ and $V(\boldsymbol{v}) = e^{-i\boldsymbol{v}\boldsymbol{Q}}$ are given by

$$(U(\boldsymbol{u})\varphi)(\boldsymbol{q}) = \varphi(\boldsymbol{q} - \hbar\boldsymbol{u}), \quad (V(\boldsymbol{v})\varphi)(\boldsymbol{q}) = e^{-i\boldsymbol{v}\boldsymbol{q}}\varphi(\boldsymbol{q}),$$

and satisfy Weyl relations (3.9). The same argument as in the proof of Proposition 3.1 shows that this representation of the Heisenberg group $\mathbf{H}_n$, called the *Schrödinger representation for n degrees of freedom*, is irreducible.

In the momentum representation, $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{p})$, where $d^n\boldsymbol{p} = dp_1 \cdots dp_n$ is the Lebesgue measure on $\mathbb{R}^n$, and

$$\hat{\boldsymbol{Q}} = i\hbar\frac{\partial}{\partial\boldsymbol{p}} = \left(i\hbar\frac{\partial}{\partial p_1}, \dots, i\hbar\frac{\partial}{\partial p_n}\right), \quad \hat{\boldsymbol{P}} = \boldsymbol{p} = (p_1, \dots, p_n).$$

Here $\mathbb{R}^n$ is the momentum space with coordinates $\boldsymbol{p}$ — a Lagrangian subspace of $\mathbb{R}^{2n}$ defined by the equations $\boldsymbol{q} = 0$.

The coordinate and momentum representations are unitarily equivalent by the Fourier transform. As in the case $n = 1$, the Fourier transform $\mathscr{F}_\hbar : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is a unitary operator defined by

$$\begin{aligned}\hat{\varphi}(\boldsymbol{p}) = \mathscr{F}_\hbar(\varphi)(\boldsymbol{p}) =& (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{q}}\varphi(\boldsymbol{q})d^n\boldsymbol{q} \\ &= \lim_{N\to\infty} (2\pi\hbar)^{-n/2} \int_{|\boldsymbol{q}|\leq N} e^{-\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{q}}\varphi(\boldsymbol{q})d^n\boldsymbol{q},\end{aligned}$$

where the limit is understood in the strong topology on $L^2(\mathbb{R}^n)$. As in the case $n = 1$, we have

$$\hat{Q}_k = \mathscr{F}_\hbar Q_k \mathscr{F}_\hbar^{-1}, \quad \hat{P}_k = \mathscr{F}_\hbar P_k \mathscr{F}_\hbar^{-1}, \quad k = 1, \dots, n.$$

In particular, since operators $\hat{P}_1, \dots, \hat{P}_n$ are obviously self-adjoint, this immediately shows that $P_1, \dots, P_n$ are also self-adjoint.

REMARK 3.5. Following Dirac, physicists denote a vector $\psi \in \mathscr{H}$ by a *ket vector* $|\psi\rangle$, a vector $\varphi \in \mathscr{H}^*$ in the dual space to $\mathscr{H}$ (by the Riesz representation theorem, $\mathscr{H}^* \simeq \mathscr{H}$ is a complex anti-linear isomorphism) by a *bra vector* $\langle\varphi|$, and their inner product by $\langle\varphi|\psi\rangle$. In standard mathematics notation,

$$(\psi, \varphi) = \langle\varphi|\psi\rangle \quad \text{and} \quad (A\psi, \varphi) = \langle\varphi|A|\psi\rangle,$$

where A is a linear operator. Dirac's notation is intuitive and convenient for working with coordinate and momentum representations. Denoting by $|\boldsymbol{q}\rangle = \delta(\boldsymbol{q} - \boldsymbol{q}')$ and $|\boldsymbol{p}\rangle = (2\pi\hbar)^{-n/2} e^{\frac{i}{\hbar}\boldsymbol{pq}}$ the set of generalized common eigenfunctions for the operators $\boldsymbol{Q}$ and $\boldsymbol{P}$, respectively, we formally get

$$\boldsymbol{Q}|\boldsymbol{q}\rangle = \boldsymbol{q}|\boldsymbol{q}\rangle, \quad \boldsymbol{P}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle,$$

where operators $\mathbf{Q}$ act on $\boldsymbol{q}'$, and

$$\langle\boldsymbol{q}|\psi\rangle = \int_{\mathbb{R}^n} \delta(\boldsymbol{q} - \boldsymbol{q}')\psi(\boldsymbol{q}') d^n\boldsymbol{q}' = \psi(\boldsymbol{q}),$$
$$\langle\boldsymbol{p}|\psi\rangle = (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}\boldsymbol{pq}}\psi(\boldsymbol{q}) d^n\boldsymbol{q} = \hat{\psi}(\boldsymbol{p}),$$

as well as $\langle\boldsymbol{q}|\boldsymbol{q}'\rangle = \delta(\boldsymbol{q} - \boldsymbol{q}')$, $\langle\boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p} - \boldsymbol{p}')$.

REMARK 3.6. Correct mathematical framework for the Dirac formalism is the notion of a rigged Hilbert space — a Hilbert space $\mathscr{H}$ with a dense linear subset $\mathscr{V}$, which is a complete topological vector space. Topology on $\mathscr{V}$ is finer than that of $\mathscr{H}$, so that the inclusion $\mathscr{V} \subset \mathscr{H}$ is a continuous map. Since $\mathscr{H}$ is self-dual, we have a triple

$$\mathscr{V} \subset \mathscr{H} \subset \mathscr{V}^*.$$

Typical example of rigged Hilbert space is $L^2(\mathbb{R}^n)$ with $\mathscr{V} = \mathscr{S}(\mathbb{R}^n)$, the Schwarz space of rapidly decaying functions. The dual space $\mathscr{V}^*$ is the space of tempered distributions and the generalized eigenfunctions $|\boldsymbol{q}\rangle$ and $\boldsymbol{p}\rangle$ are elements of $\mathscr{V}^*$.

PROBLEM 3.1. Give an example of a non-integrable representation of the Heisenberg algebra.

PROBLEM 3.2. Prove that there exists $\varphi \in \mathscr{H} = L^2(\mathbb{R}, dq)$ such that the vectors $\mathsf{P}(E)\varphi$, $E \in \mathscr{B}(\mathbb{R})$, where P is a projection-valued measure for the coordinate operator Q, are dense in $\mathscr{H}$.

PROBLEM 3.3. Find the projection-valued measure for the commutative family $\boldsymbol{P} = (P_1, \dots, P_n)$ in the coordinate representation.

CHAPTER 4

Schrödinger equation

4.1. Examples of quantum systems

Here we describe quantum systems that correspond to classical Hamiltonian systems. The phase space of these systems is a symplectic vector space $\mathbb{R}^{2n}$ with the canonical coordinates $\boldsymbol{p} = (p_1, \dots, p_n)$ and $\boldsymbol{q} = (q^1, \dots, q^n)$ and the symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$.

Example 4.1 (Free particle). A free classical particle with n degrees of freedom is described by the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{q}) = \frac{\boldsymbol{p}^2}{2m} = \frac{1}{2m}(p_1^2 + \cdots + p_n^2).$$

The Hamiltonian operator of a free quantum particle with n degrees of freedom is

$$H_0 = \frac{\boldsymbol{P}^2}{2m} = \frac{1}{2m}(P_1^2 + \cdots + P_n^2),$$

and in the coordinate representation is

$$H_0 = -\frac{\hbar^2}{2m}\Delta,$$

where

$$\Delta = \left(\frac{\partial}{\partial \boldsymbol{q}}\right)^2 = \left(\frac{\partial}{\partial q^1}\right)^2 + \cdots + \left(\frac{\partial}{\partial q^n}\right)^2$$

is the Laplace operator[1] in the Cartesian coordinates on $\mathbb{R}^n$. The Hamiltonian H_0 is a self-adjoint operator on $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ with $D(H_0) = W^{2,2}(\mathbb{R}^n)$ — the Sobolev space on $\mathbb{R}^n$.

Example 4.2 (Newtonian particle). A classical particle in $\mathbb{R}^n$ moving in a potential field $V(\boldsymbol{q})$ is described by the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{q}) = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q}).$$

[1] It is the negative of the Laplace-Beltrami operator of the standard Euclidean metric on $\mathbb{R}^n$.

The Hamiltonian operator of a Newtonian particle is

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q}),$$

in agreement with the prescription[2] $H = H_{\rm c}(\boldsymbol{P}, \boldsymbol{Q})$, so that Heisenberg equations of motion

$$\dot{\boldsymbol{P}} = \{H, \boldsymbol{P}\}_\hbar, \;\; \dot{\boldsymbol{Q}} = \{H, \boldsymbol{Q}\}_\hbar. \tag{4.1}$$

have the same form as Hamilton's equations.

In coordinate representation the Hamiltonian is the *Schrödinger operator*

$$H = -\frac{\hbar^2}{2m}\Delta + V(\boldsymbol{q}) \tag{4.2}$$

with the real-valued potential $V(\boldsymbol{q})$.

REMARK 4.1. Since the sum of two unbounded, self-adjoint operators is not necessarily self-adjoint, one needs to describe potentials $V(\boldsymbol{q})$ for which H is a self-adjoint operator on $L^2(\mathbb{R}^n, d^n\boldsymbol{q})$. If $V(\boldsymbol{q})$ is a real-valued, locally integrable function on $\mathbb{R}^n$, then differential operator (4.2) defines a symmetric operator on $C_c^2(\mathbb{R}^n)$, and admissible potentials $V(\boldsymbol{q})$ correspond to the case when this symmetric operator has zero defect indices.

EXAMPLE 4.3 (The hydrogen atom). It consists of a nucleus: a single proton[3] of mass M and charge e, and of an electron of mass m and charge $-e$. The Hamiltonian of the hydrogen atom is

$$H = -\frac{\hbar^2}{2M}\Delta_p - \frac{\hbar^2}{2m}\Delta_e - \frac{e^2}{|\boldsymbol{r}_p - \boldsymbol{r}_e|},$$

where $\boldsymbol{r}_p$ is the position of the proton and $\boldsymbol{r}_e$ is the position of the electron. As the first approximation, the proton can be considered as infinitely heavy, so that the hydrogen atom is described by an electron in an attractive Coulomb field $-e^2/|\boldsymbol{r}|$, where now $\boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_p$. The corresponding Hamiltonian operator takes the form

$$H = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|\boldsymbol{r}|}. \tag{4.3}$$

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[2]In the special case $H_{\rm c}(\boldsymbol{p}, \boldsymbol{q}) = f(\boldsymbol{p}) + g(\boldsymbol{q})$ the problem of the ordering of non-commuting operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ does not arise.

[3]In the case of hydrogen-1 or protium; it includes one or more neutrons for deuterium, tritium, and other isotopes.

EXAMPLE 4.4 (Charged particle in an electromagnetic field). A classical particle of charge e and mass m moving in the time-independent electromagnetic field with scalar and vector potentials $\varphi(\boldsymbol{r})$ and $\boldsymbol{A}(\boldsymbol{r})$, $\boldsymbol{r} \in \mathbb{R}^3$, is described by the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{r}) = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\varphi(\boldsymbol{r})$$

The corresponding classical velocity vector $\boldsymbol{v} = \{H_{\mathrm{c}}, \boldsymbol{r}\}$ is given by

$$\boldsymbol{v} = \boldsymbol{p} - \frac{e}{c}\boldsymbol{A},$$

and its components $\boldsymbol{v} = (v_1, v_2, v_3)$ have non-vanishing Poisson brackets:

$$\{v_1, v_2\} = -\frac{e}{m^2 c}B_3, \quad \{v_2, v_3\} = -\frac{e}{m^2 c}B_1, \quad \{v_3, v_1\} = -\frac{e}{m^2 c}B_2,$$

where $\boldsymbol{B} = (B_1, B_2, B_3)$ are components of the magnetic field $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$.

The Hamiltonian operator of a quantum particle is

$$H = \frac{1}{2m}\left(\boldsymbol{P} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\varphi(\boldsymbol{r}) \tag{4.4}$$

— the Schrödinger operator of a charged particle in an electromagnetic field. The corresponding quantum velocity vector $\boldsymbol{V} = \{H, \boldsymbol{Q}\}_\hbar$ is given by the same formula as in the classical case,

$$\boldsymbol{V} = \boldsymbol{P} - \frac{e}{c}\boldsymbol{A},$$

and its components $\boldsymbol{V} = (V_1, V_2, V_3)$ have non-vanishing quantum brackets:

$$\{V_1, V_2\}_\hbar = -\frac{e}{m^2 c}B_3, \quad \{V_2, V_3\}_\hbar = -\frac{e}{m^2 c}B_1, \quad \{V_3, V_1\}_\hbar = -\frac{e}{m^2 c}B_2.$$

Thus in the presence of a magnetic field the three components of a quantum velocity operator no longer commute and cannot be measured simultaneously.

4.2. Free quantum particle

The Hamiltonian of a free quantum particle with one degree of freedom

$$H_0 = \frac{P^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2}$$

is a positive operator with absolutely continuous spectrum $[0, \infty)$ of multiplicity two. Indeed, let $\mathfrak{H}_0 = L^2(\mathbb{R}_{>0}, \mathbb{C}^2; d\sigma)$ be the Hilbert space of

$\mathbb{C}^2$-valued measurable functions Ψ on the semi-line $\mathbb{R}_{>0} = (0, \infty)$, which are square-integrable with respect to the measure $d\sigma(\lambda) = \sqrt{\frac{m}{2\lambda}}\, d\lambda$,

$$\mathfrak{H}_0 = \left\{ \Psi(\lambda) = \begin{pmatrix} \psi_1(\lambda) \\ \psi_2(\lambda) \end{pmatrix} : \|\Psi\|^2 = \int_0^\infty (|\psi_1(\lambda)|^2 + |\psi_2(\lambda)|^2) d\sigma(\lambda) < \infty \right\}.$$

It follows from the unitarity of the Fourier transform that the operator $\mathscr{U}_0 : L^2(\mathbb{R}, dq) \to \mathfrak{H}_0$,

$$\mathscr{U}_0(\psi)(\lambda) = \Psi(\lambda) = \begin{pmatrix} \hat{\psi}(\sqrt{2m\lambda}) \\ \hat{\psi}(-\sqrt{2m\lambda}) \end{pmatrix},$$

is unitary, $\mathscr{U}_0^* \mathscr{U}_0 = I$ and $\mathscr{U}_0 \mathscr{U}_0^* = I_0$, where I and I_0 are, respectively, identity operators in $\mathscr{H}$ and $\mathfrak{H}_0$. The operator $\mathscr{U}_0$ establishes the isomorphism $L^2(\mathbb{R}, dq) \simeq \mathfrak{H}_0$, and since in the momentum representation H_0 is a multiplication by $\frac{1}{2m}p^2$ operator, the operator $\mathscr{U}_0 H_0 \mathscr{U}_0^{-1}$ is a multiplication by λ operator in $\mathfrak{H}_0$.

Remark 4.2. The Hamiltonian operator H_0 has no eigenvectors — the eigenvalue equation

$$H_0\psi = \lambda\psi$$

has no solutions in $L^2(\mathbb{R})$. However, for every $\lambda = \frac{1}{2m}k^2 > 0$ this differential equation has two linear independent bounded solutions

$$\psi_k^{(\pm)}(q) = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\pm \frac{i}{\hbar} kq}, \quad k > 0.$$

In the distributional sense, these eigenfunctions of the continuous spectrum combine to a Schwartz kernel of the unitary operator $\mathscr{U}_0$, which establishes the isomorphism between $\mathscr{H} = L^2(\mathbb{R}, dq)$ and the Hilbert space $\mathfrak{H}_0$, where H_0 acts as a multiplication by λ operator.

The Cauchy problem

$$i\hbar \frac{d\psi(t)}{dt} = H_0\psi(t), \quad \psi(0) = \psi, \tag{4.5}$$

is easily solved by the Fourier transform. Indeed, in the momentum representation it takes the form

$$i\hbar \frac{\partial \hat{\psi}(p,t)}{\partial t} = \frac{p^2}{2m}\hat{\psi}(p,t), \quad \hat{\psi}(p,0) = \hat{\psi}(p),$$

so that

$$\hat{\psi}(p,t) = e^{-\frac{ip^2}{2m\hbar}t}\, \hat{\psi}(p).$$

In the coordinate representation, the solution of (4.5) is given by

$$\psi(q,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}pq}\hat{\psi}(p,t)dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\chi(p,q,t)t}\hat{\psi}(p)dp, \tag{4.6}$$

where

$$\chi(p,q,t) = -\frac{p^2}{2m} + \frac{pq}{t}.$$

Formula (4.6) describes the motion of a quantum particle, and admits the following physical interpretation. Let initial condition ψ in (4.5) be such that its Fourier transform $\hat{\psi} = \mathcal{F}_\hbar(\psi)$ is a smooth function supported in a neighborhood U_0 of $p_0 \in \mathbb{R} \setminus \{0\}$, $0 \notin U_0$, and

$$\int_{-\infty}^{\infty} |\hat{\psi}(p)|^2 dp = 1.$$

Such states are called "wave packets". Then for every compact subset $E \subset \mathbb{R}$ we have

$$\lim_{|t|\to\infty}\int_E |\psi(q,t)|^2 dq = 0. \tag{4.7}$$

Since

$$\int_{-\infty}^{\infty} |\psi(q,t)|^2 dq = 1$$

for all t, it follows from (4.7) that the particle leaves every compact subset of $\mathbb{R}$ as $|t| \to \infty$ and the quantum motion is infinite. To prove (4.7), observe that the function $\chi(p,q,t)$ — the "phase" in integral representation (4.6) — has the property that $|\frac{\partial\chi}{\partial p}| > C > 0$ for all $p \in U_0$, $q \in E$ and large enough $|t|$. Integrating by parts we get

$$\begin{aligned}\psi(q,t) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{U_0} e^{\frac{i}{\hbar}\chi(p,q,t)t}\hat{\psi}(p)dp \\ &= -\frac{1}{it}\sqrt{\frac{\hbar}{2\pi}}\int_{U_0}\frac{\partial}{\partial p}\left(\frac{\hat{\psi}(p)}{\frac{\partial\chi(p,q,t)}{\partial p}}\right)e^{\frac{i}{\hbar}\chi(p,q,t)t}dp,\end{aligned}$$

so that uniformly on E,

$$\psi(q,t) = O(|t|^{-1}) \quad \text{as} \quad |t| \to \infty.$$

By repeated integration by parts, we obtain that for every $n \in \mathbb{N}$, uniformly on E,

$$\psi(q,t) = O(|t|^{-n}),$$

so that $\psi(q,t) = O(|t|^{-\infty})$.

To describe the motion of a free quantum particle in unbounded regions, we use the stationary phase method. In its simplest form it is stated as follows.

The Method of Stationary Phase. Let $f, g \in C^\infty(\mathbb{R})$, where f is real-valued and g has compact support, and suppose that f has a single non-degenerate critical point x_0, i.e., $f'(x_0) = 0$ and $f''(x_0) \neq 0$. Then

$$\int_{-\infty}^{\infty} e^{iNf(x)} g(x)dx = \left(\frac{2\pi}{N|f''(x_0)|}\right)^{\frac{1}{2}} e^{iNf(x_0) + \frac{i\pi}{4}\operatorname{sgn} f''(x_0)} g(x_0) + O\left(\frac{1}{N}\right)$$

as $N \to \infty$.

Applying the stationary phase method to the integral representation (4.6) (and setting $N = t$), we find that the critical point of $\chi(p,q,t)$ is $p_0 = \frac{mq}{t}$ with $\chi''(p_0) = -\frac{1}{m} \neq 0$, and

$$\begin{aligned}\psi(q,t) &= \sqrt{\frac{m}{t}}\hat{\psi}\left(\frac{mq}{t}\right) e^{\frac{imq^2}{2\hbar t} - \frac{\pi i}{4}} + O(t^{-1}) \\ &= \psi_0(q,t) + O(t^{-1}) \quad \text{as} \quad t \to \infty.\end{aligned}$$

Thus as $t \to \infty$, the wave function $\psi(q,t)$ is supported on $\frac{t}{m}U_0$ — a domain where the probability of finding a particle is asymptotically different from zero. At large t the points in this domain move with constant velocities $v = \frac{p}{m}$, $p \in U_0$. In this sense, the classical relation $p = mv$ remains valid in the quantum picture. Moreover, the asymptotic wave function ψ_0 satisfies

$$\int_{-\infty}^{\infty} |\psi_0(q,t)|^2 dq = \frac{m}{t}\int_{-\infty}^{\infty} \left|\hat{\psi}\left(\frac{mq}{t}\right)\right|^2 dq = 1,$$

and, therefore, describes the asymptotic probability distribution. Similarly, setting $N = -|t|$, we can describe the behavior of the wave function $\psi(q,t)$ as $t \to -\infty$.

Remark 4.3. We have $\lim_{|t|\to\infty} \psi(t) = 0$ in the weak topology on $\mathscr{H}$. Indeed, for every $\varphi \in \mathscr{H}$ we get by Parseval's identity for the Fourier integrals,

$$(\psi(t), \varphi) = \int_{-\infty}^{\infty} \hat{\psi}(p)\overline{\hat{\varphi}(p)} e^{-\frac{ip^2 t}{2m\hbar}} dp,$$

and the integral goes to zero as $|t| \to \infty$ by the Riemann-Lebesgue lemma.

Similarly, the Hamiltonian H_0 of a free quantum particle with n degrees of freedom is is a positive operator with absolutely continuous spectrum $[0, \infty)$ of infinite multiplicity. Namely, let $S^{n-1} = \{\boldsymbol{n} \in \mathbb{R}^n : \boldsymbol{n}^2 = 1\}$ be the $(n-1)$-dimensional unit sphere in $\mathbb{R}^n$, let $d\boldsymbol{n}$ be the measure on S^{n-1} induced by the Lebesgue measure on $\mathbb{R}^n$, and let

$$\mathfrak{h} = \{f : S^{n-1} \to \mathbb{C} : \|f\|_{\mathfrak{h}}^2 = \int_{S^{n-1}} |f(\boldsymbol{n})|^2 d\boldsymbol{n} < \infty\}.$$

Let $\mathfrak{H}_0^{(n)} = L^2(\mathbb{R}_{>0}, \mathfrak{h}; d\sigma_n)$ be the Hilbert space of $\mathfrak{h}$-valued measurable functions[4] Ψ on $\mathbb{R}_{>0} = (0, \infty)$, square-integrable on $\mathbb{R}_{>0}$ with respect to the measure $d\sigma_n(\lambda) = (2m\lambda)^{\frac{n}{2}} \frac{d\lambda}{2\lambda}$,

$$\mathfrak{H}_0^{(n)} = \left\{ \Psi : \mathbb{R}_{>0} \to \mathfrak{h},\ \|\Psi\|^2 = \int_0^\infty \|\Psi(\lambda)\|_{\mathfrak{h}}^2 \, d\sigma_n(\lambda) < \infty \right\}.$$

When $n = 1$, $\mathfrak{H}_0^{(1)} = \mathfrak{H}_0$ — the corresponding Hilbert space for one degree of freedom. The operator $\mathscr{U}_0 : L^2(\mathbb{R}^n, d^n\boldsymbol{q}) \to \mathfrak{H}_0^{(n)}$,

$$\mathscr{U}_0(\psi)(\lambda) = \Psi(\lambda), \quad \Psi(\lambda)(\boldsymbol{n}) = \hat{\psi}(\sqrt{2m\lambda}\, \boldsymbol{n}),$$

is unitary and establishes the isomorphism $L^2(\mathbb{R}^n, d^n\boldsymbol{q}) \simeq \mathfrak{H}_0^{(n)}$. In the momentum representation H_0 is a multiplication by $\frac{1}{2m}\boldsymbol{p}^2$ operator, so that the operator $\mathscr{U}_0 H_0 \mathscr{U}_0^{-1}$ is a multiplication by λ operator in $\mathfrak{H}_0^{(n)}$.

Remark 4.4. As in the case $n = 1$, the Hamiltonian operator H_0 has no eigenvectors — the eigenvalue equation

$$H_0\psi = \lambda\psi$$

has no solutions in $L^2(\mathbb{R}^n)$. However, for every $\lambda > 0$ this differential equation has infinitely many linearly independent bounded solutions

$$\psi_{\boldsymbol{n}}(\boldsymbol{q}) = (2\pi\hbar)^{-\frac{n}{2}} \, e^{\frac{i}{\hbar}\sqrt{2m\lambda}\,\boldsymbol{n}\boldsymbol{q}},$$

parametrized by the unit sphere S^{n-1}. These solutions do not belong to $L^2(\mathbb{R}^n)$, but in the distributional sense they combine to a Schwartz kernel of the unitary operator $\mathscr{U}_0$, which establishes the isomorphism between $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ and the Hilbert space $\mathfrak{H}_0^{(n)}$, where H_0 acts as a multiplication by λ operator.

[4]That is, for every $f \in \mathfrak{h}$ the function (f, Ψ) is measurable on $\mathbb{R}_{>0}$.

As in the case $n = 1$, the Schrödinger equation

$$i\hbar \frac{d\psi(t)}{dt} = H_0 \psi(t), \quad \psi(0) = \psi,$$

is solved by the Fourier transform

$$\psi(\boldsymbol{q}, t) = (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}(\boldsymbol{p}\boldsymbol{q} - \frac{\boldsymbol{p}^2}{2m}t)} \hat{\psi}(\boldsymbol{p}) d^n\boldsymbol{p}.$$

For a wave packet, an initial condition ψ such that its Fourier transform $\hat{\psi} = \mathscr{F}_\hbar(\psi)$ is a smooth function supported on a neighborhood U_0 of $\boldsymbol{p}_0 \in \mathbb{R}^n \setminus \{0\}$ such that $0 \notin U_0$ and

$$\int_{\mathbb{R}^n} |\hat{\psi}(\boldsymbol{p})|^2 d^n\boldsymbol{p} = 1,$$

the quantum particle leaves every compact subset of $\mathbb{R}^n$ and the motion is infinite. Asymptotically as $|t| \to \infty$, the wave function $\psi(\boldsymbol{q}, t)$ is different from 0 only when $\boldsymbol{q} = \frac{\boldsymbol{p}}{m}t$, $\boldsymbol{p} \in U_0$.

CHAPTER 5

Quantum harmonic oscillator

The simplest classical system with one degree of freedom, besides the free particle, is the harmonic oscillator. It is described by the phase space $\mathbb{R}^2$ with the canonical coordinates p, q, and the Hamiltonian function

$$H_{\mathrm{c}}(p,q) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} \tag{5.1}$$

Hamilton's equations

$$\dot{p} = \{H_{\mathrm{c}}, p\} = -m\omega^2 q, \quad \dot{q} = \{H_{\mathrm{c}}, q\} = \frac{p}{m}$$

with the initial conditions p_0, q_0 are readily solved,

$$p(t) = p_0 \cos\omega t - m\omega q_0 \sin\omega t, \tag{5.2}$$

$$q(t) = q_0 \cos\omega t + \frac{1}{m\omega} p_0 \sin\omega t, \tag{5.3}$$

and describe the harmonic motion. It is convenient to introduce complex coordinates on the phase space $\mathbb{R}^2 \simeq \mathbb{C}$,

$$z = \frac{1}{\sqrt{2\omega}}\left(\omega q + \frac{ip}{m}\right), \quad \bar{z} = \frac{1}{\sqrt{2\omega}}\left(\omega q - \frac{ip}{m}\right). \tag{5.4}$$

We have

$$\{z, \bar{z}\} = \frac{i}{m}, \quad H_{\mathrm{c}}(z,\bar{z}) = m\omega |z|^2, \tag{5.5}$$

so that Hamilton's equations decouple,

$$\dot{z} = \{H_{\mathrm{c}}, z\} = -i\omega z, \quad \dot{\bar{z}} = \{H_{\mathrm{c}}, \bar{z}\} = i\omega\bar{z}, \tag{5.6}$$

and are trivially solved,

$$z(t) = e^{-i\omega t} z_0, \quad \bar{z} = e^{i\omega t}\bar{z}_0. \tag{5.7}$$

Here

$$z_0 = \frac{1}{\sqrt{2\omega}}\left(\omega q_0 + \frac{ip_0}{m}\right), \quad \bar{z}_0 = \frac{1}{\sqrt{2\omega}}\left(\omega q_0 - \frac{ip_0}{m}\right).$$

REMARK 5.1. Equations of motion (5.6) can be also obtained from the following first order Lagrangian

$$L = m(i\bar{z}\dot{z} - \omega|z|^2). \tag{5.8}$$

Indeed, it easy to see that (5.6) are Euler-Lagrange equations of the action functional

$$S = \int_{t_0}^{t_1} L dt.$$

Moreover, conjugated momentum π to z is given by

$$\pi = \frac{\partial L}{\partial \dot{z}} = im\bar{z},$$

and we obtain canonical Poisson bracket

$$\{\pi, z\} = 1,$$

which is the bracket (5.5). At the same time, classical Hamiltonian is given by the Legendre transform:

$$H_c(z, \bar{z}) = \pi\dot{z} - L. \tag{5.9}$$

For the quantum system, the corresponding Hamiltonian operator is

$$H = \frac{P^2}{2m} + \frac{m\omega^2 Q^2}{2},$$

and in the coordinate representation $\mathscr{H} = L^2(\mathbb{R}, dq)$ it is a Schrödinger operator with a quadratic potential,

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{m\omega^2 q^2}{2}.$$

The quantum harmonic oscillator is the simplest non-trivial quantum system, besides the free particle, whose Schrödinger equation can be solved explicitly. Its exact solution has remarkable[1] algebraic and analytic properties.

[1]The algebraic structure of the exact solution of the harmonic oscillator plays a fundamental role in quantum field theory.

5.1. Exact solution

Temporarily set $m = 1$ and consider the operators

$$a = \frac{1}{\sqrt{2\omega\hbar}}\left(\omega Q + iP\right), \quad a^* = \frac{1}{\sqrt{2\omega\hbar}}\left(\omega Q - iP\right), \tag{5.10}$$

which are quantum analogs of complex coordinates (5.4). The operators a and a^* are defined on $W^{1,2}(\mathbb{R}) \cap \widehat{W}^{1,2}(\mathbb{R})$, where $\widehat{W}^{1,2}(\mathbb{R}) = \mathscr{F}(W^{1,2}(\mathbb{R}))$, and it is easy to show that a^* is the adjoint operator to a and $a^{**} = a$, so that a is a closed operator. From the Heisenberg commutation relation (3.2) we get the *canonical commutation relation*

$$[a, a^*] = I \tag{5.11}$$

on $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$, where $\widehat{W}^{2,2}(\mathbb{R}) = \mathscr{F}(W^{2,2}(\mathbb{R}))$. Indeed, we have

$$aa^* = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} + \frac{i\omega}{2\omega\hbar}[P, Q] = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} + \frac{1}{2}I,$$
$$a^*a = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} - \frac{i\omega}{2\omega\hbar}[P, Q] = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} - \frac{1}{2}I,$$

so that (5.11) holds on $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$, and

$$H = \frac{\omega\hbar}{2}(a^*a + aa^*) = \omega\hbar\left(a^*a + \tfrac{1}{2}I\right). \tag{5.12}$$

In particular, it follows from the von Neumann criterion[2] that the Hamiltonian operator H is self-adjoint.

The operators a, a^* and $N = a^*a$ satisfy the commutation relations

$$[N, a] = -a, \quad [N, a^*] = a^*, \quad [a, a^*] = I. \tag{5.13}$$

Commutation relations (5.13) allow to solve explicitly the Heisenberg equations of motion for the harmonic oscillator. Namely, we have

$$\dot{a} = \{H, a\}_\hbar = -i\omega a, \quad \dot{a}^* = \{H, a^*\}_\hbar = i\omega a^*,$$

so that

$$a(t) = e^{-i\omega t}a_0, \quad a^*(t) = e^{i\omega t}a_0^*.$$

Comparing with (5.7) we see that solutions of classical and quantum equations of motion for the harmonic oscillator have the same form!

[2]If A is a closed operator and $\overline{D(A)} = \mathscr{H}$, then $H = A^*A$ is a self-adjoint operator.

Next, using commutation relations (5.13) and positivity of the operator N, we solve the eigenvalue problem for the Hamiltonian H of the harmonic oscillator explicitly by finding its energy levels and corresponding eigenvectors. We will prove that the eigenvectors form a complete system of vectors in $\mathscr{H}$, so that the spectrum of the Hamiltonian H is the point spectrum. This is a quantum mechanical analog of the fact that classical motion of the harmonic oscillator is always finite.

The algebraic part of the exact solution is the following fundamental result.

PROPOSITION 5.1. *Suppose that there exists a non-zero* $\psi \in D(a^n) \cap D((a^*)^n)$, $n = 1, 2, \dots,$ *such that*

$$H\psi = \lambda\psi.$$

Then the following statements hold.

(i) *There exists* $\psi_0 \in \mathscr{H}$, $\|\psi_0\| = 1$, *such that*

$$H\psi_0 = \tfrac{1}{2}\hbar\omega\psi_0.$$

(ii) *The vectors*

$$\psi_n = \frac{(a^*)^n}{\sqrt{n!}}\psi_0 \in \mathscr{H}, \quad n = 0, 1, 2, \dots,$$

are orthonormal eigenvectors for H *with the eigenvalues* $\hbar\omega(n + \frac{1}{2})$,

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

(iii) *Restriction of the operator* H *to the Hilbert space* $\mathscr{H}_0$ *— a closed subspace of* $\mathscr{H}$, *spanned by the orthonormal set* $\{\psi_n\}_{n=0}^{\infty}$ *— is essentially self-adjoint.*

PROOF. Rewriting commutation relations (5.13) as

$$Na = a(N - I) \quad \text{and} \quad Na^* = a^*(N + I),$$

and putting $\lambda = \hbar\omega(\mu + \frac{1}{2})$, we get for all $n \geq 0$,

$$Na^n\psi = (\mu - n)a^n\psi \quad \text{and} \quad N(a^*)^n\psi = (\mu + n)(a^*)^n\psi. \tag{5.14}$$

Since $N \geq 0$ on $D(N)$, it follows from the first equation in (5.14) that there exists $n_0 \geq 0$ such that $a^{n_0}\psi \neq 0$ but $a^{n_0+1}\psi = 0$. Setting $\psi_0 = \dfrac{a^{n_0}\psi}{\|a^{n_0}\psi\|} \in \mathscr{H}$ we get

$$a\psi_0 = 0 \quad \text{and} \quad N\psi_0 = 0. \tag{5.15}$$

Since $H = \hbar\omega(N + \frac{1}{2}I)$, this proves part (i). To prove part (ii), we use commutation relations

$$[a, (a^*)^n] = n(a^*)^{n-1}, \tag{5.16}$$

which follow from (5.11) and the Leibniz rule. Thus for $\psi_n = \dfrac{(a^*)^n}{\sqrt{n!}}\psi_0$ we get, using (5.15)-(5.16),

$$a^*\psi_n = \sqrt{n+1}\,\psi_{n+1}, \quad a\psi_n = \sqrt{n}\,\psi_{n-1}, \tag{5.17}$$

so that

$$\|\psi_n\|^2 = \frac{1}{\sqrt{n}}(a^*\psi_{n-1}, \psi_n) = \frac{1}{\sqrt{n}}(\psi_{n-1}, a\psi_n) = \|\psi_{n-1}\|^2 = \cdots = \|\psi_0\|^2 = 1.$$

From the second equation in (5.14) it follows that $N\psi_n = n\psi_n$, so ψ_n are normalized eigenvectors of H with the eigenvalues $\hbar\omega(n + \frac{1}{2})$. The eigenvectors ψ_n are orthogonal since the corresponding eigenvalues are distinct and the operator H is symmetric. Finally, part (iii) immediately follows from the fact that, according to part (ii), the subspaces Im $(H \pm iI)|_{\mathscr{H}_0}$ are dense in $\mathscr{H}_0$, which is the criterion of essential self-adjointness. □

Remark 5.2. Since the coordinate representation of the Heisenberg commutation relations is irreducible, it is tempting to conclude, using Proposition 5.1, that $\mathscr{H}_0 = \mathscr{H}$. Namely, it follows from the construction that the linear span of vectors ψ_n — a dense subspace of $\mathscr{H}_0$ — is invariant for the operators P and Q. However, this does not immediately imply that the projection operator Π_0 onto the subspace $\mathscr{H}_0$ commutes with self-adjoint operators P and Q in the sense of the definition in Section 2.1.

Using the coordinate representation, we can immediately show the existence of the vector ψ_0 in Proposition 5.1, and prove that $\mathscr{H}_0 = \mathscr{H}$. Indeed, equation $a\psi_0 = 0$ becomes a first order linear differential equation

$$\left(\hbar\frac{d}{dq} + \omega q\right)\psi_0 = 0,$$

so that

$$\psi_0(q) = \sqrt[4]{\frac{\omega}{\pi\hbar}}\, e^{-\frac{\omega}{2\hbar}q^2},$$

and

$$\|\psi_0\|^2 = \sqrt{\frac{\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{\omega}{\hbar}q^2} dq = 1.$$

The vector ψ_0 is called the *ground state* for the harmonic oscillator. Correspondingly, the eigenfunctions

$$\psi_n(q) = \frac{1}{\sqrt{n!}} \left(\frac{1}{\sqrt{2\omega\hbar}} \left(\omega q - \hbar \frac{d}{dq} \right) \right)^n \psi_0$$

are of the form $P_n(q)e^{-\frac{\omega}{2\hbar}q^2}$, where $P_n(q)$ are polynomials of degree n. The following result guarantees that the functions $\{\psi_n\}_{n=0}^{\infty}$ form an orthonormal basis in $L^2(\mathbb{R}, dq)$.

LEMMA 5.1. *The functions* $q^n e^{-q^2}$, $n = 0, 1, 2, \ldots$, *are complete in* $L^2(\mathbb{R}, dq)$.

PROOF. Let $f \in L^2(\mathbb{R}, dq)$ is such that

$$\int_{-\infty}^{\infty} f(q) q^n e^{-q^2} dq = 0, \quad n = 0, 1, 2, \ldots.$$

The integral

$$F(z) = \int_{-\infty}^{\infty} f(q) e^{iqz - q^2} dq$$

is absolutely convergent for all $z \in \mathbb{C}$ and, therefore, defines an entire function. We have

$$F^{(n)}(0) = i^n \int_{-\infty}^{\infty} f(q) q^n e^{-q^2} dq = 0, \quad n = 0, 1, 2, \ldots,$$

so that $F(z) = 0$ for all $z \in \mathbb{C}$. This implies the function $g(q) = f(q)e^{-q^2} \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ satisfies $\mathscr{F}(g) = 0$, where $\mathscr{F}$ is the "ordinary" ($\hbar = 1$) Fourier transform. Thus we conclude that $g = 0$. □

The polynomials P_n are expressed through classical Hermite-Tchebyscheff polynomials H_n, defined by

$$H_n(q) = (-1)^n e^{q^2} \frac{d^n}{dq^n} e^{-q^2}, \quad n = 0, 1, 2, \ldots.$$

Namely, using the identity

$$e^{\frac{q^2}{2}}\frac{d^n}{dq^n}\,e^{-q^2} = -\left(q-\frac{d}{dq}\right)\left[e^{\frac{q^2}{2}}\frac{d^{n-1}}{dq^{n-1}}\,e^{-q^2}\right] = \cdots = (-1)^n\left(q-\frac{d}{dq}\right)^n e^{-\frac{q^2}{2}}$$

we obtain

$$\psi_n(q) = \sqrt[4]{\frac{\omega}{\pi\hbar}}\frac{1}{\sqrt{2^n n!}}\,e^{-\frac{\omega}{2\hbar}q^2}H_n\left(\sqrt{\frac{\omega}{\hbar}}\,q\right).$$

We summarize the obtained results as follows.

THEOREM 5.1. *The Hamiltonian*

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{m\omega^2 q^2}{2}$$

of the quantum harmonic oscillator with one degree of freedom is a self-adjoint operator on $\mathscr{H} = L^2(\mathbb{R}, dq)$ *with the domain* $D(H) = W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$. *The operator* H *has pure point spectrum*

$$H\psi_n = \lambda_n\psi_n, \quad n = 0, 1, 2, \ldots,$$

with the eigenvalues $\lambda_n = \hbar\omega(n+\frac{1}{2})$. *Corresponding eigenfunctions* ψ_n *form an orthonormal basis for* $\mathscr{H}$ *and are given by*

$$\psi_n(q) = \sqrt[4]{\frac{m\omega}{\pi\hbar}}\frac{1}{\sqrt{2^n n!}}\,e^{-\frac{m\omega}{2\hbar}q^2}H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,q\right), \tag{5.18}$$

where $H_n(q)$ *are classical Hermite-Tchebyscheff polynomials.*

PROOF. Consider the operator H defined on the Schwartz space $\mathscr{S}(\mathbb{R})$ of rapidly decreasing functions. Since the operator H is symmetric and has a complete system of eigenvectors in $\mathscr{S}(\mathbb{R})$, the subspaces $\operatorname{Im}(H \pm iI)$ are dense in $\mathscr{H}$, so that H is essentially self-adjoint. It is easy to show that self-adjoint closure of H (which we continue to denote by H) has the domain $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$. □

5.2. Holomorphic representation

Let

$$\ell^2 = \left\{c = \{c_n\}_{n=0}^{\infty} \,:\, \|c\|^2 = \sum_{n=0}^{\infty}|c_n|^2 < \infty\right\}$$

be the Hilbert ℓ^2-space. The choice of an orthonormal basis $\{\psi_n\}_{n=0}^{\infty}$ for $L^2(\mathbb{R}, dq)$, given by the eigenfunctions (5.18) of the Schrödinger operator for the harmonic oscillator, establishes the Hilbert space isomorphism $L^2(\mathbb{R}, dq) \simeq \ell^2$,

$$L^2(\mathbb{R}, dq) \ni \psi = \sum_{n=0}^{\infty} c_n \psi_n \mapsto c = \{c_n\}_{n=0}^{\infty} \in \ell^2,$$

where

$$c_n = (\psi, \psi_n) = \int_{-\infty}^{\infty} \psi(q)\psi_n(q)dq,$$

since the functions ψ_n are real-valued. Using (5.17) we get

$$a^*\psi = \sum_{n=0}^{\infty} c_n a^* \psi_n = \sum_{n=0}^{\infty} \sqrt{n+1}\, c_n \psi_{n+1} = \sum_{n=1}^{\infty} \sqrt{n}\, c_{n-1}\psi_n, \quad \psi \in D(a^*),$$

and

$$a\psi = \sum_{n=0}^{\infty} c_n a \psi_n = \sum_{n=1}^{\infty} \sqrt{n}\, c_n \psi_{n-1} = \sum_{n=0}^{\infty} \sqrt{n+1}\, c_{n+1}\psi_n, \quad \psi \in D(a),$$

so that in ℓ^2 creation and annihilation operators a^* and a are represented by the following semi-infinite matrices:

$$a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad a^* = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

As a result,

$$N = a^*a = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots \\ 0 & 0 & 0 & 3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

so that the Hamiltonian of the harmonic oscillator is represented by a diagonal matrix,

$$H = \hbar\omega(N + \tfrac{1}{2}) = \mathrm{diag}\{\tfrac{1}{2}\hbar\omega, \tfrac{3}{2}\hbar\omega, \tfrac{5}{2}\hbar\omega, \dots\}.$$

This representation of the Heisenberg commutation relations is called the *representation by occupation numbers*, and has the property that in this representation the Hamiltonian H of the harmonic oscillator is diagonal.

Another representation where H is diagonal is constructed as follows. Let $\mathscr{D}$ be the space of entire functions $f(z)$ with the inner product

$$(f,g) = \frac{1}{\pi}\int_{\mathbb{C}} f(z)\overline{g(z)}e^{-|z|^2}d^2z, \tag{5.19}$$

where $d^2z = \frac{i}{2}dz\wedge d\bar{z}$ is the Lebesgue measure on $\mathbb{C}\simeq\mathbb{R}^2$. It is easy to check that $\mathscr{D}$ is a Hilbert space with the orthonormal basis

$$f_n(z) = \frac{z^n}{\sqrt{n!}}, \quad n = 0,1,2,\dots.$$

The correspondence

$$\ell^2 \ni c = \{c_n\}_{n=0}^{\infty} \mapsto f(z) = \sum_{n=0}^{\infty} c_n f_n(z) \in \mathscr{D}$$

establishes the Hilbert space isomorphism $\ell^2 \simeq \mathscr{D}$. The realization of a Hilbert space $\mathscr{H}$ as the Hilbert space $\mathscr{D}$ of entire functions is called a *holomorphic representation*, and $\mathscr{D}$ — *holomorphic Fock-Bargmann space* for one degree of freedom. In the holomorphic representation,

$$a^* = z, \quad a = \frac{d}{dz}, \quad \text{and} \quad H = \hbar\omega\left(z\frac{d}{dz}+\frac{1}{2}\right),$$

and it is very easy to show that a^* is the adjoint operator to a. The mapping

$$\mathscr{H} \ni \psi = \sum_{n=0}^{\infty} c_n\psi_n \mapsto f(z) = \sum_{n=0}^{\infty} c_n f_n(z) \in \mathscr{D}$$

establishes the isomorphism between the coordinate and holomorphic representations. It follows from the formula for the generating function for Hermite-Tchebyscheff polynomials,

$$\sum_{n=0}^{\infty} H_n(q)\frac{z^n}{n!} = e^{2qz-z^2},$$

that the corresponding unitary operator $U:\mathscr{H}\to\mathscr{D}$ is an integral operator

$$U\psi(z) = \int_{-\infty}^{\infty} U(z,q)\psi(q)dq$$

with the kernel

$$U(z,q)=\sum_{n=0}^{\infty}\psi_n(q)f_n(z)=\sqrt[4]{\frac{m\omega}{\pi\hbar}}\,e^{\frac{m\omega}{2\hbar}q^2-\left(\sqrt{\frac{m\omega}{\hbar}}q-\frac{1}{\sqrt{2}}z\right)^2}. \tag{5.20}$$

Another useful realization is a representation in the Hilbert space $\bar{\mathscr{D}}$ of anti-holomorphic functions $f(\bar{z})$ on $\mathbb{C}$ with the inner product

$$(f,g)=\frac{1}{\pi}\int_{\mathbb{C}}f(\bar{z})\overline{g(\bar{z})}e^{-|z|^2}d^2z,$$

given by

$$a^*=\bar{z},\quad a=\frac{d}{d\bar{z}}.$$

It is straightforward to generalize these constructions to n degrees of freedom. Thus the Hilbert space $\mathscr{D}_n$ defining the holomorphic representation is the space of entire functions $f(\boldsymbol{z})$ of n complex variables $\boldsymbol{z}=(z_1,\dots,z_n)$ with the inner product

$$(f,g)=\frac{1}{\pi^n}\int_{\mathbb{C}^n}f(\boldsymbol{z})\overline{g(\boldsymbol{z})}e^{-|\boldsymbol{z}|^2}d^{2n}\boldsymbol{z}<\infty,$$

where $|\boldsymbol{z}|^2=z_1^2+\cdots+z_n^2$ and $d^{2n}\boldsymbol{z}=d^2z_1\cdots d^2z_n$ is the Lebesgue measure on $\mathbb{C}^n\simeq\mathbb{R}^{2n}$. The functions

$$f_{\boldsymbol{m}}(\boldsymbol{z})=\frac{z_1^{m_1}\dots z_n^{m_n}}{\sqrt{m_1!\dots m_n!}},\qquad m_1,\dots,m_n=0,1,2,\dots,$$

where $\boldsymbol{m}=(m_1,\dots,m_n)$ is a multi-index, form an orthonormal basis for $\mathscr{D}_n$. Corresponding creation and annihilation operators are given by

$$a_j^*=z_j,\quad a_j=\frac{\partial}{\partial z_j},\quad j=1,\dots,n$$

and satisfy the commutation relations

$$[a_k,a_l]=[a_k^*,a_l^*]=0,\quad [a_k,a_l^*]=\delta_{kl}I,\quad k,l=1,\dots,n.$$

PROBLEM 5.1. Show that $\langle H|M\rangle\geq\frac{1}{2}\hbar\omega$ for every $M\in\mathscr{S}$, where H is the Hamiltonian of the harmonic oscillator with one degree of freedom.

PROBLEM 5.2. Let $q(t)=A\cos(\omega t+\alpha)$ be the classical trajectory of the harmonic oscillator with $m=1$ and the energy $E=\frac{1}{2}\omega^2A^2$, and let μ_α be the probability measure on $\mathbb{R}$ supported at the point $q(t)$. Show that the convex linear combination of the measures μ_α, $0\leq\alpha\leq 2\pi$, is the probability measure on $\mathbb{R}$ with the distribution function $\mu(q)=\frac{\theta(A^2-q^2)}{\pi\sqrt{A^2-q^2}}$, where $\theta(q)$ is the Heavyside step function.

PROBLEM 5.3. Show that when $n \to \infty$ and $\hbar \to 0$ such that $\hbar\omega(n + \frac{1}{2}) = \frac{1}{2}\omega^2 A^2$ remains fixed, the envelope of the distribution function $|\psi_n(q)|^2$ on the interval $|q| \leq A$ coincides with the classical distribution function $\mu(q)$ from the previous problem. (*Hint:* Prove the integral representation

$$e^{-q^2} H_n(q) = \frac{2^{n+1}}{\sqrt{\pi}} \int_0^\infty e^{-y^2} y^n \cos(2qy - \tfrac{1}{2}n\pi) dy,$$

and derive the asymptotic formula

$$\psi_n(q) = \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt[4]{A^2 - q^2}} \cos\Big\{ \frac{\omega}{2\hbar}\Big(A^2 \sin^{-1} \frac{q}{A} + q\sqrt{A^2 - q^2} - \frac{1}{2}A^2\pi\Big) + O(1)\Big\}$$

when $\hbar \to 0$ and $\hbar(n + \frac{1}{2}) = \frac{1}{2}\omega A^2$, $|q| < A$.)

PROBLEM 5.4. Complete the proof of Theorem 5.1.

PROBLEM 5.5 (The N-representation theorem). Let $\psi \in \mathscr{S}(\mathbb{R})$. Show that the L^2-convergent expansion $\psi = \sum_{n=0}^\infty c_n \psi_n$, where $c_n = (\psi, \psi_n)$, converges in $\mathscr{S}(\mathbb{R})$. (*Hint*: Use $N\psi_n = n\psi_n$.)

PROBLEM 5.6. Show that the operators $E_{ij} = a_i^* a_j$, $i, j = 1, \ldots, n$, satisfy the commutation relations of the Lie algebra $\mathrm{gl}(n, \mathbb{C})$.

CHAPTER 6

Weyl quantization

6.1. Weyl transform

Let R be an irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ in the Hilbert space $\mathscr{H}$. It follows from Schur's lemma that $R(e^{\alpha c}) = e^{i\hbar\alpha}I$ for some $\hbar \in \mathbb{R}$, where I is the identity operator on $\mathscr{H}$.

If $\hbar = 0$, the n-parameter abelian groups of unitary operators $U(\boldsymbol{u}) = R(e^{\boldsymbol{u}X})$ and $V(\boldsymbol{v}) = R(e^{\boldsymbol{v}Y})$ commute, so using Schur's lemma once again we conclude that there exist $\boldsymbol{p}, \boldsymbol{q} \in \mathbb{R}^n$ such that $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{p}}I$ and $V(\boldsymbol{v}) = e^{-i\boldsymbol{v}\boldsymbol{q}}I$. Therefore, in this case the irreducible representation R is one-dimensional and is parametrized by a vector $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n}$.

In case $\hbar > 0$[1] the unitary operators $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$ satisfy the Weyl relations

$$U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar\boldsymbol{u}\boldsymbol{v}}V(\boldsymbol{v})U(\boldsymbol{u}), \tag{6.1}$$

which admit the Schrödinger representation, introduced in Sect. 3.2. It turns out that every unitary irreducible representation of the Heisenberg group $\mathbf{H}_n$ is unitarily equivalent either to a one-dimensional representation with parameters $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n}$, or to the Schrödinger representation. Namely, the following fundamental result holds.

Theorem 6.1 (Stone–von Neumann theorem). *Every irreducible unitary representation of the Weyl relations for n degrees of freedom,*

$$U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar\boldsymbol{u}\boldsymbol{v}}V(\boldsymbol{v})U(\boldsymbol{u}),$$

is unitarily equivalent to the Schrödinger representation.

Remark 6.1. Put $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{P}}$ and $V(\boldsymbol{v}) = e^{-i\boldsymbol{v}\boldsymbol{Q}}$, so that $\boldsymbol{P}$ and $\boldsymbol{Q}$ satisfy Heisenberg commutation relations. The Stone–von Neumann theorem — the statement that self-adjoint operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ are unitarily equivalent to the momenta and coordinate operators in the Schrödinger

[1]The representation with $\hbar < 0$ is given by the operators $U^{-1}(\boldsymbol{u}) = U(-\boldsymbol{u})$ and $V(\boldsymbol{v})$.

representation — is a very strong result. In particular, it implies that for the creation and annihilation operators for n degrees of freedom,

$$\boldsymbol{a}^* = \frac{1}{\sqrt{2\hbar}}(\boldsymbol{Q} - i\boldsymbol{P}) \quad \text{and} \quad \boldsymbol{a} = \frac{1}{\sqrt{2\hbar}}(\boldsymbol{Q} + i\boldsymbol{P}),$$

there always exists a ground state — a vector $\psi_0 \in \mathscr{H}$, annihilated by the operators $\boldsymbol{a} = (a_1, \dots, a_n)$. Analogous statement no longer holds for quantum systems with infinitely many degrees of freedom, described by quantum field theory, and one needs to postulate the existence of the ground state (the "physical vacuum").

Put

$$S(\boldsymbol{u}, \boldsymbol{v}) = e^{-\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v}} U(\boldsymbol{u}) V(\boldsymbol{v}) = e^{-\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v}} e^{-i\boldsymbol{u}\boldsymbol{P}} e^{-i\boldsymbol{v}\boldsymbol{Q}}.$$

Formally using the Baker-Campbell-Hausdorff formula, we get

$$S(\boldsymbol{u}, \boldsymbol{v}) = e^{-i(\boldsymbol{u}\boldsymbol{P} + \boldsymbol{v}\boldsymbol{Q})}. \tag{6.2}$$

It follows from the Weyl relations that

$$S(\boldsymbol{u}_1, \boldsymbol{v}_1) S(\boldsymbol{u}_2, \boldsymbol{v}_2) = e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2 - \boldsymbol{u}_2\boldsymbol{v}_1)} S(\boldsymbol{u}_1 + \boldsymbol{u}_2, \boldsymbol{v}_1 + \boldsymbol{v}_2). \tag{6.3}$$

The Weyl transform $W : L^1(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H})$ if defined by

$$W(f) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f(\boldsymbol{u}, \boldsymbol{v}) e^{-i(\boldsymbol{u}\boldsymbol{P} + \boldsymbol{v}\boldsymbol{Q})} d^n\boldsymbol{u}\, d^n\boldsymbol{v}$$

and can be considered as a *non-commutative Fourier transform* — an operator-valued generalization of the "ordinary" Fourier transform

$$\hat{f}(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f(\boldsymbol{u}, \boldsymbol{v}) e^{-i(\boldsymbol{u}\boldsymbol{p} + \boldsymbol{v}\boldsymbol{q})} d^n\boldsymbol{u}\, d^n\boldsymbol{v}.$$

The Weyl transform has the following properties.

WT1. For $f \in L^1(\mathbb{R}^{2n})$,

$$W(f)^* = W(f^*),$$

where

$$f^*(\boldsymbol{u}, \boldsymbol{v}) = \overline{f(-\boldsymbol{u}, -\boldsymbol{v})}.$$

WT2. For $f \in L^1(\mathbb{R}^{2n})$,

$$S(\boldsymbol{u}_1, \boldsymbol{v}_1) W(f) S(\boldsymbol{u}_2, \boldsymbol{v}_2) = W(\tilde{f}),$$

where

$$\tilde{f}(\boldsymbol{u}, \boldsymbol{v}) = e^{\frac{i\hbar}{2}\{(\boldsymbol{u}_1 - \boldsymbol{u}_2)\boldsymbol{v} - (\boldsymbol{v}_1 - \boldsymbol{v}_2)\boldsymbol{u} + \boldsymbol{u}_1\boldsymbol{v}_2 - \boldsymbol{u}_2\boldsymbol{v}_1\}} f(\boldsymbol{u} - \boldsymbol{u}_1 - \boldsymbol{u}_2, \boldsymbol{v} - \boldsymbol{v}_1 - \boldsymbol{v}_2).$$

WT3. $\operatorname{Ker} W = \{0\}$.

WT4. For $f_1, f_2 \in L^1(\mathbb{R}^{2n})$,

$$W(f_1)W(f_2) = W(f_1 *_\hbar f_2),$$

where

$$(f_1 *_\hbar f_2)(\boldsymbol{u}, \boldsymbol{v}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} e^{\frac{i\hbar}{2}(\boldsymbol{u}\boldsymbol{v}' - \boldsymbol{u}'\boldsymbol{v})} f_1(\boldsymbol{u} - \boldsymbol{u}', \boldsymbol{v} - \boldsymbol{v}') f_2(\boldsymbol{u}', \boldsymbol{v}') d^n\boldsymbol{u}' d^n\boldsymbol{v}'.$$

In the Schrödinger representation $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ the Weyl transform $W(f)$ can be explicitly described as bounded operator with an integral kernel. Namely,

$$(S(\boldsymbol{u}, \boldsymbol{v})\psi)(\boldsymbol{q}) = e^{\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v} - i\boldsymbol{v}\boldsymbol{q}} \psi(\boldsymbol{q} - \hbar\boldsymbol{u}), \quad \psi \in L^2(\mathbb{R}^n, d^n\boldsymbol{q}), \tag{6.4}$$

and for $\psi_1, \psi_2 \in L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ and $f \in L^1(\mathbb{R}^{2n}) \cap L^2(\mathbb{R}^{2n})$ we have

$$\begin{aligned}(W(f)\psi_1, \psi_2) &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f(\boldsymbol{u}, \boldsymbol{v})(S(\boldsymbol{u}, \boldsymbol{v})\psi_1, \psi_2) d^n\boldsymbol{u}\, d^n\boldsymbol{v} \\ &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \left(\int_{\mathbb{R}^n} e^{\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v} - i\boldsymbol{v}\boldsymbol{q}} f(\boldsymbol{u}, \boldsymbol{v}) \psi_1(\boldsymbol{q} - \hbar\boldsymbol{u}) \overline{\psi_2(\boldsymbol{q})} d^n\boldsymbol{q} \right) d^n\boldsymbol{u}\, d^n\boldsymbol{v} \\ &= \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} \tilde{K}(\boldsymbol{q}, \boldsymbol{q}')\psi_1(\boldsymbol{q}') d^n\boldsymbol{q}' \right) \overline{\psi_2(\boldsymbol{q})} d^n\boldsymbol{q},\end{aligned}$$

where

$$\tilde{K}(\boldsymbol{q}, \boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} f(\tfrac{\boldsymbol{q} - \boldsymbol{q}'}{\hbar}, \boldsymbol{v}) e^{-\frac{i}{2}(\boldsymbol{q} + \boldsymbol{q}')\boldsymbol{v}} d^n\boldsymbol{v}. \tag{6.5}$$

Thus $W(f)$ is an integral operator with the integral kernel $\tilde{K}(\boldsymbol{q}, \boldsymbol{q}')$,

$$(W(f)\psi)(\boldsymbol{q}) = \int_{\mathbb{R}^n} \tilde{K}(\boldsymbol{q}, \boldsymbol{q}')\psi(\boldsymbol{q}') d^n\boldsymbol{q}', \quad \psi \in L^2(\mathbb{R}^n, d^n\boldsymbol{q}).$$

By the Plancherel theorem,

$$\int_{\mathbb{R}^{2n}} |\tilde{K}(\boldsymbol{q}, \boldsymbol{q}')|^2 d^n\boldsymbol{q}\, d^n\boldsymbol{q}' = \int_{\mathbb{R}^{2n}} |f(\boldsymbol{u}, \boldsymbol{v})|^2 d^n\boldsymbol{u}\, d^n\boldsymbol{v},$$

so that $W(f)$ is a Hilbert-Schmidt operator on $\mathscr{H}$. The linear subspace $L^1(\mathbb{R}^{2n}) \cap L^2(\mathbb{R}^{2n})$ is dense in $L^2(\mathbb{R}^{2n})$ and the Weyl transform extends to the isometry $W : L^2(\mathbb{R}^{2n}) \to \mathscr{S}_2$, where $\mathscr{S}_2$ is the Hilbert space of Hilbert-Schmidt operators on $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$. Since every Hilbert-Schmidt operator on $\mathscr{H}$ is a bounded operator with the integral kernel in $L^2(\mathbb{R}^{2n})$, the mapping W is onto. Thus we have the following result.

LEMMA 6.1. *The Weyl transform W defines the isomorphism $L^2(\mathbb{R}^{2n}) \simeq \mathscr{S}_2$.*

Consider a linear map of the Schwartz space $\mathscr{S}(\mathbb{R}^{2n})$ of complex-valued functions of rapid decay on $\mathbb{R}^{2n}$ into the Banach space of bounded operators $\mathscr{L}(\mathscr{H})$, given by

$$\Phi = W \circ \mathscr{F}^{-1} : \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H}),$$

where $\mathscr{F}^{-1}$ is the inverse Fourier transform. Explicitly,

$$\Phi(f) = W(\check{f}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \check{f}(\boldsymbol{u}, \boldsymbol{v}) S(\boldsymbol{u}, \boldsymbol{v}) d^n\boldsymbol{u}\, d^n\boldsymbol{v},$$

where the integral is understood as a limit of Riemann sums in the uniform topology on $\mathscr{L}(\mathscr{H})$ and

$$\check{f}(\boldsymbol{u}, \boldsymbol{v}) = \mathscr{F}^{-1}(f)(\boldsymbol{u}, \boldsymbol{v}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f(\boldsymbol{p}, \boldsymbol{q}) e^{i(\boldsymbol{up}+\boldsymbol{vq})} d^n\boldsymbol{p}\, d^n\boldsymbol{q}.$$

From (6.5) we get that $\Phi(f)$ is an integral operator: for every $\psi \in L^2(\mathbb{R}^n, d^n\boldsymbol{q})$,

$$(\Phi(f)\psi)(\boldsymbol{q}) = \int_{\mathbb{R}^n} K(\boldsymbol{q}, \boldsymbol{q}')\psi(\boldsymbol{q}') d^n\boldsymbol{q}',$$

where

$$\begin{aligned} K(\boldsymbol{q}, \boldsymbol{q}') &= \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} \check{f}(\tfrac{\boldsymbol{q}-\boldsymbol{q}'}{\hbar}, \boldsymbol{v}) e^{-\frac{i}{2}\boldsymbol{v}(\boldsymbol{q}+\boldsymbol{q}')} d^n\boldsymbol{v} \\ &= \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} f(\boldsymbol{p}, \tfrac{\boldsymbol{q}+\boldsymbol{q}'}{2}) e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')} d^n\boldsymbol{p}. \end{aligned}$$

Since the Schwartz space is self-dual with respect to the Fourier transform, $K \in \mathscr{S}(\mathbb{R}^n \times \mathbb{R}^n) \subset L^2(\mathbb{R}^n \times \mathbb{R}^n)$, so that $\Phi(f)$ is a Hilbert-Schmidt operator. Using the property $S(\boldsymbol{u}, \boldsymbol{v})^* = S(-\boldsymbol{u}, -\boldsymbol{v})$ we get

$$\Phi(f)^* = \Phi(\bar{f}),$$

so that classical observables — real-valued functions on $\mathbb{R}^{2n}$, correspond to quantum observables — self-adjoint operators in $\mathscr{H}$. It follows from the property **WT3** that the mapping Φ is injective; its image $\operatorname{Im}\Phi$ and the inverse mapping Φ^{-1} are explicitly described as follows.

PROPOSITION 6.1. *The subspace* $\operatorname{Im}\Phi \subset \mathscr{L}(\mathscr{H})$ *consists of operators* $B \in \mathscr{S}_1$ *such that corresponding functions* $g(\boldsymbol{u},\boldsymbol{v}) = \hbar^n \operatorname{Tr}(B\,S(\boldsymbol{u},\boldsymbol{v})^{-1})$ *belong to the Schwartz class* $\mathscr{S}(\mathbb{R}^{2n})$; *in this case* $W(g) = B$. *The inverse mapping* $\Phi^{-1} = \mathscr{F}\circ W^{-1}$ *is given by the Weyl's inversion formula*

$$\check{f}(\boldsymbol{u},\boldsymbol{v}) = \hbar^n \operatorname{Tr}(\Phi(f)S(\boldsymbol{u},\boldsymbol{v})^{-1}), \quad f \in \mathscr{S}(\mathbb{R}^{2n}).$$

COROLLARY 6.2.

$$\operatorname{Tr}\Phi(f) = \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}} f(\boldsymbol{p},\boldsymbol{q})d^n\boldsymbol{p}\,d^n\boldsymbol{q}.$$

6.2. Weyl quantization

The map $\Phi : \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H})$ can be considered as a quantization of classical systems associated with the phase space $\mathbb{R}^{2n}$ and canonical symplectic form $\omega = d\boldsymbol{p}\wedge d\boldsymbol{q}$.

Namely, let $\mathcal{A}_0 = \mathscr{S}(\mathbb{R}^{2n},\mathbb{R}) \subset \mathcal{A}$ be the subalgebra of classical observables on $\mathbb{R}^{2n}$ of rapid decay, and let $\mathscr{A}_0 = \mathscr{A}\cap\mathscr{L}(\mathscr{H})$ be the space of bounded quantum observables.

PROPOSITION 6.2. *The mapping* $\mathcal{A}_0 \ni f \mapsto \Phi(f) \in \mathscr{A}_0$ *is a quantization, i.e., it satisfies*

$$\lim_{\hbar\to 0}\tfrac{1}{2}\Phi^{-1}\left(\Phi(f_1)\Phi(f_2) + \Phi(f_2)\Phi(f_1)\right) = f_1 f_2$$

and the correspondence principle

$$\lim_{\hbar\to 0}\Phi^{-1}\left(\{\Phi(f_1),\Phi(f_2)\}_\hbar\right) = \{f_1,f_2\}, \quad f_1,f_2\in\mathcal{A}_0,$$

where

$$\{\Phi(f_1),\Phi(f_2)\}_\hbar = \frac{i}{\hbar}[\Phi(f_1),\Phi(f_2)] \quad \text{and} \quad \{f_1,f_2\} = \frac{\partial f_1}{\partial\boldsymbol{p}}\frac{\partial f_2}{\partial\boldsymbol{q}} - \frac{\partial f_1}{\partial\boldsymbol{q}}\frac{\partial f_2}{\partial\boldsymbol{p}}$$

are, respectively, the quantum bracket and the Poisson bracket.

PROOF. In terms of the product $*_\hbar$ introduced in **WT4**, we have

$$\Phi^{-1}(\Phi(f_1)\Phi(f_2)) = \mathscr{F}(\check{f}_1 *_\hbar \check{f}_2),$$

and it follows from the property **WT4** that

$$\Phi^{-1}(\Phi(f_1)\Phi(f_2))(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{(2\pi)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}}\check{f}_1(\boldsymbol{u}_1,\boldsymbol{v}_1)\check{f}_2(\boldsymbol{u}_2,\boldsymbol{v}_2)\cdot \tag{6.6}$$
$$\cdot\, e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1)-i(\boldsymbol{u}_1+\boldsymbol{u}_2)\boldsymbol{p}-i(\boldsymbol{v}_1+\boldsymbol{v}_2)\boldsymbol{q}}d^n\boldsymbol{u}_1d^n\boldsymbol{u}_2d^n\boldsymbol{v}_1d^n\boldsymbol{v}_2.$$

Using the expansion

$$e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1)} = 1 + \frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2 - \boldsymbol{u}_2\boldsymbol{v}_1) + O(\hbar^2(\boldsymbol{u}_1\boldsymbol{v}_2 - \boldsymbol{u}_2\boldsymbol{v}_1)^2)$$

as $\hbar \to 0$, and the basic properties of the Fourier transform,

$$\mathscr{F}(\boldsymbol{u}\check{f}(\boldsymbol{u},\boldsymbol{v})) = i\frac{\partial f}{\partial \boldsymbol{p}}(\boldsymbol{p},\boldsymbol{q}) \quad \text{and} \quad \mathscr{F}(\boldsymbol{v}\check{f}(\boldsymbol{u},\boldsymbol{v})) = i\frac{\partial f}{\partial \boldsymbol{q}}(\boldsymbol{p},\boldsymbol{q}),$$

we get from (6.6) that as $\hbar \to 0$,

$$\Phi^{-1}(\Phi(f_1)\Phi(f_2))(\boldsymbol{p},\boldsymbol{q}) = (f_1 f_2)(\boldsymbol{p},\boldsymbol{q}) - \frac{i\hbar}{2}\{f_1, f_2\}(\boldsymbol{p},\boldsymbol{q}) + O(\hbar^2).$$

Using skew-symmetry of the Poisson bracket completes the proof. □

The quantization by the mapping $\Phi = W \circ \mathscr{F}^{-1}$ is called the *Weyl quantization*. The correspondence $f \mapsto \Phi(f)$ can be easily extended to the vector space $\widehat{L^1(\mathbb{R}^{2n})}$ — the image of $L^1(\mathbb{R}^{2n})$ under the Fourier transform, which is a subspace of $C(\mathbb{R}^{2n})$. More generally, for $f \in \mathscr{S}(\mathbb{R}^{2n})'$ — the space of tempered distributions on $\mathbb{R}^{2n}$ — the corresponding kernel

$$K(\boldsymbol{q},\boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} f(\boldsymbol{p}, \tfrac{\boldsymbol{q}+\boldsymbol{q}'}{2})e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')}d^n\boldsymbol{p}, \tag{6.7}$$

considered as a tempered distribution on $\mathbb{R}^n \times \mathbb{R}^n$, is a Schwartz kernel of the linear operator

$$\Phi(f) : \mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)'.$$

In particular, the constant function $f = 1$ corresponds to the identity operator I with $K(\boldsymbol{q},\boldsymbol{q}') = \delta(\boldsymbol{q}-\boldsymbol{q}')$. In terms of the kernel $K(\boldsymbol{q},\boldsymbol{q}')$ the Weyl inversion formula takes the form

$$f(\boldsymbol{p},\boldsymbol{q}) = \int_{\mathbb{R}^n} K(\boldsymbol{q} - \tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q} + \tfrac{1}{2}\boldsymbol{v})e^{\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{v}}d^n\boldsymbol{v}. \tag{6.8}$$

The distribution $f(\boldsymbol{p},\boldsymbol{q})$ defined by (6.8) is called the *Weyl symbol* of the operator in $L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ with the Schwartz kernel $K(\boldsymbol{q},\boldsymbol{q}')$.

Examples below describe classes of distributions f such that the operators $\Phi(f)$ are essentially self-adjoint unbounded operators on the domain $\mathscr{S}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n, d^n\boldsymbol{q})$.

EXAMPLE 6.1. Let $f = f(\boldsymbol{q}) \in L^p(\mathbb{R}^n)$ for some $1 \leq p \leq \infty$, or let f be a polynomially bounded function as $|\boldsymbol{q}| \to \infty$. We have

$$\begin{aligned} K(\boldsymbol{q}, \boldsymbol{q}') &= \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} f(\tfrac{\boldsymbol{q}+\boldsymbol{q}'}{2}) e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')} d^n\boldsymbol{p} \\ &= \delta(\boldsymbol{q}-\boldsymbol{q}') f(\tfrac{\boldsymbol{q}+\boldsymbol{q}'}{2}) = f(\boldsymbol{q})\delta(\boldsymbol{q}-\boldsymbol{q}'). \end{aligned}$$

Thus the operator $\Phi(f)$ is a multiplication by $f(\boldsymbol{q})$ operator on $L^2(\mathbb{R}^n)$. In particular, coordinates $\boldsymbol{q}$ in classical mechanics correspond to coordinate operators $\boldsymbol{Q}$ in quantum mechanics. Similarly, if $f = f(\boldsymbol{p})$, then $\Phi(f) = f(\boldsymbol{P})$. In particular, momenta $\boldsymbol{p}$ in classical mechanics correspond to the momenta operators $\boldsymbol{P}$ in quantum mechanics.

EXAMPLE 6.2. Let

$$H_{\mathrm{c}} = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$$

be the Hamiltonian function in classical mechanics. Then $H = \Phi(H_{\mathrm{c}})$ is the corresponding Hamiltonian operator in quantum mechanics,

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q}).$$

REMARK 6.2. The Weyl quantization can be considered as a way of defining a function $f(\boldsymbol{P}, \boldsymbol{Q})$ of non-commuting operators $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$, satisfying Heisenberg commutation relations, by setting

$$f(\boldsymbol{P}, \boldsymbol{Q}) = \Phi(f).$$

In particular, if $f(\boldsymbol{p}, \boldsymbol{q}) = g(\boldsymbol{p}) + h(\boldsymbol{q})$, then

$$f(\boldsymbol{P}, \boldsymbol{Q}) = g(\boldsymbol{P}) + h(\boldsymbol{Q}).$$

For $f(\boldsymbol{p}, \boldsymbol{q}) = \boldsymbol{p}\boldsymbol{q} = p_1 q^1 + \cdots + p_n q^n$ we get, using (6.7),

$$f(\boldsymbol{P}, \boldsymbol{Q}) = \frac{\boldsymbol{P}\boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{P}}{2}.$$

This shows that the Weyl quantization symmetrizes products of the non-commuting factors $\boldsymbol{P}$ and $\boldsymbol{Q}$. In general, let f be a polynomial function,

$$f(\boldsymbol{p}, \boldsymbol{q}) = \sum_{|\alpha|, |\beta| \leq N} c_{\alpha\beta}\, \boldsymbol{p}^\alpha \boldsymbol{q}^\beta, \tag{6.9}$$

where for the multi-indices $\alpha = (\alpha_1, \dots, \alpha_n)$ and $\beta = (\beta_1, \dots, \beta_n)$,

$$\boldsymbol{p}^\alpha = p_1^{\alpha_1} \dots p_n^{\alpha_n}, \quad \boldsymbol{q}^\beta = (q^1)^{\beta_1} \dots (q^n)^{\beta_n},$$

and $|\alpha| = \alpha_1 + \cdots + \alpha_n$, $|\beta| = \beta_1 + \cdots + \beta_n$. Using (6.7), we get the following formula

$$\Phi(f) = \sum_{|\alpha|,|\beta|\leq N} c_{\alpha\beta}\,\mathrm{Sym}(\boldsymbol{P}^\alpha\boldsymbol{Q}^\beta). \tag{6.10}$$

Here $\mathrm{Sym}(\boldsymbol{P}^\alpha\boldsymbol{Q}^\beta)$ is a symmetric product, defined by

$$(\boldsymbol{uP}+\boldsymbol{vQ})^k = \sum_{|\alpha|+|\beta|=k} \frac{k!}{\alpha!\beta!}\boldsymbol{u}^\alpha\boldsymbol{v}^\beta\,\mathrm{Sym}(\boldsymbol{P}^\alpha\boldsymbol{Q}^\beta), \tag{6.11}$$

where $\boldsymbol{uP}+\boldsymbol{vQ} = u^1P_1 + \cdots + u^nP_n + v_1Q^1 + \cdots + v_nQ^n$ and

$$\alpha! = \alpha_1!\dots\alpha_n!, \quad \beta! = \beta_1!\dots\beta_n!.$$

Remark 6.3. As was discussed in Chapter 3, quantization is not an algebra isomorphism, so that in general $\Phi(f_1f_2) \neq \Phi(f_1)\Phi(f_2)$. In particular, $\Phi(e^f) \neq e^{\Phi(f)}$.

6.3. The $\star$-product

The Weyl quantization $\Phi : \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H})$, studied in the previous section, defines a new bilinear operation

$$\star_\hbar : \mathscr{S}(\mathbb{R}^{2n}) \times \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{S}(\mathbb{R}^{2n})$$

on $\mathscr{S}(\mathbb{R}^{2n})$ by the formula

$$f_1 \star_\hbar f_2 = \Phi^{-1}(\Phi(f_1)\Phi(f_2)).$$

This operation is called the $\star$-product[2]. According to (6.6),

$$(f_1 \star_\hbar f_2)(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{(2\pi)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}} \check{f}_1(\boldsymbol{u}_1,\boldsymbol{v}_1)\check{f}_2(\boldsymbol{u}_2,\boldsymbol{v}_2)\cdot \\ \cdot e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1)-i(\boldsymbol{u}_1+\boldsymbol{u}_2)\boldsymbol{p}-i(\boldsymbol{v}_1+\boldsymbol{v}_2)\boldsymbol{q}}d^n\boldsymbol{u}_1d^n\boldsymbol{u}_2d^n\boldsymbol{v}_1d^n\boldsymbol{v}_2. \tag{6.12}$$

The $\star$-product on $\mathscr{S}(\mathbb{R}^{2n})$ has the following properties.

1. Associativity:

$$f_1 \star_\hbar (f_2 \star_\hbar f_3) = (f_1 \star_\hbar f_2) \star_\hbar f_3.$$

[2] Also called *Moyal product* in physics.

2. Semi-classical limit:

$$(f_1 \star_\hbar f_2)(\boldsymbol{p},\boldsymbol{q}) = (f_1 f_2)(\boldsymbol{p},\boldsymbol{q}) - \tfrac{i\hbar}{2}\{f_1, f_2\}(\boldsymbol{p},\boldsymbol{q}) + O(\hbar^2) \ \text{ as } \ \hbar \to 0.$$

3. Property of the unit:

$$f \star_\hbar \mathbf{1} = \mathbf{1} \star_\hbar f,$$

where $\mathbf{1}$ is a function which identically equals 1 on $\mathbb{R}^{2n}$.

4. The cyclic trace property:

$$\tau(f_1 \star_\hbar f_2) = \tau(f_2 \star_\hbar f_1),$$

where the $\mathbb{C}$-linear map $\tau : \mathscr{S}(\mathbb{R}^{2n}) \to \mathbb{C}$ is defined by

$$\tau(f) = \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}} f(\boldsymbol{p},\boldsymbol{q}) d^n\boldsymbol{p}\, d^n\boldsymbol{q}.$$

Property **1** follows from the corresponding property for the product $*_\hbar$, property **2** follows from Proposition 6.2, and properties **3** and **4** directly follow from the definition (6.12). The complex vector space $\mathscr{S}(\mathbb{R}^{2n}) \oplus \mathbb{C}\,\mathbf{1}$ with the bilinear operation $\star_\hbar$ is an associative algebra over $\mathbb{C}$ with unit $\mathbf{1}$ and the cyclic trace τ, satisfying the correspondence principle,

$$\lim_{\hbar\to 0} \tfrac{i}{\hbar}(f_1 \star_\hbar f_2 - f_2 \star_\hbar f_1) = \{f_1, f_2\}.$$

Finally, we get another integral representation for the $\star$-product. Applying the Fourier inversion formula to the integral over $d^n\boldsymbol{u}_1 d^n\boldsymbol{v}_1$ in (6.12), we get

$$\begin{aligned}(f_1 \star_\hbar f_2)(\boldsymbol{p},\boldsymbol{q}) &= \frac{1}{(2\pi)^n}\int_{\mathbb{R}^{2n}} f_1(\boldsymbol{p} - \tfrac{\hbar}{2}\boldsymbol{v}_2, \boldsymbol{q} + \tfrac{\hbar}{2}\boldsymbol{u}_2)\check{f}_2(\boldsymbol{u}_2,\boldsymbol{v}_2)\, \cdot \\ &\qquad \cdot e^{-i\boldsymbol{u}_2\boldsymbol{p} - i\boldsymbol{v}_2\boldsymbol{q}} d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_2 \\ &= \frac{1}{(2\pi)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}} f_1(\boldsymbol{p} - \tfrac{\hbar}{2}\boldsymbol{v}_2, \boldsymbol{q} + \tfrac{\hbar}{2}\boldsymbol{u}_2) f_2(\boldsymbol{p}_2,\boldsymbol{q}_2)\, \cdot \\ &\qquad \cdot e^{-i\boldsymbol{u}_2\boldsymbol{p} - i\boldsymbol{v}_2\boldsymbol{q} + i\boldsymbol{u}_2\boldsymbol{p}_2 + i\boldsymbol{v}_2\boldsymbol{q}_2} d^n\boldsymbol{p}_2 d^n\boldsymbol{q}_2 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_2,\end{aligned}$$

and changing variables $\boldsymbol{p}_1 = \boldsymbol{p} - \frac{\hbar}{2}\boldsymbol{v}_2$, $\boldsymbol{q}_1 = \boldsymbol{q} + \frac{\hbar}{2}\boldsymbol{u}_2$, we obtain

$$\begin{aligned}(f_1 \star_\hbar f_2)(\boldsymbol{p},\boldsymbol{q}) &= \frac{1}{(\pi\hbar)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}} f_1(\boldsymbol{p}_1,\boldsymbol{q}_1) f_2(\boldsymbol{p}_2,\boldsymbol{q}_2)\, \cdot \\ &\cdot e^{\frac{2i}{\hbar}(\boldsymbol{p}_1\boldsymbol{q} - \boldsymbol{p}\boldsymbol{q}_1 + \boldsymbol{q}_1\boldsymbol{p}_2 - \boldsymbol{q}_2\boldsymbol{p}_1 + \boldsymbol{p}\boldsymbol{q}_2 - \boldsymbol{p}_2\boldsymbol{q})} d^n\boldsymbol{p}_1 d^n\boldsymbol{q}_1 d^n\boldsymbol{p}_2 d^n\boldsymbol{q}_2.\end{aligned}$$

Let $\triangle$ be a Euclidean triangle (a 2-simplex) in the phase space $\mathbb{R}^{2n}$ with the vertices $(\boldsymbol{p},\boldsymbol{q})$, $(\boldsymbol{p}_1,\boldsymbol{q}_1)$, and $(\boldsymbol{p}_2,\boldsymbol{q}_2)$. It is easy to see that

$$\boldsymbol{p}_1\boldsymbol{q}-\boldsymbol{p}\boldsymbol{q}_1+\boldsymbol{q}_1\boldsymbol{p}_2-\boldsymbol{q}_2\boldsymbol{p}_1+\boldsymbol{p}\boldsymbol{q}_2-\boldsymbol{p}_2\boldsymbol{q}=2\int_\triangle\omega,$$

which is twice the symplectic area of $\triangle$ — the sum of oriented areas of the projections of $\triangle$ onto two-dimensional planes $(p_1,q^1),\dots,(p_n,q^n)$. Thus we have the final formula

$$(6.13)\qquad (f_1\star_\hbar f_2)(\boldsymbol{p},\boldsymbol{q})=\frac{1}{(\pi\hbar)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}}f_1(\boldsymbol{p}_1,\boldsymbol{q}_1)f_2(\boldsymbol{p}_2,\boldsymbol{q}_2)\cdot \cdot e^{\frac{4i}{\hbar}\int_\triangle\omega}d^n\boldsymbol{p}_1d^n\boldsymbol{q}_1d^n\boldsymbol{p}_2d^n\boldsymbol{q}_2.$$

PROBLEM 6.1. Prove properties **WT1–WT4**.

PROBLEM 6.2. Prove Proposition 6.1.

PROBLEM 6.3. Prove that the $\star$-product is associative using formula (6.13).

PROBLEM 6.4. Define the unitary operator $\boldsymbol{U}_\hbar$ on $L^2(\mathbb{R}^{2n})\otimes L^2(\mathbb{R}^{2n})$ by

$$\boldsymbol{U}_\hbar=e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial\boldsymbol{p}}\otimes\frac{\partial}{\partial\boldsymbol{q}}-\frac{\partial}{\partial\boldsymbol{q}}\otimes\frac{\partial}{\partial\boldsymbol{p}}\right)},$$

which means that

$$\left(\boldsymbol{U}_\hbar(f_1\otimes f_2)\right)(\boldsymbol{p}_1,\boldsymbol{q}_1,\boldsymbol{p}_2,\boldsymbol{q}_2)=\frac{1}{(2\pi)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}}\check{f}_1(\boldsymbol{u}_1,\boldsymbol{v}_1)\check{f}_2(\boldsymbol{u}_2,\boldsymbol{v}_2)\cdot \cdot e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1)-i\boldsymbol{u}_1\boldsymbol{p}_1-i\boldsymbol{u}_2\boldsymbol{p}_2-i\boldsymbol{v}_1\boldsymbol{q}_1-\boldsymbol{v}_2\boldsymbol{q}_2}d^n\boldsymbol{u}_1d^n\boldsymbol{u}_2d^n\boldsymbol{v}_1d^n\boldsymbol{v}_2,$$

and denote by $m:\mathscr{S}(\mathbb{R}^{2n})\otimes\mathscr{S}(\mathbb{R}^{2n})\to\mathscr{S}(\mathbb{R}^{2n})$ the point-wise product of functions, $(m(f_1\otimes f_2))(\boldsymbol{p},\boldsymbol{q})=f_1(\boldsymbol{p},\boldsymbol{q})f_2(\boldsymbol{p},\boldsymbol{q})$. Prove the formula

$$f_1\star_\hbar f_2=(m\circ\boldsymbol{U}_\hbar)(f_1\otimes f_2),$$

and the asymptotic expansion:

$$(f_1\star_\hbar f_2)(\boldsymbol{p},\boldsymbol{q})=\sum_{k=0}^\infty\frac{(-i\hbar)^k}{2^kk!}B_k(f_1,f_2)(\boldsymbol{p},\boldsymbol{q})+O(\hbar^\infty)\quad\text{as}\quad\hbar\to0,$$

where

$$B_k(f_1,f_2)=\left(\left(\frac{\partial^2}{\partial\boldsymbol{p}_1\partial\boldsymbol{q}_2}-\frac{\partial^2}{\partial\boldsymbol{q}_1\partial\boldsymbol{p}_2}\right)^kf_1(\boldsymbol{p}_1,\boldsymbol{q}_1)f_2(\boldsymbol{p}_2,\boldsymbol{q}_2)\right)\Big|_{\substack{\boldsymbol{p}_1=\boldsymbol{p}_2=\boldsymbol{p}\\ \boldsymbol{q}_1=\boldsymbol{q}_2=\boldsymbol{q}}}.$$

PROBLEM 6.5. For classical observable $f(\boldsymbol{p},\boldsymbol{q})$ define the $\star$-exponential (the analog of the evolution operator) by

$$\exp_\star f = \sum_{n=0}^{\infty} \frac{\hbar^{-n}}{n!} \underbrace{f \star_\hbar f \star_\hbar \cdots \star_\hbar f}_{n}.$$

Compute $\exp_\star(-itH_{\mathrm{c}})$, where $H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{q})$ is the Hamiltonian function (5.1) of the harmonic oscillator.

CHAPTER 7

Feynman path integral

7.1. The fundamental solution of the Schrödinger equation

Recall (see Chapter 2) that solution of the initial value problem for the time-dependent Schrödinger equation

$$i\hbar\frac{d\psi}{dt}(t) = H\psi(t), \tag{7.1}$$

$$\psi(t)|_{t=0} = \psi \tag{7.2}$$

is given by $\psi(t) = U(t)\psi$, where $U(t) = e^{-\frac{i}{\hbar}tH}$ is the evolution operator. For the Hamiltonian operator

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$$

of a quantum particle on $\mathbb{R}^n$ in the potential field $V(\boldsymbol{q})$, initial value problem (7.1)–(7.2) in coordinate representation takes the form

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V(\boldsymbol{q})\psi, \tag{7.3}$$

$$\psi(\boldsymbol{q}, t)|_{t=0} = \psi(\boldsymbol{q}), \tag{7.4}$$

where Δ is the Laplace operator on $\mathbb{R}^n$. Under rather general conditions[1] on the potential $V(\boldsymbol{q})$, Cauchy problem (7.3)–(7.4) has a fundamental solution — a function $K(\boldsymbol{q}, \boldsymbol{q}', t)$ that satisfies partial differential equation (7.3) with respect to the variable $\boldsymbol{q}$ in the distributional sense, and the initial condition

$$K(\boldsymbol{q}, \boldsymbol{q}', t)\big|_{t=0} = \delta(\boldsymbol{q} - \boldsymbol{q}'). \tag{7.5}$$

The solution of (7.3)–(7.4) can be formally written as

$$\psi(\boldsymbol{q}', t) = \int_{\mathbb{R}^n} K(\boldsymbol{q}', \boldsymbol{q}, t)\psi(\boldsymbol{q})d^n\boldsymbol{q}. \tag{7.6}$$

[1] I.e. when $V \in L^\infty_{\text{loc}}(\mathbb{R}^n)$ is bounded from below.

In Dirac notation (see Remark 3.5 in Chapter 3)

$$K(\boldsymbol{q}',\boldsymbol{q},t)=\langle\boldsymbol{q}'|U(t)|\boldsymbol{q}\rangle. \tag{7.7}$$

For $\psi\in L^2(\mathbb{R}^n)$ formula (7.6) should be understood as

$$\psi(\boldsymbol{q}',t)=\underset{R\to\infty}{\text{l.i.m.}}\int_{|\boldsymbol{q}|\leq R}K(\boldsymbol{q}',\boldsymbol{q},t)\psi(\boldsymbol{q})d^n\boldsymbol{q}=\text{l.i.m.}\int_{\mathbb{R}^n}K(\boldsymbol{q}',\boldsymbol{q},t)\psi(\boldsymbol{q})d^n\boldsymbol{q},$$

where l.i.m. stands for the limit in the L^2-norm. The fundamental solution $K(\boldsymbol{q},\boldsymbol{q}',t)$ is a distributional kernel (in the sense of the Schwartz kernel theorem) of the evolution operator $U(t)$.

Using the group property $U(t+t')=U(t)U(t')$, we immediately get $\psi(t')=U(t'-t)\psi(t)$, so equation (7.6) can be rewritten as

$$\psi(\boldsymbol{q}',t')=\int_{\mathbb{R}^n}K(\boldsymbol{q}',t';\boldsymbol{q},t)\psi(\boldsymbol{q},t)d^n\boldsymbol{q}, \tag{7.8}$$

where $K(\boldsymbol{q}',t';\boldsymbol{q},t)=K(\boldsymbol{q}',\boldsymbol{q},t'-t)$.

Remark 7.1. The group property of $U(t)$ in terms of the integral kernels reads

$$K(\boldsymbol{q}',\boldsymbol{q},t+t')=\int_{\mathbb{R}^n}K(\boldsymbol{q}',\boldsymbol{q}'',t)K(\boldsymbol{q}'',\boldsymbol{q},t')d^n\boldsymbol{q}''. \tag{7.9}$$

The unitarity of $U(t)$ in terms of the integral kernels reads

$$\int_{\mathbb{R}^n}K(\boldsymbol{q}',\boldsymbol{q}'',t)\overline{K(\boldsymbol{q},\boldsymbol{q}',t)}d^n\boldsymbol{q}''=\delta(\boldsymbol{q}'-\boldsymbol{q}). \tag{7.10}$$

In physics, the function $|K(\boldsymbol{q}',t';\boldsymbol{q},t)|^2$ is referred to as the conditional probability density of finding a quantum particle at position $\boldsymbol{q}'\in\mathbb{R}^n$ at time t', given that it was at position $\boldsymbol{q}\in\mathbb{R}^n$ at time t. However, it follows from (7.10) that

$$\int_{\mathbb{R}^n}|K(\boldsymbol{q}',t',\boldsymbol{q},t)|^2d^n\boldsymbol{q}'=\delta(0)=\infty.$$

This is because the state of a quantum particle at a precise position $\boldsymbol{q}\in\mathbb{R}^n$ at time t is described by the non-normalized state $|\boldsymbol{q},t\rangle$. For the normalized states, we have the following *conservation of probability*:

$$\int_{\mathbb{R}^n}|\psi(\boldsymbol{q}',t')|^2d^n\boldsymbol{q}'=1\quad\text{if}\quad\int_{\mathbb{R}^n}|\psi(\boldsymbol{q},t)|^2d^n\boldsymbol{q}=1.$$

REMARK 7.2. In physics, the distributional kernel $K(\boldsymbol{q}', t'; \boldsymbol{q}, t)$ of the evolution operator $U(t'-t)$ is called the *complex probability amplitude*, or simply the *amplitude* or *propagator*. In Dirac's notation (see Remark 3.5 tChapter 3),

$$K(\boldsymbol{q}', t'; \boldsymbol{q}, t) = \langle \boldsymbol{q}' | U(t'-t) | \boldsymbol{q} \rangle = \langle \boldsymbol{q}', t' \,|\, \boldsymbol{q}, t \rangle,$$

where we have introduced

$$|\boldsymbol{q}, t\rangle = U(-t)|\boldsymbol{q}\rangle \quad \text{and} \quad \langle \boldsymbol{q}', t'| = \langle \boldsymbol{q}'|U(t').$$

Notation $\langle \boldsymbol{q}', t' \,|\, \boldsymbol{q}, t \rangle$ for the propagator is standard in physics; one reads it from right to left: from a point $\boldsymbol{q}$ at time t to the point $\boldsymbol{q}'$ at time t'. Note that in the Heisenberg picture time evolution of observable A is $A(t) = U^{-1}(t)AU(t)$ (see formula (2.9) in Chapter 2), so $|\boldsymbol{q}, t\rangle$ are common generalized eigenfunctions of the position operators $\boldsymbol{Q}(t) = U^{-1}(t)\boldsymbol{Q}U(t)$ at time t:

$$Q^i(t)|\boldsymbol{q}, t\rangle = q^i|\boldsymbol{q}, t\rangle, \quad i = 1, \dots, n.$$

Finding the propagator of a quantum system is the main problem in quantum mechanics. When the spectral decomposition of the Hamiltonian operator H is known, the propagator can be obtained in a closed form.

Suppose for simplicity that H has a pure point spectrum, i.e., there is an orthonormal basis of the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ consisting of the eigenfunctions $\{\psi_n(\boldsymbol{q})\}_{n=0}^{\infty}$ of H with the eigenvalues E_n. We have

$$\psi(\boldsymbol{q}) = \sum_{n=0}^{\infty} c_n \psi_n(\boldsymbol{q}), \quad c_n = \int_{\mathbb{R}^n} \psi(\boldsymbol{q})\overline{\psi_n(\boldsymbol{q})} d^n\boldsymbol{q},$$

so that

$$(U(t)\psi)(\boldsymbol{q}) = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar}E_n t} c_n \psi_n(\boldsymbol{q})$$

and

$$\psi(\boldsymbol{q}', t') = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar}E_n t'} \psi_n(\boldsymbol{q}') \int_{\mathbb{R}^n} \overline{\psi_n(\boldsymbol{q})}\psi(\boldsymbol{q}) d^n\boldsymbol{q},$$

where the series and integrals converge in the L^2-sense. If the change of orders of summation and integration was justified, we could write

$$K(\boldsymbol{q}', t; \boldsymbol{q}, t) = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar}E_n T} \psi_n(\boldsymbol{q}')\overline{\psi_n(\boldsymbol{q})}, \quad T = t' - t. \tag{7.11}$$

The series (7.11) converges in the distributional sense, and gives a representation of the propagator in terms of the spectral decomposition of H.

Analogous representation for the propagator exists when the Hamiltonian H has absolutely continuous spectrum. Consider the simplest case of a free quantum particle with the Hamiltonian operator

$$H_0 = \frac{\boldsymbol{P}^2}{2m}.$$

The corresponding Schrödinger equation can be solved by the Fourier method (see Chapter 4), and we obtain

$$\begin{aligned}\psi(\boldsymbol{q}', t') &= \text{l.i.m.}(2\pi\hbar)^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}(\boldsymbol{q}'\boldsymbol{p} - \frac{\boldsymbol{p}^2}{2m}T)} \hat{\psi}(\boldsymbol{p}, t) d^n\boldsymbol{p} \\ &= \text{l.i.m.} \int_{\mathbb{R}^n} K(\boldsymbol{q}', t'; \boldsymbol{q}, t)\psi(\boldsymbol{q}, t) d^n\boldsymbol{q},\end{aligned}$$

where

$$K(\boldsymbol{q}', t'; \boldsymbol{q}, t) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}(\boldsymbol{p}(\boldsymbol{q}' - \boldsymbol{q}) - \frac{\boldsymbol{p}^2}{2m}T)} d^n\boldsymbol{p}, \quad T = t' - t. \tag{7.12}$$

Using the classical Fresnel integral formula

$$\int_{-\infty}^{\infty} e^{iax^2} dx = e^{\frac{\pi i \operatorname{sgn}(a)}{4}} \sqrt{\frac{\pi}{|a|}}, \tag{7.13}$$

and completing the square in (7.12), we obtain a closed expression for the propagator of a free quantum particle:

$$K(\boldsymbol{q}', t'; \boldsymbol{q}, t) = \Big(\frac{m}{2\pi i\hbar T}\Big)^{\frac{n}{2}} e^{\frac{im}{2\hbar T}(\boldsymbol{q} - \boldsymbol{q}')^2}, \tag{7.14}$$

where $i^{-\frac{n}{2}} = e^{-\frac{\pi i n}{4}}$ and $T = t' - t > 0$.

Remark 7.3. Formally replacing the "physical" time t in the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi$$

for a free quantum particle of mass m by the *Euclidean time* (or *pure imaginary time*) $t \mapsto -it_E$, we obtain the heat (diffusion) equation

$$\frac{1}{D}\frac{\partial u}{\partial t_E} = \Delta u$$

on $\mathbb{R}^n$ with the diffusion coefficient $D = \dfrac{\hbar}{2m}$. It is quite remarkable that in agreement with this formal procedure, the propagator (7.14) for a free quantum particle is obtained from the heat kernel on $\mathbb{R}^n$ by the analytic continuation $T \mapsto iT = T_E$. On a complex T-plane this represents a counter-clock wise rotation by 90°, called the *Wick rotation*.

REMARK 7.4. For the imaginary time the property (7.9) for a free quantum particle is called the Chapman-Kolmogorov equation for the Wiener process (Brownian motion).

7.2. Feynman path integral in the phase space

Consider classical Hamiltonian system on $\mathbb{R}^2$ with the Hamiltonian function

$$H_c(p,q) = \frac{p^2}{2m} + V(q), \tag{7.15}$$

and let

$$H = \Phi(H_c) = H_0 + V$$

be the corresponding Hamiltonian operator[2].

The main heuristic idea behind the Feynman path integral is to use the group property and to write the evolution operator $U(T) = e^{-\frac{i}{\hbar}TH}$, $T = t' - t$. as

$$U(T) = U(\Delta)^N, \quad \text{where} \quad \Delta = \frac{T}{N}.$$

For small $\Delta \ll 1$ we formally have

$$U(\Delta) = I - \frac{i\Delta}{\hbar}H + O(\Delta^2),$$

so for the propagator we obtain

$$\begin{aligned}
\langle q'|U(\Delta)|q\rangle &= \langle q'|\Phi\left(I - \frac{i\Delta}{\hbar}H_c\right)|q\rangle + O(\Delta^2) \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}p(q'-q)}\left(1 - \frac{i\Delta}{\hbar}H_c(p,q)\right)dp + O(\Delta^2) \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(p(q'-q)-\Delta H_c(p,q))}dp + O(\Delta^2).
\end{aligned}$$

[2]It is assumed that H_c is such that H is essentially self-adjoint on $D(H_0) \cap D(V)$.

Here in the second line we used[3] Example 6.1 in Chapter 6. Now it follows from (7.12) that the integral in the third line is the integral kernel of the operator $U_\Delta = e^{-\frac{i\Delta}{\hbar}H_0}e^{-\frac{i\Delta}{\hbar}V}$:

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\left\{p(q'-q)-\Delta(\frac{p^2}{2m}+v(q))\right\}}dp = \langle q'|U_\Delta|q\rangle, \tag{7.16}$$

so

$$\langle q'|U(\Delta)|q\rangle = \langle q'|U_\Delta|q\rangle + O(\Delta^2).$$

REMARK 7.5. Note that for the free quantum particle $U(\Delta) = U_\Delta$.

Next, our main assumption is that

$$U(T) = \lim_{N\to\infty} U_\Delta^N, \tag{7.17}$$

which is justified by the Lie-Kato-Trotter formula from the operator calculus:

$$\lim_{N\to\infty}\left(e^{\frac{A}{N}}\cdot e^{\frac{B}{N}}\right)^N = e^{A+B}$$

for $A, B \in \mathscr{L}(\mathscr{H})$.

Since the kernel of a product of two operators is a composition of their corresponding kernels, for the distributional kernel $\langle q'|U_\Delta^N|q\rangle$ we obtain the following representation,

$$\langle q'|U_\Delta^N|q\rangle = \underset{\mathbb{R}^{N-1}}{\int\cdots\int}\prod_{k=0}^{N-1}\langle q_{k+1}|U_\Delta|q_k\rangle\prod_{k=1}^{N-1}dq_k, \tag{7.18}$$

where $q_0 = q$, $q_N = q'$. Now replace each factor $\langle q_{k+1}|U_\Delta|q_k\rangle$ in (7.18) by its integral representation (7.16), where the corresponding variable of integration is denoted by p_k, $k = 0,\dots,N-1$. Changing the order of integrations in the resulting $(2N-1)$-fold integral, we obtain the following remarkable representation of the propagator of a quantum particle as a limit of multiple integrals when the number of integrations goes to infinity:

$$\begin{aligned}\langle q'|U(T)|q\rangle &= \lim_{N\to\infty}\langle q'|U_\Delta^N|q\rangle \\ &= \lim_{N\to\infty}\underset{\mathbb{R}^{2N-1}}{\int\cdots\int} e^{\left\{\frac{i}{\hbar}\sum_{k=0}^{N-1}(p_k(q_{k+1}-q_k)-H_c(p_k,q_k)\Delta)\right\}}\frac{dp_0}{2\pi\hbar}\prod_{k=1}^{N-1}\frac{dp_k dq_k}{2\pi\hbar}.\end{aligned} \tag{7.19}$$

[3] In general, one should use $H_c(p, \frac{q+q'}{2})$, but for the classical Hamiltonian (7.15) we can use $H_c(p,q)$.

Here $H_{\rm c}(p,q) = \dfrac{p^2}{2m} + V(q)$ is the classical Hamiltonian function, and $q_0 = q$, $q_N = q'$.

REMARK 7.6. According to Remark 7.5, for a free quantum particle we have for every N:

$$\langle q'|U(T)|q\rangle = \underset{\mathbb{R}^{2N-1}}{\int\cdots\int} e^{\left\{\frac{i}{\hbar}\sum_{k=0}^{N-1}\left(p_k(q_{k+1}-q_k)-\Delta\frac{p_k^2}{2m}\right)\right\}}\frac{dp_0}{2\pi\hbar}\prod_{k=1}^{N-1}\frac{dp_k dq_k}{2\pi\hbar}.$$

Formula (7.19) admits the following remarkable interpretation. To every point $(p_0, p_1, \dots, p_{N-1}, q_1, \dots, q_{N-1}) \in \mathbb{R}^{2N-1}$ assign a piece-wise linear path σ in the phase space $\mathbb{R}^2$ of the classical particle, defined by the following *time slicing* procedure. Let $t_k = t + k\Delta$ and $\sigma(\tau) = (p(\tau), q(\tau))$, where

$$p(\tau) = p_k, \quad q(\tau) = q_k + (\tau - t_k)\frac{q_{k+1} - q_k}{\Delta},$$

and $\tau \in [t_k, t_{k+1}]$, $k = 0, \dots, N-1$. Then for the Riemann integrable potentials $V(q)$ we have

$$\sum_{k=0}^{N-1}(p_k(q_{k+1} - q_k) - H_{\rm c}(p_k, q_k)\Delta) = S(\sigma) + o(1), \quad \text{as} \quad N \to \infty, \tag{7.20}$$

where

$$S(\sigma) = \int_\sigma (pdq - H_{\rm c}d\tau) = \int_t^{t'} (p(\tau)\dot{q}(\tau) - H_{\rm c}(p(\tau), q(\tau)))d\tau$$

is the action functional of a classical system with the Hamiltonian function $H_{\rm c}(p,q)$.

This suggests to interpret (7.19) as a kind of "integral" over the space $P(\mathbb{R}^2)_{q,t}^{q',t'}$ of all paths $\sigma(\tau) = (p(\tau), q(\tau))$, where $\tau \in [t, t']$, in the phase space $\mathbb{R}^2$ such that[4] $q(t) = q$ and $q(t') = q'$, which was used in the formulation of the principle of the least action in the phase space. Thus we put

$$\langle q', t'|q, t\rangle = \int_{P(\mathbb{R}^2)_{q,t}^{q',t'}} e^{\frac{i}{\hbar}S(\sigma)}\mathscr{D}p\mathscr{D}q, \tag{7.21}$$

[4]Note that there is no condition on the values of $p(\tau)$ at the endpoints, so $\sigma(t)$ and $\sigma(t')$ belong to Lagrangian subspaces $\mathscr{L} = \{q\} \times \mathbb{R}$ and $\mathscr{L}' = \{q'\} \times \mathbb{R}$ in $\mathbb{R}^2$.

where the "measure" $\mathscr{D}p\mathscr{D}q$ on $P(\mathbb{R}^2)_{q,t}^{q',t'}$ is given by

$$\mathscr{D}p\mathscr{D}q = \lim_{N\to\infty} \frac{dp_0}{2\pi\hbar} \prod_{k=1}^{N-1} \frac{dp_k dq_k}{2\pi\hbar}. \tag{7.22}$$

Representation (7.21)–(7.22) is the famous *Feynman path integral in the phase space* for the propagator of a quantum particle. It expresses the propagator $\langle q', t'|q, t\rangle$ as the "weighted sum" over all possible "histories" of the classical particle, the paths $\sigma \in P(\mathbb{R}^2)_{q,t}^{q',t'}$, where each path σ has a complex weight $\exp\{\frac{i}{\hbar}S(\sigma)\}$. On one hand, this representation clearly shows the fundamental difference between classical mechanics and quantum mechanics. Thus in classical mechanics, the particle moves along classical trajectories, which are the critical points (extremals) of the action functional $S(\sigma)$, whereas in quantum mechanics all possible paths contribute to the complex probability amplitude $\langle q', t'|q, t\rangle$. On the other hand, representation (7.21)–(7.22) clearly points at the relation between quantum mechanics and classical mechanics in the semi-classical limit $\hbar \to 0$. Namely, as $\hbar \to 0$ the weights $\exp\{\frac{i}{\hbar}S(\sigma)\}$ become rapidly oscillating and their contributions to (7.21) will mutually cancel, unless the action is almost constant. The latter happens near the critical points, which give the major contribution to (7.21). This is how classical trajectories of a particle emerge from its quantum description.

REMARK 7.7. The Feynman path integral in the phase space in not an integral in the sense of abstract integration theory, since the formal expression $\mathscr{D}p\mathscr{D}q$ does not define a measure[5] on the path space $P(\mathbb{R}^2)_{q,t}^{q',t'}$. Besides, the functional $\exp\{\frac{i}{\hbar}S(\sigma)\}$ has absolute value 1 and cannot be integrable with respect to any measure $d\mu$ with the property $\mu(P(\mathbb{R}^2)_{q,t}^{q',t'}) = \infty$. The rigorous mathematical meaning of (7.21)–(7.22) is the original formula (7.19), which expresses the propagator as a limit of multiple integrals as the number of integrations goes to infinity. This explains the apparent "paradox" that quantum mechanics is defined entirely in classical terms by (7.21). It is not so, since there is no "intrinsic" definition of (7.21) in classical terms, besides the time slicing procedure (7.19), which also requires the special choice of the approximation (7.20) of $S(\sigma)$ by the Riemann sums.

7.3. Feynman path integral in the configuration space

Using the Fresnel integral (7.13) for the integration over p in (7.16), we obtain the following formula for the distributional kernel of the operator

[5]In abstract measure theory the measure is non-negative and countably additive.

$e^{-\frac{i\Delta}{\hbar}H_0}\, e^{-\frac{i\Delta}{\hbar}V}$:

$$\sqrt{\frac{m}{2\pi i\hbar\Delta}}\; e^{\frac{i}{\hbar}\{\frac{m}{2}\frac{(q-q')^2}{\Delta}-V(q)\Delta t\}}.$$

Repeating the time slicing procedure from the previous section, instead of (7.19) we now get

$$\langle q',t'|q,t\rangle = \lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\Delta}\right)^{\frac{N}{2}} \times \underset{\mathbb{R}^{N-1}}{\int\cdots\int} \exp\left\{\frac{i}{\hbar}\sum_{k=0}^{N-1}\left(\frac{m}{2}\left(\frac{q_{k+1}-q_k}{\Delta}\right)^2 - V(q_k)\right)\Delta\right\}\prod_{k=1}^{N-1} dq_k. \tag{7.23}$$

Assuming that $q_k = q(t_k)$, $k = 0,\dots,N$, for some smooth path $\gamma(\tau) = q(\tau)$ in $\mathbb{R}$, where $q_0 = q$ and $q_N = q'$, we obtain as $N\to\infty$,

$$\sum_{k=0}^{N-1}\left(\frac{m}{2}\left(\frac{q_{k+1}-q_k}{\Delta}\right)^2 - V(q_k)\right)\Delta = S(\gamma) + o(1),$$

where

$$S(\gamma) = \int_t^{t'} L(\gamma'(\tau))d\tau = \int_t^{t'} L(q(\tau),\dot q(\tau))d\tau, \quad L(q,\dot q) = \tfrac{1}{2}m\dot q^2 - V(q),$$

is the action functional of a classical particle of mass m moving in the potential field $V(q)$. This suggests to interpret the limit of multiple integrals (7.23) as the *Feynman path integral in the configuration space*

$$\langle q',t'|q,t\rangle = \int_{P(\mathbb{R})_{q,t}^{q',t'}} e^{\frac{i}{\hbar}S(\gamma)}\mathscr{D}q. \tag{7.24}$$

Here $P(\mathbb{R})_{q,t}^{q',t'}$ is the space of smooth parametrized paths γ in the configuration space $\mathbb{R}$ connecting points q and q', and the "measure" $\mathscr{D}q$ on $P(\mathbb{R})_{q,t}^{q',t'}$ is given by

$$\mathscr{D}q = \lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\Delta}\right)^{\frac{N}{2}}\prod_{k=1}^{N-1} dq_k. \tag{7.25}$$

As the Feynman path integral in the phase space, the Feynman path integral in the configuration space is not actually an integral in the sense of integration theory, and the correct mathematical meaning of (7.24)-(7.25) is given by (7.23). Formula (7.24) expresses the propagator $\langle q',t'|q,t\rangle$ as the sum over all histories in the configuration space of classical particle — paths $\gamma\in P(\mathbb{R})_{q,t}^{q',t'}$, by assigning to each path γ a complex weight $\exp\{\frac{i}{\hbar}S(\gamma)\}$.

REMARK 7.8. It is said in physics textbooks that the Feynman path integral in the configuration space is obtained from the Feynman path integral in the phase space by evaluating the Fresnel integral over $\mathscr{D}p$,

$$\int\limits_{P(\mathbb{R})_{q,t}^{q',t'}} e^{\frac{i}{\hbar}\int_t^{t'}(\frac{m}{2}\dot{q}^2-V(q))d\tau}\mathscr{D}q = \int\limits_{P(\mathbb{R}^2)_{q,t}^{q',t'}} e^{\frac{i}{\hbar}\int_t^{t'}(p\dot{q}-\frac{1}{2m}p^2-V(q))d\tau}\mathscr{D}p\mathscr{D}q. \tag{7.26}$$

Note that the symbol $\mathscr{D}q$ has two different meanings: in the left-hand side of (7.26) it is defined by (7.25), whereas in the right-hand side it is defined as a part of (7.22).

7.4. Several degrees of freedom

Let

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$$

be the Hamiltonian operator of a quantum particle in $\mathbb{R}^n$ moving in the potential field $V(\boldsymbol{q})$. As in the case of one degree of freedom, the propagator $\langle \boldsymbol{q}', t'|\boldsymbol{q}, t\rangle$ is expressed as a limit of multiple integrals when the number of integrations goes to infinity,

$$\langle \boldsymbol{q}', t'|\boldsymbol{q}, t\rangle = \lim_{N\to\infty} \int\cdots\int\limits_{\mathbb{R}^{(2N-1)n}} \tag{7.27}$$

$$\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{N-1}(\boldsymbol{p}_k(\boldsymbol{q}_{k+1}-\boldsymbol{q}_k) - H_{\mathrm{c}}(\boldsymbol{p}_k,\boldsymbol{q}_k)\Delta)\right\}\frac{d^n\boldsymbol{p}_0}{(2\pi\hbar)^n}\prod_{k=1}^{N-1}\frac{d^n\boldsymbol{p}_k d^n\boldsymbol{q}_k}{(2\pi\hbar)^n}.$$

Here $H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{q}) = \dfrac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$ is the classical Hamiltonian function, and $\boldsymbol{q}_0 = \boldsymbol{q}$, $\boldsymbol{q}_N = \boldsymbol{q}'$. This representation is symbolized by the Feynman path integral in the phase space $\mathscr{M} = T^*\mathbb{R}^n$,

$$\langle \boldsymbol{q}', t'|\boldsymbol{q}, t\rangle = \int\limits_{P(\mathscr{M})_{\boldsymbol{q},t}^{\boldsymbol{q}',t'}} e^{\frac{i}{\hbar}\int_t^{t'}(\boldsymbol{p}\dot{\boldsymbol{q}}-H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{q}))d\tau}\mathscr{D}\boldsymbol{p}\mathscr{D}\boldsymbol{q}, \tag{7.28}$$

where

$$\mathscr{D}\boldsymbol{p}\mathscr{D}\boldsymbol{q} = \lim_{N\to\infty}\frac{d^n\boldsymbol{p}_0}{(2\pi\hbar)^n}\prod_{k=1}^{N-1}\frac{d^n\boldsymbol{p}_k d^n\boldsymbol{q}_k}{(2\pi\hbar)^n}$$

and $P(\mathscr{M})_{\boldsymbol{q},t}^{\boldsymbol{q}',t'}$ is the space of all admissible paths σ in the phase space $\mathscr{M}$ connecting points $\boldsymbol{q}$ at time t and $\boldsymbol{q}'$ at time t'. Equivalently, the propagator $\langle\boldsymbol{q}',t'|\boldsymbol{q},t\rangle$ can be written as

$$\langle\boldsymbol{q}',t'|\boldsymbol{q},t\rangle = \lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\Delta}\right)^{\frac{nN}{2}} \times \underbrace{\int\cdots\int}_{\mathbb{R}^{(n-1)N}} \exp\left\{\frac{i}{\hbar}\sum_{k=0}^{N-1}\left(\frac{m}{2}\left(\frac{\boldsymbol{q}_{k+1}-\boldsymbol{q}_k}{\Delta}\right)^2 - V(\boldsymbol{q}_k)\right)\Delta\right\}\prod_{k=1}^{N-1} d^n\boldsymbol{q}_k. \tag{7.29}$$

This formula is symbolized by the Feynman path integral in the configuration space,

$$\langle\boldsymbol{q}',t'|\boldsymbol{q},t\rangle = \int\limits_{P(M)_{\boldsymbol{q},t}^{\boldsymbol{q}',t'}} e^{\frac{i}{\hbar}\int_t^{t'} L(\boldsymbol{q},\dot{\boldsymbol{q}})d\tau}\mathscr{D}\boldsymbol{q}, \tag{7.30}$$

where $L(\boldsymbol{q},\dot{\boldsymbol{q}}) = \frac{1}{2}m\dot{\boldsymbol{q}}^2 - V(\boldsymbol{q})$ is the corresponding Lagrangian,

$$\mathscr{D}\boldsymbol{q} = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta}\right)^{\frac{nN}{2}}\prod_{k=1}^{N-1} d^n\boldsymbol{q}_k,$$

and $P(M)_{\boldsymbol{q},t}^{\boldsymbol{q}',t'}$ is the space of smooth parametrized paths in the configuration space M connecting points $\boldsymbol{q}$ and $\boldsymbol{q}'$. The precise mathematical meaning of formula (7.30) is the same as of (7.24).

CHAPTER 8

Gaussian path integrals

In the semi-classical limit $\hbar \to 0$ the leading contribution to the propagator $\langle q', t'|q, t\rangle$ is given by the classical trajectory $q_{\mathrm{cl}}(\tau)$. Indeed, represent the paths $\gamma = q(\tau) \in P(\mathbb{R})_{q,t}^{q',t'}$ as

$$q(\tau) = q_{\mathrm{cl}}(\tau) + y(\tau),$$

where $y(\tau)$ — the *quantum fluctuation* part — satisfies Dirichlet boundary conditions (DBC) $y(t) = y(t') = 0$. It follows from the principle of the least action that

(8.1)

$$S(q_{\mathrm{cl}} + y) = S_{\mathrm{cl}} + \tfrac{1}{2}\int_t^{t'} (m\dot{y}^2 - V''(q_{\mathrm{cl}}(\tau))y^2)d\tau + \text{higher order terms in } y,$$

where $S_{\mathrm{cl}} = S(q_{\mathrm{cl}})$ is the classical action. Similarly, for the case of several degrees of freedom,

$$S(\boldsymbol{q}_{\mathrm{cl}} + \boldsymbol{y}) = S_{\mathrm{cl}} + \tfrac{1}{2}\int_t^{t'} \mathcal{J}(\boldsymbol{y})\boldsymbol{y}\, d\tau + \text{higher order terms in } \boldsymbol{y}, \tag{8.2}$$

where $\mathcal{J}$ is the corresponding Jacobi operator associated with the Lagrangian

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \frac{m}{2}\dot{\boldsymbol{q}}^2 - V(\boldsymbol{q}).$$

It is remarkable that the Gaussian (rather Fresnel) path integral

$$\int\limits_{\mathrm{DBC}} e^{\frac{im}{2\hbar}\int_t^{t'} \mathcal{J}(\boldsymbol{y})\boldsymbol{y}\, d\tau} \mathscr{D}\boldsymbol{y} \tag{8.3}$$

over the fluctuating part can be evaluated explicitly in terms of the regularized determinant of the second order differential operator $\mathcal{J}$. Here we do this calculation for the case of the free particle and harmonic oscillator. In general, formula (8.2), with higher order terms in $\boldsymbol{y}$, and Gaussian integration over $\mathscr{D}\boldsymbol{y}$, constitute a basis of the perturbative expansion for the propagator.

8.1. Gaussian path integral for a free particle

The propagator of a free quantum particle is

$$\langle q, t'|q, t\rangle = \sqrt{\frac{m}{2\pi i\hbar T}}\; e^{\frac{im(q-q')^2}{2\hbar T}} = \int\limits_{P(\mathbb{R})_{q,t}^{q',t'}} e^{\frac{im}{2\hbar}\int_t^{t'}\dot{q}^2 d\tau}\mathscr{D}q, \tag{8.4}$$

and the corresponding classical trajectory is

$$q_{\mathrm{cl}}(\tau) = q + (\tau - t)\frac{q' - q}{T}, \quad T = t' - t.$$

Using the decomposition $q(\tau) = q_{\mathrm{cl}}(\tau) + y(\tau)$, where $y(\tau)$ satisfies Dirichlet boundary conditions $y(t) = y(t') = 0$, we obtain

$$S(q) = \tfrac{1}{2}\int_t^{t'} m\dot{q}^2 d\tau = S_{\mathrm{cl}} + S(y),$$

where

$$S_{\mathrm{cl}} = \frac{1}{2}\int_t^{t'} m\dot{q}_{\mathrm{cl}}(\tau)^2\, d\tau = \frac{m(q-q')^2}{2T}.$$

Assuming that $\mathscr{D}q = \mathscr{D}y$ under the "change of variable" $q = q_{\mathrm{cl}} + y$, we can rewrite the Feynman path integral for a free particle as

$$\langle q, t'|q, t\rangle = e^{\frac{i}{\hbar}S_{\mathrm{cl}}} \int\limits_{P(\mathbb{R})_{0,t}^{0,t'}} e^{\frac{im}{2\hbar}\int_t^{t'}\dot{y}^2 d\tau}\mathscr{D}y.$$

Remarkably, the classical contribution $e^{\frac{i}{\hbar}S_{\mathrm{cl}}} = e^{\frac{im(q-q')^2}{2\hbar T}}$ exactly reproduces the exponential factor in the propagator for a free particle. The integral over the fluctuating part — the Gaussian path integral for a free particle — does not depend on q and q' and, as we know, coincides with the prefactor in (8.4).

A more conceptual way to interpret this result is the following. Let

$$A = -D^2, \quad D = \frac{d}{d\tau},$$

be the second order differential operator on the interval $[t, t']$ with Dirichlet boundary conditions $y(t) = y(t') = 0$. The operator A is self-adjoint on $L^2(t,t')$. For any real-valued, absolutely continuous function $y(\tau)$ satisfying Dirichlet boundary conditions and $y, \dot{y} \in L^2(t,t')$, we have by using integration by parts

$$(Ay, y) = -\int_t^{t'} \ddot{y}y\, d\tau = \int_t^{t'} \dot{y}^2 d\tau.$$

The "integrand" in the fluctuation factor

$$\int\limits_{P(\mathbb{R})_{0,t}^{0,t'}} e^{\frac{im}{2\hbar}\int_t^{t'} \dot{y}^2 d\tau} \mathscr{D}y$$

is the exponent of the quadratic form of the operator A.

In the finite-dimensional case we have the formula

$$\int_{\mathbb{R}^n} e^{\frac{i}{2}(A\boldsymbol{q},\boldsymbol{q})+i(\boldsymbol{p},\boldsymbol{q})} d^n\boldsymbol{q} = e^{\frac{\pi i n}{4} - \frac{\pi i \nu}{2}} \frac{\sqrt{(2\pi)^n}}{\sqrt{|\det A|}}\, e^{-\frac{i}{2}(A^{-1}\boldsymbol{p},\boldsymbol{p})}, \tag{8.5}$$

where the integral is understood in the distributional sense as $\lim_{R\to\infty}\int_{|\boldsymbol{q}|\leq R}$ and ν is the number of negative eigenvalues of the real, non-degenerate symmetric $n \times n$ matrix A. Thus it is natural to expect that this Gaussian path integral is proportional to $(\det A)^{-\frac{1}{2}}$. The problem here is to understand what we mean by a determinant of a differential operator — a regularization of the divergent infinite product $\prod_{n=1}^{\infty} \lambda_n$, where λ_n are non-zero eigenvalues of A.

The most natural and useful regularization is given by the so-called operator zeta-function. Namely, let A be a non-negative self-adjoint operator in the Hilbert space $\mathscr{H}$ with pure point spectrum $0 \leq \lambda_1 \leq \lambda_2 \leq \dots$, such that for some $\alpha > 0$ the operator $(A+I)^{-\alpha}$ is of trace class. Then the zeta-function $\zeta_A(s)$ of the operator A is defined for $\operatorname{Re} s > \alpha$ by the following absolutely convergent series:

$$\zeta_A(s) = \sum_{\lambda_n > 0} \frac{1}{\lambda_n^s}.$$

If $\zeta_A(s)$ admits a meromorphic continuation to a larger domain containing the point $s = 0$ and is regular at $s = 0$, then we define a *regularized determinant* of A by

$$\det{}' A = \exp\Big\{ -\frac{d\zeta_A}{ds}(0)\Big\}. \tag{8.6}$$

Here the prime on the symbol det indicates that zero eigenvalues are excluded from the definition of an operator zeta-function. In the special case when 0 is not the eigenvalue of A, it is customary to denote the regularized determinant of A by $\det A$. We will also write

$$\det{}' A = \prod_{\lambda_n > 0}{}' \lambda_n,$$

where the prime indicates that the infinite product is regularized by the operator zeta-function. We have $\zeta_{cA}(s) = c^{-s}\zeta_A(s)$ for $c > 0$, so that

$$\det{}' cA = c^{\zeta_A(0)} \det{}' A,$$

which shows that $\zeta_A(0)$ plays the role of "regularized scaling dimension" of the Hilbert space $\mathscr{H}$ (with respect to the operator A). When $\dim_{\mathbb{C}} \mathscr{H} = n < \infty$ and $A > 0$, then $\zeta_A(0) = n$ and $\zeta_A'(0) = \log \lambda_1 + \cdots + \log \lambda_n$, and we recover the usual definition of $\det A$.

This basic outline works for the general case of elliptic operators on a compact manifold M. In quantum mechanics, only determinants of differential operators on one-dimensional[1] manifolds $M = [t, t']$ or $M = S^1$ appear. For the second derivative operator $A = -D^2$ the corresponding eigenvalues are $\lambda_n = \left(\frac{\pi n}{T}\right)^2$, $n = 1, 2, \dots$, and corresponding operator zeta-function is

$$\zeta_A(s) = \left(\frac{T}{\pi}\right)^{2s} \zeta(2s), \tag{8.7}$$

where $\zeta(s)$ is the Riemann zeta-function. Using classical formulas $\zeta(0) = -\frac{1}{2}$ and $\zeta'(0) = -\frac{1}{2}\log 2\pi$, we obtain

$$\zeta_A(0) = -\frac{1}{2} \quad \text{and} \quad \zeta_A'(0) = -\log\frac{T}{\pi} - \log 2\pi = -\log 2T. \tag{8.8}$$

Thus for the operator $A = -D^2$ on the interval $[t, t']$ with Dirichlet boundary conditions we have

$$\det A = 2T. \tag{8.9}$$

The formula

$$\int_{P(\mathbb{R})_{0,t}^{0,t'}} e^{\frac{im}{2\hbar}\int_t^{t'} \dot{y}^2 d\tau} \mathscr{D}y = \sqrt{\frac{m}{2\pi i\hbar T}}$$

[1]Higher-dimensional manifolds are used in quantum field theory.

agrees with our interpretation that the Gaussian path integral is proportional to $(\det A)^{-\frac{1}{2}}$. The coefficient of proportionality $c_{m,\hbar} = \sqrt{\frac{m}{\pi i \hbar}}$ is determined by comparison[2] with the actual propagator for a free particle.

8.2. Gaussian path integral for the harmonic oscillator

It is remarkable that the same method works for propagator of the quantum harmonic oscillator. Solving classical equations of motion with the boundary conditions $q(t) = q$ and $q(t') = q'$, we get

$$q_{\mathrm{cl}}(\tau) = \frac{1}{\sin \omega T} \left(q' \sin \omega(\tau - t) - q \sin \omega(\tau - t') \right), \quad T = t' - t,$$

provided $T \neq T_\nu$, where $T_\nu = \dfrac{\pi \nu}{\omega}$ and $\nu \in \mathbb{N}$. Note that T_1 is a half-period of she harmonic oscillator, so for even ν classical solution exists only when $\boldsymbol{q}' = \boldsymbol{q}$, and for odd ν — only when $\boldsymbol{q}' = -\boldsymbol{q}$. For $T \neq T_\nu$ we readily compute

$$\begin{aligned} S_{\mathrm{cl}} &= \frac{m}{2} \int_t^{t'} (\dot{q}_{\mathrm{cl}}^2 - \omega^2 q_{\mathrm{cl}}^2) d\tau \\ &= \frac{m\omega^2}{2 \sin^2 \omega T} \int_t^{t'} \left(q'^{\,2} \cos 2\omega(\tau - t) + q^2 \cos 2\omega(\tau - t') - 2qq' \cos(2\omega\tau - \omega(t + t')) \right) d\tau \\ &= \frac{m\omega}{2 \sin \omega T} \left((q^2 + q'^{\,2}) \cos \omega T - 2qq' \right). \end{aligned}$$

Thus for $T \neq T_\nu$ we obtain

$$\begin{aligned} &\langle q', t' | q, t \rangle \\ &= \exp\left\{ \frac{im\omega}{2\hbar \sin \omega T} \left((q^2 + q'^{\,2}) \cos \omega T - 2qq' \right) \right\} \int\limits_{P(\mathbb{R})_{0,t}^{0,t'}} e^{\frac{im}{2\hbar} \int_t^{t'} (\dot{y}^2 - \omega^2 y^2) d\tau} \mathscr{D}y. \end{aligned}$$

Evaluating the fluctuating factor by the same method as for the free particle, we get

$$\int\limits_{P(\mathbb{R})_{0,t}^{0,t'}} e^{\frac{im}{2\hbar} \int_t^{t'} (\dot{y}^2 - \omega^2 y^2) d\tau} \mathscr{D}y = \sqrt{\frac{m}{\pi i \hbar \det A_\omega}}.$$

Here $A_\omega = -D^2 - \omega^2$ is the second order differential operator on the interval $[t, t']$ with Dirichlet boundary conditions, and we have used the same constant $c_{m,\hbar} = \sqrt{\frac{m}{\pi i \hbar}}$ as before.

[2] For the proof, see Theorem 3.1 in Chapter 6 of the QM book.

The formula for the regularized determinant $\det A_\omega$ can be obtained by the following beautiful computation, which goes back to Euler. Namely, the eigenvalues of A_ω are $\lambda_n(\omega) = \left(\frac{\pi n}{T}\right)^2 - \omega^2$ (0 is not an eigenvalue for A_ω since $T \neq T_\nu$), and we have

$$\frac{\det A_\omega}{\det A_0} = \prod_{n=1}^{\infty} \frac{\lambda_n(\omega)}{\lambda_n(0)} = \prod_{n=1}^{\infty} \left(1 - \frac{\omega^2 T^2}{\pi^2 n^2}\right) = \frac{\sin \omega T}{\omega T}. \tag{8.10}$$

Since $\det A_0 = 2T$, we get $T \neq T_\nu$,

$$\det A_\omega = \frac{2 \sin \omega T}{\omega}.$$

Thus we obtain the following formula for the propagator of the harmonic oscillator,

$$\langle q', t' | q, t \rangle = \sqrt{\frac{m\omega}{\pi i \hbar \sin \omega T}} \exp\left\{\frac{im\omega}{2\hbar \sin \omega T}\big((q^2 + q'^{\,2}) \cos \omega T - 2qq'\big)\right\}. \tag{8.11}$$

This formula can be also obtained directly by computing finite-dimensional Gaussian integrals in the definition (7.29) in Chapter 7 of the Feynman path integral in the configuration space. In addition, one also get that for $T_\nu < T < T_{\nu+1}$

$$\sqrt{\frac{m\omega}{\pi i \hbar \sin \omega T}} = e^{-\frac{\pi i}{4} - \frac{\pi i \nu}{2}} \sqrt{\frac{m\omega}{\pi \hbar |\sin \omega T|}} \tag{8.12}$$

and

$$\lim_{T \to T_\nu} \langle q', t' | q, t \rangle = \begin{cases} e^{-\frac{\pi i \nu}{2}} \delta(q - q'), & \nu \text{ is even}, \\ e^{-\frac{\pi i \nu}{2}} \delta(q + q'), & \nu \text{ is odd}. \end{cases} \tag{8.13}$$

REMARK 8.1. Using representation (7.11) for the propagator in Chapter 7 and Theorem 5.1 in Chapter 5, one get get formula (8.11) from the well-known Mehler identity

$$\sum_{n=0}^{\infty} \frac{z^n}{2^n n!} H_n(x) H_n(y) = \frac{1}{\sqrt{1 - z^2}} \exp\left\{\frac{2xyz - (x^2 + y^2) z^2}{1 - z^2}\right\}$$

in the theory of Hermite-Tchebysheff polynomials, extended (in the distributional sense) from $|z| < 1$ to $|z| = 1$. Namely, using $E_n = \hbar\omega(n + \frac{1}{2})$

and formula (5.18) for the normalized eigenfunctions of the quantum harmonic oscillator, it is easy to see that (7.11) reduces to Mehler identity with $x = \sqrt{\frac{m\omega}{\hbar}}q$, $y = \sqrt{\frac{m\omega}{\hbar}}q'$ and $z = e^{-i\omega T}$. Moreover, we get from (7.11) that for $T = T_\nu$ for the harmonic oscillator we have

$$\langle q', T_\nu | q, 0\rangle = \sum_{n=0}^{\infty} e^{-\pi i\nu(n+\frac{1}{2})}\psi_n(q')\overline{\psi_n(q)},$$

which perfectly agrees with (8.13) since

$$\sum_{n=0}^{\infty} \psi_n(q')\overline{\psi_n(q)} = \delta(q'-q)$$

and $\psi_n(-q) = (-1)^n\psi_n(q)$.

8.3. The partition function for the harmonic oscillator

Though Hamiltonian H of the harmonic oscillator has pure discrete spectrum, the evolution operator $U(T) = e^{-\frac{i}{\hbar}TH}$ is unitary, so the formula

$$\operatorname{Tr} e^{-\frac{i}{\hbar}TH} = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar}TE_n}$$

should be considered only in the sense of distributions.

However, for pure imaginary time $T = -i\beta$ the operator $e^{-\frac{1}{\hbar}\beta H}$ is of trace class, and using $E_n = \hbar\omega(n+\frac{1}{2})$, we obtain by summing geoemtric series

$$\operatorname{Tr} e^{-\frac{1}{\hbar}\beta H} = \sum_{n=0}^{\infty} e^{-\beta\omega(n+\frac{1}{2})} = \frac{1}{2\sinh(\frac{\beta\omega}{2})}. \tag{8.14}$$

In statistical mechanics, the sum $e^{-\beta E_n}$ over all energy levels is called the *partition function*, and parameter $\beta > 0$ plays the role of inverse temperature.

Now what about the path integral formulation? According to formula (7.24), we have

$$\langle q', T | q, 0\rangle = \int\limits_{P(\mathbb{R})_{q,0}^{q',T}} e^{\frac{im}{2\hbar}\int_0^T(\dot{q}^2-\omega^2q^2)dt}\mathscr{D}q$$

so replacing T by $-i\beta$ and t by $-i\tau$, we obtain the following representation for the propagator in imaginary time:

$$\langle q', -i\beta | q, 0\rangle = \int\limits_{P(\mathbb{R})_{q,0}^{q',\beta}} e^{-\frac{m}{2\hbar}\int_0^\beta (\dot{q}^2+\omega^2 q^2)d\tau}\mathscr{D}q \tag{8.15}$$

where now we integrating over all maps $q(\tau)$ such that $q(0) = q$ and $q(\beta) = q'$. To get the partition function, the trace of $e^{-\frac{\beta}{\hbar}H}$, we need to put $q' = q$ over q integrate over q, since "the spectral trace equals to the matrix trace". Thus from (8.15) we obtain

$$\operatorname{Tr} e^{-\frac{\beta}{\hbar}H} = \int\limits_{\mathcal{L}_\beta(\mathbb{R})} e^{-\frac{m}{2\hbar}\int_0^\beta (\dot{q}^2+\omega^2 q^2)d\tau}\mathscr{D}q, \tag{8.16}$$

where $\mathcal{L}_\beta(\mathbb{R})$ is the free loop space — collection of smooth maps $q : S^1_\beta \to \mathbb{R}$, where $S^1_\beta = \mathbb{Z}/\beta\mathbb{Z}$ (in other words, $q : [0, \beta] \to \mathbb{R}$ is a smooth function satisfying periodic boundary conditions $q(0) = q(\beta)$ with all derivatives). Here the 'measure' $\mathscr{D}q$ is given by the formula (7.25), but where now the number of integrations over dq_k is also N.

Careful analysis of the finite-dimensional approximation (7.23) shows that the factor $c_{m,\hbar}$ is replaced by 1 and we have the following formula:

$$\int\limits_{\mathcal{L}_\beta(\mathbb{R})} e^{-\frac{m}{2\hbar}\int_0^\beta (\dot{q}^2+\omega^2 q^2)d\tau}\mathscr{D}q = \frac{1}{\sqrt{\det B_\omega}},$$

where $\det B_\omega$ is the zeta regularized determinant of the operator $B_\omega = -D^2+\omega^2$ on the interval $[0, \beta]$ with periodic boundary conditions (compare with the operator A_ω).

One can compute this determinant as follows. The eigenvalues of B_ω are a single eigenvalue $\lambda_0(\omega) = \omega^2$ and multiplicity two eigenvalues $\lambda_n(\omega) = \left(\frac{2\pi n}{\beta}\right)^2 + \omega^2$, $n = 1, 2, \dots$. The regularized determinant of the operator B_0 is easy to compute. As in (8.7), we have:

$$\zeta_{B_0}(s) = 2\sum_{n=1}^\infty \frac{1}{\lambda_n(0)^s} = 2\left(\frac{\beta}{2\pi}\right)^{2s}\zeta(2s),$$

and as in (8.8), we get

$$\zeta_B'(0) = -2\log\beta, \quad \text{so} \quad \det B = \beta^2.$$

Now as in (8.10), we obtain

$$\frac{\det B_\omega}{\det B_0} = \lambda_0(\omega) \prod_{n=1}^{\infty} \frac{\lambda_n(\omega)^2}{\lambda_n(0)^2} = \omega^2 \prod_{n=1}^{\infty} \left(1 + \frac{\beta^2\omega^2}{4\pi^2 n^2}\right)^2 = \frac{4}{\beta^2} \sinh^2\left(\frac{\beta\omega}{2}\right),$$

so

$$\det B_\omega = 4\sinh^2\left(\frac{\beta\omega}{2}\right).$$

Therefore we obtain

$$\operatorname{Tr} e^{-\frac{\beta}{\hbar}H} = \int\limits_{\mathcal{L}_\beta(\mathbb{R})} e^{-\frac{m}{2\hbar}\int_0^\beta(\dot{q}^2+\omega^2q^2)d\tau}\mathscr{D}q = \frac{1}{2\sinh\frac{\beta\omega}{2}},$$

which is the path integral derivation of the formula (8.14) for the partition function of the harmonic oscillator.

Problem 8.1. Show that the propagator of a particle in a constant uniform field f is given by the following formula:

$$K(q',t';q,t) = \sqrt{\frac{m}{2\pi i\hbar T}}\; e^{\frac{i}{2\hbar}\left\{\frac{m(q-q')^2}{T} + fT(q+q') - \frac{f^2T^3}{12m}\right\}}.$$

(*Hint:* Use Lagrangian function $L = \frac{1}{2}m\dot{q}^2 + fq$.)

Problem 8.2. Derive representation (8.11)–(8.12) using the definition of the Feynman path integral in the configuration space in Chapter 7 and formula (8.5).

Problem 8.3. Use representation (7.11) to prove property (8.13).

Problem 8.4. Using operator zeta function, prove that

$$\det A_{i\omega} = \frac{2\sinh\omega T}{\omega}.$$

(*Hint:* Use Jacobi inversion formula for the Jacobi theta series.)

CHAPTER 9

Fermion systems

9.1. Canonical anticommutation relations

In Sections 5.1 and 5.2 of Chapter 5 we have shown that the Hilbert space $\mathscr{H} \simeq L^2(\mathbb{R}, dq)$ of a one-dimensional quantum particle can be described in terms of the creation and annihilation operators. Namely, the operators[1]

$$a^* = \frac{1}{\sqrt{2\hbar}}\,(Q - iP) \quad \text{and} \quad a = \frac{1}{\sqrt{2\hbar}}\,(Q + iP)$$

satisfy the canonical commutation relation

$$[a, a^*] = I \tag{9.1}$$

on $W^{2,2}(\mathbb{R}) \cap \hat{W}^{2,2}(\mathbb{R})$, and the vectors

$$\psi_k = \frac{(a^*)^k}{\sqrt{k!}}\psi_0, \quad k = 0, 1, 2, \ldots,$$

where $\psi_0(q) = (\pi\hbar)^{-\frac{1}{4}} e^{-\frac{1}{2\hbar}q^2} \in \mathscr{H}$ satisfies $a\psi_0 = 0$, form an orthonormal basis for $\mathscr{H}$. The corresponding operator $N = a^*a$ is self-adjoint and has an integer spectrum,

$$N\psi_k = k\psi_k, \ \ k = 0, 1, 2, \ldots,$$

and according to formula (5.12), the Hamiltonian of the quantum harmonic oscillator is

$$H = \frac{\hbar\omega}{2}(a^*a + aa^*) = \hbar\omega\left(N + \tfrac{1}{2}I\right).$$

Similarly, for several degrees of freedom $\mathscr{H} \simeq L^2(\mathbb{R}^n, d^n\boldsymbol{q})$, the creation and annihilation operators are given by

$$a_k^* = \frac{1}{\sqrt{2\hbar}}\,(Q_k - iP_k) \quad \text{and} \quad a_k = \frac{1}{\sqrt{2\hbar}}\,(Q_k + iP_k)\,, \ \ k = 1, \ldots, n, \tag{9.2}$$

[1]Here in comparison with Section 5.1 of Chapter 5 we put $\omega = 1$.

and satisfy canonical commutation relations

$$[a_k, a_l] = [a_k^*, a_l^*] = 0 \quad \text{and} \quad [a_k, a_l^*] = \delta_{kl} I, \quad k, l = 1, \dots, n. \tag{9.3}$$

The ground state, the vector $\psi_0(\boldsymbol{q}) = (\pi\hbar)^{-\frac{n}{4}} e^{-\frac{1}{2\hbar}\boldsymbol{q}^2} \in \mathscr{H}$, has the property

$$a_k \psi_0 = 0, \quad k = 1, \dots, n,$$

and the vectors

$$\psi_{k_1,\dots,k_n} = \frac{(a_1^*)^{k_1} \dots (a_n^*)^{k_n}}{\sqrt{k_1! \dots k_n!}} \psi_0, \quad k_1, \dots, k_n = 0, 1, 2, \dots,$$

form an orthonormal basis for $\mathscr{H}$. The operator $N = \sum_{k=1}^n a_k^* a_k$ is self-adjoint and has an integer spectrum:

$$N \psi_{k_1,\dots,k_n} = (k_1 + \dots + k_n) \psi_{k_1,\dots,k_n},$$

and the Hilbert space $\mathscr{H}$ decomposes into the direct sum of invariant subspaces

$$\mathscr{H} = \bigoplus_{k=0}^{\infty} \mathscr{H}_k \tag{9.4}$$

— the eigenspaces for the operator N.

One may ask what happens if we replace commutator of operators in (12.1) and (9.3) by an anticommutator:

$$[A, B]_+ = AB + BA.$$

Thus for the case of one degree of freedom we obtain so-called *canonical anticommutation relations*:

$$[a, a]_+ = [a^*, a^*]_+ = 0 \quad \text{and} \quad [a, a^*]_+ = I. \tag{9.5}$$

It is quite remarkable, that (9.5) admit an irreducible representation in the Hilbert space $\mathscr{H} = \mathbb{C}^2$. Namely, let

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

be the famous Pauli matrices, commonly used in physics, and put

$$\sigma_+ = \frac{1}{2}(\sigma_1 + i\sigma_2), \quad \sigma_- = \frac{1}{2}(\sigma_1 - i\sigma_2).$$

Then the matrices

$$a^* = \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad a = \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

satisfies (9.5)! Moreover, it easy to see that every matrix that commutes with a^* and a is a multiple 2×2 identity matrix I_2.

The vector $e_0 = \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$ has the property $ae_0 = 0$, and together with the vector $e_1 = a^* e_0 = \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$, form an orthonormal basis of $\mathbb{C}^2$. The matrix

$$N = a^* a = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

has the eigenvectors e_0 and e_1 and the eigenvalues 0 and 1. Thus in complete analogy with the previous discussion, we say that a and a^* are *fermion creation* and *annihilation operators* for the case of one degree of freedom. The Hilbert space of a Fermi particle — a fermion — is $\mathscr{H}_F = \mathbb{C}^2$, and the vector e_0 is the ground state. In analogy with (5.12), it is natural to define the Hamiltonian of a quantum fermion oscillator by

$$H = \frac{\hbar\omega}{2}(a^* a - a a^*) = \hbar\omega \left(N - \tfrac{1}{2} I\right) = \tfrac{1}{2}\hbar\omega\sigma_3, \tag{9.6}$$

which has the eigenvectors e_0 and e_1 and the eigenvalues $-\frac{1}{2}\hbar\omega$ and $\frac{1}{2}\hbar\omega$. In Example 9.2 in Section 9.3 we explain how H can be obtained as quantization of classical Hamiltonian.

It is straightforward to generalize this construction to the case of several degrees of freedom. Namely, canonical anticommutation relations have the form

$$[a_k, a_l]_+ = [a_k^*, a_l^*]_+ = 0 \quad \text{and} \quad [a_k, a_l^*]_+ = \delta_{kl} I, \quad k, l = 1, \dots, n, \tag{9.7}$$

where I is the identity operator, and creation operators a_j^* are adjoint to annihilation operators a_j in the fermion Hilbert space $\mathscr{H}_F$. In particular, fermion operators a_j^* and a_j are nilpotent. Canonical anticommutation relations (9.7) can be realized in the Hilbert space $\mathscr{H}_F = (\mathbb{C}^2)^{\otimes n} = \mathbb{C}^{2^n}$ as follows:

$$a_k = \underbrace{\sigma_3 \otimes \cdots \otimes \sigma_3}_{k-1} \otimes a \otimes I_2 \otimes \cdots \otimes I_2, \tag{9.8}$$

$$a_k^* = \underbrace{\sigma_3 \otimes \cdots \otimes \sigma_3}_{k-1} \otimes a^* \otimes I_2 \otimes \cdots \otimes I_2, \tag{9.9}$$

$k = 1, \dots, n$. The ground state, the vector $\psi_0 = e_0 \otimes \cdots \otimes e_0 \in \mathscr{H}_F$, satisfies

$$a_k \psi_0 = 0, \quad k = 1, \dots, n, \tag{9.10}$$

and the vectors

$$\psi_{k_1,\dots,k_n} = (a_1^*)^{k_1} \dots (a_n^*)^{k_n} \psi_0, \quad k_1, \dots, k_n = 0, 1, \tag{9.11}$$

form an orthonormal basis for $\mathscr{H}_F$. The operator

$$N = \sum_{k=1}^{n} a_k^* a_k$$

is self-adjoint and has the integer spectrum:

$$N \psi_{k_1,\dots,k_n} = (k_1 + \cdots + k_n) \psi_{k_1,\dots,k_n},$$

and the Hilbert space $\mathscr{H}_F$ decomposes into the direct sum of invariant subspaces

$$\mathscr{H}_F = \bigoplus_{k=0}^{n} \mathscr{H}_k \tag{9.12}$$

— the eigenspaces of N.

REMARK 9.1. Since fermion creation a_j^* operators operators are nilpotent, we can apply them at most only once. This is a mathematical content of the famous *Pauli exclusion principle* for fermions.

As in the case of one degree of freedom, we have the following result.

LEMMA 9.1. *Realization* (9.8)–(9.9) *of canonical anticommutation relations in the fermion Hilbert space $\mathscr{H}_F$ is irreducible: every operator in $\mathscr{H}_F$, which commutes with all creation and annihilation operators a_k^* and a_k, is a multiple of the identity operator.*

REMARK 9.2. The realization of canonical anticommutation relations (9.7) in the fermion Hilbert space $\mathscr{H}_F$ is analogous to the representation of canonical commutation relations in Section 5.2 of Chapter 5, and is called representation by the occupation numbers for fermions. It should be emphasized that the algebraic structure of the former relations allows their realization in a finite-dimensional Hilbert space, while the algebraic structure of the latter relations warrants the infinite-dimensional Hilbert space.

Analogously to (9.2), coordinate and momentum operators for fermions are defined by

$$Q_k = \sqrt{\tfrac{\hbar}{2}}(a_k + a_k^*), \quad P_k = -i\sqrt{\tfrac{\hbar}{2}}(a_k - a_k^*), \quad k = 1, \dots, n. \tag{9.13}$$

As follows from (9.7), they satisfy the following anticommutation relations:

$$[Q_k, Q_l]_+ = [P_k, P_l]_+ = \hbar\delta_{kl} I \quad \text{and} \quad [P_k, Q_l]_+ = 0, \quad k, l = 1, \dots, n \tag{9.14}$$

— a fermion analog of Heisenberg commutations relations, introduced in (3.4) in Chapter 3. The following result is a fermion analog of the Stone-von Neumann theorem.

THEOREM 9.1. *Every irreducible finite-dimensional representation of canonical anticommutation relations is unitarily equivalent to the representation by occupation numbers in the fermion Hilbert space* $\mathscr{H}_F$.

PROOF. Let V be the Hilbert space which realizes the irreducible representation of canonical anticommutation relations (9.7). First of all, there is $\varphi_0 \in V$, $\|\varphi_0\| = 1$, such that

$$a_1\varphi_0 = \cdots = a_n\varphi_0 = 0.$$

Indeed, choose any non-zero $\varphi \in V$; if $a_1\varphi \neq 0$, replace it by the vector $a_1\varphi$, which obviously satisfies $a_1(a_1\varphi_1) = 0$. If $a_2(a_1\varphi) \neq 0$, replace it by $a_2a_1\varphi$, which is annihilated by a_1 and a_2, etc. In finitely many steps we arrive at a non-zero vector $\tilde{\varphi}$ annihilated by the operators $a_1, \dots, a_n$, and $\varphi_0 = \tilde{\varphi}/\|\tilde{\varphi}\|$. Now consider the subspace V_0 of V, spanned by the vectors

$$\varphi_{k_1,\dots,k_n} = (a_1^*)^{k_1} \dots (a_n^*)^{k_n}\varphi_0, \quad k_1, \dots, k_n = 0, 1.$$

It follows from (9.7) that V_0 is an invariant subspace for all operators a_k and a_k^*, so that $V_0 = V$. Since operators a_k^* and a_k are adjoint with respect to the inner product in V, it is easy to see, again using canonical anticommutation relations (9.7), that vectors $\varphi_{k_1,\dots,k_n}$ form an orthonormal basis for V. The mapping $V \ni \varphi_{k_1,\dots,k_n} \mapsto \psi_{k_1,\dots,k_n} \in \mathscr{H}_F$ establishes the Hilbert space isomorphism $V \simeq \mathscr{H}_F$. □

9.2. Clifford and Grassmann algebras

As we have seen in Section 3.1, a Heisenberg Lie algebra is the fundamental mathematical structure associated with canonical commutation relations. Similarly, the fundamental mathematical structure associated with the canonical anticommutation relations is a *Clifford algebra*.

Let V be a finite-dimensional vector space over the field k of characteristic zero, and let $Q : V \to k$ be a symmetric non-degenerate quadratic form on V, i.e., $Q(v) = \Phi(v, v),\ v \in V$, where $\Phi : V \otimes_k V \to k$ is symmetric non-degenerate bilinear form. The pair (V, Q) is called quadratic vector space.

Definition. A Clifford algebra $C(V, Q) = C(V)$ associated with a quadratic vector space (V, Q) is a k-algebra generated by the vector space V with relations

$$v^2 = Q(v) \cdot 1, \quad v \in V.$$

Equivalently, Clifford algebra is defined as a quotient algebra

$$C(V) = T(V)/J,$$

where J is a two-sided ideal in the tensor algebra $T(V)$ of V, generated by the elements $u \otimes v + v \otimes u - 2\Phi(u, v) \cdot 1$ for all $u, v \in V$, and 1 is the unit in $T(V)$. In terms of a basis $\{e_i\}_{i=1}^n$ of V, the Clifford algebra $C(V)$ is a k-algebra with the generators $e_1, \dots, e_n$, satisfying the relations

$$[e_i, e_j]_+ = e_i e_j + e_j e_i = 2\Phi(e_i, e_j) \cdot 1, \quad i, j = 1, \dots, n.$$

When $k = \mathbb{C}$ (or any algebraically closed field of characteristic zero), there always exists an orthonormal basis for V — a basis $\{e_i\}_{i=1}^n$ such that $\Phi(e_i, e_k) = \delta_{ik}$. In this case for every dimension n there is one (up to an isomorphism) Clifford algebra C_n with generators $e_1, \dots, e_n$ and relations

$$e_i e_j + e_j e_i = 2\delta_{ij} \cdot 1, \quad i, k = 1, \dots, n.$$

Remark 9.3. If $k = \mathbb{R}$, there exist non-negative integers $p + q = n$ and an isomorphism $V \simeq \mathbb{R}^n$ such that

$$Q(\boldsymbol{x}) = x_1^2 + \cdots + x_p^2 - x_{p+1}^2 - \cdots - x_n^2, \quad \boldsymbol{x} \in \mathbb{R}^n.$$

This classifies Clifford algebras over $\mathbb{R}$.

Definition. A module for a Clifford algebra $C(V)$ is a finite-dimensional k-vector space U with an algebra homomorphism $\rho : C(V) \to \operatorname{End} U$.

The fermion Hilbert space $\mathscr{H}_F = (\mathbb{C}^2)^{\otimes n}$, introduced in the previous section, is an irreducible C_{2n}-module. Indeed, it follows from canonical anticommutation relations (9.7) that the self-adjoint operators

$$\gamma_{2k-1} = a_k + a_k^*, \tag{9.15}$$

$$\gamma_{2k} = -i(a_k - a_k^*), \quad k = 1, \dots, n, \tag{9.16}$$

satisfy the following relations:

$$\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\delta_{\mu\nu}I, \quad \mu,\nu = 1,\dots,2n, \tag{9.17}$$

where I is the identity operator in $\mathscr{H}_F$. We define the action of the Clifford algebra C_{2n} on $\mathscr{H}_F$ by setting

$$\rho(1) = I \quad \text{and} \quad \rho(e_\mu) = \gamma_\mu, \quad \mu = 1,\dots,2n,$$

and extend it to a $\mathbb{C}$-algebra homomorphism $\rho : C_{2n} \to \operatorname{End}(\mathscr{H}_F)$. Relations (9.17) show that the map ρ admits such an extension.

Proposition 9.1. *The homomorphism $\rho : C_{2n} \to \operatorname{End}(\mathscr{H}_F)$ is a $\mathbb{C}$-algebra isomorphism.*

Proof. It follows from Lemma 9.1 that the representation ρ is irreducible: every operator in $\mathscr{H}_F$ which commutes with all elements of the $\mathbb{C}$-algebra $\rho(C_{2n})$ is a multiple of the identity operator. Then by Wedderburn's theorem $\rho(C_{2n}) = \operatorname{End}(\mathscr{H}_F)$, and since $\dim C_{2n} = 2^{2n} = \dim \operatorname{End}(\mathscr{H}_F)$, the map ρ is an isomorphism. □

Remark 9.4. The structure of a Clifford algebra with an odd number of generators is different. Thus the mapping $\rho(e_k) = \sigma_k$, where σ_k, $k = 1, 2, 3$, are Pauli matrices, defines an irreducible representation of C_3 in $\mathscr{H}_F = \mathbb{C}^2$. However, in this case $C_3 \simeq \operatorname{End}(\mathbb{C}^2) \otimes \mathbb{C}[\varepsilon]$, where $\varepsilon = ie_1e_2e_3$ and satisfies $\varepsilon^2 = 1$.

We define the *chirality operator* by $\Gamma = (-1)^N := e^{\pi i N}$, where $N = \sum_{j=1}^n a_j^* a_j$. Since the operator N has an integral spectrum, $\Gamma^2 = I$. Moreover, we have

$$[\Gamma, \gamma_\mu]_+ = 0, \quad \mu = 1,\dots,2n. \tag{9.18}$$

Indeed, as follows from (9.7),

$$Na_j^* = a_j^*(N + I) \quad \text{and} \quad Na_j = a_j(N - I),$$

so that

$$e^{\pi i N} a_j^* = a_j^* e^{\pi i (N+I)} = -a_j^* e^{\pi i N} \quad \text{and} \quad e^{\pi i N} a_j = a_j e^{\pi i (N-I)} = -a_j e^{\pi i N}.$$

Thus Γ anticommutes with all a_j, a_j^*, and hence with all γ_μ. Since $\Gamma^2 = I$, the operators

$$P_\pm = \frac{1}{2}(I \pm \Gamma)$$

are orthogonal projection operators and we have a decomposition

$$\mathscr{H}_F = \mathscr{H}_F^+ \oplus \mathscr{H}_F^-$$

into the subspaces of *positive* and *negative chirality spinors*. It follows from (9.18) that

$$\gamma_\mu(\mathscr{H}_F^+) = \mathscr{H}_F^-, \quad \mu = 1, \dots, 2n.$$

Also, since $e^{\pi i a_j^* a_j} = I - 2a_j^* a_j = -i\gamma_{2j-1}\gamma_{2j}$, we have

$$\Gamma = (-i)^n \gamma_1 \dots \gamma_{2n}.$$

REMARK 9.5. When $n = 2$, 4×4 matrices $\gamma_1, \gamma_2, \gamma_3, \gamma_4$ are celebrated Dirac gamma matrices (for the Euclidean metric on $\mathbb{R}^4$), and $\Gamma = \gamma_5$.

The Clifford algebras provide a mathematical tool for describing new type of quantum objects — the fermions. Their semi-classical description as $\hbar \to 0$ is described by the *Grassmann algebras*. The corresponding mathematical definition is the following.

DEFINITION. A Grassmann algebra with n generators is a $\mathbb{C}$-algebra Gr_n with the generators $\theta_1, \dots, \theta_n$ satisfying the relations

$$\theta_i\theta_j + \theta_j\theta_i = 0, \;\; i, j = 1, \dots, n.$$

In particular, these relations imply that generators of a Grassmann algebra are nilpotent: $\theta_1^2 = \dots = \theta_n^2 = 0$. Equivalently,

$$\mathrm{Gr}_n = \mathbb{C}\langle\theta_1, \dots, \theta_n\rangle/J$$

— a quotient of a free $\mathbb{C}$-algebra $\mathbb{C}\langle\theta_1, \dots, \theta_n\rangle$, generated by $\theta_1, \dots, \theta_n$, by the two-sided ideal J generated by the elements $\theta_i\theta_j + \theta_j\theta_i$, $i, j = 1, \dots, n$.

REMARK 9.6. It follows from (9.14) that in the semi-classical limit $\hbar \to 0$ fermion operators P_k and Q_k, $k = 1, \dots, 2n$, satisfy the defining relations of Grassmann algebra Gr_{2n}.

Comparison with the polynomial algebra

$$\mathbb{C}[x_1, \dots, x_n] = \mathbb{C}\langle x_1, \dots, x_n\rangle/I$$

— a quotient of a free $\mathbb{C}$-algebra $\mathbb{C}\langle x_1, \dots, x_n\rangle$ by the two-sided ideal generated by the elements $x_ix_j - x_jx_i$, $i, j = 1, \dots, n$ — shows that the Grassmann algebra Gr_n can also be considered as a *polynomial algebra in anticommuting variables* $\theta_1, \dots, \theta_n$. In what follows we will always use Roman letters for commuting variables and Greek letters for anticommuting variables, so that

$$\mathrm{Gr}_n = \mathbb{C}[\theta_1, \dots, \theta_n].$$

Needless to say, the polynomial algebra $\mathbb{C}[x_1, \dots, x_n]$ is isomorphic to the symmetric algebra of the vector space spanned by $x_1, \dots, x_n$, and the Grassmann algebra $\mathbb{C}[\theta_1, \dots, \theta_n]$ is isomorphic to the exterior algebra $\Lambda^\bullet V$ of the vector space $V = \mathbb{C}\theta_1 \oplus \cdots \oplus \mathbb{C}\theta_n$ with the basis $\theta_1, \dots, \theta_n$.

DEFINITION. An involution on $\mathrm{Gr}_n = \mathbb{C}[\theta_1, \dots, \theta_n]$ is a complex anti-linear map $* : \mathrm{Gr}_n \to \mathrm{Gr}_n$, that is an involutive anti-isomorphism of Grassmann algebras:

$$(c\alpha)^* = \bar{c}\alpha^* \quad \text{and} \quad (\alpha\beta)^* = \beta^*\alpha^* \quad \text{for all} \quad c \in \mathbb{C}, \;\; \alpha, \beta \in \mathrm{Gr}_n.$$

Thus a Grassmann algebra with $2n$ generators $\theta_1, \dots, \theta_n$ and $\bar{\theta}_1, \dots, \bar{\theta}_n$ has a natural involution given by $\theta_i^* = \bar{\theta}_i$ and $(\bar{\theta}_i)^* = \theta_i$, $i = 1, \dots, n$.

The Grassmann algebra Gr_n is a complex vector space of dimension 2^n and is $\mathbb{Z}$-graded: it admits a decomposition

$$\mathrm{Gr}_n = \bigoplus_{k=0}^{n} \mathrm{Gr}_n^k \tag{9.19}$$

into homogeneous components Gr_n^k of degree k and dimension $\binom{n}{k}$, $k = 0, \dots, n$, where $\mathrm{Gr}_n^0 = \mathbb{C} \cdot 1$. Namely, denote by $|\cdot|$ the degree of homogeneous elements in the Grassmann algebra, $|\alpha| = k$ for $\alpha \in \mathrm{Gr}_n^k$. Then multiplication in Gr_n satisfies $\mathrm{Gr}_n^k \cdot \mathrm{Gr}_n^l \subset \mathrm{Gr}_n^{k+l}$, where $\mathrm{Gr}_n^{k+l} = 0$ if $k + l > n$, and is graded-commutative:

$$\alpha\beta = (-1)^{|\alpha||\beta|}\beta\alpha \tag{9.20}$$

for homogenous elements $\alpha, \beta \in \mathrm{Gr}_n$. The elements of the Grassmann algebra Gr_n of even degree are called *even elements*, and those of odd degree — *odd elements*.

it is very convenient to think of elements

$$f = \sum_{k=0}^{n} \sum_{1 \leq i_1 < \cdots < i_k \leq n} f^{i_1 \dots i_k} \theta_{i_1} \dots \theta_{i_k} \in \mathrm{Gr}_n$$

as "function of anticommuting variables" and use a notation $f = f(\theta_1, \dots, \theta_n)$ or simply $f(\boldsymbol{\theta})$, where $\boldsymbol{\theta} = (\theta_1, \dots, \theta_n)$.

The Grassmann algebra provides us with the explicit representation of canonical anticommutation relations by multiplication and differentiation operators, which is analogous to the holomorphic representation for canonical commutation relations (see Section 5.2 of Chapter 5). Namely, let

$$\partial_i = \frac{\partial}{\partial\theta_i} : \mathrm{Gr}_n \to \mathrm{Gr}_n$$

be the left partial differentiation operators, defined on homogeneous monomials $\theta_{i_1} \dots \theta_{i_k}$ by

$$\frac{\partial}{\partial\theta_i}\theta_{i_1} \dots \theta_{i_k} = \sum_{l=1}^{k} (-1)^{l-1}\delta_{ii_l}\theta_{i_1} \dots \check{\theta}_{i_l} \dots \theta_{i_k},$$

where $\check{\theta}_{i_l}$ denotes the omission of the factor θ_{i_l}. The differentiation operators are of degree -1 and satisfy the graded Leibniz rule,

$$\frac{\partial}{\partial\theta_i}(fg) = \frac{\partial f}{\partial\theta_i}g + (-1)^{|f|}f\frac{\partial g}{\partial\theta_i}.$$

Remark 9.7. One can also introduce right partial differentiation operators by

$$(\theta_{i_1} \dots \theta_{i_k})\frac{\partial}{\partial\theta_i} = \sum_{l=1}^{k} (-1)^{k-l}\delta_{ii_l}\theta_{i_1} \dots \check{\theta}_{i_l} \dots \theta_{i_k},$$

which satisfy the following graded Leibniz rule:

$$(fg)\frac{\partial}{\partial\theta_i} = f\left(g\frac{\partial}{\partial\theta_i}\right) + (-1)^{|g|}\left(\frac{\partial}{\partial\theta_i}f\right)g.$$

To distinguish between the left and right partial derivatives of $f \in \mathrm{Gr}_n$, we will denote them, respectively, by $\frac{\partial}{\partial\theta_i}f$ and $f\frac{\partial}{\partial\theta_i}$. We have

$$f\frac{\partial}{\partial\theta_i} = -(-1)^{|f|}\frac{\partial}{\partial\theta_i}f, \tag{9.21}$$

and there is no confusion to denote the left partial derivative by $\frac{\partial f}{\partial\theta_i}$.

Remark 9.8. One can formally define the differential of a 'function' $f(\boldsymbol{\theta}) \in \mathrm{Gr}_n$ by considering Grassmann algebra Gr_{2n} with additional generators — 'differentials' $d\theta_1, \dots, d\theta_n$, and defining

$$df(\boldsymbol{\theta}) = f(\theta_1 + d\theta_1, \dots, \theta_n + d\theta_n) - f(\theta_1, \dots, \theta_n)$$

modulo higher order terms. Then using the graded Leibniz rule, it is easy to verify that

$$df(\boldsymbol{\theta}) = d\theta_1\frac{\partial f}{\partial\theta_1} + \dots + d\theta_n\frac{\partial f}{\partial\theta_n}. \tag{9.22}$$

As a complex vector space, Grassmann algebra Gr_n carries a standard inner product defined by the property that homogeneous monomials $\theta_{i_1}\dots\theta_{i_k}$, for all $1 \leq i_1 < \cdots < i_k \leq n$, form an orthonormal basis,

$$(\theta_{i_1}\dots\theta_{i_k}, \theta_{j_1}\dots\theta_{j_l}) = \delta_{kl}\delta_{i_1 j_1}\dots\delta_{i_k j_k}. \tag{9.23}$$

By checking on homogeneous monomials, it is elementary to verify that

$$(\partial_i f, g) = (f, \hat{\theta}_i g), \quad f, g \in \mathrm{Gr}_n,$$

where $\hat{\theta}_i$ are operators of the left multiplication by θ_i in Gr_n, so that $\hat{\theta}_i = \partial_i^*$. It is also easy to verify that the operators $\hat{\theta}_i$ and ∂_i satisfy the anticommutation relations

$$[\hat{\theta}_i, \hat{\theta}_j]_+ = [\partial_i, \partial_j]_+ = 0 \quad \text{and} \quad [\hat{\theta}_i, \partial_j]_+ = \delta_{ij} I, \quad i, j = 1, \dots, n,$$

where I is an identity operator in Gr_n. Thus we have the following result.

Proposition 9.2. *The assignment*

$$\mathscr{H}_F \ni \psi_{k_1,\dots,k_n} \mapsto \theta_1^{k_1}\dots\theta_n^{k_n} \in \mathrm{Gr}_n$$

establishes an isomorphism $\mathscr{H}_F \simeq \mathrm{Gr}_n$ between the fermion Hilbert space of n identical particles, and the vector space of the Grassmann algebra with n generators. It preserves decompositions (9.12) *and* (9.19) *and has the property that*

$$a_i^* \mapsto \hat{\theta}_i \quad \textit{and} \quad a_i \mapsto \frac{\partial}{\partial \theta_i}, \quad i = 1, \dots, n.$$

Using Proposition 9.2, it is also very easy to verify that the representation of canonical anticommutation relations in the fermion Hilbert space $\mathscr{H}_F$ is irreducible. Indeed, suppose that $B \in \mathrm{End}(\mathrm{Gr}_n)$ commutes with all operators $\hat{\theta}_i$ and ∂_i. Then

$$\partial_i(B(1)) = B(\partial_i(1)) = 0, \quad i = 1, \dots, n.$$

The only solution of the equations $\partial_1 f = \cdots = \partial_n f = 0$ is $f = c \cdot 1$, so that $B(1) = c \cdot 1$. Since B commutes with all creation operators $\hat{\theta}_i$, we obtain $B = cI$.

On can define an analog of Poisson bracket for anticommuting variables.

Definition. The Poisson bracket on the Grassmann algebra is a bilinear map

$$\{\ ,\ \} : \mathrm{Gr}_n \times \mathrm{Gr}_n \to \mathrm{Gr}_n$$

satisfying the following properties.

(i) (Graded skew-symmetry)

$$\{f, g\} = -(-1)^{|f||g|}\{g, f\}.$$

(ii) (Graded Leibniz rule)

$$\{fg, h\} = f\{g, h\} + (-1)^{|f||g|} g\{f, h\}.$$

(iii) (Graded Jacobi identity)

$$\{f, \{g, h\}\} + (-1)^{|f|(|g|+|h|)}\{g, \{h, f\}\} + (-1)^{|h|(|f|+|g|)}\{h, \{f, g\}\} = 0$$

for all $f, g, h \in \mathrm{Gr}_n$.

For instance, it is easy to see, using (9.21), that the formula

$$\{f, g\} = c\sum_{i=1}^{n}\left(f\frac{\partial}{\partial\theta_i}\right)\left(\frac{\partial}{\partial\theta_i}g\right) = -(-1)^{|f|}c\sum_{i=1}^{n}\frac{\partial f}{\partial\theta_i}\frac{\partial g}{\partial\theta_i} \tag{9.24}$$

with arbitrary coefficient $c \in \mathbb{C}$, defines a Poisson bracket. Another example, used in the Hamiltonian mechanics for anticommuting variables, uses the Grassmann algebra G_{2n}. Denoting its generators by $\theta_1, \dots, \theta_n$ and $\pi^1, \dots, \pi^n$, we have, in analogy with formula (1.22), the following Poisson bracket

$$\{f, g\} = -(-1)^{|f|}c\sum_{i=1}^{n}\left(\frac{\partial f}{\partial\theta_i}\frac{\partial g}{\partial\pi^i} + \frac{\partial f}{\partial\pi^i}\frac{\partial g}{\partial\theta_i}\right). \tag{9.25}$$

In particular, Poisson brackets between the generators are

$$\{\pi^i, \pi^j\} = 0, \quad \{\theta_i, \theta_j\} = 0 \quad \text{and} \quad \{\pi^i, \theta_j\} = \{\theta_j, \pi^i\} = \delta^i_j c. \tag{9.26}$$

Thus if H is an even element and $c = 1$, then

$$\{H, \pi^i\} = -\frac{\partial H}{\partial\theta_i} \quad \text{and} \quad \{H, \theta_i\} = -\frac{\partial H}{\partial\pi^i}, \quad i = 1, \dots, n. \tag{9.27}$$

Remark 9.9. For the Grassmann algebra with involution the Poisson bracket should satisfy the following compatibility condition

$$\{f, g\}^* = (-1)^{|f||g|}\{g^*, f^*\}. \tag{9.28}$$

Thus for the Grassmann algebra $\mathbb{C}[\theta_1, \dots, \theta_n]$ with involution $\theta_k^* = \theta_k$, we obtain that

$$\{\theta_k, \theta_k\}^* = -\{\theta_k, \theta_k\}, \quad k = 1, \dots, n,$$

Therefore in formula (9.24) for the Poisson bracket, the coefficient c should be pure imaginary.

PROBLEM 9.1. Formulate and prove the analog of Proposition 9.1 for Clifford algebras with an odd number of generators.

PROBLEM 9.2. Complete the proof of Proposition 9.2.

9.3. Lagrangian and Hamiltonian mechanics

Grassmann algebra $\mathrm{Gr}_n = \mathbb{R}[\theta_1, \ldots, \theta_n]$ can be considered as 'algebra of functions on configuration space' with anticommuting coordinates $\theta_1, \ldots, \theta_n$. Correspondingly, the 'paths' of a classical fermi particle can be thought of as 'functions' $\theta_1(t), \ldots, \theta_n(t)$, $t_0 \leq t \leq t_1$, with anticommuting values. Naively, this means that for each $t_0 \leq t \leq t_1$ there is a copy of the independent Grassmann algebra with generators $\theta_1(t) \ldots, \theta_n(t)$.

Recall, that for a manifold M the space all maps $\mathrm{Map}(I, M)$ of the interval $I = [t_0, t_1]$ to Mcan be described as the space of all algebra homomorphisms $C^\infty(M) \to C^\infty(I)$[2]. Indeed, to a path $\gamma \in \mathrm{Map}(I, M)$ there corresponds a homomorphism $\rho_\gamma(f) = f \circ \gamma$, $f \in C^\infty(M)$. Conversely, according to a smooth version[3] of the Gelfand-Naimark theorem, every homomorphism $\varphi : C^\infty(M) \to \mathbb{R} = C^\infty(\{\text{point}\})$ is of the form $\varphi(f) = f(q)$ for some point $q \in M$. Let $\mathrm{ev}_t : C^\infty(I) \to \mathbb{R}$ be the evaluation map at a point $t \in I$, then every homomorphism $\Phi : C^\infty(M) \to C^\infty(I)$ gives a path $\gamma = \{q(t); t \in I\}$ since $\varphi_t = \mathrm{ev}_t \circ \Phi : C^\infty(M) \to \mathbb{R}$ is evaluation map at a point $q(t) \in M$.

This is a simple example of the Grothendieck's functor of points in algebraic geometry.

However, its direct application of this construction to the Grassmann algebra $\mathrm{Gr}_n = \mathbb{R}[\theta_1, \ldots, \theta_n]$ is meaningless. Indeed, since Gr_n is generated by nilpotents, every algebra homomorphism $\mathrm{Gr}_n \to C^\infty(I)$ sends all θ to 0.

To remedy this situation, for each auxiliary Grassmann algebra $W = \mathbb{R}[\eta_1, \ldots, \eta_N]$ one should consider the *W-points* of the configuration space with anticommuting coordinates $\theta_1, \ldots, \theta_n$, defined as homomorphisms of Grassmann algebras

$$\Phi : \mathbb{C}[\theta_1, \ldots, \theta_n] \to C^\infty(I) \otimes_{\mathbb{R}} W = C^\infty(I)[\eta_1, \ldots, \eta_N],$$

[2]More generally, the space of maps between two manifolds X and Y can be described as the space of all homomorphisms $C^\infty(Y) \to C^\infty(X)$.

[3]Here one should replace the Banach algebra $C(M)$ of continuous functions on M to the algebra $C^\infty(M)$, equipped with the Fréchet topology.

which sends generators $\theta_1, \dots, \theta_n$ to odd elements $\Phi(\theta_1), \dots, \Phi(\theta_n)$ of the Grassmann algebra $C^\infty(I) \otimes_{\mathbb{R}} W$. Denoting

$$\theta_k(t) \stackrel{\text{def}}{=} \Phi(\theta_k) = \sum_I f_k^I(t)\eta_I,$$

where summation goes over the subsets $I = \{i_1, \dots, i_l\} \subseteq \{1, \dots, N\}$ with odd $\#(I) = l$ and $\eta_I = \eta_{i_1} \dots \eta_{i_l}$, we can define the time derivative by the following formula

$$\dot{\theta}_k(t) = \sum_I \dot{f}_k^I(t)\eta_I.$$

In particular, we can have

$$\theta_k(t) = f_k^1(t)\eta_1 + \cdots + f_k^N(t)\eta_N,$$

and

$$\dot{\theta}_k(t) = \dot{f}_k^1(t)\eta_1 + \cdots + \dot{f}_k^N(t)\eta_N.$$

To emphasize that Grassmann functions $\theta_j(t)$ are 'real-valued', we assume that Grassmann algebra W is the set of fixed points in a Grassmann algebra over $\mathbb{C}$ with involution, which we denote by the same symbol as complex conjugate. Thus for $\eta_I = \eta_{i_1} \dots \eta_{i_l}$ we have

$$\bar{\eta}_I = \begin{cases} (-1)^{\frac{l-1}{2}}\eta_I, & l \text{ is odd}, \\ (-1)^{\frac{l}{2}}\eta_I, & l \text{ is even}. \end{cases} \tag{9.29}$$

Then it follows from (9.29) that $\theta_k(t)$ are 'real-valued', $\bar{\theta}_k(t) = \theta_k(t)$, provided functions $f_k^I(t)$ are real-valued for $l \equiv 1 \bmod 4$, and have pure imaginary values for $l \equiv 3 \bmod 4$. Moreover, it also follows from (9.29) that functions $i\theta_k(t)\dot{\theta}_k(t)$ are real-valued.

Thus we can consider analogs of the Lagrangian 'function' — an even real function $L(\boldsymbol{\theta}, \dot{\boldsymbol{\theta}})$, the action functional

$$S(\boldsymbol{\theta}, \dot{\boldsymbol{\theta}}) = \int_{t_0}^{t_1} L(\boldsymbol{\theta}(t), \dot{\boldsymbol{\theta}}(t))dt,$$

and the Euler-Lagrange equations of motion

$$\frac{\partial L}{\partial \theta_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\theta}_i} = 0, \quad i = 1, \dots, n. \tag{9.30}$$

Correspondingly, one formally defines conjugated momenta

$$\pi^i = \frac{\partial L}{\partial \dot{\theta}_i}$$

and introduces the classical Hamiltonian by the Legendre transform

$$H(\boldsymbol{\pi}, \boldsymbol{\theta}) = \dot{\boldsymbol{\theta}}\boldsymbol{\pi} - L,$$

where $\boldsymbol{\pi} = (\pi^1, \dots, \pi^n)$ and $\dot{\boldsymbol{\theta}}\boldsymbol{\pi} = \dot{\theta}_1\pi^1 + \dots + \dot{\theta}_n\pi^n$. Note that in comparison with the formula (1.9), we choose a different ordering of the analog of $\boldsymbol{p}\dot{\boldsymbol{q}}$ term. Then it follows from (9.22), that this choice guarantees that the Euler-Lagrange equations (9.30) are equivalent to Hamilton's equations with the Poisson bracket (9.25) with $c = 1$. According to (9.27), we obtain canonical Hamilton equations for anticommuting variables:

$$\begin{aligned} \dot{\pi}^i &= -\frac{\partial H}{\partial \theta_i}, \\ \dot{\theta}_i &= -\frac{\partial H}{\partial \pi^i}. \end{aligned} \tag{9.31}$$

Note the difference in signs for the second equations in (9.31) and in (1.10).

Instead of proving these general results, we illustrate them by considering two basic examples.

Example 9.1 (Free fermion particle). In case of one degree of freedom the Lagrangian has the following form:

$$L = i\theta\dot{\theta}$$

and is real-valued.The Euler Lagrange equation gives (note the negative sign when we compute $\partial L/\partial\dot{\theta}$)

$$\frac{\partial L}{\partial \theta} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\theta}} = i\left(\dot{\theta} - \frac{d}{dt}(-\theta)\right) = 2i\dot{\theta} = 0,$$

so $\theta(t)$ is constant. Correspondingly,

$$\pi = \frac{\partial L}{\partial \dot{\theta}} = -i\theta$$

and

$$H = \dot{\theta}\pi - L = 0.$$

Thus Hamilton equations (9.31) also show that classical trajectories are constant maps. Also note that canonical Poisson bracket $\{\pi, \theta\} = 1$ gives $\{\theta, \theta\} = i$, which corresponds to the bracket (9.24), where $n = 1$ and $c = i$.

In case of several degrees of freedom we have

$$L(\boldsymbol{\theta}, \dot{\boldsymbol{\theta}}) = i\sum_{k=1}^{n} \theta_k\dot{\theta}_k,$$

and, as before, $H = 0$.

Example 9.2 (Fermion harmonic oscillator). We have seen in Section 9.1, that fermion analogs of position and momentum operators, self-adjoint operators Q and P given by formula (9.13), satisfy anticommutation relations (9.14). In the semi-classical limit $\hbar \to 0$ these operators turn into real Grassmann variables θ_1 and θ_2. Extending the correspondence principle (see Remark 3.1) to fermions, we state that in the limit $\hbar \to 0$ the anticommutator times $i/\hbar$, turns into the graded Poisson bracket. Thus the Grassmann algebra $\mathrm{Gr}_2 = \mathbb{C}[\theta_1, \theta_2]$ with an involution $\bar{\theta}_1 = \theta_1, \bar{\theta}_2 = \theta_2$ comes equipped with the Poisson brackets

$$\{\theta_1, \theta_1\} = \{\theta_2, \theta_2\} = i \quad \text{and} \quad \{\theta_1, \theta_2\} = 0$$

— the Poisson structure given by formula (9.24) for $n = 2$ and $c = i$.

Now in analogy with (5.4) (where $m = 1$ and $\omega = 1$), we put

$$\theta = \frac{1}{\sqrt{2}}(\theta_1 + i\theta_2) \quad \text{and} \quad \bar{\theta} = \frac{1}{\sqrt{2}}(\theta_1 - i\theta_2)$$

and consider the Grassmann algebra $\mathbb{C}[\theta, \bar{\theta}]$ with natural involution and with the Poisson bracket

$$\{\theta, \theta\} = \{\bar{\theta}, \bar{\theta}\} = 0 \quad \text{and} \quad \{\theta, \bar{\theta}\} = i. \tag{9.32}$$

As in (5.8), we define the Lagrangian for the the classical fermion harmonic oscillator to be

$$L = i\bar{\theta}\dot{\theta} - \omega\bar{\theta}\theta. \tag{9.33}$$

As in Remark 5.1, we see that corresponding Euler-Lagrange equations are

$$\dot{\theta} = -i\omega\theta, \quad \textit{and} \quad \dot{\bar{\theta}} = i\omega\bar{\theta}, \tag{9.34}$$

and they have exactly the same form as equations (5.6) for the commutative case. Moreover, we have

$$\pi = \frac{\partial L}{\partial \dot{\theta}} = -i\bar{\theta},$$

and canonical Poisson brackets $\{\pi, \theta\} = 1$ and $\{\pi, \pi\} = \{\theta, \theta\} = 0$ give brackets (9.32). A the same time, classical Hamiltonian is given by the Legendre transform

$$H = \dot{\theta}\pi - L = \omega\bar{\theta}\theta, \tag{9.35}$$

and corresponding Hamilton equations reproduce the Euler-Lagrange equations (9.34). Indeed, using graded Leibniz rule, we obtain

$$\dot{\theta} = \{H, \theta\} = \omega\{\bar{\theta}\theta, \theta\} = -\omega\theta\{\bar{\theta}, \theta\} = -i\omega\theta,$$
$$\dot{\bar{\theta}} = \{H, \bar{\theta}\} = \omega\{\bar{\theta}\theta, \bar{\theta}\} = \omega\bar{\theta}\{\theta, \bar{\theta}\} = i\omega\bar{\theta}.$$

PROBLEM 9.3. Prove all results in Section 9.3.

9.4. Quantum fermion harmonic oscillator

It is very easy to quantize the classical fermion harmonic oscillator — the Hamiltonian system with the phase space $\mathbb{C}[\theta, \bar{\theta}]$ equipped with Poisson brackets (9.32) and the Hamiltonian (9.35). Namely, according to the correspondence principle, the Poisson bracket $\{\ ,\ \}$ is replaced by the anticommutator $[\ ,\ ]_+$ times $\dfrac{\hbar}{i}$, and we obtain the operators $\psi = \hat{\theta}$ and $\bar{\psi} = \hat{\bar{\theta}}$, satisfying anticommutation relations

$$[\psi, \psi]_+ = [\bar{\psi}, \bar{\psi}]_+ = 0 \quad \text{and} \quad [\bar{\psi}, \psi]_+ = \hbar I$$

and the involution $\psi^* = \bar{\psi}$. It immediately follows from Theorem 9.1 that irreducible representation of these relations is realized in the Hilbert space $\mathscr{H}_F = \mathbb{C}^2$ and

$$\psi = \sqrt{\hbar}\, a,\ \bar{\psi} = \sqrt{\hbar}\, a^*.$$

For consistent quantization of the classical Hamiltonian (9.35), we observe that the problem of ordering does not arise, if we rewrite it in the following form:

$$H = \tfrac{1}{2}\omega(\bar{\theta}\theta + \theta\bar{\theta}).$$

Thus for the quantum Hamiltonian we unambiguously obtain

$$\hat{H} = \tfrac{1}{2}\omega(\bar{\psi}\psi + \psi\bar{\psi}) = \omega\left(\bar{\psi}\psi - \tfrac{\hbar}{2}I\right) = \tfrac{1}{2}\omega\hbar\sigma_3,$$

which is exactly the Hamiltonian (9.6)!

CHAPTER 10

Fermion path integrals

10.1. Berezin integral

Though there is no measure theory for anticommuting variables, there is an analog of the definite integral.

Definition. The integral on a Grassmann algebra Gr_n with an ordered set of generators $\theta_1, \dots, \theta_n$ (*Berezin integral*) is a linear functional $B : \mathrm{Gr}_n \to \mathbb{C}$, defined by

$$B(f) = f^{12\dots n},$$

where

$$f = \sum_{k=0}^{n} \sum_{1\leq i_1<\dots<i_k\leq n} f^{i_1\dots i_k}\theta_{i_1}\dots\theta_{i_k} \in \mathrm{Gr}_n.$$

It is traditional to write the Berezin integral in the form

$$B(f) = \int f(\boldsymbol{\theta})d\theta_1 \dots d\theta_n,$$

where $\boldsymbol{\theta} = (\theta_1, \dots, \theta_n)$, as if $f = f(\theta_1, \dots, \theta_n)$ was actually a "function of anticommuting variables". It follows from definition of the partial derivatives, that actually

$$\int f(\boldsymbol{\theta})d\theta_1 \dots d\theta_n = \frac{\partial}{\partial\theta_n} \cdots \frac{\partial}{\partial\theta_1} f,$$

which implies

$$\int \frac{\partial}{\partial\theta_i} f(\boldsymbol{\theta})d\theta_1 \dots d\theta_n = 0.$$

Applying this to the product fg and using graded Leibniz rule and (9.21), we get the following integration by parts formula for the Berezin integral:

$$\int \Big(f\frac{\partial}{\partial\theta_i}\Big)(\boldsymbol{\theta})g(\boldsymbol{\theta})\, d\theta_1 \dots d\theta_n = \int f(\boldsymbol{\theta})\Big(\frac{\partial}{\partial\theta_i}g\Big)(\boldsymbol{\theta})d\theta_1 \dots d\theta_n \tag{10.1}$$

for homogeneous $f, g \in \mathrm{Gr}_n$.

REMARK 10.1. The Berezin integral is not an integral in the sense of integration theory. It is defined as a linear functional on a Grassmann algebra Gr_n and it depends on the ordering of the generators $\theta_1, \dots, \theta_n$ of Gr_n, which is symbolized by $d\theta_1 \dots d\theta_n$. For each $\sigma \in \mathrm{Sym}_n$,

$$\int f(\boldsymbol{\theta}) d\theta_1 \dots d\theta_n = (-1)^{\varepsilon(\sigma)} \int f(\boldsymbol{\theta}) d\theta_{\sigma(1)} \dots d\theta_{\sigma(n)},$$

where $\varepsilon(\sigma)$ is the parity of a permutation σ.

REMARK 10.2. Using the embeddings $\mathrm{Gr}_k \subset \mathrm{Gr}_n$ for $k \leq n$, physicists usually define the Berezin integral as a "repeated integral" starting from the following "one-dimensional integrals":

$$\int d\theta_i = 0, \quad \int \theta_i d\theta_i = 1, \quad i = 1, \dots, n.$$

LEMMA 10.1 (Change of variables for Berezin integral). *Let $\theta_1, \dots, \theta_n$ and $\tilde{\theta}_1, \dots, \tilde{\theta}_n$ be two sets of generators of the Grassmann algebra Gr_n, related by $\theta_i = \sum_{j=1}^n a_{ij}\tilde{\theta}_j$, where the $n \times n$ matrix $A = \{a_{ij}\}_{i,j=1}^n$ is non-degenerate. Then*

$$\int f(\boldsymbol{\theta}) d\theta_1 \dots d\theta_n = \frac{1}{\det A} \int \tilde{f}(\tilde{\boldsymbol{\theta}}) d\tilde{\theta}_1 \dots d\tilde{\theta}_n,$$

where $\tilde{f}(\tilde{\boldsymbol{\theta}}) = f(\boldsymbol{\theta}) = f(\sum_{j=1}^n a_{1j}\tilde{\theta}_j, \dots, \sum_{j=1}^n a_{nj}\tilde{\theta}_j)$.

PROOF. By multi-linear algebra, $\tilde{f}^{12\dots n} = f^{12\dots n} \det A$. □

REMARK 10.3. According to Lemma 10.1, the "density" $d\theta_1 \dots d\theta_n$ has the transformation law

$$d\theta_1 \dots d\theta_n = \frac{1}{\det A} d\tilde{\theta}_1 \dots d\tilde{\theta}_n \tag{10.2}$$

under the change of variables $\theta_i = \sum_{j=1}^n a_{ij}\tilde{\theta}_j$. This differs from the usual change of variables formula for the Lebesgue integral

$$\int_{\mathbb{R}^n} f(x_1, \dots, x_n) dx_1 \dots dx_n = |\det A| \int_{\mathbb{R}^n} \tilde{f}(y_1, \dots, y_n) dy_1 \dots dy_n, \tag{10.3}$$

or $dx_1 \dots dx_n = |\det A| dy_1 \dots dy_n$, where $x_i = \sum_{j=1}^n a_{ij} y_j$. Of course, the Berezin integral is rather a multiple derivative than the integral with respect to a measure, which explains this profound difference.

Let $A = \{a_{ij}\}_{i,j=1}^n$ be an $n \times n$ skew-symmetric matrix. For even $n = 2m$ its *Pfaffian* $\mathrm{Pf}(A)$ is defined by

$$\mathrm{Pf}(A) = \frac{1}{m!2^m} \sum_{\sigma \in \mathrm{Sym}_n} (-1)^{\varepsilon(\sigma)} a_{\sigma(1)\sigma(2)} \dots a_{\sigma(n-1)\sigma(n)},$$

where $\varepsilon(\sigma)$ is the parity of a permutation σ. By definition, $\mathrm{Pf}(A) = 0$ when n is odd.

PROPOSITION 10.1 (Gaussian integration for anticommuting variables). *Let* $A = \{a_{ij}\}_{i,j=1}^n$ *be an* $n \times n$ *skew-symmetric matrix. Then*

(i)

$$\int \exp\left\{ \tfrac{1}{2} \sum_{i,j=1}^n a_{ij}\theta_i\theta_j \right\} d\theta_1 \dots d\theta_n = \mathrm{Pf}(A).$$

(ii) *For any non-degenerate* $n \times n$ *matrix* C

$$\mathrm{Pf}(CAC^t) = \mathrm{Pf}(A) \det C.$$

(iii)

$$\mathrm{Pf}(A)^2 = \det A.$$

PROOF. Part (i) obviously holds for odd n since the integrand is an even element of Gr_n. By the definition of the Pfaffian, we get for $n = 2m$,

$$\frac{1}{m!2^m} \Big(\sum_{i,j=1}^n a_{ij}\theta_i\theta_j \Big)^m = \mathrm{Pf}(A)\, \theta_1 \dots \theta_n,$$

and expanding the exponent into power series, we obtain

$$\int \exp\left\{ \tfrac{1}{2} \sum_{i,j=1}^n a_{ij}\theta_i\theta_j \right\} d\theta_1 \dots d\theta_n = \mathrm{Pf}(A) \int \theta_1 \dots \theta_n \, d\theta_1 \dots d\theta_n = \mathrm{Pf}(A).$$

Part (ii) follows from part (i) and Lemma 10.1. Part (iii) is a classical result, which can be proved by the Berezin integral as follows. Suppose first that A is real-valued. There exists an orthogonal matrix C with determinant 1 such that

$$CAC^{-1} = \begin{pmatrix} 0 & \lambda_1 & \cdots & 0 & 0 \\ -\lambda_1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \lambda_m \\ 0 & 0 & \cdots & -\lambda_m & 0 \end{pmatrix}$$

is a block-diagonal matrix. Using part (ii) with this matrix C, we obtain

$$\mathrm{Pf}(A) = \int e^{\lambda_1\tilde{\theta}_1\tilde{\theta}_2+\cdots+\lambda_m\tilde{\theta}_{2m-1}\tilde{\theta}_{2m}} d\tilde{\theta}_1 \dots d\tilde{\theta}_{2m} = \lambda_1 \dots \lambda_m,$$

so that $\mathrm{Pf}(A)^2 = \det A$. This relation holds for complex-valued A, since both sides are polynomials in variables a_{ij}, $1 \leq i < j \leq n$, which coincide for real a_{ij}. $\square$

REMARK 10.4. We also have

$$\exp\left\{\tfrac{1}{2}\sum_{i,j=1}^{n} a_{ij}\theta_i\theta_j\right\} = \exp\left\{\sum_{1\leq i<j\leq n} a_{ij}\theta_i\theta_j\right\} = \prod_{1\leq i<j\leq n}(1 + a_{ij}\theta_i\theta_j),$$

which gives a representation

$$\mathrm{Pf}(A) = \sum_{\sigma\in\Pi_n}(-1)^{\varepsilon(\sigma)} a_{\sigma(1)\sigma(2)} \dots a_{\sigma(n-1)\sigma(n)},$$

where Π_n consists of permutations $\sigma \in \mathrm{Sym}_n$ satisfying $\sigma(2i-1) < \sigma(2i)$ for $i = 1, \dots, m$.

For a Grassmann algebra $\mathrm{Gr}_{2n} = \mathbb{C}[\theta_1, \dots, \theta_n, \bar{\theta}_1, \dots, \bar{\theta}_n]$ with $2n$ generators denote by $\int d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}} = \int d\theta_1 d\bar{\theta}_1 \dots d\theta_n d\bar{\theta}_n$ the corresponding Berezin integral,

$$\int f(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}} = \frac{\partial}{\partial\bar{\theta}_n}\frac{\partial}{\partial\theta_n} \cdots \frac{\partial}{\partial\bar{\theta}_1}\frac{\partial}{\partial\theta_1} f, \quad f \in \mathbb{C}[\theta_1, \dots, \theta_n, \bar{\theta}_1, \dots, \bar{\theta}_n].$$

LEMMA 10.2. *For any $n \times n$ matrix $A = \{a_{ij}\}_{i,j=1}^n$,*

$$\int \exp\left\{\sum_{i,j=1}^{n} a_{ij}\theta_i\bar{\theta}_j\right\} d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}} = \det A.$$

PROOF. It follows from the definition of a matrix determinant that

$$\frac{1}{n!}\left(\sum_{i,j=1}^{n} a_{ij}\theta_i\bar{\theta}_j\right)^n = \det A\, \theta_1\bar{\theta}_1 \dots \theta_n\bar{\theta}_n. \tag{10.4}$$ $\square$

Recall that an involution on a Grassmann algebra Gr_n over $\mathbb{C}$ is a complex anti-linear mapping $\mathrm{Gr}_n \ni f \mapsto f^* \in \mathrm{Gr}_n$ satisfying $(f^*)^* = f$ and $(fg)^* = g^* f^*$ for all $f, g \in \mathrm{Gr}_n$. The Grassmann algebra $\mathbb{C}[\theta_1, \dots, \theta_n, \bar{\theta}_1, \dots, \bar{\theta}_n]$

has a natural involution defined on generators by $(\theta_1)^* = \bar{\theta}_1, (\bar{\theta}_1)^* = \theta_1, \dots, (\theta_n)^* = \bar{\theta}_n, (\bar{\theta}_n)^* = \theta_n$. In particular, for

$$f(\boldsymbol{\theta}) = \sum_{k=0}^{n} \sum_{1 \le i_1 < \cdots < i_k \le n} f^{i_1 \dots i_k}\, \theta_{i_1} \dots \theta_{i_k} \in \mathrm{Gr}_n \subset \mathrm{Gr}_{2n}$$

we have

$$f(\boldsymbol{\theta})^* = \overline{f(\boldsymbol{\theta})} = \sum_{k=0}^{n} \sum_{1 \le i_1 < \cdots < i_k \le n} \overline{f^{i_1 \dots i_k}}\, \bar{\theta}_{i_k} \dots \bar{\theta}_{i_1} \in \mathrm{Gr}_{2n}.$$

The next lemma expresses the inner product on the Grassmann algebra Gr_n, introduced in the previous section, in terms of the Berezin integral.

Lemma 10.3. *The standard inner product* (9.23) *on the Grassmann algebra* $\mathrm{Gr}_n = \mathbb{C}[\theta_1, \dots, \theta_n]$ *is given by the following Berezin integral over the Grassmann algebra* $\mathrm{Gr}_{2n} = \mathbb{C}[\theta_1, \dots, \theta_n, \bar{\theta}_1, \dots, \bar{\theta}_n]$*:*

$$(f_1, f_2) = \int f_1(\boldsymbol{\theta})\overline{f_2(\boldsymbol{\theta})} e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}}, \tag{10.5}$$

where $\bar{\boldsymbol{\theta}}\boldsymbol{\theta} = \bar{\theta}_1\theta_1 + \cdots + \bar{\theta}_n\theta_n$.

Proof. Put $f_1(\boldsymbol{\theta}) = \theta_{i_1} \dots \theta_{i_k}$ and $f_2(\boldsymbol{\theta}) = \theta_{j_1} \dots \theta_{j_l}$. It is clear that the integral (10.5) is 0, unless $k = l$ and $i_1 = j_1, \dots, i_k = j_k$, in which case we have

$$\begin{aligned}(\theta_{i_1} \dots \theta_{i_k}, \theta_{i_1} \dots \theta_{i_k}) &= \int \theta_{i_1} \dots \theta_{i_k} \bar{\theta}_{i_k} \dots \bar{\theta}_{i_1} e^{-(\bar{\theta}_1\theta_1 + \cdots + \bar{\theta}_n\theta_n)} d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}} \\ &= \int \theta_{i_1}\bar{\theta}_{i_1} \dots \theta_{i_k}\bar{\theta}_{i_k} \prod_{i=1}^{n} (1 + \theta_i\bar{\theta}_i) d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}} \\ &= \int \theta_1\bar{\theta}_1 \dots \theta_n\bar{\theta}_n\, d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}} = 1. \qquad \square\end{aligned}$$

The following result was already stated in the previous section. Lemma 10.3 allows us to prove it in a way that is reminiscent of a holomorphic representation (see Section 5.2 of Chapter 5).

Corollary 10.1. *The operators* ∂_i *and* $\hat{\theta}_i$, $i = 1, \dots, n$, *are adjoint with respect to the inner product on* Gr_n.

PROOF. Using Lemma 10.3, formulas $\partial_i\overline{f(\boldsymbol{\theta})} = 0$, $\partial_i e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}} = \bar{\theta}_i e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}}$, (9.21) and integration by parts formula (10.1), we obtain

$$\begin{aligned}(\partial_i f_1, f_2) &= \int \partial_i f_1(\boldsymbol{\theta})\overline{f_2(\boldsymbol{\theta})}e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}}d\boldsymbol{\theta}d\bar{\boldsymbol{\theta}} \\ &= -(-1)^{|f_1|+|f_2|}\int f_1(\boldsymbol{\theta})\overline{f_2(\boldsymbol{\theta})}\,\bar{\theta}_i e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}}d\boldsymbol{\theta}d\bar{\boldsymbol{\theta}} \\ &= -(-1)^{|f_1|+|f_2|}\int f_1(\boldsymbol{\theta})\overline{\theta_i f_2(\boldsymbol{\theta})}e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}}d\boldsymbol{\theta}d\bar{\boldsymbol{\theta}} \\ &= (f_1, \hat{\theta}_i f_2),\end{aligned}$$

since the last integral and $(f_1, \hat{\theta}_i f_2)$ are both 0 unless $|f_1| + |f_2|$ is odd. □

PROBLEM 10.1. Prove formula (10.4).

PROBLEM 10.2. Evaluate the Berezin integral

$$\int \exp\Big\{\tfrac{1}{2}\sum_{i,j=1}^{n} a_{ij}\theta_i\theta_j + \sum_{k=1}^{n}\eta_k\theta_k\Big\}d\theta_1\dots d\theta_n,$$

where $\eta_1,\dots,\eta_n$ are Grassmann variables.

10.2. Wick and matrix symbols

Here we describe simple calculus of Wick and matrix symbols of operators in the fermion Hilbert space $\mathscr{H}_F$. It is convenient to work in anti-holomorphic representation by using $\mathscr{H}_F = \mathbb{C}[\bar{\theta}_1,\dots,\bar{\theta}_n]$ as the fermion Hilbert space with the annihilation and creation operators

$$a_k^* = \hat{\bar{\theta}}_k \quad \text{and} \quad a_k = \frac{\partial}{\partial\bar{\theta}_k}, \quad k = 1,\dots,n. \tag{10.6}$$

The inner product (10.5) takes the form

$$(f_1, f_2) = \int f_1(\bar{\boldsymbol{\theta}})\overline{f_2(\bar{\boldsymbol{\theta}})}e^{-\boldsymbol{\theta}\bar{\boldsymbol{\theta}}}d\bar{\boldsymbol{\theta}}d\boldsymbol{\theta}, \tag{10.7}$$

and the monomials

$$f_I(\bar{\boldsymbol{\theta}}) = \bar{\theta}_{i_1}\dots\bar{\theta}_{i_k}, \quad 1 \le i_1 < \dots < i_k \le n,$$

parametrized by subsets $I = \{i_1,\dots,i_k\} \subseteq \{1,\dots,n\}$, form an orthonormal basis in $\mathscr{H}_F$.

DEFINITION. A *matrix symbol* of an operator $A:\mathscr{H}_F\to\mathscr{H}_F$ is an element $\tilde{A}(\bar{\boldsymbol{\theta}},\boldsymbol{\theta})\in\mathbb{C}[\bar{\theta}_1,\dots,\bar{\theta}_n,\theta_1,\dots,\theta_n]$, defined by

$$\begin{aligned}\tilde{A}(\bar{\boldsymbol{\theta}},\boldsymbol{\theta}) &= \sum_{I,J}(Af_J,f_I)f_I(\bar{\boldsymbol{\theta}})\overline{f_J(\bar{\boldsymbol{\theta}})}\\ &= \sum_{I,J}(Af_J,f_I)\,\bar{\theta}_{i_1}\dots\bar{\theta}_{i_k}\theta_{j_l}\dots\theta_{j_1}.\end{aligned}$$

Here summation goes over all subsets $I=\{i_1,\dots,i_k\}$ and $J=\{j_1,\dots,j_l\}$ of the set $\{1,\dots,n\}$, and as in Section 10.1, we denote by $\overline{f(\bar{\boldsymbol{\theta}})}$ a natural involution on the Grassmann algebra $\mathbb{C}[\bar{\theta}_1,\dots,\bar{\theta}_n,\theta_1,\dots,\theta_n]$,

$$\overline{f_J(\bar{\boldsymbol{\theta}})}=\theta_{j_l}\dots\theta_{j_1}\quad\text{for}\quad f_J(\bar{\boldsymbol{\theta}})=\bar{\theta}_{j_1}\dots\bar{\theta}_{j_l}.$$

According to Proposition 9.1, $C_{2n}\simeq\operatorname{End}(\mathscr{H}_F)$, so that every operator $A:\mathscr{H}_F\to\mathscr{H}_F$ can be uniquely represented in a *Wick normal form* as follows:

$$A=\sum_{I,J}K_{IJ}\,a^*_{i_1}\dots a^*_{i_k}a_{j_1}\dots a_{j_l}.$$

DEFINITION. A *Wick symbol* of an operator $A:\mathscr{H}_F\to\mathscr{H}_F$ is an element $A(\bar{\boldsymbol{\theta}},\boldsymbol{\theta})\in\mathbb{C}[\bar{\theta}_1,\dots,\bar{\theta}_n,\theta_1,\dots,\theta_n]$, defined by

$$A(\bar{\boldsymbol{\theta}},\boldsymbol{\theta})=\sum_{I,J}K_{IJ}\,\bar{\theta}_{i_1}\dots\bar{\theta}_{i_k}\theta_{j_1}\dots\theta_{j_l}.$$

To matrix and Wick symbols $\tilde{A}(\bar{\boldsymbol{\theta}},\boldsymbol{\theta})$ and $A(\bar{\boldsymbol{\theta}},\boldsymbol{\theta})$ of an operator A one canonically associates elements $\tilde{A}(\bar{\boldsymbol{\theta}},\boldsymbol{\alpha})$, $A(\bar{\boldsymbol{\theta}},\boldsymbol{\alpha})$ and $\tilde{A}(\bar{\boldsymbol{\alpha}},\boldsymbol{\theta})$, $A(\bar{\boldsymbol{\alpha}},\boldsymbol{\theta})$ in the larger Grassmann algebra

$$\mathbb{C}[\boldsymbol{\alpha},\bar{\boldsymbol{\alpha}},\boldsymbol{\theta},\bar{\boldsymbol{\theta}}]=\mathbb{C}[\alpha_1,\dots,\alpha_n,\bar{\alpha}_1,\dots,\bar{\alpha}_n,\theta_1,\dots,\theta_n\bar{\theta}_1,\dots,\bar{\theta}_n],$$

by replacing, correspondingly, θ_i by α_i and $\bar{\theta}_i$ by $\bar{\alpha}_i$. The *incomplete Berezin integral* $\int d\boldsymbol{\alpha}d\bar{\boldsymbol{\alpha}}$ on $\mathbb{C}[\boldsymbol{\alpha},\bar{\boldsymbol{\alpha}},\boldsymbol{\theta},\bar{\boldsymbol{\theta}}]$ is defined by

$$\int f d\boldsymbol{\alpha}d\bar{\boldsymbol{\alpha}}=\frac{\partial}{\partial\bar{\alpha}_n}\frac{\partial}{\partial\alpha_n}\dots\frac{\partial}{\partial\bar{\alpha}_1}\frac{\partial}{\partial\alpha_1}f,\quad f\in\mathbb{C}[\boldsymbol{\alpha},\bar{\boldsymbol{\alpha}},\boldsymbol{\theta},\bar{\boldsymbol{\theta}}],$$

and has the property

$$\int h(\boldsymbol{\theta},\bar{\boldsymbol{\theta}})g(\boldsymbol{\alpha},\bar{\boldsymbol{\alpha}})d\boldsymbol{\alpha}d\bar{\boldsymbol{\alpha}}=h(\boldsymbol{\theta},\bar{\boldsymbol{\theta}})\int g(\boldsymbol{\alpha},\bar{\boldsymbol{\alpha}})d\boldsymbol{\alpha}d\bar{\boldsymbol{\alpha}}. \tag{10.8}$$

We will also use the incomplete Berezin integral $\int d\bar{\boldsymbol{\theta}} d\boldsymbol{\theta}$, defined by

$$\int f d\bar{\boldsymbol{\theta}} d\boldsymbol{\theta} = \frac{\partial}{\partial\theta_n}\frac{\partial}{\partial\bar{\theta}_n}\cdots\frac{\partial}{\partial\theta_1}\frac{\partial}{\partial\bar{\theta}_1} f, \quad f \in \mathbb{C}[\boldsymbol{\alpha}, \bar{\boldsymbol{\alpha}}, \boldsymbol{\theta}, \bar{\boldsymbol{\theta}}].$$

The next result shows that the matrix symbol of an operator A in $\mathscr{H}_F$, which is just a $2^n \times 2^n$ matrix, can be considered as an integral kernel in anticommuting variables!

LEMMA 10.4. *Let $\tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta})$ be the matrix symbol of an operator A in $\mathscr{H}_F$. Then for every $f(\bar{\boldsymbol{\theta}}) \in \mathscr{H}_F$,*

$$(Af)(\bar{\boldsymbol{\theta}}) = \int \tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\alpha}) f(\bar{\boldsymbol{\alpha}}) e^{-\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}} d\boldsymbol{\alpha} d\bar{\boldsymbol{\alpha}}. \tag{10.9}$$

PROOF. It is sufficient to verify (10.9) for $f = f_K$, where $K = \{k_1, \dots, k_m\} \subseteq \{1, \dots, n\}$. Using (10.8) and Lemma 10.3, we get

$$\begin{aligned}\int \tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\alpha}) f_K(\bar{\boldsymbol{\alpha}}) e^{-\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}} d\boldsymbol{\alpha} d\bar{\boldsymbol{\alpha}} &= \sum_{I,J} (Af_J, f_I) f_I(\bar{\boldsymbol{\theta}}) \int \overline{f_J(\bar{\boldsymbol{\alpha}})} f_K(\bar{\boldsymbol{\alpha}}) e^{-\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}} d\boldsymbol{\alpha} d\bar{\boldsymbol{\alpha}} \\ &= \sum_I (Af_K, f_I) f_I(\bar{\boldsymbol{\theta}}) = (Af_K)(\bar{\boldsymbol{\theta}}).\end{aligned}$$

□

Next, we introduce Grassmann coherent states. Put $\Phi_{\boldsymbol{\alpha}}(\bar{\boldsymbol{\theta}}) = e^{\bar{\boldsymbol{\theta}}\boldsymbol{\alpha}}$, where $\boldsymbol{\alpha}$ are auxiliary Grassmann parameters. Expanding the exponential function, it is easy to see that

$$\begin{aligned}\Phi_{\boldsymbol{\alpha}}(\bar{\boldsymbol{\theta}}) &= \prod_{i=1}^n (1 + \bar{\theta}_i \alpha_i) = \sum_I f_I(\bar{\boldsymbol{\theta}}) \overline{f_I(\bar{\boldsymbol{\alpha}})}, \\ \Phi_{-\boldsymbol{\alpha}}(\bar{\boldsymbol{\theta}}) &= \prod_{i=1}^n (1 + \alpha_i \bar{\theta}_i) = \sum_I \overline{f_I(\bar{\boldsymbol{\alpha}})} f_I(\bar{\boldsymbol{\theta}}),\end{aligned} \tag{10.10}$$

so coherent states $\Phi_{\boldsymbol{\alpha}} \in \mathbb{C}[\boldsymbol{\alpha}, \bar{\boldsymbol{\alpha}}, \boldsymbol{\theta}, \bar{\boldsymbol{\theta}}]$ satisfy

$$a_k \Phi_{\boldsymbol{\alpha}} = \alpha_k \Phi_{\boldsymbol{\alpha}} \quad k = 1, \dots, n, \tag{10.11}$$

(recall that $a_k = \dfrac{\partial}{\partial\bar{\theta}_k}$). Moreover, $\Phi_{\boldsymbol{\alpha}}(\bar{\boldsymbol{\theta}})$, as a function of $\boldsymbol{\alpha}$, plays the role of delta function:

$$\int \Phi_{\boldsymbol{\alpha}}(\bar{\boldsymbol{\theta}}) f(\boldsymbol{\theta}) e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}} = f(\boldsymbol{\alpha}), \tag{10.12}$$

$$\int \Phi_{\bar{\boldsymbol{\alpha}}}(\boldsymbol{\theta}) f(\bar{\boldsymbol{\theta}}) e^{-\boldsymbol{\theta}\bar{\boldsymbol{\theta}}} d\bar{\boldsymbol{\theta}} d\boldsymbol{\theta} = f(\bar{\boldsymbol{\alpha}}). \tag{10.13}$$

Indeed, it is sufficient to verify these equations for $f = f_J$. Formula (10.12) follows from the first equation in (10.10), since functions f_I form an orthonormal basis in Gr_n and $f_I(\bar{\boldsymbol{\theta}})\overline{f_I(\bar{\boldsymbol{\alpha}})} = \overline{f_I(\boldsymbol{\theta})}f_I(\boldsymbol{\alpha})$, while formula (10.13) follows from the second equation in (10.10), since $\Phi_{\bar{\boldsymbol{\alpha}}}(\boldsymbol{\theta}) = \overline{\Phi_{-\boldsymbol{\alpha}}(\bar{\boldsymbol{\theta}})}$. Equation (10.13) can also be written as

$$(f, \Phi_{-\boldsymbol{\alpha}}) = f(\bar{\boldsymbol{\alpha}}), \tag{10.14}$$

which immediately implies that

$$(\Phi_{\boldsymbol{\alpha}}, \Phi_{-\boldsymbol{\alpha}}) = \Phi_{\boldsymbol{\alpha}}(\bar{\boldsymbol{\alpha}}) = e^{\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}}. \tag{10.15}$$

It is also easy to express the matrix symbol of an operator in terms of the coherent states.

LEMMA 10.5. *Let $\tilde{A}(\bar{\boldsymbol{\alpha}}, \boldsymbol{\alpha})$ be the matrix symbol of an operator A in $\mathscr{H}_F$. Then*

$$\tilde{A}(\bar{\boldsymbol{\alpha}}, \boldsymbol{\alpha}) = (A\Phi_{\boldsymbol{\alpha}}, \Phi_{-\boldsymbol{\alpha}}).$$

PROOF. Using Lemma 10.9 and formula (10.12), we obtain

$$(A\Phi_{\boldsymbol{\alpha}})(\bar{\boldsymbol{\theta}}) = \int \tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\eta})\Phi_{\boldsymbol{\alpha}}(\bar{\boldsymbol{\eta}})e^{-\bar{\boldsymbol{\eta}}\boldsymbol{\eta}}d\boldsymbol{\eta}d\bar{\boldsymbol{\eta}} = \tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\alpha}),$$

and it follows from (10.14) that

$$(A\Phi_{\boldsymbol{\alpha}}, \Phi_{-\boldsymbol{\alpha}}) = \tilde{A}(\bar{\boldsymbol{\alpha}}, \boldsymbol{\alpha}). \qquad \square$$

The next result is an important relation between matrix and Wick symbols.

LEMMA 10.6. *The matrix and Wick symbols of an operator A in $\mathscr{H}_F$ are related by*

$$\tilde{A}(\bar{\boldsymbol{\alpha}}, \boldsymbol{\alpha}) = e^{\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}}A(\bar{\boldsymbol{\alpha}}, \boldsymbol{\alpha}).$$

Moreover, $\tilde{A}(\bar{\boldsymbol{\alpha}}, \boldsymbol{\theta}) = e^{\bar{\boldsymbol{\alpha}}\boldsymbol{\theta}}A(\bar{\boldsymbol{\alpha}}, \boldsymbol{\theta})$ and $\tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\alpha}) = e^{\bar{\boldsymbol{\theta}}\boldsymbol{\alpha}}A(\bar{\boldsymbol{\theta}}, \boldsymbol{\alpha})$.

PROOF. Representing the operator A in a Wick normal form and using Lemma 10.5 and equations (10.11) and (10.14), we obtain

$$\begin{aligned}\tilde{A}(\bar{\boldsymbol{\alpha}},\boldsymbol{\alpha}) &= (A\Phi_{\boldsymbol{\alpha}},\Phi_{-\boldsymbol{\alpha}}) \\ &= \sum_{I,J} K_{IJ}(a_{i_1}^*\dots a_{i_k}^* a_{j_1}\dots a_{j_l}\Phi_{\boldsymbol{\alpha}},\Phi_{-\boldsymbol{\alpha}}) \\ &= \sum_{I,J} K_{IJ}(a_{i_1}^*\dots a_{i_k}^* \alpha_{j_1}\dots \alpha_{j_l}\Phi_{\boldsymbol{\alpha}},\Phi_{-\boldsymbol{\alpha}}) \\ &= \sum_{I,J} K_{IJ}(a_{i_1}^*\dots a_{i_k}^*\Phi_{\boldsymbol{\alpha}},\Phi_{-\boldsymbol{\alpha}})f_J(\boldsymbol{\alpha}) \\ &= \sum_{I,J} K_{IJ}(f_I(\bar{\boldsymbol{\theta}})\Phi_{\boldsymbol{\alpha}},\Phi_{-\boldsymbol{\alpha}})f_J(\boldsymbol{\alpha}) \\ &= \sum_{I,J} K_{IJ}e^{\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}}f_I(\bar{\boldsymbol{\alpha}})f_J(\boldsymbol{\alpha}) \\ &= e^{\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}}A(\bar{\boldsymbol{\alpha}},\boldsymbol{\alpha}).\end{aligned}$$

The remaining two formulas are proved similarly. □

Thus we have shown that $2^n \times 2^n$ matrices — operators in the fermion Hilbert space $\mathscr{H}_F$ — can be considered as integral operators in anticommuting variables with the integral kernels given by the matrix or Wick symbols. Recall that the trace of an operator $A \in \operatorname{End}\mathscr{H}_F$ is

$$\operatorname{Tr} A = \sum_I (Af_I, f_I).$$

In addition, since $\mathscr{H}_F$ is naturally $\mathbb{Z}_2$ graded, we define the supertrace as

$$\operatorname{Tr}_s A = \operatorname{Tr}(-1)^N A = \sum_I (-1)^{|I|}(Af_I, f_I). \tag{10.16}$$

The next result establishes the calculus of symbols for operators in $\mathscr{H}_F$.

THEOREM 10.2. *Let A_1 and A_2 be operators in $\mathscr{H}_F$ with matrix symbols $\tilde{A}_1(\bar{\boldsymbol{\theta}},\boldsymbol{\theta})$ and $\tilde{A}_2(\bar{\boldsymbol{\theta}},\boldsymbol{\theta})$ and Wick symbols $A_1(\bar{\boldsymbol{\theta}},\boldsymbol{\theta})$ and $A_2(\bar{\boldsymbol{\theta}},\boldsymbol{\theta})$. Then the following formulas hold.*

(i) *The matrix and Wick symbols of the operator $A = A_1A_2$ are given by*

$$\tilde{A}(\bar{\boldsymbol{\theta}},\boldsymbol{\theta}) = \int \tilde{A}_1(\bar{\boldsymbol{\theta}},\boldsymbol{\alpha})\tilde{A}_2(\bar{\boldsymbol{\alpha}},\boldsymbol{\theta})e^{-\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}}d\boldsymbol{\alpha}d\bar{\boldsymbol{\alpha}},$$

$$A(\bar{\boldsymbol{\theta}},\boldsymbol{\theta}) = \int A_1(\bar{\boldsymbol{\theta}},\boldsymbol{\alpha})A_2(\bar{\boldsymbol{\alpha}},\boldsymbol{\theta})e^{-(\bar{\boldsymbol{\theta}}-\bar{\boldsymbol{\alpha}})(\boldsymbol{\theta}-\boldsymbol{\alpha})}d\boldsymbol{\alpha}d\bar{\boldsymbol{\alpha}}.$$

(ii) *The trace and supertrace of an operator A in $\mathscr{H}_F$ are given by*

$$\operatorname{Tr} A = \int \tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-\boldsymbol{\theta}\bar{\boldsymbol{\theta}}} d\bar{\boldsymbol{\theta}} d\boldsymbol{\theta} = \int A(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-2\boldsymbol{\theta}\bar{\boldsymbol{\theta}}} d\bar{\boldsymbol{\theta}} d\boldsymbol{\theta},$$
$$\operatorname{Tr}_s A = \int \tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}} = \int A(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}) d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}}.$$

Proof. Part (i) for the matrix symbols is easily proved using Lemma 10.4:

$$(A_1A_2)(f)(\bar{\boldsymbol{\theta}}) = \int \tilde{A}_1(\bar{\boldsymbol{\theta}}, \boldsymbol{\alpha})(A_2 f)(\bar{\boldsymbol{\alpha}}) e^{-\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}} d\boldsymbol{\alpha} d\bar{\boldsymbol{\alpha}}$$
$$= \int \tilde{A}_1(\bar{\boldsymbol{\theta}}, \boldsymbol{\alpha}) \int \tilde{A}_2(\bar{\boldsymbol{\alpha}}, \boldsymbol{\eta}) f(\bar{\boldsymbol{\eta}}) e^{-\bar{\boldsymbol{\eta}}\boldsymbol{\eta}} d\boldsymbol{\eta} d\bar{\boldsymbol{\eta}} e^{-\bar{\boldsymbol{\alpha}}\boldsymbol{\alpha}} d\boldsymbol{\alpha} d\bar{\boldsymbol{\alpha}}$$
$$= \int \tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\eta}) f(\bar{\boldsymbol{\eta}}) e^{-\bar{\boldsymbol{\eta}}\boldsymbol{\eta}} d\boldsymbol{\eta}.$$

The corresponding formula for the Wick symbols now follows from Lemma 10.6.

The proof of part (ii) is also straightforward. We have

$$\int \tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-\boldsymbol{\theta}\bar{\boldsymbol{\theta}}} d\bar{\boldsymbol{\theta}} d\boldsymbol{\theta} = \sum_{I,J} (Af_J, f_I) \int f_I(\bar{\boldsymbol{\theta}}) \overline{f_J(\bar{\boldsymbol{\theta}})} e^{-\boldsymbol{\theta}\bar{\boldsymbol{\theta}}} d\bar{\boldsymbol{\theta}} d\boldsymbol{\theta}$$
$$= \sum_I (Af_I, f_I) = \operatorname{Tr} A.$$

Similarly,

$$\int \tilde{A}(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}} = \sum_{I,J} (Af_J, f_I) \int f_I(\bar{\boldsymbol{\theta}}) \overline{f_J(\bar{\boldsymbol{\theta}})} e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}}$$
$$= \sum_{I,J} (Af_J, f_I) \int (-1)^{|I|\cdot|J|}\, \overline{f_J(\bar{\boldsymbol{\theta}})} f_I(\bar{\boldsymbol{\theta}}) e^{-\bar{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\bar{\boldsymbol{\theta}}$$
$$= \sum_I (-1)^{|I|} (Af_I, f_I) = \operatorname{Tr}_s A,$$

where $|I|$ denotes the cardinality of the subset $I \subseteq \{1, \dots, n\}$. Corresponding formulas for the Wick symbol follow from Lemma 10.6. $\square$

COROLLARY 10.3. *Show that the Wick symbol of the product* $A = A_l \dots A_1$ *is given by*

$$A(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}) = \int \cdots \int A_l(\bar{\boldsymbol{\theta}}, \boldsymbol{\alpha}_{l-1}) \dots A_1(\bar{\boldsymbol{\alpha}}_1, \boldsymbol{\theta}) \exp\Big\{\sum_{k=1}^{l-1} \bar{\boldsymbol{\alpha}}_k(\boldsymbol{\alpha}_{k-1} - \boldsymbol{\alpha}_k) + \bar{\boldsymbol{\theta}}(\boldsymbol{\alpha}_{l-1} - \boldsymbol{\theta})\Big\} d\boldsymbol{\alpha}_1 d\bar{\boldsymbol{\alpha}}_1 \dots d\boldsymbol{\alpha}_{l-1} d\bar{\boldsymbol{\alpha}}_{l-1}$$

where $\boldsymbol{\alpha}_0 = \boldsymbol{\theta}$ *and* $A_k(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta})$ *are the Wick symbols of the operators* A_k*.*

PROOF. Indeed, according to Part (i) in Theorem 10.2, the Wick symbol $A(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta})$ is a Berezin integral over $d\boldsymbol{\alpha}_1 d\bar{\boldsymbol{\alpha}}_1 \dots d\boldsymbol{\alpha}_{l-1} d\bar{\boldsymbol{\alpha}}_{l-1}$ of the product $A_l(\bar{\boldsymbol{\theta}}, \boldsymbol{\alpha}_{l-1}) \cdots A_2(\bar{\boldsymbol{\alpha}}_2, \boldsymbol{\alpha}_1) A_1(\bar{\boldsymbol{\alpha}}_1, \boldsymbol{\theta})$ times the exponential factor

$$\begin{aligned}(\bar{\boldsymbol{\alpha}}_2 - \bar{\boldsymbol{\alpha}}_1)(\boldsymbol{\theta} - \boldsymbol{\alpha}_1) + (\bar{\boldsymbol{\alpha}}_3 - \bar{\boldsymbol{\alpha}}_2)(\boldsymbol{\theta} - \boldsymbol{\alpha}_2) + \cdots + (\bar{\boldsymbol{\theta}} - \bar{\boldsymbol{\alpha}}_{l-1})(\boldsymbol{\theta} - \boldsymbol{\alpha}_{l-1}) \\ = \sum_{k=1}^{l-1} \bar{\boldsymbol{\alpha}}_k(\boldsymbol{\alpha}_{k-1} - \boldsymbol{\alpha}_k) + \bar{\boldsymbol{\theta}}(\boldsymbol{\alpha}_{l-1} - \boldsymbol{\theta}).\end{aligned}$$ □

PROBLEM 10.3. Verify directly all results in this section for the simplest case of one degree of freedom, when $\mathscr{H}_F = \mathbb{C}^2$.

PROBLEM 10.4. Prove that the Wick symbol $\Gamma(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta})$ of the chirality operator $\Gamma = (-1)^N$ is $e^{-2\bar{\boldsymbol{\theta}}\boldsymbol{\theta}}$.

10.3. Path integral for the evolution operator

Let H be a Hamiltonian of a system of n fermions — an operator in $\mathscr{H}_F$ with the Wick symbol $H(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta})$. Here we express the Wick symbol $U(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}; T)$ of the evolution operator $U(T) = e^{-iTH}$ by using the path integral over Grassmann variables. Our exposition will be parallel to that in Section 7.2 of Chapter 7, with obvious simplification due to the fact that fermion Hilbert space $\mathscr{H}_F$ is finite-dimensional. Namely, the following elementary result replaces the assumption (7.17) in Section 7.2.

LEMMA 10.7. *Let* $\widetilde{U}(\Delta t)$ *be the operator with the Wick symbol* $e^{-iH(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta})\Delta t}$*. Then*

$$U(T) = \lim_{N\to\infty} \tilde{U}(\Delta t)^N, \quad \textit{where} \quad \Delta t = \frac{T}{N}.$$

PROOF. The Wick symbol of the operator $R(\Delta t) = I - iH\Delta t - \tilde{U}(\Delta t)$ is a polynomial in Δt with Grassmann algebra coefficients, which starts with the term $(\Delta t)^2$. It is easy to see that $\|R(\Delta t)\| \leq c(\Delta t)^2$ for some $c > 0$, and

$$U(T) = \lim_{N\to\infty} (I - iH\Delta t)^N = \lim_{N\to\infty} (U(\Delta t) + R(\Delta t))^N = \lim_{N\to\infty} \tilde{U}(\Delta t)^N. \ \square$$

Using of the Wick symbols formula in Theorem 10.2, we can represent the Wick symbol $U_N(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}; T)$ of the operator $\tilde{U}(\Delta t)^N$ as an $(N-1)$-fold Berezin integral. Namely, consider the anticommuting variables $\boldsymbol{\alpha}_k = \{\alpha_k^1, \dots, \alpha_k^n\}$, $\bar{\boldsymbol{\alpha}}_k = \{\bar{\alpha}_k^1, \dots, \bar{\alpha}_k^n\}$, $k = 1, \dots, N-1$ — generators of the Grassmann algebra with involution — and denote $\bar{\boldsymbol{\alpha}}_k\boldsymbol{\alpha}_k = \sum_{l=1}^n \bar{\alpha}_k^l \alpha_k^l$, etc. It follows from Corollary 10.3 that

$$U_N(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}; T) = \int \cdots \int \exp\Big\{ \sum_{k=1}^{N} (\bar{\boldsymbol{\alpha}}_k(\boldsymbol{\alpha}_{k-1} - \boldsymbol{\alpha}_k) + \bar{\boldsymbol{\theta}}(\boldsymbol{\alpha}_N - \boldsymbol{\theta})$$
$$-iH(\bar{\boldsymbol{\alpha}}_k, \boldsymbol{\alpha}_{k-1})\Delta t) \Big\} \prod_{k=1}^{N-1} d\boldsymbol{\alpha}_k d\bar{\boldsymbol{\alpha}}_k,$$

where $\boldsymbol{\alpha}_0 = \boldsymbol{\theta}$, and we put $\bar{\boldsymbol{\alpha}}_N = \bar{\boldsymbol{\theta}}$. It follows from Lemma 10.7 that

$$U(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}; T) = \lim_{N\to\infty} U_N(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}; T) = \lim_{N\to\infty} \int \cdots \int \tag{10.17}$$
$$\exp\Big\{ \sum_{k=1}^{N} (\bar{\boldsymbol{\alpha}}_k(\boldsymbol{\alpha}_{k-1} - \boldsymbol{\alpha}_k) + \bar{\boldsymbol{\theta}}(\boldsymbol{\alpha}_N - \boldsymbol{\theta}) - iH(\bar{\boldsymbol{\alpha}}_k, \boldsymbol{\alpha}_{k-1})\Delta t) \Big\} \prod_{k=1}^{N-1} d\boldsymbol{\alpha}_k d\bar{\boldsymbol{\alpha}}_k.$$

This formula looks quite similar to (7.19) in Chapter 7. Accordingly, we interpret the limit $N \to \infty$ as the following *Feynman path integral for Grassmann variables* (or *Grassmann path integral*):

$$U(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}; T) = \int\limits_{\left\{\substack{\bar{\boldsymbol{\alpha}}(T) = \bar{\boldsymbol{\theta}} \\ \boldsymbol{\alpha}(0) = \boldsymbol{\theta}}\right\}} e^{i\int_0^T (i\bar{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} - H(\bar{\boldsymbol{\alpha}}, \boldsymbol{\alpha}))dt + \bar{\boldsymbol{\theta}}(\boldsymbol{\alpha}(T) - \boldsymbol{\theta})} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\bar{\boldsymbol{\alpha}}. \tag{10.18}$$

Here the "integration" goes over all functions $\boldsymbol{\alpha}(t), \bar{\boldsymbol{\alpha}}(t)$ with anticommuting values[1] on the interval $[0, T]$, satisfying boundary conditions $\boldsymbol{\alpha}(0) = \boldsymbol{\theta}$, $\bar{\boldsymbol{\alpha}}(T) = \bar{\boldsymbol{\theta}}$, and

$$\mathscr{D}\boldsymbol{\alpha}\mathscr{D}\bar{\boldsymbol{\alpha}} = \prod_{0 \leq t \leq T} d\boldsymbol{\alpha}(t) d\bar{\boldsymbol{\alpha}}(t) = \lim_{N\to\infty} \prod_{k=1}^{N-1} d\boldsymbol{\alpha}_k d\bar{\boldsymbol{\alpha}}_k.$$

[1]For every $0 \leq t \leq T$ there is a copy of the independent Grassmann algebra with generators $\alpha^1(t), \dots, \alpha^n(t), \bar{\alpha}^1(t), \dots, \bar{\alpha}^n(t)$.

Here for $0 < t < T$ variables $\bar{\boldsymbol{\alpha}}(t)$ are conjugated to $\boldsymbol{\alpha}(t)$ with respect to the Grassmann algebra involution, while $\bar{\boldsymbol{\alpha}}(0)$ and $\boldsymbol{\alpha}(T)$ — also variables of integration — are not conjugated to the boundary values $\boldsymbol{\alpha}(0) = \boldsymbol{\theta}$, $\bar{\boldsymbol{\alpha}}(T) = \bar{\boldsymbol{\theta}}$.

REMARK 10.5. It should be emphasized that the only rigorous meaning of the Grassmann path integral (10.18) is the limit of multiple Berezin integrals in (10.17). However, as we have seen already in Chapter 7, it is very useful to pretend that the path integral has an independent definition, and formally work with it as if it was an actual integral.

Using Theorem 10.2, it is easy to express the supertrace of the evolution operator $U(T)$ — an operator in a finite-dimensional Hilbert space $\mathscr{H}_F$ — as a Grassmann path integral. We have

$$\begin{aligned}\operatorname{Tr}_s e^{-iTH} &= \lim_{N\to\infty}\int U_N(\bar{\boldsymbol{\theta}},\boldsymbol{\theta};T)d\boldsymbol{\theta}d\bar{\boldsymbol{\theta}} = \lim_{N\to\infty}\int\cdots\int \exp\Big\{\bar{\boldsymbol{\theta}}(\boldsymbol{\alpha}_N-\boldsymbol{\theta})\\ &+\sum_{k=1}^{N}(\bar{\boldsymbol{\alpha}}_k(\boldsymbol{\alpha}_{k-1}-\boldsymbol{\alpha}_k)-iH(\bar{\boldsymbol{\alpha}}_k,\boldsymbol{\alpha}_{k-1})\Delta t)\Big\}\prod_{k=1}^{N-1}d\boldsymbol{\alpha}_k d\bar{\boldsymbol{\alpha}}_k d\boldsymbol{\theta}d\bar{\boldsymbol{\theta}}\\ &= \int\limits_{\left\{\substack{\bar{\boldsymbol{\alpha}}(0)=\bar{\boldsymbol{\alpha}}(T)\\ \boldsymbol{\alpha}(0)=\boldsymbol{\alpha}(T)}\right\}} e^{i\int_0^T(i\bar{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}}-H(\bar{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt}\mathscr{D}\boldsymbol{\alpha}\mathscr{D}\bar{\boldsymbol{\alpha}}\end{aligned}$$

— a Grassmann path integral with periodic boundary conditions.

Here periodic boundary conditions $\boldsymbol{\alpha}(0) = \boldsymbol{\alpha}(T)$ and $\bar{\boldsymbol{\alpha}}(0) = \bar{\boldsymbol{\alpha}}(T)$ emerge from fixed ends boundary conditions $\boldsymbol{\alpha}_0 = \boldsymbol{\theta}$ and $\bar{\boldsymbol{\alpha}}_N = \bar{\boldsymbol{\theta}}$ due to the identity

$$\begin{aligned}&\sum_{k=1}^{N-1}\bar{\boldsymbol{\alpha}}_k(\boldsymbol{\alpha}_{k-1}-\boldsymbol{\alpha}_k)+\bar{\boldsymbol{\theta}}(\boldsymbol{\alpha}_{N-1}-\boldsymbol{\theta})\\ &=\sum_{k=1}^{N-1}(\bar{\boldsymbol{\alpha}}_{k+1}-\bar{\boldsymbol{\alpha}}_k)\boldsymbol{\alpha}_k+(\bar{\boldsymbol{\alpha}}_1-\bar{\boldsymbol{\theta}})\boldsymbol{\theta},\end{aligned}$$

obtained by Abel summation. Indeed, since $\bar{\boldsymbol{\theta}}$ and $\boldsymbol{\theta}$ are now integration variables, it is natural to introduce $\boldsymbol{\alpha}_N = \boldsymbol{\theta}$ and $\bar{\boldsymbol{\alpha}}_0 = \bar{\boldsymbol{\theta}}$. The Grassmann's 'integration measure' is now given by

$$\mathscr{D}\boldsymbol{\alpha}\mathscr{D}\bar{\boldsymbol{\alpha}} = \prod_{0\le t\le T}d\boldsymbol{\alpha}(t)d\bar{\boldsymbol{\alpha}}(t) = \lim_{N\to\infty}\prod_{k=1}^{N}d\boldsymbol{\alpha}_k d\bar{\boldsymbol{\alpha}}_k,$$

where $\bar{\boldsymbol{\alpha}}(0)$ are conjugated to $\boldsymbol{\alpha}(0)$ and $\boldsymbol{\alpha}(T)$ — to $\bar{\boldsymbol{\alpha}}(T)$.

Denoting by $\boldsymbol{\Lambda}$ the corresponding "Grassmann loop space" — the space of all functions with anticommuting values $\boldsymbol{\alpha}(t)$ and $\bar{\boldsymbol{\alpha}}(t)$ conjugated with respect to the Grassmann algebra involution and satisfying periodic boundary conditions $\boldsymbol{\alpha}(0) = \boldsymbol{\alpha}(T)$ and $\bar{\boldsymbol{\alpha}}(0) = \bar{\boldsymbol{\alpha}}(T)$ — we can rewrite the previous formula as

$$\operatorname{Tr}_s e^{-iTH} = \int_{\boldsymbol{\Lambda}} e^{i\int_0^T (i\bar{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} - H(\bar{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\bar{\boldsymbol{\alpha}}.$$

Replacing the physical time t by the Euclidean time $-it$ and T by $-iT$, we get the Grassmann integral representation for the Wick symbol of the operator $U(-iT) = e^{-TH}$,

$$U(\bar{\boldsymbol{\theta}}, \boldsymbol{\theta}; -iT) = \int\limits_{\left\{\substack{\bar{\boldsymbol{\alpha}}(T)=\bar{\boldsymbol{\theta}} \\ \boldsymbol{\alpha}(0)=\boldsymbol{\theta}}\right\}} e^{-\int_0^T (\bar{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} + H(\bar{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\bar{\boldsymbol{\alpha}},$$

and for the supertrace,

$$\operatorname{Tr}_s e^{-TH} = \int_{\boldsymbol{\Lambda}} e^{-\int_0^T (\bar{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} + H(\bar{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\bar{\boldsymbol{\alpha}}. \tag{10.19}$$

Problem 10.5. Express the matrix symbol of the evolution operator as the Grassmann path integral.

Problem 10.6. Show that

$$\operatorname{Tr} e^{-TH} = \int\limits_{\left\{\substack{\bar{\boldsymbol{\alpha}}(0)=-\bar{\boldsymbol{\alpha}}(T) \\ \boldsymbol{\alpha}(0)=-\boldsymbol{\alpha}(T)}\right\}} e^{-\int_0^T (\bar{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} + H(\bar{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\bar{\boldsymbol{\alpha}}$$

— the Grassmann path integral with anti-periodic boundary conditions.

10.4. Gaussian path integrals over Grassmann variables

For simplicity, here we consider only the case $n = 1$. For $u(t) \in C^1([0,T],\mathbb{R})$ put

$$u_0 = \frac{1}{T}\int_0^T u(t)dt \quad \text{and} \quad D = \frac{d}{dt},$$

and consider on the interval $[0,T]$ the first-order differential operator $D + u(t)$ with periodic boundary conditions. The following result evaluates the simplest Gaussian path integral for Grassmann variables.

THEOREM 10.4. *We have*

$$\int_\Lambda e^{-\int_0^T(\bar\alpha\dot\alpha+u(t)\bar\alpha\alpha)dt}\mathscr{D}\alpha\mathscr{D}\bar\alpha=\det(D+u(t))=1-e^{-u_0T}.$$

PROOF. Using Lemma 10.2, we get

$$\begin{aligned}&\int_\Lambda e^{-\int_0^T(\bar\alpha\dot\alpha+u(t)\bar\alpha\alpha)dt}\mathscr{D}\alpha\mathscr{D}\bar\alpha\\ &=\lim_{N\to\infty}\int\cdots\int e^{\sum_{k=1}^N\left(\bar\alpha_k(\alpha_{k-1}-\alpha_k)-u(t_k)\bar\alpha_k\alpha_{k-1}\Delta t\right)}\prod_{k=1}^N d\alpha_k d\bar\alpha_k\\ &=\lim_{N\to\infty}\det A_N.\end{aligned}$$

Here $\alpha_0=\alpha_N,\bar\alpha_0=\bar\alpha_N$, $t_k=k\Delta t$, and A_N is the following $N\times N$ matrix:

$$A_N=\begin{pmatrix}1&0&0&\cdots&0&b_N\\ b_1&1&0&\cdots&0&0\\ 0&b_2&1&\cdots&0&0\\ \vdots&\vdots&\vdots&\ddots&\vdots&\vdots\\ 0&0&0&\cdots&1&0\\ 0&0&0&\cdots&b_{N-1}&1\end{pmatrix},$$

where $b_k=-1+u(t_k)\Delta t$. We have

$$\det A_N=1-(-1)^N\prod_{k=1}^N b_k=1-\prod_{k=1}^N(1-u(t_k)\Delta t),$$

so that

$$\lim\det A_N=1-e^{-\int_0^T u(t)dt}=1-e^{-u_0T}.$$

To define the regularized determinant of the operator $D+u(t)$ we use the zeta function regularization, discussed in Section 8.1. In this simple case it is expressed in terms of the Hurwitz zeta function and we leave the equality $\det(D+u(t))=1-e^{-u_0T}$ as an exercise. $\square$

EXAMPLE 10.1 (The fermion harmonic oscillator). The fermion analog of the harmonic oscillator is the Hamiltonian

$$H=\tfrac{1}{2}\omega(a^*a-aa^*)=\omega(a^*a-\tfrac{1}{2}I)=\omega(N-\tfrac{1}{2}I),$$

where a^* and a are creation and annihilation operators in the one fermion Hilbert space $\mathscr{H}_F=\mathbb{C}^2$ (see Section 9.1). The Wick symbol H is $H(\bar\alpha,\alpha)=$

$\omega(\bar{\alpha}\alpha - \frac{1}{2})$. Now using (10.19) and Theorem 10.4, we obtain

$$\operatorname{Tr}_s e^{-TH} = \int_\Lambda e^{-\int_0^T (\bar{\alpha}\dot{\alpha} + H(\bar{\alpha},\alpha))dt} \mathscr{D}\alpha \mathscr{D}\bar{\alpha}$$
$$= e^{\frac{\omega T}{2}} \int_\Lambda e^{-\int_0^T (\bar{\alpha}\dot{\alpha} + \omega\bar{\alpha}\alpha)dt} \mathscr{D}\alpha \mathscr{D}\bar{\alpha} = e^{\frac{\omega T}{2}}(1 - e^{-\omega T}) = 2\sinh\frac{\omega T}{2}.$$

Of course, the same result can be obtained directly since e^{-TH} is just a 2×2 matrix with eigenvalues $e^{\frac{\omega T}{2}}$ and $e^{-\frac{\omega T}{2}}$ which correspond, respectively, to the eigenspaces $\mathscr{H}_F^0$ and $\mathscr{H}_F^1$. Thus

$$\operatorname{Tr}_s e^{-TH} = e^{\frac{\omega T}{2}} - e^{-\frac{\omega T}{2}} = 2\sinh\frac{\omega T}{2}.$$

PROBLEM 10.7. Show that

$$\int\limits_{\left\{\substack{\bar{\alpha}(0) = -\bar{\alpha}(T) \\ \alpha(0) = -\alpha(T)}\right\}} e^{-\int_0^T (\bar{\alpha}\dot{\alpha} + u(t)\bar{\alpha}\alpha)dt} \mathscr{D}\alpha \mathscr{D}\bar{\alpha} = 1 + e^{-u_0 T}$$

— the regularized determinant of the operator $D + u(t)$ on $[0, T]$ with anti-periodic boundary conditions.

PROBLEM 10.8. For the fermion harmonic oscillator verify that $\operatorname{Tr} e^{-TH} = 2\cosh\frac{\omega T}{2}$ directly, and also by using results of Problems 10.6 and 10.7.

Part 2

Quantum Field Theory

CHAPTER 11

Quantization of free scalar field

11.1. From particles to fields

In a nutshell, quantization of a free Newtonian particle can be described as follows. Consider the relation

$$E = \frac{\boldsymbol{p}^2}{2m} \tag{11.1}$$

between its energy E and momentum $\boldsymbol{p}$, make a replacement

$$E \mapsto i\hbar\frac{\partial}{\partial t}, \quad \boldsymbol{p} \mapsto \boldsymbol{P} = \frac{\hbar}{i}\boldsymbol{\nabla}, \quad \boldsymbol{\nabla} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right), \tag{11.2}$$

and instead of classical equation (11.1) consider the equation

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\boldsymbol{P}^2}{2m}\psi \tag{11.3}$$

for a complex-valued function $\psi(\boldsymbol{x}, t)$, the wave function.

Equation (11.3) is a Schrödinger equation for a free particle and since $H_0 = \dfrac{\boldsymbol{P}^2}{2m}$ is a self-adjoint operator on $L^2(\mathbb{R}^3)$, the corresponding evolution operator is unitary, and the L^2-norm of the wave function is preserved. In other words, if $|\psi(\boldsymbol{x})|^2 d^3\boldsymbol{x}$ was a probability measure on $\mathbb{R}^3$ at time $t = 0$ then $|\psi(\boldsymbol{x}, t)|^2 d^3\boldsymbol{x}$ is probability measure at time t, which in physics literature is called "conservation of probability". Equivalently, the "probability density" $\rho = |\psi|^2$ and the "probability current" $\boldsymbol{j} = \dfrac{1}{2m}(\bar{\psi}\boldsymbol{P}\psi - \psi\boldsymbol{P}\bar{\psi})$ satisfy the *continuity equation*

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{j} = 0, \tag{11.4}$$

which directly follows from (11.3). The conservation of probability is the statement

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^3} \rho(t, \boldsymbol{x}) d^3\boldsymbol{x} = 0, \tag{11.5}$$

which follows from (11.4) by the Stokes' theorem.

Now consider a relativistic particle of mass m, where we use the system of units $c = 1$. Its energy-momentum vector $p = (p^0, p^1, p^2, p^3)$ satisfies $p_\mu p^\mu = m^2$ or $(p^0)^2 - \boldsymbol{p}^2 = m^2$, where $\boldsymbol{p} = (p^1, p^2, p^3)$. Since $p^0 = E$, the energy of a particle, we have the following relation

$$E^2 - \boldsymbol{p}^2 = m^2 \tag{11.6}$$

between energy E and momentum $\boldsymbol{p}$ of a relativistic particle[1]. Using the same fundamental prescription (11.2) for the quantization of a relativistic particle, for a complex-valued function $\psi(x)$ we obtain the equation

$$\hbar^2 \Box \psi + m^2 \psi = 0, \tag{11.7}$$

where $x = (x^0, x^1, x^2, x^3) = (t, \boldsymbol{x}) \in \mathbb{R}^4$ and

$$\Box = \partial_\mu \partial^\mu = \frac{\partial^2}{\partial t^2} - \Delta$$

is the d'Alembertian. Here we are using relativistic notations $\partial_\mu = \dfrac{\partial}{\partial x^\mu}$ and $\partial^\mu = \eta^{\mu\nu} \partial_\nu$, $\mu = 0, 1, 2, 3$.

Equation (11.7) is known as the Klein-Gordon equation[2] for a complex-valued field ψ, and is a second-order partial differential equation. Analogously to the continuity equation (11.4) we have a conservation of a 4-current $j^\mu = \dfrac{i\hbar}{2m}(\bar{\psi} \partial^\mu \psi - \psi \partial^\mu \bar{\psi})$. Indeed, it follows from (11.7) that

$$\partial_\mu j^\mu = \frac{i\hbar}{2m}(\bar{\psi} \Box \psi - \psi \Box \bar{\psi}) = 0. \tag{11.8}$$

We have $j^\mu(x) = (\rho(x), \boldsymbol{j}(x))$, where

$$\rho(x) = \frac{i\hbar}{2m} \left(\overline{\psi}(x) \partial_0 \psi(x) - \psi(x) \partial_0 \overline{\psi}(x) \right)$$

and

$$\boldsymbol{j}(x) = \frac{i\hbar}{2m} \left(\psi(x) \boldsymbol{\nabla} \overline{\psi}(x) - \overline{\psi}(x) \boldsymbol{\nabla} \psi(x) \right)$$

---

[1] In the non-relativistic limit $\boldsymbol{p}^2 \ll m^2$ (i.e. $c \to \infty$), relation (11.6), written as $E = \sqrt{\boldsymbol{p}^2 + m^2} = m\sqrt{1 + \boldsymbol{p}^2/m^2}$, turns into (11.1).

[2] Rather it should be called Klein-Fock equation.

satisfy the continuity equation (11.4). One may think that ρ and $\boldsymbol{j}$ are the probability density and current for a quantum free relativistic particle with the conservation law (11.5).

However, since Cauchy data for the Klein-Gordon equation are independent, $\rho(0, \boldsymbol{x})$ can take positive and negative values and, therefore, cannot be used as density of a probability measure on $\mathbb{R}^3$. Thus the interpretation of the Klein-Gordon equation as a relativistic analog of single-particle Schrödinger equation with the wave function ψ should be abandoned. Moreover, if $\psi(x)$ takes only real values then $\rho(x)$ vanishes identically. Yet another problem with this interpretation is that the Klein-Gordon equation has negative energy solutions[3]. Indeed, the simplest plane-wave solution of equation (11.7) is

$$\psi(x) = e^{-i(k_0 t - \boldsymbol{k}\boldsymbol{x})/\hbar},$$

where $k_0 = \pm\sqrt{\boldsymbol{k}^2 + m^2}$ and $\boldsymbol{k} \in \mathbb{R}^3$. Since $E\psi(x) = k_0\psi(x)$, the energy of the solution $\psi(x)$ is k_0, and it has positive and negative values. However, the interaction in special relativity is described by fields and not by particles. Therefore, we should consider a classical field theory as a Hamiltonian system with infinitely many degrees of freedom and apply to it the quantization procedure, developed for the systems with finitely many degrees of freedom.

We start with the simplest example, quantization of a free massive real scalar field, and recall its Hamiltonian formulation, which allows to represent the classical field as collection of infinitely many non-interacting harmonic oscillators with frequencies $\omega_{\boldsymbol{k}} = \sqrt{\boldsymbol{k}^2 + m^2}$, parametrized by $\boldsymbol{k} \in \mathbb{R}^3$.

11.2. Normal mode decomposition

Consider a free massive real scalar field $\varphi(x)$, $x = (x^0, x^1, x^2, x^3) \in \mathbb{R}^4$, where we put $c = 1$ so that $x^0 = t$. The field $\varphi(x)$ satisfies the Klein-Gordon equation

$$(\Box + m^2)\varphi = 0, \quad \Box = \partial_\mu\partial^\mu = \partial_0^2 - \partial_1^2 - \partial_2^2 - \partial_3^2. \tag{11.9}$$

In terms of the Fourier transform

$$\varphi(x) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^4} e^{-ik\cdot x}\hat{\varphi}(k)d^4k, \quad k \cdot x = k_\mu x^\mu = k_0 x^0 - \boldsymbol{k}\boldsymbol{x}, \tag{11.10}$$

[3]The Dirac equation, which successfully resolves the problem of negative probabilities and negative energies, is not a single-particle equation. It describes the spinor field, which creates particles and antiparticles.

where $\overline{\hat{\varphi}(k)} = \hat{\varphi}(-k)$, equation (11.9) takes the form

$$(k^2 - m^2)\hat{\varphi}(k) = 0, \quad k^2 = k_\mu k^\mu = k_0^2 - \boldsymbol{k}^2.$$

Thus we get

$$\hat{\varphi}(k) = \delta(k^2 - m^2)\rho(k) = \frac{1}{2\omega_{\boldsymbol{k}}}\left(\delta(k_0 - \omega_{\boldsymbol{k}})\rho_1(\boldsymbol{k}) + \delta(k_0 + \omega_{\boldsymbol{k}})\rho_2(\boldsymbol{k})\right),$$

where $\omega_{\boldsymbol{k}} = \sqrt{\boldsymbol{k}^2 + m^2}$ and $\rho_2(\boldsymbol{k}) = \overline{\rho_1(-\boldsymbol{k})}$. Substituting the formula for $\hat{\varphi}(k)$ into (11.10), denoting $\rho_1(\boldsymbol{k}) = \sqrt{2\pi}a(\boldsymbol{k})$ and changing in the second integral $\boldsymbol{k}$ by $-\boldsymbol{k}$, we obtain

$$\varphi(x) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\left(e^{-ik\cdot x}a(\boldsymbol{k}) + e^{ik\cdot x}\bar{a}(\boldsymbol{k})\right)\frac{d^3\boldsymbol{k}}{2\omega_{\boldsymbol{k}}}, \quad k_0 = \omega_{\boldsymbol{k}} \tag{11.11}$$

and

$$(\partial_0\varphi)(x) = -\frac{i}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\omega_{\boldsymbol{k}}\left(e^{-ik\cdot x}a(\boldsymbol{k}) - e^{ik\cdot x}\bar{a}(\boldsymbol{k})\right)\frac{d^3\boldsymbol{k}}{2\omega_{\boldsymbol{k}}}, \tag{11.12}$$

where $\bar{a}(\boldsymbol{k}) = \overline{a(\boldsymbol{k})}$. Thus for the Cauchy data

$$\varphi(\boldsymbol{x}) = \varphi(x)|_{t=0}, \quad \pi(\boldsymbol{x}) = (\partial_0\varphi)(x)|_{t=0}$$

we have

$$\varphi(\boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\left(e^{i\boldsymbol{kx}}a(\boldsymbol{k}) + e^{-i\boldsymbol{kx}}\bar{a}(\boldsymbol{k})\right)\frac{d^3\boldsymbol{k}}{2\omega_{\boldsymbol{k}}}, \tag{11.13}$$

$$\pi(\boldsymbol{x}) = -\frac{i}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\omega_{\boldsymbol{k}}\left(e^{i\boldsymbol{kx}}a(\boldsymbol{k}) - e^{-i\boldsymbol{kx}}\bar{a}(\boldsymbol{k})\right)\frac{d^3\boldsymbol{k}}{2\omega_{\boldsymbol{k}}} \tag{11.14}$$

and

$$a(\boldsymbol{k}) = \omega_{\boldsymbol{k}}\hat{\varphi}(\boldsymbol{k}) + i\hat{\pi}(\boldsymbol{k}). \tag{11.15}$$

Symplectic structure on the space of Cauchy data is given by the following Poisson brackets

$$\{\pi(\boldsymbol{x}), \pi(\boldsymbol{y})\} = \{\varphi(\boldsymbol{x}), \varphi(\boldsymbol{y})\} = 0, \quad \{\pi(\boldsymbol{x}), \varphi(\boldsymbol{y})\} = \delta(\boldsymbol{x} - \boldsymbol{y}) \tag{11.16}$$

(we are referring to the last semester course for the precise meaning of these formulas). It follows from (11.15) that (11.16) are equivalent to the following Poisson brackets

$$\{a(\boldsymbol{k}), a(\boldsymbol{p})\} = \{\bar{a}(\boldsymbol{k}), \bar{a}(\boldsymbol{p})\} = 0, \quad \{a(\boldsymbol{k}), \bar{a}(\boldsymbol{p})\} = 2i\omega_{\boldsymbol{k}}\delta(\boldsymbol{k} - \boldsymbol{p}). \tag{11.17}$$

Using Plancherel's theorem for the Hamiltonian H_c and total momentum $\boldsymbol{P}_c = (P^1, P^2, P^3)$ we obtain

$$H_c = \frac{1}{2}\int_{\mathbb{R}^3} \left(\pi^2(\boldsymbol{x}) + (\boldsymbol{\nabla}\varphi)^2(\boldsymbol{x}) + m^2\varphi^2(\boldsymbol{x})\right) d^3\boldsymbol{x} = \int_{\mathbb{R}^3} \omega_{\boldsymbol{k}}\bar{a}(\boldsymbol{k})a(\boldsymbol{k})\, d\mu_{\boldsymbol{k}}$$

and

$$\boldsymbol{P}_c = -\int_{\mathbb{R}^3} \pi(\boldsymbol{x})(\boldsymbol{\nabla}\varphi)(\boldsymbol{x})d^3\boldsymbol{x} = \int_{\mathbb{R}^3} \boldsymbol{k}\bar{a}(\boldsymbol{k})a(\boldsymbol{k})\, d\mu_{\boldsymbol{k}},$$

where

$$d\mu_{\boldsymbol{k}} = \theta(k_0)\delta(k^2 - m^2) = \frac{d^3\boldsymbol{k}}{2\omega_{\boldsymbol{k}}}$$

is a restriction of the Lebesgue measure on $\mathbb{R}^4$ onto the positive energy part $\mathcal{O}_m^+ \simeq \mathbb{R}^3$ of the mass hyperboloid

$$\mathcal{O}_m = \{k \in \mathbb{R}^4 : (k^0)^2 - \boldsymbol{k}^2 = m^2\}.$$

These formulas give a *normal mode decomposition* of a solution of the Klein-Gordon equation — classical free scalar field $\varphi(x)$ of mass m. Each mode is parametrized by a "wave vector" $\boldsymbol{k} \in \mathbb{R}^3$ and is a harmonic oscillator with frequency $\omega_{\boldsymbol{k}}$, and the field $\varphi(x)$ is an integral over $\mathbb{R}^3$ with the measure $d\mu_{\boldsymbol{k}}$ of non-interacting modes.

11.3. Canonical quantization

Since the phase space of the model is a vector space (though an infinite-dimensional), for linear functions on the phase space we can apply the standard quantization rule

$$\{\ ,\ \}_\hbar = \frac{i}{\hbar}[\ ,\ ].$$

It results in replacing classical Poisson brackets (11.16) by the quantum Poisson brackets for *quantum fields*, self-adjoint operators $\boldsymbol{\pi}(\boldsymbol{x})$ and $\boldsymbol{\varphi}(\boldsymbol{x})$ satisfying

$$\{\boldsymbol{\pi}(\boldsymbol{x}), \boldsymbol{\pi}(\boldsymbol{y})\}_\hbar = \{\boldsymbol{\varphi}(\boldsymbol{x}), \boldsymbol{\varphi}(\boldsymbol{y})\}_\hbar = 0, \quad \{\boldsymbol{\pi}(\boldsymbol{x}), \boldsymbol{\varphi}(\boldsymbol{y})\}_\hbar = \delta(\boldsymbol{x} - \boldsymbol{y})I,$$

where I is the identity operator. As the result we get Heisenberg commutation relations for infinitely many degrees of freedom

$$[\boldsymbol{\pi}(\boldsymbol{x}), \boldsymbol{\pi}(\boldsymbol{y})] = [\boldsymbol{\varphi}(\boldsymbol{x}), \boldsymbol{\varphi}(\boldsymbol{y})] = 0, \quad [\boldsymbol{\pi}(\boldsymbol{x}), \boldsymbol{\varphi}(\boldsymbol{y})] = \frac{\hbar}{i}\delta(\boldsymbol{x} - \boldsymbol{y})I. \tag{11.18}$$

The presence of the delta-function $\delta(\boldsymbol{x}-\boldsymbol{y})$, is a manifestation of the fact that $\boldsymbol{\pi}(\boldsymbol{x})$ and $\boldsymbol{\varphi}(\boldsymbol{x})$ are rather *operator-valued distributions* than actual operators on some Hilbert space.

Quantum operators operators $\boldsymbol{a}(\boldsymbol{k})$ and their adjoints $\boldsymbol{a}^\dagger(\boldsymbol{k})$ are defined by the formulas analogous to (11.13)–(11.14),

$$\boldsymbol{\varphi}(\boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \left(e^{i\boldsymbol{k}\boldsymbol{x}}\boldsymbol{a}(\boldsymbol{k}) + e^{-i\boldsymbol{k}\boldsymbol{x}}\boldsymbol{a}^\dagger(\boldsymbol{k})\right) d\mu_{\boldsymbol{k}}, \tag{11.19}$$

$$\boldsymbol{\pi}(\boldsymbol{x}) = -\frac{i}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \omega_{\boldsymbol{k}} \left(e^{i\boldsymbol{k}\boldsymbol{x}}\boldsymbol{a}(\boldsymbol{k}) - e^{-i\boldsymbol{k}\boldsymbol{x}}\boldsymbol{a}^\dagger(\boldsymbol{k})\right) d\mu_{\boldsymbol{k}}. \tag{11.20}$$

Quantization of the Poisson brackets (11.17) yields the following commutations relations

$$[\boldsymbol{a}(\boldsymbol{k}), \boldsymbol{a}(\boldsymbol{p})] = [\boldsymbol{a}^\dagger(\boldsymbol{k}), \boldsymbol{a}^\dagger(\boldsymbol{p})] = 0, \quad [\boldsymbol{a}(\boldsymbol{k}), \boldsymbol{a}^\dagger(\boldsymbol{p})] = 2\hbar\omega_{\boldsymbol{k}}\delta(\boldsymbol{k}-\boldsymbol{p})I. \tag{11.21}$$

It is easy to see, using (11.19)–(11.20), that these commutation relations give back the Heisenberg commutation relations (11.18).

Commutation relations (11.21) are called *canonical commutation relations*, and play a fundamental role in quantum field theory. The operator-valued distributions $\boldsymbol{a}^\dagger(\boldsymbol{k})$ and $\boldsymbol{a}(\boldsymbol{k})$ are infinite-dimensional analogous of the creation and annihilation operators of the quantum harmonic oscillator (see Chapter 5).

Corresponding quantum field $\boldsymbol{\varphi}(x)$ in the spacetime (or rather an operator-valued distribution) is given by the same formula (11.11), where $a(\boldsymbol{k})$ and $\bar{a}(\boldsymbol{k})$ are replaced by $\boldsymbol{a}(\boldsymbol{k})$ and $\boldsymbol{a}^\dagger(\boldsymbol{k})$,

$$\boldsymbol{\varphi}(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \left(e^{-ik\cdot x}\boldsymbol{a}(\boldsymbol{k}) + e^{ik\cdot x}\boldsymbol{a}^\dagger(\boldsymbol{k})\right) d\mu_{\boldsymbol{k}}, \quad k_0 = \omega_{\boldsymbol{k}}. \tag{11.22}$$

REMARK 11.1. in physics literature this procedure is often called a *second quantization*. This reflects the fact 'first quantization' of a free relativistic particle produces a Klein-Gordon equation for a classical field $\varphi(x)$ which is 'quantized' once again to produce a quantum field $\boldsymbol{\varphi}(x)$. However, this term is a misnomer since in special relativity interaction is described by fields on the spacetime and not by particles, and we just quantize classical fields as Hamiltonian systems with infinitely many degrees of freedom.

In quantum field theory it is customary to use the system of units $c = \hbar = 1$, so-called *natural units*, and from now on we will be also using this convention.

The creation and annihilations operators are realized in the space of states, the celebrated *Fock space*, which we will rigorously introduce in the next chapter. Here we present an informal definition, which is standard in the physics textbooks. Consider a linear space $\mathcal{F}$ spanned by a vector $|0\rangle$ and vectors $|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle$ satisfying

$$|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = |\boldsymbol{k}_{\sigma(1)}, \dots, \boldsymbol{k}_{\sigma(n)}\rangle \quad \text{for all} \quad \sigma \in \mathrm{Sym}_n,$$

where $\boldsymbol{k}_i \in \mathbb{R}^3$ and $n \in \mathbb{N}$, the vector $|0\rangle$ corresponds to $n = 0$. We define the action of operators $\boldsymbol{a}(\boldsymbol{k})$ and $\boldsymbol{a}^\dagger(\boldsymbol{k})$ (or rather operator-valued distributions) by the following formulas

$$\boldsymbol{a}(\boldsymbol{k})|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = \sum_{l=1}^{n} 2\omega_{\boldsymbol{k}_l} \delta(\boldsymbol{k} - \boldsymbol{k}_l)|\boldsymbol{k}_1, \dots, \hat{\boldsymbol{k}}_l, \dots, \boldsymbol{k}_n\rangle, \tag{11.23}$$

$$\boldsymbol{a}^\dagger(\boldsymbol{k})|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = |\boldsymbol{k}, \boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle, \tag{11.24}$$

where for $n = 0$

$$\boldsymbol{a}(\boldsymbol{k})|0\rangle = 0 \tag{11.25}$$

and $\hat{\boldsymbol{k}}_l$ means that this argument is omitted. It follows from (11.24) that

$$|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = \boldsymbol{a}^\dagger(\boldsymbol{k}_1) \cdots \boldsymbol{a}^\dagger(\boldsymbol{k}_n)|0\rangle$$

and it is easy to check that operators $\boldsymbol{a}^\dagger(\boldsymbol{k})$ and $\boldsymbol{a}(\boldsymbol{k})$, defined by formulas (11.24)–(11.23), satisfy canonical commutation relations (11.21)[4]. As we will discuss in the next chapter, normalized vectors in the Fock space $\mathscr{F}$ are obtained by smearing the states $|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle$ with the smooth functions, i.e. by considering

$$\frac{1}{n!} \int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3} F_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n) \boldsymbol{a}^\dagger(\boldsymbol{k}_1) \cdots \boldsymbol{a}^\dagger(\boldsymbol{k}_n)|0\rangle \, d\mu_{\boldsymbol{k}_1} \cdots d\mu_{\boldsymbol{k}_n}.$$

Next we need to define quantum Hamiltonian $\boldsymbol{H}$ and momentum operators $\boldsymbol{P} = (\boldsymbol{P}^1, \boldsymbol{P}^2, \boldsymbol{P}^3)$. It seems natural to define them as the following quantum analogs of the corresponding classical formulas,

$$\boldsymbol{H} = H_c(\boldsymbol{\pi}, \boldsymbol{\varphi}) = \frac{1}{2} \int_{\mathbb{R}^3} \left(\boldsymbol{\pi}^2(\boldsymbol{x}) + (\boldsymbol{\nabla}\boldsymbol{\varphi})^2(\boldsymbol{x}) + m^2 \boldsymbol{\varphi}^2(\boldsymbol{x})\right) d^3\boldsymbol{x},$$

$$\boldsymbol{P} = \boldsymbol{P}_c(\boldsymbol{\pi}, \boldsymbol{\varphi}) = -\int_{\mathbb{R}^3} \boldsymbol{\pi}(\boldsymbol{x})(\boldsymbol{\nabla}\boldsymbol{\varphi})(\boldsymbol{x}) d^3\boldsymbol{x}.$$

[4]Note that $\hbar = 1$.

Using formulas (11.19)–(11.20), the identity

$$\int_{\mathbb{R}^3} e^{i\boldsymbol{kx}} d^3\boldsymbol{x} = (2\pi)^3\delta(\boldsymbol{k})$$

and carefully keeping the order when multiplying operators, we obtain

$$\boldsymbol{H} = \frac{1}{2}\int_{\mathbb{R}^3} \omega_{\boldsymbol{k}}(\boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) + \boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{k}))\, d\mu_{\boldsymbol{k}}$$

and

$$\boldsymbol{P}^j = \frac{1}{2}\int_{\mathbb{R}^3} k^j(\boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) + \boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{k}))\, d\mu_{\boldsymbol{k}}, \quad j = 1, 2, 3.$$

However, the product $\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{k})$ is ill-defined: applying it to $|0\rangle$ and using (11.23)–(11.24), we obtain a meaningless divergent formula

$$\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{k})|0\rangle = \boldsymbol{a}(\boldsymbol{k})|\boldsymbol{k}\rangle = 2\omega_{\boldsymbol{k}}\delta(0)|0\rangle,$$

since $\delta(0)$ makes no sense. A general formula is

$$\begin{aligned}\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{k})|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = \boldsymbol{a}(\boldsymbol{k})|\boldsymbol{k}, \boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle &= 2\omega_{\boldsymbol{k}}\delta(0)|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle \\ &+ \sum_{l=1}^n 2\omega_{\boldsymbol{k}_l}\delta(\boldsymbol{k} - \boldsymbol{k}_l)|\boldsymbol{k}, \boldsymbol{k}_1, \dots, \hat{\boldsymbol{k}}_l, \dots, \boldsymbol{k}_n\rangle,\end{aligned}$$

and also makes no sense.

On the other hand, the operator $\boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k})$ (rather an operator-valued distribution) is perfectly well-defined,

$$\boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k})|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = \sum_{l=1}^n 2\omega_{\boldsymbol{k}_l}\delta(\boldsymbol{k} - \boldsymbol{k}_l)|\boldsymbol{k}, \boldsymbol{k}_1, \dots, \hat{\boldsymbol{k}}_l, \dots, \boldsymbol{k}_n\rangle \tag{11.26}$$

and we obtain

$$\int_{\mathbb{R}^3} \omega_{\boldsymbol{k}}\boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k})\, d\mu_{\boldsymbol{k}}|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = \sum_{l=1}^n \omega_{\boldsymbol{k}_l}|\boldsymbol{k}_1, \dots, \boldsymbol{k}_l, \dots, \boldsymbol{k}_n\rangle. \tag{11.27}$$

The proposed naive formula for the Hamiltonian operator $\boldsymbol{H}$ is ill-defined because the last commutation relation in (11.21) becomes singular at $\boldsymbol{k} = \boldsymbol{p}$,

$$\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{k}) - \boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) = 2\omega_{\boldsymbol{k}}\delta(0)I.$$

Indeed, using this formula we obtain

$$\boldsymbol{H} = \int_{\mathbb{R}^3} \omega_{\boldsymbol{k}} \boldsymbol{a}^\dagger(\boldsymbol{k}) \boldsymbol{a}(\boldsymbol{k})\, d\mu_{\boldsymbol{k}} + \frac{1}{2}\delta(0) \int_{\mathbb{R}^3} \omega_{\boldsymbol{k}} d^3\boldsymbol{k}\, I,$$

where proportional to the identity operator second term is clearly divergent. This divergence symbolizes an infinite "vacuum energy" — the infinite sum (or rather an integral) of the ground state energies of corresponding harmonic oscillators. Similar divergence appears in the expression for $\boldsymbol{P}$. Thus there is a problem of defining quantum operators $\boldsymbol{H}$ and $\boldsymbol{P}$.

Correct definitions of $\boldsymbol{H}$ and $\boldsymbol{P}$ is very simple, one just needs to drop the divergent terms! Corresponding mathematical procedure is called the *normal ordering* of quantum creation and annihilation operators.

By definition, the normal ordering is a linear map which to every monomial in $\boldsymbol{a}(\boldsymbol{k})$ and $\boldsymbol{a}^\dagger(\boldsymbol{k})$ (considered as free variables, no commutation relations!) at arbitrary points assigns another monomial where all creation operators are just placed to the left of annihilation operators. It is denoted by a double semicolon $\boldsymbol{:}\ \boldsymbol{:}$,

$$\boldsymbol{:}\boldsymbol{a}^\dagger(\boldsymbol{p})\boldsymbol{a}(\boldsymbol{k})\boldsymbol{:}= \boldsymbol{a}^\dagger(\boldsymbol{p})\boldsymbol{a}(\boldsymbol{k}), \quad \boldsymbol{:}\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{p})\boldsymbol{:}= \boldsymbol{a}^\dagger(\boldsymbol{p})\boldsymbol{a}(\boldsymbol{k}),$$

and $\boldsymbol{:}I\boldsymbol{:}= I$.

Remark 11.2. The normal ordering is not a linear map on the quotient of a free polynomial algebra in $\boldsymbol{a}(\boldsymbol{k})$ and $\boldsymbol{a}^\dagger(\boldsymbol{k})$ modulo commutation relations! Indeed, we have

$$\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{p}) - \boldsymbol{a}^\dagger(\boldsymbol{p})\boldsymbol{a}(\boldsymbol{k}) = 2\hbar\omega_{\boldsymbol{k}}\delta(\boldsymbol{k}-\boldsymbol{p})I,$$

so assuming linearity we would have

$$\boldsymbol{:}(\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{p}) - \boldsymbol{a}^\dagger(\boldsymbol{p})\boldsymbol{a}(\boldsymbol{k}))\boldsymbol{:}=\boldsymbol{:}\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{p})\boldsymbol{:} - \boldsymbol{a}^\dagger(\boldsymbol{p})\boldsymbol{a}(\boldsymbol{k}) = 0$$

— a contradiction with $\boldsymbol{:}I\boldsymbol{:}= I$.

Thus correct definition of quantum Hamiltonian operator $\boldsymbol{H}$ and total momentum operator $\boldsymbol{P}$ is

$$\boldsymbol{H} = \boldsymbol{:}\, H_c(\boldsymbol{\pi},\boldsymbol{\varphi})\,\boldsymbol{:} = \frac{1}{2}\int_{\mathbb{R}^3} \boldsymbol{:}\big(\boldsymbol{\pi}^2(\boldsymbol{x}) + (\boldsymbol{\nabla}\boldsymbol{\varphi})^2(\boldsymbol{x}) + m^2\boldsymbol{\varphi}^2(\boldsymbol{x})\big)\boldsymbol{:}\, d^3\boldsymbol{x}, \tag{11.28}$$

$$\boldsymbol{P} = \boldsymbol{:}\, \boldsymbol{P}_c(\boldsymbol{\pi},\boldsymbol{\varphi})\,\boldsymbol{:} = -\int_{\mathbb{R}^3} \boldsymbol{:}\boldsymbol{\pi}(\boldsymbol{x})(\boldsymbol{\nabla}\boldsymbol{\varphi})(\boldsymbol{x})\boldsymbol{:}\, d^3\boldsymbol{x}. \tag{11.29}$$

As the result, in terms of creation and annihilation operators we obtain the following formulas for $\boldsymbol{H}$ and $\boldsymbol{P}$,

$$\boldsymbol{H} = \int_{\mathbb{R}^3} \omega_{\boldsymbol{k}} \boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) d\mu_{\boldsymbol{k}}, \tag{11.30}$$

$$\boldsymbol{P} = \int_{\mathbb{R}^3} \boldsymbol{k}\boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) d\mu_{\boldsymbol{k}}. \tag{11.31}$$

It follows from (11.25) that

$$\boldsymbol{H}|0\rangle = 0 \quad \text{and} \quad \boldsymbol{P}^j|0\rangle = 0, \quad j = 1, 2, 3.$$

Moreover, using (11.26) we readily obtain

$$\boldsymbol{H}|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = \sum_{l=1}^{n} \omega_{\boldsymbol{k}_l} |\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle, \tag{11.32}$$

$$\boldsymbol{P}|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = \sum_{l=1}^{n} \boldsymbol{k}_l |\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle. \tag{11.33}$$

These formulas show that the state $|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle$ describes n identical relativistic particles of mass m with the momenta $\boldsymbol{k}_1, \dots, \boldsymbol{k}_n$ and the energies $\omega_{\boldsymbol{k}_1}, \dots, \omega_{\boldsymbol{k}_n}$. Also introducing the following

$$N = \int_{\mathbb{R}^3} \boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) d\mu_{\boldsymbol{k}}$$

we get

$$N|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle = n|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle, \tag{11.34}$$

so that operator N plays the role of *number of particles* operator.

In relativistic notations, let $\boldsymbol{P}^\mu$ be the quantum energy-momentum operator, where $\boldsymbol{P}^0 = \boldsymbol{H}$ and $\mu = 0, 1, 2, 3$. Using canonical commutation relations (11.21) and formulas (11.22) and (11.30)–(11.31) we obtain

$$[\boldsymbol{\varphi}(x), \boldsymbol{P}^\mu] = i\partial^\mu \boldsymbol{\varphi}(x). \tag{11.35}$$

CHAPTER 12

The Fock space

12.1. Exponential Hilbert space

Let $\mathfrak{h}$ be a Hilbert space. Following Friedrichs[1], define the exponential of $\mathfrak{h}$ — the Hilbert space $\mathfrak{H} = e^{\mathfrak{h}}$ — as the following direct sum of Hilbert spaces,

$$\mathfrak{H} = \bigoplus_{n=0}^{\infty} \mathfrak{H}_n, \quad \text{where} \quad \mathfrak{H}_0 = \mathbb{C} \text{ and } \mathfrak{H}_n = \frac{1}{n!}\mathfrak{h}^{\otimes n}.$$

The factor $1/n!$ symbolizes that the norm in $\mathfrak{H}_n$ is defined by

$$\|u_1 \otimes \cdots \otimes u_n\|^2_{\mathfrak{H}_n} = \frac{1}{n!}\|u_1\|^2_{\mathfrak{h}} \cdots \|u_n\|^2_{\mathfrak{h}}.$$

In particular, let $\mathfrak{h} = L^2(X, d\mu)$, where $(X, d\mu)$ is a measure space. Since

$$\mathfrak{h}^{\otimes n} \simeq L^2(\underbrace{X \times \cdots \times X}_{n}, \underbrace{d\mu \times \cdots \times d\mu}_{n}) = L^2(X^n, d^n\mu)$$

every $F \in \mathfrak{H}$ is represented by an infinite vector

$$F = (F_0, F_1, \ldots, F_n, \ldots), \quad \text{where} \quad F_n \in \mathfrak{H}_n = L^2(X^n, d^n\mu)$$

and

$$\|F\|^2 = |F_0|^2 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{X^n} |F_n(x_1, \ldots, x_n)|^2 d\mu(x_1) \cdots d\mu(x_n) < \infty. \tag{12.1}$$

The symmetric group Sym_n acts on $\mathfrak{h}^{\otimes n}$ by

$$\sigma(u_1 \otimes \cdots \otimes u_n) = u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(n)},$$

and we denote by S_n orthogonal projection of $\mathfrak{H}_n$ onto the symmetric subspace of $\mathfrak{h}^{\otimes n}$,

$$\mathrm{S}_n(u_1 \otimes \cdots \otimes u_n) = \frac{1}{n!} \sum_{\sigma \in \mathrm{Sym}_n} u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(n)}.$$

[1]See K. O. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields*, Interscience, New York, 1953.

Definition. The *bosonic Fock space* $\mathscr{F}_B$ associated with the Hilbert space $\mathfrak{h}$ is a graded Hilbert space

$$\mathscr{F}_B = \bigoplus_{n=0}^{\infty} \mathscr{F}_n, \quad \text{where} \quad \mathscr{F}_n = \mathrm{S}_n \mathfrak{H}_n.$$

We denote by $(\ ,\ )_{\mathfrak{h}}$ the inner product in $\mathfrak{h}$, by $(\ ,\ )_{\mathscr{F}_n}$ — the inner product in $\mathscr{F}_n$ and by $(\ ,\ )$ — the inner product in $\mathscr{F}_B$. It is given by formula (12.1), where F_n are symmetric functions of their arguments.

For the case of free scalar relativistic particle of mass m we have

$$\mathfrak{h} = L^2(\mathcal{O}_m^+, d\mu), \quad d\mu_{\boldsymbol{k}} = \frac{d^3\boldsymbol{k}}{2\sqrt{\boldsymbol{k}^2 + m^2}},$$

so that $\mathfrak{h}$ is a one-particle Hilbert space and $\mathscr{F}_n$ is the n-particle space. The Fock space $\mathscr{F}_B$ contains a nuclear subspace $\mathscr{S}$ consisting of finite sequences $F = (F_0, F_1, \dots, F_n, \dots)$ with Schwartz class functions f_n, and we have a Gelfand triple

$$\mathscr{S} \subsetneqq \mathscr{F}_B \subsetneqq \mathscr{S}'.$$

Similarly, one defines

Definition. The *fermion Fock space* $\mathscr{F}_F$ associated with the Hilbert space $\mathfrak{h}$ is a graded Hilbert space

$$\mathscr{F}_F = \bigoplus_{n=0}^{\infty} \mathscr{A}_n,$$

where $\mathscr{A}_n = \mathrm{Alt}_n \mathfrak{H}_n$ is the orthogonal projection of $\mathfrak{H}_n$ onto the totally anti-symmetric subspace of $\mathfrak{h}^{\otimes n}$,

$$\mathrm{Alt}_n(u_1 \otimes \cdots \otimes u_n) = \frac{1}{n!} \sum_{\sigma \in \mathrm{Sym}_n} (-1)^{\varepsilon(\sigma)} u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(n)}.$$

In the next chapter, we describe the fermion Fock space for the spinor field, associated with the Dirac equation.

12.2. Creation and annihilation operators

We start with the bosonic Fock space, denoted here simply by $\mathscr{F}$. For $f \in \mathfrak{h}$ define operators $\boldsymbol{a}(f)$ and $\boldsymbol{a}^\dagger(f)$ on $\mathscr{F}$ by the following formulas

$$(\boldsymbol{a}(f)F)_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n) = \int_{\mathbb{R}^3} f(\boldsymbol{k}) F_{n+1}(\boldsymbol{k}, \boldsymbol{k}_1, \dots, \boldsymbol{k}_n) d\mu_{\boldsymbol{k}}, \tag{12.2}$$

$$(\boldsymbol{a}^\dagger(f)F)_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n) = \sum_{l=1}^{n} f(\boldsymbol{k}_l) F_{n-1}(\boldsymbol{k}_1, \dots, \hat{\boldsymbol{k}}_l, \dots, \boldsymbol{k}_n). \tag{12.3}$$

Domains of $\boldsymbol{a}(f)$ and $\boldsymbol{a}^\dagger(f)$ contain the dense subspace $\mathscr{F}_c$ of finite sequences. The operators $\boldsymbol{a}^\dagger(f)$ have graded degree $+1$, i.e. they satisfy $\boldsymbol{a}^\dagger(f) : \mathscr{F}_n \to \mathscr{F}_{n+1}$, while operators $\boldsymbol{a}(f)$ satisfy $\boldsymbol{a}(f) : \mathscr{F}_n \to \mathscr{F}_{n-1}$ and have degree -1.

The vector

$$\Phi = (1, 0, \dots, 0, \dots) \in \mathscr{F}$$

— the *vacuum vector* — has the property

$$\boldsymbol{a}(f)\Phi = 0 \quad \text{for all} \quad f \in \mathfrak{h}.$$

Conversely, if a vector $F \in \mathscr{F}$ satisfies $\boldsymbol{a}(f)F = 0$ for all $f \in \mathfrak{h}$ then it follows from (12.2) that $F = c\Phi$, where $c \in \mathbb{C}$. It follows from (12.3) that

$$\boldsymbol{a}^\dagger(f_1)\cdots\boldsymbol{a}^\dagger(f_n)\Phi = n!\mathrm{S}_n\left(f_1 \otimes \cdots \otimes f_n\right) = f_1 \odot \cdots \odot f_n \tag{12.4}$$

— a commutative product in the symmetric algebra of $\mathfrak{h}$. Therefore, a linear span of the vectors $\boldsymbol{a}^\dagger(f_1)\cdots\boldsymbol{a}^\dagger(f_n)\Phi$ is dense in $\mathscr{F}_n$. We also have

$$(\boldsymbol{a}^\dagger(f_1)\cdots\boldsymbol{a}^\dagger(f_n)\Phi, \boldsymbol{a}^\dagger(g_1)\cdots\boldsymbol{a}^\dagger(g_n)\Phi) = (F_n, G_n)_{\mathscr{F}_n}, \tag{12.5}$$

where $F_n = f_1 \odot \cdots \odot f_n$, $G_n = g_1 \odot \cdots \odot g_n$. Also note, that according to (12.1),

$$(F_n, G_n)_{\mathscr{F}_n} = \frac{1}{n!}\int_{R^{3n}} F_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n)\overline{G_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n)}d\mu_{\boldsymbol{k}_1}\cdots d\mu_{\boldsymbol{k}_n} = \mathrm{perm}(A)$$

— the permanent of the matix $a_{ij} = (f_i, g_j)_{\mathfrak{h}}$.

Remark 12.1. In physics textbooks, it is customary to ignore the factors $n!$ in the definition (12.1) of the norm in the Hilbert space $\mathfrak{H} = e^{\mathfrak{h}}$. Correspondingly, the operators $\boldsymbol{a}(f)$ and $\boldsymbol{a}^\dagger(f)$ are then defined by the formulas

$$(\boldsymbol{a}(f)F)_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n) = \sqrt{n+1}\int_{\mathbb{R}^3} f(\boldsymbol{k})F_{n+1}(\boldsymbol{k}, \boldsymbol{k}_1, \dots, \boldsymbol{k}_n)d\mu_{\boldsymbol{k}},$$
$$(\boldsymbol{a}^\dagger(f)F)_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n) = \frac{1}{\sqrt{n}}\sum_{l=1}^{n} f(\boldsymbol{k}_l)F_{n-1}(\boldsymbol{k}_1, \dots, \hat{\boldsymbol{k}}_l, \dots, \boldsymbol{k}_n).$$

Also, in this normalization, the functions $F_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n) = \mathrm{perm}\{(f_i(\boldsymbol{k}_j)\}$ are replaced by $\mathrm{perm}\{(f_i(\boldsymbol{k}_j)\}/\sqrt{n!}$.

Proposition 12.1. *The following properties hold.*

(i) *On the domain* $\mathscr{F}_c$ *the operators* $\boldsymbol{a}(f)$ *and* $\boldsymbol{a}^\dagger(f)$ *satisfy commutation relations*

$$[\boldsymbol{a}(f),\boldsymbol{a}(g)]=0,\quad [\boldsymbol{a}^\dagger(f),\boldsymbol{a}^\dagger(g)]=0,\quad [\boldsymbol{a}(f),\boldsymbol{a}^\dagger(g)]=(f,\bar{g})_{\mathfrak{h}}I, \tag{12.6}$$

where I *is the identity operator on* $\mathscr{F}$.

(ii) *Symmetric operators*

$$\boldsymbol{Q}(f)=\frac{1}{\sqrt{2}}(\boldsymbol{a}(f)+\boldsymbol{a}^\dagger(\bar{f}))\quad\textit{and}\quad \boldsymbol{P}(f)=\frac{1}{i\sqrt{2}}(\boldsymbol{a}(f)-\boldsymbol{a}^\dagger(\bar{f}))$$

on $\mathscr{F}_c$ *have defect indices* $(0,0)$ *and thus admit unique self-adjoint extensions. In particular,* $\boldsymbol{a}^\dagger(\bar{f})$ *is the adjoint operator to* $\boldsymbol{a}(f)$.

Proof. The first two commutation relations in (12.6) are trivial. To prove the third relation we compute, using (12.2)–(12.3),

$$\begin{aligned}(\boldsymbol{a}^\dagger(g)\boldsymbol{a}(f)F)_n(\boldsymbol{k}_1,\dots,\boldsymbol{k}_n)&=\sum_{l=1}^n g(\boldsymbol{k}_l)(\boldsymbol{a}(f)F)_{n-1}(\boldsymbol{k}_1,\dots,\hat{\boldsymbol{k}}_l,\dots,\boldsymbol{k}_n)\\&=\sum_{l=1}^n g(\boldsymbol{k}_l)\int_{\mathbb{R}^3} f(\boldsymbol{k})F_n(\boldsymbol{k},\boldsymbol{k}_1,\dots,\hat{\boldsymbol{k}}_l,\dots,\boldsymbol{k}_n)d\mu_{\boldsymbol{k}}\end{aligned}$$

and

$$\begin{aligned}(\boldsymbol{a}(f)\boldsymbol{a}^\dagger(g)F)_n(\boldsymbol{k}_1,\dots,\boldsymbol{k}_n)&=\int_{\mathbb{R}^3} f(\boldsymbol{k})(\boldsymbol{a}^\dagger(g)F)_{n+1}(\boldsymbol{k},\boldsymbol{k}_1,\dots,\boldsymbol{k}_n)d\mu_{\boldsymbol{k}}\\&=\int_{\mathbb{R}^3} f(\boldsymbol{k})g(\boldsymbol{k})d\mu_{\boldsymbol{k}}\cdot F_n(\boldsymbol{k}_1,\dots,\boldsymbol{k}_n)\\&\quad+\sum_{l=1}^n g(\boldsymbol{k}_l)\int_{\mathbb{R}^3} f(\boldsymbol{k})F_n(\boldsymbol{k},\boldsymbol{k}_1,\dots,\hat{\boldsymbol{k}}_l,\dots,\boldsymbol{k}_n)d\mu_{\boldsymbol{k}},\end{aligned}$$

which yields

$$[\boldsymbol{a}(f),\boldsymbol{a}^\dagger(g)](F)=(f,\bar{g})_{\mathfrak{h}}F.$$

Next we check that for $F,G\in\mathscr{F}_c$

$$(\boldsymbol{a}(f)F,G)=(F,\boldsymbol{a}^\dagger(\bar{f})G). \tag{12.7}$$

Indeed we have

$$\begin{aligned}
&(\boldsymbol{a}(f)F, G) = \\
&\sum_{n=0}^{\infty} \frac{1}{n!} \int_{\mathbb{R}^{3(n+1)}} f(\boldsymbol{k}) F_{n+1}(\boldsymbol{k}, \boldsymbol{k}_1, \ldots, \boldsymbol{k}_n) \overline{G_n(\boldsymbol{k}_1, \ldots, \boldsymbol{k}_n)} d\mu_{\boldsymbol{k}} \prod_{j=1}^{n} d\mu_{\boldsymbol{k}_j} \\
&= \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \int_{\mathbb{R}^{3n}} f(\boldsymbol{k}_1) F_n(\boldsymbol{k}_1, \ldots, \boldsymbol{k}_n) \overline{G_{n-1}(\boldsymbol{k}_2, \ldots, \boldsymbol{k}_n)} \prod_{j=1}^{n} d\mu_{\boldsymbol{k}_j} \\
&= \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{R}^{3n}} F_n(\boldsymbol{k}_1, \ldots, \boldsymbol{k}_n) \sum_{l=1}^{n} \overline{\bar{f}(\boldsymbol{k}_l) G_{n-1}(\boldsymbol{k}_1, \ldots, \hat{\boldsymbol{k}}_l, \ldots \boldsymbol{k}_n)} \prod_{j=1}^{n} d\mu_{\boldsymbol{k}_j} \\
&= (F, \boldsymbol{a}^{\dagger}(\bar{f})G),
\end{aligned}$$

where we used that the functions F_n, G_n are symmetric. The rest of the proof of (ii) is left as an exercise[2]. □

COROLLARY 12.1. *Formula* (12.5) *can also be derived from canonical commutation relations* (12.6), *equation* (12.7), *and the normalization* $\|\Phi\| = 1$.

PROOF. It is sufficient to consider the special case when $f_1 = g_1, \ldots, f_n = g_n$ are mutually orthogonal. Then since $a(\bar{f}_i)$ commutes with $a^{\dagger}(f_j)$ for $i \neq j$, we have

$$\begin{aligned}
&(\boldsymbol{a}^{\dagger}(f_1) \cdots \boldsymbol{a}^{\dagger}(f_n)\Phi, \boldsymbol{a}^{\dagger}(f_1) \cdots \boldsymbol{a}^{\dagger}(f_n)\Phi) \\
&= (\Phi, \boldsymbol{a}(\bar{f}_n) \cdots \boldsymbol{a}(\bar{f}_1)\boldsymbol{a}^{\dagger}(f_1) \cdots \boldsymbol{a}^{\dagger}(f_n)\Phi) \\
&= \|f_1\|^2 (\Phi, \boldsymbol{a}(\bar{f}_n) \cdots \boldsymbol{a}(\bar{f}_2)\boldsymbol{a}^{\dagger}(f_2) \cdots \boldsymbol{a}^{\dagger}(f_n)\Phi) \\
&= \|f_1\|^2 \cdots \|f_n\|^2 = \|f_1 \odot \cdots \odot f_n)\|^2_{\mathscr{F}_n}.
\end{aligned}$$ □

For an orthonormal basis $\{e_i\}_{i=1}^{\infty}$ in $\mathfrak{h}$ consider an operator

$$\boldsymbol{N} = \sum_{i=1}^{\infty} \boldsymbol{a}^{\dagger}(e_i)\boldsymbol{a}(\bar{e}_i). \tag{12.8}$$

We have $\boldsymbol{N}F_0 = 0$ and

$$(\boldsymbol{N}F)_1(\boldsymbol{k}) = \sum_{i=1}^{\infty} e_i(\boldsymbol{k}) \int_{\mathbb{R}^3} F_1(\boldsymbol{k})\overline{e_i(\boldsymbol{k})} d\mu_{\boldsymbol{k}} = F_1(\boldsymbol{k}).$$

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[2]See F.A. Berezin, *The method of second quantization*, Academic Press, 1966.

In general, denoting

$$c_i(\boldsymbol{k}_1,\ldots,\hat{\boldsymbol{k}}_l,\ldots,\boldsymbol{k}_n)=\int_{\mathbb{R}^3}F_n(\boldsymbol{k},\boldsymbol{k}_1,\ldots,\hat{\boldsymbol{k}}_l,\ldots,\boldsymbol{k}_n)\overline{e_i(\boldsymbol{k})}d\mu_{\boldsymbol{k}},$$

we obtain

$$\begin{aligned}(\boldsymbol{N}F)_n(\boldsymbol{k}_1,\ldots,\boldsymbol{k}_n)&=\sum_{i=1}^{\infty}\sum_{l=1}^{n}e_i(\boldsymbol{k}_l)c_i(\boldsymbol{k}_1,\ldots,\hat{\boldsymbol{k}}_l,\ldots,\boldsymbol{k}_n)\\&=nF_n(\boldsymbol{k}_1,\ldots,\boldsymbol{k}_n).\end{aligned}$$

Thus we see that $\boldsymbol{N}$ is a number of a particles operator and does not depend on the choice of an orthonormal basis for $\mathfrak{h}$. It is a self-adjoint operator on $\mathscr{F}$ such that

$$\boldsymbol{N}|_{\mathscr{F}_n}=nI|_{\mathscr{F}_n},$$

and its domain consists of $F\in\mathscr{F}$ with the property

$$\sum_{n=1}^{\infty}\frac{n^2}{n!}\|f_n\|^2_{\mathscr{F}_n}<\infty$$

Remark 12.2. It follows from (12.2)–(12.3) that common domain of operators $\boldsymbol{a}^\dagger(f),\boldsymbol{a}(f)$ contains $F\in\mathscr{F}$ such that

$$\langle F,\boldsymbol{N}F\rangle<\infty.$$

Similarly, fermion creation-annihilation operators in $\mathscr{F}_F$ are defined by the same formulas (12.2)–(12.3), where now all functions F_n are totally anti-symmetric and into the sum in (12.3) we need to insert alternating sign $(-1)^{l-1}$. Thus we have

$$\boldsymbol{a}^\dagger(f_1)\cdots\boldsymbol{a}^\dagger(f_n)\Phi=n!\mathrm{Alt}_n(f_1\otimes\cdots\otimes f_n)=f_1\wedge\cdots\wedge f_n. \tag{12.9}$$

Equivalently, we can define creation and annihilation operators by the following explicit formulas

$$\boldsymbol{a}(f)(u_1\wedge\cdots\wedge u_n)=\sum_{i=1}^{n}(-1)^{i-1}(f,\bar{u}_i)u_1\wedge\cdots\wedge\widehat{u_i}\wedge\cdots\wedge u_n, \tag{12.10}$$

$$\boldsymbol{a}^\dagger(f)(u_1\wedge\cdots\wedge u_n)=f\wedge u_1\wedge\cdots\wedge u_n. \tag{12.11}$$

The following analog of the Proposition 12.1 holds.

PROPOSITION 12.2. *The operators* $a(f)$ *and* $a^{\dagger}(f)$ *are bounded operators on* $\mathscr{F}_F$*,* $a^*(f) = a^{\dagger}(\bar{f})$*, that satisfy canonical anticommutation relations*

$$\begin{aligned} [\boldsymbol{a}(f), \boldsymbol{a}(g)]_+ = 0, \quad [\boldsymbol{a}^{\dagger}(f), \boldsymbol{a}^{\dagger}(g)]_+ = 0, \\ [\boldsymbol{a}(f), \boldsymbol{a}^{\dagger}(g)]_+ = (f, \bar{g})_{\mathfrak{h}} I, \end{aligned} \tag{12.12}$$

where I *is the identity operator on* $\mathscr{F}_F$*.*

PROOF. Indeed, using formulas (12.2)–(12.3) with totally anti-symmetric functions F_n, the same arguments as in the proof of Proposition 12.1 show that (12.2) are valid on the dense subset of finite sequences F in $\mathscr{F}_F$. Also we have $(a(f)F, G) = (F, a^{\dagger}(\bar{f})G)$ for such vectors F and G. Using this formula and the the relation

$$a(f)a^{\dagger}(\bar{f})F + a^{\dagger}(\bar{f})a(f)F = F$$

for finite sequence F and $\|f\|_{\mathfrak{h}} = 1$, we obtain

$$\|a^{\dagger}(\bar{f})F\|^2 + \|a(f)F\|^2 = \|F\|^2,$$

so $\|a^{\dagger}(\bar{f})F\|, \|a(f)F\| \leq \|F\|$ on the dense linear subspace in $\mathscr{F}_F$. Therefore, $a(f)$ and $a^{\dagger}(f)$ extend to bounded operators on $\mathscr{F}_F$. □

12.3. Representations of canonical commutation relations

PROPOSITION 12.3. *Every bounded operator* B *on* $\mathscr{F}$ *which commutes with all* $\boldsymbol{a}(f)$ *and* $\boldsymbol{a}^{\dagger}(f)$ *is a multiple of the identity operator* I*.*

PROOF. By definition, we have

$$Be^{s\boldsymbol{Q}(f)} = e^{s\boldsymbol{Q}(f)}B \quad \text{and} \quad Be^{s\boldsymbol{P}(f)} = e^{s\boldsymbol{P}(f)}B$$

for all $s \in \mathbb{R}$ and $f \in \mathfrak{h}$. By Stone theorem, this implies that if $F \in D(\boldsymbol{Q}(f))$ then also $BF \in D(\boldsymbol{Q}(f))$ and $B\boldsymbol{Q}(f)F = \boldsymbol{Q}(f)BF$, and similar statement holds for operators $\boldsymbol{P}(f)$. Thus if $F \in D(\boldsymbol{a}(f))$ then also $BF \in D(\boldsymbol{a}(f))$ and $B\boldsymbol{a}(f)F = \boldsymbol{a}(f)BF$ and similar statement holds for operators $\boldsymbol{a}^{\dagger}(f)$. in particular, $B\Phi \in D(\boldsymbol{a}(f))$ and

$$\boldsymbol{a}(f)B\Phi = B\boldsymbol{a}(f)\Phi = 0.$$

However, it follows from the definition (12.2) that the only solution of the equation $\boldsymbol{a}(f)F = 0$ is $F = c\Phi$, $c \in \mathbb{C}$, so that

$$B\Phi = c\Phi$$

and we obtain

$$B\boldsymbol{a}^{\dagger}(f_1)\cdots\boldsymbol{a}^{\dagger}(f_n)\Phi=\boldsymbol{a}^{\dagger}(f_1)\cdots\boldsymbol{a}^{\dagger}(f_n)B\Phi=c\boldsymbol{a}^{\dagger}(f_1)\cdots\boldsymbol{a}^{\dagger}(f_n)\Phi.$$

Since the linear span of the vectors $\boldsymbol{a}^{\dagger}(f_1)\cdots\boldsymbol{a}^{\dagger}(f_n)F_0$ is dense in $\mathscr{F}_n$, $B=cI$. □

Such representation of canonical commutation relations (12.6) is called *irreducible*. Unlike the case of finitely many degrees of the freedom, the analog of Stone-von Neumann theorem does not hold for infinitely many degrees of freedom[3]. However, the following statement remedies the situation.

THEOREM 12.2. *Every irreducible representation of canonical commutation relations* (12.6) *with a vacuum vector is unitary equivalent to the Fock space representation.*

PROOF. Suppose that $\mathscr{H}$ is a Hilbert space in which a representation of canonical commutation relations (12.6) with creation-annihilation operators $\tilde{\boldsymbol{a}}(f)$ and $\tilde{\boldsymbol{a}}^{\dagger}(f)$ is realized, and let $\tilde{\Phi}$ be a vacuum vector. Since this representation is irreducible, the closure of a linear span of vectors

$$\tilde{\boldsymbol{a}}^{\dagger}(f_1)\cdots\tilde{\boldsymbol{a}}^{\dagger}(f_n)\tilde{\Phi} \tag{12.13}$$

is the n-particle space $\mathscr{H}_n$. To each such vector consider the vector $F_n=S_n(f_1\otimes\cdots\otimes f_n)\in\mathscr{F}_n$. As in the derivation of (12.5), from the canonical commutation relations and normalization $\|\tilde{\Phi}\|=1$ we obtain

$$(\tilde{\boldsymbol{a}}^{\dagger}(f_1)\cdots\tilde{\boldsymbol{a}}^{\dagger}(f_n)\tilde{\Phi},\tilde{\boldsymbol{a}}^{\dagger}(g_1)\cdots\tilde{\boldsymbol{a}}^{\dagger}(g_n)\tilde{\Phi})_{\mathscr{H}_n}=(F_n,G_n)_{\mathscr{F}_n}, \tag{12.14}$$

where $G_n=S_n(g_1\otimes\cdots\otimes g_n)\in\mathscr{F}_n$. This allows to define a unitary operator $U:\mathscr{H}_n\to\mathscr{F}_n$ by

$$U(\tilde{\boldsymbol{a}}^{\dagger}(f_1)\cdots\tilde{\boldsymbol{a}}^{\dagger}(f_n)\tilde{\Phi})=F_n.$$

Indeed, property (12.14) shows that if $c_1v_1+\cdots+c_mv_m=0$, where v_i are given by (12.13), then $c_1U(v_1)+\cdots+c_mU(v_m)=0$, so that the map U is well-defined. □

Same results hold for the representations of canonical anti-commutation relations (12.12).

[3]See the papers L. Gårding and A. Wightman, *Representations of the commutation relations*, Proc. Nat. Acad. Sci. USA, **40** №7 (1954), 622–62 and I.E. Segal, *Distributions in Hilbert space and canonical systems of operators*, Trans. Amer. Math. Soc. **88** №1 (1958), 12–76 and the book I.M. Gelfand and N.Ya. Vilenkin, *Generalized functions*, vol. **4**, 1964.

12.4. In physics notations

Here we make a connection with operator-valued distributions $\boldsymbol{a}^\dagger(\boldsymbol{k})$ and $\boldsymbol{a}(\boldsymbol{k})$, introduced in Chapter 11. We have

$$\boldsymbol{a}(f) = \int_{\mathbb{R}^3} f(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k})d\mu_{\boldsymbol{k}},$$
$$\boldsymbol{a}^\dagger(f) = \int_{\mathbb{R}^3} f(\boldsymbol{k})\boldsymbol{a}^\dagger(\boldsymbol{k})d\mu_{\boldsymbol{k}}$$

so that the vacuum state $|0\rangle$ corresponds to the vector Φ and smeared n-particle states

$$\frac{1}{n!}\int_{\mathbb{R}^{3n}} F_n(\boldsymbol{k}_1,\dots,\boldsymbol{k}_n)\boldsymbol{a}^\dagger(\boldsymbol{k}_1)\cdots\boldsymbol{a}^\dagger(\boldsymbol{k}_n)|0\rangle d\mu_{\boldsymbol{k}_1}\cdots d\mu_{\boldsymbol{k}_n}$$

correspond to the vectors

$$F = (0,\dots,0,\underbrace{F_n(\boldsymbol{k}_1,\dots,\boldsymbol{k}_n)}_{n\text{-th place}},0,\dots) \in \mathscr{F}.$$

Conversely, the operator-valued distributions $\boldsymbol{a}^\dagger(\boldsymbol{k})$ and $\boldsymbol{a}(\boldsymbol{k})$ can be formally defined by

$$\boldsymbol{a}^\dagger(\boldsymbol{k}) = \boldsymbol{a}^\dagger(f_{\boldsymbol{k}}) \quad\text{and}\quad \boldsymbol{a}(\boldsymbol{k}) = \boldsymbol{a}(f_{\boldsymbol{k}}), \tag{12.15}$$

where $f_{\boldsymbol{k}}(\boldsymbol{p}) = 2\omega_{\boldsymbol{k}}\delta(\boldsymbol{k}-\boldsymbol{p})$. Formulas (12.2)–(12.3) give

$$(\boldsymbol{a}(\boldsymbol{k})F)_n(\boldsymbol{k}_1,\dots,\boldsymbol{k}_n) = F_{n+1}(\boldsymbol{k},\boldsymbol{k}_1,\dots,\boldsymbol{k}_n), \tag{12.16}$$

$$(\boldsymbol{a}^\dagger(\boldsymbol{k})F)_n(\boldsymbol{k}_1,\dots,\boldsymbol{k}_n) = 2\sum_{l=1}^n \omega_{\boldsymbol{k}}\delta(\boldsymbol{k}-\boldsymbol{k}_l)F_{n-1}(\boldsymbol{k}_1,\dots,\hat{\boldsymbol{k}}_l,\dots,\boldsymbol{k}_n), \tag{12.17}$$

so that $\boldsymbol{a}^\dagger(\boldsymbol{k})$ can be thought of as an operator from $\mathscr{S}$ to $\mathscr{S}'$ and $\boldsymbol{a}(\boldsymbol{k})$ — as an operator-valued distribution. The states

$$|\boldsymbol{k}_1,\dots,\boldsymbol{k}_n\rangle = \boldsymbol{a}^\dagger(\boldsymbol{k}_1)\cdots\boldsymbol{a}^\dagger(\boldsymbol{k}_n)|0\rangle$$

correspond to the vectors

$$F(\boldsymbol{k}_1,\dots,\boldsymbol{k}_n) = (0,\dots,0,\underbrace{F_n(\boldsymbol{k}_1,\dots,\boldsymbol{k}_n;\boldsymbol{p}_1,\dots,\boldsymbol{p}_n)}_{n\text{-th place}},0,\dots) \in \mathscr{S}'$$

where

$$F_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n; \boldsymbol{p}_1, \dots, \boldsymbol{p}_n) = \sum_{\sigma \in \mathrm{Sym}_n} \prod_{l=1}^{n} 2\omega_{\boldsymbol{p}_l} \delta(\boldsymbol{p}_l - \boldsymbol{k}_{\sigma(l)})$$

are distributions, parameterized by $\boldsymbol{k}_1, \dots, \boldsymbol{k}_n$. Evaluating $\boldsymbol{a}(k)|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle$ and $\boldsymbol{a}^\dagger(k)|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle$ by formulas (12.16)–(12.17) gives back formulas (11.23)–(11.24) in Lecture 11.

As another example, using (12.16)–(12.17) we get

$$\begin{aligned}(\boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k})F)_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n) &= 2\sum_{l=1}^{n} \omega_{\boldsymbol{k}} \delta(\boldsymbol{k} - \boldsymbol{k}_l) F_n(\boldsymbol{k}, \boldsymbol{k}_1, \dots, \hat{\boldsymbol{k}}_l, \dots, \boldsymbol{k}_n) \\ &= 2\sum_{l=1}^{n} \omega_{\boldsymbol{k}} \delta(\boldsymbol{k} - \boldsymbol{k}_l) F_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n),\end{aligned}$$

so that the product in the opposite order $\boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k})$ of creation and annihilation operators at coincident points makes sense as an operator-valued distribution.

Quantum Hamiltonian

$$\begin{aligned}\boldsymbol{H} &= \frac{1}{2}\int_{\mathbb{R}^3} \boldsymbol{:}\big(\boldsymbol{\pi}^2(\boldsymbol{x}) + (\boldsymbol{\nabla}\boldsymbol{\varphi})^2(\boldsymbol{x}) + m^2\boldsymbol{\varphi}^2(\boldsymbol{x})\big)\boldsymbol{:}\, d^3\boldsymbol{x} \\ &= \int_{\mathbb{R}^3} \omega_{\boldsymbol{k}} \boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) d\mu_{\boldsymbol{k}},\end{aligned}$$

introduced in Lecture 11, is a well-defined operator on $\mathscr{F}$. Indeed,

$$(\boldsymbol{H}F)_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n) = \sum_{l=1}^{n} \omega_{\boldsymbol{k}_l} F_n(\boldsymbol{k}_1, \dots, \boldsymbol{k}_n)$$

so that $\boldsymbol{H}$ is a multiplication by the function $\sum_{l=1}^{n} \omega_{\boldsymbol{k}_l}$ operator on $\mathscr{F}_n$. Similarly, the total momentum operator components

$$\boldsymbol{P}^j = \int_{\mathbb{R}^3} \boldsymbol{:}\boldsymbol{\pi}(\boldsymbol{x})\partial^j\boldsymbol{\varphi}(\boldsymbol{x})\boldsymbol{:}\, d^3\boldsymbol{x} = \int_{\mathbb{R}^3} k^j \boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k})\, d\mu_{\boldsymbol{k}}$$

are well-defined on $\mathscr{F}$, preserve the grading and act as multiplication by the functions $\sum_{l=1}^{n} k_l^j$ operators on $\mathscr{F}_n$. The states $|\boldsymbol{k}_1, \dots, \boldsymbol{k}_n\rangle$ are generalized eigenfunctions for the operators $\boldsymbol{H}$ and $\boldsymbol{P}$. Finally, operator (12.8) coincides with the introduced in in Lecture 11 the number of particles operator

$$\boldsymbol{N} = \int_{\mathbb{R}^3} \boldsymbol{a}^\dagger(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k})\, d\mu_{\boldsymbol{k}}.$$

PROBLEM 12.1. Prove Corollary 12.1.

PROBLEM 12.2. Show that $\boldsymbol{P}^\mu$ and $\boldsymbol{M}^{\mu\nu}$, $\mu,\nu = 0,1,2,3$, where $\boldsymbol{P}^0 = \boldsymbol{H}$ and

$$\boldsymbol{M}^{ij} = \int_{\mathbb{R}^3} \boldsymbol{:} (x^i \boldsymbol{\pi}(\boldsymbol{x})\partial^j \boldsymbol{\varphi}(\boldsymbol{x}) - x^j \boldsymbol{\pi}(\boldsymbol{x})\partial^i \boldsymbol{\varphi}(\boldsymbol{x})) \boldsymbol{:} d^3\boldsymbol{x},$$
$$\boldsymbol{M}^{0i} = \frac{1}{2}\int_{\mathbb{R}^3} x^i \boldsymbol{:} \big(\boldsymbol{\pi}^2(\boldsymbol{x}) + (\boldsymbol{\nabla}\boldsymbol{\varphi})^2(\boldsymbol{x}) + m^2\boldsymbol{\varphi}^2(\boldsymbol{x})\big) \boldsymbol{:} d^3\boldsymbol{x},$$

$\boldsymbol{M}^{i0} = -\boldsymbol{M}^{0i}$, define a representation of the Poincaré algebra in $\mathscr{F}$ (from the last semester course on the classical field theory).

CHAPTER 13

Correlation functions of free quantum fields

13.1. Free quantum field

Recall that the free scalar quantum field $\boldsymbol{\varphi}(x)$ of mass m is given by formula (11.22) from Chapter 11,

$$\begin{aligned}\boldsymbol{\varphi}(x) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \left(e^{ik\cdot x} \boldsymbol{a}^\dagger(\boldsymbol{k}) + e^{-ik\cdot x} \boldsymbol{a}(\boldsymbol{k}) \right) d\mu_{\boldsymbol{k}} \\ &= \boldsymbol{\varphi}^+(x) + \boldsymbol{\varphi}^-(x), \quad k_0 = \omega_{\boldsymbol{k}} = \sqrt{\boldsymbol{k}^2 + m^2},\end{aligned}$$

where

$$\boldsymbol{\varphi}^+(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{ik\cdot x} \boldsymbol{a}^\dagger(\boldsymbol{k}) d\mu_{\boldsymbol{k}}, \tag{13.1}$$

and

$$\boldsymbol{\varphi}^-(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-ik\cdot x} \boldsymbol{a}(\boldsymbol{k}) d\mu_{\boldsymbol{k}} \tag{13.2}$$

are, respectively, positive and negative frequency components of the quantum field $\boldsymbol{\varphi}(x)$. Component $\boldsymbol{\varphi}^+(x)$ creates a particle at $\boldsymbol{x}$ at time x^0, while component $\boldsymbol{\varphi}^-(x)$ annihilates it[1]. The quantum fields $\boldsymbol{\varphi}^\pm(x)$ satisfy

$$\boldsymbol{\varphi}^-(x)|0\rangle = 0 \tag{13.3}$$

and

$$\boldsymbol{\varphi}^-(x)^\dagger = \boldsymbol{\varphi}^+(x), \tag{13.4}$$

[1]Our notations $\boldsymbol{\varphi}^\pm(x)$ are the same as in the textbook by N.N. Bogoliubov and D.V. Shirkov, *Quantum Fields*, Benjamin/Cummings Co., 1982. They reflect the fundamental fact that $\boldsymbol{\varphi}^+(x)$ creates particles while $\boldsymbol{\varphi}^-(x)$ destroys them. In modern textbooks these components are often denoted by $\boldsymbol{\varphi}^\mp(x)$ since because of $E = i\partial_0$ our field $\boldsymbol{\varphi}^+(x)$ corresponds to negative energy solutions of the Klein-Gordon equation, and $\boldsymbol{\varphi}^-(x)$— to positive energy solutions.

so that $\boldsymbol{\varphi}(x) = \boldsymbol{\varphi}^{+}(x)+\boldsymbol{\varphi}^{-}(x)$ is a self-adjoint operator (rather an operator-valued distribution).

The following result is fundamental.

LEMMA 13.1. *Quantum field satisfy commutation relations*

$$[\boldsymbol{\varphi}(x), \boldsymbol{\varphi}(y)] = -iD(x-y)I, \tag{13.5}$$

where

$$\begin{aligned} D(x) &= \frac{i}{(2\pi)^3}\int_{\mathbb{R}^3}(e^{-ik\cdot x} - e^{ik\cdot x})d\mu_{\boldsymbol{k}} \\ &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\sin\omega_{\boldsymbol{k}}x^0 e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\frac{d^3\boldsymbol{k}}{\omega_{\boldsymbol{k}}} \end{aligned} \tag{13.6}$$

is the Pauli-Jordan function. In particular, when $x, y \in \mathbb{R}^4$ are spacelike separated, i.e. $(x-y)^2 < 0$,

$$[\boldsymbol{\varphi}(x), \boldsymbol{\varphi}(y)] = 0.$$

The latter property is called local commutativity *or* microscopic causality.

PROOF. It follows from (11.22) and canonical commutation relations that

$$\begin{aligned} [\boldsymbol{\varphi}(x), \boldsymbol{\varphi}(y)] &= [\boldsymbol{\varphi}^{+}(x), \boldsymbol{\varphi}^{-}(y)] + [\boldsymbol{\varphi}^{-}(x), \boldsymbol{\varphi}^{+}(y)] \\ &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} e^{i(k\cdot x - p\cdot y)}[\boldsymbol{a}^{\dagger}(\boldsymbol{k}), \boldsymbol{a}(\boldsymbol{p})]d\mu_{\boldsymbol{k}}d\mu_{\boldsymbol{p}} \\ &+ \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} e^{-i(k\cdot x - p\cdot y)}[\boldsymbol{a}(\boldsymbol{k}), \boldsymbol{a}^{\dagger}(\boldsymbol{p})]d\mu_{\boldsymbol{k}}d\mu_{\boldsymbol{p}} \\ &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}(e^{-ik\cdot(x-y)} - e^{ik\cdot(x-y)})d\mu_{\boldsymbol{k}}\cdot I \\ &= -iD(x-y)I. \end{aligned}$$

To prove the local commutativity observe that the Pauli-Jordan function is Lorentz invariant. Since by an appropriate Lorentz transformation any two space-like separated $x, y \in \mathbb{R}^4$ can be put in the form $x = (t, \boldsymbol{x}), y = (t, \boldsymbol{y})$, it follows from (13.6) that $D(x-y) = 0$. □

REMARK 13.1. Local commutativity reflects causal independence of events separated by spacelike intervals.

Local commutativity is often referred as *locality* in the following sense.

Definition. Operator-valued distributions $\boldsymbol{A}(x)$ and $\boldsymbol{B}(y)$ are called *mutually local* if

$$[\boldsymbol{A}(x), \boldsymbol{B}(y)] = 0 \quad \text{for} \quad (x-y)^2 < 0.$$

Corollary 13.1. *We have*

$$[\boldsymbol{\varphi}^-(x), \boldsymbol{\varphi}^+(y)] = -iD^-(x-y)I,$$
$$[\boldsymbol{\varphi}^+(x), \boldsymbol{\varphi}^-(y)] = -iD^+(x-y)I,$$

where

$$D^-(x) = \frac{i}{(2\pi)^3}\int_{\mathbb{R}^3} e^{-ik\cdot x}d\mu_{\boldsymbol{k}} \quad \textit{and} \quad D^+(x) = -D^-(-x), \tag{13.7}$$

so that

$$D(x) = D^+(x) + D^-(x).$$

We have

$$\overline{D^-(x)} = D^+(x),$$

so that $D(x)$ is real-valued[2].

It follows from the integral representation (13.6) that the Pauli-Jordan function has the following properties.

1. $D(x)$ is an odd function,

$$D(-x) = -D(x).$$

2. $D(x)$ satisfies the Klein-Gordon equation

$$(\Box + m^2)D(x) = 0.$$

3. $D(x)$ satisfies boundary conditions at $t = 0$,

$$D(0, \boldsymbol{x}) = 0,$$
$$\frac{\partial D}{\partial t}(0, \boldsymbol{x}) = \delta(\boldsymbol{x}),$$

and it follows from **2** that

$$\frac{\partial^2 D}{\partial t^2}(0, \boldsymbol{x}) = 0.$$

[2]Our notations for the propagators $D(x)$ and $D^{\pm}(x)$ are the same as in Bogoliubov-Shirkov, *ibid.*

The Pauli-Jordan function is the fundamental solution of the Cauchy problem for the Klein-Gordon equation

$$(\square + m^2)\varphi(x) = 0,$$
$$\varphi(0, \boldsymbol{x}) = \varphi(\boldsymbol{x}), \quad \frac{\partial \varphi}{\partial t}(0, \boldsymbol{x}) = \pi(\boldsymbol{x})$$

with rapidly decaying $\varphi(\boldsymbol{x})$ and $\pi(\boldsymbol{x})$. Namely, it follows from **1-3** that solution $\varphi(x)$ of the Cauchy problem is

$$\varphi(x) = \int_{\mathbb{R}^3} \left(\frac{\partial D}{\partial t}(x - y)\varphi(\boldsymbol{y}) + D(x - y)\pi(\boldsymbol{y}) \right) d^3\boldsymbol{y}, \quad \text{where} \quad y = (0, \boldsymbol{y}).$$

REMARK 13.2. In relativistic notations,

$$D(x) = \frac{i}{(2\pi)^3} \int_{\mathbb{R}^4} e^{-ik\cdot x} \varepsilon(k_0)\delta(k^2 - m^2) d^4k,$$

where $\varepsilon(k_0) = \operatorname{sgn}(x_0)$. As a distribution, the Pauli-Jordan function is

$$D(x) = \frac{\varepsilon(x^0)\delta(\lambda)}{2\pi} - \frac{m}{4\pi\sqrt{\lambda}} \varepsilon(x^0)\theta(\lambda)J_1(m\sqrt{\lambda}), \tag{13.8}$$

where $\lambda = x^2 = (x^0)^2 - \boldsymbol{x}^2$, J_1 is the Bessel function, $\theta(\lambda) = 1$ for $\lambda > 0$ and is 0 otherwise. Similarly,

$$D^-(x) = \frac{i}{(2\pi)^3} \int_{\mathbb{R}^4} e^{-ik\cdot x} \theta(k_0)\delta(k^2 - m^2) d^4k$$

and as a distribution,

$$\begin{aligned} D^-(x) = {} & \frac{\varepsilon(x^0)\delta(\lambda)}{4\pi} - \frac{m\theta(\lambda)}{8\pi\sqrt{\lambda}} \left(\varepsilon(x^0)J_1(m\sqrt{\lambda}) - iY_1(m\sqrt{\lambda}) \right) \\ & + \frac{\theta(-\lambda)mi}{4\pi^2\sqrt{-\lambda}} K_1(m\sqrt{-\lambda}), \end{aligned} \tag{13.9}$$

where Y_1 is the Bessel function of the second kind (Neumann function) and K_1 is the modified Bessel function of the second kind (Macdonald function).

13.2. Correlation functions and Wick's theorem

For any operator A in the Fock space $\mathscr{F}$ its *vacuum expectation value* is the inner product $(A\Phi, \Phi)$. Using standard physics terminology and notation, we define the *vacuum expectation value* of an operator A by

$$\langle 0|A|0\rangle = (A\Phi, \Phi).$$

We have $(A\Phi, \Phi) = (\Phi, A^{\dagger}\Phi)$, so that in the formula $\langle 0|A|0\rangle$ we can interpret the left action $\langle 0|A$ as $A^{\dagger}|0\rangle$, where $A^{\dagger}$ is the adjoint operator. Similarly, for any $F, G \in \mathscr{F}$ such that $G \in D(A)$ we define *matrix elements* of A by

$$\langle F|A|G\rangle = (AG, F)$$

Since the linear span of the vectors $\boldsymbol{a}^{\dagger}(f_1)\cdots\boldsymbol{a}^{\dagger}(f_n)\Phi$ is dense in $\mathscr{F}$, we see from (11.22) that to know all matrix elements of the quantum field — operator-valued distribution $\boldsymbol{\varphi}(x)$ — it is sufficient to know all *n-point correlations functions of the quantum fields*. By definition, they are the vacuum expectation values of the product $\boldsymbol{\varphi}(x_1)\cdots\boldsymbol{\varphi}(x_n)$ of operator-valued distributions[3],

$$W_n(x_1, \dots, x_n) = \langle 0|\boldsymbol{\varphi}(x_1)\cdots\boldsymbol{\varphi}(x_n)|0\rangle \in \mathscr{S}(\mathbb{R}^4 \times \cdots \times \mathbb{R}^4)'. \tag{13.10}$$

In axiomatic approach to QFT these distributions are called *Wightman functions*.

It follows from (13.3)–(13.4) that

$$W_1(x) = \langle 0|\boldsymbol{\varphi}(x)|0\rangle = \langle 0|\boldsymbol{\varphi}^{+}(x)|0\rangle + \langle 0|\boldsymbol{\varphi}^{-}(x)|0\rangle = 0,$$

so that the one-point correlation function of a free quantum field vanishes. To compute the two-point correlation function we use Corollary 13.1 and observe that

$$\begin{aligned}\langle 0|\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)|0\rangle &= \langle 0|\boldsymbol{\varphi}^{+}(x)\boldsymbol{\varphi}^{+}(y)|0\rangle + \langle 0|\boldsymbol{\varphi}^{+}(x)\boldsymbol{\varphi}^{-}(y)|0\rangle \\ &\quad + \langle 0|\boldsymbol{\varphi}^{-}(x)\boldsymbol{\varphi}^{+}(y)|0\rangle + \langle 0|\boldsymbol{\varphi}^{-}(x)\boldsymbol{\varphi}^{-}(y)|0\rangle \\ &= \langle 0|\boldsymbol{\varphi}^{-}(x)\boldsymbol{\varphi}^{+}(y)|0\rangle \\ &= \langle 0|[\boldsymbol{\varphi}^{-}(x), \boldsymbol{\varphi}^{+}(y)]|0\rangle.\end{aligned}$$

Thus

$$W_2(x, y) = -iD^{-}(x - y). \tag{13.11}$$

Equivalently, since

$$:\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y):= \boldsymbol{\varphi}^{+}(x)\boldsymbol{\varphi}^{+}(y) + \boldsymbol{\varphi}^{+}(x)\boldsymbol{\varphi}^{-}(y) + \boldsymbol{\varphi}^{+}(y)\boldsymbol{\varphi}^{-}(x) + \boldsymbol{\varphi}^{-}(x)\boldsymbol{\varphi}^{-}(y)$$

we have

$$\langle 0| :\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y): |0\rangle = 0,$$

[3] Though we call it a product, it is really a tensor product of distributions.

and

$$\begin{aligned}\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y) &= :\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y): + [\boldsymbol{\varphi}^-(x), \boldsymbol{\varphi}^+(y)] \\ &= :\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y): - iD^-(x-y)I\end{aligned}$$

immediately gives back (13.11).

REMARK 13.3. Using elementary estimate

$$\int_{-\infty}^{\infty} e^{iur} \frac{du}{\sqrt{u^2+m^2}} = O(e^{-mr}), \quad r>0,$$

it is easy to show that for $(x-y)^2 < 0$

$$\langle 0|\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)|0\rangle = O(e^{-m|\boldsymbol{x}-\boldsymbol{y}|}) \quad \text{as} \quad |\boldsymbol{x}-\boldsymbol{y}| \to \infty.$$

The distribution $D^-(x)$ has remarkable analytic properties. Namely, consider the *past tube*, the domain $\mathbb{R}^4 + iV^-$ in $\mathbb{C}^4$, where V^- is the interior of the past light cone,

$$V^- = \{x \in \mathbb{R}^4 : x^0 < 0,\ x^2 > 0\}.$$

The following result holds.

THEOREM 13.2. *The 2-point Wightman function $W_2(x)$ of a free quantum field is a boundary value on $\mathbb{R}^4$ of the analytic function $W_2(\zeta)$ in the the past tube $\mathbb{R}^4 + iV^-$.*

PROOF. For $\zeta = x + i\eta \in \mathbb{R}^4 + iV^-$ put

$$W_2(\zeta) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{-i\omega_{\boldsymbol{k}}\zeta^0 + i\boldsymbol{k}\cdot\boldsymbol{\zeta}} \frac{d^3\boldsymbol{k}}{2\omega_{\boldsymbol{k}}}.$$

Since $|\boldsymbol{\eta}| < -\eta^0$ for $\eta \in V^-$ and $\omega_{\boldsymbol{k}} = \sqrt{\boldsymbol{k}^2+m^2}$, we have

$$|\boldsymbol{k}\cdot\boldsymbol{\eta}| \le |\boldsymbol{k}||\boldsymbol{\eta}| < -\omega_{\boldsymbol{k}}\eta^0,$$

so that

$$\mathrm{Re}(-i\omega_k\zeta^0 + i\boldsymbol{k}\cdot\boldsymbol{\zeta}) = \omega_{\boldsymbol{k}}\eta^0 - \boldsymbol{k}\cdot\boldsymbol{\eta} < 0.$$

Thus the integral for $W_2(\zeta)$ is absolutely convergent for $\zeta \in \mathbb{R}^4 + iV^-$, uniformly on compact subsets, and defines an analytic function there. Whence, in the distributional sense,

$$W_2(x) = \lim_{\eta\to 0} W_2(x+i\eta). \quad \square$$

REMARK 13.4. In fact, $W_2(x)$ admits an analytic continuation to a larger domain[4], which contains Euclidean $\mathbb{R}^4 \simeq i\mathbb{R} \times \mathbb{R}^3$ in the complexified Minkowski space $\mathbb{C}^4$. Restriction of W_2 to this domain is the *Schwinger function* S_2, which has the form

$$S_2(x) = \frac{1}{(2\pi)^4} \int_{\mathbb{R}^4} \frac{e^{ik_4 x^4 + i\boldsymbol{k}\cdot\boldsymbol{x}}}{k_4^2 + \boldsymbol{k}^2 + m^2} d^4 k, \quad x \in \mathbb{R}^4. \tag{13.12}$$

Indeed, we have for $a, v > 0$,

$$\int_{-\infty}^{\infty} \frac{e^{iuv}}{u^2 + a^2} du = \frac{\pi}{a} e^{-av}.$$

Thus in our case for $x = (-ix^4, \boldsymbol{x})$, where $x^4 > 0$, we obtain, putting $a = \omega_{\boldsymbol{k}}$ and $u = k_4$,

$$\begin{aligned} W_2(-ix^4, \boldsymbol{x}) &= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{-\omega_k x^4 + i\boldsymbol{k}\cdot\boldsymbol{x}} \frac{d^3\boldsymbol{k}}{2\omega_{\boldsymbol{k}}} \\ &= \frac{1}{(2\pi)^4} \int_{\mathbb{R}^4} \frac{e^{ik_4 x^4 + i\boldsymbol{k}\cdot\boldsymbol{x}}}{k_4^2 + \boldsymbol{k}^2 + m^2} d^4 k. \end{aligned}$$

Whence $W_2(x)$ admits analytic continuation to Euclidean $\mathbb{R}^4 \simeq i\mathbb{R} \times \mathbb{R}^3$ and coincides there with $S_2(x)$. Schwinger functions play a fundamental role in Euclidean formulation of QFT.

Representation

$$\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y) = \boldsymbol{:}\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)\boldsymbol{:} - iD^-(x-y)I \tag{13.13}$$

shows that though the limit $y \to x$ of the operator-valued distribution $\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)$ is singular and not defined, the formula

$$\boldsymbol{:}\boldsymbol{\varphi}^2(x)\boldsymbol{:} = \lim_{y\to x} \boldsymbol{:}\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)\boldsymbol{:} = \lim_{y\to x} \big(\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y) + iD^-(x-y)I\big) \tag{13.14}$$

gives a well-defined operator-valued distribution.

Formula (13.13) can also be used for a computation of multi-point correlation functions of operator-valued distributions $\boldsymbol{A}(x)$ which are linear combinations of $\boldsymbol{\varphi}^+(x)$ and $\boldsymbol{\varphi}^-(x)$, called *linear operators*. It follows from (13.13) that for two-such operators $\boldsymbol{A}(x)$ and $\boldsymbol{B}(y)$ the product $\boldsymbol{A}(x)\boldsymbol{B}(y)$

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[4]The so-called *symmetrized tube*; see Ch. 9 of the monograph "General Principles of Quantum Field Theory" by N.N. Bogolyubov, A.A. Logunov, A.I. Oksak and I.T. Todorov, Kluwer, 1990, for the detailed exposition.

differs from the normal product $:\boldsymbol{A}(x)\boldsymbol{B}(y):$ by a certain number times the identity operator. In physics literature this number is called a *pairing* between $\boldsymbol{A}(x)$ and $\boldsymbol{B}(y)$ and is denoted by bracketing below the line,

$$\boldsymbol{A}(x)\boldsymbol{B}(y) = :\boldsymbol{A}(x)\boldsymbol{B}(y): + \underbracket{\boldsymbol{A}(x)\boldsymbol{B}}(y). \tag{13.15}$$

Since the vacuum expectation value of the normal product is zero, unless it is a multiple of the identity operator, we can also define the pairing as a vacuum expectation value of the ordinary product,

$$\underbracket{\boldsymbol{A}(x)\boldsymbol{B}}(y) = \langle 0|\boldsymbol{A}(x)\boldsymbol{B}(y)|0\rangle. \tag{13.16}$$

One can also define the normal product of n linear operators with pairing by

$$\begin{aligned} &:\boldsymbol{A}_1(x_1)\cdots \underbracket{\boldsymbol{A}_i(x_i)\cdots \boldsymbol{A}}_j(x_j)\cdots \boldsymbol{A}_n(x_n): \\ &= \underbracket{\boldsymbol{A}_i(x_i)\boldsymbol{A}}_j(x_j) :\boldsymbol{A}_1(x_1)\cdots \hat{\boldsymbol{A}}_i(x_i)\cdots \hat{\boldsymbol{A}}_j(x_j)\cdots \boldsymbol{A}_n(x_n):, \end{aligned}$$

the normal product with arbitrary number of pairings is defined similarly. The following theorem allows to compute the normal product of arbitrary number of linear operators.

THEOREM 13.3 (Wick's first theorem). *The product of linear operators is equal to the sum of their normal product with arbitrary number of pairings, including the normal product withour pairing,*

$$\begin{aligned} \boldsymbol{A}_1\cdots\boldsymbol{A}_n &= :\boldsymbol{A}_1\cdots\boldsymbol{A}_n: + \sum_{i\neq j} :\boldsymbol{A}_1\cdots \underbracket{\boldsymbol{A}_i\cdots\boldsymbol{A}}_j\cdots\boldsymbol{A}_n: \\ &+ \sum_{i,k,j,l} :\boldsymbol{A}_1\cdots \underbracket{\boldsymbol{A}}_i\cdots\underbracket{\boldsymbol{A}}_j\cdots\underbracket{\boldsymbol{A}}_k\cdots\underbracket{\boldsymbol{A}}_l\cdots\boldsymbol{A}_n: + \ldots \end{aligned}$$

PROOF. We prove this formula by induction on n, starting with case $n = 2$. Now suppose that the theorem is true for $\boldsymbol{A}_2, \ldots, \boldsymbol{A}_n$, so that

$$\begin{aligned} \boldsymbol{A}_2\cdots\boldsymbol{A}_n &= :\boldsymbol{A}_2\cdots\boldsymbol{A}_n: + \sum_{i\neq j} :\boldsymbol{A}_2\cdots \underbracket{\boldsymbol{A}_i\cdots\boldsymbol{A}}_j\cdots\boldsymbol{A}_n: \\ &+ \sum_{i,k,j,l} \boldsymbol{A}_1 :\boldsymbol{A}_2\cdots \underbracket{\boldsymbol{A}}_i\cdots\underbracket{\boldsymbol{A}}_j\cdots\underbracket{\boldsymbol{A}}_k\cdots\underbracket{\boldsymbol{A}}_l\cdots\boldsymbol{A}_n: + \ldots \end{aligned} \tag{13.17}$$

Since $\boldsymbol{A}_1$ is a linear operator, $\boldsymbol{A}_1 = \boldsymbol{A}_1^+ + \boldsymbol{A}_1^-$, where $\boldsymbol{A}_1$ is a linear in $\boldsymbol{\varphi}^+(x)$, and $\boldsymbol{A}_1^-$ is a linear in $\boldsymbol{\varphi}^-(x)$. Since

$$\boldsymbol{A}_1^+ \,\boldsymbol{:}\boldsymbol{A}_2 \cdots \boldsymbol{A}_n\boldsymbol{:} = \boldsymbol{:}\boldsymbol{A}_1^+ \boldsymbol{A}_2 \cdots \boldsymbol{A}_n\boldsymbol{:} \quad \text{and} \quad \underbracket{\boldsymbol{A}_1^+ \boldsymbol{A}}_i = 0, \quad i = 2, \dots, n,$$

we get the Wick formula for $\boldsymbol{A}_1^+, \boldsymbol{A}_2 \dots, \boldsymbol{A}_n$ by left multiplying formula (13.17) by $\boldsymbol{A}_1^+$. For the operator $\boldsymbol{A}_1^-$ we observe that

$$\boldsymbol{:}\boldsymbol{A}_2 \cdots \boldsymbol{A}_n\boldsymbol{:}\, \boldsymbol{A}_1^- = \boldsymbol{:}\boldsymbol{A}_1^- \boldsymbol{A}_2 \cdots \boldsymbol{A}_n\boldsymbol{:} \quad \text{and} \quad [\boldsymbol{A}_1^-, \boldsymbol{A}_i] = \underbracket{\boldsymbol{A}_1^- \boldsymbol{A}}_i \, I.$$

Right multiplying formula (13.17) by $\boldsymbol{A}_1^-$ and using that commutator is a derivation with respect to the operator product,

$$\begin{aligned}[\boldsymbol{A}_1^-, \boldsymbol{A}_2 \cdots \boldsymbol{A}_n] = [\boldsymbol{A}_1^-, \boldsymbol{A}_2]\boldsymbol{A}_3 \cdots \boldsymbol{A}_n + \boldsymbol{A}_2[\boldsymbol{A}_1^-, \boldsymbol{A}_3] \cdots \boldsymbol{A}_n + \dots \\ + \boldsymbol{A}_2 \cdots \boldsymbol{A}_{n-1}[\boldsymbol{A}_1^-, \boldsymbol{A}_n],\end{aligned}$$

we get the Wick formula for $\boldsymbol{A}_1^-, \boldsymbol{A}_2 \dots, \boldsymbol{A}_n$. □

REMARK 13.5. The first Wick's theorem is also applicable when some of the factors appear as normal products, like

$$\boldsymbol{A}_1 \cdots \boldsymbol{A}_j \,\boldsymbol{:}\boldsymbol{A}_{j+1} \cdots \boldsymbol{A}_{j+l}\boldsymbol{:}\, \boldsymbol{A}_{j+l+1} \cdots \boldsymbol{A}_n.$$

In this case one does not take into the account pairings inside the same normal product.

COROLLARY 13.4. *For the multi-point Wightman functions of a free scalar field we have*

$$\begin{aligned}&W_{2n+1}(x_1, \dots, x_{2n+1}) = 0, \\ &\quad W_{2n}(x_1, \dots, x_{2n}) = \frac{1}{n!} \sum_{\sigma \in \mathrm{Sym}_{2n}}{}' W_2(x_{\sigma(1)}, x_{\sigma(2)}) \cdots W_2(x_{\sigma(2n-1)}, x_{\sigma(2n)}),\end{aligned}$$

where summation goes over permutations $\sigma \in \mathrm{Sym}_{2n}$ *with the property* $\sigma(2l-1) < \sigma(2l)$, $l = 1, \dots, n,$.

Wick theorem allows to compute all possible correlation functions *descendant* of quantum fields — operator valued distributions like $\partial_\mu \boldsymbol{\varphi}(x)$, $\boldsymbol{:}\boldsymbol{\varphi}^2(x)\boldsymbol{:}$ and so on. Thus it follows from (13.14) and Corollary 13.4 (or the above remark), that

$$\langle 0|\, \boldsymbol{:}\boldsymbol{\varphi}^2(x)\boldsymbol{:}\boldsymbol{:}\varphi^2(y)\boldsymbol{:}\, |0\rangle = 2W_2^2(x - y). \tag{13.18}$$

PROBLEM 13.1. Prove all properties of the Pauli-Jordan function.

PROBLEM 13.2. Derive formulas (13.8)–(13.9).

PROBLEM 13.3. Prove formula (13.18).

CHAPTER 14

Chronological product and causal propagator

14.1. Time-ordered product

The vacuum expectation $\langle 0|\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)|0\rangle$ value of the product of quantum fields can be written as

$$\langle 0|\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)|0\rangle = \langle 0|\boldsymbol{\varphi}^{-}(x)\boldsymbol{\varphi}^{+}(y)|0\rangle$$

and is a complex amplitude of creating a particle at point $\boldsymbol{y}$ at time y^0, and destroying it at $\boldsymbol{x}$ at time x^0. This means that $|\langle 0|\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)|0\rangle|^2$ is the probability density of this event and causality implies that one should have $x^0 > y^0$. In case $x^0 < y^0$ similar role is played by $\langle 0|\boldsymbol{\varphi}(y)\boldsymbol{\varphi}(x)|0\rangle$. Note that the notion of time ordering makes sense only when x and y are timelike, $(x-y)^2 > 0$. However, microscopic causality implies that quantum fields $\boldsymbol{\varphi}(x)$ and $\boldsymbol{\varphi}(y)$ commute when x and y are spacelike, $(x-y)^2 < 0$, and $\langle 0|\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)|0\rangle = \langle 0|\boldsymbol{\varphi}(y)\boldsymbol{\varphi}(x)|0\rangle$. This motivates the following definition.

Definition. *Chronological product* of local operators $\boldsymbol{A}_1(x_1), \dots, \boldsymbol{A}_n(x_n)$ is given by

$$T(\boldsymbol{A}_1(x_1)\cdots \boldsymbol{A}_n(x_n)) = \boldsymbol{A}_{i_1}(x_{i_1})\cdots \boldsymbol{A}_{i_n}(x_{i_n}),$$

where $i_1, \dots, i_n$ is a permutation of $1, \dots, n$ such that $x_{i_1} \gtrsim \cdots \gtrsim x_{i_n}$. Here $x \gtrsim y$ means that either the vector x lies in the future light cone of y, or x and y are spacelike separated.

Remark 14.1. The product $\boldsymbol{A}(x_i)\boldsymbol{A}(x_j)$ is singular when $(x_i - x_j)^2 = 0$ and the time-ordered product for such arguments is not defined. It follows from locality that for all other values of $x_1, \dots, x_n$ the chronological product is Lorentz invariant.

The *Stueckelberg-Feynman propagator*[1], or *casual Green's function*, is defined by

$$\langle 0|T(\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y))|0\rangle = -iD^c(x-y). \tag{14.1}$$

To obtain a Lorentz invariant integral representation for $D^c(x-y)$, we note

$$T(\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)) = \theta(x^0-y^0)\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y) + \theta(y^0-x^0)\boldsymbol{\varphi}(y)\boldsymbol{\varphi}(x),$$

so that

$$D^c(x-y) = \theta(x^0-y^0)D^-(x-y) - \theta(y^0-x^0)D^+(x-y). \tag{14.2}$$

Using formulas (13.7) and the formula

$$\theta(v) = \frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{e^{iuv}}{u-i0}du \overset{\text{def}}{=} \frac{1}{2\pi i}\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}\frac{e^{iuv}}{u-i\varepsilon}du, \tag{14.3}$$

where the contour of integration is depicted on Fig. 1

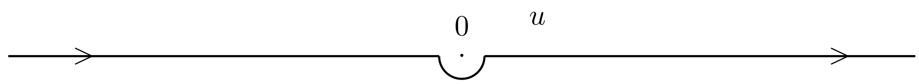

Fig. 1

and bypasses the point 0 by the lower part of a semi-circle of radius ε, we obtain

$$\begin{aligned} D^c(x) &= \frac{1}{(2\pi)^4}\int_{\mathbb{R}^3}\int_{-\infty}^{\infty}\left(\frac{e^{i(u-\omega_{\boldsymbol{k}})x^0+i\boldsymbol{k}\cdot\boldsymbol{x}}}{u-i0} + \frac{e^{-i(u-\omega_{\boldsymbol{k}})x^0-i\boldsymbol{k}\cdot\boldsymbol{x}}}{u-i0}\right)du\frac{d^3\boldsymbol{k}}{2\omega_{\boldsymbol{k}}} \\ &= \frac{1}{(2\pi)^4}\int_{\mathbb{R}^4}e^{-ik\cdot x}\left(\frac{1}{\omega_{\boldsymbol{k}}-k_0-i0} + \frac{1}{\omega_{\boldsymbol{k}}+k_0-i0}\right)\frac{dk_0d^3\boldsymbol{k}}{2\omega_{\boldsymbol{k}}} \\ &= \frac{1}{(2\pi)^4}\int_{\mathbb{R}^4}\frac{e^{-ik\cdot x}}{m^2-k^2-i0}\,d^4k. \end{aligned} \tag{14.4}$$

[1]In most physics textbooks it is called a Feynman propagator. Our terminology reflects Stueckelberg's 1942 paper and is historically accurate: see, e.g. the textbook G. Sterman, *An introduction to quantum field theory*, Cambridge University Press, 1993, p. 48. Our notation and terminology follows Bogoliubov-Shirkov, *ibid.*

Here we put $u-\omega_{\boldsymbol{k}} = -k_0$ in the first integral, and $u-\omega_{\boldsymbol{k}} = k_0$ and change $\boldsymbol{k} \to -\boldsymbol{k}$ in the second integral.

The contour integration over k_0 in formula (14.4) is over the *Feynman contour*, which bypasses the poles at $-\omega_{\boldsymbol{k}}$ from below and the pole at $\omega_{\boldsymbol{k}}$ from above, as depicted on Fig. 2

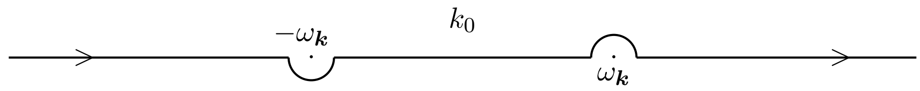

Fig. 2

As a distribution,

$$D^c(x) = \frac{mi}{4\pi^2}\frac{K_1(m\sqrt{-\lambda+i0})}{\sqrt{-\lambda+i0}}, \tag{14.5}$$

where $\sqrt{-a+i0} = i\sqrt{a}$ for $a > 0$.

Properties of the causal Green's function can be summarized as follows.

1. $D^c(x)$ is an even function,

$$D^c(x) = D^c(-x).$$

2. $D^c(x)$ is a complex-valued function,

$$\overline{D^c(x)} = D^c(x) + D^+(x) - D^-(x).$$

3. $D^c(x)$ satisfies the Klein-Gordon equation with delta-function source,

$$(\Box + m^2)D^c(x) = \delta(x),$$

as immediately follows from integral representation (14.4).

4. The Fourier transform of $D^c(x)$ has a pole at $k^2 = m^2$, which identifies the mass of the particle associated with the free quantum scalar field $\boldsymbol{\varphi}(x)$ as m.

Remark 14.2. The Stueckelberg-Feynman propagator does not vanish for $(x-y)^2 < 0$. This does not contradict that the particle travels from y to x faster then the light. Indeed, after an appropriate Lorentz transformation we can assume that $x = (0, \boldsymbol{x})$ and $y = (0, \boldsymbol{y})$, and creation of a particle at $\boldsymbol{y}$ and its simultaneous annihilation at $\boldsymbol{x}$ does not represent a causal dependence between $\boldsymbol{x}$ and $\boldsymbol{y}$. One thinks of this process as emission of a "virtual particle" at $\boldsymbol{y}$ and its absorption at $\boldsymbol{x}$.

REMARK 14.3. Non-homogeneous equation

$$(\Box + m^2)G(x) = \delta(x) \tag{14.6}$$

also has real-valued solutions, so-called *retarded* and *advanced Green's functions*,

$$D^{\text{ret}}(x) = \theta(x^0)D(x), \quad D^{\text{adv}}(x) = -\theta(-x^0)D(x),$$

so that $D(x) = D^{\text{ret}}(x) - D^{\text{adv}}(x)$.

The causal Green's function has the property that for each $f \in \mathscr{S}(\mathbb{R}^4)$ the function

$$\varphi(x) = \int_{\mathbb{R}^4} D^c(x-y)f(y)d^4y,$$

which satisfies the non-homogeneous Klein-Gordon equation

$$(\Box + m^2)\varphi(x) = f(x),$$

also satisfies the so-called *Feynman boundary conditions*, which reflect the large time behavior of $\varphi(x)$,

$$\varphi(x) = \varphi_\pm(x) + o(1) \quad \text{as} \quad t = x^0 \to \pm\infty, \tag{14.7}$$

where

$$\varphi_\pm(x) = \frac{i}{2\pi}\int_{\mathbb{R}^3} e^{\mp i\omega_{\boldsymbol{k}}t + i\boldsymbol{k}\cdot\boldsymbol{x}}\hat{f}(\pm\omega_{\boldsymbol{k}}, \boldsymbol{k})d\mu_{\boldsymbol{k}}, \tag{14.8}$$

and $\hat{f}(k)$ is the Fourier transform of $f(x)$.

Indeed, assuming for simplicity that $f(y_0, \boldsymbol{y}) = 0$ for $|y_0| > a$ and all $\boldsymbol{y} \in \mathbb{R}^3$, we get from (14.2) and (13.7) that as $t \to \infty$,

$$\begin{aligned}\varphi(x) &= \int_{\mathbb{R}^4} D^-(x-y)f(y)d^4y \\ &= \frac{i}{(2\pi)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^4} e^{-ik\cdot(x-y)}f(y)d^4y d\mu_{\boldsymbol{k}} \\ &= \frac{i}{2\pi}\int_{\mathbb{R}^3} e^{-ik\cdot x}\hat{f}(\omega_{\boldsymbol{k}}, \boldsymbol{k})d\mu_{\boldsymbol{k}}.\end{aligned}$$

The case $t \to -\infty$ is considered similarly.

Since $\varphi_\pm(x)$ are, correspondingly, positive/negative energy solutions of the Klein-Gordon equation, we see that casual Green's function has characteristic property: positive energy solutions propagate forward in time, while negative energy solutions propagate backwards in time. Thus Feynman boundary conditions (14.7)–(14.8) distinguish the causal Green's function among all other solutions of equation (14.6).

14.2. Chronological pairing

In accordance with the definition of ordinary pairing in Lecture 13, for local operators $\boldsymbol{A}(x)$ and $\boldsymbol{B}(y)$ we get

$$T(\boldsymbol{A}(x)\boldsymbol{B}(y)) = \begin{cases} :\boldsymbol{A}(x)\boldsymbol{B}(y): + \underbracket{\boldsymbol{A}(x)\boldsymbol{B}}(y)I, & x^0 > y^0, \\ :\boldsymbol{A}(x)\boldsymbol{B}(y): + \underbracket{\boldsymbol{B}(y)\boldsymbol{A}}(x)I, & y^0 > x^0. \end{cases}$$

This allows to define a *chronological pairing* of local operators by

$$\overbracket{\boldsymbol{A}(x)\boldsymbol{B}}(y) = \begin{cases} \underbracket{\boldsymbol{A}(x)\boldsymbol{B}}(y), & x^0 > y^0, \\ \underbracket{\boldsymbol{B}(y)\boldsymbol{A}}(x), & y^0 > x^0, \end{cases} \tag{14.9}$$

so that

$$T(\boldsymbol{A}(x)\boldsymbol{B}(y)) =: \boldsymbol{A}(x)\boldsymbol{B}(y): +. \overbracket{\boldsymbol{A}(x)\boldsymbol{B}}(y)I \tag{14.10}$$

and we have

$$\overbracket{\boldsymbol{A}(x)\boldsymbol{B}}(y) = \langle 0|T(\boldsymbol{A}(x)\boldsymbol{B}(y))|0\rangle. \tag{14.11}$$

Similarly to the first Wick's theorem, we have the following result for the chronological products of local operators.

THEOREM 14.1 (Wick's second theorem). *The chronological product of local operators is equal to the sum of their normal product with arbitrary number of chronological pairings, including the normal product withour pairing,*

$$T(\boldsymbol{A}_1 \cdots \boldsymbol{A}_n) =: \boldsymbol{A}_1 \cdots \boldsymbol{A}_n: + \sum_{i\neq j} :\boldsymbol{A}_1 \cdots \overbracket{\boldsymbol{A}_i \cdots \boldsymbol{A}_j} \cdots \boldsymbol{A}_n:$$
$$+ \sum_{i,k,j,l} :\boldsymbol{A}_1 \cdots \overbracket{\boldsymbol{A}_i \cdots \boldsymbol{A}_j \cdots \boldsymbol{A}_k} \cdots \boldsymbol{A}_l \cdots \boldsymbol{A}_n: + \cdots$$
$$\text{(pairings } \boldsymbol{A}_i\text{–}\boldsymbol{A}_k \text{ and } \boldsymbol{A}_j\text{–}\boldsymbol{A}_l\text{)}$$

The following result allows to compute the vacuum expectation value of the chronological product of local operators.

THEOREM 14.2 (Wick's third theorem). *The vacuum expectation value of the time-ordered product of* $n+1$ *linear operators* $\boldsymbol{A}, \boldsymbol{B}_1, \ldots, \boldsymbol{B}_n$ *is equal to the sum of* n *vacuum expectation values of these same time-ordered products* *with all possible pairings of one of these operators (for instance, $\boldsymbol{A}$) with all the remaining ones,*

$$\langle 0|T(\boldsymbol{A}\boldsymbol{B}_1\cdots\boldsymbol{B}_n|0\rangle = \sum_{i=1}^{n}\langle 0|T(\overbracket{\boldsymbol{A}\boldsymbol{B}_1\cdots\boldsymbol{B}}_i\cdots\boldsymbol{B}_n)|0\rangle.$$

Proof. The result directly follows directly from the second Wick's theorem. Indeed, since the vacuum expectation value of the normal product of an arbitrary nonzero number of unpaired operators vanishes, the left-hand side is the sum of all possible total pairings of the operators $\boldsymbol{A}, \boldsymbol{B}_1, \dots, \boldsymbol{B}_n$ — the pairings where each operator is paired with some other operator. Similarly, the i-th term in the right-hand side is

$$\overbracket{\boldsymbol{A}\boldsymbol{B}}_i\langle 0|T(\boldsymbol{B}_1\cdots\hat{\boldsymbol{B}}_i\cdots\boldsymbol{B}_n|0\rangle,$$

which a product of $\overbracket{\boldsymbol{A}\boldsymbol{B}}_i$ with the sum of all possible total pairings of the operators $\boldsymbol{B}_1, \dots, \boldsymbol{B}_{i-1}, \boldsymbol{B}_{i+1}, \dots, \boldsymbol{B}_n$. □

Corollary 14.3. *For the n-point functions — the vacuum expectation value of the chronological product of quantum fields,*

$$G_n(x_1, \dots, x_n) = \langle 0|T(\boldsymbol{\varphi}(x_1)\cdots\boldsymbol{\varphi}(x_n))|0\rangle,$$

we have

$$\begin{aligned} &G_{2n+1}(x_1, \dots, x_{2n+1}) = 0, \\ &\qquad G_{2n}(x_1, \dots, x_{2n}) = \frac{1}{n!}\sum_{\sigma\in\mathrm{Sym}_{2n}}{}' G_2(x_{\sigma(1)}, x_{\sigma(2)})\cdots G_2(x_{\sigma(2n-1)}, x_{\sigma(2n)}), \end{aligned}$$

where summation goes over permutations $\sigma \in \mathrm{Sym}_{2n}$ with the property $\sigma(2l-1) < \sigma(2l)$, $l = 1, \dots, n$, and

$$G_2(x_1, x_2) = -iD^c(x_1 - x_2).$$

Clearly third Wick's theorem and Corollary 14.3 also hold for the vacuum expectation values of ordinary products.

One can also define a generating function of the multi-point correlation functions by

$$Z[J] = \langle 0|T(\exp i\int_{\mathbb{R}^4} J(x)\boldsymbol{\varphi}(x)d^4x)|0\rangle, \tag{14.12}$$

where

$$T(\exp i \int_{\mathbb{R}^4} J(x)\boldsymbol{\varphi}(x) d^4x)$$
$$\stackrel{\text{def}}{=} \sum_{n=0}^{\infty} \frac{i^n}{n!} \int_{\mathbb{R}^4} \cdots \int_{\mathbb{R}^4} J(x_1) \cdots J(x_n) T(\boldsymbol{\varphi}(x_1) \cdots \boldsymbol{\varphi}(x_n)) d^4x_1 \cdots d^4x_n.$$

Then

$$G_n(x_1, \ldots, x_n) = \frac{1}{i^n} \left. \frac{\delta^n Z[J]}{\delta J(x_1) \cdots \delta J(x_n)} \right|_{J=0}. \tag{14.13}$$

One can also consider *connected n-point correlation functions*, defined inductively by

$$G_1^{\text{con}}(x_1) = G_1(x_1),$$
$$G_2^{\text{con}}(x_1, x_2) = G_2(x_1, x_2) - G_1(x_1) G_2(x_2),$$
$$G_n^{\text{con}}(x_1, \ldots, x_n) = G_n(x_1, \ldots, x_n) - \sum_{r=2}^{n} \sum_{I_1, \ldots, I_r} G_{I_1}^{\text{con}} \cdots G_{I_r}^{\text{con}},$$

where the sum runs over all partitions $I_1, \ldots, I_r$ of the set $\{x_1, \ldots, x_n\}$ and for $I = \{x_{i_1}, \ldots, x_{i_l}\}$

$$G_I^{\text{con}} = G_l^{\text{con}}(x_{i_1}, \ldots, x_{i_l}).$$

It is quite remarkable that

$$W[J] = \log Z[J] \tag{14.14}$$

is a generating function of connected correlation functions,

$$G_n^{\text{con}}(x_1, \ldots, x_n) = \frac{1}{i^n} \left. \frac{\delta^n W[J]}{\delta J(x_1) \cdots \delta J(x_n)} \right|_{J=0}. \tag{14.15}$$

In our case we have

$$G_1^{\text{con}}(x_1) = 0, \quad G_2^{\text{con}}(x_1, x_2) = G_2(x_1, x_2)$$

and

$$G_n^{\text{con}}(x_1, \ldots, x_n) = 0, \quad n > 2.$$

Thus all correlation functions reduce to 2-point functions, which is a characteristic feature of a free quantum field theory.

14.3. Euclidean formulation

The contour of integration over k_0 for the Stuekelberg-Feynman propagator, depicted in Fig. 2, has a remarkable property that it can be rotated counter-clockwise by an angle $\theta > 0$ in the complex k_0-plane without crossing the poles of the denominator! Setting $k_0 = ue^{i\theta}$ we see that $D^c(x)$ admits an analytic continuation in the variable x^0 to the values $x^0 = e^{-i\theta}v$, $v \in \mathbb{R}$, by the formula

$$D^c(x^0, \boldsymbol{x}) = \frac{e^{i\theta}}{(2\pi)^4} \int_{\mathbb{R}^4} \frac{e^{-iue^{i\theta}x^0 + i\boldsymbol{k}\cdot\boldsymbol{x}}}{\boldsymbol{k}^2 + m^2 - u^2 e^{2i\theta}} \, du d^3\boldsymbol{k}.$$

In particular, rotation by the angle $\theta = \pi/2$, called *Wick rotation*, transforms Minkowski spacetime $\mathbb{R}^4$ with Minkowski metric into $\mathbb{R}^4$ with the Euclidean metric.

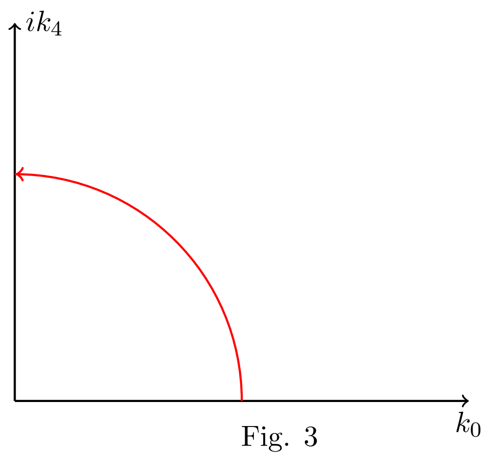

Fig. 3

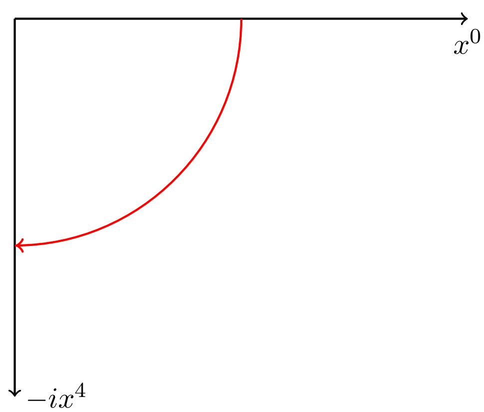

Fig. 4

Denoting $k_0 = ik_4$ and $x^0 = -ix^4$ (see Fig. 3–4), where $k_4, x^4 \in \mathbb{R}$, and changing $\boldsymbol{k}$ to $-\boldsymbol{k}$ we obtain

$$D^c(-ix^4, \boldsymbol{x}) = \frac{i}{(2\pi)^4} \int_{\mathbb{R}^4} \frac{e^{-ik_4x^4 - i\boldsymbol{k}\cdot\boldsymbol{x}}}{k_4^2 + \boldsymbol{k}^2 + m^2} \, dk_4 d^3\boldsymbol{k}.$$

As the result, we have in Euclidean notations $k_E = (\boldsymbol{k}, k_4)$ and $x_E = (\boldsymbol{x}, x^4)$ we get the following formula

(14.16)

$$-iD^c(-ix^4, \boldsymbol{x}) = G(x_E) = \frac{1}{(2\pi)^4} \int_{\mathbb{R}^4} \frac{e^{-ik_E\cdot x_E}}{k_E^2 + m^2} \, d^4k_E, \quad k_E^2 = k_4^2 + \boldsymbol{k}^2.$$

Here $G(x_E)$ is the Green's function for the operator $-\Delta + m^2$, where Δ is Euclidean Laplace operator on $\mathbb{R}^4$,

$$\Delta = \left(\frac{\partial}{\partial x^1}\right)^2 + \left(\frac{\partial}{\partial x^2}\right)^2 + \left(\frac{\partial}{\partial x^3}\right)^2 + \left(\frac{\partial}{\partial x^4}\right)^2.$$

In other words, Wick rotation — analytic continuation of the casual Green's function $D^c(x)$ to "imaginary" time $x^0 = -ix^4$ — gives *Euclidean Green's function* $G(x_E)$, which satisfies

$$(-\Delta + m^2)G(x_E) = \delta(x_E).$$

Comparing with formula (13.12) in Lecture 13, we see that Euclidean Green's function G coincides with Schwinger function S_2.

Remark 14.4. Since $D^-(x)$ admits analytic continuation to the past tube $\mathbb{R}^4 + iV^-$ (see Theorem 13.2 in Chapter 13), and $D^+(x) = -D^-(-x)$ — to the future tube $\mathbb{R}^4 + iV^+$, the analytic continuation of $D^c(x)$ follows from (14.2).

Remembering the definition of the Schwinger function (see Remark 13.4 in Chapter 13), we see that the time-ordered correlation function

$$G_2(x - y) = \langle 0|T(\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y))|0\rangle$$

can be obtained by analytic continuation of the Wightman function $W_2(x - y)$ to the Schwinger function $S_2(x - y)$ on the Euclidean spacetime $\mathbb{R}^4$ and coming back to the Minkowski spacetime $\mathbb{R}^4$ by the inverse Wick rotation.

Problem 14.1. Prove the following relation between chronological and normal products

$$T(\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)) =\mathbf{:}\, \boldsymbol{\varphi}(x)\boldsymbol{\varphi}(y)\, \mathbf{:} - iD^c(x - y).$$

PROBLEM 14.2. Derive formula (14.5).

PROBLEM 14.3. Prove formulas (14.14)–(14.15).

PROBLEM 14.4. Put $z = x^0 e^{-i\theta}$, where $x^0 \in \mathbb{R}$ and $0 < \theta < \pi/2$, and consider

$$G(z) = \int_{-\infty}^{\infty} \frac{e^{i\theta - ik_0 x^0}}{k_0^2 e^{2i\theta} - a^2} dk_0,$$

where $a > 0$. Differentiating under the integral sign, verify that for such z

$$\frac{\partial G}{\partial \bar{z}} = 0.$$

CHAPTER 15

Green's functions and Feynman path integral

15.1. Correlation functions in QM

In Chapter 7 we introduced Dirac notations

$$\langle q', t'| = \langle q'|e^{-\frac{i}{\hbar}t'H} \quad \text{and} \quad |q,t\rangle = e^{\frac{i}{\hbar}tH}|q\rangle, \tag{15.1}$$

and expressed the quantum-mechanical amplitude

$$\langle q', t'|q,t\rangle \overset{\text{def}}{=} \langle q'|e^{-\frac{i}{\hbar}(t'-t)H}|q\rangle \tag{15.2}$$

— the integral kernel of the evolution operator $U(t'-t) = e^{-\frac{i}{\hbar}(t'-t)H}$ — in terms of the Feynman path integral (7.30) in the configuration space. For simplicity, here we consider the case of one degree of freedom.

Let Q be the coordinate operator in $\mathscr{H} = L^2(\mathbb{R}, dq)$. In the Heisenberg picture, complex amplitude (15.2) can be interpreted as the inner product of generalized eigenfunctions of the operator

$$Q(t) = U(t)^{-1}QU(t) = e^{\frac{i}{\hbar}tH}Qe^{-\frac{i}{\hbar}tH}$$

at different times. Namely, $|q\rangle$ is a generalized eigenfunction[1] of the operator Q, that is, $Q|q\rangle = q|q\rangle$, so $|q,t\rangle$ is a generalized eigenfunction of $Q(t)$, $Q(t)|q,t\rangle = q|q,t\rangle$, and the complex amplitude $\langle q',t'|q,t\rangle$ is their inner product.

Similar to (15.2),consider the "matrix element"

$$\begin{aligned}\langle q',t'|Q(t_1)|q,t\rangle &= \langle q',t'|e^{\frac{i}{\hbar}t_1H}Qe^{-\frac{i}{\hbar}t_1H}|q,t\rangle, \\ &\overset{\text{def}}{=} \langle q'|e^{-\frac{i}{\hbar}(t'-t_1)H}Qe^{-\frac{i}{\hbar}(t_1-t)H}|q\rangle,\end{aligned}$$

where $t < t_1 < t'$.

It is remarkable that $\langle q',t'|O(t_1)|q,t\rangle$ can be also expressed through the path integral. Namely, denote by $\langle q'|e^{-\frac{i}{\hbar}(t'-t_1)H}Q|q_1\rangle$ and $\langle q_1|e^{-\frac{i}{\hbar}(t_1-t)H}|q\rangle$

[1] As a function of q' it is the Dirac delta function, $|q\rangle(q') = \delta(q-q') \in \mathscr{S}(\mathbb{R})'$.

the integral kernels of the operators $e^{-\frac{i}{\hbar}(t'-t_1)H}Q$ and $e^{-\frac{i}{\hbar}(t_1-t)H}$. Using $Q|q\rangle = q|q\rangle$ and the formula for the integral kernel of the operator product, we get

$$\begin{aligned}\langle q', t'|Q(t_1)|q, t\rangle &= \int_{-\infty}^{\infty} \langle q'|e^{-\frac{i}{\hbar}(t'-t_1)H}Q|q_1\rangle\langle q_1|e^{-\frac{i}{\hbar}(t_1-t)H}|q\rangle dq_1 \\ &= \int_{-\infty}^{\infty} \langle q', t'|q_1, t_1\rangle q_1 \langle q_1, t_1|q, t\rangle dq_1.\end{aligned}$$

(In physics literature this is called "inserting a complete set of states"). Using (7.30), we obtain

$$\begin{aligned}&\int_{-\infty}^{\infty} \langle q', t'|q_1, t_1\rangle q_1 \langle q_1, t_1|q, t\rangle dq_1 \\ &= \int_{-\infty}^{\infty} q_1 \left(\int\limits_{\substack{q(t')=q' \\ q(t_1)=q_1}} e^{\frac{i}{\hbar}\int_{t_1}^{t'} L(q,\dot{q})d\tau}\mathscr{D}q \int\limits_{\substack{q(t_1)=q_1 \\ q(t)=q}} e^{\frac{i}{\hbar}\int_{t}^{t_1} L(q,\dot{q})d\tau}\mathscr{D}q \right) dq_1 \\ &= \int\limits_{\substack{q(t')=q' \\ q(t)=q}} q(t_1) e^{\frac{i}{\hbar}\int_{t}^{t'} L(q,\dot{q})d\tau}\mathscr{D}q,\end{aligned}$$

so that

$$\langle q', t'|Q(t_1)|q, t\rangle = \int\limits_{P(\mathbb{R})_{q,t}^{q',t'}} q(t_1) e^{\frac{i}{\hbar}\int_{t}^{t'} L(q,\dot{q})d\tau}\mathscr{D}q. \tag{15.3}$$

REMARK 15.1. In physics literature it is customary to use $q(t_1)$ in both sides of (15.3), where in the left hand side it is understood as an operator $e^{\frac{i}{\hbar}t_1 H}Qe^{-\frac{i}{\hbar}t_1 H}$, and in the right had side — as a value of a function $q(\tau) \in P(\mathbb{R})_{q,t}^{q',t'}$ at $\tau = t_1$.

Repeating these time-slicing arguments for the definition of path integral, for $t' > t_1 > t_2 > t$ we get

$$\langle q', t'|Q(t_1)Q(t_2)|q, t\rangle = \int\limits_{P(\mathbb{R})_{q,t}^{q',t'}} q(t_1)q(t_2) e^{\frac{i}{\hbar}\int_{t}^{t'} L(q,\dot{q})d\tau}\mathscr{D}q.$$

However, if $t' > t_2 > t_1 > t$, then, according to the time-slicing procedure, the right hand side of this formula is equal to $\langle q', t'|Q(t_2)Q(t_1)|q, t\rangle$.

Combining these two cases, we obtain

$$\langle q', t'|T(Q(t_1)Q(t_2))|q, t\rangle = \int\limits_{P(\mathbb{R})_{q,t}^{q',t'}} q(t_1)q(t_2)e^{\frac{i}{\hbar}\int_t^{t'} L(q,\dot{q})d\tau}\mathscr{D}q, \tag{15.4}$$

where

$$T(Q(t_1)Q(t_2)) = \begin{cases} (Q(t_1)Q(t_2) & \text{if} \quad t_1 > t_2, \\ (Q(t_2)Q(t_1) & \text{if} \quad t_2 > t_1 \end{cases}$$

"puts earlier times on the right".

In general, n-point matrix elements

$$\langle q', t'|T(Q(t_1)\cdots Q(t_n))|q, t\rangle = \int\limits_{P(\mathbb{R})_{q,t}^{q',t'}} q(t_1)\cdots q(t_n)e^{\frac{i}{\hbar}\int_t^{t'} L(q,\dot{q})d\tau}\mathscr{D}q \tag{15.5}$$

can be combined into a single path integral by introducing an "external source" $j(t)$ and adding the term $\int_t^{t'} j(\tau)q(\tau)d\tau$ to the action. Namely, introduce a generating functional

$$z[j] = \int\limits_{P(\mathbb{R})_{q,t}^{q',t'}} e^{\frac{i}{\hbar}\int_t^{t'}(L(q,\dot{q})+\hbar j(\tau)q(\tau))d\tau}\mathscr{D}q, \tag{15.6}$$

so that $z[0] = \langle q', t'|q, t\rangle$. Then we obtain

$$\langle q', t'|T(Q(t_1)\cdots Q(t_n))|q, t\rangle = i^{-n}\frac{\delta^n z[j]}{\delta j(t_1)\cdots\delta j(t_n)}\bigg|_{j=0} z(0).$$

15.2. Green's functions in QFT

Our goal is to express the generating function[2] $Z[J]$ of multi-point correlation functions of quantum fields, introduced in Chapter 14, in terms of the path integral. Namely, similarly to (15.6), we formally consider a path integral[3]

$$\boldsymbol{Z}[J] = \int e^{iS(\varphi)+i\int_{\mathbb{R}^4} J(x)\varphi(x)d^4x}\mathscr{D}\varphi, \tag{15.7}$$

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[2]Here we put $\hbar = 1$.

[3]One can define $\boldsymbol{Z}[J]$ (up to an infinite J-independent constant) as a limit of multiple Fresnel type integrals when the number of integrations goes to infinity.

where

$$S(\varphi) = \int_{\mathbb{R}^4} \mathscr{L}(\varphi, \partial_\mu \varphi) d^4x = \frac{1}{2} \int_{\mathbb{R}^4} \left(\partial_\mu \varphi \partial^\mu \varphi - m^2 \varphi^2\right) d^4x$$

is the action functional of a free scalar field, $J(x)$ is rapidly decaying real-valued function on $\mathbb{R}^4$,

$$\mathscr{D}\varphi = \prod_{x \in \mathbb{R}^4} d\varphi(x)$$

and "integration" goes over all smooth fields $\varphi(x)$ that decay fast as $(x^0)^2 + \boldsymbol{x}^2 \to \infty$. Since in QFT we have $Z[0] = \langle 0|0 \rangle = 1$, it is natural to define

$$Z[J] = \frac{\boldsymbol{Z}[J]}{\boldsymbol{Z}[0]},$$

which 'cancels' the infinite constant in the definition of $\boldsymbol{Z}[J]$.

One can formally understand what kind of objects $\boldsymbol{Z}[0]$ and $\boldsymbol{Z}[J]$ are, and explicitly compute their ratio. For this aim, recall the finite-dimensional Gaussian integral

$$\int_{\mathbb{R}^n} e^{-\frac{1}{2}(A\boldsymbol{x}, \boldsymbol{x}) + (\boldsymbol{b}, \boldsymbol{x})} d^n \boldsymbol{x} = \sqrt{\frac{\pi^n}{\det A}} e^{\frac{1}{2}(A^{-1}\boldsymbol{b}, \boldsymbol{b})}, \tag{15.8}$$

where A is positive-definite $n \times n$ symmetric matrix, $\boldsymbol{b} \in \mathbb{R}^n$ and $(\, , \,)$ stands for the Euclidean inner product in $\mathbb{R}^n$. Formula (15.8) is easily proved by "completing the square" — a change variables $\boldsymbol{x} \mapsto \boldsymbol{x} + \boldsymbol{x}_0$, where $\boldsymbol{x}_0$ satisfies $A\boldsymbol{x}_0 = \boldsymbol{b}$, after which it reduces to pure Gaussian integral. Similar formula holds for the F integral (see Chapter 8),

$$\int_{\mathbb{R}^n} e^{-\frac{i}{2}(A\boldsymbol{q}, \boldsymbol{q}) + i(\boldsymbol{p}, \boldsymbol{q})} d^n \boldsymbol{q} = e^{-\frac{\pi i n}{4} + \frac{\pi i \nu}{2}} \frac{\sqrt{(2\pi)^n}}{\sqrt{|\det A|}} \, e^{\frac{i}{2}(A^{-1}\boldsymbol{p}, \boldsymbol{p})}, \tag{15.9}$$

where the integral is understood in as $\lim_{R \to \infty} \int_{|\boldsymbol{q}| \leq R}$ and ν is the number of negative eigenvalues of a real, non-degenerate symmetric $n \times n$ matrix A.

It follows from the Stokes theorem,

$$S(\varphi) = -\frac{1}{2} \int_{\mathbb{R}^4} \varphi(x)(\Box + m^2)\varphi(x) d^4x,$$

so that we can write

$$\boldsymbol{Z}[J] = \int e^{-\frac{i}{2} \int \varphi(x)(\Box + m^2)\varphi(x) d^4x + i \int_{\mathbb{R}^4} J(x)\varphi(x) d^4x} \mathscr{D}\varphi.$$

This formula shows remarkable similarity with formula (15.9), where the operator $\Box + m^2$ plays the role of a matrix A, the source $J(x)$ — the role of a vector $\boldsymbol{b}$, and the inner product in $\mathbb{R}^n$ — the role of an inner product in the real Hilbert space $L^2(\mathbb{R}^4, d^4x)$. Correspondingly, the role of a vector $\boldsymbol{x}_0$ is played by the function $\varphi_0(x)$, which satisfies the equation

$$(\Box + m^2)\varphi_0(x) = J(x). \tag{15.10}$$

Assuming that the "measure of integration" is invariant under translations, $\mathscr{D}(\varphi + \varphi_0) = \mathscr{D}\varphi$, by the analogy with (15.9) we get

$$\boldsymbol{Z}[J] = \frac{C}{\sqrt{\det(\Box + m^2)}} \exp\left\{\frac{i}{2}\int_{\mathbb{R}^4} \varphi_0(x)J(x)d^4x\right\},$$

where $\det(\Box + m^2)$ is suitably defined determinant of the differential operator $\Box + m^2$, and C is some (possibly infinite!) constant. Since also

$$\boldsymbol{Z}[0] = \frac{C}{\sqrt{\det(\Box + m^2)}},$$

we see that the ratio

$$Z[J] = \exp\left\{\frac{i}{2}\int_{\mathbb{R}^4} \varphi_0(x)J(x)d^4x\right\}$$

is well-defined and does not depend on the definition of $\det(\Box + m^2)$!

However, solution $\varphi_0(x)$ of equation (15.10) depends on the choice of a Green's function for the operator $\Box + m^2$. As we seen in Chapter 14, correct choice should reflect causality and is given by the causal Green's function $D^c(x - y)$. As it follows from formula (14.4), the replacement $m^2 \mapsto m^2 - i\varepsilon$ makes the inverse operator $(\Box + m^2 - i\varepsilon)^{-1}$ well-defined, and the causal propagator is obtained in the limit $\varepsilon \to 0^+$. Thus for the generating functional we finally obtain

$$\begin{aligned} Z[J] &= \lim_{\varepsilon\to 0^+} \exp\left\{\frac{i}{2}\int_{\mathbb{R}^4} J(x)(\Box + m^2 - i\varepsilon)^{-1}J(x)d^4x\right\} \\ &= \exp\left\{\frac{i}{2}\int_{\mathbb{R}^4}\int_{\mathbb{R}^4} D^c(x-y)J(x)J(y)d^4xd^4y\right\}. \end{aligned} \tag{15.11}$$

As before, from here we immediately get

$$W[J] = \frac{i}{2}\int_{\mathbb{R}^4}\int_{\mathbb{R}^4} D^c(x-y)J(x)J(y)d^4xd^4y, \tag{15.12}$$

so all correlation functions reduce to the 2-point function.