Lectures on Quantum Mechanics

Leon A. Takhtajan

Department of Mathematics, Stony Brook University, Stony Brook, NY 11794-3651, USA

E-mail address: leontak@math.sunysb.edu

Contents

CHAPTER 1

Classical Mechanics

1. Lagrangian Mechanics

1.1. Generalized coordinates. Classical mechanics describes systems of finitely many interacting particles[1]. The position of a system is specified by positions of its particles and defines a point in a smooth, finite-dimensional manifold M, the *configuration space* of a system. Coordinates on M are called *generalized coordinates* of a system, and the dimension $n = \dim M$ is called the *number of degrees of freedom*. Classical mechanics describes systems with finitely many degrees of freedom, while systems with infinitely many degrees of freedom are described by classical field theory.

The state of a system at any fixed moment of time is described by a point $q \in M$, and by a tangent vector $v \in T_qM$ at this point. The basic principle of classical mechanics is *Newton-Laplace determinacy principle*, which asserts that the state of a system at a given moment completely determines its motion at all times t (in the future and in the past), defining a *classical trajectory* — a path $q(t)$ in M. In generalized coordinates $q(t)$ is given by $(q_1(t), \dots, q_n(t))$, and corresponding derivatives $\dot{q}_i = \frac{dq_i}{dt}$ are called *generalized velocities*. Newton-Laplace principle is a fundamental experimental fact, which is valid in the world around us. It implies that *generalized accelerations* $\ddot{q}_i = \frac{d^2q_i}{dt^2}$ are uniquely defined by generalized coordinates q_i and generalized velocities $\dot{q}_i$, so that classical trajectories satisfy a system of second order differential equations, called *equations of motion*. In the next section we formulate the most general principle governing the motion of mechanical systems.

1.1.1. *Notations.* We use standard notations from differential geometry. All manifolds, maps and functions are smooth (i.e., C^∞) and real-valued, unless it is specified explicitly otherwise. Local coordinates $\mathbf{q} = (q_1, \dots, q_n)$ on a smooth n-dimensional manifold M at a point $q \in M$ are Cartesian coordinates on $\phi(U) \subset \mathbb{R}^n$, where (U, ϕ) is a coordinate chart on M centered at $q \in U$. For $f : U \to \mathbb{R}^n$ we denote $(f \circ \phi^{-1})(q_1, \dots, q_n)$ by $f(\mathbf{q})$. If U is a domain in $\mathbb{R}^n$ then for $f : U \to \mathbb{R}$ we denote by

$$\frac{\partial f}{\partial \mathbf{q}} = \left(\frac{\partial f}{\partial q_1}, \dots, \frac{\partial f}{\partial q_n}\right)$$

[1]A particle is a material body whose dimensions may be neglected in describing its motion.

the gradient of a function f at a point $\mathbf{q} \in \mathbb{R}^n$ with Cartesian coordinates $(q_1, \dots, q_n)$. We denote by

$$\mathsf{A}^\bullet(M) = \bigoplus_{k=0}^{n} \mathsf{A}^k(M)$$

the graded algebra of smooth differential forms on M, and by d its deRham differential — a graded derivation of $\mathsf{A}^\bullet(M)$ of degree 1, such that for $f \in \mathsf{A}^0(M) = C^\infty(M)$ it is a differential df of a function f. By $\mathrm{Vect}(M)$ we denote the Lie algebra of smooth vector fields on M and for $X \in \mathrm{Vect}(M)$ we denote, respectively, by $\mathcal{L}_X$ and i_X the Lie derivative along X and the inner product with X. The inner product is a graded derivation of $\mathsf{A}^\bullet(M)$ of degree -1 such that $i_X(df) = X(f) = df(X)$ for $f \in \mathsf{A}^0(M)$. The derivations $\mathcal{L}_X$ and i_X satisfy Cartan formulas

$$\begin{aligned} \mathcal{L}_X =& i_X \circ d + d \circ i_X = (d + i_X)^2 \\ i_{[X,Y]} =& \mathcal{L}_X \circ i_Y - i_Y \circ \mathcal{L}_X \end{aligned}$$

If $f : M \to N$ is a smooth mapping of manifolds, then $f_* : TM \to TN$ and $f^* : T^*N \to T^*M$ denote, respectively, the induced mappings on tangent and cotangent bundles. Other notations, including those traditional for classical mechanics, will be introduced in the main text.

1.2. The principle of the least action. The main assumption of Lagrangian mechanics is that a mechanical system with a configuration space M is completely characterized by its *Lagrangian* L — a smooth, real-valued function on the direct product $TM \times \mathbb{R}$ of the tangent bundle of M and the time axis[2]. The fundamental problem is to derive the differential equations for generalized coordinates, which describe the motion of the system (M, L) starting from the initial state $q_i, \dot{q}_i$. According to the *principle of the least action* (or *Hamilton's principle*), the equations of motion are completely characterized by specifying the motion of the system between position $q_0 \in M$ at $t = t_0$ and position $q_1 \in M$ at $t = t_1$.

Namely, let

$$\Omega(M; q_0, t_0, q_1, t_1) = \{\gamma : [t_0, t_1] \to M,\ \gamma(t_0) = q_0,\ \gamma(t_1) = q_1\}$$

be the space of smooth paths in M connecting points q_0 and q_1. The path space $\Omega(M) = \Omega(M; q_0, t_0, q_1, t_1)$ is a real infinite-dimensional Fréchet manifold, and the tangent space $T_\gamma\Omega(M)$ to $\Omega(M)$ at a point $\gamma \in \Omega(M)$ consists of all smooth vector fields along the path $\gamma(t)$ in M which vanish at the endpoints. Following tradition, we call a smooth path in $\Omega(M)$, passing through the point $\gamma \in \Omega(M)$, a *variation with fixed endpoints* of the path $\gamma(t)$ in M. Explicitly, variation is a smooth family $\gamma_\varepsilon(t) = \Gamma(t, \varepsilon)$ of paths in M, given by a smooth map

$$\Gamma : [t_0, t_1] \times [-\varepsilon_0, \varepsilon_0] \to M,$$

[2]It follows from Newton-Laplace principle that L could depend only on generalized coordinates and velocities, and on time.

such that $\Gamma(t,0) = \gamma(t)$ for all $t \in [t_0, t_1]$, and $\Gamma(t_0, \varepsilon) = q_0, \Gamma(t_1, \varepsilon) = q_1$ for all $\varepsilon \in [-\varepsilon_0, \varepsilon_0]$. The tangent vector to $\Omega(M)$ at γ corresponding to the variation $\gamma_\varepsilon(t)$ is also called *infinitesimal variation* and is given by

$$\delta\gamma = \left.\frac{\partial \Gamma}{\partial \varepsilon}\right|_{\varepsilon=0} \in T_\gamma \Omega(M), \ \ \delta\gamma(t) = \Gamma_*(\tfrac{\partial}{\partial \varepsilon})(t,0) \in T_{\gamma(t)}M.$$

For every $\gamma \in \Omega(M)$ let $\gamma'(t) = \gamma_*(\frac{\partial}{\partial t}) \in T_{\gamma(t)}M$, where $\frac{\partial}{\partial t}$ is the tangent vector to the interval $[t_0, t_1]$ at a point t. The path $\gamma'(t)$ in TM is the tangential lift of the path $\gamma(t)$ in M.

Definition. The *action functional* $S : \Omega(M) \to \mathbb{R}$ of the system $(M; L)$ is

$$S(\gamma) = \int_{t_0}^{t_1} L(\gamma'(t), t)dt.$$

Equivalently, the action functional can be defined as the evaluation of the 1-form Ldt on $TM \times \mathbb{R}$ over the 1-chain $\tilde{\gamma}$ on $TM \times \mathbb{R}$,

$$S(\gamma) = \int_{\tilde{\gamma}} Ldt,$$

where $\tilde{\gamma} = \{(\gamma'(t), t); t_0 \leq t \leq t_1\} \subset TM \times \mathbb{R}$ and

$$Ldt\left(w, c\tfrac{\partial}{\partial t}\right) = cL(q, v), \ \ w \in T_{(q,v)}TM, \ c \in \mathbb{R}.$$

Principle Of The Least Action (Hamilton's Prinicple). The path $\gamma \in \Omega(M)$ describes the motion of the system (M, L) between the position $q_0 \in M$ at time t_0 and the position $q_1 \in M$ at time t_1 if and only if it is a critical point (an *extremal*) of the action functional S,

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

for all variations $\gamma_\varepsilon(t)$ of $\gamma(t)$.

Remark. Note that this principle does not state that a classical trajectory connecting points q_0 and q_1 always exists or is unique, nor does it state that corresponding trajectory is a minimum of the action functional. The principle just states that the system (M, L) moves along the extremals of the action functional.

The following choice of local coordinates on TM will be very convenient for writing down equations of motion.

Definition. Let (U, ϕ) be a coordinate chart on M with local coordinates $\mathbf{q}$. Coordinates

$$(\mathbf{q}, \mathbf{v}) = (q_1, \ldots, q_n, v_1, \ldots, v_n)$$

on a chart TU on TM are called *standard coordinates*, if for $(q, v) \in TU$ and $f \in C^\infty(U)$,

$$v(f) = \sum_{i=1}^{n} v_i \frac{\partial f}{\partial q_i}(q) = \mathbf{v}\frac{\partial f}{\partial \mathbf{q}}.$$

Equivalently, standard coordinates on TU are uniquely characterized by the condition that $\mathbf{v} = (v_1, \dots, v_n)$ are coordinates in the fiber corresponding to the basis $\frac{\partial}{\partial q_1}, \dots, \frac{\partial}{\partial q_n}$ for T_qM. In other words, standard coordinates are Cartesian coordinates on $\phi_*(TU) \subset T\mathbb{R}^n \simeq \mathbb{R}^n \times \mathbb{R}^n$.

The tangential lift $\gamma'(t)$ of a path $\gamma(t)$ in M in standard coordinates on TU is $(\mathbf{q}(t), \dot{\mathbf{q}}(t)) = (q_1(t), \dots, q_n(t), \dot{q}_1(t), \dots, \dot{q}_n(t))$, where dot stands for the time derivative, so that

$$L(\gamma'(t), t) = L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t).$$

Following a centuries long tradition, we will denote standard coordinates as

$$(\mathbf{q}, \dot{\mathbf{q}}) = (q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n),$$

where the dot here *does not* stand for the time derivative. Since we only consider curves in TM that are tangential lifts of curves in M, there will be no confusion[3] .

THEOREM 1.1. *In standard coordinates, extremals $\mathbf{q}(t)$ of the action functional satisfy the Euler-Lagrange equations*

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

PROOF. Suppose first that the extremal $\gamma(t)$ lies in a coordinate chart U of M. Then a simple computation in standard coordinates, using integration by parts, gives

$$\begin{aligned} 0 &= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} S(\gamma_\varepsilon) \\ &= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \int_{t_0}^{t_1} L\left(\mathbf{q}(t,\varepsilon), \dot{\mathbf{q}}(t,\varepsilon), t\right) dt \\ &= \sum_{i=1}^{n} \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta \dot{q}_i\right) dt \\ &= \sum_{i=1}^{n} \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}\right) \delta q_i dt + \sum_{i=1}^{n} \left.\frac{\partial L}{\partial \dot{q}_i}\delta q_i\right|_{t_0}^{t_1}. \end{aligned}$$

The second sum in the last line vanishes due to the property $\delta q_i(t_0) = \delta q_i(t_1) = 0$, $i = 1, \dots, n$. The first sum is zero for arbitrary smooth functions

[3]We reserve notation $(\mathbf{q}(t), \mathbf{v}(t))$ for general curves in TM.

δq_i on $[t_0, t_1]$ which vanish at the endpoints. This implies that for each term in the sum the integrand is identically zero,

$$\frac{\partial L}{\partial q_i}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\right) = 0, \; i = 1, \dots, n.$$

Since the restriction of an extremal of the action functional on a coordinate chart on M is again an extremal, each extremal in standard coordinates satisfies Euler-Lagrange equations. □

1.2.1. *Examples.* Mathematically, one can consider mechanical systems on a configuration space M with arbitrary smooth functions on $TM \times \mathbb{R}$ as Lagrangians. However, Lagrangians describing physical systems satisfy additional properties which can be deduced from basic physical principles. The first basic principle describes the nature of the *space-time* in classical mechanics. It states that the space-time is a direct product $\mathbb{R}^3 \times \mathbb{R}$, where $\mathbb{R}^3$ carries standard Euclidean product and has a fixed orientation. The second is Galileo's relativity principle[4].

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

$$\mathbf{r} \mapsto \mathbf{r} + \mathbf{r}_0 + \mathrm{g}\mathbf{r}, \;\; t \mapsto t + t_0,$$

where $\mathbf{r} \in \mathbb{R}^3$ and $\mathrm{g} : \mathbb{R}^3 \to \mathbb{R}^3$ is an orthogonal transformation.

Example 1.1 (Free particle). Configuration space for a free particle is $M = \mathbb{R}^3$, and it can deduced from Galileo's relativity principle that the Lagrangian for a free particle is

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

Here $m > 0$ is the mass of a particle and $\dot{\mathbf{r}}^2 = |\dot{\mathbf{r}}|^2$ is the square of the length of the velocity vector $\dot{\mathbf{r}} \in T_{\mathbf{r}}\mathbb{R}^3 \simeq \mathbb{R}^3$. Euler-Lagrange equations give *Newton's law of inertia*,

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

If the Lagrangian does not explicitly depend on time, i.e., L is a function on TM, then the system (M, L) is called *closed.*

Example 1.2 (Interacting particles). Closed system of N interacting particles in $\mathbb{R}^3$ with masses $m_1, \dots, m_N$, is described by the configuration space

$$M = \mathbb{R}^{3N} = \underbrace{\mathbb{R}^3 \times \cdots \times \mathbb{R}^3}_{N}$$

[4]These principles are valid only in the non-relativistic limit of special relativity, when the speed of light in the vacuum is assumed to be infinite.

with a position vector $\mathbf{r} = (\mathbf{r}_1, \dots, \mathbf{r}_N)$, where $\mathbf{r}_a \in \mathbb{R}^3$ is the position vector of a-th particle, $a = 1, \dots, N$. It is found that the Lagrangian is given by

$$L = \sum_{a=1}^{N} \tfrac{1}{2} m_a \dot{\mathbf{r}}_a^2 - U(\mathbf{r}) = T - U,$$

where

$$T = \sum_{a=1}^{N} \tfrac{1}{2} m_a \dot{\mathbf{r}}_a^2$$

is called the *kinetic energy* and $U(\mathbf{r})$ — the *potential energy.* The Euler-Lagrange equations give *Galileo-Newton's equations*

$$m_a \ddot{\mathbf{r}}_a = \mathbf{F}_a,$$

where

$$\mathbf{F}_a = -\frac{\partial U}{\partial \mathbf{r}_a}$$

is a *force* on a-th particle, $a = 1, \dots, N$. Forces of this form are called *conservative.*

Example 1.3 (Universal gravitation). It follows from the Galileo's relativity principle that the potential energy $U(\mathbf{r})$ of the closed system of N interacting particles with conservative forces depends only on relative positions of the particles. The principle of *equality of action and reaction forces*[5] leads to the following form for the potential energy

$$U(\mathbf{r}) = \sum_{1 \le a < b \le N} U_{ab}(\mathbf{r}_a - \mathbf{r}_b).$$

A fundamental example is universal gravitation. According to the *Newton's law of gravitation*, the potential energy of the gravitational force between two particles with masses m_a and m_b is

$$U(\mathbf{r}_a - \mathbf{r}_b) = G \frac{m_a m_a}{|\mathbf{r}_a - \mathbf{r}_b|},$$

where G is the gravitational constant. In this case, the configuration space of N particles is

$$M = \{(\mathbf{r}_1, \dots, \mathbf{r}_N) \in \mathbb{R}^{3N} \,|\, \mathbf{r}_a \neq \mathbf{r}_b \text{ for } a \neq b, a, b = 1, \dots, N\}.$$

Example 1.4 (Riemannian geometry). Let M be a Riemannian manifold with a Riemannian metric $\langle\ ,\ \rangle : T_q M \otimes T_q M \to \mathbb{R}$,

$$\langle u, v \rangle = \sum_{i,j=1}^{n} g^{ij}(q) u_i v_j, \;\; u, v \in T_q M.$$

The Lagrangian

$$L(q, v) = \frac{1}{2} \|v\|^2 = \frac{1}{2} \langle v, v \rangle, \; v \in T_q M$$

[5]This principle is independent from Galileo's relativity principle.

gives rise to the action functional in Riemannian geometry, and corresponding Euler-Lagrange equations are geodesic equations written with respect to the natural parameter. Another choice of the Langrangian is

$$\tilde{L}(q,v) = \|v\|,\ v \in T_qM.$$

It gives rise to the length functional in Riemannian geometry and corresponding Euler-Lagrange equations are geodesic equations written in a reparameterization invariant way.

1.2.2. *Exercises.* (Later) Examples of Lagrangians and first and second variations for the action functional in Riemannian geometry; invariant formulation of Euler-Lagrange equations (following Bryant lectures), etc.

1.3. Symmetries and Noether theorem. Since during the motion of a mechanical system its generalized coordinates and velocities vary with time, of particular interest are the functions of these quantities which remain constant during the motion.

Definition. A smooth function $I : TM \to \mathbb{R}$ is the *integral of motion* (*first integral*, or *conservation law*) for the system (M, L) if

$$\frac{d}{dt} I(\gamma'(t)) = 0$$

for all extremals γ of L.

Definition. The *energy* of a system (M, L) is a function E on $TM \times \mathbb{R}$ defined in standard coordinates on TM by

$$E(\mathbf{q}, \dot{\mathbf{q}}, t) = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i}(\mathbf{q}, \dot{\mathbf{q}}, t)\dot{q}_i - L(\mathbf{q}, \dot{\mathbf{q}}, t).$$

Lemma 1.1. *The energy* $E = \frac{\partial L}{\partial \dot{\mathbf{q}}}\dot{\mathbf{q}} - L$ *is a well-defined function on* $TM \times \mathbb{R}$.

Proof. Let (U, ϕ) and (U', ϕ') be coordinate charts on M such that $\mathbb{R}^n \supset \phi(U \cap U') \ni \mathbf{q} \mapsto \mathbf{q}' = f(\mathbf{q}) \in \phi'(U \cap U') \subset \mathbb{R}^n$. It follows from the definition of standard coordinates that

$$\dot{q}'_i = \sum_{j=1}^{n} \frac{\partial f_i}{\partial q_j}\dot{q}_j,\ \ i = 1, \dots, n,$$

or $\dot{\mathbf{q}}' = f_*(\mathbf{q})\dot{\mathbf{q}}$, where $f_*(\mathbf{q}) = \left\{\frac{\partial f_i}{\partial q_j}\right\}_{i,j=1}^{n}$ is a matrix-valued function on $\phi'(U \cap U')$. Similarly,

$$d\mathbf{q}' = f_*(\mathbf{q})d\mathbf{q} \quad \text{and} \quad d\dot{\mathbf{q}}' = g(\mathbf{q}, \dot{\mathbf{q}})d\mathbf{q} + f_*(\mathbf{q})d\dot{\mathbf{q}},$$

where $g(\mathbf{q},\dot{\mathbf{q}})$ is a matrix-valued function. We have

$$\begin{aligned} dL =& \frac{\partial L}{\partial \mathbf{q}'} d\mathbf{q}' + \frac{\partial L}{\partial \dot{\mathbf{q}}'} d\dot{\mathbf{q}}' \\ =& \left(\frac{\partial L}{\partial \mathbf{q}'} f_*(\mathbf{q}) + \frac{\partial L}{\partial \dot{\mathbf{q}}'} g(\mathbf{q},\dot{\mathbf{q}}) \right) d\mathbf{q} + \frac{\partial L}{\partial \dot{\mathbf{q}}'} f_*(\mathbf{q}) d\dot{\mathbf{q}} \\ =& \frac{\partial L}{\partial \mathbf{q}} d\mathbf{q} + \frac{\partial L}{\partial \dot{\mathbf{q}}} d\dot{\mathbf{q}}. \end{aligned}$$

Thus under the change of variables $\mathbf{q}' = f(\mathbf{q}), \dot{\mathbf{q}}' = f_*(\mathbf{q})\dot{\mathbf{q}}$

$$\frac{\partial L}{\partial \dot{\mathbf{q}}'} f_*(\mathbf{q}) = \frac{\partial L}{\partial \dot{\mathbf{q}}} \quad \text{and} \quad \frac{\partial L}{\partial \dot{\mathbf{q}}'} \dot{\mathbf{q}}' = \frac{\partial L}{\partial \dot{\mathbf{q}}} \dot{\mathbf{q}},$$

so that two expressions for E in coordinates $(\mathbf{q},\dot{\mathbf{q}})$ and $(\mathbf{q}',\dot{\mathbf{q}}')$ agree on $\phi'_*(TU \cap TU')$. □

COROLLARY 1.1. *Standard coordinates $(\mathbf{q},\dot{\mathbf{q}})$ on TM have the property that under the change of coordinates $\mathbf{q}$ on M components of*

$$\frac{\partial L}{\partial \dot{\mathbf{q}}}(\mathbf{q},\dot{\mathbf{q}}) = \left(\frac{\partial L}{\partial \dot{q}_1}, \dots, \frac{\partial L}{\partial \dot{q}_n} \right)$$

transform like components of a 1-form on M, and components of $\dot{\mathbf{q}} = (\dot{q}_1, \dots, \dot{q}_n)$ — like components of a tangent vector on M.

PROPOSITION 1.1 (Conservation of energy). *The energy of a closed system is an integral of motion.*

PROOF. For an extremal γ set $E(t) = E(\gamma(t))$. We have, according to the Euler-Lagrange equations,

$$\begin{aligned} \frac{dE}{dt} =& \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}} \right) \dot{\mathbf{q}} + \frac{\partial L}{\partial \dot{\mathbf{q}}} \ddot{\mathbf{q}} - \frac{\partial L}{\partial \mathbf{q}} \dot{\mathbf{q}} - \frac{\partial L}{\partial \dot{\mathbf{q}}} \ddot{\mathbf{q}} - \frac{\partial L}{\partial t} \\ =& \left(\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}} \right) - \frac{\partial L}{\partial \mathbf{q}} \right) \dot{\mathbf{q}} - \frac{\partial L}{\partial t} = -\frac{\partial L}{\partial t}. \end{aligned}$$

Since for the closed system $\frac{\partial L}{\partial t} = 0$, the energy is conserved. □

Conservation of energy for a closed mechanical system is a basic law of physics, which follows from the fundamental principle of *homogenuity of time*. By virtue of this principle, the Lagrangian of a closed system is invariant under time translations, i.e., it does not explicitly depend on time. For the closed system of N interacting particles considered in the previous example,

$$E = \sum_{a=1}^{N} m_a \dot{\mathbf{r}}_a^2 - L = \sum_{a=1}^{N} \tfrac{1}{2} m_a \dot{\mathbf{r}}_a^2 + U(\mathbf{r}).$$

The total energy is the sum of the kinetic energy and the potential energy, $E = T + U$.

DEFINITION. A Lagrangian $L : TM \to \mathbb{R}$ for a closed system is invariant with respect to the diffeomorphism $h : M \to M$, if $L(h_*(w)) = L(w)$ for all $w \in TM$. The diffeomorphism h is called the *symmetry* of the system (M, L).

The following theorem asserts that continuous symmetries of a mechanical system give rise to conservation laws.

THEOREM 1.2 (Noether). *Suppose that the Lagrangian L of a closed system is invariant under a one-parameter group $\{h^s\}_{s\in\mathbb{R}}$ of diffeomorphisms of M. Then the system (M, L) admits an integral of motion I, given in the standard coordinates by*

$$I(\mathbf{q}, \dot{\mathbf{q}}) = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i}(\mathbf{q}, \dot{\mathbf{q}}) \left(\left.\frac{dh_i^s(\mathbf{q})}{ds}\right|_{s=0} \right) = \frac{\partial L}{\partial \dot{\mathbf{q}}}\mathbf{q}'.$$

PROOF. Since

$$\mathbf{q}' = \left(\left.\frac{dh_1^s(\mathbf{q})}{ds}\right|_{s=0}, \dots, \left.\frac{dh_n^s(\mathbf{q})}{ds}\right|_{s=0} \right)$$

are components of the vector field on M associated with the one-parameter group $\{h^s\}_{s\in\mathbb{R}}$, it follows from Corollary 1.1 that I is a well-defined function on TM. We get, differentiating $L(h_*^s w) = L(w)$ with respect to s at $s = 0$ and using the Euler-Lagrange equations,

$$0 = \frac{\partial L}{\partial \mathbf{q}}\mathbf{q}' + \frac{\partial L}{\partial \dot{\mathbf{q}}}\dot{\mathbf{q}}' = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)\mathbf{q}' + \frac{\partial L}{\partial \dot{\mathbf{q}}}\frac{d\mathbf{q}'}{dt} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\mathbf{q}'\right).$$

□

REMARK. Conservation of energy does not follow from Noether's theorem, which was formulated for closed systems. One can extend it to general systems as follows. For a Lagrangian $L : TM \times \mathbb{R} \to \mathbb{R}$ define the *extended configuration space* $M_1 = M \times \mathbb{R}$ and set $L_1 : TM_1 \to \mathbb{R}$

$$L_1(\mathbf{q}, \tau, \dot{\mathbf{q}}, \dot{\tau}) = L\left(\mathbf{q}, \frac{\dot{\mathbf{q}}}{\dot{\tau}}, \tau\right)\dot{\tau},$$

where $(\mathbf{q}, \tau)$ are local coordinates on M_1 and we are using standard coordinates on TM_1. The Noether integral of motion I_1 for a system (M_1, L_1) give rise to the integral of motion I for the system (M, L),

$$I(\mathbf{q}, \dot{\mathbf{q}}, t) = I_1(\mathbf{q}, t, \dot{\mathbf{q}}, 1).$$

In particular, if L does not depend on time, Lagrangian L_1 is invariant under the one-parameter group of translations $\tau \mapsto \tau + s$ and corresponding Noether integral $I_1 = \frac{\partial L_1}{\partial \dot{\tau}}\dot{\tau}$ gives rise to $I = -E$, where E is the energy of the system (M, L).

The main applications of Noether theorem are the following.

EXAMPLE 1.5 (Conservation of momentum). Let $M = V$ — a vector space, and suppose that the Lagrangian L is invariant with respect to the one-parameter group $h^s(q) = q+sa$, $a \in V$. According to Noether's theorem,

$$I = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i} a_i$$

is an integral of motion. For the system of N interacting particles, considered in Example 1.2, $V = \mathbb{R}^{3N}$. Another fundamental principle of classical mechanics is *homogenuity of space.* By virtue of this principle, Lagrangian of a closed system of N particles is invariant under simultaneous translation of coordinates $\mathbf{r}_a = (r_{a1}, r_{a2}, r_{a3})$ of all particles by the same vector $\mathbf{c} \in \mathbb{R}^3$. Thus $a = (\mathbf{c}, \dots, \mathbf{c}) \in \mathbb{R}^{3N}$, and for every $\mathbf{c} = (c_1, c_2, c_3) \in \mathbb{R}^3$

$$I = \sum_{a=1}^{N} \left(\frac{\partial L}{\partial \dot{r}_{a1}} c_1 + \frac{\partial L}{\partial \dot{r}_{a2}} c_2 + \frac{\partial L}{\partial \dot{r}_{a3}} a_3 \right) = P^1 c_1 + P^2 c_2 + P^3 c_3$$

is an integral of motion. The integrals of motion P^1, P^2, P^3 define the vector

$$\mathbf{P} = \sum_{a=1}^{N} \frac{\partial L}{\partial \dot{\mathbf{r}}_a} \in \mathbb{R}^3$$

(or rather a vector in the dual space to $\mathbb{R}^3$), called the *momentum vector.* Explicitly,

$$\mathbf{P} = \sum_{a=1}^{N} m_a \dot{\mathbf{r}}_a,$$

so that the total momentum of a closed system is the sum of momenta of individual particles.

EXAMPLE 1.6 (Conservation of angular momentum). Let $M = V$ be the vector space with Euclidean inner product and let $G = \mathrm{SO(V)} \subset \mathrm{GL(V)}$ be the connected Lie group of automorphisms of V preserving the inner product, and let $\mathfrak{g} = \mathrm{so(V)} \subset \mathfrak{gl}(\mathrm{V})$ be its Lie algebra. Suppose that Lagrangian L is invariant with respect to the action of the one-parameter subgroup $h^s(q) = e^{s\mathrm{x}}(q)$ of G on V, where $\mathrm{x} \in \mathfrak{g}$ and e^{x} is the exponential map. According to Noether's theorem,

$$I = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i} (\mathrm{x}(q))_i$$

is an integral of motion. For the system of N interacting particles, considered in Example 1.2, $V = \mathbb{R}^{3N}$ and it is equipped with the standard Euclidean inner product.

Another fundamental principle of classical mechanics is the *isotropy of space.* By virtue of this principle, Lagrangian of a closed system is invariant under simultaneous rotation of coordinates $\mathbf{r}_a$ of all particles by the same orthogonal transformation in $\mathbb{R}^3$. Thus $\mathrm{x} = (x, \dots, x) \in \underbrace{\mathrm{so}(3) \oplus \cdots \oplus \mathrm{so}(3)}_{N}$, and for every $x \in \mathrm{so}(3)$

$$I = \sum_{a=1}^{N} \left(\frac{\partial L}{\partial \dot{r}_{a1}} x(\mathbf{r}_a)_1 + \frac{\partial L}{\partial \dot{r}_{a2}} x(\mathbf{r}_a)_2 + \frac{\partial L}{\partial \dot{r}_{a3}} x(\mathbf{r}_a)_3 \right)$$

is an integral of motion. Using the standard basis in $\mathrm{so}(3) \simeq \mathbb{R}^3$ (i.e., identifying $\mathbb{R}^3 \wedge \mathbb{R}^3 \simeq \mathbb{R}^3$), we get the *angular momentum vector*

$$\mathbf{M} = \sum_{a=1}^{N} \mathbf{r}_a \wedge \frac{\partial L}{\partial \dot{\mathbf{r}}_a} \in \mathbb{R}^3$$

(or rather a vector in the dual space to so(3)), whose components are integrals of motion. Explicitly,

$$\mathbf{M} = \sum_{a=1}^{N} m_a \mathbf{r}_a \wedge \dot{\mathbf{r}}_a,$$

so that the total angular momentum of a closed system is the sum of angular momenta of individual particles.

Combining the principle of equality of action and reaction forcess with homogenuity and isotropy of space, we see that the most general form of a Lagrangian for a closed system of N interacting particles is

$$L = \sum_{a=1}^{N} \tfrac{1}{2} m_a \dot{\mathbf{r}}_a^2 - \sum_{1 \leq a < b \leq N} U_{ab}(|\mathbf{r}_a - \mathbf{r}_b|).$$

1.4. Integration of equations of motion.

1.4.1. *One-dimensional motion.*

1.4.2. *The motion in a central field.*

1.4.3. *The Kepler problem.*

1.5. Legendre transformation. In standard coordinates $(\mathbf{q}, \dot{\mathbf{q}})$ at $(q, v) \in TM$ the Euler-Lagrange equations can be written explicitly as the following system of second order differential equations

$$\begin{aligned} \frac{\partial L}{\partial q_i}(\mathbf{q}, \dot{\mathbf{q}}) =& \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}(\mathbf{q}, \dot{\mathbf{q}}) \right) \\ =& \sum_{j=1}^{n} \left(\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}(\mathbf{q}, \dot{\mathbf{q}})\, \ddot{q}_j + \frac{\partial^2 L}{\partial \dot{q}_i \partial q_j}(\mathbf{q}, \dot{\mathbf{q}})\, \dot{q}_j \right), \quad i = 1, \dots, n. \end{aligned}$$

In order for this system to be solvable for the highest derivatives, the matrix

$$H_L = \left(\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}(\mathbf{q}, \dot{\mathbf{q}}) \right)$$

should be invertible in the neighborhood of a point (q, v) in TM.

DEFINITION. A system (M, L) is called non-degenerate if the matrix $H_L(q, v)$ is invertible for all $(q, v) \in TM$.

The last definition uses standard coordinates. For an invariant formulation, consider the 1-form θ_L on TM, defined in standard coordinates on TM by

$$\theta_L = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i} dq_i = \frac{\partial L}{\partial \dot{\mathbf{q}}} d\mathbf{q}.$$

It follows from Corollary 1.1 that the 1-form θ_L is well-defined.

LEMMA 1.2. *A system (M, L) is non-degenerate if and only if the 2-form $d\theta_L$ on TM is non-degenerate.*

PROOF. In standard coordinates,

$$d\theta_L = \sum_{i,j=1}^{n} \left(\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} d\dot{q}_j \wedge dq_i + \frac{\partial^2 L}{\partial \dot{q}_i \partial q_j} dq_j \wedge dq_i \right).$$

□

DEFINITION. Let (U, ϕ) be a coordinate chart on M. Coordinates

$$(\mathbf{q}, \mathbf{p}) = (q_1, \dots, q_n, p^1, \dots, p^n)$$

on the chart T^*U on the cotangent bundle T^*M are called *standard coordinates* if for $(q, p) \in T^*U$ and $f \in C^\infty(U)$

$$p^i(df) = \frac{\partial f}{\partial q_i}, \; i = 1, \dots, n.$$

Equivalently, standard coordinates on T^*U are uniquely characterized by the condition that $(p^1, \dots, p^n)$ are coordinates in the fiber corresponding to the basis $dq_1, \dots, dq_n$ for T_q^*M, which is dual to the basis $\frac{\partial}{\partial q_1}, \dots, \frac{\partial}{\partial q_n}$ for T_qM.

DEFINITION. The 1-form θ on T^*M, defined in standard coordinates by

$$\theta = \sum_{i=1}^{n} p^i dq_i = \mathbf{p} d\mathbf{q},$$

is called the *canonical Liouville 1-form.*

Corollary 1.1 shows that θ is a well-defined 1-form on T^*M. Equivalently, the 1-form θ can be defined as follows. Let $\pi : T^*M \to M$ be the canonical projection and $u \in T_{(q,p)}T^*M$. Then $\theta(u) = p(\pi_*(u))$.

DEFINITION. A fibre-wise mapping $\tau_L : TM \to T^*M$ is called a *Legendre transformation* associated with the Lagrangian L, if

$$\theta_L = \tau_L^*(\theta).$$

Equivalently, the Legendre transformation in standard coordinates is defined by

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

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

Definition. Suppose that the Legendre transformation τ_L is a diffeomorphism. The *Hamiltonian* $H : T^*M \to \mathbb{R}$, associated with the Lagrangian $L : TM \to \mathbb{R}$, is defined by

$$H \circ \tau_L = E = \frac{\partial L}{\partial \dot{\mathbf{q}}}\dot{\mathbf{q}} - L.$$

In standard coordinates,

$$H(\mathbf{q},\mathbf{p}) = \left.(\mathbf{p}\dot{\mathbf{q}} - L(\mathbf{q},\dot{\mathbf{q}}))\right|_{\mathbf{p}=\frac{\partial L}{\partial \dot{\mathbf{q}}}},$$

where $\dot{\mathbf{q}}$ is expressed in terms of $\mathbf{q},\mathbf{p}$ through the inverse of the Legendre transformation.

Theorem 1.3. *Suppose that the Legendre transformation τ_L is a diffeomorphism. Then the Euler-Lagrange equations in standard coordinates on TM,*

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{q}}} - \frac{\partial L}{\partial \mathbf{q}} = 0$$

are equivalent to the canonical Hamilton's equations in standard coordinates on T^*M,

$$\dot{q}_i = \frac{\partial H}{\partial p^i}, \quad \dot{p}^i = -\frac{\partial H}{\partial q_i}, \quad i = 1,\dots,n.$$

Proof. We have

$$\begin{aligned} dH =& \frac{\partial H}{\partial \mathbf{q}}d\mathbf{q} + \frac{\partial H}{\partial \mathbf{p}}d\mathbf{p} \\ =& \left.\left(\mathbf{p}d\dot{\mathbf{q}} + \dot{\mathbf{q}}d\mathbf{p} - \frac{\partial L}{\partial \mathbf{q}}d\mathbf{q} - \frac{\partial L}{\partial \dot{\mathbf{q}}}d\dot{\mathbf{q}}\right)\right|_{\mathbf{p}=\frac{\partial L}{\partial \dot{\mathbf{q}}}} \\ =& \left.\left(\dot{\mathbf{q}}d\mathbf{p} - \frac{\partial L}{\partial \mathbf{q}}d\mathbf{q}\right)\right|_{\mathbf{p}=\frac{\partial L}{\partial \dot{\mathbf{q}}}}. \end{aligned}$$

Thus under the Legendre transform $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$,

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}} \quad \text{and} \quad \frac{\partial L}{\partial \mathbf{q}} = -\frac{\partial H}{\partial \mathbf{q}}.$$

The second half of Hamilton's equations follows from the Euler-Lagrange equations,

$$\frac{\partial L}{\partial \mathbf{q}} = \frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{q}}} = \dot{\mathbf{p}}.$$

□

COROLLARY 1.2. *The Hamiltonian function H is constant on the solutions of the Hamilton equations, e.g., it is an integral of motion.*

PROOF. On the solution $(q(t), p(t))$ we have for $H(t) = H(q(t), p(t))$,

$$\frac{dH}{dt} = \frac{\partial H}{\partial \mathbf{q}}\dot{\mathbf{q}} + \frac{\partial H}{\partial \mathbf{p}}\dot{\mathbf{p}} = \frac{\partial H}{\partial \mathbf{q}}\frac{\partial H}{\partial \mathbf{p}} - \frac{\partial H}{\partial \mathbf{p}}\frac{\partial H}{\partial \mathbf{q}} = 0.$$

□

The cotangent bundle T^*M is called the *phase space* of the Hamiltonian system associated with (M, L).

EXAMPLES 1.4.

1. The Lagrangian of a particle of mass m with the potential energy $U(\mathbf{r})$ is

$$L = \frac{m\dot{\mathbf{r}}^2}{2} - U(\mathbf{r}),\ \mathbf{r} \in \mathbb{R}^3.$$

We have

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{r}}} = m\dot{\mathbf{r}},$$

so that the Legendre transformation is global diffeomorphism linear on the fibers, and

$$H = (\mathbf{p}\dot{\mathbf{r}} - L)|_{\dot{\mathbf{r}}=\frac{\mathbf{p}}{m}} = \frac{\mathbf{p}^2}{2m} + U(\mathbf{r}).$$

The Hamilton's equations

$$\dot{\mathbf{r}} = \frac{\partial H}{\partial \mathbf{p}} = \frac{\mathbf{p}}{m},$$
$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{r}} = -\frac{\partial U}{\partial \mathbf{r}},$$

are equivalent to Newton's equations with the force $\mathbf{F} = -\frac{\partial U}{\partial \mathbf{r}}$.

2. Consider the Lagrangian

$$L = \sum_{i,j=1}^{n} \tfrac{1}{2}a^{ij}(\mathbf{q})\dot{q}_i\dot{q}_j - U(\mathbf{q}),\ \mathbf{q} \in \mathbb{R}^n,$$

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

$$p^i = \sum_{j=1}^{n} a^{ij}\dot{q}_j,$$

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

$$H = (\mathbf{p}\dot{\mathbf{q}} - L)\big|_{\mathbf{p}=\frac{\partial L}{\partial \dot{\mathbf{q}}}} = \sum_{i,j=1}^{n} \tfrac{1}{2}a_{ij}(\mathbf{q})p^ip^j + U(\mathbf{q}),$$

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

1.6. The action functional in the phase space. With every function H on the phase space T^*M we associate a 1-form

$$\theta - Hdt = \mathbf{p}d\mathbf{q} - Hdt$$

on the extended phase space $T^*M \times \mathbb{R}$, called the *Poincaré-Cartan form.* Let $\Omega(T^*M \times \mathbb{R}; q_0, t_0, q_1, t_1)$ be the space of all smooth paths $\sigma : [t_0, t_1] \to T^*M \times \mathbb{R}$ such that $\pi_1(\sigma(t_0)) = q_0$, $\pi_1(\sigma(t_1)) = q_1$, and $\pi_2(\sigma(t)) = t$ for all $t \in [t_0, t_1]$. Here π_1 and π_2 are, respectively, canonical projections of $T^*M \times \mathbb{R}$ onto M and $\mathbb{R}$. Such path σ is called an *admissible path* in $T^*M \times \mathbb{R}$. A variation of an admissible path σ is a smooth family of admissible paths $\sigma_\varepsilon, \varepsilon \in [-\varepsilon_0, \varepsilon_0]$, such that $\sigma_0 = \sigma$, and the corresponding infinitesimal variation is

$$\delta\sigma = \left.\frac{\partial \sigma_\varepsilon}{\partial \varepsilon}\right|_{\varepsilon=0} \in T_\sigma \Omega(T^*M \times \mathbb{R}; q_0, t_0, q_1, t_1).$$

The principle of the least action in the phase space is the following statement.

THEOREM 1.5 (Poincaré). *The admissible path σ in $T^*M \times \mathbb{R}$ is an extremal for the action functional*

$$S(\sigma) = \int\limits_\sigma (\mathbf{p}d\mathbf{q} - Hdt)$$

if and only if its projection onto T^*M is a solution of canonical Hamilton's equations.

PROOF. As for the derivation of Euler-Lagrange equations, using integration by parts we compute in standard coordinates

$$\begin{aligned}\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} S(\sigma_\varepsilon) = &\int_{t_0}^{t_1} \sum_{i=1}^n \left(\dot{q}_i \delta p^i - \dot{p}^i \delta q_i - \frac{\partial H}{\partial q_i}\delta q_i - \frac{\partial H}{\partial p^i}\delta p^i\right) dt \\ &+ \sum_{i=1}^n p^i \left.\delta q_i\right|_{t_0}^{t_1}.\end{aligned}$$

Since $\delta\mathbf{q}(t_0) = \delta\mathbf{q}(t_1) = 0$, we conclude that the path σ is critical if and only if $\mathbf{q}(t), \mathbf{p}(t)$ satisfy canonical Hamilton's equations. □

2. Hamiltonian Mechanics

2.1. Canonical Hamilton's equations. The canonical Hamilton's equations on T^*M with a Hamiltonian $H : T^*M \to \mathbb{R}$ in standard coordinates on T^*U have the form

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \ \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}.$$

and define a vector field X_H on T^*U by

$$X_H = \sum_{i=1}^n \left(\frac{\partial H}{\partial p^i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p^i}\right) = \frac{\partial H}{\partial \mathbf{p}}\frac{\partial}{\partial \mathbf{q}} - \frac{\partial H}{\partial \mathbf{q}}\frac{\partial}{\partial \mathbf{p}}.$$

As it follows from the definition of standard coordinates, this gives rise to a well-defined vector field X_H on T^*M, called the *Hamiltonian vector field.* Suppose that the vector field X_H is complete, i.e., its integral curves exist for all times (this is the case when level sets of the Hamiltonian H are compact submanifolds on T^*M). The corresponding one-parameter group $\{g^t\}_{t\in\mathbb{R}}$ of diffeomorphisms of T^*M generated by X_H is defined by $g^t : (q(0), p(0)) \mapsto (q(t), p(t))$ and is called *Hamiltonian phase flow.*

DEFINITION. The *canonical symplectic form* on T^*M is $\omega = d\theta$.

In standard coordinates (q, p) on T^*M the 2-form ω is

$$\omega = \sum_{i=1}^{n} dp^i \wedge dq_i = d\mathbf{p} \wedge d\mathbf{q},$$

and is non-degenerate. The symplectic form ω defines an isomorphism between tangent and cotangent bundles of T^*M,

$$J : T^*(T^*M) \to T(T^*M),$$

such that for every $(q, p) \in T^*M$

$$\omega(u_1, u_2) = J^{-1}(u_2)(u_1),\ \ u_1, u_2 \in T_{(q,p)}(T^*M).$$

In standard coordinates on T^*M and TM,

$$J(d\mathbf{q}) = -\frac{\partial}{\partial \mathbf{p}},\ \ J(d\mathbf{p}) = \frac{\partial}{\partial \mathbf{q}} \quad \text{and} \quad X_H = J(dH).$$

THEOREM 2.1. *The Hamiltonian phase flow on T^*M preserves canonical symplectic form.*

PROOF. We need to proof that $(g^t)^*\omega = \omega$. Since g^t is a one-parameter group of diffeomorphisms, it is sufficient to show that

$$\left.\frac{d}{dt}(g^t)^*\omega\right|_{t=0} = \mathcal{L}_{X_H}\omega = 0,$$

where $\mathcal{L}_{X_H}$ stands for the Lie derivative along the vector field X_H. For every vector field X

$$d\mathcal{L}_X(f) = \mathcal{L}_X(df),$$

we have

$$\mathcal{L}_{X_H}(dq_i) = d(X_H(q_i)) = d\left(\frac{\partial H}{\partial p^i}\right) \text{ and } \mathcal{L}_{X_H}(dp^i) = d(X_H(p_i)) = -d\left(\frac{\partial H}{\partial q^i}\right).$$

Thus

$$\begin{aligned}\mathcal{L}_{X_H}\omega &= \sum_{i=1}^{n} \left(\mathcal{L}_{X_H}(dp^i) \wedge dq_i + dp^i \wedge \mathcal{L}_{X_H}(dq_i)\right) \\ &= \sum_{i=1}^{n} \left(-d\left(\frac{\partial H}{\partial q_i}\right) \wedge dq_i + dp^i \wedge d\left(\frac{\partial H}{\partial p^i}\right)\right) = -d(dH) = 0.\end{aligned}$$

$\square$

The canonical symplectic form ω on T^*M defines the volume form $\omega^n = \underbrace{\omega \wedge \cdots \wedge \omega}_{n}$ — *the Liouville volume form* on T^*M.

COROLLARY 2.1 (Liouville's Theorem). *The Hamiltonian phase flow on T^*M preserves the Liouville volume form.*

The configuration space M has the property that the restriction of the symplectic form ω to M vanishes. Generalizing this property we have the following

DEFINITION. A submanifold $\mathscr{L}$ of the phase space is called *Lagrangian submanifold* if $\dim \mathscr{L} = \dim M$ and $\omega|_{\mathscr{L}} = 0$.

It follows from the theorem that under the Hamiltonian phase flow the image of a Lagrangian submanifold is a Lagrangian submanifold.

2.2. The action as a function of coordinates. For a system (M, L) let $\gamma(t; \mathbf{q}_0, \dot{\mathbf{q}}_0)$ be the solution of Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{q}}} - \frac{\partial L}{\partial \mathbf{q}} = 0$$

with the initial conditions $\gamma(t_0; \mathbf{q}_0, \dot{\mathbf{q}}_0) = \mathbf{q}_0$, $\dot{\gamma}(t_0; \mathbf{q}_0, \dot{\mathbf{q}}_0) = \dot{\mathbf{q}}_0$. Fix $\mathbf{q}_0 \in M$ and t suppose that a self-mapping of M defined in standard coordinates by $\dot{\mathbf{q}}_0 \mapsto \gamma(t; \mathbf{q}_0, \dot{\mathbf{q}}_0)$ is a diffeomorphism. Then for every $\mathbf{q} \in M$ there is a unique extremal $\gamma(\tau; \mathbf{q}_0, \mathbf{q})$ connecting points $\mathbf{q}_0$ and $\mathbf{q}$ at times t_0 and t, and we define the *action as functions of coordinates* by

$$S(\mathbf{q}, t; \mathbf{q}_0, t_0) = \int_{t_0}^{t} L(\gamma'(\tau; \mathbf{q}_0, \mathbf{q}))d\tau.$$

REMARK. If the mapping $\dot{\mathbf{q}}_0 \mapsto \gamma(t; \mathbf{q}_0, \dot{\mathbf{q}}_0)$ is a local diffeomorphism, i.e., a diffeomorphism between some domains U_0 and U, then $S(\mathbf{q}, t; \mathbf{q}_0, t_0)$ is defined on U. For each extremal $\gamma(t; \mathbf{q}_0, \dot{\mathbf{q}}_0)$ with $|t - t_0|$ small enough, there always exists such a domain U containing $\mathbf{q} = \gamma(t, \mathbf{q}_0, \dot{\mathbf{q}}_0)$. In this case it is said that the extremal connecting $\mathbf{q}_0$ at t_0 and $\mathbf{q}$ at t is *included into a central field of extremals.*

THEOREM 2.2. *Differential of the action as a function of coordinates (with fixed initial point) is given by*

$$dS = \mathbf{p}d\mathbf{q} - H dt$$

where $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$ *and* $H = \mathbf{p}\dot{\mathbf{q}} - L$ *are defined by* $\dot{\mathbf{q}} = \dot{\gamma}(t; \mathbf{q}_0, \mathbf{q})$.

PROOF. Fix $\mathbf{v} \in T_{\mathbf{q}}M \simeq \mathbb{R}^n$ using standard cooridnates. For the family of extremals $\gamma_\varepsilon(\tau) = \gamma(\tau; \mathbf{q}_0, \mathbf{q} + \varepsilon\mathbf{v})$ the corresponding infinitesimal variation $\delta\gamma$ satisfies $\delta\gamma(t_0) = 0$ and $\delta\gamma(t) = \mathbf{v}$. Repeating the computation in the proof of Theorem 1.1 and using the fact that γ_ε satisfy Euler-Lagrange equations, we get for fixed t,

$$dS(\mathbf{v}) = \frac{\partial L}{\partial \dot{\mathbf{q}}}\mathbf{v},$$

so that $\dfrac{\partial S}{\partial \mathbf{q}} = \mathbf{p}$. Now along the extremal $\gamma(t; \mathbf{q}_0, \mathbf{q})$,

$$\frac{d}{dt}S(\mathbf{q}(t), t; \mathbf{q}_0, t_0) = \frac{\partial S}{\partial \mathbf{q}}\dot{\mathbf{q}} + \frac{\partial S}{\partial t} = L,$$

so that $\dfrac{\partial S}{\partial t} = L - \mathbf{p}\dot{\mathbf{q}} = -H$. □

Corollary 2.2. *The classical action satisfies the following nonlinear partial differential equation*

$$\frac{\partial S}{\partial t} + H\left(\frac{\partial S}{\partial \mathbf{q}}, \mathbf{q}\right) = 0. \tag{2.1}$$

This equation is called the *Hamilton-Jacobi equation.* Hamilton's equations can be used for solving the Cauchy problem

$$S(\mathbf{q}, t)|_{t=t_0} = s(\mathbf{q}) \tag{2.2}$$

for Hamilton-Jacobi equation (2.1) by the method of characteristics. Namely, let g^t be the Hamiltonian phase flow in the phase space $\mathscr{M} = T^*M$ and let

$$\mathscr{L} = \left\{(\mathbf{q}, \mathbf{p}) \in T^*M : \mathbf{p} = \frac{\partial s(\mathbf{q})}{\partial \mathbf{q}}\right\}$$

be the Lagrangian submanifold — a graph of the section ds of the cotangent bundle $\pi : T^*M \to M$. The submanifold $\mathscr{L}$ has an addition property that the mapping $\pi|_{\mathscr{L}}$ is one to one. For the Lagrangian submanifold $\mathscr{L}^t = g^{t-t_0}\mathscr{L}$ the restriction of the projection mapping π to $\mathscr{L}^t$ will remain one to one provided that $t - t_0$ is sufficiently small. For such t we consider the mapping $\pi^t = \pi \circ g^t \circ (\pi|_{\mathscr{L}})^{-1} : M \to M$ is a diffeomorphism. This is the statement that for $t_0 \leq \tau \leq t$ the extremals $\gamma(\tau, \mathbf{q}_0, \dot{\mathbf{q}}_0)$ in the extended configuration space $M \times \mathbb{R}$, where $\dot{\mathbf{q}}_0 = \dfrac{\partial H}{\partial \mathbf{q}}(\mathbf{q}_0, \mathbf{p}_0)$ for $(\mathbf{q}_0, \mathbf{p}_0) \in \mathscr{L}$, called *characteristics* of the Hamilton-Jacobi equation, do not intersect.

Proposition 2.1. *Under the above assumptions, the solution $S(\mathbf{q}, t)$ to the Cauchy problem* (2.1)-(2.2) *is given by*

$$S(\mathbf{q}, t) = s(\mathbf{q}_0) + \int_{t_0}^{t} L(\gamma'(\tau))d\tau.$$

Here $\gamma(\tau)$ is the characteristic which ends at a given point $(\mathbf{q}, t) \in M \times \mathbb{R}$ and starts at some point $(\mathbf{q}_0, t_0) \in M \times \mathbb{R}$, uniquely determined by $\mathbf{q} \in M$.

Proof. By the same computation as in the proof of the previous theorem, with the only difference that $\mathbf{q}_0$ now depends on $\mathbf{q}$, we get that along the characteristic,

$$\frac{\partial S}{\partial \mathbf{q}}(\mathbf{q}) = \frac{\partial s}{\partial \mathbf{q}_0}(\mathbf{q}_0)\frac{\partial \mathbf{q}_0}{\partial \mathbf{q}} + \frac{\partial L}{\partial \dot{\mathbf{q}}}(\mathbf{q}) - \frac{\partial L}{\partial \dot{\mathbf{q}}}(\mathbf{q}_0)\frac{\partial \mathbf{q}_0}{\partial \mathbf{q}} = \mathbf{p},$$

where we have used Theorem 2.1 and definition of $\mathscr{L}$. Since along the characteristic

$$\frac{\partial S}{\partial t} = -H(\mathbf{p}, \mathbf{q}),$$

we get the result. □

We can also consider the action $S(\mathbf{q}, t; \mathbf{q}_0, t_0)$ as a function of both variables $\mathbf{q}$ and $\mathbf{q}_0$. The analog of Theorem 2.3 is the following statement, where notations and conditions should be clear from the content.

PROPOSITION 2.2. *Differential of the action as a function of initial and final points is given by*

$$dS = \mathbf{p}d\mathbf{q} - \mathbf{p}_0 d\mathbf{q}_0 - H dt + H_0 dt_0.$$

2.3. Classical observables and Poisson bracket. The vector space $C^\infty(T^*M)$ of smooth real-valued functions on T^*M is an $\mathbb{R}$-algebra — an associative algebra with a unit over $\mathbb{R}$, with a multiplication given by the point-wise product of functions. The $\mathbb{R}$-algebra $C^\infty(T^*M)$ is called the algebra of *classical observables.* The time evolution of every observable $f \in C^\infty(T^*M)$ is determined by the Hamiltonian phase flow and is given by

$$f_t(q,p) = f(g^t(q,p)), \ (q,p) \in T^*M.$$

Equivalently, the evolution is described by Hamilton's equations of motion for classical observables,

$$\begin{aligned} \frac{df_t}{dt} &= \frac{df_{s+t}}{ds}\bigg|_{s=0} = \frac{d(f_t \circ g^s)}{ds}\bigg|_{s=0} = X_H(f_t) \\ &= \sum_{i=1}^{n} \left(\frac{\partial H}{\partial p^i}\frac{\partial f_t}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial f_t}{\partial p^i} \right) = \frac{\partial H}{\partial \mathbf{p}}\frac{\partial f_t}{\partial \mathbf{q}} - \frac{\partial H}{\partial \mathbf{q}}\frac{\partial f_t}{\partial \mathbf{p}}. \end{aligned}$$

This motivates the following definiton.

DEFINITION. *The canonical Poisson bracket* of classical observables on T^*M is a linear[6] mapping $\{\ ,\ \} : C^\infty(T^*M) \otimes C^\infty(T^*M) \to C^\infty(T^*M)$, given by

$$\{f, g\} = X_f(g) = \frac{\partial f}{\partial \mathbf{p}}\frac{\partial g}{\partial \mathbf{q}} - \frac{\partial f}{\partial \mathbf{q}}\frac{\partial g}{\partial \mathbf{p}},$$

where $\otimes$ stands for the tensor product of vector spaces.

THEOREM 2.3. *The canonical Poisson bracket on T^*M has the following properties.*

(i) *(Relation with the symplectic form)*

$$\{f, g\} = \omega(Jdf, Jdg) = \omega(X_f, X_g).$$

(ii) *(Skew-symmetry)*

$$\{f, g\} = -\{g, f\}.$$

[6]Equivalently, a bilinear mapping $\{\ ,\ \} : C^\infty(T^*M) \times C^\infty(T^*M) \to C^\infty(T^*M)$.

(iii) *(Leibniz rule)*

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

(iv) *(Jacobi identity)*

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

for all $f, g, h \in C^\infty(T^*M)$.

PROOF. Property (i) immediately follows from the definitions of the canonical symplectic form ω and linear operator J. Properties (ii)-(iii) are obvious. As we will prove in the next section, the Jacobi identity follows from the property

$$\mathcal{L}_{X_H}\omega = 0 \quad \text{for all} \quad H \in C^\infty(T^*M).$$

For the canonical Poisson bracket the Jacobi identity can be also verified by a straightforward computation. Another elegant argument is the following. The Poisson bracket $\{f, g\}$ is a bilinear first order differential operator, and analyzing each term of the left hand side of the Jacobi identity, we conclude that it is a linear homogenous function of second partial derivatives of the functions f, g, h. The only terms in the Jacobi identity that may contain second derivatives of h (say) are of the form

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} = (X_f X_g - X_g X_f)(h).$$

However, this expression does not contain second derivatives of h since a commutator of two differential operators of the first order is again an operator of the first order! □

This theorem motivates the following definition.

DEFINITION. A commutative $\mathbb{R}$-algebra A is called a *Poisson algebra* if it has a Lie algebra structure such that the Lie bracket $[\ ,\ ]$ is a derivation with respect to the multiplication in A,

$$[ab, c] = a\,[b, c] + b\,[a, c] \text{ for all } a, b, c \in A.$$

The algebra $C^\infty(T^*M)$ of classical observables on T^*M is a Poisson algebra with a Lie bracket given by the canonical Poisson bracket. In addition, the Poisson bracket preserves supports of functions. Derivations on $C^\infty(T^*M)$ with these property are called *local derivations*.

2.4. Symplectic and Poisson manifolds. Here we formulate Hamiltonian mechanics on manifolds by generalizing Hamiltion's canonical formalism developed for the cotangent bundle T^*M.

2.4.1. *Symplectic manifolds.* The natural symplectic structure on the cotangent bundle T^*M admits the following generalization.

Definition. A non-degenerate, closed 2-form ω on a manifold $\mathscr{M}$ is called *symplectic form.* A pair $(\mathscr{M},\omega)$, where ω is a symplectic form, is called a *symplectic manifold.*

Since symplectic form is non-degenerate, a symplectic manifold $\mathscr{M}$ is necessarily even-dimensional, $\dim\mathscr{M}=2n$. Every non-degenerate 2-form ω on $\mathscr{M}$ defines the bundle isomorphism

$$J : T^*\mathscr{M}\to T\mathscr{M},$$

where for every $x\in\mathscr{M}$,

$$\omega(v_1,v_2)=J^{-1}(v_2)(v_1),\;\; v_1,v_2\in T_x\mathscr{M}.$$

Let $\mathbf{x}=(x_1,\dots,x_{2n})$ be local coordinates on $\mathscr{M}$ associated with the coordinate chart (U,ϕ) centered at $x\in\mathscr{M}$. In these coordinates the 2 form ω is given by

$$\omega=\tfrac{1}{2}\sum_{i,j=1}^{2n}\omega^{ij}(\mathbf{x})\,dx_i\wedge dx_j,$$

where $\{\omega^{ij}(\mathbf{x})\}_{i,j=1}^{2n}$ is non-degenerate, skew-symmetric matrix-function on $\phi(U)$. Denoting the inverse matrix by $\{\omega_{ij}(\mathbf{x})\}_{i,j=1}^{2n}$, we have in standard coordinates on T^*U and TU

$$Jdx_i=\sum_{j=1}^{2n}\omega_{ij}(\mathbf{x})\frac{\partial}{\partial x_j},\;\; i=1,\dots,2n.$$

Symplectic manifolds form a category. A morphism between $(\mathscr{M}_1,\omega_1)$ and $(\mathscr{M}_2,\omega_2)$ is a mapping $f:\mathscr{M}_1\to\mathscr{M}_2$ of smooth manifolds such that $\omega_1=f^*(\omega_2)$. Such mapping f is called a *symplectomorphism.* The direct product of symplectic manifolds $(\mathscr{M}_1,\omega_1)$ and $(\mathscr{M}_2,\omega_2)$ is a symplectic manifold

$$(\mathscr{M}_1\times\mathscr{M}_2,\pi_1^*(\omega_1)+\pi_2^*(\omega_2)),$$

where π_1 and π_2 are, respectively, projections of $\mathscr{M}_1\times\mathscr{M}_2$ onto the first and second factors.

Definition. A mechanical system on a symplectic manifold $(\mathscr{M},\omega)$ is given by a *Hamiltonian* H — a smooth real-valued function on $\mathscr{M}$. The time evolution of the system $(\mathscr{M},H)$ is described by a *Hamiltonian vector field* X_H on $\mathscr{M}$ associated with the Hamiltonian function H,

$$X_H=JdH.$$

The manifold $\mathscr{M}$ is called the called *phase space* of a mechanical system and the algebra $\mathsf{A}=\mathsf{A}^0(\mathscr{M})=C^\infty(\mathscr{M})$ is called the algebra of classical observables on the phase space $\mathscr{M}$. Time evolution of classical observables is given by the Hamilton's equations of motion

$$\frac{df}{dt} = X_H(f) = \omega(X_H, X_f), \; f \in \mathsf{A}.$$

The following statement shows that Hamiltonian mechanics on a symplectic manifold locally can be described by canonical Hamiltonian formalism on the cotangent bundle.

THEOREM 2.4 (Darboux' Theorem). *Let* $(\mathscr{M}, \omega)$ *be a symplectic manifold,* $\dim \mathscr{M} = 2n$. *For every point* $x \in \mathscr{M}$ *there is a neighborhood* U *of* x *with local coordinates* $(\mathbf{q}, \mathbf{p}) = (q_1, \dots, q_n, p^1, \dots, p^n)$ *such that on* U

$$\omega = \sum_{i=1}^{n} dp^i \wedge dq_i = d\mathbf{p} \wedge d\mathbf{q}.$$

The proof of Darboux's Theorem will be sketched in the exercises.

Now we assume that the vector field X_H on $\mathscr{M}$ is complete. The *phase flow* on $\mathscr{M}$ associated with a Hamiltonian H is a one-parameter group $\{g^t\}_{t \in \mathbb{R}}$ of diffeomorphisms of $\mathscr{M}$ generated by X_H. The following statement generalizes Theorem 2.1.

THEOREM 2.5. *The Hamiltonian phase flow on a symplectic manifold preserves the symplectic form.*

PROOF. It is sufficient to show that $\mathcal{L}_{X_H}\omega = 0$ for every $H \in \mathsf{A}$. Using Cartan's formula

$$\mathcal{L}_X = i_X \circ d + d \circ i_X$$

and $d\omega = 0$, we get

$$\mathcal{L}_X\omega = (d \circ i_X)(\omega)$$

for every $X \in \mathrm{Vect}(\mathscr{M})$. Since

$$i_X(\omega)(Y) = \omega(X, Y)$$

for every $Y \in \mathrm{Vect}(\mathscr{M})$, we have for $X = X_H$,

$$i_{X_H}(\omega)(Y) = \omega(JdH, Y) = -dH(Y).$$

Thus $i_{X_H}(\omega) = -dH$, and the statement follows from $d^2 = 0$. $\square$

It follows from the proof that a vector field X on $\mathscr{M}$ is Hamiltonian if and only if the 1-form $i_X(\omega)$ on $\mathscr{M}$ is exact. Similarly, a vector field X on $\mathscr{M}$ is called *symplectic* if the 1-form $i_X(\omega)$ is closed.

Since Hamilton's equations for observables

$$\frac{df}{dt} = X_H(f) = \omega(JdH, Jdf)$$

have the same form as Hamilton's equations on $\mathscr{M} = T^*M$, this justifies the following definition.

Definition. A Poisson bracket on the algebra $\mathsf{A} = C^\infty(\mathscr{M})$ of classical observables on a symplectic manifold $(\mathscr{M}, \omega)$ is a linear mapping $\{\ ,\ \} : \mathsf{A} \otimes \mathsf{A} \to \mathsf{A}$, defined by

$$\{f, g\} = X_f(g) = \omega(Jdf, Jdg) = \omega(X_f, X_g),\ \ f, g \in \mathsf{A}.$$

In local coordinates $\mathbf{x} = (x_1, \ldots, x_{2n})$ on $\mathscr{M}$,

$$\{f, g\}(x) = \sum_{i,j=1}^{2n} \omega_{ij}(\mathbf{x}) \frac{\partial f(\mathbf{x})}{\partial x_i} \frac{\partial g(\mathbf{x})}{\partial x_j}.$$

Theorem 2.6. *The bracket mapping $\{\ ,\ \}$ on a symplectic manifold $(\mathscr{M}, \omega)$ is a Poisson bracket, i.e., it is skew-symmetric and satisfies Leibniz rule and the Jacobi identity.*

Proof. The first two properties are obvious. The Jacobi identity is equivalent to from the property

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

since

$$\{\{f, g\}, h\} = X_{\{f,g\}}(h) = (X_g X_f - X_f X_g)(h) = \{g, \{f, h\}\} - \{f, \{g, h\}\}.$$

To prove this property, let X and Y be symplectic vector fields on $\mathscr{M}$. Using

$$\mathcal{L}_X \circ i_Y - i_Y \circ \mathcal{L}_X = i_{[X,Y]},$$

Cartan's formula and Theorem 2.7, we get

$$\begin{aligned} i_{[X,Y]}(\omega) =& \mathcal{L}_X(i_Y(\omega)) - i_Y(\mathcal{L}_X(\omega)) \\ =& d(i_X \circ i_Y(\omega)) + i_X d(i_Y(\omega)) \\ =& d(\omega(X, Y)) = -d(\omega(Y, X)) = i_{X_{\omega(X,Y)}}(\omega). \end{aligned}$$

Since 2-form ω is non-degenerate, $i_X(\omega) = i_Y(\omega)$ implies $X = Y$, and we get

$$[X, Y] = X_{\omega(X,Y)}.$$

Setting $X = X_f, Y = X_g$ and using $\{f, g\} = \omega(X_f, X_g)$ we get the assertion. □

The property $[X_f, X_g] = X_{\{f,g\}}$ means that the vector space $\mathrm{Ham}(\mathscr{M})$ of Hamiltonian vector fields on $\mathscr{M}$ is a Lie subalgebra of the Lie algebra $\mathrm{Vect}(\mathscr{M})$ and the mapping $\mathsf{A} \to \mathrm{Ham}(\mathscr{M})$ given by $f \mapsto X_f$ is a Lie algebra homomorphism. The kernel of this mapping consists of locally constant functions on $\mathscr{M}$ (and is $\mathbb{R}$ if $\mathscr{M}$ is connected).

In the Lagrangian mechanics, the function I on $\mathscr{M}$ is called an *integral of motion* (*first integral*) for the mechanical system $(\mathscr{M}, H)$ if it is constant along the Hamiltonian phase flow. Equivalently, I is the first integral if

$$\{H, I\} = 0.$$

This condition is also stated that observables H and I *are in involution.* From the Jacobi identity for the Poisson bracket we get the following

COROLLARY 2.3 (Poisson's Theorem). *The Poisson bracket of two integrals of motion is an integral of motion.*

PROOF. If $\{H, I_1\} = \{H, I_2\} = 0$, then

$$\{H, \{I_1, I_2\}\} = \{\{H, I_1\}, I_2\} - \{\{H, I_2\}, I_1\} = 0.$$

∎

Below we give several examples of symplectic manifolds, compact and non compact.

EXAMPLE 2.1 (Cotangent bundles). $\mathscr{M} = T^*M$, with the canonical symplectic form $\omega = d\theta$.

EXAMPLE 2.2 (Kähler manifolds). $\mathscr{M} = X_{\mathbb{R}}$ — a real form of a Kähler manifold X with Kähler form as a symplectic form.

EXAMPLE 2.3 (Projective varieties). Real forms of complex projective varities, with a pull-back of Fubini-Study metric on $\mathbb{CP}^n$ as a symplectic form.

EXAMPLE 2.4 (Coadjont orbits). $\mathscr{M} = \mathscr{O}_u$ — a coadjoint orbit of a finite-dimensional Lie group G with a Lie algebra $\mathfrak{g}$, where $u \in \mathfrak{g}^*$ is the dual space to $\mathfrak{g}$. The symplectic form is the Kirillov-Kostant 2-form on the orbit.

EXAMPLE 2.5 (Symplectic quotients). Let $(\mathscr{M}, \omega)$ be a connected symplectic manifold on which a Lie group G acts by symplectomorphisms. The action is called Hamiltonian if the Lie algebra $\mathfrak{g}$ of G acts on $\mathscr{M}$ by Hamiltonian vector fields,

$$\mathfrak{g} \ni \xi \mapsto X_{H_\xi} \in \mathrm{Vect}(\mathscr{M}).$$

The action is called Poisson if

$$\{H_\xi, H_\eta\} = H_{[\xi,\eta]} \quad \text{for all} \quad \xi, \eta \in \mathfrak{g}.$$

For a Poisson action define the moment map $P : \mathscr{M} \to \mathfrak{g}^*$ by

$$P(x)(\xi) = H_\xi(x),\ \xi \in \mathfrak{g}, x \in \mathscr{M}.$$

The for every regular value $p \in \mathfrak{g}^*$ of the moment map P such that a stabilizer G_p of p acts freely and proper on $\mathscr{M}_p = P^{-1}(p)$, the quotient $M_p = G_p \backslash \mathscr{M}_p$ is called a reduced phase space. It is a symplectic manifold and the symplectic form on M_p is uniquely characterized by the condition that its pull-back to $\mathscr{M}_p$ coincides with the restriction to $\mathscr{M}_p$ of the symplectic form ω.

In general a quotient of a symplectic manifold by a symplectic group action is not symplectic. The usefullness of the last example is that it provides a systematic way of producing a family of quotient symplectic manifolds parameterized by $\mathfrak{g}^*$. In the exercises we will give a more detailed information about the last two examples.

For the example $\mathscr{M} = T^*M$ the configuration space M is the base of the fibration $\pi : T^*M \to M$ and has the property that $\omega|_M = 0$. Generalizing this we get the following

DEFINITION. A submanifold M of a symplectic manifold $(\mathscr{M}, \omega)$ is call *Lagrangian submanifold* if $\dim M = \frac{1}{2}\dim \mathscr{M}$ and the restriction of the symplectic form ω to M is 0.

EXAMPLE 2.6. Configuration space M is a Lagrangian submanifold in $\mathscr{M} = T^*M$.

2.4.2. *Poisson manifolds.* The Poisson bracket on a symplectic manifold $(\mathscr{M}, \omega)$ has the property that only locally constant obervables are in involution with the whole algebra A. Relaxing this condition, we get an important notion of a Poisson manifold.

DEFINITION. *A Poisson manifold* is a smooth manifold $\mathscr{M}$ equipped with a Poisson structure: a skew-symmetric linear mapping $\{\ ,\ \} : C^\infty(\mathscr{M}) \otimes C^\infty(\mathscr{M}) \to C^\infty(\mathscr{M})$, which preserves supports, satisfies the Leibniz rule and Jacobi identity.

Equivalently, $\mathscr{M}$ is a Poisson manifold if algebra $\mathsf{A} = C^\infty(\mathscr{M})$ of classical observables on $\mathscr{M}$ has a structure of a Poisson algebra such that a Lie bracket is a local derivation. Due to this property, in local coordinates at $x \in \mathscr{M}$ the Poisson bracket has the form

$$\{f, g\}(x) = \sum_{i,j=1}^{N} \eta_{ij}(\mathbf{x}) \frac{\partial f(\mathbf{x})}{\partial x_i} \frac{\partial g(\mathbf{x})}{\partial x_j}.$$

The 2-tensor $\eta_{ij}(\mathbf{x})$ defines a section over $\mathscr{M}$ of the exterior square $\Lambda^2 T\mathscr{M}$ of the tangent bundle $T\mathscr{M}$, called the Poisson tensor.

The evolution of classical observables on a Poisson manifold is given by Hamilton's equations of motion

$$\frac{df}{dt} = X_H(f) = \{H, f\}.$$

The phase flow g^t for a complete Hamiltonian vector field $X_H = \{H, \cdot\}$ defines an evolution operator

$$U_t(f)(x) = f(g^t(x)),\ \ f \in \mathsf{A}.$$

THEOREM 2.7. *Suppose that every Hamiltonian vector field on a Poisson manifold $(\mathscr{M}, \{\ ,\ \})$ is complete. Then for every Hamiltonian $H \in \mathsf{A}$, the evolution operator U_t is an isomorphism of the Poisson algebra A,*

$$U_t(\{f, g\}) = \{U_t(f), U_t(g)\} \quad \textit{for all} \quad f, g \in \mathsf{A}.$$

PROOF. Since U_t is a one-parameter group, it is sufficient to verify this statement infinitesimally. Applying $\frac{d}{dt}$ at $t = 0$ to both sides of the equation we see that it is equivalent to the Jacobi identity for the observables H, f, g. $\square$

COROLLARY 2.4. *A smooth section η of $\Lambda^2 T\mathscr{M}$ is a Poisson tensor if and only if*

$$\mathcal{L}_{X_f}\eta = 0 \quad \textit{for all} \quad f \in \mathsf{A}.$$

REMARK. The above result is the counter-part of Theorem 2.4 for Poisson manifolds.

DEFINITION. The *center* of a Poisson manifold $(\mathscr{M}, \{\ ,\ \})$ is

$$\mathcal{Z}(\mathscr{M}) = \{f \in C^\infty(\mathscr{M}) : \{f, g\} = 0 \quad \text{for all} \quad g \in C^\infty(\mathscr{M})\}.$$

A Poisson manifold is called *non-degenerate* if $\mathcal{Z}(\mathscr{M}) = \mathbb{R}$.

Equivalently, a Poisson manifold $(\mathscr{M}, \{\ ,\ \})$ is non-degenerate if the Poisson tensor $\eta \in \mathrm{Vect}(\mathscr{M}) \wedge \mathrm{Vect}(\mathscr{M})$ gives rise to a bundle isomorphism $J : T^*\mathscr{M} \to T\mathscr{M}$.

Poisson manifolds form a category. A morphism between $(\mathscr{M}_1, \{\ ,\ \}_1)$ and $(\mathscr{M}_2, \{\ ,\ \}_2)$ is a mapping $\phi : \mathscr{M}_1 \to \mathscr{M}_2$ of smooth manifolds such that

$$\{f \circ \phi, g \circ \phi\}_1 = \{f, g\}_2 \circ \phi \quad \forall f, g \in C^\infty(\mathscr{M}_2).$$

Non-degenerate Poisson manifolds form a subcategory of the category of Poisson manifolds. A direct product of Poisson manifolds $(\mathscr{M}_1, \{\ ,\ \}_1)$ and $(\mathscr{M}_1, \{\ ,\ \}_1)$ is a Poisson manifold $(\mathscr{M}_1 \times \mathscr{M}_2, \{\ ,\ \}_{12})$ defined by the property that natural projections maps $\pi_1 : \mathscr{M}_1 \times \mathscr{M}_2 \to \mathscr{M}_1$ and $\pi_2 : \mathscr{M}_1 \times \mathscr{M}_2 \to \mathscr{M}_2$ are Poisson mappings. Identifying $C^\infty(\mathscr{M}_1 \times \mathscr{M}_2) \simeq C^\infty(\mathscr{M}_1) \otimes C^\infty(\mathscr{M}_2)$, we have

$$\{f_1 \otimes f_2, g_1 \otimes g_2\}_{12} = \{f_1, g_1\}_1 \otimes f_2 g_2 + f_1 g_1 \otimes \{f_2, g_2\}_2,$$

where $f_1, g_1 \in C^\infty(\mathscr{M}_1)$, $f_2, g_2 \in C^\infty(\mathscr{M}_2)$.

THEOREM 2.8. *The category of symplectic manifolds is (anti-) isomorphic to the category of non-degenerate Poisson manifolds.*

PROOF. We already have proved that every symplectic manifold is a non-degenerate Poisson manifold. Conversely, let $(\mathscr{M}, \{\ ,\ \})$ be a non-degenerate Poisson manifold and define the 2-form ω on $\mathscr{M}$ by

$$\omega(X, Y) = J^{-1}(Y)(X) \ X, Y \in \mathrm{Vect}(\mathscr{M}).$$

Clearly, the 2-form ω is skew-symmetric and non-degenerate. For every $f \in \mathsf{A}$ define $X_f \in \mathrm{Vect}(\mathscr{M})$ by

$$X_f(g) = \{f, g\}, \ g \in \mathsf{A}.$$

The Jacobi identity for the Poisson bracket $\{\ ,\ \}$ is equivalent to the condition $\mathcal{L}_{X_f}\eta = 0$ for every $f \in \mathsf{A}$ so that

$$\mathcal{L}_{X_f}\omega = 0.$$

Since $X_f = Jdf$, we have

$$\omega(X, Jdf) = df(X), \ X \in \mathrm{Vect}(\mathscr{M})$$

and

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

Now using another one of Cartan's formulas,

$$\begin{aligned}d\omega(X,Y,Z) =&\tfrac{1}{3}\left(\mathcal{L}_X\omega(X,Y)-\mathcal{L}_Y\omega(X,Z)+\mathcal{L}_Z\omega(X,Y)\right.\\&\left.-\omega([X,Y],Z)+\omega([X,Z],Y)-\omega([Y,Z],X)\right),\quad X,Y,Z\in\operatorname{Vect}(\mathscr{M})\end{aligned}$$

and setting $X = Jdf, Y = Jdg, Z = Jdh$, we get

$$\begin{aligned}d\omega(Jdf,Jdg,Jdh) =&\tfrac{1}{3}\left(\omega(X_h,[X_f,X_g])+\omega(X_f,[X_g,X_h])+\omega(X_g,[X_h,X_f])\right)\\=&\tfrac{1}{3}\left(\omega(X_h,X_{\{f,g\}})+\omega(X_f,X_{\{g,h\}})+\omega(X_g,X_{\{h,f\}})\right)\\=&\tfrac{1}{3}\left(\{h,\{f,g\}\}+\{f,\{g,h\}\}+\{g,\{h,f\}\}\right)\\=&0\end{aligned}$$

by the Jacobi identity.

Since 1-forms df, $f\in\mathsf{A}$, generate $\mathsf{A}^1(\mathscr{M})$ as a module over A, Hamiltonian vector vector fields Jdf generate $\operatorname{Vect}(\mathscr{M})$ as a module over A, so that $d\omega = 0$. Thus $(\mathscr{M},\omega)$ is a symplectic manifold corresponding to the Poisson manifold $(\mathscr{M},\{\ ,\ \})$. Now from $\omega(X_f,X_g)=\{f,g\}$ it follows that Poisson mappings of non-degenerate Poisson manifolds correspond to symplectomorphisms. □

Remark. One can also prove the theorem by a straightforward computation in local coordinates at $x\in\mathscr{M}$. Namely, define

$$\omega = -\sum_{1\leq i<j\leq N}\eta^{ij}(\mathbf{x})\,dx_i\wedge dx_j,$$

where $\{\eta^{ij}(\mathbf{x})\}_{i,j=1}^N$ is the inverse matrix to $\eta_{ij}(\mathbf{x})$. Then the condition

$$\frac{\partial\eta^{ij}}{\partial x_l}+\frac{\partial\eta^{jl}}{\partial x_i}+\frac{\partial\eta^{li}}{\partial x_j}=0$$

for all $i,j,l=1,\dots,N$, which is a coordinate form of $d\omega=0$, follows from the condition

$$\sum_{j=1}^N\left(\eta_{ij}\frac{\partial\eta_{kl}}{\partial x_j}+\eta_{lj}\frac{\partial\eta_{ik}}{\partial x_j}+\eta_{kj}\frac{\partial\eta_{li}}{\partial x_j}\right)=0,$$

which is a coordinate form of the Jacobi identity, by multiplying it three times by the inverse matrix using

$$\sum_{p=1}^N\left(\eta_{ip}\frac{\partial\eta^{pj}}{\partial x_m}+\frac{\partial\eta_{ip}}{\partial x_m}\eta^{pj}\right)=0.$$

Below are two examples of Poisson manifolds.

Example 2.7 (Dual space to a Lie algebra). Let $\mathfrak{g}$ be a finite-dimensional Lie algebra with a Lie bracket $[\ ,\ ]$ and let $\mathfrak{g}^*$ be its dual space. The vector space $\mathscr{M}=\mathfrak{g}^*$ has a natural Poisson structure, which goes back to Sophus

Lie, and is defined as follows. For $f, g \in C^\infty(\mathscr{M})$ the differentials df and dg at $u \in \mathscr{M}$ are[7] elements in $(\mathfrak{g}^*)^* = \mathfrak{g}$, and we set

$$\{f, g\}(u) = u\left([df, dg]\right).$$

The Jacobi identity for the Poisson bracket $\{\ ,\ \}$ follows from the Jacobi identity for the Lie bracket $[\ ,\ ]$. When $f(u) = u(x), g(u) = u(y)$, $x, y \in \mathfrak{g}$ are linear functions on $\mathscr{M}$, then $\{f, g\}(u) = u\left([x, y]\right)$, so that Lie-Poisson bracket on $\mathscr{M}$ is linear. Let $x_1, \dots, x_n$ be a basis for $\mathfrak{g}$ with the structure constants c_{ij}^k,

$$[x_i, x_j] = \sum_{k=1}^n c_{ij}^k x_k,\ \ i, j = 1, \dots, n,$$

and let $x^1, \dots, x^n$ be the corresponding dual basis for $\mathfrak{g}^*$. Denote by $\mathbf{u} = (u_1, \dots, u_n)$ the coordinates on $\mathfrak{g}^*$, $u = \sum_{i=1}^n u_i x^i \in \mathfrak{g}^*$. Then

$$\{f, g\}(u) = \sum_{i,j,k=1}^n c_{ij}^k u_k \frac{\partial f(\mathbf{u})}{\partial u_i} \frac{\partial g(\mathbf{u})}{\partial u_j},$$

and the Poisson tensor for the Lie-Poisson bracket is

$$\eta_{ij}(\mathbf{u}) = \sum_{k=1}^n c_{ij}^k u_k,\ \ i, j = 1, \dots, n.$$

The center $\mathcal{Z}(\mathsf{A})$ of the Poisson algebra consists of functions f on $\mathfrak{g}^*$ satisfying

$$\sum_{k,j=1}^n c_{ij}^k u_k \frac{\partial f(\mathbf{u})}{\partial u_j} = 0,\ \ i = 1, \dots, n,$$

and is generated by *Casimir elements*. The phase space $\mathscr{M}$ is a degenerate Poisson manifold, foliated by symplectic leaves of the Lie-Poisson bracket, which are coadjoint orbits of G.

Example 2.8 (Poisson-Lie groups). Let G be a Lie group with a Lie algebra $\mathfrak{g}$. It is called a Lie-Poisson group if it has a structure of a Poisson manifold $(G, \{\ ,\ \})$ such that the group multiplication $G \times G \to G$ is a Poisson mapping (when $G \times G$ is equipped with the product Poisson structure). For $x \in \mathfrak{g}$ denote by ∂_x the left-invariant vector field on G,

$$(\partial_x f)(g) = \left.\frac{d}{ds}\right|_{s=0} f(ge^{tx}),$$

where e^x stands for the exponential map. For every choice of the basis $x_1, \dots, x_n$ for $\mathfrak{g}$ denote by $\partial_1, \dots, \partial_n$ corresponding left-invariant vector fields. The Poisson bracket on G can be written as

$$\{f_1, f_2\}(g) = \sum_{i,j=1}^n \eta^{ij}(g) \partial_i f_1 \partial_j f_2,$$

[7] We are identifying $T_u\mathscr{M}$ with $\mathscr{M}$ at every $u \in \mathscr{M}$.

where 2-tensor $\eta^{ij}(g)$ defines a mapping

$$\eta : G \to \Lambda^2\mathfrak{g}.$$

The bracket $\{\ ,\ \}$ equips G with a Lie-Poisson structure if and only if the following properties are satisfied.

1. The mapping η is a group 1-cocycle with the adjoint action on $\Lambda^2\mathfrak{g}$,

$$\eta(g_1g_2) = \mathrm{Ad}^{-1}g_2\,\eta(g_1) + \eta(g_2),\ \ g_1, g_2 \in G$$

2. For all $g \in G$, the 3-tensor

$$\xi^{ijk}(g) = \sum_{l=1}^{n} \Big(\eta^{il}(g)\partial_l\eta^{jk}(g) + \eta^{jl}(g)\partial_l\eta^{ki}(g) + \eta^{kl}(g)\partial_l\eta^{ij}(g)\Big)$$
$$+ \sum_{l,p=1}^{n} \Big(c^i_{lp}\eta^{pj}(g)\eta^{kl}(g) + c^j_{lp}\eta^{pk}(g)\eta^{il}(g) + c^k_{lp}\eta^{pi}(g)\eta^{jl}(g)\Big)$$

vanishes.

The first condition is trivially satisfied when η is a coboundary, $\eta(g) = -r + \mathrm{Ad}^{-1}g\,r$ for some $r \in \Lambda^2\mathfrak{g}$. The second condition is fulfilled when r satisfies the so-called *classical Yang-Baxter equation.*

2.5. Hamilton and Liouville representations. In order to complete our description of classical mechanics, we need to understand the process of *measurement.* In physics, by the measurement we understand the result of a physical experiment which gives numerical values for classical observables of a mechanical system. The experiment consists of creating certain conditions for the system and it is always assumed that these conditions can be repeated over and over. The conditions of the experiment define a *state* of the system, if repeating these conditions results in probability distributions for the values of all observables of the system.

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

$$\mathsf{A} \ni f \mapsto \mu_f, \text{ a probability measure on } \mathbb{R}.$$

Here for every Borel set $E \subset \mathbb{R}$ the number $0 \le \mu_f(E) \le 1$ is the probability that in the state μ the values of the observable f are in E. The *expectation value* of the 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 the distribution function. The assignment $f \mapsto \mu_f$ should should satisfy the following natural properties.

S1. The integral $\mathsf{E}_\mu(f)$ is convergent for bounded observables $f \in \mathsf{A}$.
S2. $\mathsf{E}_\mu(1) = 1$, where 1 is the unit in A.

S3. If $f_1 = \varphi \circ f_2$ with smooth $\varphi : \mathbb{R} \to \mathbb{R}$, then for every Borel set $E \subset \mathbb{R}$,

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

S4. For all $a, b \in \mathbb{R}$ and $f, g \in \mathsf{A}$,

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

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

It follows from property **S3** and definition of the Lebesgue-Stieltjes integral, that

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

In particular, $\mathsf{E}_\mu(f^2) \geq 0$ for all $f \in \mathsf{A}$. It follows from these properties that states define normalized, positive, linear functionals on the subalgebra of bounded observables of the algebra A.

Assuming that the functional E_μ can be extended to a bounded, piecewise continuous functions on $\mathscr{M}$, one can recover the distribution function from the expectation values by the formula

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

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

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

Indeed, setting $\theta_\lambda(x) = \theta(\lambda - x)$, we get

$$\mu_{\theta_\lambda(f)}((-\infty, s]) = \mu_f\left(\theta_\lambda^{-1}(-\infty, s]\right) = \begin{cases} 1, & s \geq 1, \\ \mu_f((\lambda, \infty)), & 0 \leq s < 1, \\ 0, & s < 0, \end{cases}$$

so that

$$\mathsf{E}_\mu(\theta(\lambda - f)) = \int_{-\infty}^{\infty} s d\mu_{\theta_\lambda(f)}(s) = 1 - \mu_f((\lambda, \infty)) = \mu_f(\lambda).$$

Conversely, a probability measure $d\mu$ on $\mathscr{M}$ defines for every observable f a probability measure on $\mathbb{R}$ with the distribution function

$$\mu_f(\lambda) = \int\limits_{\mathscr{M}} \theta(\lambda - f) d\mu = \int\limits_{\{f \leq \lambda\}} d\mu,$$

and by definition of the Lebesque-Stieltjes integral,

$$\int_{-\infty}^{\infty} \lambda d\mu_f(\lambda) = \int\limits_{\mathscr{M}} f d\mu.$$

When the phase space $\mathscr{M}$ is compact, the classical Riesz representation theorem asserts that for every positive, continuous, linear functional l on the Banach space $C(\mathscr{M})$ of continuous functions on $\mathscr{M}$ there exists a unique measure $d\mu$, defined on the σ-algebra of all Borel subsets of $\mathscr{M}$, such that

$$l(f) = \int_{\mathscr{M}} f d\mu.$$

We summarize this discussion in the following definition.

Definition. The set of states $\mathcal{S}$ for a mechanical system with the phase space $\mathscr{M}$ is the set $\mathsf{P}(\mathscr{M})$ of all probability measures on $\mathscr{M}$. For every $\mu \in \mathcal{S}$ and $f \in \mathsf{A}$ the distribution function μ_f is defined by

$$\mu_f(\lambda) = \int_{\mathscr{M}} \theta(\lambda - f) d\mu = \int_{\{f \leq \lambda\}} d\mu,$$

and the expectation value of f in the state μ is

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

The states corresponding to Dirac measures $d\mu_x$ supported at points $x \in \mathscr{M}$ are called *pure states*; all other states are called *mixed states*.

Physically, pure states are characterized by the property that a measurement of every observable in the pure state gives a well-defined result. Mathematically this can be expressed as follows. Let

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

be the *dispersion* of the observable f in the state μ. By the Cauchy-Schwarz inequality, $\sigma^2_\mu(f) \geq 0$, and equality holds if only if f is constant on the support of a probability measure $d\mu$. Thus pure states are the only states in which every observable has zero dispersion. In particular, a *mixture* of two pure states $d\mu_x$ and $d\mu_y$, $x, y \in \mathscr{M}$, is a mixed state with the measure

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

and $\sigma^2_\mu(f) > 0$ for every observable f such that $f(x) \neq f(y)$.

For a system consisting of few interacting particles (say, a motion of planets in celestian mechanics) it is possible to measure all coordinates and momenta, so one considers only pure states. Mixed states necessarily appear for *macroscopic* systems, when it is impossible to measure all coordinates and momenta[8]. Macroscopic systems are studied in *classical statistical mechanics*.

[8]Typically, a macroscopic system consists of $N \sim 10^{23}$ molecules.

2.5.1. *Hamilton's description of dynamics.* Consider a mechanical system with the phase space $(\mathscr{M}, \{\ ,\ \})$, algebra of observables A, set of states $\mathcal{S}$, and Hamiltonian H. In Hamilton's picture, states do not depend on time and time evolution of observables is given by Hamilton's equations of motion,

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

Assuming that Hamiltonian vector field X_H is complete, the expectation value of an observable f in the state μ at time t is

$$\mathsf{E}_\mu(f_t) = \int\limits_{\mathscr{M}} f\left(g^t(x)\right) d\mu(x).$$

In particular, the expectation value of f in the pure state corresponding to the point $x \in \mathscr{M}$ is $f(g^t(x))$.

2.5.2. *Liouville's description of dynamics.* Here we assume that the phase space $\mathscr{M}$ of the mechanical system has a volume form invariant under the phase flow with Hamiltonian H. In particular, this is the case when Poisson structure on $\mathscr{M}$ is non-degenerate. Denoting this volume form by dx, we can write a probability measure $d\mu$ as $d\mu(x) = \rho(x)dx$, where $\rho(x)$ is a positive distribution (generalized function) on $\mathscr{M}$. This is the usual description of states in statistical mechanics by distribution functions on the phase space. For the pure state supported at $x_0 \in \mathscr{M}$ we have $\rho(x) = \delta(x - x_0)$ — Dirac δ-function. Since the volume form is invaraint under the phase flow, we have by the change of variables,

$$\mathsf{E}_\mu(f_t) = \int\limits_{\mathscr{M}} f(x)\rho\left(g^{-t}(x)\right) dx.$$

This representation introduces Liouville's picture, in which observables do not depend on time

$$\frac{df}{dt} = 0,\ \ f \in \mathsf{A},$$

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

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

which is understood in the distributional sense. Liouiville's picture is commonly used in statistical mechanics. The equality

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

expresses the equivalence between Liouville's and Hamilton's descriptions of dynamics.

CHAPTER 2

Foundations of Quantum Mechanics

1. Observables and States

1.1. Physical principles. Quantum mechanics studies the physical laws of the microworld at the atomic scale. The properties of the microworld are so different from our everyday's experience that there is no surprise that its laws seem to contradict the common sense. The need for a quantum mechanics is the breakdown of classical mechanics, its inadequacy to describe the properties of atomic systems. Thus classical mechanics and classical electrodynamics can not explain 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.

We will not discuss here these and other basic experimental facts, referring the interested reader to physics textbooks. Nor will we follow the historic path of the theory. Instead, we show how to formulate quantum mechanics using the general notions of states, observables and time evolution. The departure from classical mechanics is that we will realize these notions differently. The fundamental difference between microworld and the world around us is that in the microworld every experiment results in interaction with the system and thus disturbs its properties, whereas in classical physics it is always assumed that one can neglect the disturbances the measurement brings upon a system. This imposes a limitation on our powers of observation and leads to a conclusion that there exist observables which can not be measured simultaneously.

Mathematically, this means that observables in quantum mechanics no longer form a commutative algebra. Indeed, according to Gelfand's theorem, every semi-simple commutative Banach algebra is an algebra of continuous functions on a compact topological space, the spectrum of the algebra, and the values of all these functions at a given point can be "measured simultaneously". An example of a non-commutative algebra is given by the Banach algebra of bounded operators on a complex Hilbert space, and it is this passage from functions on the phase space to operators on the Hilbert space that lies at the heart of quantum mechanics. Below we formulate the basic principles of quantum mechanics in a convenient form. At this point it should be noted that one can not verify directly the principles lying in the foundation of quantum mechanics. Nevertheless, the validity of quantum mechanics is continuously being confirmed by numerous experimental facts which perfectly agree with predictions of the theory.

1.1.1. *Notations.* We use standard notations and basic facts from the theory of self-adjoint operators on Hilbert spaces. Let $\mathscr{H}$ be a separable Hilbert space with an inner product $(\, , \,)$ and let A be a linear operator in $\mathscr{H}$ with the domain $D(A) \subset \mathscr{H}$ — a linear subset of $\mathscr{H}$. If domain of A is dense[1] in $\mathscr{H}$, i.e., $\overline{D(A)} = \mathscr{H}$, the adjoint operator A^* is an operator with the domain

$$D(A^*) = \{\varphi \in \mathscr{H} \mid \exists \, \eta \in \mathscr{H} \text{ such that } (A\psi, \varphi) = (\psi, \eta) \; \forall \, \psi \in D(A)\},$$

defined by $\eta = A^*\varphi$. Operator A is called symmetric if

$$(A\varphi, \psi) = (\varphi, A\psi) \quad \text{for all} \quad \varphi, \psi \in D(A).$$

The regular set of a closed operator A with a dense domain $D(A)$ is the set

$$\rho(A) = \{\lambda \in \mathbb{C} \,|\, A - \lambda I : D(A) \to \mathscr{H} \text{ is a bijection with a bounded inverse}^2\}.$$

If $\lambda \in \rho(A)$, the bounded operator $R_\lambda(A) = (A - \lambda I)^{-1}$ is called the resolvent of A at λ. The resolvent set $\rho(A)$ is closed and its complement $\sigma(A) = \mathbb{C} \setminus \rho(A)$ is called the spectrum of A. The set of all eigenvalues of A is called the point spectrum.

An operator A is called self-adjoint if $A = A^*$ (i.e., A is symmetric and $D(A) = D(A^*)$), and for such operators $\sigma(A) \subset \mathbb{R}$. A symmetric operator A is called essentially self-adjoint if its closure $\bar{A} = A^{**}$ is self-adjont. A symmetric operator A with $D(A) = \mathscr{H}$ is bounded and self-adjoint. An operator A is called positive if $(A\varphi, \varphi) \geq 0$ for all $\phi \in D(A)$, which we denote by $A \geq 0$. Positive operators satisfy the Cauchy-Schwarz inequality

$$|(Ax, y)|^2 \leq (Ax, x)(Ay, y) \quad \text{for all} \quad x, y \in D(A).$$

In particular, $(Ax, x) = 0$ implies that $Ax = 0$. Every bounded positive operator is self-adjoint[3]. We denote by $\mathscr{L}(\mathscr{H})$ the Banach algebra of bounded operators on $\mathscr{H}$. Compact operator A is of trace class, if

$$\sum_{n=1}^{\infty} \mu_n(A) < \infty,$$

where $\mu_n(A)$ are singular values of A, $\mu_n(A) = \sqrt{\lambda_n(A)} \geq 0$, where $\lambda_n(A)$ are eigenvalues for A^*A. A bounded operator A is of trace class if and only

$$\sum_{n=1}^{\infty} |(Ae_n, e_n)| < \infty$$

for every orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$. Since a permutation of an orthonormal basis is again an orthonormal basis, this condition is equivalent

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[1]We consider only linear operators with dense domains.

[2]By the closed-graph theorem, the last condition is redundant.

[3]This is true only for complex Hilbert spaces.

to

$$\sum_{n=1}^{\infty}(Ae_n, e_n) < \infty$$

for every orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$. By definition, for a trace class operator A,

$$\operatorname{Tr} A = \sum_{n=1}^{\infty}(Ae_n, e_n),$$

and does not depend on the choice of a basis. Operators of trace class form a two-sided ideal $\mathscr{S}_1$ (Schatten ideal) in the Banach algebra $\mathscr{L}(\mathscr{H})$ and

$$\operatorname{Tr} AB = \operatorname{Tr} BA \quad \text{for all} \quad A \in \mathscr{S}_1,\ B \in \mathscr{L}(\mathscr{H})$$

— the cyclic property of the trace. Bounded positive operator A is of trace class if there is an orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$ such that

$$\sum_{n=1}^{\infty}(Ae_n, e_n) < \infty.$$

1.2. Basic axioms.

A1. With every quantum system there is an associated separable complex Hilbert space $\mathscr{H}$, in physics terminology called the *space of states*[4].

A2. The set of *observables* $\mathscr{A}$ of a quantum system with the Hilbert space $\mathscr{H}$ consists of all self-adjoint operators on $\mathscr{H}$.

A3. Set of *states* $\mathscr{S}$ of a quantum system with a Hilbert space $\mathscr{H}$ consists of all positive (and hence self-adjoint) $M \in \mathscr{S}_1$ such that $\operatorname{Tr} M = 1$. *Pure states* are projection operators onto one-dimensional subspaces of $\mathscr{H}$. For $\psi \in \mathcal{H}$, $\|\psi\| = 1$, the corresponding projection is denoted by P_ψ. All other states are called *mixed states.*

A4. The expectation value of an observable $A \in \mathscr{A}$ in a state $M \in \mathscr{S}$ is

$$\langle A|M\rangle = \operatorname{Tr} AM,$$

and it exists whenever AM is a trace class operator (a nesessary condition is $M(\mathcal{H}) \subset D(A)$). In particular, if $M = P_\psi$ and $\psi \in D(A)$, then

$$\langle A|M\rangle = (A\psi, \psi).$$

A5. A state $M \in \mathscr{S}$ assigns to every observable $A \in \mathscr{A}$ a probability measure μ_A on $\mathbb{R}$. For a quantum system in the state M, the probability that the value of a measurement of the observable A lies in the Borel set $E \subset \mathbb{R}$ is $0 \leq \mu_A(E) \leq 1$. The correspondence $\mathscr{S} \ni M \mapsto \mu_A \in \mathscr{P}(\mathbb{R})$ satisfies

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

[4]Space of pure states, to be precise.

where $\mu_A(\lambda) = \mu_A((-\infty, \lambda])$ is the distribution function associated with the measure μ_A.

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

Definition. A mapping $\mathsf{P} : \mathscr{B}(\mathbb{R}) \to \mathscr{L}(\mathscr{H})$ of the σ-algebra $\mathscr{B}(\mathbb{R})$ of Borel subsets of $\mathbb{R}$ into the Banach algebra of bounded operators on $\mathscr{H}$ is called a projection-valued measure on $\mathbb{R}$ if the following properties are satisfied.

1. For every Borel set $E \subset \mathbb{R}$, $\mathsf{P}(E)$ is an orthogonal projection, i.e., $\mathsf{P}(E) = \mathsf{P}(E)^2$ and $\mathsf{P}(E) = \mathsf{P}(E)^*$.

2. $\mathsf{P}(\emptyset) = 0,\ \mathsf{P}(\mathbb{R}) = I$, the identity operator on $\mathscr{H}$.

3. For every disjoint union of Borel sets,

$$E = \coprod_{n=1}^{\infty} E_n, \quad \mathsf{P}(E) = \lim_{n\to\infty} \sum_{i=1}^{n} \mathsf{P}(E_i)$$

in the strong topology on $\mathscr{L}(\mathscr{H})$.

In particular, it follows from properties **1-3** that

$$\mathsf{P}(E_1)\mathsf{P}(E_2) = \mathsf{P}(E_1 \cap E_2).$$

With every projection-valued measure P we associate a projection-valued function

$$\mathsf{P}(\lambda) = \mathsf{P}((-\infty, \lambda]),$$

called the projection-valued decomposition of unity. It is characterized by the properties

1′.

$$\mathsf{P}(\lambda)\mathsf{P}(\mu) = \mathsf{P}(\min\{\lambda, \mu\}).$$

2′.

$$\lim_{\lambda\to-\infty} \mathsf{P}(\lambda) = 0, \quad \lim_{\lambda\to\infty} \mathsf{P}(\lambda) = I.$$

3′.

$$\lim_{\mu\to\lambda+0} \mathsf{P}(\mu) = \mathsf{P}(\lambda).$$

For every $\varphi \in \mathscr{H}$ the decomposition of unity $\mathsf{P}(\lambda)$ defines a distribution function $(\mathsf{P}(\lambda)\varphi, \varphi)$ of the bounded measure on $\mathbb{R}$ (probability measure when $\|\varphi\| = 1$). By the polarization identity

$$\begin{aligned}(\mathsf{P}(\lambda)\varphi, \psi) = \tfrac{1}{4}\{&(\mathsf{P}(\lambda)(\varphi + \psi), \varphi + \psi) - (\mathsf{P}(\lambda)(\varphi - \psi), \varphi - \psi) \\ &+ i(\mathsf{P}(\lambda)(\varphi + i\psi), \varphi + i\psi) - i(\mathsf{P}(\lambda)(\varphi - i\psi), \varphi - i\psi)\},\end{aligned}$$

so that $(\mathsf{P}(\lambda)\varphi, \psi)$ corresponds to a complex measure — a complex linear combination of measures.

A measurable function f on $\mathbb{R}$ is called finite almost everywhere (a.e.) with respect to the projection-valued measure P, if it is finite a.e. with respect to the measures $(\mathsf{P}\psi, \psi)$ for all $\psi \in \mathscr{H}$. According to von Neumann theorem, for a separable Hilbert space $\mathscr{H}$ there exists an element $\varphi \in \mathscr{H}$ such that f is finite a.e. with respect to the projection-valued measure P if and only if it is finite a.e. with respect to the measure $(\mathsf{P}\varphi, \varphi)$.

THEOREM 1.1 (von Neumann). *For every self-adjoint operator A on the Hilbert space $\mathscr{H}$ there exists a unique projection-valued decomposition of unity $\mathsf{P}(\lambda)$, satisfying the following properties.*

(i)
$$D(A) = \left\{ \varphi \in \mathscr{H} \;\middle|\; \int_{-\infty}^{\infty} \lambda^2 d(\mathsf{P}(\lambda)\varphi, \varphi) < \infty \right\}$$
and for every $\varphi \in D(A)$
$$A\varphi = \int_{-\infty}^{\infty} \lambda \, d\mathsf{P}(\lambda)\varphi$$
as the limit of Riemann sums in the strong topology on $\mathscr{H}$.

(ii) *For every continuous function f on $\mathbb{R}$*
$$D(f(A)) = \left\{ \varphi \in \mathcal{H} \;\middle|\; \int_{-\infty}^{\infty} f(\lambda)^2 d(\mathsf{P}(\lambda)\varphi, \varphi) < \infty \right\}$$
is a dense linear subspace of $\mathscr{H}$ and
$$f(A) = \int_{-\infty}^{\infty} f(\lambda) d\mathsf{P}(\lambda)$$
is a linear operator on $\mathscr{H}$, understood as a limit of Riemann sums in strong operator topology on $\mathscr{H}$. Operator $f(A)$ satisfies
$$f(A)^* = \bar{f}(A),$$
where $\bar{f}$ is the complex conjugate function to f, and operator $f(A)$ is bounded if and only if f is bounded. For bounded continuous functions f and g,
$$f(A)g(A) = \int_{-\infty}^{\infty} f(\lambda)g(\lambda) d\mathsf{P}(\lambda).$$

(iii) *For every measurable function f on $\mathbb{R}$, finite a.e. with respect to the projection-valued measure P, $f(A)$ is a linear operator on $\mathscr{H}$ with a dense domain $D(f(A))$ defined as in (ii), understood in the weak sense: for every $\varphi \in D(f(A))$ and $\psi \in \mathscr{H}$,*
$$(f(A)\varphi, \psi) = \int_{-\infty}^{\infty} f(\lambda) d(\mathsf{P}(\lambda)\varphi, \psi)$$
is a linear combination of Lebesgue-Stieltjes integrals. The correspondence $f \mapsto f(A)$ satisfies the same properties as in (ii).

(iv) *For every bounded operator B which commutes with A, that is, $B(D(A)) \subset D(A)$ and $AB = BA$ on $D(A)$, operator B commutes with the decomposition of unity $\mathsf{P}(\lambda)$ and, therefore, with every operator $f(A)$.*

We will denote the decomposition of unity for a self-adjoint operator A given by the spectral theorem by $\mathsf{P}_A(\lambda)$. Conversely, every decomposition of unity $\mathsf{P}(\lambda)$ as defined by properties $\mathbf{1}'$-$\mathbf{3}'$, by virtue of (i)-(ii) is a decomposition of unity for a self-adjoint operator.

According to the spectral theorem, $\lambda \in \sigma(A)$ if and only if $\mathsf{P}(\lambda-\varepsilon, \lambda+\varepsilon) \neq 0$ for all $\varepsilon > 0$. For $\psi \in \mathscr{H}$ let μ_ψ is a Borel measure on $\mathbb{R}$ defined by $\mu_\psi(E) = (\mathsf{P}(E)\psi, \psi)$ for $E \in \mathscr{B}(\mathbb{R})$. The next result is used for more detailed classification of the spectra.

THEOREM 1.2. *Let $A = A^*$ on $\mathscr{H}$. Then*

$$\mathscr{H} = \mathscr{H}_{pp} \oplus \mathscr{H}_{ac} \oplus \mathscr{H}_{sc}$$

is a direct sum of closed invariant subspaces[5] *for A,where*

$$\mathscr{H}_{pp} = \{\psi \in \mathscr{H} \mid \mu_\psi \textit{ is a pure point measure with countable support on } \mathbb{R}\},$$

$$\mathscr{H}_{ac} = \{\psi \in \mathscr{H} \mid \mu_\psi \textit{ is absolutely continuous w.r.t. Lebesgue measure on } \mathbb{R}\},$$

$$\mathscr{H}_{sc} = \{\psi \in \mathscr{H} \mid \mu_\psi \textit{ is continuous singular w.r.t. Lebesgue measure on } \mathbb{R}\}.$$

By definition, the point spectrum of A is $\sigma_p(A) = \sigma(A|_{\mathscr{H}_{pp}})$, the absolutely continuous spectrum of A is $\sigma_{ac}(A) = \sigma(A|_{\mathscr{H}_{ac}})$, and the singular spectrum of A is $\sigma_{sing}(A) = \sigma(A|_{\mathscr{H}_{sc}})$, so that

$$\sigma(A) = \sigma_p(A) \cup \sigma_{ac}(A) \cup \sigma_{sing}(A).$$

In virtue of the spectral theorem, two (possibly unbounded) self-adjoint operators A and B commute if corresponding projection-valued measures P_A and P_B commute. The following three statements are equivalent.

- Self-adjoint operators A and B commute.
- For all $\lambda, \mu \in \mathbb{C}, \operatorname{Im}\lambda, \operatorname{Im}\mu \neq 0$,
$$R_\lambda(A)R_\mu(B) = R_\mu(B)R_\lambda(A),$$
where $R_\lambda(A) = (A-\lambda I)^{-1}$ and $R_\mu(B) = (B-\mu I)^{-1}$ are resolvents.
- For all $u, v \in \mathbb{R}$,
$$e^{iuA}e^{ivB} = e^{ivB}e^{iuA}.$$

The correspondence $\mathscr{S} \times \mathscr{A} \to \mathscr{P}(\mathbb{R})$ is defined by $(M, A) \mapsto \mu_A$, where

$$\mu_A(\lambda) = \operatorname{Tr} \mathsf{P}_A(\lambda)M,$$

and P_A is decomposition of unity for the self-adjoint operator A. It immediately follows from the spectral theorem that $\mu_A(\lambda)$ is a distribution function of a probability measure on $\mathbb{R}$ and

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

if AM is of trace class. In particular, for $M = P_\psi$

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

[5] A subspace V is invariant for the unbounded operator A, if $A(D(A) \cap V) \subset V$.

and

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

if $\psi \in D(A)$.

Mixed and pure states can be characterized as follows.

LEMMA 1.1. *Every mixed state is a convex linear combination of pure states. A state is pure if and only if it can not be represented as a non-trivial convex linear combination of states.*

PROOF. It follows from Hilbert-Schmidt theorem for compact operators that for every state M there exists (finite or infinite) orthonormal set $\{\psi_n\}_{n=1}^N$ in $\mathscr{H}$ such that

$$M = \sum_{n=1}^{N} \alpha_n P_{\psi_n},$$

where $\alpha_n > 0$ are corresponding non-zero eigenvalues of M. Such representation is called canonical decomposition for self-adjoint compact operator. Since $M \in \mathscr{S}_1$ and

$$\operatorname{Tr} M = \sum_{n=1}^{N} \alpha_n = 1,$$

the state M is a convex linear combination of pure states. To prove the second statement we need to show that if

$$P_\psi = aM_1 + (1-a)M_2,$$

for some states M_1, M_2 and $0 < a < 1$, than $M_1 = M_2 = P_\psi$. Let

$$\mathscr{H} = \mathbb{C}\psi \oplus \mathscr{H}_1$$

be the orthogonal sum decomposition. Since M_1 and M_2 are positive operators, for $\varphi \in \mathscr{H}_1$ we have

$$a(M_1\varphi, \varphi) \leq (P_\psi\varphi, \varphi) = 0,$$

so that $(M_1\varphi, \varphi) = 0$ for all $\varphi \in \mathscr{H}_1$ and $M_1|_{\mathscr{H}_1} = 0$. Since M_1 is self-adjoint, it leaves the complimentary subspace $\mathbb{C}\psi$ invariant, and from $\operatorname{Tr} M_1 = 1$ it follows that $M_1 = P_\psi$. □

1.3. Heisenberg's uncertainty principle. The dispersion of the observable A in the state M is defined as

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

provided the expectation values $\langle A^2|M\rangle$ and $\langle A|M\rangle$ exist. For every $M \in \mathscr{S}$ let

$$M = \sum_{n=1}^{N} \alpha_n P_{\psi_n}$$

be its Hilbert-Schmidt decomposition of the operator M and let P_M be the orthogonal projection onto the closed subspace $\mathscr{H}_M$ in $\mathscr{H}$ spanned by $\{\psi_n\}_{n=1}^N$ ($\mathscr{H}_M$ is the orthogonal complement to $\operatorname{Ker} M$ in $\mathscr{H}$).

LEMMA 1.2. *For every $M \in \mathscr{S}$ and $A \in \mathscr{A}$ the dispersion $\sigma_M^2(A) \geq 0$. The dispersion $\sigma_M(A) = 0$ if and only if $\mathscr{H}_M$ is an eigenspace for the operator A. In particular, if $M = P_\psi$, then ψ is an eigenvector of A.*

PROOF. First of all, it is sufficient to prove the statement for bounded operators A since by the spectral theorem

$$\operatorname{Tr} MA = \lim_{n\to\infty} \operatorname{Tr} MA_n,$$

where $A_n = f_n(A)$ and

$$f_n(\lambda) = \begin{cases} \lambda, & |\lambda| \leq n, \\ 0, & |\lambda| > n. \end{cases}$$

Thus assuming $A \in \mathscr{L}(\mathscr{H})$ and completing, if necessary, the set $\{\psi_n\}_{n=1}^N$ to an orthonormal basis $\{e_n\}_{n=1}^\infty$ for $\mathscr{H}$, we have

$$\begin{aligned} \langle A^2|M\rangle = \operatorname{Tr} A^2M &= \sum_{n=1}^N \alpha_n(A^2\psi_n, \psi_n) = \sum_{n=1}^N \alpha_n(A\psi_n, A\psi_n) \\ &= \sum_{n=1}^N \sum_{m=1}^\infty \alpha_n(A\psi_n, e_m)(e_m, A\psi_n) = \sum_{n=1}^N \sum_{m=1}^\infty \alpha_n|(A\psi_n, e_m)|^2. \end{aligned}$$

Thus

$$\langle A^2|M\rangle \geq \sum_{n=1}^N \alpha_n|(A\psi_n, \psi_n)|^2 \geq \left(\sum_{n=1}^N \alpha_n(A\psi_n, \psi_n)\right)^2 = \langle A|M\rangle^2$$

by the Cauchy-Schwarz inequality, since $\sum_{n=1}^N \alpha_n = 1$. Now $\sigma_M^2(A) = 0$ if and only if $A\psi_n \perp e_m$ for all $m \neq n$ and $(A\psi_1, \psi_1) = \cdots = (A\psi_N, \psi_N)$. Thus there is $\lambda \in \mathbb{R}$ such that $A\psi_n = \lambda\psi_n$ for $n = 1, \dots, N$ and $\mathscr{H}_M$ is an eigenspace for A. $\square$

Now we formulate generalized *Heisenberg uncertainty principle.*

PROPOSITION 1.1 (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 all $M \in \mathscr{S}$, where by definition $\langle i[A, B]|M\rangle = \lim_{n\to\infty}\langle i[A_n, B_n]|M\rangle$.

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 $\alpha \in \mathbb{R}$,

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

so that necessarily $4(A^2\psi, \psi)(B^2\psi, \psi) \geq (i[A, B]\psi, \psi)$. The same argument works for the mixed states. As in the proof of Lemma 1.2, it is sufficient to prove the inequality for bounded A and B. Then using the cyclic property of the trace we have for all $\alpha \in \mathbb{R}$,

$$
\begin{aligned}
& 0 \leq \operatorname{Tr}((A + i\alpha B)M(A + i\alpha B)^*) = \operatorname{Tr}((A + i\alpha B)M(A - i\alpha B)) \\
=& \alpha^2 \operatorname{Tr} BMB + i\alpha \operatorname{Tr} BMA - i\alpha \operatorname{Tr} AMB + \operatorname{Tr} AMA \\
=& \alpha^2 \operatorname{Tr} MB^2 + \alpha \operatorname{Tr}(i[A, B]M) + \operatorname{Tr} MA^2,
\end{aligned}
$$

and the inequality follows. □

A consequence of the Heisenberg's uncertainty principle is that in quantum mechanics there are observables which can not be measured simultaneously, even in a pure state. This is a fundamental difference between classical and quantum mechanics.

1.4. Dynamics. Though quantum observables $\mathscr{A}$ do not form an algebra in any sense[6], a subspace $\mathscr{A}_0 = \mathscr{A} \cap \mathscr{L}(\mathscr{H})$ of $\mathscr{A}$ carries a natural structure of a Lie algebra with respect to the bracket

$$i[A, B] = i(AB - BA).$$

In analogy with classical mechanics, the time evolution is defined by choosing an observable $H \in \mathscr{A}$, called the *Hamiltonian operator* (Hamiltonian for brevitiy). The corresponding quantum equations of motion are

$$\frac{dM}{dt} = 0,\ M \in \mathscr{S}, \quad \hbar \frac{dA}{dt} = i[H, A],\ A \in \mathscr{A}_0$$

and define the *Heisenberg picture* in quantum mechanics. Here the positive number $\hbar$ is called *Planck constant*; numerical value of $\hbar$ is determined from experiment[7].

One should be careful with the commutator $[H, A]$ when H is not bounded, since $\operatorname{Im} A$ is not necessarily a subspace of $D(H)$. To avoid this complication, and to extend the time evolution for all observables (not necessarily bounded), we pass from a self-adjoint operator H to a one-parameter group $U(t)$ fo unitary operators,

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

Conversely, according to the Stone theorem, every self-adjoint operator comes from a one-parameter group. Namely, the following statement is valid.

---

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

[7]The Planck constant has physical dimension of the action. The value $\hbar = 1.054 \times 10^{-27}$ erg $\times$ sec manifests that quantum mechanics is a microscopic theory.

THEOREM 1.3 (Stone's theorem). *Let $U(t)$ be a strongly continuous one-parameter group of unitary operators on $\mathscr{H}$. Then there exists a self-adjoint operator A on $\mathscr{H}$, called an infinitesimal generator of $U(t)$, such that $U(t) = e^{itA}$.*

Explicitly,

$$D(A) = \left\{ \varphi \in \mathscr{H} \;\middle|\; \lim_{t\to 0} \frac{U(t)\varphi - \varphi}{it} = \psi \in \mathscr{H} \right\},$$

and $A\varphi = \psi$.

REMARK. A theorem of von Neumann asserts that for a separable Hilbert space every weakly measurable one-parameter group of unitary operators is strongly continuous, so in this case the conditions of Stone theorem can be relaxed.

The evolution operator $U_t : \mathscr{A} \to \mathscr{A}$ is defined by

$$U_t(A) = U(t)^{-1}AU(t) = e^{\frac{i}{\hbar}tH}Ae^{-\frac{i}{\hbar}tH}.$$

This formula justifies the introduction of *Heisenberg equation for quantum observables*

$$\frac{dA}{dt} = \{H, A\}_\hbar,\ A \in \mathscr{A},$$

where

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

is called *quantum bracket.*

Similarly to the Liouville's picture in classical mechanics, we can consider the quantum mechanical evolution where observables do not depend on time. It is called *Schrödinger picture* and dynamics is given by

$$\frac{dA}{dt} = 0,\ A \in \mathscr{A},\ \frac{dM}{dt} = -\{H, M\}_h,\ M \in \mathscr{S}.$$

Thus

$$M(t) = U(t)MU^{-1}(t) = e^{-\frac{i}{\hbar}tH}Me^{\frac{i}{\hbar}tH}$$

and

$$\langle A(t)|M\rangle = \mathrm{Tr}(U^{-1}(t)AU(t)M) = \mathrm{Tr}(AU(t)MU^{-1}(t)) = \langle A|M(t)\rangle$$

by the cyclic property of the trace. This shows that Heisenberg and Schrödinger pictures are equivalent.

In particular, for a pure state $M = P_\psi$ we get $M(t) = P_{\psi(t)}$ where $\psi(t) = U(t)\psi$, so that $\psi(t)$ satisfies Schrödinger equation

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

A state $M \in \mathscr{S}$ is called *stationary* if $M(t)$ does not depend on time, i.e. if $[M, U(t)] = 0$ so that, by definition, $[M, H] = 0$.

LEMMA 1.3. *The pure state $M = P_\psi$ is statiionary if and only if ψ is the eigenvector for H,*

$$H\psi = E\psi.$$

Corresponding eigenvalue E is called the energy and

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

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, $U(t)\psi = c(t)\psi$. Since $U(t)$ is strongly continuous (weak continuity would be enough), there exists $E \in \mathbb{R}$ such that $c(t) = e^{-\frac{i}{\hbar}tE}$. □

Eigenvalue equation $H\psi = E\psi$ is called *stationary Schrödinger equation.*

2. Heisenberg's commutation relations

Many quantum mechanical systems have classical analogs. Here we start to consider the *quantization* problem, which can be heuristically formulated as follows. Given classical system with the phase space $(\mathscr{M}, \{\ ,\ \})$ and algebra of classical observables $\mathcal{A}$, one needs to construct a Hilbert space $\mathscr{H}$ and a one-to-one correspondence $\mathcal{A} \ni f \mapsto A_f \in \mathscr{A}$ between classical and quantum observables. This correspondence depends on a parameter $\hbar > 0$ and satisfies

$$\tfrac{1}{2}(A_f A_g + A_g A_f) \to fg, \ \{A_f, A_g\}_\hbar \to \{f, g\} \quad \text{as} \quad \hbar \to 0$$

for all $f, g \in \mathcal{A}$. The correspondence $f \mapsto A_f$ is called *quantization* and Hamiltonian operator for a quantum system is a quantization of a Hamiltonian function for the classical system. Later we will formulate quantization problem mathematically. Here we consider several basic examples which will help to state it in a closed form.

2.1. Free particle. Consider first the simplest case of a free quantum particle with one degree of freedom. Corresponding classical phase space is $\mathscr{M} = T^*\mathbb{R} \simeq \mathbb{R}^2$ with canonical Poisson bracket

$$\{f, g\} = \frac{\partial f}{\partial p}\frac{\partial g}{\partial q} - \frac{\partial f}{\partial q}\frac{\partial g}{\partial p}, \quad f, g \in \mathcal{A} = C^\infty(\mathbb{R}^2),$$

wriitten in standard coordinates q, p on $\mathscr{M}$. The Hamiltonian function of a free particle is

$$h = \frac{p^2}{2m}.$$

Poisson bracket of standard coordinates have the following simple form

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

It is another postulate of quantum mechanics that there is a correspondence $q \mapsto Q$ and $p \mapsto P$ between classical and quantum observables such that self-adjoint operators P and Q on a Hilbert space $\mathscr{H}$ satisfy the following commutation relation,

$$\{P, Q\}_\hbar = I \quad \text{on} \quad D(P) \cap D(Q),$$

called *Heisenberg's (canonical) commutation relation.* Mathematically, operators P and Q realize a representation of a Heisenberg Lie algebra. The latter is a 3-dimensional Lie algebra $\mathfrak{h}$ with the generators x, y, c satisfying the relations $[x, y] = c$, $[x, c] = [y, c] = 0$, where now $[\ ,\ ]$ stands for the Lie bracket on $\mathfrak{h}$. The correspondence $x \mapsto -iP, y \mapsto -iQ$ and $c \mapsto i\hbar I$ defines a representation of $\mathfrak{h}$ on the Hilbert space $\mathscr{H}$. It is natural to assume, in addition, that this representation is irreducible, i.e., every bounded operator on $\mathscr{H}$ which commutes with P and Q is a multiple of the identity operator.

Remark. It is well-known that there are no bounded operators on a Hilbert space which satisfy $[A, B] = I$ (which is trivial in the finite-dimensional case). Thus operators P and Q should be necessarily unbounded. Defining a representation of a Lie algebra by unbounded operators requires a caution. However, later we will bypass all these ramifications by considering unitary representations of the corresponding Lie group to $\mathfrak{h}$ — the Heisenberg group.

We we consider two natural realizations of the Heisenberg's commutation relation, 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).

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

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

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

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

Operator Q is called a *coordinate operator* and it is obviously self-adjoint. Its decomposition of unity is given by

$$(\mathsf{P}(\lambda)\varphi)(q) = \begin{cases} \varphi(q), & q \leq \lambda, \\ 0, & q > \lambda. \end{cases}$$

Self-adjoint operator Q has a simple continuous spectrum $\sigma(Q) = \mathbb{R}$ and every bounded operator which commutes with Q is a function of Q, i.e., is a multiplication by a function operator on $\mathscr{H}$. Indeed, a bounded operator B on $\mathscr{H}$ commutes with Q if it commutes with projections $\mathsf{P}(E)$ for all $E \in \mathscr{B}(\mathbb{R})$. In particular, for every interval $[a, b]$

$$B(\chi_{[a,b]}) = f_{a,b}\chi_{[a,b]}$$

for some measurable function $f_{a,b}$ on $[a,b]$, where $\chi_{[a,b]}$ is a characteristic function of the interval $[a,b]$. Using the property $\mathsf{P}(E)B = B\mathsf{P}(E)$ once again we see that for $[c,d] \subset [a,b]$,

$$f_{a,b}|_{[c,d]} = f_{c,d},$$

so that $f_{a,b}$ patch to a measurable function f on $\mathbb{R}$. Since characteristic function are dense in $\mathscr{H}$ we get that B is a multiplication by $f(q)$ operator. Another version of this proof (now at a physical level of rigor) is the following. Represent B as an integral operator with a Schwarz kernel — a distribution $K(q,q')$ (by Schwarz kernel theorem this is legitimate on the linear subspace $\mathscr{S}(\mathbb{R}) \subset L^2(\mathbb{R})$ of Schwarz class functions). Then the commutativity $BQ = QB$ implies that in the distibutional sense

$$(q - q')K(q,q') = 0.$$

Thus K is "proportional" to the Dirac delta-function, i.e.,

$$K(q,q') = f(q)\delta(q - q'),$$

with some bounded measurable function f on $\mathbb{R}$.

REMARK. Operator Q on $\mathscr{H}$ has no eigenfunctions: equation

$$Q\varphi = q_0\,\varphi$$

has no solutions in $L^2(\mathbb{R})$. However, in a distributional sense for every $q_0 \in \mathbb{R}$ it has a unique (up to a constant) solution $\phi_{q_0}(q) = \delta(q - q_0)$. These "generalized eigenfunctions" combine to Schwarz kernel $\delta(q - q_0)$ of the identity operator I on $L^2(\mathbb{R})$. This reflects the fact that operator Q is diagonal in the coordinate representation.

For every pure state $M = P_\psi$, $\|\psi\| = 1$, denote by μ_ψ the probability measure on $\mathbb{R}$ corresponding to Q. We have

$$\mu_\psi(E) = \int_E |\psi(q)|^2 dq$$

for every Borel subset $E \subset \mathbb{R}$. Physically, this is interpreted that in the state P_ψ with the "wave function" $\psi(q)$, the probability of finding quantum mechanical particle in the interval $[q, q + dq]$ is $|\psi(q)|^2 dq$. In other words, the modulus square of a wave function is the probability distribution for the coordinate of a particle.

Corresponding operator P is a differential operator

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

with $D(P) = W^{1,2}(\mathbb{R})$ — a Sobolev space of absolutely continuous functions f on $\mathbb{R}$ such that f and its derivative f' (defined almost everywhere) are in $L^2(\mathbb{R})$. Thus defined operator P is self-adjoint and is called *momentum* *operator*. It is now straightforward to verify that on $D(P) \cap D(Q)$ (which is a dense linear subspace in $\mathscr{H}$)

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

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

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

REMARK. Operator P on $\mathscr{H}$ has no eigenvectors: the equation

$$P\varphi = p\,\varphi, \;\; p \in \mathbb{R},$$

has a solution

$$\varphi(q) = \text{const} \times e^{ipq/\hbar}$$

which does not belong to $\mathscr{H}$. However the family of "normalized generalized eigenfunctions"

$$\varphi_p(q) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipq/\hbar}$$

combines to a Schwarz kernel of the inverse Fourier transform operator. As it will be shown below, this operator diagonalizes the momentum operator P. The choice of the constant is such that

$$\int_{-\infty}^{\infty} \varphi_p(q)\overline{\varphi_{p'}(q)}dq = \delta(p - p').$$

The following fundamental fact asserts that coordinate representation is irreducible.

PROPOSITION 2.1. *Every bounded operator on $\mathscr{H}$ which commutes with coordinate and momentum operators Q and P in coordinate representation $\mathscr{H} \simeq L^2(\mathbb{R}, dq)$ is a multiple of the identity operator I.*

PROOF. Let T be such operator. By part (iv) of Theorem 1.1, operator T commutes with the projection-valued measure P_Q so that T is a function of Q, $T = f(Q)$ for some bounded measurable function f on $\mathbb{R}$. Similarly, commutativity between T and P means that T commutes with the one-parameter group $U(u) = e^{-iuP}$ of unitary operators. It follows from the definition of the derivative that in coordinate representation $(U(u)\psi)(q) = \psi(q - \hbar u)$ for all $\psi \in \mathscr{H}$. Thus

$$TU(u) = U(u)T \quad \text{for all} \quad u \in \mathbb{R}$$

is equivalent to $f(q - \hbar u) = f(q)$ for all $q, u \in \mathbb{R}$, and $f = \text{const}$ a.e. $\square$

The Hamiltonian operator of a free quantum particle on $\mathbb{R}$ is

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

It is a self-adjoint operator on $\mathscr{H}$ with $D(H) = W^{2,2}(\mathbb{R})$ — a Sobolev space of functions in $L^2(\mathbb{R})$ whose generalized first and second derivatives are in $L^2(\mathbb{R})$.

2.1.2. *Momentum representation.* It 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 coordinate p, which is a Lagrangian subspace of $\mathscr{M}$ defined by the equation $q = 0$. Now the coordinate and momentum operators are

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

and satisfy Heisenberg's commutation relation. In momentum representation, the wave function ψ of a pure state $M = P_\psi$ defines the probability distribution for the momentum of the quantum particle: its modulus square $|\psi(p)|^2 dp$ is the probability that momentum of a particle is between p and $p + dp$.

Coordinate and momentum representations are unitary equivalent. Namely, let $\mathscr{F}_\hbar : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the $\hbar$-dependent Fourier transform operator, defined by

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

Here 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

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

It is well-known that $\mathscr{F}$ is a unitary operator on $L^2(\mathbb{R})$ and

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

In particular, since operator $\hat{P}$ is obviously self-adjoint, this immediately shows that P is self-adjoint.

It follows from Heisenberg uncertainty principle that for any pure state $M = P_\psi$ satisfying conditions of the Lemma,

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

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

2.1.3. *Motion of free quantum particle.* The Schrödinger equation

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

in momentum representation becomes

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

so that

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

and

$$\psi(q,t)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{i\left(qp-\frac{p^2}{2m}t\right)/\hbar}\hat{\psi}(p)dp.$$

This formula admits a simple physical interpretation. Suppose that the initial condition $\hat{\psi}(p)$ is smooth function supported in a neighborhood U_0 of $p_0\neq 0$ such that $0\notin U_0$ and

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

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

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

Since

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

for all t, it follows that as $|t|\to\infty$, quantum particle "leaves" every compact subset of $\mathbb{R}$, so that the motion is unbounded. To prove this observe that the function $\chi(p,q,t)=-\frac{p^2}{2m}+\frac{qp}{t}$ has the property that $|\frac{\partial\chi}{\partial p}|>C>0$ for all $p\in U_0$ and $q\in E$, provided that $|t|$ is large enough. Integrating by parts in the representation for $\psi(q,t)$ gives

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

so that uniformly on E,

$$|\psi(q,t)|\leq\frac{C}{t}\quad\text{for } |t| \text{ large enough.}$$

To describe the motion of the particle as $|t|\to\infty$ in the unbounded regions, we use the stationary phase method. In its simplest form it is the following statement.

THE METHOD OF STATIONARY PHASE. Let $f, g \in C^\infty(\mathbb{R})$, where f is real-valued and g has compact support $\mathrm{Supp}(g)$, and suppose that f has a single non-degenerate critical $x_0 \in \mathrm{Supp}(g)$, i.e., $f'(x_0) = 0$ and $f''(x_0) \neq 0$. Then

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

as $N \to \infty$.

Setting $N = t$ we find that the critical point of $\chi(q,p,t)$ is $p_0 = mq/t$ and $\chi''(p_0) = \frac{1}{m\hbar} \neq 0$. Thus as $t \to \infty$,

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

Asymptotically 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 $v = \frac{p}{m}$, $p \in U_0$. Thus the classical relation $p = mv$ remains valid in the quantum picture. Moreover, the asymptotic wave function ψ_0 satisfies

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

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

Moreover, in the weak topology on $\mathscr{H}$ the vector $\psi(t) \to 0$ as $|t| \to \infty$. Indeed, for every $\varphi \in \mathscr{H}$ we get by the Parseval identity

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

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

2.1.4. *Several degrees of freedom.* We start with the phase space $\mathscr{M} = T^*\mathbb{R}^n \simeq \mathbb{R}^{2n}$ with coordinates $\mathbf{q} = (q_1, \dots, q_n)$ and $\mathbf{p} = (p^1, \dots, p^n)$, and with canonical Poisson bracket $\{\ ,\ \}$, coming from canonical symplectic form $\omega = d\mathbf{p} \wedge d\mathbf{q}$. The Poisson brackets between coordinates $\mathbf{q}$ and $\mathbf{p}$ are

$$\{q_k, q_l\} = 0,\ \{p^k, p^l\} = 0,\ \{p^k, q_l\} = \delta^k_l,\ k, l = 1, \dots, n.$$

The Hamiltonian function of a free particle is

$$h = \frac{\mathbf{p}^2}{2m} = \frac{(p^1)^2 + \cdots + (p^n)^2}{2m}.$$

Corresponding quantum coordinate and momenta operators $\mathbf{Q} = (Q_1, \dots, Q_n)$ and $\mathbf{P} = (P^1, \dots, P^n)$ satisfy Heisenberg commutation relations for n degrees of freedom,

$$\{Q_k, Q_l\}_\hbar = 0,\ \{P^k, P^l\}_\hbar = 0,\ \{P^k, Q_l\}_\hbar = \delta^k_l I,\ k, l = 1, \dots, n.$$

REMARK. These are commutation relations of the Heisenberg Lie algebra $\mathfrak{h}$ — a Lie algebra with generators $x^k, \dots, x^n, y_1, \dots, y_n, c$ and relations

$$[x^k, c] = 0, \ [y_k, c] = 0, \ [x^k, y_l] = \delta^k_l c, \ k, l = 1, \dots, n.$$

The correspondence $x^k \mapsto -iP^k, y_k \mapsto -iQ_k$ and $c \mapsto i\hbar I$ defines a representation of a Heisenberg Lie algebra.

In coordinate representation, $\mathscr{H} \simeq L^2(\mathbb{R}^n, d^n\mathbf{q})$, where $d^n\mathbf{q} = dq_1 \dots dq_n$ is the Lebesgue measure on $\mathbb{R}^n$, and

$$\mathbf{Q} = \mathbf{q} = (q_1, \dots, q_n), \quad \mathbf{P} = \frac{\hbar}{i}\frac{\partial}{\partial \mathbf{q}} = \left(\frac{\hbar}{i}\frac{\partial}{\partial q_1}, \dots, \frac{\hbar}{i}\frac{\partial}{\partial q_n}\right).$$

The coordinate and momenta operators are self-adjoint and satisfy Heisenberg's commutation relations. Corresponding decompositions of unity for operators Q_k are defined as before,

$$(\mathsf{P}_k(\lambda)\varphi)(\mathbf{q}) = \begin{cases} \varphi(\mathbf{q}), & q_k \leq \lambda, \\ 0, & q_k > \lambda. \end{cases}$$

$k = 1, \dots, n$. Coordinate operators $Q_1, \dots, Q_n$ form a complete system of commuting operators on $\mathscr{H}$. This means that none of coordinate operators is the function of the other coordinate operators and every operator commuting with $Q_1, \dots, Q_n$ is a function of these operators, i.e., is a multiplication by a function operator on $\mathscr{H}$. The proof repeats verbatim the proof in the case of one degree of freedom. For the pure state $M = P_\psi$ the modulus square $|\psi(\mathbf{q})|^2$ of the wave function is the density of joint distribution function μ_ψ for $Q_1, \dots, Q_n$. In the state with the wave function $\psi(\mathbf{q})$ the probability of finding a particle in the Borel subset $E \subset \mathbb{R}^n$

$$\mu_\psi(E) = \int_E |\psi(\mathbf{q})|^2 d^n\mathbf{q}.$$

The Hamiltonian operator of a free particle in coordinate representation is $\frac{\hbar^2}{2m}$ times the Laplace operator of the Euclidean metric on $\mathbb{R}^n$,

$$H = \frac{\mathbf{P}^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial q_1^2} + \dots + \frac{\partial^2}{\partial q_n^2}\right),$$

and is a self-adjoint operator with domain $D(H) = W^{2,2}(\mathbb{R}^n)$ — the Sobolev space on $\mathbb{R}^n$.

In momentum representation $\mathscr{H} \simeq L^2(\mathbb{R}^n, d^n\mathbf{p})$, where $d^n\mathbf{p} = dp^1 \dots dp^n$, and

$$\hat{\mathbf{Q}} = i\hbar\frac{\partial}{\partial \mathbf{p}}, \quad \hat{\mathbf{P}} = \mathbf{p}.$$

The Hamiltonian operator

$$H = \frac{\mathbf{p}^2}{2m}$$

is a multiplication by a function operator on $\mathscr{H}$.

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

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

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

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

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.

The Schrödinger equation for free particle,

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

is solved, as in the case $n = 1$, by using the Fourier transform

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

where $\hat{\psi} = \mathscr{F}_\hbar(\psi)$. For a wave packet — a smooth function $\hat{\psi}(\mathbf{p})$ supported on a neighborhood U_0 of $0 \neq \mathbf{p}_0 \in \mathbb{R}^n$ such that $0 \notin U_0$ and

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

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

2.2. Quantization of Newtonian particle. As in the previous section, we consider the phase space $\mathscr{M} = \mathbb{R}^{2n} \simeq T^*\mathbb{R}^n$ with canonical Poisson bracket. Newtonian particle — a particle in a potential field $V(\mathbf{q})$ is described by the Hamiltonian

$$h = \frac{\mathbf{p}^2}{2m} + v(\mathbf{q}).$$

Corresponding quantum system has a Hamiltonian

$$H = \frac{\mathbf{P}^2}{2m} + V$$

for some operator V and corresponding coordinate and momenta operators satisfy Heisenberg equations of motion

$$\dot{\mathbf{P}} = \{H, \mathbf{P}\}_\hbar, \ \dot{\mathbf{Q}} = \{H, \mathbf{Q}\}_\hbar.$$

The explicit form of operator V can obtained by requiring that classical relation $\dot{\mathbf{q}} = \mathbf{p}/m$ between velocity and momentum is preserved under the quantization, i.e.,

$$\dot{\mathbf{Q}} = \frac{\mathbf{P}}{m}.$$

Indeed, since $\{\mathbf{P}^2, \mathbf{Q}\}_\hbar = 2\mathbf{P}$, it follows from Heisenberg equations of motion that this condition is equivalent to $[V, Q_k] = 0$ for $k = 1, \dots, n$. Thus V is a function of the commuting operators $Q_1, \dots, Q_n$ and it is natural to suppose that $V = v(\mathbf{Q})$ and is a self-adjoint operator on $\mathscr{H}$ (for real-valued v). Thus Hamiltonian operator of a Newtonian particle is

$$H = \frac{\mathbf{P}^2}{2m} + v(\mathbf{Q}).$$

Note that though both terms in the expression for H are self-adjoint operators, it is not true that the sum of (unbounded) self-adjoint operators is self-adjoint. Admissible classes of potential functions $v(\mathbf{q})$ are determined by the requirement that H is (essentially) self-adjoint. In coordinate representation H has the standard form

$$H = \frac{\hbar^2}{2m}\Delta + V,$$

where Δ is the Laplacian of the standard Eucildean metric on $\mathbb{R}^n$,

$$\Delta = -\sum_{k=1}^{n} \frac{\partial^2}{\partial q_k^2},$$

and $V = v(\mathbf{q})$ is a multiplication by $v(\mathbf{q})$ operator.

3. Harmonic oscillator and holomorphic representation

3.1. Harmonic oscillator. In classical mechanics the simplest system with one degree of freedom is harmonic oscillator. Its phase space $\mathscr{M} = \mathbb{R}^2$ carries canonical Poisson bracket and corresponding Hamiltonian function is

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

where $\omega > 0$ has a physical meaning of frequency of the oscillations. Hamilton's equations of motion describe harmonic motion.

In quantum mechanics, corresponding Hamiltonian operator is

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

where P and Q satisfies Heisenberg's commutation relation. In coordinate representation it is a Schrödinger operator with quadratic potential,

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

on the Hilbert space $\mathscr{H} = L^2(\mathbb{R})$. The significance of this quantum system is that we can explicitly diagonalize the operator H, i.e., find its eigenvalues and eigenvectors, where the latter form a complete set. In particular, it follow from here that operator H, which is obviously symmetric on $\mathscr{S}(\mathbb{R})$, is a self-adjoint operator with $D(H) = W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$.

Namely, set temporarily $m = 1$ and consider the operators

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

defined on $W^{1,2}(\mathbb{R}) \cap \widehat{W}^{1,2}(\mathbb{R})$. It is easy to verify that a^* is the adjoint operator to a. It follows from Heisenberg commutation relations that

$$[a, a^*] = I$$

on $W^{2,2}(\mathbb{R}) \cap \hat{W}^{2,2}(\mathbb{R})$. Indeed, we have

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

and

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

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

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

It follows from this representation that operators a, a^* and $N = a^*a$ generate a nilpotent Lie algebra:

$$[N, a] = -a, \quad [N, a^*] = a^*, \quad [a, a^*] = I. \tag{3.1}$$

It is this Lie-algebraic structure of the harmonic oscillator which is responsible for the exact solution of the Schrödinger equation. Namely, suppose that

I. There exists $\psi \in \mathscr{H}$ such that

$$H\psi = E\psi.$$

II. For all $n \in \mathbb{N}$, $\psi \in D(a^n) \cap D((a^*)^n)$.

Then we have the following.

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

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

— the *ground state vector* for the harmonic oscillator.

(b) The vectors $\psi_n = \frac{1}{\sqrt{n!}}(a^*)^n\psi_0 \in \mathscr{H}$ are orthonormal eigenvectors for H with eigenvalues $\omega\hbar(n + \frac{1}{2})$, i.e.,

$$H\psi_n = \omega\hbar(n + \tfrac{1}{2})\psi_n, \quad n \in \mathbb{N} \cup \{0\}.$$

(c) Operator H is essentially self-adjoint on the Hilbert subspace $\mathscr{H}_0$ of $\mathscr{H}$, spanned by the orthonormal set $\{\psi_n\}_{n=0}^{\infty}$.

It is easy to prove these statements. If $\psi \in \mathscr{H}$ satisfies properties **I-II**, then rewriting commutation relations (3.1) as

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

we get for all $n \geq 0$,

$$Na^n\psi = (E - n)a^n\psi \quad \text{and} \quad N(a^*)^n\psi = (E + n)(a^*)^n\psi. \tag{3.2}$$

Since $N \geq 0$ on $D(N)$, it follows from the first equation in (3.2) that there exists $n_0 \geq 0$ such that $a^{n_0}\psi \neq 0$ but $a^{n_0+1}\psi = 0$. Setting $\psi_0 = a^{n_0}\psi \in \mathscr{H}$ we get

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

Since $H = \omega\hbar(N + \frac{1}{2}I)$, this proves (a). To prove (b) we observe that it follows from the commutation relation $[a, a^*] = I$ by Leibniz rule that

$$[a, (a^*)^n] = n(a^*)^{n-1}.$$

Using this relation, we have

$$\begin{aligned}
\|(a^*)^n\psi_0\|^2 &= ((a^*)^n\psi_0, (a^*)^n\psi_0) = (\psi_0, a^{n-1}a(a^*)^n\psi_0) \\
&= n(\psi_0, a^{n-1}(a^*)^{n-1}\psi_0) + (\psi_0, a^{n-1}(a^*)^n a\psi_0) \\
&= n\|(a^*)^{n-1}\psi_0\|^2 = \cdots = n!\|\psi_0\|^2 = n!
\end{aligned}$$

From the second equation in (3.2) it now follows that ψ_n are normalized eigenvectors of H with the eigenvalues $\omega\hbar(n + \frac{1}{2})$. These eigenvectors are orthogonal since these eigenvalues are distinct and H is symmetric. Finally, property (c) immediately follows from the fact that, according to (b), the closure of $\operatorname{Im}(H|_{\mathscr{H}_0} + iI)$ is $\mathscr{H}_0$.

Remark. Since coordinate representation of Heisenberg's commutation relation is irreducible it is tempting to conclude from the properties (a)-(c) that $\mathscr{H}_0 = \mathscr{H}$. However, though it folllows from construction of the Hilbert subspace $\mathscr{H}_0$ that the linear subspace $(D(P) \cap D(Q)) \cap \mathscr{H}_0)$ is invariant for the operators P and Q, we can not immediately conclude from here that projection operator P_0 onto the subspace $\mathscr{H}_0$ commutes with operators P and Q. Namely, we still need to prove that $P_0(D(P)) \subset D(P)$ and $P_0(D(Q)) \subset D(Q)$.

However, we can prove that $\mathscr{H}_0 = \mathscr{H}$ using the coordinate representation explicitly. Namely, 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

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

and

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

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 $P_n(q)e^{-\frac{\omega q^2}{2\hbar}}$, where $P_n(q)$ are polynomials of degree n. Thus to prove that the functions $\{\psi_n\}_{n=0}^{\infty}$ form an orthonormal basis in $L^2(\mathbb{R})$, it is sufficient to show that the system of functions $\{q^n e^{-q^2}\}_{n=0}^{\infty}$ is complete. Suppose that $f \in L^2(\mathbb{R})$ is such that

$$\int_{-\infty}^{\infty} f(q)q^n e^{-q^2}\, dq = 0 \quad \text{for all} \quad n \geq 0.$$

For $z \in \mathbb{C}$ introduce

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

Clearly, this integral absolutely converges for all $z \in \mathbb{C}$ and defines an entire function. We have for all $n \geq 0$,

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

so that $F(z) = 0$ for all $z \in \mathbb{C}$. In particular, setting $z = -ip, p \in \mathbb{R}$ and $g(q) = f(q)e^{-q^2} \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$, we get $\mathscr{F}(g) = 0$, where $\mathscr{F}$ stands for the ordinary ($\hbar = 1$) Fourier transform, so that $g = 0$.

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

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

Namely, using the identity

$$\begin{aligned} e^{q^2/2}\frac{d^n}{dq^n}\left(e^{-q^2}\right) &= -\left(q - \frac{d}{dq}\right)\left[e^{q^2/2}\frac{d^{n-1}}{dq^{n-1}}\left(e^{-q^2}\right)\right] \\ &= \cdots = (-1)^n \left(q - \frac{d}{dq}\right)^n e^{-q^2/2} \end{aligned}$$

we obtain

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

We summarize everything in the following statement.

THEOREM 3.1. *Hamiltonian*

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

of harmonic oscillator, defined on $\mathscr{S}(\mathbb{R})$*, is essentially self-adjoint operator on* $L^2(\mathbb{R})$ *with pure point spectrum. The complete system of eigenfunctions is*

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

where $H_n(q)$ *are classical Hermite polynomials, and*

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

The closure $\bar{H}$ *of* H *is self-adjoint and* $D(\bar{H}) = W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$*.*

PROOF. The operator H is symmetric and has a complete system of eigenvectors, so that

$$\overline{\operatorname{Im}(H + iI)} = \overline{\operatorname{Im}(H - iI)} = \mathscr{H}.$$

This proves that H is essentially self-adjoint. The proof that $D(\bar{H}) = W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$ is left to the reader. □

3.2. 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 the basic $\{\psi_n\}_{n=0}^\infty$ for $L^2(\mathbb{R})$ defines the isomorphism $L^2(\mathbb{R}) \simeq \ell^2$,

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

where

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

since functions ψ_n are real-valued. Using $[a, (a^*)^n] = n(a^*)^{n-1}$, we obtain

$$a^*\psi = \sum_{n=0}^\infty c_n a^*\psi_n = \sum_{n=0}^\infty c_n \frac{(a^*)^{n+1}}{\sqrt{n!}}\psi_0 = \sum_{n=1}^\infty \sqrt{n}\, c_{n-1}\psi_n, \quad \psi \in D(a^*),$$

and

$$a\psi = \sum_{n=0}^{\infty} c_n a\psi_n = \sum_{n=0}^{\infty} c_n \frac{a(a^*)^n}{\sqrt{n!}}\psi_0 = \sum_{n=0}^{\infty} \sqrt{n+1}\, c_{n+1}\psi_n, \quad \psi \in D(a).$$

Thus creation and annihilations operators a^* and a in the Hilbert space ℓ^2 can be represented by the following semi-infinite matrices:

$$a = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & . \\ 0 & 0 & \sqrt{2} & 0 & . \\ 0 & 0 & 0 & \sqrt{3} & . \\ . & . & . & . & . \end{bmatrix}, \quad a^* = \begin{bmatrix} 0 & 0 & 0 & 0 & . \\ \sqrt{1} & 0 & 0 & 0 & . \\ 0 & \sqrt{2} & 0 & 0 & . \\ 0 & 0 & \sqrt{3} & 0 & . \\ . & . & . & . & . \end{bmatrix},$$

and

$$N = a^*a = \begin{bmatrix} 0 & 0 & 0 & 0 & . \\ 0 & 1 & 0 & 0 & . \\ 0 & 0 & 2 & 0 & . \\ 0 & 0 & 0 & 3 & . \\ . & . & . & . & . \end{bmatrix}.$$

Thus in this representation the Hamiltonian of the harmonic oscillator is represented by a diagonal matrix,

$$H = \omega\hbar\left(N + \frac{1}{2}\right) = \operatorname{diag}\left\{\frac{\omega\hbar}{2}, \frac{3\omega\hbar}{2}, \frac{5\omega\hbar}{2}, \dots\right\}.$$

Let $\mathscr{D}$ be the Hilbert space of entire functions,

$$\mathscr{D} = \left\{ f \text{ entire function } : \|f\|^2 = \frac{1}{\pi}\iint_{\mathbb{C}} |f(z)|^2 e^{-|z|^2} d^2z \right\},$$

where $d^2z = \frac{i}{2}dz \wedge d\bar{z}$. The functions

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

form an orthonormal basis for $\mathscr{D}$, and the assignment

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

establishes the isomorphism $\ell^2 \simeq \mathscr{D}$. The realization of the Hilbert space $\mathscr{H}$ as the Hilbert space $\mathscr{D}$ of entire functions is called *holomorphic representation.* It follows from the matrix representations of creation-annihilation operators that in the holomorphic representation

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

and

$$H = \omega\hbar\left(z\frac{d}{dz} + \frac{1}{2}\right).$$

The holomorphic representation is characterized by the property that Hamiltonian H of the harmonic oscillator is diagonal. Moreover, since H has a simple spectrum, every bounded operator which commutes with H is a function of H.

The assignment

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

establishes the isomorphism between the coordinate and momentum representations. Using the generating function for Hermite polynomials,

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

corresponding unitary operator $U : \mathscr{H} \to \mathscr{D}$ can be specified explicitly as the integral operator

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

with the kernel

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

3.2.1. *Wick symbols of operators.*

4. Stone-von Neumann theorem

4.1. Weyl commutation relations. As we discussed before, Heisenberg commutation relations realize irreducible representation of Heisenberg Lie algebra $\mathfrak{h}$ by skew self-adjoint operators on the Hilbert space,

$$x^k \mapsto -iP^k,\ y_k \mapsto -iQ_k,\ k = 1, \dots, n, \quad c \mapsto i\hbar I.$$

It is a non-trivial mathematical problem to define a commutator of unbounded operators. It can be completely bypassed by considering corresponding unitary representation of the Heisenberg group G. The latter is a connected, simply-connected Lie group with the Lie algebra $\mathfrak{h}$. It is a unipotent Lie group of $(n+2)\times(n+2)$ matrices, defined by

$$G = \left\{ g = \begin{bmatrix} 1 & u_1 & u_2 & \dots & u_n & c \\ 0 & 1 & 0 & \dots & 0 & v^1 \\ 0 & 0 & 1 & \dots & 0 & v^2 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 1 & v^n \\ 0 & 0 & 0 & \dots & 0 & 1 \end{bmatrix} \in \mathrm{SL}(n+2,\mathbb{R}) \right\}.$$

The Heisenberg group G generated by n-parameter abelian subgroups $e^{\mathbf{u}X} = e^{\sum_{k=1}^{n} u_k x^k}$, $e^{\mathbf{v}Y} = e^{\sum_{k=1}^{n} v^k y_k}$ and a one-parameter center $e^{\alpha c}$, which satisfy the relations

$$e^{\mathbf{u}X}e^{\mathbf{v}Y} = e^{\mathbf{uv}c}e^{\mathbf{v}Y}e^{\mathbf{u}X}, \quad \text{where} \quad \mathbf{uv} = \sum_{k=0}^{n} u_k v^k.$$

The exponential map $\mathfrak{h} \to G$ is onto, so by Schur lemma in order to describe the irreducible unitary representation $\rho : G \to \mathscr{U}(\mathscr{H})$, it is sufficient to define strongly continuous n-parameter abelian groups of unitary operators

$$U(\mathbf{u}) = \rho(e^{\mathbf{u}X}),\ \ V(\mathbf{v}) = \rho(e^{\mathbf{v}Y})$$

satisfying *Hermann Weyl commutation relations*

$$U(\mathbf{u})V(\mathbf{v}) = e^{i\hbar\mathbf{uv}}V(\mathbf{v})U(\mathbf{u}).$$

Here parameter $\hbar$ is determined by $\rho(e^c) = e^{i\hbar}I$. Thus mathematically the Planck constant parameterizes irreducible unitary representations of the Heisenberg Lie group. In coordinate representation, $U(\mathbf{u}) = e^{-i\mathbf{uP}}$ and $V(\mathbf{v}) = e^{-i\mathbf{vQ}}$ are given by the unitary operators

$$U(\mathbf{u})\psi(\mathbf{q}) = \psi(\mathbf{q} - \hbar\mathbf{u}), \quad V(\mathbf{v}) = e^{-i\mathbf{vq}}\psi(\mathbf{q}),$$

which satisfy Weyl relations. This realization of Weyl relations is called *Schrödinger representation*. We proved in Section 2.1.1 that Schrödinger representation is irreducible, so that irreducible unitary representations of Heisenberg group exist for all real $\hbar \neq 0$.

REMARK. It should be noted that neither Weyl relations can be obtained from Heisenberg commutation relations, nor Heisenberg commutation relations can be obtained from Weyl relations. However, there is a heuristic (at the physical level of rigor) derivation of Weil relaions. Consider, for simplicity, the case of one degree of freedom and start with the Heisenberg commutation relation

$$\{P, Q\}_\hbar = I.$$

Since quantum bracket satisfies the Leibniz rule, i.e., is a derivation, we have (for a "suitable" function f) that

$$\{f(P), Q\}_\hbar = f'(P).$$

In particular, choosing $f(P) = e^{-iuP} = U(u)$, we obtain

$$U(u)Q - QU(u) = \hbar u U(u) \quad \text{or} \quad U(u)QU(u)^{-1} = Q + \hbar u I.$$

In turn, we get from here (for a "suitable" function g)

$$U(u)g(Q) = g(Q + \hbar u I)U(u).$$

Setting $g(Q) = e^{-ivQ} = V(v)$, we get from here Weyl relation. Another formal derivation of Weyl relation is based on the Campbell-Baker-Hausdorff formula. Namely, since $[P, Q] = \frac{\hbar}{i}I$, we get

$$e^{-iuP}e^{-ivQ} = e^{\frac{uv}{2}[P,Q]}e^{-i(uP+vQ)}$$

and

$$e^{-ivQ}e^{-iuP} = e^{-\frac{uv}{2}[P,Q]}e^{-i(uP+vQ)}.$$

4.2. Stone-von Neumann theorem. It turns out that Schrodinger representation, for real $\hbar \neq 0$, and trivial (one-dimensional) representation are the only unitary irreducible representations of the Heisenberg group.

THEOREM 4.1. *(Stone-von Neumann Theorem) Every irreducible unitary representation of Weyl commutation relations for n degrees of freedom*

,

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

is unitary equivalent to the Schrodinger representation.

COROLLARY 4.1. *Generators $\mathbf{P} = (P^1, \dots, P^n)$ and $\mathbf{Q} = (Q_1, \dots, Q_n)$ of n-parameter abelian groups $U(\mathbf{u})$ and $V(\mathbf{v})$, realizing irreducible representation of Weyl commutation relations, satisfy Heisenberg commutation relations.*

REMARK. The Stone-von Neumann theorem is a very strong statement. In particular, it guarantees that for creation-annihilation operators $\mathbf{a}$ and $\mathbf{a}^*$, constructed from the infinitesimal generators $\mathbf{P}$ and $\mathbf{Q}$, there exists a ground state — a vector $\psi_0 \in \mathscr{H}$, annihilated by all operators $\mathbf{a}$. Corresponding statement does not hold for the systems with infinitely many degrees of freedom, where in addition one postulates the existence of the ground state ("physical vacuum"). This reflects a fundamental difference between quantum mechanics (systems with finitely many degrees of freedom) and quantum field theory (systems with infinitely many degrees of freedom),

Now we will give a proof of Stone-von Neumann theorem. For simplicity, we consider the case of $n = 1$. Later we interprete corresponding constructions from the symplectic geometry point of view.

PROOF. Set

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

Unitary operator $S(u,v)$ satisfies

$$S(u,v)^* = S(-u,-v)$$

and it follows from Weyl relation that

$$S(u_1,v_1)S(u_2,v_2) = e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1)}S(u_1+u_2,v_1+v_2).$$

Define a linear map $W : L^1(\mathbb{R}^2) \to \mathscr{B}(\mathscr{H})$ by

$$W(f) = \frac{1}{2\pi}\iint_{\mathbb{R}^2} f(u,v)S(u,v)dudv,$$

where integral is understood in the weak sense: for every $\psi_1, \psi_2 \in \mathscr{H}$,

$$(W(f)\psi_1, \psi_2) = \frac{1}{2\pi} \iint\limits_{\mathbb{R}^2} f(u,v)(S(u,v)\psi_1, \psi_2)dudv.$$

It follows from this definition that the integral is convergent for all $\psi_1, \psi_2 \in \mathscr{H}$ and

$$\|W(f)\| \leq \frac{1}{2\pi}\|f\|_{L^1}.$$

The map W is called *Weyl transfrom.* From the above relations we have

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

where

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

and

$$S(u_1,v_1)W(f)S(u_2,v_2) = W(\tilde{f}),$$

where

$$\tilde{f}(u,v) = e^{\frac{\hbar}{2}\{(u_1-u_2)v-(v_1-v_2)u+u_2v_1-u_1v_2\}} f(u-u_1-u_2, v-v_1-v_2).$$

The Weyl transfrom has the following properties.

1. $\ker W = \{0\}$.
2. For $f_1, f_2 \in L^1(\mathbb{R}^2)$,

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

where

$$(f_1 *_\hbar f_2)(u,v) = \frac{1}{2\pi} \iint\limits_{\mathbb{R}^2} e^{-\frac{i\hbar}{2}(u'v-uv')} f_1(u-u', v-v') f_2(u',v')du'dv'.$$

To prove the first property, suppose that $W(f) = 0$. Then for all for all $u', v' \in \mathbb{R}$ we have

$$S(-u',-v')W(f)S(u',v') = \frac{1}{2\pi} \iint\limits_{\mathbb{R}^2} e^{-\frac{i\hbar}{2}(u'v-uv')} f(u,v)S(u,v)dudv = 0,$$

which implies that for every $\psi_1, \psi_2 \in \mathscr{H}$ and every trigonometric polynomial $p(u,v)$ we have

$$\iint\limits_{\mathbb{R}^2} p(u,v)f(u,v)(S(u,v)\psi_1, \psi_2)dudv = 0.$$

Therefore, $f(u,v)(S(u,v)\psi_1,\psi_2)=0$ for all $\psi_1,\psi_2\in\mathscr{H}$, so that $f=0$. To prove the second property, we compute

$$\begin{aligned}(W(f_1)W(f_2)\psi_1,\psi_2)&=(W(f_2)\psi_1,W(f_1)^*\psi_2)\\ &=\frac{1}{2\pi}\iint\limits_{\mathbb{R}^2} f_2(u_2,v_2)(S(u_2,v_2)\psi_1,W(f_1)^*\psi_2)du_2dv_2\\ &=\frac{1}{2\pi}\iint\limits_{\mathbb{R}^2} f_2(u_2,v_2)(W(f_1)S(u_2,v_2)\psi_1,\psi_2)du_2dv_2\end{aligned}$$

$$=\frac{1}{(2\pi)^2}\iint\limits_{\mathbb{R}^4} f_1(u_1-u_2,v_1-v_2)f_2(u_2,v_2)e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1)}(S(u_1,v_1)\psi_1,\psi_2)du_1dv_1du$$

$$=\frac{1}{2\pi}\iint\limits_{\mathbb{R}^2}(f_1*_\hbar f_2)(u,v)(S(u,v)\psi_1,\psi_2)dudv,$$

where $f_1*_\hbar f_2\in L^1(\mathbb{R}^2)$. The linear mapping

$$*_\hbar: L^1(\mathbb{R}^2)\times L^1(\mathbb{R}^2)\to L^1(\mathbb{R}^2)$$

is associative,

$$f_1*_\hbar(f_2*_\hbar f_3)=(f_1*_\hbar f_2)*_\hbar f_3\quad\text{for all}\quad f_1,f_2,f_3\in L^1(\mathbb{R}^2),$$

which immediately follows from associativity of the operator product. When $\hbar=0$, the product $*_\hbar$ becomes the usual convolution product of functions in $L^1(\mathbb{R}^2)$.

For every $\psi\in\mathscr{H},\psi\neq 0$, denote by $\mathscr{H}_\psi$ the closed subspace of $\mathscr{H}$ spanned by the vectors $S(u,v)\psi$ for all $u,v\in\mathbb{R}$. The subspace $\mathscr{H}_\psi$ is an invariant subspace for the operators $U(u)$ and $V(v)$ for all $u,v\in\mathbb{R}$. Since the representation of Weyl commutation relations is irreducible, $\mathscr{H}_\psi=\mathscr{H}$. It turns out that there is a vector $\psi_0\in\mathscr{H}$ for which all the scalar products of the generating elements $S(u,v)\psi_0$ of the subspace $\mathscr{H}_{\psi_0}$ can be explicitly computed. For this aim, we let

$$f_0(u,v)=\hbar\, e^{-\frac{\hbar(u^2+v^2)}{4}}$$

and set

$$W_0=W(f_0).$$

Then $W_0^*=W_0$ and

$$W_0S(u,v)W_0=e^{-\frac{\hbar}{4}(u^2+v^2)}W_0.$$

In particular, $W_0^2=W_0$, so that W_0 is an orthogonal projection. Indeed, using property **2**, we have

$$W_0S(u,v)W_0=W(f_0*_\hbar\tilde{f}_0),$$

where

$$\tilde{f}_0(u',v')=e^{-\frac{i\hbar}{2}(u'v-uv')}f_0(u'-u,v'-v).$$

Thus

$$(f_0 *_\hbar \tilde{f}_0)(u', v') = \hbar e^{-\frac{\hbar}{4}(u^2+v^2+{u'}^2+{v'}^2)} I(u', v'),$$

where

$$I(u', v') = \frac{\hbar}{2\pi} \iint\limits_{\mathbb{R}^2} e^{-\frac{\hbar}{2}\{(u''-u-u'+iv+iv')^2+(v''-v-v'-iu-iu')^2\}} du'' dv''.$$

Shifting contours of integration to $\operatorname{Im} u'' = -v - v', \operatorname{Im} v'' = u + u'$ and substituting $\xi = u'' - u - u' + iv + iv', \eta = v'' - v - v' - iu - iu$, we get

$$I(u', v') = \frac{\hbar}{2\pi} \iint\limits_{\mathbb{R}^2} e^{-\frac{\hbar}{2}(\xi^2+\eta^2)} d\xi d\eta = 1.$$

Now let $\mathscr{H}_0$ be the image of the projection operator W_0, a closed subspace of $\mathscr{H}$. By the property **1**, $\mathscr{H} \neq \{0\}$. For every $\psi_1, \psi_2 \in \mathscr{H}_0$ we have $W_0\psi_1 = \psi_1, W_0\psi_2 = \psi_2$ and

$$\begin{aligned}
(S(u_1, v_1)\psi_1, S(u_2, v_2)\psi_2) &= (S(u_1, v_1)W_0\psi_1, S(u_2, v_2)W_0\psi_2) \\
&= (W_0 S(-u_2, -v_2) S(u_1, v_1) W_0\psi_1, \psi_2) \\
&= e^{\frac{i\hbar}{2}(u_1v_2 - u_2v_1)} (W_0 S(u_1 - u_2, v_1 - v_2) W_0 \psi_1, \psi_2) \\
&= e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1) - \frac{\hbar}{4}\{(u_1-u_2)^2+(v_1-v_2)^2\}} (W_0\psi_1, \psi_2) \\
&= e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1) - \frac{\hbar}{4}\{(u_1-u_2)^2+(v_1-v_2)^2\}} (\psi_1, \psi_2).
\end{aligned}$$

Now we claim the subspace $\mathscr{H}_0$ is one-dimensional. Indeed, by the above formula, for every $\psi_1, \psi_2 \in \mathscr{H}_0$ such that $(\psi_1, \psi_2) = 0$ the corresponding subspaces $\mathscr{H}_{\psi_1}$ and $\mathscr{H}_{\psi_2}$ are orthogonal. Since $\mathscr{H}_\psi = \mathscr{H}$ for every $\psi \neq 0$, at least one of the vectors ψ_1, ψ_2 is 0. Let $\mathscr{H}_0 = \mathbb{C}\,\psi_0, \|\psi_0\| = 1$, and set

$$\psi_{\alpha,\beta} = S(\alpha, \beta)\psi_0, \quad \alpha, \beta \in \mathbb{R}.$$

The closure of the linear span of the vectors $\psi_{\alpha,\beta}$ for all $\alpha, \beta \in \mathbb{R}$ is $\mathscr{H}$. We have

$$(\psi_{\alpha,\beta}, \psi_{\gamma,\delta}) = e^{\frac{i\hbar}{2}(\alpha\delta-\beta\gamma) - \frac{\hbar}{4}\{(\alpha-\gamma)^2+(\beta-\delta)^2\}}$$

and

$$S(u, v)\psi_{\alpha,\beta} = e^{\frac{i\hbar}{2}(u\beta - v\alpha)} \psi_{\alpha+u,\beta+v}.$$

Now consider Schrödinger representation of Weyl commutation relations in the Hilbert space $L^2(\mathbb{R})$:

$$\begin{aligned}
(\mathsf{U}(u)\psi)(q) &= \psi(q - \hbar u), \\
(\mathsf{V}(v)\psi)(q) &= e^{-ivq}\psi(q), \\
(\mathsf{S}(u, v)\psi)(q) &= e^{\frac{i\hbar uv}{2} - ivq}\psi(q - \hbar u).
\end{aligned}$$

For the corresponding projection operator W_0 we have

$$\begin{aligned}(\mathsf{W}_0\psi)(q) &= \frac{\hbar}{2\pi}\iint\limits_{\mathbb{R}^2} e^{-\frac{\hbar}{4}(u^2+v^2)}e^{\frac{i\hbar uv}{2}-ivq}\psi(q-\hbar u)dudv \\ &= \sqrt{\frac{\hbar}{\pi}}\int_{-\infty}^{\infty} e^{-\frac{\hbar}{4}(u^2+(u-\frac{2q}{\hbar})^2)}\psi(q-\hbar u)du \\ &= \frac{1}{\sqrt{\hbar\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2\hbar}(q^2+q'^2)}\psi(q')dq',\end{aligned}$$

where we have performed Gaussian integration with respect to the variable v. Thus W_0 is a projection operator onto the one-dimensional subspace of $L^2(\mathbb{R})$ spanned by the Gaussian exponential $\varphi_0 = \frac{1}{\sqrt[4]{\pi\hbar}}e^{-q^2/2\hbar}$, $\|\varphi_0\| = 1$. Now set

$$\varphi_{\alpha,\beta} = \mathsf{S}(\alpha,\beta)\varphi_0.$$

Since Schrödinger representation of Weyl commutation relations is irreducible, the closure of the linear span of the functions $\varphi_{\alpha,\beta}$ for all $\alpha,\beta\in\mathbb{R}$ is the Hilbert space $L^2(\mathbb{R})$. (This also can be proved directly from the completeness of Hermite functions, since $\varphi_{\alpha,\beta}(q) = \frac{1}{\sqrt[4]{\pi\hbar}}e^{\frac{i\hbar\alpha\beta}{2}-i\beta q-(q-\hbar\alpha)^2/2\hbar}$). We have

$$(\varphi_{\alpha,\beta},\varphi_{\gamma,\delta}) = e^{\frac{i\hbar}{2}(\alpha\delta-\beta\gamma)-\frac{\hbar}{4}\{(\alpha-\gamma)^2+(\beta-\delta)^2\}}$$

and

$$\mathsf{S}(u,v)\varphi_{\alpha,\beta} = e^{\frac{i\hbar}{2}(u\beta-v\alpha)}\varphi_{\alpha+u,\beta+v}.$$

For $\psi = \sum_{i=1}^n c_i\psi_{\alpha_i,\beta_i}\in\mathscr{H}$ define

$$\mathscr{U}(\psi) = \sum_{i=1}^n c_i\varphi_{\alpha_i,\beta_i}\in L^2(\mathbb{R}).$$

Since the inner products between vectors $\psi_{\alpha,\beta}$ coincide with the inner products between the vectors $\varphi_{\alpha,\beta}$, we have

$$\|\mathscr{U}(\psi)\|^2_{L^2(\mathbb{R})} = \|\psi\|^2_{\mathscr{H}},$$

so that $\mathscr{U}$ is well-defined unitary operator between the linear spans of the systems of vectors $\{\psi_{\alpha,\beta}\}_{\alpha,\beta\in\mathbb{R}}$ and $\{\varphi_{\alpha,\beta}\}_{\alpha,\beta\in\mathbb{R}}$. Thus $\mathscr{U}$ extends to the unitary operator $\mathscr{U}:\mathscr{H}\to L^2(\mathbb{R})$ satisfying

$$\mathscr{U}S(\alpha,\beta) = \mathsf{S}(\alpha,\beta)\mathscr{U}\quad\text{for all}\quad\alpha,\beta\in\mathbb{R}.$$

This completes the proof of Stone-von Neumann theorem. □

Corollary 4.2. *The Weyl transform W extends to the isomorphism between $L^2(\mathbb{R}^2)$ and the Hilbert space $\mathscr{S}_2(\mathscr{H})$ of Hilbert-Schmidt operators on $\mathscr{H}$.*

PROOF. It follows from the proof of Stone-von Neumann theorem that for $f \in L^1(\mathbb{R}^2)$ operator $W(f)$ on $L^2(\mathbb{R})$ is an integral operator with the kernel

$$K(q,q') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} f(\tfrac{q-q'}{\hbar}, v)e^{-\frac{i(q+q')v}{2}}dv,$$

i.e., for every $\psi \in L^2(\mathbb{R})$,

$$(W(f)\psi)(q) = \int_{-\infty}^{\infty} K(q,q')\psi(q')dq'.$$

For $f \in \mathscr{S}(\mathbb{R}^2)$ we have by elementary theory of Fourier transform that

$$\iint\limits_{\mathbb{R}^2} |K(q,q')|^2 dq dq' = \|f\|^2_{L^2(\mathbb{R}^2)}.$$

Thus for such f the operator $W(f)$ is Hilbert-Schmidt and since $\mathscr{S}(\mathbb{R}^2)$ is dense in $L^2(\mathbb{R}^2)$, we get the isometry $W : L^2(\mathbb{R}^2) \to \mathscr{S}_2(\mathscr{H})$. Since every Hilbert-Scmidt operator on $L^2(\mathbb{R})$ is an integral operator with square-summable kernel, the mapping W is onto. $\square$

4.3. Invariant formulation of Stone-von Neumann theorem. Let (V,ω) be a finite-dimensional symplectic vector space, $\dim V = 2n$. Corresponding Heisenberg Lie algebra $\mathfrak{h}$ is a one-dimensional central extension of the abelian Lie algebra V by the two-cocycle given by the symplectic form ω. As a vector space,

$$\mathfrak{h} = V \oplus \mathbb{R}c,$$

and the Lie bracket is

$$[u+\alpha c, v+\beta c] = \omega(u,v)c, \quad u,v \in V, \ \ \alpha,\beta \in \mathbb{R}.$$

Choosing the symplectic basis $x^1,\dots,x^n,y_1,\dots,y_n$ for V (that is, $\omega(x^k,x^l) = \omega(y_k,y_l) = 0$, $\omega(x^k,y_l) = \delta^k_l$) we see that this definition agrees with the one given in Section 2.1.4. Every Lagrangian subspace ℓ of V defines an abelian subalgebra $\ell \oplus \mathbb{R}c$ of $\mathfrak{h}$. Let ℓ' be a complimentary Lagrangian subspace to ℓ in V,

$$\ell \oplus \ell' = V.$$

Then

$$\mathfrak{h}/(\ell \oplus \mathbb{R}c) \simeq \ell'.$$

Let G be the Heisenberg group — connected and simply-connected Lie group such that $\mathrm{Lie}(G) = \mathfrak{h}$. Under the exponential map, Lie group G is identified with the $(2n+1)$-vector space $V \oplus \mathbb{R}c$ with the group law

$$\exp(v_1+\alpha_1 c)\exp(v_2+\alpha_2 c) = \exp\left(v_1+v_2+\left(\alpha_1+\alpha_2+\tfrac{1}{2}\omega(v_1,v_2)\right)c\right),$$

where $v_1,v_2 \in V$, $\alpha_1,\alpha_2 \in \mathbb{R}$. The volume form $d^{2n}\mathbf{v}\wedge dc$, where $d^{2n}\mathbf{v} \in \Lambda^{2n}V^\vee$ is a non-zero volume form on V (here $V^\vee$ is a dual vector space to V), defines a bi-invariant Haar measure on G. Let $L = \exp(\ell \oplus \mathbb{R}c)$ be abelian subgroup of G defined by the Lagrangian subspace ℓ. Since every $g \in G$ can be uniquely represented as $g = \exp v' \exp(v + \alpha c)$, where $v \in \ell, v' \in \ell'$,

$$G/L \simeq \ell'.$$

The isomorphism $\Lambda^{2n}V^\vee \simeq \Lambda^n \ell^\vee \wedge \Lambda^n \ell'^\vee$ gives rise to the volume form $d^n\mathbf{v}'$ on ℓ' and defines on the homogeneous space G/L the measure dg, invariant under the left G-action. The measure dg does not depend on the choice of the complimentary Lagrangian subspace ℓ'.

For a given $\hbar \in \mathbb{R}$, the function $\chi : G \to \mathbb{C}$,

$$\chi(\exp(v + \alpha c)) = e^{i\hbar\alpha} \quad \text{for} \quad v \in V, \, \alpha \in \mathbb{R},$$

defines a unitary character of L,

$$\chi(l_1 l_2) = \chi(l_1)\chi(l_2) \quad \text{for} \quad l_1, l_2 \in L.$$

Definition. Schrödinger representation $S(\ell)$ of the Heisenberg group G, associated with a Lagrangian subspace ℓ, is a representation of G induced by the one-dimensional representation χ of L,

$$S(\ell) = \operatorname{Ind}_L^G \chi.$$

Explicitly, the representation $S(\ell)$ is realized in the Hilbert space $\mathscr{H}(\ell)$ of functions $f : G \to \mathbb{C}$ satisfying

$$f(gl) = \chi(l)^{-1} f(g) \quad \text{for all} \quad g \in G, \; l \in \ell,$$

and

$$\|f\|^2 = \int\limits_{G/L} |f(g)|^2 dg < \infty.$$

The representation $S(\ell)$ of the Heisenberg group G on $\mathscr{H}(\ell)$ acts by left translations,

$$(S(\ell)(g)f)(g') = f(g^{-1}g') \quad \text{for all} \quad f \in \mathscr{H}(\ell), \; g \in G.$$

In particular,

$$(S(\ell)(\exp \alpha c)f)(g) = f(\exp(-\alpha c)g) = f(g \exp(-\alpha c)) = e^{i\hbar\alpha} f(g),$$

so that $S(\ell)(\exp \alpha c) = e^{i\hbar\alpha} I$, where I is the identity operator on $\mathscr{H}(\ell)$.

Every choice of a complimentary Lagrangian subspace ℓ' gives rise to the decomposition $g = \exp v' \exp(v + \alpha c)$ for all $g \in G$. For $f \in \mathscr{H}(\ell)$ we get,

$$f(g) = f(\exp v' \exp(v + \alpha c)) = e^{-i\hbar\alpha} f(\exp v'), \quad v \in \ell, \, v' \in \ell', \, \alpha \in \mathbb{R},$$

so that $f \in \mathscr{H}(\ell)$ is completely determined by its restriction on $\exp \ell' \simeq \ell'$. Thus the mapping

$$\mathscr{H} \ni f \mapsto \psi \in L^2(\ell', d^n\mathbf{v}'), \quad \psi(v') = f(\exp \tfrac{v'}{\hbar}), \quad v' \in \ell',$$

defines the isomorphism $\mathscr{H}(\ell) \simeq L^2(\ell', d^n\mathbf{v}')$. In this realization, the representation $S(\ell)$ is given by

$$(S(\ell)(\exp v)\psi)(v') = e^{i\omega(v,v')}\psi(v'), \quad v \in \ell,\ v' \in \ell'$$
$$(S(\ell)(\exp u')\psi)(v') = \psi(v' - \hbar u'), \quad u',\ v' \in \ell'.$$

In particular, choose a symplectic basis $x^1, \dots, x^n, y_1, \dots, y_n$ for V and set

$$d^{2n}\mathbf{v} = dx^1 \wedge \cdots \wedge dx^n \wedge dy_n \wedge \cdots \wedge dy_n.$$

For $\ell = \mathbb{R}y_1 \oplus \cdots \oplus \mathbb{R}y_n$ choosing $\ell' = \mathbb{R}x^1 \oplus \cdots \oplus \mathbb{R}x^n$ we see that the representation $S(\ell)$ becomes coordinate representation of Weyl commutation relations. Namely, for $u = \sum_{k=1}^n u_k x^k \in \ell'$ and $v = \sum_{k=1}^n v^k y_k \in \ell$ we get

$$S(\ell)(\exp u) = U(\mathbf{u}) \quad \text{and} \quad S(\ell)(\exp v) = V(\mathbf{v}).$$

Similarly, choosing $\ell = \mathbb{R}x^1 \oplus \cdots \oplus \mathbb{R}x^n$ and $\ell' = \mathbb{R}y_1 \oplus \cdots \oplus \mathbb{R}y_n$, we recover the momentum representation (with $\mathbf{P}, \mathbf{Q}$ replaced by $-\mathbf{P}, -\mathbf{Q}$).

Finally, we explain the invariant meaning of the $*_\hbar$ operation. Namely, consider the complex vector space $C_0(G, \chi_\hbar)$ of all continuous functions f on G with compact support satisfying

$$f(g \exp \alpha c) = e^{-i\hbar\alpha} f(g) \quad \text{for all} \quad g \in G,\ \alpha \in \mathbb{R}.$$

Let $B_\hbar = G/\Gamma_\hbar$, where $\Gamma_\hbar$ is discrete central subgroup in G,

$$\Gamma_\hbar = \{g = \exp(\tfrac{2\pi n}{\hbar} c) \in G \,|\, n \in \mathbb{Z}\},$$

and let db be the left-invariant Haar measure on $B_\hbar$,

$$db = d^{2n}\mathbf{v} \wedge d\alpha, \quad ,\alpha \in \mathbb{R}/\tfrac{2\pi}{\hbar}\mathbb{Z}.$$

The complex vector space $C_0(B_\hbar)$ of continuous functions on $B_\hbar$ with compact support has an algebra structure with respect to the convolution operation,

$$(\varphi_1 *_{B_\hbar} \varphi_2)(b) = \int_{B_\hbar} \varphi_1(b_1)\varphi_2(b_1^{-1}b)db_1 \quad \text{for} \quad \varphi_1, \varphi_2 \in C_0(B_\hbar).$$

The convolution operator also defines the algebra structure on the Banach space $L^1(B_\hbar, db)$, as well as on the space of distributions on $B_\hbar$ with compact support.

The natural inclusion $C_0(G, \chi_\hbar) \hookrightarrow C_0(B_\hbar)$ has the property that the image of $C_0(G, \chi_\hbar)$ is a subalgebra of $C_0(B_\hbar)$ under the convolution. From the other side, the isomorphism $\exp V \simeq V$ allows to identify the vector space $C_0(G, \chi_\hbar)$ with $C_0(V)$. We have

$$\begin{aligned}(\varphi_1 *_{B_\hbar} \varphi_2)(\exp v) &= \int_V \varphi_1(\exp u)\varphi_2(\exp(-u)\exp v)d^{2n}\mathbf{v}\\ &= \int_V \varphi_1(\exp u)\varphi_2(\exp(v-u)\exp(-\tfrac{1}{2}\omega(u,v)c))d^{2n}\mathbf{v}\\ &= \int_V \varphi_1(\exp u)\varphi_2(\exp(v-u))e^{\frac{i\hbar}{2}\omega(u,v)}d^{2n}\mathbf{v}.\end{aligned}$$

Under the correspondence $f(v) = \varphi(\exp v)$ we get

$$(\phi_1 *_{B_\hbar} \varphi_2)(\exp v) = (f_1 *_\hbar f_2)(v), \quad v \in V,$$

where $*_\hbar$ was introduced in the proof of Stone-von Neumann theorem. Thus the $*_\hbar$ operation from the Weyl transform is nothing but the convolution operator on $C_0(B_\hbar)$ restricted to $C_0(G, \chi_\hbar)$. Moreover, the Weyl transfrom is an injective homomorphism of the algebra $L^1(V, d^{2n}\mathbf{v})$ with the operation $*_\hbar$ into the algebra $\mathscr{L}(\mathscr{H})$ of bounded operators on the Hilbert space $\mathscr{H}$.

5. Quantization

Here we consider the quantization problem of classical system $(\mathscr{M}, \{\ ,\ \})$, outlined in the beginning of Section 2.

5.1. Weyl quantization. The quantization of the classical system with the phase space $\mathscr{M} = \mathbb{R}^{2n}$ and the canonical Poisson bracket associated with the symplectic form $\omega = d\mathbf{p} \wedge d\mathbf{q}$ can be described by the help of the Weyl transform. Namely, consider the linear mapping

$$\Phi : \mathscr{A} \to \mathscr{L}(\mathscr{H})$$

of the subalgebra of classical observables of rapid decay $\mathscr{A}_0 = \mathscr{S}(\mathbb{R}^{2n})$ into the algebra of bounded operators $\mathscr{L}(\mathscr{H})$ on the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^n)$, defined by

$$\mathscr{A} \ni f \mapsto W(\mathscr{F}^{-1}(f)) \in \mathscr{L}(\mathscr{H}),$$

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

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

Explicitly,

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

The linear mapping Φ is one-to-one. Its image and the inverse mapping are described by the following

LEMMA 5.1. *For every $f \in \mathscr{A}$ the operator $\Phi(f)$ is of trace class and*

$$\check{f}(\mathbf{u}, \mathbf{v}) = \hbar^n \operatorname{Tr}(\Phi(f)S(\mathbf{u}, \mathbf{v})^{-1}).$$

PROOF. First, the operator $\Phi(f)$ on $L^2(\mathbb{R}^n)$ in an integral operator: for every $\psi \in L^2(\mathbb{R}^n)$,

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

where

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

Since $K \in \mathscr{S}(\mathbb{R}^n \times \mathbb{R}^n) \subset L^2(\mathbb{R}^n \times \mathbb{R}^n)$, the operator $\Phi(f)$ is Hilbert-Schmidt.

To prove that $\Phi(f)$ is of trace class, we first consider the case $n = 1$. Let

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

be the Hamiltonian of the harmonic oscillator with $m = 1$ and $\omega = 1$. Operator H has a complete system of eigenfunctions

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

with the eigenvalues $\hbar(n + \frac{1}{2})$, $n = 0, 1, 2 \dots$. The inverse operator H^{-1} is Hilbert-Schmidt. Using integration by parts, it is easy to show that the operator $\Phi(f)H$ is an integral operator with the kernel

$$\frac{1}{2}\left(-\frac{\partial^2}{\partial q'^2} + q'^2\right) K(q, q'),$$

which is a Schwarz class function on $\mathbb{R}^2$. Thus the operator $\Phi(f)H$ is Hilbert-Schmidt, so that the operator

$$\Phi(f) = \Phi(f)HH^{-1}$$

is of the trace class. Since $\{\psi_n(q)\}_{n=0}^{\infty}$ is an orthonormal basis for $\mathscr{H} = L^2(\mathbb{R})$, we have

$$K(q, q') = \sum_{m,n=0}^{\infty} c_{mn}\psi_n(q)\overline{\psi_m(q')},$$

where

$$c_{mn} = \int_{\mathbb{R}^2} K(q, q')\overline{\psi_n(q)}\psi_m(q')dqdq',$$

and convergence is in the $L^2(\mathbb{R}^2)$-topology. Since $K \in \mathscr{S}(\mathbb{R}^2)$, this series is also convergent in the $\mathscr{S}(\mathbb{R}^2)$-topology. Setting $q' = q$, we get the expansion

$$K(q,q) = \sum_{m,n=0}^{\infty} c_{mn}\psi_n(q)\overline{\psi_m(q)},$$

convergent in the $\mathscr{S}(\mathbb{R})$-topology. This allows to interchange the order of the summation and the integration over q, and we obtain

$$\operatorname{Tr}\Phi(f) = \sum_{n=0}^{\infty}(\Phi(f)\psi_n,\psi_n) = \sum_{n=0}^{\infty} c_{nn} = \int_{-\infty}^{\infty} K(q,q)dq.$$

The general case $n > 1$ is similar: consider the operator

$$H = \frac{\mathbf{P}^2 + \mathbf{Q}^2}{2}$$

and use the fact that operators KH^n and H^{-n} are Hilbert-Schmidt. To prove the formula

$$\operatorname{Tr}\Phi(f) = \int\limits_{\mathbb{R}^n} K(\mathbf{q},\mathbf{q})d^n\mathbf{q},$$

expand the kernel K with respect to the orthonormal basis $\{\psi_{\mathbf{k}}(\mathbf{q})\psi_{\mathbf{k}'}(\mathbf{q}')\}_{\mathbf{k},\mathbf{k}'=0}^{\infty}$ for $L^2(\mathbb{R}^n \times \mathbb{R}^n)$, where

$$\psi_{\mathbf{k}}(\mathbf{q}) = \psi_{k_1}(q_1)\cdots\psi_{k_n}(q_n), \quad \mathbf{k} = (k_1,\dots,k_n).$$

Using the explicit form of the kernel K, we get

$$\operatorname{Tr}\Phi(f) = \frac{1}{(2\pi\hbar)^n}\int\limits_{\mathbb{R}^n}\int\limits_{\mathbb{R}^n}\check{f}(0,\mathbf{v})e^{-i\mathbf{v}\mathbf{q}}d^n\mathbf{v}d^n\mathbf{q} = \hbar^{-n}\check{f}(0,0).$$

Finally, using $S(\mathbf{u},\mathbf{v})^{-1} = S(\mathbf{u},\mathbf{v})^* = S(-\mathbf{u},-\mathbf{v})$ and the property

$$W(\check{f})S(-\mathbf{u},-\mathbf{v}) = W(\check{f}_{\mathbf{u},\mathbf{v}}),$$

where

$$\check{f}_{\mathbf{u},\mathbf{v}}(\mathbf{u}',\mathbf{v}') = \check{f}(\mathbf{u}+\mathbf{u}',\mathbf{v}+\mathbf{v}')e^{\frac{i\hbar}{2}(\mathbf{v}'\mathbf{u}-\mathbf{u}'\mathbf{v})},$$

we get the inversion formula. □

Corollary 5.1.

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

Remark. Formally, the operator $S(\mathbf{u},\mathbf{v})$ is an integral operator with the kernel

$$e^{\frac{i\hbar\mathbf{u}\mathbf{v}}{2} - i\mathbf{v}\mathbf{q}}\delta(\mathbf{q}-\mathbf{q}'-\hbar\mathbf{u})$$

(which could be properly understood by Schwarz kernel theorem), so that

$$\operatorname{Tr}S(\mathbf{u},\mathbf{v}) = \left(\frac{2\pi}{\hbar}\right)^n\delta(\mathbf{u})\delta(\mathbf{v}).$$

Thus (at a physical level of rigor)

$$\operatorname{Tr}\Phi(f)=\hbar^{-n}\int\limits_{\mathbb{R}^n}\check{f}(\mathbf{u},\mathbf{v})\delta(\mathbf{u})\delta(\mathbf{v})d^n\mathbf{u}d^n\mathbf{v}=\hbar^{-n}\check{f}(0,0).$$

The linear mapping $\Phi:\mathscr{A}_0\to\mathscr{L}(\mathscr{H})$ which assigns quantum observables to (rapidly decaying) classical observables, is called *Weyl quantization.* Clearly, it can be extended to the complex vector space of continuous functions which are inverse Fourier transforms of the L^1 functions on $\mathbb{R}^{2n}$. More generally, it follows from the explicit formula for the kernel K, that for $f\in\mathscr{S}(\mathbb{R}^{2n})'$ — the space of L. Schwarz (tempered) distributions on $\mathbb{R}^{2n}$, corresponding $K\in\mathscr{S}(\mathbb{R}^n\times\mathbb{R}^n)'$. Such kernels K correspond to linear operators from the Schwarz space $\mathscr{S}(\mathbb{R}^n)$ to the space of tempered distributions $\mathscr{S}(\mathbb{R}^n)'$. In particular, the constant function $f=1$ corresponds to the identity operator I. In many cases, as the examples below show, Schwarz kernels K correspond to an unbounded self-adjoint operators on $\mathscr{H}=L^2(\mathbb{R}^n)$.

EXAMPLE 5.1. Let $f=f(\mathbf{q})\in L^p(\mathbb{R}^n)$ for some $p\geq 1$, or f be a polynomially bounded function as $|\mathbf{q}|\to\infty$. Considered as a tempered distribution on $\mathbb{R}^{2n}$,

$$\check{f}(\mathbf{u},\mathbf{v})=(2\pi)^{n/2}\delta(\mathbf{u})\check{f}(\mathbf{v}),$$

so that

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

This is the Schwarz kernel of a multiplication by $f(\mathbf{q})$ operator on $L^2(\mathbb{R}^n)$. In particular, coordinates $\mathbf{q}$ in classical mechanics correspond to coordinate operators $\mathbf{Q}$ in quantum mechanics. Similarly, if $f=f(\mathbf{p})$ then $\Phi(f)=f(\mathbf{P})$. In particular, momenta $\mathbf{p}$ in classical mechanics correspond to the momenta operators $\mathbf{P}$ in quantum mechanics.

EXAMPLE 5.2. Let

$$h=\frac{\mathbf{p}^2}{2m}+v(\mathbf{q})$$

be the Hamiltonian function in classical mechanics. Then $H=\Phi(h)$ is the corresponding Hamiltonian operator in quantum mechanics,

$$H=\frac{\mathbf{P}^2}{2m}+v(\mathbf{Q})$$

REMARK. The Weyl quantization can be considered as a way of defining, for $f\in\mathscr{A}_0$, a function $f(\mathbf{Q},\mathbf{P})$ of non-commuting operators $\mathbf{P}=(P^1,\dots,P^n)$ and $\mathbf{Q}=(Q_1,\dots,Q_n)$ by setting

$$f(\mathbf{P},\mathbf{Q})=\Phi(f).$$

In particular, if $f(\mathbf{p},\mathbf{q})=g(\mathbf{p})+h(\mathbf{q})$, then

$$f(\mathbf{P},\mathbf{Q})=g(\mathbf{P})+h(\mathbf{Q}).$$

For $f(\mathbf{p},\mathbf{q})=\mathbf{pq}=p^1q_1+\dots+p^nq_n$, it is easy to compute

$$f(\mathbf{P},\mathbf{Q})=\frac{\mathbf{PQ}+\mathbf{QP}}{2},$$

so that Weil quantization gives a symmetrized form of the non-commuting factors $\mathbf{P}$ and $\mathbf{Q}$. In general, let f is a polynomial function,

$$f(\mathbf{p},\mathbf{q})=\sum_{|\alpha|,|\beta|\leq N}c_{\alpha\beta}\,\mathbf{p}^{\alpha}\mathbf{q}^{\beta},$$

where for the multi-indices $\alpha=(\alpha_1,\dots,\alpha_n)$ and $\beta=(\beta_1,\dots,\beta_n)$,

$$\mathbf{p}^{\alpha}=(p^1)^{\alpha_1}\dots(p^n)^{\alpha_n},\quad q^{\beta}=q_1^{\beta_1}\dots q_n^{\beta_n},$$

and $|\alpha|=\alpha_1+\dots+\alpha_n,\quad|\beta|=\beta_1+\dots+\beta_n$. Then

$$\Phi(f)=\sum_{|\alpha|,|\beta|\leq N}c_{\alpha\beta}\operatorname{Sym}(\mathbf{P}^{\alpha}\mathbf{Q}^{\beta}),$$

where the symmetric product $\operatorname{Sym}(\mathbf{P}^{\alpha}\mathbf{Q}^{\beta})$ is defined by

$$(\mathbf{uP}+\mathbf{vQ})^k=\sum_{|\alpha|+|\beta|=k}\frac{k!}{\alpha!\beta!}\mathbf{u}^{\alpha}\mathbf{v}^{\beta}\operatorname{Sym}(\mathbf{P}^{\alpha}\mathbf{Q}^{\beta}),$$

with $\mathbf{uP}+\mathbf{vQ}=u_1P^1+\dots+u_nP^n+v^1Q_1+\dots+v^nQ_n$ and

$$\alpha!=\alpha_1!\dots\alpha_n!,\quad\beta!=\beta_1!\dots\beta_n!.$$

As another example, consider the pure state P_ψ, where $\psi\in\mathscr{H}$, $\|\psi\|=1$ and find the classical observable f such that

$$\Phi(f)=P_\psi.$$

Since P_ψ is an integral operator with the kernel $\psi(\mathbf{q})\overline{\psi(\mathbf{q}')}$, we get

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

so that introducing $\mathbf{q}_+=\frac{\mathbf{q}+\mathbf{q}'}{2},\mathbf{q}_-=\frac{\mathbf{q}-\mathbf{q}'}{2}$, we get

$$\check{f}(\tfrac{2\mathbf{q}_-}{\hbar},\mathbf{v})=\hbar^n\int_{\mathbb{R}^n}\psi(\mathbf{q}_-+\mathbf{q}_+)\overline{\psi(\mathbf{q}_+-\mathbf{q}_-)}e^{i\mathbf{v}\mathbf{q}_+}d^n\mathbf{q}_+,$$

or

$$\check{f}(\mathbf{u},\mathbf{v})=\hbar^n\int_{\mathbb{R}^n}\psi(\mathbf{q}+\tfrac{\hbar\mathbf{u}}{2})\overline{\psi(\mathbf{q}-\tfrac{\hbar\mathbf{u}}{2})}e^{i\mathbf{v}\mathbf{q}}d^n\mathbf{q}.$$

Setting

$$\check{\rho}(\mathbf{u},\mathbf{v})=\lim_{\hbar\to0}\frac{1}{(2\pi\hbar)^n}\check{f}(\mathbf{u},\mathbf{v})=\frac{1}{(2\pi)^n}\int_{\mathbb{R}^n}|\psi(\mathbf{q})|^2e^{i\mathbf{v}\mathbf{q}}d^n\mathbf{v},$$

we see that in the classical limit $\hbar \to 0$ the pure state P_ψ in quantum mechanics corresponds to the mixed state in classical mechanics with the density

$$\rho(\mathbf{p}, \mathbf{q}) = \delta(\mathbf{p})|\psi(\mathbf{q})|^2.$$

Corresponding probability measure $d\mu = \rho(\mathbf{p}, \mathbf{q})d^n\mathbf{p}d^n\mathbf{q}$ describes the classical state of the particle at rest ($\mathbf{p} = 0$) with the coordinates distribution $|\psi(\mathbf{q})|^2 d^n\mathbf{q}$.

5.2. The $\star$-product. As in Section 4.2, the assignment $\mathscr{A}_0^{\mathbb{C}} \ni f \mapsto \Phi(f) \in \mathscr{L}(\mathscr{H})$ defines a new bilinear operation

$$\star_\hbar : \mathscr{A}_0^{\mathbb{C}} \times \mathscr{A}_0^{\mathbb{C}} \to \mathscr{A}_0^{\mathbb{C}}$$

by

$$f_1 \star_\hbar f_2 = \Phi^{-1}(\Phi(f_1)\Phi(f_2)),$$

or

$$f_1 \star_\hbar f_2 = \mathscr{F}\left(\mathscr{F}^{-1}(f_1) *_\hbar \mathscr{F}^{-1}(f_2)\right).$$

Explicitly, as it follows from the computation in Section 4.2,

$$(f_1 \star_\hbar f_2)(\mathbf{p}, \mathbf{q}) = \frac{1}{(2\pi)^{2n}} \int\limits_{\mathbb{R}^{2n}} \int\limits_{\mathbb{R}^{2n}} \check{f}_1(\mathbf{u}_1, \mathbf{v}_1)\check{f}_2(\mathbf{u}_2, \mathbf{v}_2)$$
$$e^{\frac{i\hbar}{2}(\mathbf{u}_1\mathbf{v}_2 - \mathbf{u}_2\mathbf{v}_1) - i(\mathbf{u}_1+\mathbf{u}_2)\mathbf{p} - i(\mathbf{v}_1+\mathbf{v}_2)\mathbf{q}} d^n\mathbf{u}_1 d^n\mathbf{u}_2 d^n\mathbf{v}_1 d^n\mathbf{v}_2. \tag{5.1}$$

The $\star_\hbar$-operation has the following properties.

1. Associativity

$$f_1 \star_\hbar (f_2 \star_\hbar f_3) = (f_1 \star_\hbar f_2) \star_\hbar f_3 \quad \text{for all} \quad f_1, f_2, f_3 \in \mathscr{A}_0.$$

2. Semi-classical limit

$$(f_1 \star_\hbar f_2)(\mathbf{p}, \mathbf{q}) = f_1(\mathbf{p}, \mathbf{q})f_2(\mathbf{p}, \mathbf{q}) - \frac{i\hbar}{2}\{f_1, f_2\}(\mathbf{p}, \mathbf{q}) + O(\hbar^2) \text{ as } \hbar \to 0.$$

3. Property of the unit

$$f \star_\hbar \mathbf{1} = \mathbf{1} \star_\hbar f \quad \text{for all} \quad f \in \mathscr{A}_0^{\mathbb{C}},$$

where $\mathbf{1}$ is the constant function equal to 1 on $\mathbb{R}^{2n}$.

4. The $\mathbb{C}$-linear mapping $\tau : \mathscr{A}_0^{\mathbb{C}} \to \mathbb{C}$, defined by

$$\tau(f) = \frac{1}{(2\pi\hbar)^n} \int\limits_{\mathbb{R}^{2n}} f(\mathbf{p}, \mathbf{q})d^n\mathbf{p}d^n\mathbf{q},$$

satisfies the cyclic trace property

$$\tau(f_1 \star_\hbar f_2) = \tau(f_2 \star_\hbar f_1) \quad \text{for all} \quad f_1, f_2 \in \mathscr{A}_0^{\mathbb{C}}.$$

These properties imply that the complex vector space $\mathscr{A}_1^{\mathbb{C}} = \mathscr{A}_0^{\mathbb{C}} \oplus \mathbb{C}\mathbf{1}$ with bilinear operation $\star_\hbar$ is an associative algebra over $\mathbb{C}$ with a unit $\mathbf{1}$ and the cyclic trace τ, satisfying the celebrated *correspondence principle*,

$$\lim_{\hbar\to 0} \frac{i}{\hbar}(f_1 \star_\hbar f_2 - f_2 \star_\hbar f_1) = \{f_1, f_2\} \quad \text{for all} \quad f_1, f_2 \in \mathscr{A}_0^{\mathbb{C}}.$$

The operation $\star_\hbar$ is called the $\star$*-product*.

Properties **1**, **3** and **4** immediately follow from the corresponding properties for the operator product. To prove property **2**, it is sufficient to expand

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

where the 0-term is uniform on compact subsets of $\mathbb{R}^{2n}$, and to use

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

Since $\check{f}_1, \check{f}_2 \in \mathscr{S}(\mathbb{R}^{2n})$, the estimate follows.

Next, consider the tensor product of Hilbert spaces,

$$L^2(\mathbb{R}^{2n}) \otimes L^2(\mathbb{R}^{2n}) \simeq L^2(\mathbb{R}^{2n} \times \mathbb{R}^{2n}),$$

and the unitary operator $\mathbf{U}_1$ on $L^2(\mathbb{R}^{2n}) \otimes L^2(\mathbb{R}^{2n})$, defined by

$$\mathbf{U}_1 = e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial\mathbf{p}}\otimes\frac{\partial}{\partial\mathbf{q}}\right)},$$

where

$$\frac{\partial}{\partial\mathbf{p}} \otimes \frac{\partial}{\partial\mathbf{q}} = \sum_{l=1}^{n} \frac{\partial}{\partial p^l} \otimes \frac{\partial}{\partial q_l}.$$

It follows from the theory of Fourier transform that for $f_1, f_2 \in \mathscr{S}(\mathbb{R}^{2n})$,

$$(\mathbf{U}_1(f_1 \otimes f_2))(\mathbf{p}_1,\mathbf{q}_1,\mathbf{p}_2,\mathbf{q}_2) = \frac{1}{(2\pi)^{2n}} \int\limits_{\mathbb{R}^{2n}}\int\limits_{\mathbb{R}^{2n}} \check{f}_1(\mathbf{u}_1,\mathbf{v}_1)\check{f}_2(\mathbf{u}_2,\mathbf{v}_2)$$
$$e^{\frac{i\hbar}{2}\mathbf{u}_1\mathbf{v}_2 - i\mathbf{u}_1\mathbf{p}_1 - i\mathbf{u}_2\mathbf{p}_2 - i\mathbf{v}_1\mathbf{q}_1 - i\mathbf{v}_2\mathbf{q}_2} d^n\mathbf{u}_1 d^n\mathbf{u}_2 d^n\mathbf{v}_1 d^n\mathbf{v}_2.$$

Similarly, introducing the unitary operator $\mathbf{U}_2$ on $L^2(\mathbb{R}^{2n}) \otimes L^2(\mathbb{R}^{2n})$,

$$\mathbf{U}_2 = e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial\mathbf{q}}\otimes\frac{\partial}{\partial\mathbf{p}}\right)},$$

we get

$$(\mathbf{U}_2(f_1 \otimes f_2))(\mathbf{p}_1,\mathbf{q}_1,\mathbf{p}_2,\mathbf{q}_2) = \frac{1}{(2\pi)^{2n}} \int\limits_{\mathbb{R}^{2n}}\int\limits_{\mathbb{R}^{2n}} \check{f}_1(\mathbf{u}_1,\mathbf{v}_1)\check{f}_2(\mathbf{u}_2,\mathbf{v}_2)$$
$$e^{\frac{i\hbar}{2}\mathbf{u}_2\mathbf{v}_1 - i\mathbf{u}_1\mathbf{p}_1 - i\mathbf{u}_2\mathbf{p}_2 - i\mathbf{v}_1\mathbf{q}_1 - \mathbf{v}_2\mathbf{q}_2} d^n\mathbf{u}_1 d^n\mathbf{u}_2 d^n\mathbf{v}_1 d^n\mathbf{v}_2.$$

Introducing the unitary operator $\mathbf{U}_\hbar$ on $L^2(\mathbb{R}^{2n}) \otimes L^2(\mathbb{R}^{2n})$,

$$\mathbf{U}_\hbar = \mathbf{U}_1\mathbf{U}_2^{-1} = e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial\mathbf{p}}\otimes\frac{\partial}{\partial\mathbf{q}} - \frac{\partial}{\partial\mathbf{q}}\otimes\frac{\partial}{\partial\mathbf{p}}\right)},$$

and defining the linear operator $m : \mathscr{A}_0^{\mathbb{C}} \otimes \mathscr{A}_0^{\mathbb{C}} \to \mathscr{A}_0^{\mathbb{C}}$ by[8]

$$(m(f_1 \otimes f_2))(\mathbf{p}, \mathbf{q}) = f_1(\mathbf{p}, \mathbf{q}) f_2(\mathbf{p}, \mathbf{q}),$$

we can rewrite the $\star$-product in the following succinct form:

$$f_1 \star_\hbar f_2 = (m \circ \mathbf{U}_\hbar)\,(f_1 \otimes f_2).$$

Now remembering that the canonical Poisson bracket on the phase space $\mathbb{R}^{2n}$ has the form

$$\{f_1, f_2\} = \frac{\partial f}{\partial \mathbf{p}} \frac{\partial g}{\partial \mathbf{q}} - \frac{\partial f}{\partial \mathbf{q}} \frac{\partial g}{\partial \mathbf{p}},$$

and introducing the notation

$$\{\ \overset{\otimes}{,}\ \} = \frac{\partial}{\partial \mathbf{p}} \otimes \frac{\partial}{\partial \mathbf{q}} - \frac{\partial}{\partial \mathbf{q}} \otimes \frac{\partial}{\partial \mathbf{p}} = \frac{\partial^2}{\partial \mathbf{p}_1 \partial \mathbf{q}_2} - \frac{\partial^2}{\partial \mathbf{q}_1 \partial \mathbf{p}_2},$$

we get for all $f_1, f_2 \in \mathscr{A}_0^{\mathbb{C}}$,

$$(f_1 \star_\hbar f_2)(\mathbf{p}, \mathbf{q}) = \left(e^{-\frac{i\hbar}{2}\{\ \overset{\otimes}{,}\ \}} f_1(\mathbf{p}_1, \mathbf{q}_1) f_2(\mathbf{p}_2, \mathbf{q}_2) \right) \Big|_{\substack{\mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p} \\ \mathbf{q}_1 = \mathbf{q}_2 = \mathbf{q}}} . \tag{5.2}$$

The formula (5.2) for the $\star$-product is equivalent to (5.1). Its has an advantage of formally expanding the exponential $e^{-\frac{i\hbar}{2}\{\ \overset{\otimes}{,}\ \}}$ to get an asymptotic expansion of the $\star$-product as $\hbar \to 0$. Namely, for $k \in \mathbb{N}$ define the bidifferential operators

$$B_k : \mathscr{S}(\mathbb{R}^{2n}) \otimes \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{S}(\mathbb{R}^{2n})$$

by $B_k = m \circ \{\ \overset{\otimes}{,}\ \}^k$ and set $B_0 = m$ — the point-wise multiplication of functions. Repeating the proof of property **2** and expanding the exponential function $e^{\frac{i\hbar}{2}(\mathbf{u}_1 \mathbf{v}_2 - \mathbf{u}_2 \mathbf{v}_1)}$ into Taylor series, we obtain the following result.

Lemma 5.2. *For every $f_1, f_2 \in \mathscr{A}_0^{\mathbb{C}}$, there is the asymptotic expansion*

$$(f_1 \star_\hbar f_2)(\mathbf{p}, \mathbf{q}) = \sum_{k=0}^{\infty} \frac{(-i\hbar)^k}{2^k k!} B_k(f_1, f_2)(\mathbf{p}, \mathbf{q}) + O(\hbar^\infty) \quad \textit{as} \quad \hbar \to 0,$$

i.e., for every $N \in \mathbb{N}$ the exists $C > 0$ (depending on $\mathbf{p}, \mathbf{q}$ and functions f_1, f_2) such that

$$\left| (f_1 \star_\hbar f_2)(\mathbf{p}, \mathbf{q}) - \sum_{k=0}^{N} \frac{(-i\hbar)^k}{2^k k!} B_k(f_1, f_2)(\mathbf{p}, \mathbf{q}) \right| \leq C \hbar^{N+1}.$$

[8]This is the definition of the point-wise product of functions as a restriction on the diagonal in the tensor product.

Finally, let us obtain another integral representation for the $\star$-product. Consider again formula (5.1) and apply Fourier inversion formula to the integral over $d^n\mathbf{u}_1 d^n\mathbf{v}_1$. We obtain

$$(f_1 \star_\hbar f_2)(\mathbf{p},\mathbf{q}) = \frac{1}{(2\pi)^n}\int\limits_{\mathbb{R}^{2n}} f_1(\mathbf{p}-\tfrac{\hbar}{2}\mathbf{v}_2, \mathbf{q}+\tfrac{\hbar}{2}\mathbf{u}_2)\check{f}_2(\mathbf{u}_2,\mathbf{v}_2)e^{-i\mathbf{u}_2\mathbf{p}-i\mathbf{v}_2\mathbf{q}}d^n\mathbf{u}_2 d^n\mathbf{v}_2$$
$$= \frac{1}{(2\pi)^{2n}}\int\limits_{\mathbb{R}^{2n}}\int\limits_{\mathbb{R}^{2n}} f_1(\mathbf{p}-\tfrac{\hbar}{2}\mathbf{v}_2, \mathbf{q}+\tfrac{\hbar}{2}\mathbf{u}_2)f_2(\mathbf{p}_2,\mathbf{q}_2)$$
$$e^{-i\mathbf{u}_2\mathbf{p}-i\mathbf{v}_2\mathbf{q}+i\mathbf{u}_2\mathbf{p}_2+i\mathbf{v}_2\mathbf{q}_2}d^n\mathbf{p}_2 d^n\mathbf{q}_2 d^n\mathbf{u}_2 d^n\mathbf{v}_2.$$

Introducing new variables

$$\mathbf{p}_1 = \mathbf{p} - \frac{\hbar}{2}\mathbf{v}_2, \quad \mathbf{q}_1 = \mathbf{q} + \frac{\hbar}{2}\mathbf{u}_2,$$

we obtain

$$(f_1 \star_\hbar f_2)(\mathbf{p},\mathbf{q}) = \frac{1}{(\pi\hbar)^{2n}}\int\limits_{\mathbb{R}^{2n}}\int\limits_{\mathbb{R}^{2n}} f_1(\mathbf{p}_1,\mathbf{q}_2)f_2(\mathbf{p}_2,\mathbf{q}_2)$$
$$e^{\frac{2i}{\hbar}(\mathbf{p}_1\mathbf{q}-\mathbf{p}\mathbf{q}_1+\mathbf{q}_1\mathbf{p}_2-\mathbf{q}_2\mathbf{p}_1+\mathbf{p}\mathbf{q}_2-\mathbf{p}_2\mathbf{q})}d^n\mathbf{p}_1 d^n\mathbf{q}_1 d^n\mathbf{p}_2 d^n\mathbf{q}_2.$$

Consider now Euclidean triangle $\triangle$ in the phase space $\mathbb{R}^{2n}$ (a 2-simplex) with the vertices $(\mathbf{p},\mathbf{q})$, $(\mathbf{p}_1,\mathbf{q}_1)$ and $(\mathbf{p}_2,\mathbf{q}_2)$. It is easy to see that

$$\mathbf{p}_1\mathbf{q}-\mathbf{p}\mathbf{q}_1+\mathbf{q}_1\mathbf{p}_2-\mathbf{q}_2\mathbf{p}_1+\mathbf{p}\mathbf{q}_2-\mathbf{p}_2\mathbf{q} = 2\int\limits_{\triangle}\omega,$$

which is twice the oriented area of a triangle for $n=1$. For $n>1$ this is twice the symplectic area of a triangle $\triangle$ — 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

$$(f_1 \star_\hbar f_2)(\mathbf{p},\mathbf{q}) = \frac{1}{(\pi\hbar)^{2n}}\int\limits_{\mathbb{R}^{2n}}\int\limits_{\mathbb{R}^{2n}} f_1(\mathbf{p}_1,\mathbf{q}_2)f_2(\mathbf{p}_2,\mathbf{q}_2)e^{\frac{4i}{\hbar}\int_{\triangle}\omega}$$
$$d^n\mathbf{p}_1 d^n\mathbf{q}_1 d^n\mathbf{p}_2 d^n\mathbf{q}_2.$$

5.3. Deformation quantization. We start with an elementary introduction to the deformation theory of algebras. Let $\mathcal{A}$ be a $\mathbb{C}$-algebra (or an associative algebra with unit over any field k of characteristic zero) with a multiplication map

$$m : \mathcal{A}\otimes_{\mathbb{C}}\mathcal{A}\to\mathcal{A}.$$

Here $\otimes_{\mathbb{C}}$ stands for a tensor product of vector spaces over $\mathbb{C}$. Let $\mathbb{C}[[t]]$ be a ring of formal power series in the variable t, i.e.,

$$\mathbb{C}[[t]] = \left\{\sum_{n=0}^{\infty} z_n t^n \mid z_n\in\mathbb{C}\right\},$$

and let

$$\mathcal{A}_t = \mathbb{C}[[t]] \otimes_{\mathbb{C}} \mathcal{A}$$

be the $\mathbb{C}[[t]]$-algebra of formal power series over $\mathcal{A}$ (formal power series in t with coefficients in $\mathcal{A}$). The multiplication in $\mathcal{A}_t$ is a $\mathbb{C}[[t]]$-linear extension of the multiplication m in $\mathcal{A}$, which we continue to denote by m. For $a, b \in \mathcal{A}$ (or in $\mathcal{A}_t$) we also denote $ab = m(a \otimes b)$. The algebra $\mathcal{A}_t$ is $\mathbb{Z}$-graded,

$$\mathcal{A}_t = \bigoplus_{n=0}^{\infty} A_n,$$

where $A_n = t^n \mathcal{A}$, so that $A_m A_m \subset A_{m+n}$.

Definition. A deformation of the $\mathbb{C}$-algebra $\mathcal{A}$ is a pair $(\mathcal{A}_t, m_t)$ with a $\mathbb{C}[[t]]$-linear map

$$m_t : \mathcal{A}_t \otimes_{\mathbb{C}} \mathcal{A}_t \to \mathcal{A}_t,$$

satisfying the associativity property

$$m_t \circ (m_t \otimes_{\mathbb{C}} \mathrm{id}) = m_t \circ (\mathrm{id} \otimes_{\mathbb{C}} m_t)$$

(as mappings from $\mathcal{A}_t \otimes_{\mathbb{C}} \mathcal{A}_t \otimes_{\mathbb{C}} \mathcal{A}_t$ into $\mathcal{A}_t$), and such that

$$m_t|_{\mathcal{A}\otimes_{\mathbb{C}}\mathcal{A}} = m + t\mu_1 + t^2\mu_2 + \dots,$$

where $\mu_n : \mathcal{A} \otimes_{\mathbb{C}} \mathcal{A} \to \mathcal{A}$ are $\mathbb{C}$-linear mappings, $n \geq 0$.

Definition. Two deformations m_t and m_t' of the $\mathbb{C}$-algebra $\mathcal{A}$ are equivalent, if there is a $\mathbb{C}[[t]]$-linear mapping $F_t : \mathcal{A}_t \to \mathcal{A}_t$ of the form

$$F_t|_{\mathcal{A}} = \mathrm{id} + tf_1 + t^2 f_2 + \dots,$$

where $f_n : \mathcal{A} \to \mathcal{A}$ are $\mathbb{C}$-linear mappings, such that

$$F_t \circ m_t' = m_t \circ (F_t \otimes_{\mathbb{C}} F_t).$$

The mapping F_t with the property $f_0 = \mathrm{id}$ is a $\mathbb{C}[[t]]$-modules isomorphism, so that the equivalence of deformations is an equivalence relation.

The $\mathbb{C}$-linear mappings μ_n should satisfy infinitely many relations obtained by the expanding the associativity condition

$$m_t(a, m_t(b, c)) = m_t(m_t(a, b), c) \quad \text{for all} \quad a, b, c \in \mathcal{A}$$

into the formal power series in t. The first two of them, arising from comparing the coefficients at powers t and t^2, are

$$\mu_1(a, bc) + a\mu_1(b, c) = \mu_1(ab, c) + \mu_1(a, b)c$$

$$\mu_2(a, bc) + a\mu_2(b, c) + \mu_1(a, \mu_1(b, c)) = \mu_2(ab, c) + \mu_2(a, b)c + \mu_1(\mu_1(a, b), c),$$

and in general

$$\begin{aligned} &a\mu_n(b, c) - \mu_n(ab, c) + \mu_n(a, bc) - \mu_n(a, b)c \\ &= \sum_{j=1}^{n-1} \left(\mu_j(\mu_{n-j}(a, b), c) - \mu_j(a, \mu_{n-j}(b, c))\right). \end{aligned}$$

For the proper algebraic interpretation of these equations one needs to introduce the notion of *Hochschild cohomology.*

Let M be $\mathcal{A}$-bimodule, i.e., M is left and right module with respect to the $\mathbb{C}$-algebra $\mathcal{A}$.

DEFINITION. Hochschild cochain complex $(\mathsf{C}^\bullet(\mathcal{A}, M), d)$ of a $\mathbb{C}$-algebra $\mathcal{A}$ with coefficients in $\mathcal{A}$-bimodule M is defined by the cochains $\mathsf{C}^n(\mathcal{A}, M) = \operatorname{Hom}_{\mathbb{C}}(\mathcal{A}^{\otimes^n}, M)$ and the differential $d_n : \mathsf{C}^n(\mathcal{A}, M) \to \mathsf{C}^{n+1}(\mathcal{A}, M)$,

$$(d_n f)(a_1, a_2, \dots, a_{n+1}) = a_1 f(a_2, \dots, a_{n+1}) + \sum_{j=1}^{n} (-1)^j f(a_1, \dots, a_j a_{j+1}, \dots, a_{n+1}$$
$$+ (-1)^{n+1} f(a_1, \dots, a_n) a_{n+1}.$$

It is clear that $d^2 = 0$, i.e., $d_{n+1} \circ d_n = 0$. The cohomology of the Hochschild complex $(\mathsf{C}^\bullet(\mathcal{A}, M), d)$ is called Hochschild cohomology and is denoted by $H^\bullet(\mathcal{A}, M)$,

$$H^n(\mathcal{A}, M) = \ker d_n / \operatorname{Im} d_{n-1}.$$

The simplest non-trivial example of $\mathcal{A}$-bimodule is $M = \mathcal{A}$ with the left and right actions of $\mathcal{A}$. It follows from the associativity equations that $\mu_1 \in \mathsf{C}^2(\mathcal{A}, \mathcal{A})$ is a Hochschild 2-cocycle, $d_2\mu_1 = 0$, and

$$(d_2\mu_n)(a, b, c) = \sum_{j=1}^{n-1} \left(\mu_j(\mu_{n-j}(a, b), c) - \mu_j(a, \mu_{n-j}(b, c))\right).$$

It turns out that the right-hand side of this equation defines another operation on Hochschild cochains for the case $M = \mathcal{A}$. Namely, for $f \in \mathsf{C}^m(\mathcal{A}, \mathcal{A}), g \in \mathsf{C}^n(\mathcal{A}, \mathcal{A})$ set

$$(f \circ g)(a_1, \dots, a_{m+n-1})$$
$$= \sum_{j=0}^{m-1} (-1)^j f(a_1, \dots, a_j, g(a_{j+1}, \dots, a_{j+n}), a_{j+n+1}, \dots, a_{m+n-1}),$$

and define

$$[f, g]_G = f \circ g - (-1)^{(m+1)(n+1)} g \circ f.$$

The linear mapping $[\ ,\ ]_G : \mathsf{C}^m(\mathcal{A}, \mathcal{A}) \times \mathsf{C}^n(\mathcal{A}, \mathcal{A}) \to \mathbb{C}^{m+n-1}(\mathcal{A}, \mathcal{A})$ is called the *Gershtenhaber bracket* and it defines the structure of a *graded Lie differential Lie algebra* on $\mathsf{C}^\bullet(\mathcal{A}.\mathcal{A})$. In terms of Gershtenhaber bracket, the associativity condition can be written succinctly as

$$dm_t = \tfrac{1}{2}[m_t - m, m_t - m]_G.$$

This gives the way of solving this equation. Suppose we already solved it mod t^n, starting with the case $n = 1$. Then it can be shown that the right-hand side mod t^{n+1} is always a Hochschild 2-cocycle and we need to ensure that it is zero in Hochschild cohomology.

Now we will concentrate on the case when the $\mathbb{C}$-algebra $\mathcal{A}$ is commutative, and let $\mathcal{A}_t$ be a deformation of $\mathcal{A}$. Define $\{\ ,\ \} : \mathcal{A} \times \mathcal{A} \to \mathcal{A}$ by

$$\{a, b\} = \mu_1(a, b) - \mu_1(b, a), \quad a, b \in \mathcal{A}.$$

LEMMA 5.3. *Any deformation $\mathcal{A}_t$ of a commutative $\mathbb{C}$-algebra $\mathcal{A}$ equippes $\mathcal{A}$ with the structure of a Poisson algebra with the Poisson bracket $\{\ ,\ \}$.*

PROOF. First, consider the equation $d\mu_1(a, b, c) = 0$. Subtracting from it the equation with a and c interchanged and using the commutativity of the product in $\mathcal{A}$, we get the following equation for the 2-cochain $\{\ ,\ \}$:

$$\{ab, c\} - \{a, bc\} = a\{b, c\} - c\{a, b\}.$$

Interchanging b and c, we get

$$\{ac, b\} - \{a, bc\} = a\{c, b\} - b\{a, c\},$$

and interchanging a and c in this equation we obtain

$$\{ac, b\} - \{c, ab\} = c\{a, b\} - b\{c, a\}.$$

Now adding the first and third equations and subtracting the second equation we obtain

$$\{ab, c\} = a\{a, c\} + b\{a, c\},$$

so that skew-symmetric 2-cochain $\{\ ,\ \}$ satisfies the Leibniz rule. To prove the Jacobi identity, observe that

$$\{a, b\} = \frac{a \star_t b - b \star_t a}{t} \bmod t,$$

where we have set $m_t(a, b) = a \star_t b$. Using that the product $\star_t$ is associative modulo t^2 (which is expressed by the equation $d\mu_2 = \frac{1}{2}[\mu_1, \mu_1]_G$), we get

$$\begin{gathered}\{\{a, b\}, c\} + \{\{c, a\}, b\} + \{\{b, c\}, a\} = \frac{1}{t^2}\Big((a \star_t b - b \star_t a) \star_t c \\ -c \star_t (a \star_t b - b \star_t a) + (c \star_t a - a \star_t c) \star_t b - b \star_t (c \star_t a - a \star_t c) \\ +(b \star_t c - c \star_t b) \star_t a - a \star_t (b \star_t c - c \star_t b)\Big) \bmod t = 0.\end{gathered}$$

$\square$

This result motivates the following

DEFINITION. A deformation of the Poisson algebra $(\mathcal{A}, \{\ ,\ \})$ with the commutative product $m : \mathcal{A} \otimes \mathcal{A} \to \mathcal{A}$, $m(a \otimes b = ab$, is an associate algebra $\mathcal{A}_t$ over $\mathbb{C}[[t]]$ with the $\mathbb{C}[[t]]$-linear product $m_t : \mathcal{A}_t \otimes \mathcal{A}_t \to \mathcal{A}_t$, $m_t(a \otimes b) = a \star_t b$, such that for all $a, b \in \mathcal{A}$

1.

$$a \star_t b = ab \bmod t\mathcal{A}_t$$

2.

$$\frac{a \star_t b - b \star_t a}{t} = \{a, b\} \bmod t\mathcal{A}_t$$

3.

$$a \star_t 1 = 1 \star_t a = a.$$

The Weyl quantization provides the example of a deformation of the Poisson algebra of classical observables on the phase space $\mathscr{M} = \mathbb{R}^{2n}$ with the canonical Poisson bracket. The algebraic nature of the Weyl quantization is revealed by the following

THEOREM 5.1 (Universal deformation). *Let $\mathcal{A}$ be a commutative $\mathbb{C}$-algebra and let $\varphi_1, \varphi_2 \in \operatorname{Hom}_{\mathbb{C}}(\mathcal{A}, \mathcal{A})$ be two commuting derivations of $\mathcal{A}$, i.e., φ_1, φ_2 satisfy Leibniz rule and*

$$\varphi_1 \circ \varphi_2 = \varphi_2 \circ \varphi_1.$$

The $\{a, b\} = \varphi_1(a)\varphi_2(b) - \varphi_2(a)\varphi_1(b)$, $a, b \in \mathcal{A}$, is a Poisson bracket and the deformation of the Poisson algebra $(\mathcal{A}, \{\ ,\ \})$ is given by the universal deformation formula

$$m_t = m \circ e^{t\varphi_1 \otimes \varphi_2}.$$

PROOF. It is sufficient to verify the associativity of the product m_t, since the properties **1-3** are obvious. Let $\Phi = \varphi_1 \otimes \varphi_2 : \mathcal{A} \otimes \mathcal{A} \to \mathcal{A}$ and let $\Delta : \mathcal{A} \to \mathcal{A} \otimes \mathcal{A}$ be the coproduct map,

$$\Delta(a) = a \otimes 1 + 1 \otimes a, \quad a \in \mathcal{A}.$$

The coproduct map extends to a $\mathbb{C}$-linear mapping from $\operatorname{Hom}_{\mathbb{C}}(\mathcal{A}, \mathcal{A})$ to $\operatorname{Hom}_{\mathbb{C}}(\mathcal{A}^{\otimes^2}, \mathcal{A}^{\otimes^2})$, which we continue to denote by Δ,

$$\Delta(\varphi) = \varphi \otimes \mathrm{id} + \mathrm{id} \otimes \varphi, \quad \varphi \in \operatorname{Hom}_{\mathbb{C}}(\mathcal{A}, \mathcal{A}).$$

For $a, b \in \mathcal{A}$ set $a \star_t b = m_t(a \otimes b)$. It is sufficient to verify that for all $a, b, c \in \mathcal{A}$,

$$a \star_t (b \star_t c) = (a \star_t b) \star_t c. \tag{5.3}$$

It follows from Leibniz rule that a derivation φ of $\mathcal{A}$ satisfies the following identity in $\mathcal{A}_t$,

$$e^{t\varphi}(ab) = m\left(e^{t\varphi}(a \otimes b)\right).$$

Thus we obtain,

$$\begin{aligned}
a \star_t (b \star_t c) &= m(e^{t\Phi}(a \otimes m(e^{t\Phi}(b \otimes c)))) \\
&= (m \circ (\mathrm{id} \otimes m))(e^{t(\mathrm{id} \otimes \Delta)(\Phi)} e^{t\, \mathrm{id} \otimes \Phi}(a \otimes b \otimes c)) \\
&= (m \circ (\mathrm{id} \otimes m))(e^{t(\mathrm{id} \otimes \Delta)(\Phi) + t\, \mathrm{id} \otimes \Phi}(a \otimes b \otimes c)),
\end{aligned}$$

where we have also used commutativity of φ_1 and φ_2. Similarly,

$$(a \star_t b) \star_t c = (m \circ (m \otimes \mathrm{id}))(e^{t(\Delta \otimes \mathrm{id})(\Phi) + t\Phi \otimes \mathrm{id}}(a \otimes b \otimes c)).$$

Since $m \circ (\mathrm{id} \otimes m) = m \circ (m \otimes \mathrm{id})$ due to the associativity of the product m, it is sufficient to prove that

$$\Delta \otimes \mathrm{id})(\Phi) + \Phi \otimes \mathrm{id} = id \otimes \Delta)(\Phi) + \mathrm{id} \otimes \Phi,$$

which reduces to the identity

$$(\varphi_1 \otimes \mathrm{id} + \mathrm{id} \otimes \varphi_1) \otimes \varphi_2 + \varphi_1 \otimes \varphi_2 \otimes \mathrm{id} = \varphi_1 \otimes (\varphi_2 \otimes \mathrm{id} + \mathrm{id} \otimes \varphi_2) + \mathrm{id} \otimes \varphi_1 \otimes \varphi_2.$$

$\square$

CHAPTER 3

Schrödinger Equation

To be completed during the semester.

1. General properties

The Schrödinger operator is defined the formal differential expression

$$H = -\Delta + v(\mathbf{q}).$$

Here we present general conditions on the potential $v(\mathbf{q})$ guaranteeing that has a unique extension to a self-adjoint operator on the Hilbert state $\mathscr{H} = L^2(\mathbb{R}^n)$, i.e., when H is essentially self-adjoint. In this case we, slightly abusing notations, will continue to denote the closure by H. We know that self-adjointness is a fundamental property of quantum observables. Uniqueness of the self-adjoint extension is also fundamental: there are no physical principles distinguishing between different extentions (which exist if the defect indices of H are equal and non-zero). We also will present different criteria for the absence of the singular spectrum of H, for the spectrum to be purely discrete and other possibilities.

1.1. Self-adjointness. First we consider the case when v is a real-valued measurable locally bounded function on $\mathbb{R}^n$, i.e., $v \in L^\infty_{loc}(\mathbb{R}^n, \mathbb{R})$. The operator H defined by the formal differential expression, is symmetric on $C_0^\infty(\mathbb{R}^n) \subset \mathscr{H}$, and we are interested in sufficient conditions for H being essentially self-adjoint. The simplest one is stated as follows.

Theorem 1.1. *If $v(\mathbf{q})$ is bounded from below, $v(\mathbf{q}) \geq C$ for almost all $\mathbf{q} \in \mathbb{R}^n$, then H is essentially self-adjoint on $\mathscr{H}$.*

In fact, a much more general statement holds.

Theorem 1.2 (Sears). *Suppose that the potential $v(\mathbf{q})$ for all $\mathbf{q} \in \mathbb{R}^n$ satisfies the condition*

$$v(\mathbf{q}) \geq -Q(|\mathbf{q}|),$$

where $Q(r)$ is an increasing continuous positive function on $\mathbb{R}_{\geq 0}$ such that

$$\int_0^\infty \frac{dr}{\sqrt{Q(r)}} = \infty.$$

Then H is essentially self-adjoint on $\mathscr{H}$.

1.2. Discreteness of the spectrum. The simplest result is the following statement.

THEOREM 1.3. *Suppose that*

$$\lim_{|\mathbf{q}|\to\infty} v(\mathbf{q}) = \infty.$$

Then operator H has a point spectrum, i.e., there exists an orthonormal basis $\{\psi_n\}_{n\in\mathbb{N}}$ for $\mathscr{H}$ consisting of eigenfunctions of H,

$$H\psi_n = E_n\psi_n,\ n \in \mathbb{N}.$$

2. One-dimensional Schrödinger equation

3. Angular momentum and SO(3)

4. Two-body problem

5. Hydrogen atom and S0(4)

6. Semi-classical asymptotics

CHAPTER 4

Path Integral Formulation of Quantum Mechanics

1. Feynman path integral for the evolution operator

Here we develop another approach toward Schrödinger equation

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

(see Chapter 2, Section 1.4). Namely every solution of the initial value problem

$$\psi(t)|_{t=0} = \psi$$

for the Schrödinger equation (assuming $\psi \in D(H)$) can be written in terms of the evolution operator $U(t) = e^{-\frac{i}{\hbar}tH}$ as $\psi(t) = U(t)\psi$. Choosing coordinate representation (see Chapter 2, Section 2.1.2) and assuming that $U(t)$ is an integral operator with the kernel $K(\mathbf{q}, \mathbf{q}', t)$, we can write

$$\psi(\mathbf{q}', t') = \int_{\mathbb{R}^n} K(\mathbf{q}', t'; \mathbf{q}, t)\psi(\mathbf{q}, t)d^n\mathbf{q},$$

where $K(\mathbf{q}', t'; \mathbf{q}, t) = K(\mathbf{q}', \mathbf{q}, T)$ and we have set $T = t' - t$. The function $|K(\mathbf{q}', t' \,|\, \mathbf{q}, t)|^2$ has a physical meaning of the conditional probability distribution of finding quantum mechanical particle at $\mathbf{q}' \in \mathbb{R}^n$ at time t' provided the particle was at $\mathbf{q} \in \mathbb{R}^n$ at time t. Our goal is to give a representation for the propagator.

Of course, when the spectral decomposition of the Hamiltonian operator is known, the propagator can be obtained in a closed form. Suppose, for simplicity, that H has a pure discrete spectrum, i.e., there is an orthonormal basis of the Hilbert space $\mathscr{H} \simeq L^2(\mathbb{R}^n, d^n\mathbf{q})$ consisting of the eigenfunctions $\{\psi_n(\mathbf{q})\}_{n\in\mathbb{N}}$ of H with the eigenvalues E_n. Then for

$$\psi(\mathbf{q}) = \sum_{n=1}^{\infty} c_n\psi_n(\mathbf{q})$$

we have

$$(U(T)\psi)(\mathbf{q}) = \sum_{n=1}^{\infty} e^{-\frac{i}{\hbar}E_nT}c_n\psi_n(\mathbf{q}).$$

Thus

$$\psi(\mathbf{q}', t) = \sum_{n=1}^{\infty} e^{-\frac{i}{\hbar}E_nT}\psi_n(\mathbf{q}')\int\limits_{\mathbb{R}^n}\overline{\psi_n(\mathbf{q})}\psi(\mathbf{q})d^n\mathbf{q},$$

where all the series converge in L^2 sense. If the change of orders of summation and integration was justified, we could write

$$K(\mathbf{q}',t;\mathbf{q},t)=\sum_{n=1}^{\infty}e^{-\frac{i}{\hbar}E_nT}\psi_n(\mathbf{q}')\overline{\psi_n(\mathbf{q})}. \tag{1.1}$$

This is what happen in many cases and the series (1.1) converges in the distributional sense, thus providing a representation for the propogator in terms of the spectral decomposition of H. Similar representation exists when Hamiltonian H has continuous spectrum. In general, the integral kernel $K(\mathbf{q},\mathbf{q}',t)$ of the evolution operator is the *fundamental solution* of the Schrödinger equation, considered as a partial differential equation. Namely, when

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

then in coordinate representation $K(\mathbf{q},\mathbf{q}',t)$ satisfies the Schrödinger equation

$$i\hbar\frac{\partial K}{\partial t}=-\frac{\hbar^2}{2m}\Delta\,K+v(\mathbf{q})K \tag{1.2}$$

with the initial condition

$$K(\mathbf{q},\mathbf{q}',t)\big|_{t=0}=\delta(\mathbf{q}-\mathbf{q}'), \tag{1.3}$$

where

$$\Delta=\sum_{i=1}^{n}\frac{\partial^2}{\partial q_i^2}$$

is the classical Laplace operator (minus of the Laplace operator of the Euclidean metric on $\mathbb{R}^n$).

It is remarkable that one can get another representation for the propagator in terms of the corresponding classical system. We start with the case $n=1$ and consider

$$H=\frac{P^2}{2m}+v(Q)=-\frac{\hbar^2}{2m}\frac{d^2}{dq^2}+v(q).$$

1.1. Free particle. It is easy to give an explicit representation for the propagator of the free particle. Namely, using explicit representation for the solution of the Schrödinger equation we get

$$\psi(q',t')=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}\left(q'p-\frac{p^2}{2m}t'\right)}\hat{\psi}(p,t)dp=\int_{-\infty}^{\infty}K(q',t';q,t)\psi(q,t)dq,$$

where

$$K(q',t';q,t)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}\left(p(q'-q)-\frac{p^2}{2m}T\right)}dp. \tag{1.4}$$

Using the Gaussian integral

$$\int_{-\infty}^{\infty} e^{-iax^2} dx = e^{-\frac{\pi i}{4}} \sqrt{\frac{\pi}{a}}, \quad a > 0,$$

(understood as analytic continuation in the distributional sense, or, which is equivalent, as $\lim_{R\infty} \int_{|q|\leq R}$), we obtain

$$K(q', t'; q, t) = \sqrt{\frac{m}{2\pi i\hbar T}}\, e^{\frac{im(q-q')^2}{2\hbar T}}. \tag{1.5}$$

Thus the propagator for the free quantum mechanical particle on $\mathbb{R}$ is obtained from the heat kernel on $\mathbb{R}$ (with respect to Euclidean metric) by analytic continuation $T \mapsto iT$ to "imaginary time".

1.2. Path integral in the phase space. No such simple formula exists for a propagator of the quantum particle in a potential $v(q)$. Indeed, $H = A+B$, where the operators $A = \dfrac{P^2}{2m}$ and $B = v(Q)$ no longer commute, so that $e^{i(A+B)} \neq a^{iA}e^{iB}$. However, there is a way of expressing the exponential $e^{i(A+B)}$ in terms of the individual exponentials e^{iA} and e^{iB}, given by the Trotter product formula.

THEOREM 1.1 (The Trotter product formula). *Let A and B be self-adjoint operators on $\mathscr{H}$ such that $A+B$ is essentially self-adjoint on $D(A)\cap D(B)$. Then for $\psi \in \mathscr{H}$,*

$$e^{i(A+B)}\psi = \lim_{n\to\infty} (e^{iA/n}e^{iB/n})^n\psi.$$

PROOF. When $A, B \in \mathscr{B}(\mathscr{H})$, this is the classical theorem of S. Lie. Namely, set $C_n = e^{i(A+B)/n}$ and $D_n = e^{iA/n}e^{iB/n}$. Then

$$C_n^n - D_n^n = \sum_{k=0}^{n-1} C_n^{n-k-1}(C_n - D_n)D_n^k.$$

Since $\|C_n - D_n\| \leq \dfrac{c}{n^2}$ for some constant $c > 0$, we have

$$\|C_n^n - D_n^n\| \leq \frac{c}{n},$$

and the result follows (with the convergence in the uniform topology). For the proof of the general case, see Reed and Simon, v. 1. $\square$

Using the Trotter formula, we have (in the strong operator topology)

$$e^{-\frac{i}{\hbar}TH} = \lim_{n\to\infty} \left(e^{-\frac{i\Delta t}{\hbar}A}\, e^{-\frac{i\Delta t}{\hbar}B}\right)^n, \quad \Delta t = \frac{T}{n} = \frac{t'-t}{n}.$$

In the Schrödinger representation the operator $e^{-\frac{i\Delta t}{\hbar}B}$ is a multiplication by $e^{-\frac{i}{\hbar}v(q)\Delta t}$ operator, and the integral kernel of the operator $e^{-\frac{i\Delta t}{\hbar}A}$ is given by (1.4), where T is replaced by Δt. Thus the integral kernel of the operator $e^{-\frac{i\Delta t}{\hbar}A}e^{-\frac{i\Delta t}{\hbar}B}$ is given by

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\left(p(q'-q)-\left(\frac{p^2}{2m}+v(q)\right)\Delta t\right)}dp. \tag{1.6}$$

As the result, we obtain the representation of the propagator of quantum mechanical particle as the limit of multiple integrals,

(1.7)

$$K(q',t';q,t)=\lim_{n\to\infty}\underset{\mathbb{R}^{2n-1}}{\int\cdots\int}\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{n-1}(p_k(q_{k+1}-q_k)-h(p_k,q_k)\Delta t)\right\}$$
$$\frac{dp_0}{2\pi\hbar}\prod_{k=1}^{n-1}\left(\frac{dp_k dq_k}{2\pi\hbar}\right).$$

Here $h(p,q)=\dfrac{p^2}{2m}+v(q)$ is the corresponding classical Hamiltonian function, and $q_0=q$, $q_n=q'$.

This formula admits a remarkable interpretation which which exhibits the deep relation between quantum and classical mechanics. Namely, 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 curve $\sigma:[t,t']\to\mathbb{R}^2\times\mathbb{R}$ by $\sigma(\tau)=(p(\tau),q(\tau),\tau)$, $\tau\in[t,t']$, defined by dividing interval $[t,t']$ into n subintervals $[t_k,t_{k+1}]$ of length Δt, and setting

$$p(\tau)=p_k,\quad q(\tau)=q_k+(\tau-t_k)\frac{q_{k+1}-q_k}{t_{k+1}-t_k},$$

for $\tau\in[t_k,t_{k+1}]$, where $t_0=t_1$ and $t_n=t'$. Then (provided that $v(q)$ is Riemann integrable) we have

$$\sum_{k=0}^{n-1}(p_k(q_{k+1}-q_k)-h(p_k,q_k)\Delta t)=A(\sigma)+o(1)$$

as $n\to\infty$, where $S(\sigma)=\displaystyle\int_\sigma(pdq-hdt)$ is the action functional of the classical system with the Hamiltonian function $h(p,q)$ (see Chapter 1, Section 1.5). Following Feynman, we rewrite representation (1.7) in the following form:

$$K(q',t';q,t)=\int_{\boldsymbol{\Omega}_{q,t}^{q',t'}} e^{\frac{i}{\hbar}S(\sigma)}\mathscr{D}p\mathscr{D}q. \tag{1.8}$$

Here $\boldsymbol{\Omega}_{q,t}^{q',t'}=\Omega(T^*\mathbb{R}\times\mathbb{R},q,t,q',t')$ is the space of all admissible paths in extended phase space $T^*\mathbb{R}\times\mathbb{R}$ connecting points (q,t) and (q',t') (see Chapter 1, Section 1.5), and $\mathscr{D}p\mathscr{D}q$ "symbolizes" the "measure" on the path space of $\mathbf{\Omega}_{q,t}^{q',t'}$, naively defined as

$$\mathscr{D}p\mathscr{D}q = \lim_{n\to\infty} \frac{dp_0}{2\pi\hbar} \prod_{k=1}^{n-1} \left(\frac{dp_k dq_k}{2\pi\hbar} \right),$$

by "approximating by piece-wise linear paths" introduced above.

Of course, correct mathematical meaning of formula (1.8) is just (1.7). Still, the form (1.8), called *Feynman path integral in the phase space* provides a profound interpretation of the quantum mechanical propagator $K(q', t', q, t)$ as an "average" of the exponential of $\frac{i}{\hbar} \times$ classical action functional over all admissible paths in the extented phase space connecting (q, t) and (q', t').

Of course, "integrating" over smooth paths is rather naive; in cases when we make a precise meaning of Feynman path integral (when the time difference $T = t' - t$ has a non-zero positive imaginary part) the corresponding measure will be supported on the set of nowhere differentiable paths.

1.3. Path integral in the configuration space. We can remove the integration over p in (1.6) by using Gaussian integral (1.5). The resulting expression

$$K(q', t'; q, t) = \lim_{n\to\infty} \left(\frac{m}{2\pi\hbar i \Delta t} \right)^{n/2} \underset{\mathbb{R}^{n-1}}{\int \cdots \int} \exp\left\{ \frac{i}{\hbar} \sum_{k=0}^{n-1} \left(\frac{m}{2} \left(\frac{q_{k+1} - q_k}{\Delta t} \right)^2 - v(q_k)\Delta t \right) \right\} \prod_{k=1}^{n-1} dq_k \tag{1.9}$$

admits the following interpretation as *Feynman path integral in the configuration space*. Suppose that there exists a smooth path $\gamma : [t, t'] \to M$ such that $\gamma(t) = q, \gamma(t') = q'$ and $\gamma(t_k) = q_k$ for remaining $k = 1, \ldots, n-1$. Then

$$\sum_{k=0}^{n-1} \left(\frac{m}{2} \left(\frac{q_{k+1} - q_k}{\Delta t} \right)^2 - v(q_k)\Delta t \right) = \int_t^{t'} L(\gamma'(\tau))d\tau + o(1),$$

where $L(q, \dot{q}) = \dfrac{m\dot{q}^2}{2} - v(q)$ is the Lagrangian of the corresponding classical system. Thus as before, we can interpret (1.9) as

$$K(q', t'; q, t) = \int\limits_{\substack{q(t')=q' \\ q(t)=q}} e^{\frac{i}{\hbar}\int_t^{t'} L(q,\dot{q})d\tau} \mathscr{D}q, \tag{1.10}$$

where now the "integration" goes over the space of paths $\Omega(\mathbb{R}, q, t; q', t')$ in the configuration space $\mathbb{R}$ connecting points q and q' (see Chapter 1, Section 1.2), and $\mathscr{D}q$ "symbolizes" the "measure" on the path space, naively defined as

$$\mathscr{D}q = \lim_{n\to\infty} \left(\frac{m}{2\pi\hbar i \Delta t} \right)^{n/2} \prod_{k=1}^{n-1} dq_k$$

by "approximating by piece-wise linear paths". Again, correct mathematical meaning of (1.10) is given by (1.9).

Heuristically, the Feynman path integral (1.10) in the configuration space is obtained from the Feynman path integral (1.8) in the phase space by "evaluating the Gaussian integral over $\mathscr{D}p$":

$$\int\limits_{\substack{q(t')=q'\\ q(t)=q}} \exp\left\{\frac{i}{\hbar}\int_t^{t'}\left(\frac{m\dot{q}^2}{2}-v(q)\right)d\tau\right\}\mathscr{D}q$$

$$=\int\limits_{\boldsymbol{\Omega}(q,t;q',t')} \exp\left\{\frac{i}{\hbar}\int_t^{t'}(p\dot{q}-h(p,q))d\tau\right\}\mathscr{D}p\mathscr{D}q.$$

1.4. Harmonic oscillator. By definition, Feynman path integral is a limit of multiple integrals with the number of integrations tending to infinity, so it does not seem to be very practical. However, Feynman integrals play a profound role in formulation of quantum mechanics and can be computed exactly in several cases.

Obviously, Feynman path integral for free particle gives the same answer (1.5) for the propogator. This is because in this case Trotter product formula reduces to $e^A=(e^{A/n})^n$, which is valid for all n. The first nontrivial example is provided by the harmonic oscillator — the classical system with the Lagrangian $L(q,\dot{q})=\dfrac{m(\dot{q}^2-\omega^2q^2)}{2}$. In this case the $(n-1)$-fold integral in (1.9) is Gaussian and can be computed exactly.

Namely, start with the basic formula of the Gaussian integration

$$\int\limits_{\mathbb{R}^n}\exp\left\{-\frac{\langle A\mathbf{q},\mathbf{q}\rangle}{2}+\langle\mathbf{p},\mathbf{q}\rangle\right\}d^n\mathbf{q}=\frac{(2\pi)^{n/2}}{\sqrt{\det A}}\exp\{\langle A^{-1}\mathbf{p},\mathbf{p}\rangle\}, \tag{1.11}$$

where A is positive-definite symmetric $n\times n$ matrix and $\langle\ ,\ \rangle$ stands for the standard inner product in $\mathbb{R}^n$. By analytic continuation, the formula remains valid when $A=iB$, where B is positive-definite and symmetric. In this case the integral is understood in the distributional sense as $\lim_{R\to\infty}\int_{\|\mathbf{q}\|\leq R}$, where $\|\mathbf{q}\|^2=\langle\mathbf{q},\mathbf{q}\rangle$, and $\sqrt{\det A}=e^{i\pi/4}\sqrt{\det B}$. For the harmonic oscillator,we apply (1.11) with the following thrice-diagonal $(n-1)\times(n-1)$ matrix

$$A=\frac{m}{i\hbar\Delta t}\begin{bmatrix} 2-(\omega\Delta t)^2 & -1 & 0 & \dots & 0 & 0\\ -1 & 2-(\omega\Delta t)^2 & -1 & \dots & 0 & 0\\ 0 & -1 & 2-(\omega\Delta t)^2 & \dots & 0 & 0\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ 0 & 0 & 0 & \dots & 2-(\omega\Delta t)^2 & -1\\ 0 & 0 & 0 & \dots & -1 & 2-(\omega\Delta t)^2 \end{bmatrix}.$$

and

$$\mathbf{p} = \frac{m}{i\hbar\Delta t}\begin{bmatrix} q \\ 0 \\ \cdot \\ \cdot \\ 0 \\ q' \end{bmatrix} \in \mathbb{R}^{n-1}.$$

Using mathematical induction, it is easy to compute that

$$\det A = \left(\frac{m}{i\hbar\Delta t}\right)^{n-1}\frac{\sin n\theta}{\sin\theta}, \quad \text{where} \quad 2-(\omega\Delta t)^2 = 2\cos\theta,$$

and

$$\langle A^{-1}\mathbf{p},\mathbf{p}\rangle = -\frac{m}{2i\hbar\Delta t}\frac{\sin(n-1)\theta}{\sin n\theta}(q^2+{q'}^2) + \frac{m\sin\theta}{i\hbar\Delta t\sin n\theta}qq'.$$

Using that $\theta = \omega\Delta t + o(1)$ as $n\to\infty$, we get

$$K(q',t';q,t) = \lim_{n\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{n}{2}}\frac{(2\pi)^{\frac{n-1}{2}}}{\sqrt{\det A}}\exp\left\{\frac{im(q^2+{q'}^2)}{2\hbar\Delta t} + \langle A^{-1}\mathbf{p},\mathbf{p}\rangle\right\}$$

$$= \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\exp\left\{\frac{im\omega}{2\hbar\sin\omega T}\left((q^2+{q'}^2)\cos\omega T - 2qq'\right)\right\}. \tag{1.12}$$

Thus we obtained a closed expression for the propagator of harmonic oscillator. It is instructive to compare it with the series (1.1). Using the explicit representation for the wave functions $\psi_n(q)$ of the harmonic oscillator in terms of the Hermite polynomials (see Chapter 2, Section 3.1), we get the series

$$K(q',t';q,t) = \sqrt{\frac{\omega}{\pi\hbar}}\sum_{n=0}^{\infty}\frac{e^{-\frac{\omega}{2\hbar}\{(q^2+{q'}^2)-i\omega T(2n+1)\}}}{2^n n!}H_n\left(\sqrt{\frac{\omega}{\hbar}}q'\right)H_n\left(\sqrt{\frac{\omega}{\hbar}}q\right)$$

which converge in the distributional sense. Setting $x=\sqrt{\frac{\omega}{\hbar}}q\,, y=\sqrt{\frac{\omega}{\hbar}}q'$ and $z=e^{-\omega(t'-t)/2}$ and comparing with (1.12), we obtain

$$\sum_{n=0}^{\infty}\frac{z^n}{2^n n!}H_n(x)H_n(y) = \frac{1}{\sqrt{1-z^2}}\exp\left\{\frac{2xyz-(x^2+y^2)z^2}{1-z^2}\right\}.$$

When $|z|<1$, this is classical Mehler identity from the theory of Hermite polynomials. Two ways of computing the propagator of the harmonic oscillator give a proof of this identity, in the distributional sense, for $|z|=1$.

Expression (1.12) becomes singular when $\sin\omega T = 0$, i.e., when $T = T_k = \dfrac{\pi k}{\omega}$. The eigenvalues of the evolution operator $U(T_k)$ are $e^{-\pi ik(n+\frac{1}{2})}$, so that when k is even $U(T_k) = e^{-\frac{\pi ik}{2}}I$, and

$$K(q',t+T_k,q,t) = e^{-\frac{\pi ik}{2}}\delta(q-q').$$

For odd k we have

$$e^{-\frac{i}{\hbar}HT_k} = e^{-\frac{\pi i k}{2}}\sum_{n=0}(-1)^n P_n,$$

where P_n are projection operators on the eigenspaces $\mathbb{C}\psi_n$ of H. Since $H_n(-q) = (-1)^n H_n(q)$, we have in this case

$$K(q', t+T_k, q, t) = e^{-\frac{\pi i k}{2}}\delta(q+q').$$

1.5. Several degrees of freedom. In general, consider the classical mechanical system (M, L). At a physical level of rigor, its quantization is described by the propagator $K(\mathbf{q}', t'; \mathbf{q}, t)$ given by the Feynman path integral in the configuration space,

$$K(\mathbf{q}', t'; \mathbf{q}, t) = \int\limits_{\substack{\mathbf{q}(t')=\mathbf{q}' \\ \mathbf{q}(t)=\mathbf{q}}} e^{\frac{i}{\hbar}\int_t^{t'} L(\mathbf{q},\dot{\mathbf{q}})d\tau}\mathscr{D}\mathbf{q}, \tag{1.13}$$

For the case when $M = \mathbb{R}^n$ and $L(\mathbf{q}, \dot{\mathbf{q}}) = \dfrac{m\dot{\mathbf{q}}^2}{2} - v(\mathbf{q})$, the mathematical meaning of (1.13) is the same as (1.10): it gives the representation of the propagator for a quantum Hamiltonian $H = \dfrac{\mathbf{P}^2}{2m} + v(\mathbf{Q})$ as the limit of multiple integrals using Trotter product formula. In general, this formula serves as a heuristic tool which enables, in some cases, to understand what a quantization of a classical system (M, L) should be.

Analogously, for a Hamiltonian system with the phase space $\mathscr{M} = T^*M$ with the canonical symplectic form $\omega = d\mathbf{p}\wedge d\mathbf{q}$ and a hamiltonian function h, its quantization is described by the propagator $K(\mathbf{q}', t'; \mathbf{q}, t)$ given by the Feynman path integral in the phase space,

$$K(\mathbf{q}', t'; \mathbf{q}, t) = \int\limits_{\mathbf{\Omega}_{\mathbf{q},t}^{\mathbf{q}',t'}} e^{\frac{i}{\hbar}\int_\sigma(\mathbf{p}d\mathbf{q}-hdt)}\mathscr{D}\mathbf{p}\mathscr{D}\mathbf{q}. \tag{1.14}$$

Here $\mathbf{\Omega}_{\mathbf{q},t}^{\mathbf{q}',t'} = \Omega(T^*M\times\mathbb{R}, \mathbf{q}, t, \mathbf{q}', t')$ is the space of all admissible paths σ in $T^*M\times\mathbb{R}$ connecting points $(\mathbf{q}, t)$ and $(\mathbf{q}', t')$ (see Section 1.5). Again, when $\mathscr{M} = T^*\mathbb{R}^n$ and $h(\mathbf{p}, \mathbf{q}) = \dfrac{\mathbf{p}^2}{2m} + v(\mathbf{q})$, the precise mathematical meaning of (1.14) is the same as (1.8): it gives the representation of the propagator for a quantum Hamiltonian $H = \dfrac{\mathbf{P}^2}{2m} + v(\mathbf{Q})$ as the limit of multiple integrals using Trotter product formula. In this case formulas (1.13) and (1.14) are equivalent. We note that for Lagrangian functions $\mathbb{R}^n$ which are not quadratic in $\dot{\mathbf{q}}$ the formulas eqreffeynman-several-config and (1.14) are not necessarily equivalent.

In general, this formula serves as a heuristic tool which enables, in some cases, to understand what a quantization of a classical system $(\mathscr{M}, \omega, h)$ is.

This is a very non-trivial problem, especially when the phase space $\mathscr{M}$ is a compact manifold.

1.6. Path integral in the holomorphic representation. Let $H(\bar{z}, z)$ be the Wick symbol of a Hamiltonian operator. Here we find a formula for the symbol $K_t(\bar{z}, z)$ of the evolution operator $U_t = e^{-\frac{it}{\hbar}H}$. Let $\tilde{U}_{\Delta t}$ be the operator with the Wick symbol $e^{-\frac{i\Delta t}{\hbar}H(\bar{z},z)}$. We have

$$U_t = \lim_{N\to\infty} (\tilde{U}_{\Delta t})^N.$$

Using formulas for the composition of Wick symbols, we obtain the following representation for the Wick of the evolution operator:

$$U_t(\bar{z}, z) = \int\limits_{\substack{\bar{a}(t)=\bar{z} \\ a(0)=z}} \exp\left\{\int_0^t (\dot{a}\bar{a} - iH(\bar{a}, a))d\tau + \bar{z}\, a(t) - \bar{z}z\right\} \mathscr{D}\bar{a}\mathscr{D}a,$$

which is the Feynman path integral in holomorphic representation. Using relation between the trace and Wick symbols we obtain that in Euclidean time

$$\operatorname{Tr} e^{-TH} = \int\limits_{\substack{\bar{a}(0)=\bar{a}(T) \\ a(0)=a(T)}} \exp\left\{\int_0^T (\dot{a}\bar{a} - iH(\bar{a}, a))d\tau\right\} \mathscr{D}\bar{a}\mathscr{D}a.$$

2. Gaussian path integrals and determinants

2.1. Free particle and harmonic osicllator revisited. It turns out that formulas (1.5) and (1.12) for the propagators for the free particle and harmonic oscillator admits a very nice interpretation which shows the importance of Feynman path integrals.

2.1.1. *Gaussian integral for the free particle.* We know that for the free quantum particle

$$K_{free}(q', t'; q, t) = \sqrt{\frac{m}{2\pi i\hbar T}}\; e^{\frac{im(q-q')^2}{2\hbar T}} = \int\limits_{\substack{q(t')=q' \\ q(t)=q}} e^{\frac{im}{2\hbar}\int_t^{t'} \dot{q}^2 d\tau} \mathscr{D}q. \tag{2.1}$$

Here we will establish this formula differently by computing the Feynman path integral as if it was defined independently of the limit as $n \to \infty$. Let

$$q_{cl}(\tau) = q + (\tau - t)\frac{q' - q}{T}, \quad T = t' - t,$$

be the classical trajectory connecting points q and q'. For any other path $q(\tau)$ connecting these points we set $q(\tau) = q_{cl}(\tau) + y(\tau)$, where $y : [t, t'] \to \mathbb{R}$ satisfies $y(t) = y(t') = 0$. Since the classical trajectory is the extremal of the action functional (see Chapter 1, Section 1.1) and for the free particle this functional is quadratic, we have

$$S(q) = \int_t^{t'} \frac{m}{2}\dot{q}^2 d\tau = S_{cl} + S(y).$$

Here $S_{cl} = S(q_{cl})$ is called the *classical action* and is given by

$$S_{cl} = \int_t^{t'} \frac{m\dot{q}_{cl}^{\,2}}{2} d\tau = \frac{m}{2}\frac{(q-q')^2}{T}.$$

Assuming (which is quite natural) that under the "change of variable" $q = q_{cl} + y$ we have $\mathscr{D}q = \mathscr{D}y$, we can rewrite the Feynman path integral as

$$K_{free}(q',t';q,t) = e^{\frac{i}{\hbar}S_{cl}} \int\limits_{\substack{y(t')=0\\ y(t)=0}} e^{\frac{im}{2\hbar}\int_t^{t'}\dot{y}^2 d\tau}\mathscr{D}y.$$

Remarkably, $e^{\frac{i}{\hbar}S_{cl}} = e^{\frac{im(q-q')^2}{2\hbar T}}$ — the exponential factor in the propagator for the free particle. The remaining path integral does not depend on q and q' and, as we know, coincides with the prefactor in (2.1).

Another, more "profound" way to interpret this result is the following. Let A be the self-adjoint operator on $L^2([t,t'])$ defined by the differential expression $-\dfrac{d^2}{d\tau^2}$ with Dirichlet boundary conditions $y(t) = 0$, $y(t') = 0$. Then for any real-valued, absolutely continuous function $y(\tau)$ satisfying Dirichlet boundary conditions and such that $y, \dot{y} \in L^2([t,t'])$, we have by integrating by parts

$$\langle Ay, y\rangle_{L^2} = \int_t^{t'} \dot{y}^2 d\tau.$$

Thus the "integrand" in the path integral

$$\int\limits_{\substack{y(t')=0\\ y(t)=0}} e^{-\int_t^{t'}\dot{y}^2 d\tau}\mathscr{D}y.$$

can be interpret as the quadratic form of the operator A and, in accordance with (1.11) it natural to expect that this Gaussian path integral is proportional to $\dfrac{1}{\sqrt{\det A}}$. Of course, we need to understand what we mean by the determinant of a differential operator. Clearly, it should be defined by some regularization of the divergent product $\prod_{n=1}^{\infty}\lambda_n$, where λ_n are eigenvalues of A.

The most convenient regularization is given by considering the operator zeta-function. Namely, let A be a non-negative self-adjoint operator on the Hilbert space $\mathscr{H}$ with pure discrete 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 $\zeta_A(s)$ is defined for $\operatorname{Re} s > \alpha$ by the following absolutely convergent series

$$\zeta_A(s) = \sum_{\lambda_n > 0} \frac{1}{\lambda_n^s}.$$

Provided $\zeta_A(s)$ can be meromorphically continued to the larger domain containing $s = 0$ and is regular at this point, we define the regularized determinant by

$$\det{}' A = e^{-\zeta_A(0)}.$$

Here $\zeta'_A(s)$ stands for the derivative with respect to s, and the prime on det symbolizes that we omit zero eigenvalues. We will also use convenient notation

$$\det{}' A = \prod_{\lambda_n > 0}{}' \lambda_n,$$

where the prime indicates that the infinite product is regularized by the operator zeta-function.

Since $\zeta_{cA}(s) = c^{-s}\zeta_A(s)$ for $c > 0$, we get

$$\det{}' cA = c^{\zeta_A(0)} \det{}' A,$$

so 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 $\zeta'_A(0) = \log\lambda_1 + \cdots + \log\lambda_n$, so that we recover the usual definition of $\det A$.

This outline works for the general case of elliptic operators on compact manifold M. Here we will be dealing only with the cases when $M = [t, t']$ or $M = S^1$ and will prove all the statements above. The case of free particle provides the simplest example. Indeed, the corresponding eigenvalues are $\lambda_n = \left(\frac{\pi n}{T}\right)^2$ and we have

$$\zeta_A(s) = \left(\frac{T}{\pi}\right)^{2s} \zeta(2s),$$

where $\zeta(s)$ is Riemann zeta-function. Using classical formulas $\zeta(0) = -\frac{1}{2}$ and $\zeta'(0) = -\frac{1}{2}\log 2\pi$, we obtain

$$\zeta_A(0) = -\frac{1}{2} \quad \text{and} \quad \zeta'_A(0) = -\log\frac{T}{\pi} - \log 2\pi = -\log 2T. \tag{2.2}$$

Thus for the operator $A = -\dfrac{d^2}{d\tau^2}$ on the interval $[t, t']$ with Dirichlet boundary conditions we have

$$\det{}' A = 2T. \tag{2.3}$$

The formula

$$\int\limits_{\substack{y(t')=0\\ y(t)=0}} e^{\frac{im}{2\hbar}\int_t^{t'}\dot{y}^2 d\tau}\mathscr{D}y = \sqrt{\frac{m}{2\pi i\hbar T}}$$

is in agreement with the intepretation that Gaussian path integral is proportional to $\dfrac{1}{\sqrt{\det' A}}$. The coefficient of proportionality $\sqrt{\dfrac{m}{\pi i\hbar}}$ is determined by comparison with the definition of the path integral as a limit as $n\to\infty$.

2.1.2. *Gaussian integral for harmonic oscillator.* The propagator for harmonic oscillator

$$\begin{aligned}K_{osc}(q',t';q,t) &= \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\exp\left\{\frac{im\omega}{2\hbar\sin\omega T}\left(\left(q^2+{q'}^2\right)\cos\omega T-2qq'\right)\right\}\\ &= \int\limits_{\substack{q(t')=q'\\ q(t)=q}}\exp\left\{\frac{im}{2\hbar}\int_t^{t'}\left(\dot{q}^2-\omega^2q^2\right)d\tau\right\}\mathscr{D}q\end{aligned}$$

admits similar interpretation. Indeed, solving classical equations of motion we readily compute that

$$S_{cl} = \frac{im\omega}{2\sin\omega T}\left(\left(q^2+{q'}^2\right)\cos\omega T-2qq'\right),$$

and we would have

$$\int\limits_{\substack{y(t')=0\\ y(t)=0}}\exp\left\{\frac{im}{2\hbar}\int_t^{t'}\left(\dot{y}^2-\omega^2y^2\right)d\tau\right\}\mathscr{D}y = \sqrt{\frac{m}{\pi i\hbar\det' A_\omega}},$$

where A_ω is the self-adjoint operator on $L^2[t,t']$, defined by the differential expression $-\dfrac{d^2}{d\tau^2}-\omega^2$ with Dirichlet boundary conditions. The interpration holds provided we can show that $\det' A_\omega = \dfrac{2\sin\omega T}{\omega}$.

It is easy to get convinced that it is indeed the case. The eigenvalues of A_ω are $\lambda_n(\omega) = \left(\dfrac{\pi n}{T}\right)^2-\omega^2$, and (provided 0 is not an eigenvalue for A_ω) we have the following heuristic computation, which goes back to Euler:

$$\frac{\det' A_\omega}{\det' A_0} = \prod_{n=1}^{\infty}\frac{\lambda_n(\omega)}{\lambda_n(0)} = \prod_{n=1}^{\infty}\left(1-\frac{\omega^2T^2}{\pi^2n^2}\right) = \frac{\sin\omega T}{\omega T}.$$

The claim would follow since we already know that $\det' A_0 = 2T$.

For the rigorous derivation, it more convenient to consider the operator $A_{i\omega}$ for $\omega\in\mathbb{R}_{\geq 0}$ since it is positive-definite.

Lemma 2.1.

$$\det' A_{i\omega} = \frac{\sinh\omega T}{\omega T}.$$

PROOF. Denoting $\zeta_{i\omega}(s)=\zeta_{A_{i\omega}}(s)$, we have for $\operatorname{Re}s>\frac{1}{2}$,

$$
\begin{aligned}
\zeta_{i\omega}(s) &= \frac{1}{\Gamma(s)}\int_0^\infty e^{-\omega^2 x}\sum_{n=1}^\infty e^{-\frac{\pi^2 n^2}{T^2}x}x^s\frac{dx}{x} \\
&= \frac{1}{2\Gamma(s)}\int_0^\infty e^{-\omega^2 x}\vartheta\left(\frac{\pi x}{T^2}\right)x^s\frac{dx}{x}-\frac{1}{2\omega^s},
\end{aligned}
$$

where

$$\vartheta(x)=\sum_{n\in\mathbb{Z}}e^{-\pi n^2 x}$$

is Jacobi theta series. Using Jacobi inversion formula

$$\vartheta\left(\frac{1}{x}\right)=\sqrt{x}\,\vartheta(x),\quad x>0,$$

we get the following representation

$$
\begin{aligned}
\zeta_{i\omega}(s) &= -\frac{1}{2\omega^s}+\frac{T}{2\sqrt{\pi}\Gamma(s)}\int_0^\infty e^{-\omega^2 x}\vartheta\left(\frac{T^2}{\pi x}\right)x^{s-\frac{1}{2}}\frac{dx}{x} \\
&= -\frac{1}{2\omega^s}+\frac{T\Gamma(s-\frac{1}{2})}{2\sqrt{\pi}\omega^{2s-1}\Gamma(s)}+\frac{T}{\sqrt{\pi}\Gamma(s)}\int_0^\infty e^{-\omega^2 x}\sum_{n=1}^\infty e^{-\frac{n^2T^2}{x}}x^{s-\frac{1}{2}}\frac{dx}{x}
\end{aligned}
$$

$$
= -\frac{1}{2\omega^s}+\frac{T\Gamma(s-\frac{1}{2})}{2\sqrt{\pi}\omega^{2s-1}\Gamma(s)}+\frac{T}{\sqrt{\pi}\Gamma(s)}\sum_{n=1}^\infty\left(\frac{nT}{\omega}\right)^{s-\frac{1}{2}}K_{s-\frac{1}{2}}(\omega nT), \tag{2.4}
$$

where

$$K_s(x)=\int_0^\infty e^{-x(u+u^{-1})}u^s\frac{du}{u},\quad x>0,$$

is Macdonald's K-function (modified Bessel function). Since for $K_s(x)=O(e^{-x})$ as $x\to\infty$, for every $s\in\mathbb{C}$, uniformly on compact subsets, representation (2.4) establishes meromorphic continuation of $\zeta_{i\omega}(s)$ to the entire s-plane with simple poles at $s\in-\frac{1}{2}+\mathbb{Z}_{\geq 0}$. Since $\lim_{s\to 0}s\Gamma(s)=1$, we obtain $\zeta_{i\omega}(0)=-\frac{1}{2}$. Using classical formulas

$$K_{\frac{1}{2}}(x)=K_{-\frac{1}{2}}(x)=\sqrt{\frac{\pi}{x}}\,e^{-2x},$$

and $\Gamma(\frac{1}{2})=\sqrt{\pi}$, we also obtain from (2.4)

$$
\begin{aligned}
\zeta_{i\omega}'(0) &= \log\omega-\omega T+\sum_{n=1}^\infty\frac{1}{n}e^{-2n\omega T} \\
&= \log\omega-\omega T-\log(1-e^{-2\omega T}),
\end{aligned}
$$

so that $\det{}'A_{i\omega}=e^{-\zeta_{i\omega}'(0)}=\dfrac{2\sinh\omega T}{\omega}$. $\square$

Now we will show how to define a "characteristic polynomial" of the operator $A=A_0$ — an entire function $\det(A-\lambda I)$ on λ-plane, whose zeros are the eighenvalues $\lambda_n = \lambda_n(0)$. First we note that for $\mathrm{Re}(\lambda_N - \lambda) > 0$ the truncated zeta-function

$$\zeta^{(N)}_{A-\lambda I}(s) = \sum_{n=N+1}^{\infty} \frac{1}{(\lambda_n - \lambda)^s},$$

where the principal branch of of the logarithm is used, is absolutely convergent for $\mathrm{Re}\, s > \frac{1}{2}$, admits a meromorphic continuation to the s-plane and is regular at $s = 0$. Indeed, setting

$$\vartheta_N(x) = \vartheta(x) - 2\sum_{n=1}^{N} e^{-\lambda_n x} - 1,$$

we have

$$\zeta^{(N)}_{A-\lambda I}(s) = \frac{1}{2\Gamma(s)} \int_1^{\infty} e^{-\lambda x}\vartheta_N(x) x^s \frac{dx}{x} + \frac{1}{2\Gamma(s)} \int_0^1 e^{-\lambda x}\vartheta_N(x) x^s \frac{dx}{x}.$$

Since $\mathrm{Re}(\lambda_n - \lambda) >$ for all $n > N$, the first integral in this formula is absolutely convergent for all $s \in \mathbb{C}$ and represents a holomorphic function. Using Jacobi inversion formula and expanding $e^{-\lambda x}, e^{-\lambda_1 x}, \dots, e^{-\lambda_N x}$ into power series in x, we conclude just as before that the second integral admits a meromorphic continuation to the s-plane with simple poles at $s \in -\frac{1}{2} + \mathbb{Z}_{\geq 0}$. For $\mathrm{Re}(\lambda_N - \lambda) > 0$ we set

$$\prod_{n=N+1}^{\infty}{}' (\lambda_n - \lambda) = e^{-\zeta^{(N)}_{A-\lambda I}{}'(0)}$$

and define

$$\det(A - \lambda I) = \prod_{k=1}^{N} (\lambda_k - \lambda) \prod_{n=N+1}^{\infty}{}' (\lambda_n - \lambda).$$

Since for $M > N$

$$\prod_{n=N+1}^{\infty}{}' (\lambda_n - \lambda) = \prod_{k=N+1}^{M} (\lambda_k - \lambda) \prod_{n=M+1}^{\infty}{}' (\lambda_n - \lambda),$$

$\det(A - \lambda I)$ is well-defined and is an entire function with zeros at λ_n. For $\lambda = -\omega^2 < 0$ we have $\det(A - \lambda I) = \det{}' A_{i\omega}$, which is given by Lemma 2.1.2. Thus for all $\lambda \in \mathbb{C}$,

$$\det(A - \lambda I) = \frac{2 \sin \sqrt{\lambda}\, T}{\sqrt{\lambda}}.$$

2.2. Determinants. Here define and evaluate the characteristic determinant $\det(A - \lambda I)$ of the Sturm-Liouville operator

$$A = -\frac{d^2}{dx^2} + u(x)$$

on the interval $[0, T]$ with Dirichlet or periodic boundary conditions.

2.2.1. *Dirichlet boundary conditions.* Namely, suppose that $u \in C^1([0,T],\mathbb{R})$. It is known that A is a self-adjoint operator on $L^2[0,T]$ with the domain $D(A)$ consisting of $y(x) \in W_2^2[0,T]$ satisfying $y(0)=0$, $y(T)=0$. Moreover, in this case operator A has a pure discrete spectrum with simple eigenvalues $\lambda_1 < \lambda_2 \cdots < \lambda_n < \dots$ such that

$$\lambda_n = \frac{\pi^2 n^2}{T^2} + c + O\left(\frac{1}{n^2}\right) \tag{2.5}$$

as $n \to \infty$, where $c = \dfrac{\pi}{T^2}\displaystyle\int_0^T u(x)dx$. Assume first that $A > 0$. Setting

$$\vartheta_A(t) = \sum_{n=1}^{\infty} e^{-\lambda_n t},$$

we have for $\operatorname{Re} s > \frac{1}{2}$,

$$\begin{aligned}\zeta_A(s) &= \frac{1}{\Gamma(s)}\int_0^\infty \vartheta_A(t)t^s\,\frac{dt}{t} \\ &= \frac{1}{\Gamma(s)}\int_1^\infty \vartheta_A(t)t^s\,\frac{dt}{t} + \frac{1}{\Gamma(s)}\int_0^1 \vartheta_A(t)t^s\,\frac{dt}{t}. \end{aligned} \tag{2.6}$$

Since $\vartheta_A(t) = O(e^{-\lambda_1 t})$ as $t \to \infty$ and, by assumption $\lambda_1 > 0$, the first integral converges absolutely for all $s \in \mathbb{C}$ and represents an entire function. Using asymptotics (2.5) and Jacobi inversion formula we get

$$\vartheta_A(t) = \frac{1}{2}e^{ct}\left(\vartheta\left(\frac{\pi t}{T^2}\right) - 1\right)(1 + O(t)) = \frac{a_{-\frac{1}{2}}}{\sqrt{t}} + a_0 + \widetilde{\vartheta}_A(t),$$

where

$$a_{-\frac{1}{2}} = \frac{T}{2\sqrt{\pi}}, \quad a_0 = -\frac{1}{2} \quad \text{and} \quad \widetilde{\vartheta}_A(t) = O(\sqrt{t})$$

as $t \to 0$. Thus for the second integral in (2.6) we have

$$\frac{1}{\Gamma(s)}\int_0^1 \vartheta_A(t)t^s\,\frac{dt}{t} = \frac{a_{-\frac{1}{2}}}{(s-\frac{1}{2})\Gamma(s)} + \frac{a_0}{s\Gamma(s)} + \frac{1}{\Gamma(s)}\int_0^1 \widetilde{\vartheta}_A(t)t^s\,\frac{dt}{t},$$

which shows that it admits a meromorphic continuation to the half-plane $\operatorname{Re} s > -\frac{1}{2}$ and is regular at $s=0$. This completes the proof that for the case $A > 0$ the zeta-function $\zeta_A(s)$ admits a meromorphic continuation to $\operatorname{Re} s > -\frac{1}{2}$ and is regular at $s = 0$.

Thus

$$\det{}' A = \prod_{n=1}^{\infty}{}' \lambda_n = e^{-\zeta_A'(0)}$$

is well-defined. Repeating verbatim the arguments at the end of the previous section we get that for $\operatorname{Re}(\lambda_N - \lambda) > 0$ the truncated zeta-function $\zeta^{(N)}_{A-\lambda I}(s)$

admits a meromorphic continuation to $\operatorname{Re} s > -\frac{1}{2}$ and is regular at $s = 0$. This defines

$$\det(A - \lambda I) = \prod_{k=1}^{N} (\lambda_k - \lambda) \prod_{n=N+1}^{\infty}{}' (\lambda_n - \lambda)$$

as an entire function of λ with simple zeros at λ_n. Finally we can remove the assumption $A > 0$ by replacing A by $\tilde{A} = A + (1 - \lambda_1)I > 0$ and defining

$$\det{}' A = \begin{cases} \det(\tilde{A} - (1 - \lambda_1)I) & \text{if } 0 \text{ is not an eigenvalue of } A, \\ \dfrac{d}{d\lambda} \det(\tilde{A} - (1 - \lambda_1)I) & \text{if } 0 \text{ is an eigenvalue of } A. \end{cases}$$

Let $y_1(x, \lambda)$ be the solution of the Sturm-Liouville boundary value problem

$$-y'' + u(x)y = \lambda y, \tag{2.7}$$

satisfying initial conditions

$$y(0, \lambda) = 0, \quad y'(0, \lambda) = 1.$$

It is well-known that $y_1(x, \lambda)$, for every x, is entire function of λ of order $\frac{1}{2}$ and

$$y_1(x, \lambda) = \frac{\sin \sqrt{\lambda} x}{\sqrt{\lambda}} + O\left(\frac{e^{|\operatorname{Re} \sqrt{\lambda}| x}}{|\lambda|} \right). \tag{2.8}$$

The entire function $d(\lambda) = y_1(T, \lambda)$ has simple zeros at the eigenvalues λ_n of the operator A and is represented by the absolutely convergent product,

$$d(\lambda) = \text{const}\, \lambda^{\delta} \prod_{\lambda_n \neq 0} \left(1 - \frac{\lambda}{\lambda_n}\right),$$

where $\delta = 1$ if 0 is an eigenvalue of A, and $\delta = 0$ otherwise. The following theorem expresses the characteristic determinant $\det(A - \lambda I)$ of the operator A in terms of the function $d(\lambda)$.

THEOREM 2.1. *One has*

$$\det(A - \lambda I) = 2d(\lambda)$$

and

$$\frac{\det(A - \lambda I)}{\det' A} = \lambda^{\delta} \prod_{\lambda_n \neq 0} \left(1 - \frac{\lambda}{\lambda_n}\right).$$

PROOF. By what was said above, it is sufficient to prove the identity $\det(A - \lambda I) = 2d(\lambda)$ for $\operatorname{Re}(\lambda_1 - \lambda) > 0$. In this case, using

$$\zeta_{A - \lambda I}(s) = \frac{1}{\Gamma(s)} \int_0^{\infty} \operatorname{Tr} e^{-(A - \lambda I)t} t^s \frac{dt}{t}$$

for $\operatorname{Re} s > \frac{1}{2}$, and differentiating under the integral sign we get

$$\frac{\partial}{\partial\lambda}\zeta_{A-\lambda I}(s) = \frac{1}{\Gamma(s)}\int_0^\infty \operatorname{Tr} e^{-(A-\lambda I)t} t^s dt,$$

which is now absolutely convergent for $\operatorname{Re} s > -\frac{1}{2}$. Thus we obtain

$$\frac{\partial}{\partial\lambda}\zeta_{A-\lambda I}(0) = \int_0^\infty \operatorname{Tr} e^{-(A-\lambda I)t} dt = \operatorname{Tr}(A-\lambda I)^{-1}.$$

It follows from (2.5) that the operator $R_\lambda = (A-\lambda I)^{-1}$ — the resolvent of A — is of trace class. Thus all our manipulations are justified and we arrive at the formula

$$\frac{d}{d\lambda}\log\det(A-\lambda I) = -\operatorname{Tr} R_\lambda, \tag{2.9}$$

which generalizes the familiar property of finite-dimensional determinants.

To compute this trace, we use the representation of R_λ as an integral operator with the continuous kernel

$$R_\lambda(x,x') = \begin{cases} \dfrac{1}{d(\lambda)}\, y_1(x,\lambda)y_2(x',\lambda) & \text{if } x \leq x', \\ \dfrac{1}{d(\lambda)}\, y_1(x',\lambda)y_2(x,\lambda) & \text{if } x \geq x'. \end{cases} \tag{2.10}$$

where $y_2(x,\lambda)$ is another solution of (2.7) satisfying initial conditions

$$y(T,\lambda) = 0, \quad y'(T,\lambda) = -1,$$

so that

$$W(y_1,y_2)(\lambda) = y_1(x,\lambda)y_2'(x,\lambda) - y_1'(x,\lambda)y_2(x,\lambda) = d(\lambda).$$

Since R_λ is a trace class operator on $L^2[0,T]$ with the integral kernel $R_\lambda(x,x')$ continuous on $[0,T]\times[0,T]$, we have by Lidskij theorem,

$$\operatorname{Tr} R_\lambda = \int_0^T R_\lambda(x,x)dx = \frac{1}{d(\lambda)}\int_0^T y_1(x,\lambda)y_2(x,\lambda)dx.$$

We evaluate this integral by the following beautiful computation. Let $\dot{y}(x,\lambda) = \dfrac{\partial y}{\partial\lambda}(x,\lambda)$ and consider the following pair of equations:

$$\begin{aligned} -\dot{y}_1'' + u(x)\dot{y}_1 &= \lambda\dot{y}_1 + y_1, \\ -y_2'' + u(x)y_2 &= \lambda y_2. \end{aligned}$$

Multiplying the first equation by $y_2(x,\lambda)$, the second equation by $\dot{y}_1(x,\lambda)$ and subtracting, we obtain

$$y_1y_2 = \dot{y}_1\, y_2'' - \dot{y}_1''\, y_2 = \left(\dot{y}_1\, y_2' - \dot{y}_1'\, y_2\right)'.$$

Using the initial conditions for y_1 and y_2, we finally get

$$\begin{aligned} \int_0^T y_1(x,\lambda)y_2(x,\lambda)dx &= \left[\dot{y}_1(x,\lambda)y_2'(x,\lambda) - \dot{y}_1'(x,\lambda)y_2(x,\lambda)\right]\Big|_0^T \\ &= -\dot{y}_1(T,\lambda). \end{aligned} \tag{2.11}$$

Thus we have proved that for $\mathrm{Re}(\lambda_1 - \lambda) > 0$,

$$\operatorname{Tr} R_\lambda = -\frac{d}{d\lambda}\log d(\lambda),$$

from which it follows that

$$\det(A - \lambda I) = C\, d(\lambda) \tag{2.12}$$

for all $\lambda \in \mathbb{C}$ and some constant C. Using the product representation for for $d(\lambda)$ we get from here the second formula in the theorem.

Now we will determine the constant C in (2.12). It follows from (2.8) that it is sufficient to compute the asymptotics of $\det(A - \lambda I)$ as $\lambda \to -\infty$. Setting $\lambda = -\mu$ we have

$$\zeta_{A+\mu I}(s) = \frac{1}{\Gamma(s)}\int_1^\infty \vartheta_A(t)e^{-\mu t}\, t^s\,\frac{dt}{t} + \frac{1}{\Gamma(s)}\int_0^1 \vartheta_A(t)e^{-\mu t}\, t^s\,\frac{dt}{t}.$$

As before, the first integral is an entire function of s whose derivative at $s=0$ exponentially decays as $\mu \to +\infty$. For the second integral we have

$$\begin{aligned}\frac{1}{\Gamma(s)}\int_0^1 \vartheta_A(t)e^{-\mu t}\, t^s\,\frac{dt}{t} &= \frac{1}{\Gamma(s)}\int_0^1 \widetilde{\vartheta}_A(t)e^{-\mu t}\, t^s\,\frac{dt}{t} \\ &\quad + \frac{1}{\Gamma(s)}\int_0^1 \left(\frac{a_{-\frac{1}{2}}}{\sqrt{t}} + a_0\right) e^{-\mu t}\, t^s\,\frac{dt}{t}.\end{aligned}$$

Since $\widetilde{\vartheta}_A(t) = O(\sqrt{t})$ as $t \to 0$, the first integral is absolutely convergent for $\operatorname{Re} s > -\frac{1}{2}$ and it derivative at $s=0$ is $O(\mu^{-\frac{1}{2}})$ as $\mu \to +\infty$. For the remaining integral we have

$$\begin{aligned}\frac{1}{\Gamma(s)}\int_0^1 \left(\frac{a_{-\frac{1}{2}}}{\sqrt{t}} + a_0\right) e^{-\mu t}\, t^s\,\frac{dt}{t} &= \frac{a_{-\frac{1}{2}}\,\mu^{\frac{1}{2}-s}}{\Gamma(s)}\left(\Gamma(s-\tfrac{1}{2}) - \int_\mu^\infty e^{-t}t^{s-\frac{1}{2}}\frac{dt}{t}\right) \\ &\quad + \frac{a_0\,\mu^{-s}}{\Gamma(s)}\left(\Gamma(s) - \int_\mu^\infty e^{-t}t^s\frac{dt}{t}\right).\end{aligned}$$

Now it is elementary to show that s-derivative of this integral at $s=0$ has an asymptotics $-2\sqrt{\pi}a_{-\frac{1}{2}}\sqrt{\mu} - a_0\log\mu + O(e^{-\mu/2})$ as $\mu \to +\infty$. Using the expression for the Seeley coefficients obtained in the previous section, we finally get

$$\det(A + \mu I) = \frac{e^{\sqrt{\mu}T}}{\sqrt{\mu}}\left(1 + O\left(\frac{1}{\sqrt{\mu}}\right)\right)$$

as $\mu \to +\infty$. Comparing this with (2.8) at $x = T$ we conclude that $C = 2$, which completes the proof. □

Similar results hold for for the matrix-valued Sturm-Liouville operator with Dirichlet boundary conditions. Namely, let $U(x) = \{u_{ij}(x)\}_{i,j=1}^n$ be a C^1-function on $[0,T]$ with values in real, symmetric n by n matrices, and let

$$\mathbf{A} = -\frac{d^2}{dx^2} + U(x)$$

be the corresponding differential operator with Dirichlet boundary conditions. As in the case $n = 1$, $\mathbf{A}$ is a self-adjoint operator on the Hilbert space $L^2([0, T], \mathbb{C}^n)$ of $\mathbb{C}^n$-valued functions, and has a pure discrete spectrum accumulating to ∞. Its regularized determinant $\det'\mathbf{A}$ and characteristic determinant $\det(\mathbf{A} - \lambda I)$ are defined as before and have similar properties. Let $\mathbf{Y}(x, \lambda)$ be the solution of the differential equation

$$-\mathbf{Y}'' + U(x)\mathbf{Y} = \lambda\mathbf{Y}$$

satisfying initial conditions

$$\mathbf{Y}(0, \lambda) = 0, \quad \mathbf{Y}'(0, \lambda) = I_n,$$

where I_n is n by n identity matrix, and define $\mathbf{D}(\lambda) = \det \mathbf{Y}(T, \lambda)$. The entire function $\mathbf{D}(\lambda)$ has similar properties to that of $d(\lambda)$. Namely, the analog of Theorem 2.1 is the following statement.

PROPOSITION 2.1. *One has*

$$\det(\mathbf{A} - \lambda I) = 2^n \mathbf{D}(\lambda)$$

and

$$\frac{\det(\mathbf{A} - \lambda I)}{\det'\mathbf{A}} = \lambda^\delta \prod_{\lambda_n \neq 0} \left(1 - \frac{\lambda}{\lambda_n}\right),$$

where $\delta \in \mathbb{Z}_{\geq 0}$ *is the multiplicity of the the eigenvalue* $\lambda = 0$.

2.2.2. *Periodic boundary conditions.* The Sturm-Liouville operator

$$A = -\frac{d^2}{dx^2} + u(x)$$

with periodic boundary conditions is a self-adjoint operator on $L^2[0, T]$ with the domain consisting of $y(x) \in W_2^2[0, T]$ satisfying $y(0) = y(T)$ and $y'(0) = y'(T)$. In case $u(x) \in C^1[0, T]$ the operator A has a pure discrete spectrum with the eigenvalues $\lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots$ such that as $n \to \infty$,

$$\lambda_{2n-1} = \frac{4\pi^2 n^2}{T^2} + c + O\left(\frac{1}{n^2}\right),$$
$$\lambda_{2n} = \frac{4\pi^2 n^2}{T^2} + c + O\left(\frac{1}{n^2}\right),$$

where c is the same as in (2.5). Assume that $\lambda_0 > 0$ (which can be always achieved by replacing A by $A - \lambda_0 + \varepsilon$ with $\varepsilon > 0$) and set

$$\vartheta_A(t) = \sum_{n=0}^{\infty} e^{-\lambda_n t}, \quad t > 0.$$

As in the previous section, using the asymptotic for λ_n we get that as $t \to 0$,

$$\vartheta_A(t) = c^{ct}\vartheta\left(\frac{4\pi t}{T^2}\right) = \frac{a_{-\frac{1}{2}}}{\sqrt{t}} + O(\sqrt{t}),$$

where as for the Dirichlet boundary conditions, $a_{-\frac{1}{2}} = \dfrac{T}{2\sqrt{\pi}}$, but now $a_0 = 0$. This allows to define the regularized determinant $\det' A$ and the characteristic determinant $\det(A - \lambda I)$ exactly as in the previous section. Due to the property $a_0 = 0$ we now get, as in the end of the proof of Theorem 2.1, that

$$\det(A + \mu I) = e^{\sqrt{\mu}T}(1 + O(\mu^{-1/2})) \tag{2.13}$$

as $\mu \to +\infty$.

Here we denote by $y_1(x, \lambda)$ and $y_2(x, \lambda)$ solutions of the Sturm-Liouville equation (2.7) with the initial conditions $y_1(0, \lambda) = 1$, $y_1'(0, \lambda) = 0$ and $y_2(0, \lambda) = 0$, $y_2'(0, \lambda) = 1$. Solutions y_1 and y_2 are linear independent for all λ and the matrix

$$Y(x, \lambda) = \begin{pmatrix} y_1(x, \lambda) & y_2(x, \lambda) \\ y_1'(x, \lambda) & y_2'(x, \lambda) \end{pmatrix}$$

satisfies the initial condition $Y(0, \lambda) = I_2$, where I_2 is 2×2 identity matrix, and has the property $\det Y(x, \lambda) = 1$. For fixed x the matrix $Y(x, \lambda)$ is an entire matrix-valued function of λ having the following asymptotic as $\lambda \to \infty$

$$Y(x, \lambda) = \begin{pmatrix} \cos\sqrt{\lambda}T & \dfrac{\sin\sqrt{\lambda}T}{\sqrt{\lambda}} \\ \sqrt{\lambda}\sin\sqrt{\lambda}T & \cos\sqrt{\lambda}T \end{pmatrix} \left(I_2 + O\left(\frac{e^{|\sqrt{\lambda}|x}}{\lambda}\right)\right). \tag{2.14}$$

By definition, the *monodromy matrix* of the periodic Sturm-Liouville problem is the matrix

$$T(\lambda) = Y(T, \lambda).$$

The monodromy matrix satisfies $\det T(\lambda) = 1$ and is an entire matrix-valued function. The following result is the analog of Theorem 2.1 for the periodic boundary conditions.

THEOREM 2.2. *One has*

$$\det(A - \lambda I) = -\det(T(\lambda) - I_2) = y_1(T, \lambda) + y_2'(T, \lambda) - 2,$$

where det *in the right hand side is a matrix determinant, and*

$$\frac{\det(A - \lambda I)}{\det' A} = \lambda^{\delta} \prod_{\lambda_n \neq 0} \left(1 - \frac{\lambda}{\lambda_n}\right),$$

where $\{\lambda_n\}_{n=1}^{\infty}$ *are non-zero eigenvalues of* A *and* $\delta = 0, 1, 2$ *is the multiplicity of the eigenvalue* $\lambda = 0$.

PROOF. it follows very closely the proof of Theorem 2.1 and we will assume that $A > 0$. First, in precise analogy with (2.9) we obtain,

$$\frac{d}{d\lambda} \log\det(A - \lambda I) = -\operatorname{Tr} R_{\lambda},$$

where $\det(T(\lambda)-I_2)\neq 0$. Similar to (2.10), the resolvent R_λ is an integral operator with the symmetric kernel $R_\lambda(x,x')=R_\lambda(x',x)$, given for $x<x'$ by the following formula

$$\begin{aligned}R_\lambda(x,x') &= \big(y_1(x,\lambda),y_2(x,\lambda)\big)\,(T(\lambda)-I_2)^{-1}T(\lambda)\begin{pmatrix}-y_2(x',\lambda)\\ y_1(x',\lambda)\end{pmatrix}\\ &= -\operatorname{Tr}\left((T(\lambda)-I_2)^{-1}T(\lambda)Z(x,x')\right),\end{aligned}$$

where Tr in the last formula is the matrix trace and

$$Z(x,x')=\begin{pmatrix}-y_1(x,\lambda)y_2(x',\lambda) & y_2(x,\lambda)y_2(x',\lambda)\\ y_1(x,\lambda)y_2(x',\lambda) & y_2(x,\lambda)y_1(x',\lambda)\end{pmatrix}.$$

One can verify this formula directly by solving the non-homogeneous differential equation

$$-y''+u(x)y=f(x)$$

with the boundary conditions $y(0)=y(T)=c_1$, $y'(0)=y'(T)=c_2$ for some uniquely determined c_1 and c_2 by variation of parameter method.

As in the proof of Theorem 2.1, we need to compute $\displaystyle\int_0^T Z(x,x)dx$. It readily follows from (2.11) that

$$\int_0^T Z(x,x)dx=T^{-1}(\lambda)\frac{d}{d\lambda}T(\lambda)$$

and we obtain

$$\frac{d}{d\lambda}\log\det(A-\lambda I)=\operatorname{Tr}\left((T(\lambda)-I_2)^{-1}\frac{d}{d\lambda}T(\lambda)\right)=\frac{d}{d\lambda}\log\det(T(\lambda-I_2).$$

Thus $\det(A-\lambda I)=C\det(T(\lambda)-I_2)$. To determine the constant C we set $\lambda=-\mu\to+\infty$ and compare the asymptotic (2.13) with the asymptotic

$$\begin{aligned}\det(T(-\mu)-I_2) &= 2-\operatorname{Tr}T(-\mu)=2-2\cosh\sqrt{\mu}T(1+O(\mu^{-1/2}))\\ &= -e^{\sqrt{\mu}T}(1+O(\mu^{-1/2})),\end{aligned}$$

which follows from (2.14). Thus $C=-1$. □

In particular, when $u(x)=\omega^2>0$, we have

$$y_1(x,0)=\cosh\omega x\quad\text{and}\quad y_2(x,0)=\frac{\sinh\omega x}{\omega},$$

so that for the operator $A_{i\omega}=-\dfrac{d^2}{dx^2}+\omega^2$ we have

$$\det{}'A_{i\omega}=2(\cosh\omega T-1)=4\sinh^2\frac{\omega T}{2}. \tag{2.15}$$

The smallest eigenvalue of $A_{i\omega}$ is $\lambda_0=\omega^2$ and it tends to 0 as when $\omega\to 0$, so that for the operator $A_0=-\dfrac{d^2}{dx^2}$ we get

$$\det{}'A_0=\lim_{\omega\to 0}\frac{\det{}'A_{i\omega}}{\omega^2}=T^2.$$

One can also derive these formulas directly, as it was done in Section 2.1.2 of Chapter 4 for Dirichlet boundary conditions.

Similar results hold for for the matrix-valued Sturm-Liouville operator with periodic boundary conditions. Namely, let $U(x) = \{u_{ij}(x)\}_{i,j=1}^n$ be a C^1-function on $[0,T]$ with values in real, symmetric n by n matrices, and let

$$\mathbf{A} = -\frac{d^2}{dx^2} + U(x)$$

be the corresponding differential operator with periodic boundary conditions. As in the case $n=1$, $\mathbf{A}$ is a self-adjoint operator on the Hilbert space $L^2([0,T],\mathbb{C}^n)$ of $\mathbb{C}^n$-valued functions, and has a pure discrete spectrum accumulating to ∞. Its regularized determinant $\det{}'\mathbf{A}$ and characteristic determinant $\det(\mathbf{A}-\lambda I)$ are defined as before and have similar properties. Let $\mathbf{Y}_1(x,\lambda)$ and $\mathbf{Y}_2(x,\lambda)$ be the solutions of the differential equation

$$-\mathbf{Y}'' + U(x)\mathbf{Y} = \lambda\mathbf{Y}$$

satisfying, respectively, the initial conditions

$$\mathbf{Y}_1(0,\lambda) = I_n, \quad \mathbf{Y}_1'(0,\lambda) = 0 \quad \text{and} \quad \mathbf{Y}_2(0,\lambda) = 0, \quad \mathbf{Y}_2'(0,\lambda) = I_n,$$

where I_n is $n\times n$ identity matrix. The monodromy matrix $\mathbf{T}(\lambda)$ is defined as the following $2n\times 2n$ block mathrix,

$$\mathbf{T}(\lambda) = \begin{pmatrix} \mathbf{Y}_1(T,\lambda) & \mathbf{Y}_2(T,\lambda) \\ \mathbf{Y}_1'(T,\lambda) & \mathbf{Y}_2'(T,\lambda) \end{pmatrix},$$

and is entire matrix-valued function. The analog of Theorem 2.2 is the following statement.

Proposition 2.2. *One has*

$$\det(\mathbf{A}-\lambda I) = (-1)^n \det(\mathbf{T}(\lambda) - I_{2n})$$

and

$$\frac{\det(\mathbf{A}-\lambda I)}{\det{}'\mathbf{A}} = \lambda^\delta \prod_{\lambda_n\neq 0}\left(1-\frac{\lambda}{\lambda_n}\right),$$

where $\delta\in\mathbb{Z}_{\geq 0}$ is the multiplicity of the the eigenvalue $\lambda = 0$.

2.2.3. *First order differential operators.* Here we assume that $u(x)$ is smooth real-valued periodic function with period T and study first-order differential operators

$$A = \frac{d}{dx} + u(x)$$

on the interval $[0,T]$ with periodic boundary conditions $y(T) = y(0)$. The equation

$$y' + u(x)y = \lambda y$$

has an explicit solution $y(x) = Ce^{\lambda x - \int_0^x u(\tau)d\tau}$ has a periodic solution if and only if $\lambda = \lambda_n$, where

$$\lambda_n = u_0 + \frac{2\pi i n}{T}, \quad n \in \mathbb{Z}, \quad \text{and} \quad u_0 = \frac{1}{T}\int_0^T u(x)dx.$$

Thus the spectrum of the operator A coincides with the spectrum of the operator A_0 with the constant coefficient u_0. This is because $A = UA_0U^{-1}$, where $U : L^2[0,T] \to L^2[0,T]$ is a multiplication operator by a periodic function $e^{-U(x)}$ with $U(x) = \int_0^x (u(\tau) - u_0)d\tau$. Set $D = \dfrac{d}{dx}$.

PROPOSITION 2.3. *For* $u_0 \neq 0$,

$$\det{}'(D + u(x)) = 1 - e^{-u_0 T},$$

and $\det{}' D = T$ *for* $u_0 = 0$.

PROOF. The zeta-function of the operator A with $u_0 \neq 0$ is given by the following series

$$\zeta_A(s) = \sum_{n=-\infty}^{\infty} \frac{1}{\lambda_n^s},$$

where $\lambda_n^{-s} = e^{-s \log \lambda_n}$ with the principal branch of log for $n \neq 0$. The series is absolutely convergent for $\operatorname{Re} s > 1$. Introducing the *Hurwitz zeta-function*

$$\zeta(s,a) = \sum_{n=0}^{\infty} \frac{1}{(n+a)^s},$$

where $\operatorname{Re} a > 0$ and $\operatorname{Re} s > 1$, we can rewrite $\zeta_A(s)$ as follows

$$\zeta_A(s) = \left(\frac{2\pi}{T}\right)^{-s} \left(e^{-\frac{\pi i s}{2}}\zeta(s,a) + e^{\frac{\pi i s}{2}}\zeta(s,\bar{a})\right) + \frac{1}{u_0^s}, \quad a = 1 - \frac{u_0 T}{2\pi} i.$$

It is well-known that Hurwitz zeta-function admits a meromorphic continuation to the whole s-plane with single simple pole at $s = 1$ with residue 1, and

$$\zeta(0,a) = \frac{1}{2} - a, \quad \frac{\partial \zeta}{\partial s}(0,a) = \log \Gamma(a) - \frac{1}{2}\log 2\pi.$$

Thus using the classical formula

$$\Gamma(1+z)\Gamma(1-z) = \frac{\pi z}{\sin \pi z},$$

we get

$$\begin{aligned} \frac{\partial \zeta_A}{\partial s}(0) &= \log|\Gamma(a)|^2 - \log u_0 T + \frac{u_0 T}{2} \\ &= -\log(e^{\frac{u_0 T}{2}} - e^{-\frac{u_0 T}{2}}) + \frac{u_0 T}{2}, \end{aligned}$$

and $\det{}'(D + u_0(x)) = 1 - e^{-u_0 T}$. Finally, $\zeta_D(s) = \lim_{u_0 \to 0}(\zeta_A(s) - u_0^{-s})$, so that

$$\det{}' D = \lim_{u_0 \to 0} \frac{\det{}'(D + u_0)}{u_0} = T.$$

□

REMARK. Since operators $D+u(x)$ and $-D+u(x)$ with periodic boundary conditions have the same spectrum, $\det'(-D+u(x)) = 1 - e^{-u_0 T}$.

One can also consider the operator $A = D + u(x)$ on the interval $[0, T]$ with periodic function $u(x)$ and anti-periodic boundary conditions $y(T) = -y(0)$. Since corresponding eigenvalues are

$$\lambda_n = u_0 + \frac{\pi i(2n+1)}{T}, \quad n \in \mathbb{Z},$$

we see the the passage from periodic to anti-periodic boundary conditions amounts to replacing u_0 by $u_0 + \frac{\pi i}{T}$. From Proposition 2.3 we get

PROPOSITION 2.4. *For the anti-periodic boundary conditions on* $[0, T]$,

$$\det'(D + u(x)) = 1 + e^{-u_0 T}.$$

2.3. Semi-classical asymptotics. Here for the quantum mechanical system with the Hamiltonian

$$H = \frac{P^2}{2m} + v(Q)$$

with the one degree of freedom we consider the asymptotics of the propagator $K_\hbar(q', t'; q, t)$ as $\hbar \to \infty$, called *semi-classical asymptotics*, where we indicated explicitly the dependence on $\hbar$. We will compare the heuristic method based on Feynman path integral with the rigorous asymptotic analysis.

2.3.1. *Using Feynman path integral.* The Feynman path integral representation (1.10) allows to derive this asymptotics easily (albeit at a heuristic level). Namely, suppose that an analog of the stationary phase method is valid for the path integrals. Examples of Gaussian path integrals considered in the previous sections confirm this point of view.

Thus we are assuming that the leading contribution to the Feynman integral (1.13) comes from a critical point point of the action functional — the classical trajectory $q_{cl}(\tau)$ connecting points q and q' at times t and t' (we are assuming that such trajectory exists and is unique; compare with the discussion in Section 2.2 in Chapter 1). Then the leading term of the semi-classical asymptotics will be given by the factor $e^{\frac{i}{\hbar}S_{cl}}$, where

$$S_{cl} = S(q', t'; q, t) = \int_t^{t'} L(q_{cl}, \dot{q}_{cl}) d\tau$$

is the classical action — the critical value of the action functional (see Section 2.2 in Chapter 1). To compute the prefactor, we set in eqreffeynman-several-config

$$q(\tau) = q_{cl}(\tau) + y(\tau),$$

where $y(\tau)$ — the *quantum fluctuation* — satisfies Dirichlet boundary conditions $y(t) = y(t') = 0$, and expand the action functional around the critical point, keeping only quadratic terms in y. Using Dirichlet boundary conditions we obtain

$$S(q) = S_{cl} + \int_t^{t'} \left(\frac{m}{2}\dot{y}^2 - \frac{v''(q_{cl}(\tau))}{2} y^2 \right) d\tau + O(y^3).$$

Following the convention in previous sections and setting $u(\tau) = \dfrac{1}{m} v''(q_{cl}(\tau))$, we get

$$\int\limits_{\substack{y(t')=0\\ y(t)=0}} \exp\left\{ \frac{im}{2\hbar} \int_t^{t'} \left(\dot{y}^2 + u(\tau)y^2\right) d\tau \right\} \mathscr{D}y = \sqrt{\frac{m}{\pi i\hbar \det' A}},$$

where A is a self-adjoint operator on $L^2[t,t']$ defined by the differential expression

$$A = -\frac{d^2}{d\tau^2} + u(\tau)$$

and Dirichlet boundary conditions. (We assume that $v \in C^3([t,t'],\mathbb{R})$, so that $u \in C^1([t,t'],\mathbb{R})$ and A has a pure discrete spectrum.) Differential operator A is the operator of the second variation of the action functional S.

Thus we arrive at the following asymptotic behavior

$$K_\hbar(q',t';q,t) \simeq \sqrt{\frac{m}{\pi i\hbar \det' A}}\, e^{\frac{i}{\hbar}S(q',t';q,t)} \tag{2.16}$$

as $\hbar \to 0$. This formula is remarkably simple and shows a deep relation between semi-classical asymptotic of a quantum mechanical propagator and classical motion. Of course, our derivation was heuristic.

Remark. According to Theorem 2.1, we have $\det' A = 2y_1(t',0)$, where the function $y_1(\tau) = y_1(\tau,0)$ is the solution of the differential equation $Ay_1 = 0$ with the initial condition

$$y_1(t) = 0, \quad \dot{y}_1(t) = 1.$$

When $u(\tau) = \dfrac{1}{m} v''(q_{cl}(\tau))$, the function $y_1(\tau)$ can be easily expressed in terms of the classical solution $q_{cl}(\tau)$. Indeed, setting $f(\tau) = \dot{q}_{cl}(\tau)$ and differentiating the Newton's equation

$$m\ddot{q}_{cl} = -v'(q_{cl}),$$

we get that f satisfies the differential equation $Af = 0$, so that the Wronskian $\dot{y}_1 f - \dot{f} y_1$ of its two solutions is constant on $[t,t']$. Using the initial conditions for y_1 we get $\dot{y}_1 f - \dot{f} y_1 = f(t)$. Assuming that $f(t) \neq 0$ we obtain

$$y_1(\tau) = f(\tau) f(t) \int_t^\tau \frac{ds}{f^2(s)}$$

and

$$\det{}' A = 2f(t)f(t')\int_t^{t'}\frac{d\tau}{f^2(\tau)}.$$

If $f(t)=0$, then $\dot f(t)\neq 0$ (unless $q_{cl}=\text{const}$), so that

$$y_1(\tau)=\frac{f(\tau)}{\dot f(t)}=-m\frac{f(\tau)}{v'(q_{cl}(t))}$$

and

$$\det{}' A=-m\frac{\dot q_{cl}(t')}{v'(q)}.$$

As the result, we have expressed $\det' A$ — a contribution from the quantum fluctuations around the classical solution — in terms of the classical motion.

Similarly, for the case of n degrees of freedom, when

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

and $v\in C^3(\mathbb{R}^n,\mathbb{R})$, we obtain

$$K_\hbar(\mathbf{q}',t';\mathbf{q},t)\simeq\left(\frac{m}{\pi i\hbar}\right)^{n/2}\frac{1}{\sqrt{\det'\mathbf{A}}}\,e^{\frac{i}{\hbar}S(\mathbf{q}',t';\mathbf{q},t)}\tag{2.17}$$

as $\hbar\to 0$, where $\mathbf{A}=-\dfrac{d^2}{d\tau^2}+U(\tau)$ and

$$U(\tau)=\frac{\partial^2 v}{\partial\mathbf{q}^2}(\mathbf{q}_{cl}(\tau))=\left\{\frac{\partial^2 v}{\partial q_i\partial q_j}(\mathbf{q}_{cl}(\tau))\right\}_{i,j=1}^n.$$

2.3.2. *Rigorous derivation.* The rigorous approach is based on the fact that integral kernel $K_\hbar(q,q',t)$ is the fundamental solution of the Schrödinger equation — the Cauchy problem (1.2)–(1.3). Since $K_\hbar(q',t';q,t)=K_\hbar(q',q,T)$, where $T=t'-t$, we need to find the asymptotics of a fundamental solution $K_\hbar(q,q',t)$ as $\hbar\to 0$. This problem can be solved in two steps.

1. Finding *short-wave asymptotics* — asymptotics as $\hbar\to 0$ of the solution $\psi_\hbar(q,t)$ of the Cauchy problem for the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^2}+v(q)\psi$$

with the initial condition

$$\psi_\hbar(q,t)|_{t=0}=\varphi(q)e^{\frac{i}{\hbar}s(q)},$$

where $s(q),\varphi(q)\in C^\infty(\mathbb{R},\mathbb{R})$ and the "amplitude" $\varphi(q)$ has compact support.

2. For fixed $q'=q_0$ use the representation

$$\delta(q-q_0)=\frac{\varphi(q)}{2\pi\hbar}\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}\xi(q-q_0)}d\xi,$$

where φ has compact support and satisfies $\varphi(q_0)=1$, and use the "superposition principle" to express the kernel $K(q,q_0,t)$ as an integral over $d\xi$ of solutions of the Schr'odinger equation with initial amplitude $\varphi(q)$ and initial "phases" $s(q, \xi) = \xi(q - q_0)$. Use asymptotics from part **1** and evaluate the resulting integral by the stationary phase method as $\hbar \to 0$.

To realize the first step, we set $\psi_\hbar(q, t) = e^{\frac{i}{\hbar}\mathcal{S}(q,t,\hbar)}$ and substitute this "Ansatz" into the Schrödinger equation. For the function $\mathcal{S}$ we obtain the following nonlinear partial differential equation,

$$\frac{\partial \mathcal{S}}{\partial t} + \frac{1}{2m}\left(\frac{\partial \mathcal{S}}{\partial q}\right)^2 + v(q) = \frac{i\hbar}{2m}\frac{\partial^2 \mathcal{S}}{\partial q^2}, \tag{2.18}$$

which is equivalent to the Schrödinger equation. The advantage of (2.18) is that it is more convenient for determining the asymptotic expansion of $\mathcal{S}(q, t, \hbar)$ as $\hbar \to 0$. Namely, substituting

$$\mathcal{S}(q, t, \hbar) = \sum_{n=0}^{\infty} (-i\hbar)^n S_n(q, t)$$

into (2.18) and equating terms with the same powers of $\hbar$, we obtain that $S_0(q, t)$ satisfies the following initial value problem

$$\frac{\partial S_0}{\partial t} + \frac{1}{2m}\left(\frac{\partial S_0}{\partial q}\right)^2 + v(q) = 0 \tag{2.19}$$

and

$$S_0(q, t)|_{t=0} = s(q), \tag{2.20}$$

whereas $S_1(q, t)$ satisfies

$$\frac{\partial S_1}{\partial t} + \frac{1}{m}\frac{\partial S_0}{\partial q}\frac{\partial S_1}{\partial q} = -\frac{1}{2m}\frac{\partial^2 S_0}{\partial q^2} \tag{2.21}$$

and

$$S_1(q, t)|_{t=0} = \varphi(q). \tag{2.22}$$

For $n > 1$ the functions $S_n(q, t)$ satisfy differential equations similar to (2.21).

It is remarkable that (2.19)–(2.20) is the Cauchy problem for the Hamilton-Jacobi equation with the Hamiltonian $h(p, q) = \dfrac{p^2}{2m} + v(q)$ considered in Section 2.2 in Chapter 1! According to Proposition 2.1 in Section 2.2 of Chapter 1, solution of (2.19)–(2.20) is given by the method of characteristics as follows:

$$S_0(q, t) = s(q_0) + \int_0^t L(\gamma'(\tau))d\tau. \tag{2.23}$$

Here $\gamma(\tau)$ is the characteristic: the classical trajectory which at $\tau = 0$ starts at q_0 with the momentum $p_0 = \dfrac{\partial s}{\partial q}(q_0)$ and at $\tau = t$ ends at q, where q_0 is uniquely determined by q. (Here we assume that the Hamiltonian phase flow

g^t satisfies the assumptions made in Section 2.2.) It follows from Theorem 2.2 in Section 2.2 of Chapter 1 that along the characteristic,

$$\frac{\partial S_0}{\partial q}(q,t) = m\frac{d\gamma}{dt}(t),$$

so that

$$\left(\frac{\partial}{\partial t} + \frac{\partial S_0}{\partial q}\right) S_1(\gamma(t),t) = \frac{d}{dt} S_1(\gamma(t),t). \tag{2.24}$$

Now we can solve the Cauchy problem (2.21)–(2.22) for the transport equation explicitly. For this aim, consider the flow $\pi^t : \mathbb{R} \to \mathbb{R}$, defined in Section 2.2 of Chapter 1, set $Q = \pi^t(q)$[1], and denote by $\gamma(Q,q;\tau)$ the characteristic connecting points q at $\tau = 0$ and Q at $\tau = t$. Differentiating the equation

$$\frac{\partial S_0}{\partial Q}(Q,t) = m\frac{\partial \gamma}{\partial t}(Q,q;t)$$

with respect to q we obtain

$$\frac{\partial^2 S_0}{\partial Q^2}(Q,t)\frac{\partial Q}{\partial q} = m\frac{\partial^2 \gamma}{\partial q \partial t}(Q,q;t) = m\frac{d}{dt}\left(\frac{\partial Q}{\partial q}\right),$$

so that we can rewrite (2.21) as

$$\frac{d}{dt} S_1(Q,t) = -\frac{1}{2}\frac{d}{dt}\log\frac{\partial Q}{\partial q}.$$

Using (2.22), this equation (under the assumptions made in Section 2.2. of Chapter 1) is easily solved as follows,

$$S_1(Q,t) = \varphi(q)\left|\frac{\partial Q}{\partial q}(q)\right|^{-1/2}.$$

Thus we obtain

$$\psi_\hbar(Q,t) = \varphi(q)\left|\frac{\partial Q}{\partial q}(q)\right|^{-1/2} e^{\frac{i}{\hbar}(S(Q,q;t)+s(q))}(1+O(\hbar)), \tag{2.25}$$

where $S(Q,q;t)$ is the classical action along the characteristic that ends at Q. Under our assumption the flow π^t is a diffeomorphism so that the mapping $q \mapsto Q$ is one to one. Here we did not prove that (2.25) is an asymptotic expansion as $\hbar \to 0$. This can be shown using the assumptions made in Section 2.2 of Chapter 1.

The asymptotics (2.25) is consistent with the *conservation of probability*: for any Borel subset $E \subset \mathbb{R}$,

$$\int_{E^t} |\psi_\hbar(Q,t)|^2 dQ = \int_E |\varphi(q)|^2 dq + O(\hbar)$$

as $\hbar \to 0$, where $E^t = \pi^t(E)$.

[1] There should not be any confusion with the quantum coordinate operator Q.

Remark. When assumptions made in Section 2.2 of Chapter 1 are not satisfied, the situation becomes more complicated. Namely, in this case there may be several characteristics $\gamma_j(\tau)$ which end at Q at $\tau = t$ having q_j as their corresponding initial points. In this case,

$$\psi_\hbar(Q,t) = \sum_j \varphi(q_j)\left|\frac{\partial Q}{\partial q}(q_j)\right|^{-1/2} e^{\frac{i}{\hbar}(S(Q,q_j;t)+s(q_j))-\frac{\pi i}{2}\mu_j}(1+O(\hbar)),$$

where $\mu_j \in \mathbb{Z}$ is the Morse index of the characteristic γ_j. It is defined as the number of focal points of the phase curve $(q(\tau), p(\tau))$ with inital data q_j and $p_j = \dfrac{\partial s}{\partial q}(q_j)$ with respect to the configuration space $\mathbb{R}$. It is a special case of a more general Maslov index.

Now we proceed to the second step. For every $\xi \in \mathbb{R}$ let $\psi_\hbar(q,t;\xi)$ be the solution to the Schrödinger equation with the initial amplitude $\varphi(q)$ and the initial phase $s(q) = \xi(q-q_0)$. In this case $p(q) = \dfrac{\partial s}{\partial q} = \xi$, so the characteristic ending at Q has the initial momentum ξ and the initial coordinate $q = q(\xi, Q)$ Using (2.25), we obtain

$$K_\hbar(Q,q_0;t) \simeq \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\varphi(q(\xi,Q))\left|\frac{\partial Q}{\partial q}(q(\xi,Q))\right|^{-1/2} e^{\frac{i}{\hbar}(S(Q,q(\xi,Q);t)+\xi(q(\xi,Q)-q_0)}d\xi.$$

To this expression we apply the stationary phase method (see Section 2.1.3 of Chapter II). To find the critical points of the function $S(Q,q(\xi,Q);t) + \xi(q(\xi,Q)-q_0)$, we use Proposition 2.2 in Section 2.2 of Chapter 1 that

$$\frac{\partial S}{\partial q}(Q,q;t) = -p$$

— the initial momentum. Thus

$$\begin{aligned}\frac{\partial}{\partial \xi}(S(Q,q(\xi,Q);t)+\xi(q(\xi,Q)-q_0)) &= -\xi\frac{\partial q}{\partial \xi}(\xi,Q) + q(\xi,Q) - q_0 + \xi\frac{\partial q}{\partial \xi}(\xi,Q)\\ &= q(\xi,Q)-q_0.\end{aligned}$$

Thus (under our assumptions) we have a single critical point ξ_0 determined by the equation $q(\xi_0,Q) = q_0$. To find the prefactor, we use the equation

$$\frac{\partial Q}{\partial \xi} + \frac{\partial Q}{\partial q}\frac{\partial q}{\partial \xi} = 0,$$

which follows from the equation $Q(\xi, q(\xi,Q)) = Q$. Thus we arrive at the expression

$$K_\hbar(Q,q_0;t) \simeq \frac{1}{\sqrt{2\pi i\hbar}}\left|\frac{\partial Q}{\partial \xi}(q_0,\xi_0)\right|^{-1/2} e^{\frac{i}{\hbar}S(Q,q_0;t)}. \tag{2.26}$$

Since $K_\hbar(q',t';q,t) = K_\hbar(q',q;t'-t)$, formula (2.26) would be the same as (2.16), provided we can express $\dfrac{\partial Q}{\partial \xi}(q_0,\xi_0)$ in terms of the determinant of the operator A from the previous section. To this aim we use Theorem

2.1. Namely, differentiating Euler-Lagrange equation for the characteristic $\gamma(Q, q; \tau)$ with respect to $\dot{q}$ — the velocity at $\tau = 0$, which is a function of Q and q — we get that $y(\tau) = \dfrac{\partial\gamma}{\partial\dot{q}}(Q, q, \tau)$ satisfies the differential equation $Ay = 0$ and the initial conditions

$$y(0) = 0, \;\; \dot{y}(0) = 1.$$

Since $\xi = m\dot{q}_0$, we have

$$\frac{\partial Q}{\partial\xi}(q_0) = \frac{y(t)}{m} = \frac{1}{2m}\det{}' A.$$

Substituting this into the representation (2.26) we get exactly the representaion (2.16).

As in the case of short-wave asymptotics for the Schrödinger equation, when assumptions made in Section 2.2 of Chapter 1 are not satisfied, there are several characteristics $\gamma_j(\tau)$ connecting points q_0 and Q and initial momenta having ξ_j. In this case we have,

$$K_\hbar(Q, q_0, t) \simeq \sum_j \frac{1}{\sqrt{2\pi i\hbar}}\left|\frac{\partial Q}{\partial\xi}(q_0, \xi_j)\right|^{-1/2} e^{\frac{i}{\hbar}(S(Q, q_0, \xi_j; t) - \frac{\pi i}{2}\mu_j},$$

where μ_j is the Morse index of γ_j.

Remark. One can get yet another formula for the pre-factor in representation (2.26). Namely, differentiating $\dfrac{\partial S}{\partial q}(Q, q; t) = -\xi$ with respect to Q we get

$$\frac{\partial^2 S}{\partial q\partial Q} = -\frac{\partial\xi}{\partial Q},$$

so that (2.26) can be rewritten entirely in terms of the classical action

$$K_\hbar(Q, q_0; t) \simeq \frac{1}{\sqrt{2\pi i\hbar}}\left|\frac{\partial^2 S}{\partial q\partial Q}(Q, q_0; t)\right|^{1/2} e^{\frac{i}{\hbar}S(Q, q_0; t)}.$$

The case of n degrees of freedom, under assumptions made is Section 2.2 of Chapter 1, is considered similarly. The solution $\psi_\hbar(\mathbf{q}, t)$ of the Cauchy problem for the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + v(\mathbf{q})\psi,$$

$$\psi_\hbar(\mathbf{q}, t)|_{t=0} = \varphi(\mathbf{q})e^{\frac{i}{\hbar}s(\mathbf{q})},$$

with smooth $s(\mathbf{q}), \varphi(\mathbf{q})$ and compactly supported $\varphi(\mathbf{q})$, has the the following asymptotics as $\hbar \to 0$:

$$\psi_\hbar(\mathbf{Q}, t) = \varphi(\mathbf{q})\left|\det\left(\frac{\partial\mathbf{Q}}{\partial\mathbf{q}}(\mathbf{q})\right)\right|^{-1/2} e^{\frac{i}{\hbar}(S(\mathbf{Q}, \mathbf{q}; t) + s(\mathbf{q}))}(1 + O(\hbar)),$$

and the asymptotics of the fundamental solution is given by

$$K_\hbar(\mathbf{Q},\mathbf{q}_0,t) \simeq (2\pi i\hbar)^{-n/2}\left|\det\left(\frac{\partial\mathbf{Q}}{\partial\boldsymbol{\xi}}(\mathbf{q}_0,\boldsymbol{\xi}_0)\right)\right|^{-1/2} e^{\frac{i}{\hbar}(S(\mathbf{Q},\mathbf{q}_0,\boldsymbol{\xi}_0;t)}.$$

Using the equation

$$\frac{\partial\boldsymbol{\xi}}{\partial\mathbf{Q}} = -\frac{\partial^2 S}{\partial\mathbf{q}\partial\mathbf{Q}} = \left\{\frac{\partial^2 S}{\partial q_i\partial Q_j}\right\}_{i,j=1}^{n},$$

this asymptotics can be rewritten as

$$K_\hbar(\mathbf{Q},\mathbf{q}_0;t) \simeq (2\pi i\hbar)^{-n/2}\left|\det\left(\frac{\partial^2 S}{\partial\mathbf{q}\partial\mathbf{Q}}(\mathbf{Q},\mathbf{q}_0;t)\right)\right|^{1/2} e^{\frac{i}{\hbar}S(\mathbf{Q},\mathbf{q}_0;t)}.$$

Here $\det\dfrac{\partial^2 S}{\partial\mathbf{q}\partial\mathbf{Q}}$ is known as *van Vleck determinant.*

CHAPTER 5

Integration in Functional Spaces

1. Gaussian measures

Here we will study classical Gaussian measures.

1.1. Finite-dimensional case. Let A be symmetric, positive-definite, real $n \times n$ matrix. As we know in Section 1.4 of Chapter 4,

$$\int_{\mathbb{R}^n} e^{-\langle A\mathbf{q},\mathbf{q}\rangle} d^n\mathbf{q} = \sqrt{\frac{(2\pi)^n}{\det A}}$$

is the basic formula of Gaussian integration. We use it to define a *Gaussian measure* μ_A on $\mathbb{R}^n$ by

$$d\mu_A(\mathbf{q}) = \sqrt{\frac{\det A}{\pi^n}}\, e^{-\frac{1}{2}\langle A\mathbf{q},\mathbf{q}\rangle} d^n\mathbf{q}, \tag{1.1}$$

so that $\mu_A(\mathbb{R}^n) = 1$. The measure μ_A is a mean-zero probability measure on $\mathbb{R}^n$ with the covariance $G = A^{-1}$. When $A = I_n$ — $n \times n$ identity matrix — the corresponding measure is denoted by μ_n.

As it follows from (1.11) in Section 1.4 of Chapter 4,

$$\int_{\mathbb{R}^n} e^{\langle \mathbf{p},\mathbf{q}\rangle} d\mu_A(\mathbf{q}) = e^{\frac{1}{2}\langle G\mathbf{p},\mathbf{p}\rangle}, \tag{1.2}$$

and by analytic continuation,

$$\int_{\mathbb{R}^n} e^{i\langle \mathbf{p},\mathbf{q}\rangle} d\mu_A(\mathbf{q}) = e^{-\frac{1}{2}\langle G\mathbf{p},\mathbf{p}\rangle}. \tag{1.3}$$

The function $(2\pi)^{-n/2}e^{-\frac{1}{2}\langle G\mathbf{p},\mathbf{p}\rangle}$ is the Fourier transform of the measure μ_A (in the distributional sense).

Applying to (1.2) the directional derivative with respect to $\mathbf{v} \in \mathbb{R}^n$ — the differential operator

$$\partial_{\mathbf{v}} = \mathbf{v}\frac{\partial}{\partial \mathbf{p}} = \sum_{k=1}^{n} v_k \frac{\partial}{\partial p_k}$$

(the differentiation under the integral sign is clearly legitimate), we obtain

$$\int_{\mathbb{R}^n} \langle \mathbf{v},\mathbf{q}\rangle e^{\langle \mathbf{p},\mathbf{q}\rangle} d\mu_A(\mathbf{q}) = \langle G\mathbf{v},\mathbf{p}\rangle e^{\frac{1}{2}\langle G\mathbf{p},\mathbf{p}\rangle}. \tag{1.4}$$

Setting here $\mathbf{p} = 0$ we get

$$\int\limits_{\mathbb{R}^n} \langle \mathbf{v}, \mathbf{q} \rangle d\mu_A(\mathbf{q}) = 0,$$

while applying to (1.4) another $\partial_{\mathbf{v}'}$ and setting $\mathbf{p} = 0$ afterwards, we obtain

$$\int\limits_{\mathbb{R}^n} \langle \mathbf{v}, \mathbf{q} \rangle \langle \mathbf{v}', \mathbf{q} \rangle d\mu_A(\mathbf{q}) = \langle G\mathbf{v}, \mathbf{v}' \rangle.$$

Repeating this procedure, we arrive at the following very important and useful formula, the so-called *Wick's theorem*:

(1.5)

$$\int\limits_{\mathbb{R}^n} \langle \mathbf{v}_1, \mathbf{q} \rangle \dots \langle \mathbf{v}_N, \mathbf{q} \rangle d\mu_A(\mathbf{q}) = \begin{cases} 0 & \text{if } N \text{ is odd} \\ \sum \langle G\mathbf{v}_{i_1}, \mathbf{v}_{j_1} \rangle \dots \langle G\mathbf{v}_{i_{N/2}}, \mathbf{v}_{j_{N/2}} \rangle & \text{if } N \text{ is even.} \end{cases}$$

Here the sum goes over all possible pairings $(i_1, j_1), \dots, (i_{N/2}, j_{N/2})$ of the set $\{1, 2, \dots, N\}$.

1.2. Infinite-dimensional case. Let

$$\mathscr{H} = \ell^2(\mathbb{R}) = \left\{ x = \{x_i\}_{i=1}^{\infty} : \|x\|^2 = \sum_{i=1}^{\infty} x_i^2 < \infty \right\}$$

be the real Hilbert space with the scalar product $\langle x, y \rangle = \sum_{i=1}^{\infty} x_i y_i$, and let $\mathscr{V} = \mathbb{R}^\infty$ be the Cartesian product over $\mathbb{N}$ of copies of $\mathbb{R}$ equipped with Tychonoff topology, so that $\mathscr{H} \subset \mathscr{V}$. The element $x \in \mathscr{V}$ is said to have finite support if $x_i = 0$ for sufficiently large i.

The Gaussian measure μ on $\mathscr{V}$ is defined by the direct porduct of the Gaussian measures μ_1, $\mu = \mu_\infty = \mu_1 \times \mu_1 \times \cdots$, and can be heuristically represented as

$$d\mu = \pi^{-\infty} e^{-\frac{1}{2}\|x\|^2} \prod_{i=1}^{\infty} dx_i.$$

Here "divergent to 0 product $\pi^{-\infty} e^{-\frac{1}{2}\|x\|^2}$" compensates "divergent to ∞ product" $\prod_{i=1}^{\infty} dx_i$. More precisely, the measure μ first is defined for "cylindrical sets $C = E_1 \times \cdots \times E_n \times \mathbb{R} \times \cdots$" with $E_1, \dots, E_n \in \mathscr{B}(\mathbb{R})$ by $\mu(C) = \mu_1(E_1) \dots \mu_1(E_n)$, and then extending it to the whole σ-algebra generated by the cylindrical sets by using Kolmogoroff theorem. In particular, if $F(x) = f(x_1, \dots, x_n)$, where f is bounded measurable function on $\mathbb{R}^n$, then

$$\int\limits_{\mathscr{V}} F d\mu = \int\limits_{\mathbb{R}^n} f d\mu_n. \tag{1.6}$$

Conversely, the following statement holds.

Lemma 1.1. *There exists a unique probability measure μ on $\mathscr{V}$ such that for all $v \in \mathscr{V}$ with finite support,*

$$\int_{\mathscr{V}} e^{i\langle v,x\rangle} d\mu(x) = e^{-\frac{1}{2}\|v\|^2}.$$

Proof. Immediately follows from (1.3) since the measure μ_n on $\mathbb{R}^n$ is uniquely determined by its Fourier transform. □

Now for $\alpha = \{\alpha_i\} \in \mathscr{V}$ let

$$\mathscr{H}_\alpha = \left\{ x \in \mathscr{V} : \sum_{i=1}^{\infty} \alpha_i^2 x_i^2 < \infty \right\}.$$

Proposition 1.1 ("0-1 law").

$$\mu(\mathscr{H}_\alpha) = \begin{cases} 0 & \text{if } \alpha \notin \mathscr{H}, \\ 1 & \text{if } \alpha \in \mathscr{H}. \end{cases}$$

In particular, $\mu(\mathscr{H}) = 0$.

Proof. Let χ_α be the characteristic function of the set $\mathscr{H}_\alpha \subset \mathscr{V}$,

$$\chi_\alpha(x) = \lim_{\varepsilon \to 0} \exp\{-\varepsilon^2 \sum_{i=1}^{\infty} \alpha_i^2 x_i^2\}.$$

Twice applying the dominated convergence theorem, we get

$$\begin{aligned} \mu(\mathscr{H}_\alpha) &= \int_{\mathscr{V}} \chi_\alpha d\mu \\ &= \lim_{\varepsilon \to 0} \int_{\mathscr{V}} \exp\{-\varepsilon^2 \sum_{i=1}^{\infty} \alpha_i^2 x_i^2\} d\mu(x) \\ &= \lim_{\varepsilon \to 0} \lim_{n \to \infty} \int_{\mathbb{R}^n} \exp\{-\varepsilon^2 \sum_{i=1}^{n} \alpha_i^2 x_i^2\} d\mu_n(x) \\ &= \lim_{\varepsilon \to 0} \lim_{n \to \infty} \prod_{i=1}^{n} (1 + \varepsilon^2 \alpha_i^2)^{-1/2}. \end{aligned}$$

The product $\prod_{i=1}^{\infty}(1 + \varepsilon^2\alpha_i^2)$ is convergent if and only if the series $\sum_{i=1}^{\infty} \alpha_i^2$ is convergent, and the statement follows. □

For $v \in \mathscr{H}$ let $v^{(n)} = (v_1, \dots, v_n, 0, 0 \dots)$. It follows from (1.6) that

$$\int_{\mathscr{V}} \langle v^{(n)}, x\rangle^2 d\mu(x) = \|v^{(n)}\|^2,$$

so that the sequence of functions $F_n(x) = \langle v^{(n)}, x\rangle$ is a Cauchy sequence in $L^2(\mathscr{V}, d\mu)$ and converges in L^2 to the function $F(x)$. Abusing notation, we write $F(x) = \langle v, x\rangle$. This shows that though $\mu(\mathscr{H}) = 0$, $\langle v, x\rangle$ is still a well-defined element in $L^2(\mathscr{V}, d\mu)$. Moreover, Lemma 1.1 and, consequently, Wick's theorem, hold for $v \in \mathscr{H}$.

2. Wiener measure and Wiener integral

In the previous chapter we considered the one-parameter group of unitary operators $U(t) = e^{-\frac{it}{\hbar}H}$ for the quantum Hamiltonian operator $H = H_0 + V$. Corresponding propagator $K_\hbar(\mathbf{q}', t'; \mathbf{q}, t)$ — the integral kernel of the operator $U(t'-t)$ — has been expressed in a form reminiscent, at a heuristic level, of an integral over the space of paths — the Feynman path integral. Here we replace the physical time t by "Euclidean time" $-it$ and consider the semigroup $e^{-\frac{t}{\hbar}H}$ of contracting operators (when $H > 0$) for $t > 0$. In this case all constructions can be made rigorous with Wiener integral replacing the Feynman integral.

2.1. Definition of the Wiener measure. Here we define the probability measure on the space $C([0,\infty), \mathbb{R}^n; 0)$ of continuous paths in $\mathbb{R}^n$ starting at the origin, called the Wiener measure. In physical terminology, it is related to the Brownian motion — the diffusion process in $\mathbb{R}^n$ with diffusion coefficient $D = \dfrac{\hbar}{2m}$. Mathematically, it is described by the probability density

$$P(\mathbf{q}', \mathbf{q}; t) = (4\pi D t)^{n/2} e^{-(\mathbf{q}-\mathbf{q}')^2/4Dt} \tag{2.1}$$

that a particle with initial certainty of being at $\mathbf{q}$ is diffused in time t to point $\mathbf{q}'$.

For compactness argument, It will be convenient to use one-point compactification $\widehat{\mathbb{R}}^n \simeq S^n$ of $\mathbb{R}^n$ that allows paths to pass through ∞. Let

$$\Omega = \prod_{0 \le t < \infty} \widehat{\mathbb{R}}^n$$

be the Cartesian product of copies of $\widehat{\mathbb{R}}^n$ parameterized by the $\mathbb{R}_{\geq 0}$. Equipped with the Tychonoff topology Ω is compact topological space — the space of all paths in $\widehat{\mathbb{R}}^n$. For every partition $\mathbf{t} = \{0 \le t_1 \le \cdots \le t_m\}$ and every $F \in C(\prod_{i=1}^m \widehat{\mathbb{R}}^n)$, define $\varphi \in C(\Omega)$ by

$$\varphi(\gamma) = F(\gamma(t_1), \dots, \gamma(t_m)) \quad \text{for all} \quad \gamma \in \Omega.$$

Denote by $C_{fin}(\Omega)$ the subspace of $C(\Omega)$ spanned by functions φ for all partitions $\mathbf{t}$ for all m and all continuous functions F. Define a linear functional l on $C_{fin}(\Omega)$ by the following formula:

$$\begin{aligned} l(\varphi) = \int_{\mathbb{R}^n} \cdots \int_{\mathbb{R}^n} & F(\mathbf{q}_1, \dots, \mathbf{q}_m) P(\mathbf{q}_m, \mathbf{q}_{m-1}; t_m - t_{m-1}) \dots \\ & \dots P(\mathbf{q}_1, 0; t_1) d^n\mathbf{q}_1 \dots d^n\mathbf{q}_m. \end{aligned} \tag{2.2}$$

It follows from the semi-group property

$$\int_{\mathbb{R}^n} P(\mathbf{q}', \mathbf{q}_1; t' - t_1) P(\mathbf{q}_1, \mathbf{q}; t_1 - t) d^n \mathbf{q}_1 = P(\mathbf{q}', \mathbf{q}; t' - t)$$

that the functional l is well-defined. The functional l is positive: $l(\varphi) \geq 0$ for $\varphi \geq 0$, satisfies $l(1) = 1$ and

$$|l(\varphi)| \leq |\varphi\|_\infty = \sup_{\gamma \in \Omega} |\varphi(\gamma)|.$$

By Stone-Weierstrass theorem, $C_{fin}(\Omega)$ is dense in $C(\Omega)$, and l has a unique extension to a continuous positive linear functional on $C(\Omega)$ with norm 1. By Riesz-Markoff theorem, there exists a unique regular Borel measure μ_W on Ω with $\mu_W(\Omega) = 1$ such that

$$l(\varphi) = \int_\Omega \varphi \, d\mu_W$$

The measure μ_W is called the Wiener measure.

Remark. The Riesz-Markoff theorem is the usual way the measures arise in functional analysis. Actually, the theorem guarantees an existence of the Baire measure — a measure defined on the σ-algebra of Baire sets. However, for compact spaces a Baire measure has a unique extension to a regular Borel measure — a measure defined on the σ-algebra generated by all open subsets. A Borel measure μ is regular if for for every Borel set $E \subset \Omega$,

$$\mu(E) = \begin{cases} \inf\{\mu(U) : E \subset U, & U \text{ is open}\} \\ \sup\{\mu(K) : K \subset E, & K \text{ is compact and Borel }\}. \end{cases}$$

The space Ω is "so large" that its σ-algebras of Baire and Borels sets are different.

Thus constructed Wiener measure is supported on continuous paths starting at the origin, i.e., $\mu_W(C) = 1$ for $C = C([0,\infty), \mathbb{R}^n; 0)$. The support μ_W can be characterized more precisely as follows. For $0 < \alpha \leq 1$ let Ω_α be the subspace of Ω of Holder continuous path of order α:

$$\Omega_\alpha = \left\{ \gamma \in \Omega : \sup_{t,t' \geq 0} \frac{\|\gamma(t) - \gamma(t')\|}{|t - t'|^\alpha} < \infty \right\}.$$

Then

$$\mu_W(\Omega_\alpha) = \begin{cases} 1, & \text{if } 0 < \alpha < \frac{1}{2}, \\ 0, & \text{if } \frac{1}{2} \leq \alpha \leq 1. \end{cases}$$

Replacing in the definition (2.2) $P(\mathbf{q}_1, 0; t_1)$ by $P(\mathbf{q}_1, \mathbf{q}_0; t_1)$ for a fixed $\mathbf{q}_0 \in \mathbb{R}^n$, we obtain a Wiener measure supported on continuous paths that start at $\mathbf{q}_0$.

REMARK. One could try to define the Wiener measure by the following construction. Set, for simplicity, $n = 1$ and for every partition $\mathbf{t}$ and intervals $(\alpha_1, \beta_1) \dots, (\alpha_m, \beta_m)$ consider the *cylindrical sets*

$$C_{\mathbf{t}} = \{\gamma \in \Omega : \alpha_1 < \gamma(t_1) < \beta_1, \dots, \alpha_m < \gamma(t_m) < \beta_m\},$$

and assign to them the measure

$$\mu(C_{\mathbf{t}}) = \int_{\alpha_1}^{\beta_1} \dots \int_{\alpha_m}^{\beta_m} P(q_m, q_{m-1}; t_m - t_{m-1}) \dots P(q_1, 0; t_1) dq_1 \dots dq_m.$$

By Kolmogoroff extension theorem and the semi-group property, μ extends to a measure on the σ-algebra of Ω generated by the cylindrical sets, which we continue to denote by μ. However, the set C of continuous path starting at 0 turns out to be non-measurable! Specifically, one can show that

$$\mu_*(C) = 0 \quad \text{and} \quad \mu^*(C) = 1.$$

To remedy this situation, one should define cylindrical sets as consisting of continuous functions only with the measure defined as above. This measure extends to the σ-algebra of C generated by cylindrical sets and coincides with the Wiener measure μ_W.

PROPOSITION 2.1. *Let $v \in C(\mathbb{R}^n, \mathbb{R})$ be bounded below. Then for every $t \geq 0$ the function $\mathcal{F}_t : C \to \mathbb{R}$, defined by*

$$\mathcal{F}_t(\gamma) = e^{-\int_0^t v(\gamma(\tau))d\tau},$$

is integrable with respect to the Wiener measure, and

$$\int\limits_C \mathcal{F}_t d\mu_W = \lim_{N\to\infty} \int\limits_{\mathbb{R}^n} \dots \int\limits_{\mathbb{R}^n} \exp\{-\tfrac{t}{N} \sum_{k=1}^N v(\mathbf{q}_k)\} P(\mathbf{q}_N, \mathbf{q}_{N-1}; \tfrac{t}{N}) \dots$$
$$\dots P(\mathbf{q}_1, 0; \tfrac{t}{N}) d^n\mathbf{q}_1 \dots d^n\mathbf{q}_N.$$

PROOF. For $\gamma \in C$,

$$\int_0^t v(\gamma(\tau))d\tau = \lim_{N\to\infty} \sum_{k=1}^N v(\gamma(t_k))\Delta t,$$

where $t_k = \frac{kt}{N}$ and $\Delta t = \frac{t}{N}$. Since by definition every function $\sum_{k=1}^N v(\gamma(t_k))\Delta t$ is measurable with respect to the Wiener measure on C, the function $\mathcal{F}_t$ is measurable as a point-wise limit of a sequence of measurable functions. The function $\mathcal{F}_t$ is bounded and, therefore, is integrable on C with respect to the Wiener measure. Finally, by the dominated convergence theorem,

$$\int\limits_C \mathcal{F}_t d\mu_W = \lim_{N\to\infty} \int\limits_C \exp\left\{-\sum_{k=1}^N v(\gamma(t_k))\Delta t\right\} d\mu_W(\gamma),$$

and the result follows. $\square$

REMARK. Note the limit in Proposition 2.1 exists because the function $\mathcal{F}_t$ is integrable, and not the other way around. This is similar to an elementary calculus argument that the limit

$$\lim_{n\to\infty}(1+2+\cdots+n-\log n)$$

exists since the integral

$$\int_0^1\left(\frac{1}{x}-\left[\frac{1}{x}\right]\right)dx$$

is convergent. Here $[x]$ stands for the largest integer not greater then x.

2.2. Conditional Wiener measure and Feynman-Kac formula. Let

$$\Omega_{t,t'}^{\mathbf{q},\mathbf{q}'}=\{\gamma\in\prod_{t\leq\tau\leq t'}\widehat{\mathbb{R}}^n:\gamma(t)=\mathbf{q},\gamma(t')=\mathbf{q}'\}$$

be space of all paths which start at $\mathbf{q}\in\mathbb{R}^n$ at time t and end at $\mathbf{q}'\in\mathbb{R}^n$ at t', and let $C_{t,t'}^{\mathbf{q},\mathbf{q}'}$ be the subspace of continuous paths. Conditional Wiener measure $\mu_W^{\mathbf{q},\mathbf{q}'}$ on $\Omega_{t,t'}^{\mathbf{q},\mathbf{q}'}$ is defined analogously. We replace a positive linear functional l on $C(\Omega)$ by a positive linear functional $l_{t,t'}^{\mathbf{q},\mathbf{q}'}$ on $C(\Omega_{t,t'}^{\mathbf{q},\mathbf{q}'})$, which for $\varphi\in C_{fin}(\Omega_{t,t'}^{\mathbf{q},\mathbf{q}'})$ is defined by

$$l_{t,t'}^{\mathbf{q},\mathbf{q}'}(\varphi)=\int\limits_{\Omega_{t,t'}^{\mathbf{q},\mathbf{q}'}}\varphi\,d\mu_W^{\mathbf{q},\mathbf{q}'}=\int\limits_{\mathbb{R}^n}\dots\int\limits_{\mathbb{R}^n}F(\mathbf{q}_1,\dots,\mathbf{q}_m)P(\mathbf{q}',\mathbf{q}_m;t'-t_m)\dots$$

$$\dots P(\mathbf{q}_1,\mathbf{q};t_1-t)d^n\mathbf{q}_1\dots d^n\mathbf{q}_m,$$

where $t\leq t_1\leq\cdots\leq t_m\leq t'$ and $\varphi(\gamma)=F(\gamma(t_1),\dots,\gamma(t_m))$. As in the case of Wiener measure, conditional Wiener measure is supported on continuous paths and

$$\mu_W^{\mathbf{q},\mathbf{q}'}(C(\Omega_{t,t'}^{\mathbf{q},\mathbf{q}'}))=P(\mathbf{q}',\mathbf{q};t'-t).$$

Now it is easy to define a Wiener measure μ_W^{loop} on the space $\mathcal{L}_{t,t'}$ of based loops in $\widehat{\mathbb{R}}^n$, parameterized by $[t,t']$. Namely, the space $\mathcal{L}_{t,t'}$ is a disjoint union of the spaces $C(\Omega_{t,t'}^{\mathbf{q},\mathbf{q}})$ of closed paths starting and ending at $\mathbf{q}\in\widehat{\mathbb{R}}^n$. By definition, a function $\varphi:\mathcal{L}_{t,t'}\to\mathbb{C}$ is integrable, if $\varphi|_{C(\Omega_{t,t'}^{\mathbf{q},\mathbf{q}})}$ is measurable with respect to $\mu_W^{\mathbf{q},\mathbf{q}}$ for all $\mathbf{q}\in\widehat{\mathbb{R}}^n$, and if the function $\int_{C(\Omega_{t,t'}^{\mathbf{q},\mathbf{q}})}\varphi\,d\mu_W^{\mathbf{q},\mathbf{q}}:\mathbb{R}^n\to\mathbb{C}$ is Lebesgue integrable on $\mathbb{R}^n$. Then

$$\int\limits_{\mathcal{L}_{t,t'}}\varphi\,d\mu_W^{loop}=\int\limits_{\mathbb{R}^n}\int\limits_{C(\Omega_{t,t'}^{\mathbf{q},\mathbf{q}})}\varphi\,d\mu_W^{\mathbf{q},\mathbf{q}}\,d^n\mathbf{q}.$$

Let

$$H=H_0+V=\frac{\hbar^2}{2m}\mathbf{P}^2+v(\mathbf{Q})$$

be the Schrödinger operator on $L^2(\mathbb{R}^n, d^n\mathbf{q})$ with continuous, bounded below and real-valued potential $v(\mathbf{q})$. Let $L_\hbar(\mathbf{q}', \mathbf{q}; t', t)$, $t' > t$, be the integral kernel of the operator $e^{-\frac{t'-t}{\hbar}H}$. Here is the meain result of this section.

THEOREM 2.1 (Feynman-Kac formula).

$$L_\hbar(\mathbf{q}', \mathbf{q}; t', t) = \int\limits_{C_{t,t'}^{\mathbf{q},\mathbf{q}'}} e^{-\frac{1}{\hbar}\int_t^{t'} v(\gamma(\tau))d\tau} d\mu_W^{\mathbf{q},\mathbf{q}'}(\gamma).$$

PROOF. Setting $T = t' - t$ and $\Delta t = \frac{T}{N}$, we have by Trotter product formula

$$e^{-\frac{T}{\hbar}H} = \lim_{N\to\infty} (e^{-\frac{\Delta t}{\hbar}H_0} e^{-\frac{\Delta t}{\hbar}V})^N.$$

Let $L_\hbar^{(N)}(\mathbf{q}', \mathbf{q}; t', t)$ be the integral kernel of the operator $(e^{-\frac{\Delta t}{\hbar}H_0} e^{-\frac{\Delta t}{\hbar}V})^N$. Computing this kernel as in Sections 1.2-1.3 of Chapter 4, and using the definition of the conditional Wiener measure we obtain

$$L_\hbar^{(N)}(\mathbf{q}', \mathbf{q}; t', t) = \int\limits_{C_{t,t'}^{\mathbf{q},\mathbf{q}'}} \exp\left\{-\frac{1}{\hbar}\sum_{k=1}^N v(\gamma(t_k))\Delta t\right\} d\mu_W^{\mathbf{q},\mathbf{q}'}(\gamma),$$

and applying the dominated convergence theorem completes the proof. $\square$

It is very instructive to compare Feynman and Wiener integrals. Informally, conditional Wiener measure can be written as

$$\mathscr{D}\mathbf{q}_W = e^{-\frac{m}{2\hbar}\int_t^{t'} \dot{\mathbf{q}}^2 d\tau} \mathscr{D}_\hbar\mathbf{q},$$

where

$$\mathscr{D}_\hbar\mathbf{q} = \lim_{N\to\infty} \left(\frac{m}{2\pi\hbar\Delta t}\right)^{N/2} \prod_{k=1}^{N-1} d^n\mathbf{q}_k.$$

Of course, neither the "measure" $\mathscr{D}\mathbf{q}$ exists: the product is divergent, nor the trajectory $\mathbf{q}(\tau)$ is differentiable: the integral $\int_t^{t'} \dot{\mathbf{q}}^2 d\tau$ is divergent. However, due to the presence of the negative sign in the exponential we get "the ratio of infinities" and the resulting expression for the Wiener measure makes a precise sense! The corresponding "measure" for the Feynman path integral is obtained by replacing $\hbar$ by $i\hbar$. In this case the exponential factor can not compensate for the divergence of $\mathscr{D}_{i\hbar}\mathbf{q}$ since it is a complex number of modulus 1 for differentiable trajectories and has no meaning for non-differentiable ones.

Still, the advantage of Feynman path integral, besides having a rigorous definition as limit of multiple integrals, is that the corresponding representation for the propagator

$$K_\hbar(\mathbf{q}', t'; \mathbf{q}, t) = \int\limits_{\substack{\mathbf{q}(t')=\mathbf{q}' \\ \mathbf{q}(t)=\mathbf{q}}} e^{\frac{i}{\hbar}\int_t^{t'} L(\mathbf{q},\dot{\mathbf{q}})d\tau} \mathscr{D}_{i\hbar}\mathbf{q},$$

where $L(\mathbf{q},\dot{\mathbf{q}})=\dfrac{\mathbf{p}^2}{2m}-v(\mathbf{q})$, shows a deep relation between quantum and classical mechanics, which manifests itself as $\hbar\to 0$. Similarly, the Feynman-Kac formula can formally rewritten as

$$L_\hbar(\mathbf{q}',t';\mathbf{q},t)=\int\limits_{\substack{\mathbf{q}(t')=\mathbf{q}'\\ \mathbf{q}(t)=\mathbf{q}}} e^{-\frac{1}{\hbar}\int_t^{t'} h(\mathbf{q},\dot{\mathbf{q}})d\tau}\mathscr{D}_\hbar\mathbf{q},$$

where $h(\mathbf{q},\dot{\mathbf{q}})=\dfrac{\mathbf{p}^2}{2m}+v(\mathbf{q})$, and we no longer see the presence of the action functional of the corresponding classical system.

2.3. Relation between Wiener and Feynman integrals. The simplest example which illustrates the nature of the relation between Wiener and Feynman integrals is the following. Let f be a smooth bounded function on $\mathbb{R}$ such that $f'(x)=O(x^{-1})$ as $x\to\infty$. The Gaussian integral $\int_{-\infty}^{\infty}f(x)e^{-x^2}dx$ is absolutely convergent, whereas the integral $\int_{-\infty}^{\infty}f(x)e^{ix^2}dx$ is convergent only as $\lim_{M,N\to\infty}\int_{-M}^{N}f(x)e^{ix^2}dx$, as simple integration by parts shows. We also have

$$\int_{-\infty}^{\infty}f(x)e^{ix^2}dx=\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}f(x)e^{(i-\varepsilon)x^2}dx,$$

so that conditionally convergent integral $\int_{-\infty}^{\infty}f(x)e^{ix^2}dx$ is interpreted as as a limit $\varepsilon\to\infty$ of an integral of bounded function $f(x)$ with respect respect to the complex-valued Gaussian measure $e^{(i-\varepsilon)x^2}dx$.

It is tempting to extend this interpretation for Wiener in integrals and for a complex diffusion coefficient D with $\operatorname{Re}D>0$ define a complex-valued Wiener measure by the same formula (2.2). However, a theorem of Cameron states that corresponding linear function l is no longer bounded on $C_{fin}(\Omega)$, so that this approach does not work. However, under our assumptions on a potential $v(\mathbf{q})$ it easy to show by using the profuct Trotter formula that $L_\hbar(\mathbf{q}',t';\mathbf{q},t)$, defined for $\hbar>0$, admits an analytic continuation into the half-plane $\operatorname{Re}\hbar>0$ and

$$K_\hbar(\mathbf{q}',t';\mathbf{q},t)=\lim_{\varepsilon\to 0^+}L_{i\hbar-\varepsilon}(\mathbf{q}',t';\mathbf{q},t).$$

This establishes the precise relation between Wiener and Feynman integrals for the case of quantum particle.

2.4. Gaussian Wiener integrals. In Section 2 of Chapter 4 we evaluated Gaussian Feynman integrals in terms of the zeta-function regularized determinants. Here we consider the corresponding problem for Gaussian Wiener integrals.

2.4.1. *Dirichlet boundary conditions.* Let $A = -\dfrac{d^2}{dx^2} + u(x)$ with $u \in C^1[0,T]$, $u \geq 0$, be the Sturm-Liouville operator on $[0,T]$ with Dirichlet boundary conditions. We have the following result.

THEOREM 2.2.

$$\int\limits_{C_{0,T}^{0,0}} e^{-\frac{m}{2\hbar}\int_0^T u(x)y^2(x)dx} d\mu_W^{0,0}(y) = \sqrt{\frac{m}{\pi\hbar \det' A}}.$$

PROOF. Using the dominated convergence theorem and finite-dimensional Gaussian integration formula we get

$$\int\limits_{C_{0,T}^{0,0}} e^{-\frac{m}{2\hbar}\int_0^T u(x)y^2(x)dx} d\mu_W^{0,0}(y) = \lim_{n\to\infty} \left(\frac{m}{2\pi\hbar\Delta t}\right)^{n/2} \int\limits_{\mathbb{R}^{n-1}} \cdots \int$$

$$\exp\left\{-\frac{m}{2\hbar}\sum_{k=0}^{n-1}\left(\left(\frac{y_{k+1}-y_k}{\Delta t}\right)^2 + u(t_k)y_k^2\right)\Delta t\right\}\prod_{k=1}^{n-1} dy_k$$

$$= \lim_{n\to\infty}\sqrt{\frac{m}{2\pi\hbar\,\det A^{(n)}}},$$

where $y_0 = y_n = 0$, $\Delta t = \frac{T}{n}$, and

$$A^{(n)} = \begin{pmatrix} b_1 & c_1 & 0 & \dots & 0 & 0 \\ a_1 & b_2 & c_2 & \dots & 0 & 0 \\ 0 & a_2 & b_3 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & b_{n-2} & c_{n-2} \\ 0 & 0 & 0 & \dots & a_{n-2} & b_{n-1} \end{pmatrix},$$

where $a_1 = -1$, $b_1 = 2\Delta t + u(t_1)(\Delta t)^3$, $c_1 = -\Delta t$ and $a_k = c_k = -1$, $b_k = 2 + u(t_k)(\Delta t)^2$, $k = 2,\dots,n-1$. Denote by $y_k^{(n)}$, $k = 2,\dots,n$, the $(k-1)\times(k-1)$ minor of $A^{(n)}$ corresponding to the upper-left corner of $A^{(n)}$, so that $\det A^{(n)} = y_n^{(n)}$.The sequence $y_k^{(n)}$ satisfies the recurrence relation

$$y_{k+1}^{(n)} = (2 + u(t_k)(\Delta t)^2)y_k^{(n)} - y_{k-1}^{(n)}, \quad k = 3,\dots,n-1,$$

with the initial conditions

$$y_2^{(n)} = 2\Delta t + u(t_1)(\Delta t)^3, \quad y_3^{(n)} = 3\Delta t + 2(u(t_1)+u(t_2))(\Delta t)^3 + u(t_1)u(t_2)(\Delta t)^5.$$

We rewrite the recurrence relation as

$$\frac{y_{k+1}^{(n)} + y_{k-1}^{(n)} - 2y_k^{(n)}}{(\Delta t)^2} = u(t_k), \quad k = 3,\dots,n-1. \tag{2.3}$$

According the method of finite-differences for solving initial value problems for ordinary differential equations, we obtain that when

$$\lim_{k,n\to\infty}\frac{k}{n}T = x \in [0,T],$$

then

$$\lim_{k,n\to\infty} y_k^{(n)} = y(x),$$

where $y(x)$ satisfies the differential equation

$$-y'' + u(x)y = 0,$$

and the initial conditions

$$y(0) = \lim_{n\to\infty} y_2^{(n)} = 0, \quad y'(0) = \lim_{n\to\infty} \frac{y_3^{(n)} - y_2^{(n)}}{\Delta t} = 1.$$

Using Theorem 2.1 in Chapter 4, we obtain from here that $\lim_{n\to\infty} \det A^{(n)} = \frac{1}{2}\det' A$. $\square$

2.4.2. *Periodic boundary conditions.* Let $A = -\dfrac{d^2}{dx^2} + u(x)$ with $u \in C^1[0,T]$, $u(0) = u(T)$, $u \geq 0$, be the Sturm-Liouville operator on $[0,T]$ with periodic boundary conditions. We have the following result.

THEOREM 2.3.

$$\int\limits_{\mathcal{L}_{[0,T]}} e^{-\frac{m}{2\hbar}\int_0^T u(x)y^2(x)dx} d\mu_W^{loop}(y) = \frac{1}{\sqrt{\det' A}}.$$

PROOF. As in the proof of Theorem 2.2, we have

$$\int\limits_{\mathcal{L}_{0,T}} e^{-\frac{m}{2\hbar}\int_0^T u(x)y^2(x)dx} d\mu_W^{loop}(y) = \lim_{n\to\infty} \left(\frac{m}{2\pi\hbar\Delta t}\right)^{n/2} \int\cdots\int\limits_{\mathbb{R}^n}$$

$$\exp\left\{-\frac{m}{2\hbar}\sum_{k=0}^{n-1}\left(\left(\frac{y_{k+1}-y_k}{\Delta t}\right)^2 + u(t_k)y_k^2\right)\Delta t\right\}\prod_{k=1}^{n} dy_k$$

$$= \lim_{n\to\infty} \frac{1}{\sqrt{\det A_n}},$$

where $y_0 = y_n$, $\Delta t = \frac{T}{n}$ and A_n is the following $n \times n$ matrix

$$A_n = \begin{pmatrix} b_0 & -1 & 0 & \dots & 0 & -1 \\ -1 & b_1 & -1 & \dots & 0 & 0 \\ 0 & -1 & b_2 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & b_{n-2} & -1 \\ -1 & 0 & 0 & \dots & -1 & b_{n-1} \end{pmatrix},$$

where $b_k = 2 + u(t_k)(\Delta t)^2$, $k = 0, 1, \dots, n-1$. We compute $\det A_n$ by the following elegant argument. First, note that the real λ is an eigenvalue of A_n if only if the system of linear algebraic equations

$$y_{k+1} + y_{k-1} - (2 + u(t_k)(\Delta t)^2)y_k = \lambda y_k, \quad k = 0, \dots, n-1, \tag{2.4}$$

with "initial conditions" y_{-1} and y_0 has a "periodic solution" — a solution $\{y_k\}_{k=1}^n$ satisfying $y_{n-1} = y_{-1}$ and $y_n = y_0$. Now for given λ let $v_k^{(1)}(\lambda)$

and $v_k^{(2)}(\lambda)$ be the solutions of (2.4) with corresponding initial conditions $v_{-1}^{(1)}(\lambda)=1$, $v_0^{(1)}(\lambda)=0$ and $v_{-1}^{(2)}(\lambda)=0$, $v_0^{(2)}(\lambda)=1$, and let

$$T_n(\lambda)=\begin{pmatrix} v_{n-1}^{(1)}(\lambda) & v_{n-1}^{(2)}(\lambda)\\ v_n^{(1)}(\lambda) & v_n^{(2)}(\lambda)\end{pmatrix}.$$

It is easy to show that "Wronskian" $v_{k-1}^{(1)}(\lambda)v_k^{(2)}(\lambda)-v_k^{(1)}(\lambda)v_{k-1}^{(1)}(\lambda)$ does not depend on k, so that $\det T_n(\lambda)=1$. Since every solution y_k of the initial value problem for (2.4) is a linear combination of solutions $v_k^{(1)}(\lambda)$ and $v_k^{(2)}(\lambda)$,

$$\begin{pmatrix} y_{n-1}\\ y_n\end{pmatrix}=T_n(\lambda)\begin{pmatrix} y_{-1}\\ y_0\end{pmatrix}.$$

This shows that λ is an eigenvalue of A_n if and only if $\det(T_n(\lambda)-I_2)=0$. Moreover, the multiplicity of λ as the eigenvalue of A_n is the same as the eigenvalue of $T_n(\lambda)-I_2$. Finally, it is easy to show that $v_{n-1}^{(1)}(\lambda)=O(\lambda^{n-1})$, $v_n^{(2)}(\lambda)=\lambda^n+O(\lambda^{n-1})$ as $\lambda\to\infty$, so that

$$\det(A_n-\lambda I_n)=-\det(T_n(\lambda)-I_2)=v_{n-1}^{(1)}(\lambda)+v_n^{(2)}(\lambda)-2.$$

To compute $\lim_{n\to\infty}\det A_n$, denote by $y_k^{(1)}(\lambda)$ and $y_k^{(2)}(\lambda)$ two solutions of (2.4) with initial conditions

$$\begin{pmatrix} y_{-1}^{(1)}(\lambda)\\ y_0^{(1)}(\lambda)\end{pmatrix}=\begin{pmatrix} 1\\ 1+(\Delta t)^2\end{pmatrix}\quad\text{and}\quad\begin{pmatrix} y_{-1}^{(2)}(\lambda)\\ y_0^{(2)}(\lambda)\end{pmatrix}=\begin{pmatrix} \Delta t\\ \Delta t\end{pmatrix}$$

correspondingly. Expressing solutions $v_k^{(1)}(\lambda)$ and $v_k^{(2)}(\lambda)$ through $y_k^{(1)}(\lambda)$ and $y_k^{(2)}(\lambda)$, we get

$$\det(A_n-\lambda I_n)=y_{n-1}^{(1)}(\lambda)-\Delta t\,y_{n-1}^{(2)}(\lambda)+\frac{y_n^{(2)}(\lambda)-y_{n-1}^{(1)}(\lambda)}{\Delta t}-2.$$

Now it follows from the method of finite differences that

$$\lim_{n\to\infty}\det(A_n-\lambda I_n)=y_1(T,\lambda)+y_2'(T,\lambda)-2=\det(A-\lambda I)$$

by Theorem 2.2 in Chapter 4. □

2.4.3. *Traces.* Here we assume that the Hamiltonian operator $H=H_0+V$ has a pure discrete spectrum and that $\operatorname{Tr}e^{-\frac{T}{\hbar}H}$ exists. For instance, this is the case when $v(\mathbf{q})\to\infty$ as $\mathbf{q}\to\infty$ "fast enough".

PROPOSITION 2.2.

$$\operatorname{Tr}e^{-\frac{T}{\hbar}H}=\int_{\mathcal{L}_{0,T}} e^{-\frac{1}{\hbar}\int_0^T v(\gamma(t))dt}d\mu_W^{loop}(\gamma).$$

PROOF. It immediately follows from Feynman-Kac formula and Lidskij theorem. □

As an illustration, we use this result to compute $\operatorname{Tr} e^{-\frac{T}{\hbar}H}$ when $H = H_{osc} = \dfrac{m}{2}$ Since the eigenvalues of H_{osc} are $E_n = \hbar\omega(n+\frac{1}{2})$, we have

$$\operatorname{Tr} e^{-\frac{T}{\hbar}H_{osc}} = \sum_{n=0}^{\infty} e^{-\frac{T}{\hbar}E_n} = e^{-\frac{\omega T}{2}} \sum_{n=0}^{\infty} e^{-\omega T n} = \frac{1}{2\sinh\frac{\omega T}{2}}.$$

The same result can be also obtained without using the explicit form of the eigenvalues of the harmonic oscillator. Namely, using Proposition 2.2, Theorem 2.3 and formula (2.15) in Chapter 4, we get

$$\operatorname{Tr} e^{-\frac{T}{\hbar}H_{osc}} = \frac{1}{\sqrt{\det' A_{i\omega}}} = \frac{1}{2\sinh\frac{\omega T}{2}}.$$

CHAPTER 6

Spin and Identical Particles

1. Spin

So far we have tacitly assumed that the Hilbert space space for a quantum mechanical particle is $\mathscr{H} = L^2(\mathbb{R}^3)$. Based on this assumption, in Chapter 3 we found the energy levels of the hydrogen atom. In particular, in the ground state the quantum angular momentum operator M_3 has eigenvalue 0. However, the famous Stern-Gerlach experiment has shown that the hydrogen atom also has a "magnetic angular momentum", whose third component in the ground state may take two values which differ by a sign. Therefore in addition to the "mechanical" angular momentum operator $\mathbf{M}$ with components M_1, M_2, M_3, the electron also has the "internal angular momentum" operator $\mathbf{S}$ with components S_1, S_2, S_3, called *spin*, which is independent of its position in the space. The spin describes internal degrees of freedom of the electron. As the result, the number of the states is doubled and the Hilbert space of states is $\mathscr{H}_S = \mathscr{H} \otimes \mathbb{C}^2$. Equivalently, $\mathscr{H}_S$ consists of two-component vectors

$$\Psi = \begin{pmatrix} \psi_1(\mathbf{q}) \\ \psi_2(\mathbf{q}) \end{pmatrix}$$

and

$$\|\Psi\|^2 = \int_{\mathbb{R}^3} |\psi_1(\mathbf{q})|^2 d^3\mathbf{q} + \int_{\mathbb{R}^3} |\psi_2(\mathbf{q})|^2 d^3\mathbf{q}.$$

To every observable A in $\mathscr{H}$ there corresponds an observable $A \otimes I_2$ in $\mathscr{H}_S$, given by the 2×2 block-diagonal matrix $\left(\begin{smallmatrix} A & 0 \\ 0 & A \end{smallmatrix}\right)$. Observables of the form $I \otimes S$, where I is the identity operator in $\mathscr{H}$ and S is a self-adjoint operator in $\mathbb{C}^2$, characterized the inner degrees of freedom and commute with all observables $A \otimes I_2$. The complete set of the observables in $\mathscr{H}_S$ consists of the operators $Q_1 \otimes I_2, Q_2 \otimes I_2, Q_3 \otimes I_2$ and $I \otimes S_1, I \otimes S_2, I \otimes S_3$, where S_j are the spin operators — the traceless self-adjoint operators on $\mathbb{C}^2$ satisfying the same commutation relations as the quantum operators of the angular momentum, i.e.,

$$[S_1, S_2] = i\hbar S_3, \quad [S_2, S_3] = i\hbar S_1, \quad [S_3, S_1] = i\hbar S_2.$$

In terms of the standard basis $e_1 = \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$, $e_2 = \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$ of $\mathbb{C}^2$, $S_j = \frac{\hbar}{2}\sigma_j$, $j = 1, 2, 3$, where σ_j are popular in physics Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

It is convenient to represent $\Psi = \left(\begin{smallmatrix}\psi_1\\ \psi_2\end{smallmatrix}\right) \in \mathscr{H}_S$ as a function $\psi(\mathbf{q},\sigma)$, where $\mathbf{q}\in\mathbb{R}^3$ and σ takes two values $\frac{1}{2}$ and $-\frac{1}{2}$, by setting $\psi(\mathbf{q},\frac{1}{2}) = \psi_1(\mathbf{q})$ and $\psi(\mathbf{q},-\frac{1}{2}) = \psi_2(\mathbf{q})$. Then the operator S_3 becomes a multiplication by $\hbar\sigma$ operator,

$$S_3\psi(\mathbf{q},\sigma) = \hbar\sigma\psi(\mathbf{q},\sigma),$$

and

$$S_1\psi(\mathbf{q},\sigma) = \hbar|\sigma|\psi(\mathbf{q},-\sigma), \quad S_2\psi(\mathbf{q},\sigma) = i\hbar\sigma\psi(\mathbf{q},-\sigma).$$

Here and in what follows we will always assume that the spin operators act on the variable σ and will often write S_j instead of $I\otimes S_j$. The operator $S^2 = S_1^2 + S_2^2 + S_3^2$ is called the square of the total splin operator and $S^2 = \hbar^2 s(s+1)I_2$, where $s = |\sigma| = \frac{1}{2}$. In physics terminology, electron has spin $\frac{1}{2}$.

Mathematical interpretation of spin is provided by the representation theory of the Lie algebra su(2). Namely operators

$$x_\pm = \frac{1}{\hbar}(S_1 \pm iS_2) = \frac{\sigma_1 \pm i\sigma_2}{2}$$

and $h = \frac{2S_3}{\hbar} = \sigma_3$ satisfy su(2) commutations relations

$$[h, x_\pm] = \pm 2x_\pm, \quad [x_+, x_-] = h,$$

and thus define an irreducible an irreducible two-dimensional representation of su(2). The highest weight of the representation — the maximal eigenvalue of the generator h of the Cartan subalgebra of su(2) — is $2s = 1$. This representation is said to be spin $\frac{1}{2}$ representation and is denoted by $D_{\frac{1}{2}}$. It is known that all irreducible representations of su(2) are highest weight finite-dimensional representations D_s of dimension $2s+1$, parameterized by the highest weight — the spin $s = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$. The representation D_s can be described as the vector space of polynomials $f(z)$ of degree not greater than $2s$ with the inner product

$$\langle f, g\rangle = \frac{(2s+1)!}{\pi}\int_{\mathbb{C}} \frac{f(z)\overline{g(z)}}{(1+|z|^2)^{2s+2}} d^2z, \tag{1.1}$$

with the generators $h, x_\pm$ represented by the operators

$$h = z\frac{d}{dz}, \quad x_+ = \frac{d}{dz}, \quad x_- = z^2\frac{d}{dz} - 2sz.$$

It is easy to verify that $h^* = h$ and $x_+ = x_-^*$ with respect to the inner product (1.1). This representation of the Lie algebra su(2) is associated with the representation of the Lie group $G = \mathrm{SU}(2)$, defined by

$$\rho_s(g)(f)(z) = (\bar\beta z + \alpha)^{2s} f\left(\frac{\bar\alpha z - \beta}{\bar\beta z + \alpha}\right),$$

where $g = \left(\begin{smallmatrix}\alpha & \beta\\ -\bar\beta & \bar\alpha\end{smallmatrix}\right) \in \mathrm{SU}(2)$ and $f \in D_s$.

Now we can specify the first axiom **A1** in Section 1.1 of Chapter 2 for the case of particles with spin.

DEFINITION. A quantum mechanical particle with a spin $s \in \{0, \frac{1}{2}, 1, \frac{3}{2}, \dots\}$ is associated with a Hilbert space of states $\mathscr{H}_S = L^2(\mathbb{R}^3) \otimes D_s$, where D_s is the irreducible representation of su(2) of spin s. Corresponding spin operators are given by $I \otimes S_j$, $j = 1, 2, 3$, where

$$S_1 = \frac{\hbar}{2}(x_+ + x_-), \quad S_2 = \frac{i\hbar}{2}(x_+ - x_-), \quad S_3 = \frac{\hbar}{2}h,$$

and h, x_+, x_- are self-adjoint operators in $\mathbb{C}^{2s+1}$ corresponding to the standard generators su(2). Particles with integer spin are called *bosons*, and particle with half-integer spin are called *fermions*.

As in the case $s = \frac{1}{2}$, the complete set of observables for a quantum particle of spin s consists of position operators $Q_1 \otimes I_{2s+1}, Q_2 \otimes I_{2s+1}, Q_3 \otimes I_{2s+1}$, and spin operators $I \otimes S_1, I \otimes S_2, I \otimes S_3$. The total operators of angular momentum in $\mathscr{H}_S$ are

$$J_j = M_j \otimes I_{2s+1} + I \otimes S_j, \quad j = 1, 2, 3,$$

which satisfy the commutation relations

$$[J_j, J_k] = i\hbar\varepsilon_{jkl}J_l, \quad j, k, l = 1, 2, 3.$$

As the spin operators S_j, the operatorsJ_j of total angular momentum are related with self-adjoint operators corresponding to the representation of the Lie algebra su(2) is the Hilbert space $\mathscr{H}_S$, which is associated with the unitary representation $R \otimes \rho_s$ of the Lie group SU(2) in $\mathscr{H}_S = L^2(\mathbb{R}^3) \otimes D_s$. Here R is the unitary representation of SU(2) in $L^2(\mathbb{R}^3)$, defined by

$$(R(g)\psi)(\mathbf{q}) = \psi(\mathrm{Ad}g^{-1}\mathbf{q}), \quad \mathbf{q} \in \mathbb{R}^3,$$

where $\psi \in L^2(\mathbb{R}^3)$, $g \in \mathrm{SU}(2)$, and Ad is the adjoint representation of SU(2) in $\mathrm{su}(2) \simeq \mathbb{R}^3$. For $\mathbf{a} = (a_1, a_2, a_3) \in \mathbb{R}^3$ setting $g(\mathbf{a}) = e^{-i\hbar(a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3)} \in \mathrm{SU}(2)$, we have

$$\frac{\partial}{\partial a_i}(R \otimes \rho_s)(g(\mathbf{a}))\bigg|_{\mathbf{a}=0} = iJ_j, \quad j = 1, 2, 3.$$

2. Charged spin particle in the magnetic field

2.1. Pauli Hamiltonian.

2.2. Electron in a magnetic field.

3. System of Identical Particles

Consider a quantum system of n particles of spins $s_1, \dots, s_n$. According to the basic principles of quantum mechanics, the Hilbert space of states of the system is given by

$$\mathscr{H} = \mathscr{H}_{s_1} \otimes \cdots \otimes \mathscr{H}_{s_n} = L^2(\mathbb{R}^3) \otimes D_{s_1} \cdots \otimes L^2(\mathbb{R}^3) \otimes D_{s_n}.$$

Introducing the variables $\boldsymbol{\xi}_i = (\mathbf{q}_i, \sigma_i)$, where $\mathbf{q}_i \in \mathbb{R}^3$ and $\sigma_i \in \{-s_i, -s_i + 1, \dots, s_i - 1, s_i\}$, the wave function of the system can be written as $\Psi(\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_n)$. Corresponding n-particle Hamiltonian (without the spin interaction) in the Schrödinger representation can be written as

$$H = -\sum_{i=1}^{n} \frac{\hbar^2}{2m_i} \Delta_i + \sum_{i=1}^{n} V_i(\mathbf{q}_i) + \sum_{1 \leq i < k \leq n} U_{ik}(\mathbf{q}_i - \mathbf{q}_k),$$

where the first term is the operator of kinetic energy of the system of n particles, the second term describes the interaction of the particles with the corresponding external fields, and the last term describes the pair-wise interaction of particles.

When the particles are identical, i.e., when $m_1 = \cdots = m_n = m$ and $s_1 = \cdots = s_n = s$, the symmetric group Sym_n on n elements acts on $\mathscr{H}$ by

$$P_\pi \Psi(\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_n) = \Psi(\boldsymbol{\xi}_{\pi_1}, \dots, \boldsymbol{\xi}_{\pi_n}), \quad \pi \in \mathrm{Symm}(n).$$

Since in this case it is natural to assume that $V_i = V$ and $U_{ik} = U$ for all $i = 1, \dots, n$ and $1 \leq i < k \leq n$, the Hamiltonian H commutes with the $\mathrm{Symm}(n)$-action:

$$[H, P_\pi] = 0 \quad \text{for all} \quad \pi \in \mathrm{Symm}(n).$$

As the result, H can be restricted to the Sym_n-invariant subspaces of $\mathscr{H}$, in particular to the subspace $\mathscr{H}_{sym}$ of totally symmetric functions $\Psi(\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_n)$, and to the subspace $\mathscr{H}_{alt}$ of totally antisymmetric functions. It turns out that in the case of identical particles the Hilbert space of states is defined as follows.

The Pauli Principle of Identical Particles. The Hilbert space of states for the system of n identical particles of spin s is the totally symmetric subspace $\mathscr{H}_{sym}$ of $(L^2(\mathbb{R}^3) \otimes D_s)^{\otimes^n}$ for the case of bosons (integer spin), and the totally antisymmetric subspace $\mathscr{H}_{alt}$ for the case of fermions (half-integer spin).

This is another postulate of quantum mechanics, also known as *Pauli exclusion principle for fermions.*

CHAPTER 7

Fermion Systems and Supersymmetry

1. Canonical Anticommutation Relations

1.1. Motivation. As was discussed in Section 3.1 of Chapter 2, the Hilbert space $\mathscr{H} = L^2(\mathbb{R})$ for the one-dimensional quantum particle can be described in terms of the creation and annihilation operators. Namely, the operators

$$a = \frac{1}{\sqrt{2\hbar}}(\omega Q + iP) \quad \text{and} \quad a^* = \frac{1}{\sqrt{2\hbar}}(\omega Q - iP)$$

satisfy the canonical commutation relation

$$[a, a^*] = I$$

on $W^{2,2}(\mathbb{R}) \cap \hat{W}^{2,2}(\mathbb{R})$, and the vectors

$$\psi_k = \frac{(a^*)^k}{\sqrt{k!}}\psi_0, \quad k \in \mathbb{Z}_{\geq 0},$$

where $\psi_0 \in \mathscr{H}$ satisfies $a\psi_0 = 0$, form an orthonormal basis for $\mathscr{H}$. Corresponding operator $N = a^*a$ is self-adjoint and has an integer spectrum,

$$N\psi_k = k\psi_k, \ \ k \in \mathbb{Z}_{\geq 0}.$$

Similarly, for several degrees of freedom, $\mathscr{H} = L^2(\mathbb{R}^n)$ and the creation and annihilation operators

$$a_k^* = \frac{1}{\sqrt{2\hbar}}(\omega Q_k - iP_k) \quad \text{and} \quad a_k = \frac{1}{\sqrt{2\hbar}}(\omega Q_k + iP_k), \ \ k = 1, \dots, n,$$

satisfy canonical commutation relations

$$[a_k, a_l^*] = \delta_{kl} I \quad \text{and} \quad [a_k, a_l] = [a_k^*, a_l^*] = 0, \ \ k, l = 1, \dots, n. \tag{1.1}$$

There exists a vector $\psi_0 \in \mathscr{H}$ such that $a_k\psi_0 = 0$, $k = 1, \dots, n$ ($\psi_0(\mathbf{q}) = (\pi\hbar)^{-n/4} e^{-\frac{\mathbf{q}^2}{2\hbar}}$), and the vectors

$$\psi_{k_1,\dots,k_n} = \frac{(a_1^*)^{k_1} \dots (a_n^*)^{k_n}}{\sqrt{k_1! \dots k_n!}}\psi_0, \quad (k_1, \dots, k_n) \in \mathbb{Z}_{\geq 0}^n,$$

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:

$$N\psi_{k_1,\dots,k_n} = (k_1 + \cdots + k_n)\psi_{k_1,\dots,k_n},$$

and the Hilbert space $\mathscr{H}$ decomposes into the direct sum of invariant subspaces

$$\mathscr{H} = \bigoplus_{k=0}^{\infty} \mathscr{H}_k, \tag{1.2}$$

where $N|_{\mathscr{H}_k} = kI|_{\mathscr{H}_k}$.

While studying the spin operators in the previous chapter, we found that for the quantum particle of spin $\frac{1}{2}$ the operators $\sigma_\pm = 2S_\pm/\hbar$ have the form

$$\sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \sigma_- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

are nilpotent, $\sigma_\pm^2 = 0$, and satisfy the following *anticommutation* relation

$$\sigma_+\sigma_- + \sigma_-\sigma_+ = I_2.$$

Introducing the notion of an anticommutator of two operators,

$$[A, B]_+ = AB + BA,$$

we can say that the operators $a = \sigma_-$ and $a^* = \sigma_+$ satisfy *canonical anticommutation relations*

$$[a,a^*]_+ = I \quad \text{and} \quad [a, a]_+ = [a^*, a^*]_+ = 0.$$

The vectors $e_0 = \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$ and $a^*e_0 = \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$ form an orthonormal basis of $\mathbb{C}^2$, and

$$N = a^*a = \frac{1}{2}(\sigma_3 + I_2) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

In addition, the vector e_0 has the property $ae_0 = 0$. We thus say that the Hilbert space of a fermion particle with one degree of freedom is $\mathscr{H}_F = \mathbb{C}^2$, and it is generated by the creation and annihilation operators a and a^* satisfying canonical anticommutation relations.

Similarly, canonical anticommutation relations for several degrees of freedom have the form

$$[a_k, a_l^*]_+ = \delta_{kl}I \quad \text{and} \quad [a_k, a_l]_+ = [a_k^*, a_l^*]_+ = 0, \quad k, l = 1, \dots, n, \tag{1.3}$$

where operators a_j^* are adjoint to a_j, $j = 1, \dots, n$. These relations can be realized in the Hilbert space $\mathscr{H}_F = \underbrace{\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2}_{n} = \mathbb{C}^{2^n}$ as follows

$$a_j = \underbrace{\sigma_3 \otimes \cdots \otimes \sigma_3}_{j-1} \otimes a \otimes I_2 \otimes \cdots \otimes I_2, \tag{1.4}$$

$$a_j^* = \underbrace{\sigma_3 \otimes \cdots \otimes \sigma_3}_{j-1} \otimes a^* \otimes I_2 \otimes \cdots \otimes I_2, \tag{1.5}$$

$j = 1, \dots, n$. It is easy to see that this representation is irreducible, i.e., in there are no nontrivial subspaces of $\mathscr{H}_F$, invariant with respect to the operators a_j and a_j^*, $j = 1, \dots, n$. Moreover, the vector $\psi_0 = e_0 \otimes \cdots \otimes e_0 \in \mathscr{H}_F$ satisfies $a_j\psi_0 = 0$, $j = 1, \dots, n$, and the vectors

$$\psi_{k_1 \dots k_n} = (a_1^*)^{k_1} \dots (a_n^*)^{k_n}\psi_0, \quad (k_1, \dots, k_n) \in \{0, 1\}^n,$$

form an orthonormal basis for $\mathscr{H}_F$. The operator

$$N = \sum_{k=1}^{n} a_k^* a_k$$

is self-adjoint and has an integer spectrum:

$$N\psi_{k_1,\dots,k_n} = (k_1 + \cdots + k_n)\psi_{k_1,\dots,k_n},$$

and the Hilbert space $\mathscr{H}_F$ decomposes into the direct sum of invariant subspaces

$$\mathscr{H}_F = \bigoplus_{k=0}^{n} \mathscr{H}_k, \tag{1.6}$$

where $N|_{\mathscr{H}_k} = kI|_{\mathscr{H}_k}$.

1.2. Clifford algebras. 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 a 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 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 $\mathrm{Cl}(V, Q)$ is a $\mathbb{C}$-algebra with the generators $e_1, \dots, e_n$, satisfying the relations

$$[e_i, e_j]_+ = e_ie_j + e_je_i = 2\Phi(e_i, e_j), \quad i, j = 1, \dots, n.$$

The Clifford algebra $C(V)$ is a superalgebra with the $\mathbb{Z}_2$ grading descended from the tensor algebra $T(V)$. The natural map $V \hookrightarrow C(V)$ is injective and V is identified with its image in $C(V)$. The elements in V are odd. The definition of $C(V)$ is compatible with the field change: if $k \subset K$ is a field extension and $V_K = K \otimes_k V_k$, then

$$C(V_K) = K \otimes_k C(V_k).$$

If the field k is algebraically closed (e.g., $k = \mathbb{C}$), there always exists an orthonormal basis for V — a basis $\{e_i\}_{i=1}^n$ such that

$$\Phi(e_i, e_k) = \delta_{ik}, \quad i, k = 1, \dots, n.$$

In this case there is essentially one Clifford algebra C_n for every dimension n. If $k = \mathbb{R}$, there exists non-negative integers p, q such that $p + q = n$ and there is an isomorphism $V \simeq \mathbb{R}^n$ such that

$$Q(x) = x_1^2 + \cdots + x_p^2 - x_{p+1}^2 - \cdots - x_n^2, \;\; x \in \mathbb{R}^n.$$

This classifies Cliffords algebras over $\mathbb{R}$.

A (left) module S for a Clifford algebra $C(V)$ is superalgebra module — a finite-dimensional superspace S over k with a map $\rho : C(V) \otimes S \to S$ such that

$$|\rho(a \otimes s)| = |a| + |s|$$

and

$$\rho(ab \otimes s) = \rho(a \otimes \rho(b \otimes s))$$

for all $a, b \in C(V)$ and $s \in S$.

The fermion Hilbert space $\mathscr{H}_F$ from the previous section is an irreducible C_{2n} module. Indeed, it follows from the canonical anticommutation relations (1.3) that the operators

$$\gamma_{2k-1} = a_k + a_k^* \tag{1.7}$$

$$\gamma_{2k} = -i(a_k - a_k^*) \tag{1.8}$$

$k = 1, \dots, n$, satisfy the relations

$$[\gamma_\mu, \gamma_\nu]_+ = 2\delta_{\mu\nu} I,$$

where I is the identity operator on $\mathscr{H}_F = \mathbb{C}^{2^n}$. Thus the Clifford algebra C_{2n} acts on $\mathscr{H}_F$ and $\rho(1) = I$. The representation $\rho : C_{2n} \to \operatorname{End}(\mathscr{H}_F)$ is irreducible and is analogous to the Schrödinger representation for the canonical anticommutation relations.

Set $N = \sum_{j=1}^n a_j^* a_j$ and define the *chirality operator* $\Gamma = e^{\pi i N}$. Since the operator N has an integral spectrum, $\Gamma^2 = I$. Moreover, we have that

$$[\Gamma, \gamma_\mu]_+ = 0, \;\; \mu = 1, \dots, 2n$$

Indeed, it follows from (1.3) that

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

so that

$$e^{\pi i N} a_j^* = a_j^* e^{\pi i (N+I)} \quad \text{and} \quad e^{\pi i N} a_j = a_j e^{\pi i (N-I)}.$$

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

$$\mathscr{H}_F = \mathscr{H}_+ \oplus \mathscr{H}_-$$

into the subspaces of positive and negative *spinors*, and $\gamma_\mu(\mathscr{H}_+) = \mathscr{H}_-$. Also, since $e^{\pi i a_j^* a_j} = I - 2a_j^* a_j = -i\gamma_{2j-1}\gamma_{2j}$, we have

$$\Gamma = (-i)^n \gamma_1 \dots \gamma_{2n}.$$

When $n = 2$, matrices $\gamma_1, \gamma_2, \gamma_3, \gamma_4$ are famous γ-matrices of Dirac with $\Gamma = \gamma_5$.

The analog of Stone-von Neumann theorem for canonical anticommutation relations is the following statement.

THEOREM 1.1. *Let $C(V)$ be a Clifford algebra over a $\mathbb{C}$-vector space V.*

(i) *If* $\dim V = 2n$, *then*

$$C(V) \simeq \underline{\mathrm{End}}(S) \quad \textit{where} \quad S \simeq \mathbb{C}^{2^{n-1}|2^{n-1}}.$$

(ii) *If* $\dim V = 2n+1$, *then*

$$C(V) \simeq D \otimes \mathrm{End}(S_0), \quad \textit{where} \quad D = \mathbb{C}[\varepsilon]/\{\varepsilon^2 - 1\} \;\; \textit{and} \;\; S_0 \simeq \mathbb{C}^{2^n}.$$

PROOF. If $\dim V = 2n$, the quadratic vector space (V, Q) is isomorphic to $U \oplus U^\vee$ with the quadratic form $Q(u + \alpha) = \alpha(u)$, where $U^\vee$ is the dual vector space to U, $\dim U = n$. (Indeed, using the orthonormal basis $\{e_i\}_{i=1}^{2n}$, set U to be the linear span of the vectors $\frac{1}{\sqrt{2}}(e_k + \sqrt{-1}e_{k+n})$, $k = 1, \dots, n$, and $U^\vee$ be the subspace spanned by the vectors $\frac{1}{\sqrt{2}}(e_k - \sqrt{-1}e_{k+n})$, $k = 1, \dots, n$.) Set $S = \Lambda^\bullet U^\vee$ and define the mapping

$$\rho : C(U \oplus U^\vee) \to \underline{\mathrm{End}}(S)$$

by

$$\rho(u)s = i_u s, \quad \rho(\alpha)s = \alpha \wedge s,$$

where $u \in U, \alpha \in U^\vee$ and $s \in S$. It is easy to see that the mapping ρ is an isomorphism of superalgebras.

When $\dim V = 2n+1$, the quadratic vector space (V, Q) is isomorphic to the $U \otimes U^\vee \oplus \mathbb{C} \cdot e_{2n+1}$, where $Q(u + \alpha + ae_{2n+1}) = \alpha(u) + a^2$. Since $C(\mathbb{C} \cdot e_{2n+1}) \simeq D$, we have, setting $S_0 = \Lambda U^\vee$,

$$C(V) \simeq \underline{\mathrm{End}}(S) \otimes D \simeq D \otimes \mathrm{End}(S_0).$$

$\square$

REMARK. Part (i) of the Theorem is a fermion analog of Stone-von Neumann theorem. Choosing a polarization of V given by the orthonormal basis $\{e_j\}_{j=1}^{2n}$ of V, we see that $S \simeq \mathscr{H}_F$ with $1 \mapsto \psi_0$ and the operators $\alpha_k \wedge$ and i_{u_k} become, correspondingly, creation and annihilation operators $\hat{a}_k^*$, $\hat{a}_k$, $k = 1, \dots, n$.

2. Grassmann algebras

A Grassmann algebra Gr_n with n generators is a $\mathbb{C}$-algebra with the generators $\theta_1, \dots, \theta_n$ satisfying the relations

$$\theta_i\theta_j + \theta_j\theta_i = 0, \quad i, j = 1, \dots, n.$$

Of course, Gr_n is nothing but the exterior algebra $\Lambda^\bullet V$ of an n-dimensional vector space V with a choice of a basis of V. In this form it can be considered as counterpart of a polynomial algebra $\mathbb{C}[x_1, \dots, x_n]$ — a symmetric algebra $\mathrm{Sym}(V)$ of an n n-dimensional vector space V with a choice of a basis.

The Grassmann algebra Gr_n is a vector space of dimension 2^n and it admits a decomposition

$$\mathrm{Gr}_n = \mathbb{C} \oplus \mathrm{Gr}_n^1 \oplus \cdots \oplus \mathrm{Gr}_n^n \tag{2.1}$$

into grades components Gr_n^k of degree k and dimension $\binom{n}{k}$, $k = 0, \dots, n$. The multiplication in Gr_n is graded-commutative:

$$\alpha\beta = (-1)^{|\alpha||\beta|}\beta\alpha$$

for homogenous elements $\alpha, \beta \in \mathrm{Gr}_n$.

The advantage of using Grassmann algebra is that we can realize the representation ρ of a Clifford algebra associated with canonical anticommutation relations, considered in the previous section, by an analogs of multiplication and differentiation operators, quite similar to the ones used for canonical commutation relations. Namely, let $\hat{\theta}_i$ be a left-multiplication by θ_i operator in Gr_n, and let $\dfrac{\partial}{\partial\theta_i}$ be a left derivative operator,

$$\frac{\partial}{\partial\theta_i}\theta_{i_1}\dots\theta_{i_k} = \sum_{l=1}^{k}(-1)^{l-1}\delta_{ii_l}\theta_{i_1}\dots\check{\theta}_{i_l}\dots\theta_{i_k}.$$

The derivative operators satisfy the graded Leibniz rule

$$\frac{\partial}{\partial\theta_i}(\alpha\beta) = \frac{\partial\alpha}{\partial\theta_i}\beta + (-1)^{|\alpha|}\alpha\frac{\partial\beta}{\partial\theta_i},$$

and it is easy to verify that the operators $\widehat{\theta}_i, \dfrac{\partial}{\partial\theta_i}$ satisfy

$$\left[\widehat{\theta}_i, \widehat{\theta}_j\right]_+ = \left[\frac{\partial}{\partial\theta_i}, \frac{\partial}{\partial\theta_j}\right]_+ = 0$$

and

$$\left[\widehat{\theta}_i, \frac{\partial}{\partial\theta_j}\right]_+ = \delta_{ij}I, \quad i, j = 1, \dots, n.$$

Moreover, operators $\widehat{\theta}_i, \dfrac{\partial}{\partial\theta_i}$ are Hermitian conjugate with respect to the standard inner product in Gr_n with the orthonormal basis given by the monomials $\theta_{i_1}\dots\theta_{i_k}$ for all $1 \le i_1 < \cdots < i_k \le n$.

These arguments prove the following result.

PROPOSITION 2.1. *The assigment* $\mathscr{H}_F \ni \psi_{i_1\dots i_k} \mapsto \theta_{i_1}\dots\theta_{i_k} \in \mathrm{Gr}_n$ *establish an isometric isomorphism* $\mathscr{H}_F \simeq \mathrm{Gr}_n$ *between the fermion Hilbert space of* n *identical particles and the vector space of Grassmann algebra which preserves decompositions* (1.6) *and* (2.1) *and such that* $a_i^* \mapsto \hat{\theta}_i$ *and* $a_i \mapsto \dfrac{\partial}{\partial\theta_i}$, $i = 1, \dots, n$.

Thus in analogy the holomorphic representation of canonical commutation relations (1.1), we obtain a realization of the operators a_i, a_i^* satisfying canonical anticommutation relations (1.3) as derivation and multiplication operators in Gr_n. In Section 1.5 we will develop the notion of an integral over the Grassmann variables and will show that the inner product in Gr_n can be also written in a form similar to the holomorphic representation.

2.1. Commutative superalgebras. The notion of a commutative superalgebra allows to consider exterior and symmetric algebras (or Grassmann and polynomial algebras) on the same footing.

DEFINITION. A graded ($\mathbb{Z}/2$-graded) vector space over $\mathbb{C}$ is a vector space W with a decomposition

$$W = W^0 \oplus W^1$$

into *even* and *odd* subspaces. The elements in $W^0 \cup W^1 \setminus \{0\}$ are called homogeneous and the parity is a map $|\cdot| : W^0 \cup W^1 \setminus \{0\} \to \{0, 1\}$ such that $|w| = 0$ for $w \in W^0$ and $|w| = 1$ for $w \in W^1$.

We reserve the notation V for ordinary (even) vector spaces, denoting graded vector spaces by W.

A tensor product of graded vector spaces is defined in the same way as for ordinary vector spaces. However, the difference between ordinary and graded vector spaces becomes transparent for the corresponding tensor categories. Namely, the associativity morphism

$$c_{W_1W_2W_3} : W_1 \otimes (W_2 \otimes W_3) \to (W_1 \otimes W_2) \otimes W_3$$

for graded vector spaces is defined by the same formula

$$c_{W_1W_2W_3}(w_1 \otimes (w_2 \otimes w_3)) = (w_1 \otimes w_2) \otimes w_3$$

as in the case of ordinary vector spaces, whereas the commutativity morphism

$$\sigma_{W_1W_2} : W_1 \otimes W_2 \to W_2 \otimes W_1$$

is defined by

$$\sigma_{W_1W_2}(w_1 \otimes w_2) = (-1)^{|w_1||w_2|} w_2 \otimes w_1.$$

The tensor algebra $T(W)$ of a graded vector space W is defined using the associativity morphism. The exterior algebra $\Lambda^\bullet W$ and symmetric algebra $\mathrm{Sym}(W)$ of W are defined as a quotient algebras of $T(W)$ by using the commutativity morphism.

DEFINITION. A *superalgebra* over $\mathbb{C}$ is a graded vector space $A = A^0 \oplus A^1$ with a $\mathbb{C}$-algebra structure such that $1 \in A^0$ and

$$A^0 \cdot A^0 \subset A^0, \quad A^0 \cdot A^1 \subset A^1, \quad A^1 \cdot A^1 \subset A^0.$$

A superalgebra A is a *commutative superalgebra*, if

$$a \cdot b = (-1)^{|a||b|} b \cdot a$$

for homogeneous elements $a, b \in A$.

Exterior $\Lambda^\bullet V$ and symmetric $\mathrm{Sym}(V)$ algebras of a vector space V are obvious examples of commutative superalgebras.

DEFINITION. Let $W = W^0 \oplus W^1$ be a graded vector space. A *parity-reversed* vector space ΠW is a graded vector space with $(\Pi W)^0 = W^1$ and $(\Pi W)^1 = W^0$.

It immediately follows from the above definitions that

$$\Lambda^\bullet(V) = \mathrm{Sym}(\Pi V).$$

Thus the Grassmann algebra Gr_n can be considered as polynomial algebra on odd generators,

$$\mathrm{Gr}_n = \mathbb{C}[\theta_1, \dots, \theta_n].$$

To avoid the confusion, in what follows we always use the Greek letters for the odd generators.

2.2. Differential calculus on Grassmann algebra.

2.3. Grassmann integration. Every element $f \in \mathbb{C}[\theta_1, \dots, \theta_n]$ can be uniquely written as

$$f = \sum_{k=0}^{n} \sum_{1 \le i_1 < \dots < i_k \le n} f^{i_1 \dots i_k} \theta_{i_1} \dots \theta_{i_k}.$$

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

$$B(f) = f^{12\dots n}.$$

It is a tradition to write the Berezin integral as

$$B(f) = \int f(\theta_1, \dots, \theta_n) d\theta_1 \dots d\theta_n.$$

It follows from the definition of the partial derivatives on Grassmann algebra that

$$\int f(\theta_1, \dots, \theta_n) d\theta_1 \dots d\theta_n = \frac{\partial}{\partial \theta_n} \cdots \frac{\partial}{\partial \theta_1} f,$$

so that

$$\int \frac{\partial}{\partial \theta_i} f(\theta_1, \dots, \theta_n) d\theta_1 \dots d\theta_n = 0.$$

This leads to the following *integration by parts* formula

$$\int\left(\frac{\partial f}{\partial\theta_i}g\right)(\theta_1,\dots,\theta_n)\,d\theta_1\dots d\theta_n=-(-1)^{|f|}\int\left(f\frac{\partial g}{\partial\theta_i}\right)(\theta_1,\dots,\theta_n)\,d\theta_1\dots d\theta_n$$

for homogeneous $f\in\mathrm{Gr}_n$ and $g\in\mathrm{Gr}_n$.

Remark. Berezin integral is not an integral in the sense of integration theory. It is defined as linear functional on a Grassmann algebra Gr_n and it depends on the choice of the ordered generators for Gr_n, which is symbolized by $d\theta_1\dots d\theta_n$. In particular, for any permutation $\sigma\in\mathrm{Sym}_n$,

$$\int f(\theta_1,\dots,\theta_n)d\theta_1\dots d\theta_n=(-1)^{\varepsilon(\sigma)}\int f(\theta_1,\dots,\theta_n)d\theta_{\sigma(1)}\dots d\theta_{\sigma(n)},$$

where σ is the parity of a permutation σ.

Remark. Using the embeddings $\mathrm{Gr}_k\subset\mathrm{Gr}_n$ for $k\le n$, physicists usually define the Berezin integral as a "repeated integral" starting from the following "one-dimensional integrals"

$$\int d\theta_j=0,\quad\int\theta_j d\theta_j=1,\ \ j=1,\dots,n.$$

Lemma 2.1 (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*,* $\theta_i=\sum_{j=1}^n a_{ij}\tilde\theta_j$*,* $j=1,\dots,n$*, with a non-degenerate* $n\times n$ *matrix* $A=\{a_{ij}\}_{i,j=1}^n$*. Then*

$$\int f(\theta_1,\dots,\theta_n)d\theta_1\dots d\theta_n=\frac{1}{\det A}\int\tilde f(\tilde\theta_1,\dots,\tilde\theta_n)d\tilde\theta_1\dots d\tilde\theta_n,$$

where $\tilde f(\tilde\theta_1,\dots,\tilde\theta_n)=f(\sum_{j=1}^n a_{1j}\tilde\theta_j,\dots,\sum_{j=1}^n a_{nj}\tilde\theta_j)$*.*

Proof. By multi-linear algebra, $\tilde f^{12\dots n}=f^{12\dots n}\det A$. □

Remark. Informally, the lemma states that under the change of variables $\theta_i=\sum_{j=1}^n a_{ij}\tilde\theta_j$,

$$d\theta_1\dots d\theta_n=\frac{1}{\det A}\,d\tilde\theta_1\dots d\tilde\theta_n.$$

This differs from the usual change of variables formula for Lebesgue integral

$$\int\limits_{\mathbb{R}^n}f(x_1,\dots,x_n)dx_1\dots dx_n=|\det A|\int\limits_{\mathbb{R}^n}\tilde f(y_1,\dots,y_n)dy_1\dots dy_n,$$

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, Berezin integral is not an integral with respect to any measure but rather is a multiple derivative, which explains this difference.

Let $A=\{a_{ij}\}_{i,j=1}^n$ be $n\times n$ skew-symmetric matrix. Its *Pfaffian* $\mathrm{Pf}(A)$ is defined by

$$\mathrm{Pf}(A)=\frac{1}{n!2^n}\sum_{\sigma\in\mathrm{Sym}_{2n}}(-1)^{\varepsilon(\sigma)}a_{\sigma(1)\sigma(2)}\dots a_{\sigma(2n-1)\sigma(2n)},$$

where $\varepsilon(\sigma)$ is the parity of a permutation σ. Clearly $\mathrm{Pf}(A) = 0$ when n is odd.

PROPOSITION 2.2 (Gaussian integrals for Grassmann variables). *Let $A = \{a_{ij}\}_{i,j=1}^{n}$ be $n \times n$ skew-symmetric matrix. Then*

(i)

$$\int \exp\left\{\frac{1}{2}\sum_{i,j=1}^{n} a_{ij}\theta_i\theta_j\right\} d\theta_1 \dots d\theta_n = \mathrm{Pf}(A).$$

(ii)

$$\mathrm{Pf}(A)^2 = \det A.$$

PROOF. It is sufficient to prove part (i) for $n = 2m$. It follows from the definition of the Pfaffian

$$Pf(A)\theta_1 \dots \theta_n = \frac{1}{n!2^n}\left(\sum_{i,j=1}^{n} \theta_i\theta_j\right)^m,$$

and from the definition of Berezin integral. Part (ii) is a classical result, which can be proved by Berezin integral as follows. Suppose first that A is real-valued. There exists an orthogonal matric C, $\det C = 1$, such that

$$CAC^{-1} = \begin{pmatrix} 0 & \lambda_1 & \dots & 0 & 0 \\ -\lambda_1 & 0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 & \lambda_m \\ 0 & 0 & \dots & -\lambda_m & 0 \end{pmatrix}$$

is a block-diagonal matrix. Since

$$\int e^{\lambda_1\theta_1\theta_2 + \dots + \lambda_m\theta_{2m-1}\theta_{2m}} d\theta_1 \dots d\theta_{2m} = \lambda_1 \dots \lambda_m,$$

using part (i) and change of variables formula we obtain $\mathrm{Pf}(A)^2 = \det A$. For complex-valued A the relation holds since both sides are polynomials in variables a_{ij}, $1 \le i < j \le n$, which coincide for real values of a_{ij}. $\square$

For a Grassmann algebra $\mathrm{Gr}_{2n} = \mathbb{C}[\theta_1, \bar\theta_1 \dots, \theta_n, \bar\theta_n]$ with $2n$ generators denote by $\int d\bar\theta d\theta$ the corresponding Berezin integral,

$$\int f(\theta,\bar\theta)d\bar\theta d\theta = \frac{\partial}{\partial\bar\theta_n}\frac{\partial}{\partial\theta_n}\cdots\frac{\partial}{\partial\bar\theta_1}\frac{\partial}{\partial\theta_1}f, \quad f \in \mathbb{C}[\theta_1, \bar\theta_1 \dots, \theta_n, \bar\theta_n].$$

We also set

$$\int f(\theta,\bar\theta)d\theta d\bar\theta = \frac{\partial}{\partial\theta_n}\frac{\partial}{\partial\bar\theta_n}\cdots\frac{\partial}{\partial\theta_1}\frac{\partial}{\partial\bar\theta_1}f = (-1)^n\int f(\theta,\bar\theta)d\bar\theta d\theta.$$

LEMMA 2.2. *For an $n \times n$ matrix $A = \{a_{ij}\}_{i,j=1}^{n}$ set $(A\theta, \bar\theta) = \sum_{i,j=1}^{n} a_{ij}\theta_i\bar\theta_j$. Then*

$$\int e^{(A\theta,\bar\theta)} d\bar\theta d\theta = \det A.$$

PROOF. According to Proposition 2.2,

$$\int e^{(A\theta,\bar{\theta})} d\bar{\theta} d\theta = \mathrm{Pf}(\mathbf{A}),$$

where $\mathbf{A} = \left(\begin{smallmatrix} 0 & A \\ -A^t & 0 \end{smallmatrix} \right)$ is a $2n \times 2n$ skew-symmetric matrix. We have $\mathrm{Pf}(\mathbf{A})^2 = \det \mathbf{A} = (\det A)^2$, so that $\mathrm{Pf}(\mathbf{A}) = \pm \det A$, and checking for $A = I_n$ determines the correct sign. $\square$

DEFINITION. An involution on a Grassmann algebra Gr over $\mathbb{C}$ is a complex anti-linear mapping $\mathrm{Gr} \ni f \mapsto f^* \in \mathrm{Gr}$ such that $(f^*)^* = f$ and $(fg)^* = g^* f^*$ for all $f, g \in \mathrm{Gr}$.

The Grassmann algebra $\mathbb{C}[\theta_1, \bar{\theta}_1 \dots, \theta_n, \bar{\theta}_n]$ 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

$$f(\theta) = \sum_{k=0}^{n} \sum_{1 \le i_1 < \cdots < i_k \le n} f^{i_1 \dots i_k} \, \theta_{i_1} \dots \theta_{i_k} \in \mathrm{Gr}_n \subset \mathrm{Gr}_{2n}$$

we have

$$f^*(\theta) = \overline{f(\theta)} = \sum_{k=0}^{n} \sum_{1 \le i_1 < \cdots < i_k \le n} \overline{f^{i_1 \dots i_k}} \, \bar{\theta}_{i_1} \dots \bar{\theta}_{i_k} \in \mathrm{Gr}_{2n}.$$

LEMMA 2.3. *The standard inner product on the Grassmann algebra* $\mathrm{Gr}_n = \mathbb{C}[\theta_1, \dots, \theta_n]$ *is expressed as the following Berezin integral over the Grassmann algebra* $\mathrm{Gr}_{2n} = \mathbb{C}[\theta_1, \bar{\theta}_1 \dots, \theta_n, \bar{\theta}_n]$

$$\langle f_1, f_2 \rangle = \int f_1(\theta) \overline{f_2(\theta)} e^{-\bar{\theta}\theta} d\bar{\theta} d\theta,$$

where $\bar{\theta}\theta = \bar{\theta}_1 \theta_1 + \cdots + \bar{\theta}_n \theta_n$.

PROOF. It sufficient to prove the lemma for monomials. It is clear that for $f_1(\theta) = \theta_{i_1} \dots \theta_{i_k}$ and $f_2(\theta) = \theta_{j_1} \dots \theta_{j_l}$ the integral is 0 unless $k = l$ and $i_1 = j_1, \dots, i_k = j_k$. In this case we have

$$\begin{aligned} \langle \theta_{i_1} \dots \theta_{i_k}, \theta_{i_1} \dots \theta_{i_k} \rangle &= \int \theta_{i_1} \dots \theta_{i_k} \bar{\theta}_{i_k} \dots \bar{\theta}_{i_1} e^{-(\bar{\theta}_1 \theta_1 + \cdots + \bar{\theta}_n \theta_n)} d\bar{\theta} d\theta \\ &= \int \theta_1 \dots \theta_n \bar{\theta}_n \dots \bar{\theta}_1 d\bar{\theta} d\theta = 1. \end{aligned}$$

$\square$

COROLLARY 2.1. *The operators* $\dfrac{\partial}{\partial \theta_i}$ *and* $\widehat{\theta}_i$, $i = 1, \dots, n$, *are adjoint with respect to the inner product on* Gr_{2n}.

Proof. It follows from Lemma 2.3 the integration by parts formula that

$$\begin{aligned}\left\langle \frac{\partial f}{\partial\theta_i}, f_2\right\rangle &= \int \frac{\partial f_1}{\partial\theta_i}(\theta)\overline{f_2(\theta)}e^{-\bar\theta\theta}d\bar\theta d\theta \\ &= -(-1)^{|f_1|+|f_2|}\int f_1(\theta)\overline{f_2(\theta)}\bar\theta_i e^{-\bar\theta\theta}d\bar\theta d\theta \\ &= -(-1)^{|f_1|+|f_2|}\int f_1(\theta)\overline{\theta_i f_2(\theta)}e^{-\bar\theta\theta}d\bar\theta d\theta \\ &= \langle f_1, \widehat{\theta}_i f_2\rangle,\end{aligned}$$

since $\dfrac{\partial}{\partial\theta_i}e^{-\bar\theta\theta} = \bar\theta_i e^{-\bar\theta\theta}$ and the integrals are different from 0 if and only if $|f_1| + |f_2|$ is odd. □

2.4. Functions with anticommuting values.

2.5. Supermanifolds. A supercommutative superalgebra $\mathsf{A}(M)$ of differential forms on the manifold M can be also considered as a superalgebra of functions on a supermanifold ΠTM. Namely, to every $\omega_p \in \mathsf{A}^p(M)$, given in local coordinates on $U \subset M$ by

$$\omega_p = \sum_{i_1<\cdots<i_p} a_{i_1\ldots i_p}(x)dx_{i_1}\wedge\cdots\wedge dx_{i_p},$$

we assign

$$\omega_p(x,\eta) = \sum_{i_1<\cdots<i_p} a_{i_1\ldots i_p}(x)\eta_{i_1}\ldots\eta_{i_p} \in C^\infty(U)[\eta_1,\ldots,\eta_n].$$

Since under a change of coordinates $a_{i_1\ldots i_p}(x)$ transform like coefficients of differential forms, and $\eta_1,\ldots,\eta_n$ — like components of tangent vectors, $\omega_p(x,\eta)$ is a well-defined function on the supermanifold ΠTM. The de Rham differential d gives rise to an odd vector field δ on ΠTM,

$$\delta = \sum_{k=1}^n \eta_k \frac{\partial}{\partial x_k}$$

with the property that $\delta^2 = 0$. Integration of a top form over M reduces to the integration of a corresponding function over ΠTM with respect to the canonical volume form $dxd\eta = dx_1\ldots dx_n d\eta_1\ldots d\eta_n$:

$$\int_M \omega_n = \int_{\Pi TM} \omega_n(x,\eta)dxd\eta.$$

The volume form $dxd\eta$ is well-defined due the opposite change of variables formulas for the ordinary and Berezin's integrals.

2.6. Classical mechanics on supermanifolds.

EXAMPLE 2.1 (Free spin $\frac{1}{2}$ particle). The configuration space is the supermanifold $M = \Pi T\mathbb{R}^n \simeq \mathbb{R}^{n|n}$ — the tangent bundle to $\mathbb{R}^n$ with the reversed parity of the fibres, with even and odd real coordinates $q_1, \dots, q_n$ and $\psi_1, \dots, \psi_n$. Denote by $\pi : M \to \mathbb{R}^n$ the corresponding projection and let $\pi^*(T\mathbb{R}^n)$ be the pull-back to M by the mapping π of the tangent bundle $T\mathbb{R}^n$ over $\mathbb{R}^n$. For every $\gamma \in \Omega_I(\mathbb{R}^n)$ — the space of smooth maps of $I = [t_0, t_1]$ to $\mathbb{R}^n$, let $\boldsymbol{\psi}$ be the odd vector field along the path $\gamma = \mathbf{q}(t)$ in $\mathbb{R}^n$ — a global section over I of the bundle $\gamma^*(\Pi T\mathbb{R}^n)$, and let $\frac{d}{dt}$ be the connection in $\gamma^*(\Pi T\mathbb{R}^n)$ corresponding to the Euclidean metric on $\mathbb{R}^n$ — the Levi-Civita connection. Explicitly,

$$\boldsymbol{\psi}(t) = \sum_{k=1}^{n} \psi_k(t) \frac{\partial}{\partial q_k}, \quad t \in I.$$

Every pair $(\mathbf{q}(t), \boldsymbol{\psi}(t))$ — a path in M, lifts to a path $\boldsymbol{\gamma}(t) = (\mathbf{q}(t), \dot{\mathbf{q}}(t), \boldsymbol{\psi}(t))$ in $\pi^* T\mathbb{R}^n$, and we define the Lagrangian (with values in auxiliary Grassmann algebra) along this path by

$$L = \frac{m\dot{\mathbf{q}}^2}{2} + \frac{i}{2}\langle \boldsymbol{\psi}, \dot{\boldsymbol{\psi}} \rangle = \sum_{k=1}^{n} \frac{m\dot{q}_k^2}{2} + i\sum_{k=1}^{n} \frac{\psi_k \dot{\psi}_k}{2}$$

and the corresponding action functional by

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

The Euler-Lagrange equations are

$$\ddot{\mathbf{q}} = 0 \quad \text{and} \quad \dot{\boldsymbol{\psi}} = 0.$$

Corresponding Legendre transformation introduces canonically conjugated momenta as follows

$$p_j = \frac{\partial L}{\partial \dot{q}_j} = m\dot{q}_j \quad \text{and} \quad \pi_j = \frac{\partial L}{\partial \dot{\psi}_j} = -\frac{i}{2}\psi_j, \ \ j = 1, \dots, n.$$

Thus the phase space is a supermanifold $\mathbb{R}^{2n|n}$ with real coordinates $\mathbf{p}, \mathbf{q}, \boldsymbol{\psi}$ and the symplectic form

$$\omega = d\mathbf{p} \wedge d\mathbf{q} + \frac{i}{2} d\boldsymbol{\psi} d\boldsymbol{\psi},$$

and the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m}. \tag{2.2}$$

EXAMPLE 2.2 (Spin $\frac{1}{2}$ particle in a constant magnetic field). On the configuration space $\mathbb{R}^{3|3}$ with real coordinates $\mathbf{q}, \boldsymbol{\psi}$ consider the Lagrangian

$$L = \frac{m}{2}\dot{\mathbf{q}}^2 + \frac{i}{2}\boldsymbol{\psi}\dot{\boldsymbol{\psi}} + \frac{i}{2}(\mathbf{B} \times \boldsymbol{\psi})\boldsymbol{\psi}.$$

The corresponding phase space is $\mathbb{R}^{6|3}$ with real coordinates $\mathbf{p}, \mathbf{q}, \boldsymbol{\psi}$ and the symplectic form

$$\omega = d\mathbf{p} \wedge d\mathbf{q} + \frac{i}{2} d\boldsymbol{\psi} d\boldsymbol{\psi},$$

and the Hamiltonian is

$$H = \frac{\mathbf{p}^2}{2m} - \frac{i}{2}(\mathbf{B} \times \boldsymbol{\psi})\boldsymbol{\psi}. \tag{2.3}$$

3. Quantization of classical systems on supermanifolds

Quantization of the phase space $\mathbb{R}^{2n|n}$ with the symplectic form

$$\omega = d\mathbf{p} \wedge d\mathbf{q} + \frac{i}{2} d\boldsymbol{\psi} d\boldsymbol{\psi}$$

is the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^n) \otimes \mathbb{C}^{2^d}$, where $d = \left[\frac{n}{2}\right]$, where now $\hat{\psi}_k$ satisfy Clifford algebra relations

$$[\hat{\psi}_k, \hat{\psi}_l]_+ = \delta_{kl} I,$$

and P_k, Q_k satisfy Heisenberg commutation relations. The Hamiltonian operator corresponding to (2.2) is

$$\hat{H} = \frac{\mathbf{P}^2}{2m}$$

and describes free quantum particle of spin $\frac{1}{2}$.

Similarly, Hamiltonian operator corresponding to (2.3)

$$\hat{H} = \frac{\mathbf{P}^2}{2m} - \frac{\mathbf{B} \cdot \boldsymbol{\sigma}}{2}$$

in $\mathscr{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$, which describes quantum particle of spin $\frac{1}{2}$ in a constant magnetic field. The second term in this formula is called *Pauli Hamiltonian.*

4. Path Integrals for Anticommuting Variables

4.1. Matrix and Wick symbols of operators. Let $\hat{a}_k^*, \hat{a}_k$, $k = 1, \dots, n$ be fermion creation and annihilation operators of n identical particles, let

$$\mathscr{H}_F = \bigoplus_{k=0}^{n} \mathscr{H}_k \tag{4.1}$$

be the decomposition of the fermion Hilbert space into a direct sum of invariant subspaces of the operator $N = \sum_{k=1}^n \hat{a}_k^* \hat{a}_k$, and denote by P_k corresponding orthogonal projection operators onto $\mathscr{H}_k$. According to the decomposition (4.1), every operator A in $\mathscr{H}_F$ can be represented in a follwoing block-matrix form

$$A = \begin{pmatrix} A_{00} & A_{01} & \dots & A_{0n} \\ A_{10} & A_{11} & \dots & A_{1n} \\ \dots & \dots & \dots & \dots \\ A_{n0} & A_{n1} & \dots & A_{nn} \end{pmatrix},$$

where $A_{ij} : \mathscr{H}_j \to \mathscr{H}_i$ is the operator $P_i A P_j$.

DEFINITION. The *supertrace* of an operator A on $\mathscr{H}_F$ is defined by

$$\operatorname{Tr}_s A = \operatorname{Tr} \Gamma A = \sum_{k=0}^{n} (-1)^k \operatorname{Tr}|_{\mathscr{H}_k} P_k A,$$

where Γ is the chirality operator in $\mathscr{H}_F$.

Let $\mathrm{Gr}_{2n} = \mathbb{C}[a_1, \bar{a}_1 \ldots, a_n, \bar{a}_n]$ be the Grassmann algebra with $2n$ generators.

DEFINITION. A *matrix symbol* of an operator $A : \mathscr{H}_F \to \mathscr{H}_F$ is a element $\mathcal{A}(\bar{a}, a) \in \mathrm{Gr}_{2n}$, defined by

$$\mathcal{A}(\bar{a}, a) = \sum_{i,j=0}^{n} \sum_{\substack{0 \le k_1 < \cdots < k_i \le n \\ 0 \le l_1 < \cdots < l_j \le n}} A_{ij}(k_1, \ldots, k_i; l_1, \ldots, l_j) \bar{a}_{k_1} \ldots \bar{a}_{k_i} a_{l_j} \ldots a_{l_1},$$

where $A_{ij}(k_1, \ldots, k_i; l_1, \ldots, l_j) = \langle A\psi_{l_1 \ldots l_j}, \psi_{k_1 \ldots k_i} \rangle$.

Since $\mathrm{Cl}_{2n} \simeq \mathrm{End}(\mathscr{H}_F)$, every operator $A : \mathscr{H}_F \to \mathscr{H}_F$ can be uniquely represented in a *normal form* as follows

$$A = \sum_{i,j=0}^{n} \sum_{\substack{0 \le k_1 < \cdots < k_i \le n \\ 0 \le l_1 < \cdots < l_j \le n}} K_{ij}(k_1, \ldots, k_i; l_1, \ldots, l_j) \hat{a}^*_{k_1} \ldots \hat{a}^*_{k_i} \hat{a}_{l_j} \ldots \hat{a}_{l_1}.$$

DEFINITION. A *Wick symbol* of an operator $A : \mathscr{H}_F \to \mathscr{H}_F$ is a element $A(\bar{a}, a) \in \mathrm{Gr}_{2n}$, defined by

$$A(\bar{a}, a) = \sum_{i,j=0}^{n} \sum_{\substack{0 \le k_1 < \cdots < k_i \le n \\ 0 \le l_1 < \cdots < l_j \le n}} K_{ij}(k_1, \ldots, k_i; l_1, \ldots, l_j) \bar{a}_{k_1} \ldots \bar{a}_{k_i} a_{l_j} \ldots a_{l_1}.$$

When $n = 1$, every operator A in $\mathscr{H}_F \simeq \mathbb{C}^2$ is represented by

$$A = \begin{pmatrix} \alpha_{00} & \alpha_{01} \\ \alpha_{10} & \alpha_{11} \end{pmatrix},$$

so that

$$\mathcal{A}(\bar{a}, a) = \alpha_{00} + \alpha_{01} a + \alpha_{10} \bar{a} + \alpha_{11} \bar{a} a \in \mathbb{C}[a, \bar{a}].$$

On the other hand,

$$A = \alpha_{00} \hat{a} \hat{a}^* + \alpha_{01} \hat{a} + \alpha_{10} \hat{a}^* + \alpha_{11} \hat{a}^* \hat{a} = \alpha_{00} I + \alpha_{01} \hat{a} + \alpha_{10} \hat{a}^* + (\alpha_{11} - \alpha_{00}) \hat{a}^* \hat{a},$$

so that

$$A(\bar{a}, a) = \alpha_{00} + \alpha_{01} a + \alpha_{10} \bar{a} + (\alpha_{11} - \alpha_{00}) \bar{a} a \in \mathbb{C}[a, \bar{a}].$$

In this case it is elementary to verify that $\mathcal{A}(\bar{a}, a) = A(\bar{a}, a) e^{\bar{a} a}$ and, in fact, this relation holds in general.

LEMMA 4.1. *Matrix and Wick symbols of an operator* $A : \mathscr{H}_F \to \mathscr{H}_F$ *in the Hilbert space of* n *identical fermions are related by*

$$\mathcal{A}(\bar{a}, a) = A(\bar{a}, a)e^{\bar{a}a},$$

where $\bar{a}a = \sum_{k=1}^{n} \bar{a}_k a_k$.

PROOF. It is sufficient to compute the matrix symbol of the operator $A = \hat{a}^*_{k_1} \dots \hat{a}^*_{k_i} \hat{a}_{l_j} \dots \hat{a}_{l_1}$. Denote by $K = \{k_1, \dots, k_i\}$ and $L = \{l_1, \dots, l_j\}$ the ordered subsets of the set $\{1, \dots, n\}$, and let $S = \{s_1, \dots, s_p\}$ and $T = \{t_1, \dots, t_q\}$ be two other ordered subsets of $\{1, \dots, n\}$. Then the inner product

$$\langle A\psi_{s_1 \dots s_p}, \psi_{t_1 \dots t_q} \rangle = \langle \hat{a}_{l_j} \dots \hat{a}_{l_1} \psi_{s_1 \dots s_p}, \hat{a}_{k_i} \dots \hat{a}_{k_1} \psi_{t_1 \dots t_q} \rangle$$

is different from 0 if and only if $L \subset S$, $K \subset T$ and the corresponding set complements coincide: $S \setminus L = T \setminus K$. In this case,

$$\langle A\psi_{s_1 \dots s_p}, \psi_{t_1 \dots t_q} \rangle = (-1)^{\varepsilon(L,S)+\varepsilon(K,T)}.$$

Here for any pair of ordered subsets L and S of $\{1, \dots, n\}$ such that $L \subset S$, we denote by $\varepsilon(L, S)$ the parity of a permutation that sends $L \sqcup (S \setminus L)$ to S. Thus the matrix symbol of A is given by

$$\mathcal{A}(\bar{a}, a) = \sum_{S,T} (-1)^{\varepsilon(L,S)+\varepsilon(K,T)} \bar{a}_{t_1} \dots \bar{a}_{t_q} a_{s_p} \dots a_{s_1},$$

where the summation goes over the subsets S and T satisfying the above condition. Setting $\{r_1, \dots, r_m\} = S \setminus L = T \setminus K$, we get

$$\begin{aligned}
\mathcal{A}(\bar{a}, a) &= \sum_{m=0}^{n} \sum_{1 \le r_1 < \dots < r_m \le n} \bar{a}_{k_1} \dots \bar{a}_{k_i} \bar{a}_{r_1} \dots \bar{a}_{r_m} a_{r_m} \dots a_{r_1} a_{l_j} \dots a_{l_1} \\
&= \bar{a}_{k_1} \dots \bar{a}_{k_i} a_{l_j} \dots a_{l_1} \sum_{m=0}^{n} \sum_{1 \le r_1 < \dots < r_m \le n} \bar{a}_{r_1} a_{r_1} \dots \bar{a}_{r_m} a_{r_m} \\
&= \bar{a}_{k_1} \dots \bar{a}_{k_i} a_{l_j} \dots a_{l_1} e^{\bar{a}_1 a_1 + \dots + \bar{a}_n a_n}.
\end{aligned}$$

□

To matrix symbol $\mathcal{A}(\bar{a}, a)$ of an operator A on $\mathscr{H}_F$ (respectively, Wick symbol $A(\bar{a}, a)$) one canonically associates the elements $\mathcal{A}(\bar{a}, \eta)$ and $\mathcal{A}(\bar{\eta}, a)$ (respectively $A(\bar{a}, \eta)$ and $A(\bar{\eta}, a)$) in the larger Grassmann algebra $\mathrm{Gr}_{4n} = \mathbb{C}[a_1, \bar{a}_1, \dots, a_n, \bar{a}_n, \eta_1, \bar{\eta}_1, \dots, \eta_n, \bar{\eta}_n]$ by replacing, correspondingly, Grassmann variables a_i by η_i and $\bar{a}_i$ by $\bar{\eta}_i$. We define the incomplete Berezin integral as the following linear mapping $\int d\bar{\eta} d\eta : \mathrm{Gr}_{4n} \to \mathrm{Gr}_{2n}$:

$$\int f(a, \bar{a}, \eta, \bar{\eta}) d\bar{\eta} d\eta = \frac{\partial}{\partial \bar{\eta}_n} \frac{\partial}{\partial \eta_n} \dots \frac{\partial}{\partial \bar{\eta}_1} \frac{\partial}{\partial \eta_1} f, \quad f \in \mathrm{Gr}_{4n}.$$

The following result shows the usefulness of matrix and Wick symbols.

THEOREM 4.1. *Let* A *and* B *be two operators in* $\mathscr{H}_F$ *with matrix symbols* $\mathcal{A}(\bar{a}, a)$ *and* $\mathcal{B}(\bar{a}, a)$. *Then the following formulas hold.*

(i) *The matrix and Wick symbols of $C = AB$ are given by*

$$\mathcal{C}(\bar{a}, a) = \int \mathcal{A}(\bar{a}, \eta)\mathcal{B}(\bar{\eta}, a)e^{-\bar{\eta}\eta}d\bar{\eta}d\eta,$$
$$C(\bar{a}, a) = \int A(\bar{a}, \eta)B(\bar{\eta}, a)e^{-(\bar{\eta}-\bar{a})(\eta-a)}d\bar{\eta}d\eta.$$

(ii) *The trace and supertrace of an operator A are given by*

$$\operatorname{Tr} A = \int \mathcal{A}(\bar{a}, a)e^{\bar{a}a}dad\bar{a} = \int A(\bar{a}, a)e^{2\bar{a}a}dad\bar{a},$$
$$\operatorname{Tr}_s A = \int \mathcal{A}(\bar{a}, a)e^{-\bar{a}a}d\bar{a}da = \int A(\bar{a}, a)d\bar{a}da.$$

PROOF. The first formula in part (i) follows from

$$\int \eta_{l_j} \dots \eta_{l_1}\bar{\eta}_{k_1} \dots \bar{\eta}_{k_i}e^{-\bar{\eta}\eta}d\bar{\eta}d\eta = \delta_{ij}\delta_{k_1l_1} \dots \delta_{k_il_i}$$

and the rules of matrix multiplication. The second formula in part (i) is obtained using Lemma 4.1. The first and second formulas in part (ii) follow, correspondingly, from

$$\int \bar{a}_{k_1} \dots \bar{a}_{k_i}a_{l_j} \dots a_{l_1}e^{\bar{a}a}dad\bar{a} = \delta_{ij}\delta_{k_1l_1} \dots \delta_{k_il_i}$$

and

$$\int \bar{a}_{k_1} \dots \bar{a}_{k_i}a_{l_j} \dots a_{l_1}e^{-\bar{a}a}d\bar{a}da = (-1)^i\delta_{ij}\delta_{k_1l_1} \dots \delta_{k_il_i}.$$

□

REMARK. Note the difference between formulas for $\operatorname{Tr} A$ and $\operatorname{Tr}_s A$.

REMARK. Since $\Gamma = e^{\pi i\hat{a}^*\hat{a}} = \prod_{k=1}^n(1 - 2\hat{a}_k^*\hat{a}_k)$ (see Section 1.2), for the Wick symbol of Γ we have

$$\Gamma(\bar{a}, a) = \prod_{k=1}^{n}(1 - 2\bar{a}_k a_k) = e^{-2\bar{a}a},$$

so that

$$\operatorname{Tr}_s \Gamma = \operatorname{Tr} I = \int e^{-2\bar{a}a}d\bar{a}da = 2^n = \dim \mathscr{H}_F.$$

Here is another derivation of the formula for $\operatorname{Tr}_s A = \operatorname{Tr} A\Gamma$ based on the formulas for $\operatorname{Tr} A$, Part (i) of Theorem 4.1 and the expression $\Gamma(\bar{a}, a) =$

$e^{-2\bar{a}a}$. We have

$$\begin{aligned}\operatorname{Tr} A\Gamma &= \int\int A(\bar{a},\eta)e^{-2\eta a-(\bar{\eta}-\bar{a})(\eta-a)+2\bar{a}a}d\bar{\eta}d\eta da d\bar{a} \\ &= \int\int A(\bar{a},\theta+a)e^{-2\bar{\theta}a-\bar{\theta}\theta}d\bar{\theta}d\theta da d\bar{a} \\ &= \int A(\bar{a},\theta-a)e^{-\bar{\theta}\theta}d\bar{\theta}d\theta da d\bar{a} \\ &= \int A(\bar{a},-a)da d\bar{a} = \int A(\bar{a},a)d\bar{a}da.\end{aligned}$$

Here in the second line we changed variables $\eta = \theta + a$, $\bar{\eta} = \bar{\theta} + \bar{a}$, changed θ by $\theta + 2a$ in the third line, and have used that

$$\int f(\theta)e^{-\bar{\theta}\theta}d\bar{\theta}d\theta = f(0)$$

in the fourth line.

4.2. Path integral for the evolution operator. Let $\hat{H}$ be an Hamiltonian of a system of n identical fermions — an operator in $\mathscr{H}_F$ with Wick symbol $H(\bar{a},a)$. Here we express the Wick symbol $U_T(\bar{a},a)$ of the evolution operator $\hat{U}_T = e^{-iT\hat{H}}$ using the path integral over Grassmann variables. Set $\Delta t = \frac{T}{N}$, and let $\widetilde{U}_{\Delta t}$ be the operator with the Wick symbol $e^{-iH(\bar{a},a)\Delta t}$. The following elementary fact replaces Trotter's product formula for bosons.

LEMMA 4.2.

$$\hat{U}_T = \lim_{N\to\infty} \widetilde{U}_{\Delta t}^N,$$

where the convergence in the Grassmann algebra $\mathrm{Gr}_{2n} = \mathbb{C}[a_1, \bar{a}_1, \dots, a_n, \bar{a}_n]$ *is understood in the topology of the underlying vector space* $\mathrm{Gr}_{2n} \simeq \Lambda^\bullet\mathbb{C}^{2n}$.

PROOF. We have

$$\hat{U}_T = \lim_{N\to\infty}\left(I - i\hat{H}\Delta t\right)^N.$$

The Wick symbol of the operator $\hat{R}_{\Delta t} = I - i\hat{H}\Delta t - \widetilde{U}_{\Delta t}$, as a polynomial in Δt with Grassmann algebra coefficients which starts with the term $(\Delta t)^2$. Therefore, $\|\hat{R}_{\Delta t}\| = O((\Delta t)^2)$, and

$$\hat{U}_T = \lim_{N\to\infty}(\widetilde{U}_{\Delta t} + \hat{R}_{\Delta t})^N = \lim_{N\to\infty}\widetilde{U}_{\Delta t}^N.$$

□

Using Theorem 4.1, we can represent the Wick symbol $\widetilde{U}_{\Delta t}^N(\bar{a},a)$ of the operator $\widetilde{U}_{\Delta t}^N$ as a $(N-1)$-fold Berezin integral over the Grassmann variables $\{a_1^{(k)}, \bar{a}_1^{(k)}, \dots, a_n^{(k)}, \bar{a}_n^{(k)}\}$, $k = 1, \dots, N-1$. We set for brevity $a^{(k)} =$

$\{a_1^{(k)}, \dots, a_n^{(k)}\}$, $\bar{a}^{(k)} = \{\bar{a}_1^{(k)}, \dots, \bar{a}_n^{(k)}\}$, and denote $\bar{a}^{(k)}a^{(k)} = \sum_{l=1}^n \bar{a}_l^{(k)} a_l^{(k)}$, etc. Then

$$\widetilde{U}^N_{\Delta t}(\bar{a}, a) = \int \cdots \int \exp\left\{\frac{1}{2}\sum_{k=1}^{N-1}((\bar{a}^{(k+1)} - \bar{a}^{(k)})a^{(k)} + (a^{(k)} - a^{(k-1)})\bar{a}^{(k)})\right.$$
$$\left. + \frac{1}{2}((\bar{a}^{(1)} - \bar{a})a + (a - a^{(N-1)})\bar{a}) - i\sum_{k=0}^{N-1} H(\bar{a}^{(k+1)}, a^{(k)})\Delta t\right\} \prod_{k=1}^{N-1} d\bar{a}^{(k)} da^{(k)},$$

where we set $a^{(0)} = a$ and $\bar{a}^{(N)} = \bar{a}$. (Note that in this formula there are no variables $\bar{a}^{(0)}$ and $a^{(N)}$!).

It follows from Lemma 4.2 that

$$U_T(\bar{a}, a) = \lim_{N\to\infty} \widetilde{U}^N_{\Delta t}(\bar{a}, a) \tag{4.2}$$
$$= \lim_{N\to\infty} \int \cdots \int \exp\left\{\frac{1}{2}\sum_{k=1}^{N-1}((\bar{a}^{(k+1)} - \bar{a}^{(k)})a^{(k)} + (a^{(k)} - a^{(k-1)})\bar{a}^{(k)})\right.$$
$$\left. + \frac{1}{2}((\bar{a}^{(1)} - \bar{a})a + (a - a^{(N-1)})\bar{a}) - i\sum_{k=0}^{N-1} H(\bar{a}^{(k+1)}, a^{(k)})\Delta t\right\} \prod_{k=1}^{N-1} d\bar{a}^{(k)} da^{(k)}.$$

Now following the analogy with the boson case considered in Section 1.5 in Chapter 4, we pretend that as $N \to \infty$, the piece-wise constant functions

$$a_i(t) = a_i^{(k)}, \;\; \bar{a}(t) = \bar{a}_i^{(k)}, \quad k\Delta t \le t \le (k+1)\Delta t, \;\; k = 0, \dots, N-1,$$

with anticommuting values "converge" to the functions $a_i(t)$, $\bar{a}_i(t)$ on $[0, T]$ satisfying boundary conditions $a_i(0) = a_i$, $\bar{a}_i(T) = \bar{a}_i$, $i = 1, \dots, n$, and, respectively,

$$\frac{a_i^{(k)} - a_i^{(k-1)}}{\Delta t}, \quad \frac{\bar{a}_i^{(k)} - \bar{a}_i^{(k-1)}}{\Delta t} \;\text{ “converge” to }\; \dot{a}_i(t) = \frac{da_i}{dt}, \quad \dot{\bar{a}}_i(t) = \frac{d\bar{a}_i}{dt}.$$

Extending the analogy further we pretend that

$$\lim_{N\to\infty}\left\{\frac{1}{2}\sum_{k=1}^{N-1}((\bar{a}^{(k+1)} - \bar{a}^{(k)})a^{(k)} + (a^{(k)} - a^{(k-1)})\bar{a}^{(k)})\right.$$
$$\left. + \frac{1}{2}((\bar{a}^{(1)} - \bar{a})a + (a - a^{(N-1)})\bar{a}) - i\sum_{k=0}^{N-1} H(\bar{a}^{(k+1)}, a^{(k)})\Delta t\right\}$$
$$= \int_0^T \left(\tfrac{1}{2}(\dot{\bar{a}}a + \dot{a}\bar{a}) - iH(\bar{a}, a)\right) dt + \tfrac{1}{2}(\bar{a}(0)a + \bar{a}a(T)) - \bar{a}a)$$
$$= \int_0^T (\dot{a}\bar{a} - iH(\bar{a}, a))dt + \bar{a}a(T) - \bar{a}a,$$

where in the last line we have used "integration by parts"

$$\int_0^T \dot{\bar{a}}a\, dt = \int_0^T \dot{a}\bar{a}\, dt + \bar{a}a(T) - \bar{a}(0)a.$$

We can summarize everything by writing

$$U_T(\bar{a}, a) = \int\limits_{\substack{\bar{a}(T)=\bar{a}\\ a(0)=a}} \exp\left\{\int_0^T (\dot{a}\bar{a} - iH(\bar{a}, a))dt + \bar{a}\,a(T) - \bar{a}a\right\} \mathscr{D}\bar{a}\mathscr{D}a, \tag{4.3}$$

where the symbol on the right hand-side is, by definition, the *path integral over Grassmann variables.* Here the "integration" goes over all functions $a_l(t), \bar{a}_l(t)$ with anticommuting values on the interval $[0, T]$, satisfying boundary conditions $a_l(0) = a_l$, $\bar{a}_l(T) = \bar{a}_l$, $l = 1, \dots, n$, and

$$\mathscr{D}\bar{a}\mathscr{D}a = \prod_{0 \le t \le T} d\bar{a}(t)da(t) = \prod_{0 \le t \le T} \prod_{l=1}^{n} d\bar{a}_l(t)da_l(t),$$

where the integration goes over $a(T)$ and $\bar{a}(0)$ as well.

Remark. We emphasize that the rigorous definition of the Grassmann path integral is given by the limit $N \to \infty$ in (4.2). Still, in many interesting cases the heuristic reasoning presented above can be made into rigorous arguments.

Using Theorem 4.1, we can also express the trace and the supertrace of the evolution operator $U_T = e^{-iT\hat{H}}$ as a Grassmann path integral. We have

$$\operatorname{Tr} e^{-iT\hat{H}} = \int U_T(\bar{a}, a)e^{2\bar{a}a}dad\bar{a}$$

$$= \lim_{N\to\infty} \int \cdots \int \exp\left\{\tfrac{1}{2}\sum_{k=1}^{N-1}((\bar{a}^{(k+1)} - \bar{a}^{(k)})a^{(k)} + (a^{(k)} - a^{(k-1)})\bar{a}^{(k)})\right.$$

$$\left. + \tfrac{1}{2}((\bar{a}^{(1)} + \bar{a})a - (a + a^{(N-1)})\bar{a}) - i\sum_{k=0}^{N-1} H(\bar{a}^{(k+1)}, a^{(k)})\Delta t\right\} \prod_{k=1}^{N-1} d\bar{a}^{(k)}da^{(k)}dad\bar{a},$$

where $a^{(0)} = a$ and $\bar{a}^{(N)} = \bar{a}$. The terms $(\bar{a}^{(1)} + \bar{a})a$ and $-(a + a^{(N-1)})\bar{a}$ can be included into the respective sums $\sum_{k=0}^{N-1}$ and $\sum_{k=1}^{N}$ if we set $\bar{a}^{(0)} = -\bar{a}$ and $a^{(N)} = -a$. In the limit $N \to \infty$ we arrive to the anti-periodic boundary conditions for $a(t)$ and $\bar{a}(t)$ and

$$\operatorname{Tr} e^{-iT\hat{H}} = \int\limits_{\substack{\bar{a}(0)=-\bar{a}(T)\\ a(0)=-a(T)}} \exp\left\{\int_0^T (\dot{a}\bar{a} - iH(\bar{a}, a))\,dt\right\} \mathscr{D}\bar{a}\mathscr{D}a.$$

For the supertrace we have

$$\operatorname{Tr}_s e^{-iT\hat{H}} = \int U_T(\bar{a}, a) d\bar{a} da$$

$$= \lim_{N\to\infty} \int \cdots \int \exp\left\{ \tfrac{1}{2} \sum_{k=1}^{N-1} ((\bar{a}^{(k+1)} - \bar{a}^{(k)}) a^{(k)} + (a^{(k)} - a^{(k-1)}) \bar{a}^{(k)}) \right.$$

$$\left. + \tfrac{1}{2}((\bar{a}^{(1)} - \bar{a})a + (a - a^{(N-1)})\bar{a}) - i \sum_{k=0}^{N-1} H(\bar{a}^{(k+1)}, a^{(k)}) \Delta t \right\} \prod_{k=1}^{N-1} d\bar{a}^{(k)} da^{(k)} d\bar{a} da,$$

where $a^{(0)} = a$ and $\bar{a}^{(N)} = \bar{a}$. In this case the inclusion of the terms $(\bar{a}^{(1)} - \bar{a})a$ and $(a - a^{(N-1)})\bar{a})$ into the corresponding sums imposes the conditions $\bar{a}(0) = \bar{a}$ and $a^{(N)} = a$. In the limit $N \to \infty$ we arrive to the periodic boundary conditions in the Grassmann path integral,

$$\operatorname{Tr}_s e^{-iT\hat{H}} = \int\limits_{\substack{\bar{a}(0)=\bar{a}(T)\\ a(0)=a(T)}} \exp\left\{ \int_0^T (\dot{a}\bar{a} - iH(\bar{a}, a))\, dt \right\} \mathscr{D}\bar{a}\mathscr{D}a.$$

Remark. Formulas for the trace and supertrace of the evolution operator $e^{-iT\hat{H}}$ make sense because it is an operator in a finite-dimensional Hilbert space $\mathscr{H}_F$.

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 $U_{-iT} = e^{-T\hat{H}}$,

$$U_{-iT}(\bar{a}, a) = \int\limits_{\substack{\bar{a}(T)=\bar{a}\\ a(0)=a}} \exp\left\{ -\int_0^T (-\dot{a}\bar{a} + H(\bar{a}, a)) dt + \bar{a}\, a(T) - \bar{a}a \right\} \mathscr{D}\bar{a}\mathscr{D}a,$$

and for its trace and superstrace,

$$\operatorname{Tr} e^{-T\hat{H}} = \int\limits_{\substack{\bar{a}(0)=-\bar{a}(T)\\ a(0)=-a(T)}} \exp\left\{ -\int_0^T (-\dot{a}\bar{a} + H(\bar{a}, a))\, dt \right\} \mathscr{D}\bar{a}\mathscr{D}a, \tag{4.4}$$

$$\operatorname{Tr}_s e^{-T\hat{H}} = \int\limits_{\substack{\bar{a}(0)=\bar{a}(T)\\ a(0)=a(T)}} \exp\left\{ -\int_0^T (-\dot{a}\bar{a} + H(\bar{a}, a))\, dt \right\} \mathscr{D}\bar{a}\mathscr{D}a. \tag{4.5}$$

4.3. Gaussian path integrals over Grassmann variables. We start with the case $n = 1$. Let $u(t)$ be smooth periodic function on the interval $[0, T]$. We set

$$u_0 = \frac{1}{T} \int_0^T u(t) dt$$

and consider the first-order differential operator

$$D + u(t), \quad D = -\frac{d}{dt},$$

on the interval $[0, T]$. Similarly to the corresponding result for the bosons, we have the following statement for the corresponding Gaussian path integrals over Grassmann variables.

THEOREM 4.2. *We have*

$$\int\limits_{\substack{\bar{a}(0)=\bar{a}(T)\\ a(0)=a(T)}} e^{-\int_0^T(-\dot{a}\bar{a}+u(t)\bar{a}a)dt}\mathscr{D}\bar{a}\mathscr{D}a = \det{}'(-D+u(t))\big|_{\text{pbc}} = 1 - e^{-u_0T}$$

and

$$\int\limits_{\substack{\bar{a}(0)=-\bar{a}(T)\\ a(0)=-a(T)}} \exp^{-\int_0^T(-\dot{a}\bar{a}+u(t)\bar{a}a))dt}\mathscr{D}\bar{a}\mathscr{D}a = \det{}'(-D+u(t))\big|_{\text{apbc}} = 1 + e^{-u_0T},$$

where pbc *and* apbc *stand, correspondingly, for the periodic and anti-periodic boundary conditions for the differential operator $D + u(t)$ on the interval $[0, T]$.*

PROOF. We repeat the arguments for the bosonic case and prove the first formula; the second formula is proved analogously. Using (4.2) and Lemma 2.2 we get

$$\int\limits_{\substack{\bar{a}(0)=\bar{a}(T)\\ a(0)=a(T)}} e^{-\int_0^T(-\dot{a}\bar{a}+u(t)\bar{a}a)dt}\mathscr{D}\bar{a}\mathscr{D}a$$

$$= \lim_{N\to\infty}\int\cdots\int e^{-\sum_{k=0}^{N-1}((\bar{a}_k-\bar{a}_{k+1})a_k+u(t_k)\bar{a}_{k+1}a_k\Delta t)}\prod_{k=0}^{N-1}d\bar{a}_kda_k$$

$$= \lim_{N\to\infty}\det A_N,$$

where $a_N = a_0, \bar{a}_N = \bar{a}_0$, $t_k = \frac{kT}{N}$, and A_N is the following $N\times N$ matrix:

$$A_N = \begin{pmatrix} 1 & 0 & \dots & 0 & -1+u(t_{N-1})\Delta t \\ -1+u(t_0)\Delta t & 1 & \dots & 0 & 0 \\ 0 & -1+u(t_1)\Delta t & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & -1+u(t_{N-2})\Delta t & 1 \end{pmatrix}$$

It is elementary to compute that

$$\det A_N = 1 - \prod_{k=0}^{N-1}(1-u(t_k)\Delta t),$$

so that

$$\lim \det A_N = 1 - e^{-\int_0^T u(t)dt} = 1 - e^{-u_0 T}.$$

Using Proposition 2.3 in Chapter 4 completes the proof. □

EXAMPLE 4.1 (The fermion harmonic oscillator). The Hamiltonian

$$\hat{H} = \frac{\omega}{2}(\hat{a}^*\hat{a} - \hat{a}\hat{a}^*) = \omega\hat{a}^*\hat{a} - \frac{\omega}{2}I$$

has Wick symbol $H(\bar{a}, a) = \omega\bar{a}a - \frac{\omega}{2}$, so that using (4.4) and Theorem 4.2 we get,

$$\operatorname{Tr} e^{-T\hat{H}} = e^{\frac{\omega T}{2}} \int\limits_{\substack{\bar{a}(0)=-\bar{a}(T)\\ a(0)=-a(T)}} \exp^{-\int_0^T(-\dot{a}\bar{a}+\omega\bar{a}a))dt} \mathscr{D}\bar{a}\mathscr{D}a = e^{\frac{\omega T}{2}}(1+e^{-\omega T}) = 2\cosh\frac{\omega T}{2}$$

Of course, in this case $\mathscr{H}_F = \mathbb{C}^2$ and $\hat{H} = -\frac{\omega}{2}\sigma_3$, so that

$$\operatorname{Tr} e^{-T\hat{H}} = e^{\frac{\omega T}{2}} + e^{-\frac{\omega T}{2}} = 2\cosh\frac{\omega T}{2}.$$

— a different derivation of the same result.

Similarly, using (4.5) and Theorem 4.2 we get

$$\operatorname{Tr}_s e^{-T\hat{H}} = e^{\frac{\omega T}{2}} \int\limits_{\substack{\bar{a}(0)=\bar{a}(T)\\ a(0)=a(T)}} \exp^{-\int_0^T(-\dot{a}\bar{a}+\omega\bar{a}a))dt} \mathscr{D}\bar{a}\mathscr{D}a = e^{\frac{\omega T}{2}}(1-e^{-\omega T}) = 2\sinh\frac{\omega T}{2},$$

Using that for $\mathscr{H}_F = \mathbb{C}^2$ we have $\Gamma = \sigma_3$, the same result is obtained by

$$\operatorname{Tr}_s e^{-T\hat{H}} = \operatorname{Tr}\sigma_3 e^{-T\hat{H}} = e^{\frac{\omega T}{2}} - e^{-\frac{\omega T}{2}} = 2\sinh\frac{\omega T}{2}.$$

5. Supersymmetry

5.1. The basic example. We start with the Lagrangian of a free particle in $\mathbb{R}^n$ of spin $\frac{1}{2}$, considered in Example 2.2 in Section 2.6:

$$L = \frac{m}{2}\langle\dot{\mathbf{q}}, \dot{\mathbf{q}}\rangle + \frac{i}{2}\langle\boldsymbol{\psi}, \dot{\boldsymbol{\psi}}\rangle.$$

5.1.1. *Total angular momentum.* This Lagrangian is invariant with respect to the action of the orthogonal group $G = \mathrm{SO}(n)$ on the configuration space $\mathbb{R}^{n|n}$,

$$L(g\cdot\mathbf{v}) = L(\mathbf{v}), \quad \mathbf{v} \in T\mathbb{R}^{n|n}, \tag{5.1}$$

where the action of G on an tangent bundle $T\mathbb{R}^{n|n}$ extends the diagonal action on $\mathbb{R}^{n|n}$, defined by $(\mathbf{q}, \boldsymbol{\psi}) \mapsto (g\cdot\mathbf{q}, g\cdot\boldsymbol{\psi})$, $g \in G$. Corresponding conserved quantity — the Noether charge $\mathbf{J} \in \mathfrak{g}^*$ — the dual space to the Lie algebra $\mathfrak{g} = \mathrm{so}(n)$, can be obtained as follows (c.f. the proof of Theorem 1.2 in Chapter 1).

Consider arbitrary infinitesimal change of coordinates

$$\mathbf{q} \mapsto \tilde{\mathbf{q}} = \mathbf{q} + \delta\mathbf{q}, \quad \boldsymbol{\psi} \mapsto \tilde{\boldsymbol{\psi}} = \boldsymbol{\psi} + \delta\boldsymbol{\psi},$$

and compute $\delta L = L(\tilde{\mathbf{v}}) - L(\mathbf{v})$, up to the second order terms in $\delta\mathbf{q}, \delta\boldsymbol{\psi}$ as follows:

$$\begin{aligned}\delta L &= m\langle\dot{\mathbf{q}}, \delta\dot{\mathbf{q}}\rangle + \frac{i}{2}\Big(\langle\delta\boldsymbol{\psi}, \dot{\boldsymbol{\psi}}\rangle + \langle\boldsymbol{\psi}, \delta\dot{\boldsymbol{\psi}}\rangle\Big)\\ &= -m\langle\ddot{\mathbf{q}}, \delta\mathbf{q}\rangle + m\frac{d}{dt}\langle\dot{\mathbf{q}}, \delta\mathbf{q}\rangle + \frac{i}{2}\Big(\langle\delta\boldsymbol{\psi}, \dot{\boldsymbol{\psi}}\rangle - \langle\dot{\boldsymbol{\psi}}, \delta\boldsymbol{\psi}\rangle\Big) + \frac{i}{2}\frac{d}{dt}\langle\boldsymbol{\psi}, \delta\boldsymbol{\psi}\rangle\\ &= -m\langle\ddot{\mathbf{q}}, \delta\mathbf{q}\rangle + m\frac{d}{dt}\langle\dot{\mathbf{q}}, \delta\mathbf{q}\rangle + i\langle\delta\boldsymbol{\psi}, \dot{\boldsymbol{\psi}}\rangle + \frac{i}{2}\frac{d}{dt}\langle\boldsymbol{\psi}, \delta\boldsymbol{\psi}\rangle,\end{aligned}$$

where we have used that $\langle\dot{\boldsymbol{\psi}}, \delta\boldsymbol{\psi}\rangle = -\langle\delta\boldsymbol{\psi}, \dot{\boldsymbol{\psi}}\rangle$. Thus on solutions of the Euler-Lagrange equations $\ddot{\mathbf{q}} = 0$, $\dot{\boldsymbol{\psi}} = 0$ we have

$$\delta L = \frac{d}{dt}\left(m\langle\dot{\mathbf{q}}, \delta\mathbf{q}\rangle + \frac{i}{2}\langle\boldsymbol{\psi}, \delta\boldsymbol{\psi}\rangle\right).$$

Now using (5.1) with $g = e^{\varepsilon\mathbf{x}}$, where $\mathbf{x} \in \mathfrak{g}$, for $\delta\mathbf{q} = \varepsilon\mathbf{x}\cdot\mathbf{q}$ and $\delta\boldsymbol{\psi} = \varepsilon\mathbf{x}\cdot\boldsymbol{\psi}$ we obtain $\delta L = 0$, so that

$$-\mathbf{J}(\mathbf{x}) = m\langle\dot{\mathbf{q}}, \mathbf{x}\cdot\mathbf{q}\rangle + \frac{i}{2}\langle\boldsymbol{\psi}, \mathbf{x}\cdot\boldsymbol{\psi}\rangle$$

is an integral of motion:

$$\frac{d}{dt}\mathbf{J}(\mathbf{x}) = 0$$

on solutions of the Euler-Lagrange equations. Choosing a standard basis $\mathbf{x}_{kl}$, $1 \leq k < l \leq n$ of so(n) consisting of skew-symmetric $n \times n$ matrices corresponding to the roots of $\mathfrak{g}$, we get Noether integrals of motion

$$J_{kl} = q_k p_l - q_l p_k - i\psi_k\psi_l, \quad 1 \leq k < l \leq n,$$

which are components of the total angular momentum of a classical particle of spin $\frac{1}{2}$. In particular, for $n = 3$ we get

$$\begin{aligned}J_1 &:= J_{23} = M_1 - i\psi_2\psi_3,\\ J_2 &:= J_{31} = M_2 - i\psi_3\psi_1,\\ J_3 &:= J_{12} = M_3 - i\psi_1\psi_2,\end{aligned}$$

where M_1, M_2, M_3 are components of the angular momentum $\mathbf{M}$ of a particle in $\mathbb{R}^3$ (see Section 1.3 in Chapter 1).

REMARK. In fact, Lagrangian L of a free particle with spin $\frac{1}{2}$ is invariant under the action of $G \times G$ on $\mathbb{R}^{n|n}$, so that both the angular momentum $q_k p_l - q_l p_k$ in $\mathbb{R}^n$ and the "Grassmann angular momentum" $-i\psi_k\psi_l$ in $\mathbb{R}^{0|n}$ are conserved.

As we know, the Hilbert space for a corresponding quantum system is $\mathscr{H} = L^{\mathbb{R}^n} \otimes \mathbb{C}^{2^d}$, where $d = \left[\frac{n}{2}\right]$, and Noether charges J_{kl} correspond to the operators

$$\hat{J}_{kl} = Q_k P_l - Q_l P_k - i\hat{\psi}_k\hat{\psi}_l,$$

where the operators $\hat{\psi}_k$ satisfy

$$[\hat{\psi}_k, \hat{\psi}_l]_+ = \delta_{kl}I, \quad k, l = 1, \ldots, n.$$

In particular, for $n = 3$ we have $\hat{\psi}_j = \frac{1}{\sqrt{2}}\sigma_j$, and

$$\hat{\mathbf{J}} = \hat{\mathbf{M}} + \tfrac{1}{2}\boldsymbol{\sigma}$$

— the total angular momentum of a quantum particle in $\mathbb{R}^3$ of spin $\frac{1}{2}$.

5.1.2. *Supersymmetry transformation.* It is remarkable that Lagrangian L is also invariant under another transformations on $\mathbb{R}^{n|n}$ that mix even and odd coordinates. Namely, for $\gamma \in \Omega_I(\mathbb{R}^n)$ let $\boldsymbol{\psi}(t) \in \Pi T_\gamma \Omega_I(\mathbb{R}^n)$ — a global section over I of the pull-back by γ of the tangent bundle of $T\mathbb{R}^n$ with the reverse parity of the fibres,

$$\boldsymbol{\psi}(t) = \sum_{k=1}^{n} \psi_k(t) \frac{\partial}{\partial q_k}.$$

Now let ε be an odd real element and for every $(\gamma, \boldsymbol{\psi}) \in \Pi T\Omega_I(\mathbb{R}^n)$ consider

$$\delta_\varepsilon \mathbf{q}(t) = i\varepsilon\boldsymbol{\psi}(t) \in T_\gamma\Omega_I(\mathbb{R}^n) \;\text{ and }\; \delta_\varepsilon\boldsymbol{\psi}(t) = -m\varepsilon\dot{\mathbf{q}}(t) \in \Pi T_\gamma\Omega_I(\mathbb{R}^n).$$

Then for

$$\delta_\varepsilon L = L(\mathbf{q} + \delta_\varepsilon\mathbf{q}, \boldsymbol{\psi} + \delta_\varepsilon\boldsymbol{\psi}) - L(\mathbf{q}, \boldsymbol{\psi})$$

we obtain

$$\begin{aligned}\delta_\varepsilon L &= im\langle\dot{\mathbf{q}}, \varepsilon\boldsymbol{\psi}\rangle - \frac{im}{2}(\langle\varepsilon\dot{\mathbf{q}}, \dot{\boldsymbol{\psi}}\rangle + \langle\boldsymbol{\psi}, \varepsilon\ddot{\mathbf{q}}\rangle) \\ &= \frac{im}{2}(\langle\dot{\mathbf{q}}, \varepsilon\boldsymbol{\psi}\rangle + \langle\varepsilon\boldsymbol{\psi}, \ddot{\mathbf{q}}\rangle) \\ &= \frac{im\varepsilon}{2}\frac{d}{dt}\langle\boldsymbol{\psi}, \dot{\mathbf{q}}\rangle.\end{aligned}$$

Introducing $Q = i\langle\boldsymbol{\psi}, m\dot{\mathbf{q}}\rangle = i\langle\boldsymbol{\psi}, \mathbf{p}\rangle = i\sum_{k=1}^{n}\psi_k p_k$ — the *generator of supersymmetry*, we get that along every $\gamma \in \Omega_I(\mathbb{R}^n)$, $\boldsymbol{\psi} \in \gamma^*(\Pi T\mathbb{R}^n)$,

$$\delta_\varepsilon L = \frac{\varepsilon}{2}\frac{dQ}{dt} \tag{5.2}$$

This means that $\delta_\varepsilon S = 0$ for all periodic boundary conditions (and not only on equations of motion)!

Another remarkable property is the Lagrangian L can be recovered from "supercharge "Q. Namely, the computation

$$\begin{aligned}\delta_\varepsilon Q &= im(\langle\delta_\varepsilon\boldsymbol{\psi}, \dot{\mathbf{q}}\rangle + \langle\boldsymbol{\psi}, \delta_\varepsilon\dot{\mathbf{q}}\rangle) \\ &= im\varepsilon(-m\langle\dot{\mathbf{q}}, \dot{\mathbf{q}}\rangle - i\langle\boldsymbol{\psi}, \dot{\boldsymbol{\psi}}\rangle),\end{aligned}$$

gives

$$-2im\varepsilon L = \delta_\varepsilon Q. \tag{5.3}$$

The Hamiltonian can also be recovered from Q by

$$\{Q, Q\} = \mathbf{p}^2 = 2mH,$$

which shows that all properties of a free particle of spin $\frac{1}{2}$ are contained in the supercharge Q.

The invariant meaning of the supersymmetry transformation is related to the geometry of a path space. Namely, set $m = 1$ and consider the Wick rotation $t \mapsto -it$ to Euclidean time, so that the sypersymmetry transformation becomes

$$\delta_\varepsilon \mathbf{q}(t) = i\varepsilon\boldsymbol{\psi}(t), \quad \delta_\varepsilon \boldsymbol{\psi}(t) = -i\varepsilon\dot{\mathbf{q}}(t). \tag{5.4}$$

Now consider the infinite-dimensional supermanifold $\Pi T\Omega_I(\mathbb{R}^n)$ with coordinates $(\mathbf{q}(t), \boldsymbol{\psi}(t))$, $t \in I$. The supersymmetry transformation (5.4) (up to an overall factor of i) corresponds to the following vector field on $\Pi T\Omega_I(\mathbb{R}^n)$,

$$\mathscr{X} = \sum_{k=1}^{n} \int_{t_0}^{t_1} \left(\psi_k(t) \frac{\delta}{\delta q_k(t)} - \dot{q}_k(t) \frac{\delta}{\delta \psi_k(t)} \right) dt.$$

Setting

$$\mathscr{Q} = \int_{t_0}^{t_1} \langle \boldsymbol{\psi}(t), \dot{\mathbf{q}}(t) \rangle dt,$$

we get

$$\begin{aligned}
\mathscr{X}(\mathscr{Q}) &= \int_{t_0}^{t_1} (-\langle \dot{\mathbf{q}}(t), \dot{\mathbf{q}}(t) \rangle dt + \int_{t_0}^{t_1} \int_{t_0}^{t_1} \frac{d}{ds} \delta(s-t) \langle \boldsymbol{\psi}(t), \boldsymbol{\psi}(s) \rangle dt ds \\
&= -\int_{t_0}^{t_1} (\langle \dot{\mathbf{q}}(t), \dot{\mathbf{q}}(t) \rangle + \langle \boldsymbol{\psi}(t), \dot{\boldsymbol{\psi}}(t) \rangle) dt \\
&= -2S(\mathbf{q}(t), \boldsymbol{\psi}(t)),
\end{aligned}$$

where now S stands for the Euclidean action. Interpreting functions on $\Pi T\Omega_I(\mathbb{R}^n)$ as differential forms on $\Omega_I(\mathbb{R}^n)$, we also get that

$$\mathscr{X} \circ \mathscr{X} = -\sum_{k=1}^{n} \int_{t_0}^{t_1} \left(\dot{q}_k(t) \frac{\delta}{\delta q_k(t)} + \dot{\psi}_k(t) \frac{\delta}{\delta \psi_k(t)} \right) dt = -\mathcal{L}_V$$

— a first order differential operator on functions on $\Pi T\Omega_I(\mathbb{R}^n)$ which corresponds to a Lie derivative of the vector field V on $\Omega_I(\mathbb{R}^n)$, defined by $V_\gamma = \dot{\gamma} \in T_\gamma \Omega_I(\mathbb{R}^n)$. Also, we have

$$\mathscr{X}(S) = -2 \int_{t_0}^{t_1} \frac{dQ}{dt} dt = -2\, Q(t)|_{t_0}^{t_1},$$

where $Q(t) = \langle \boldsymbol{\psi}(t), \dot{\mathbf{q}}(t) \rangle$ is Euclidean supercharge.

After the quantization,

$$\hat{Q} = i \sum_{k=1}^{n} \hat{\psi}_k P_k,$$

where

$$P_k = \frac{\hbar}{i} \frac{\partial}{\partial q_k} \quad \text{and} \quad \hat{\psi}_k = \frac{1}{\sqrt{2}} \gamma_k, \quad k = 1, \dots, n,$$

so that

$$\hat{Q} = \frac{1}{\sqrt{2}} \eth$$

where $\eth$ is a Dirac operator for the Euclidean metric on $\mathbb{R}^n$. We have

$$[\hat{Q}, \hat{Q}]_+ = 2\hat{Q}^2 = \Delta = 2m\hat{H},$$

where Δ is the Laplace operator on $\mathbb{R}^n$.

5.1.3. *Spin $\frac{1}{2}$ particle on a Riemannian manifold.* Let M be n-dimensional Riemannian manifold with a Riemannian metric ds^2. In local coordinates $\mathbf{q} = (q_1, \dots, q_n)$,

$$ds^2 = \sum_{i,j=1}^{n} g^{ij}(\mathbf{q}) dq_i \otimes dq_j.$$

Let ΠTM be the tangent bundle of M with the reverse parity on the fibres. For a path $\gamma \in \Omega_I(M)$ denote by $\boldsymbol{\psi}(t)$ the section of the pull-back bundle $\gamma^*(\Pi TM)$ over I. In local coordinates,

$$\boldsymbol{\psi}(t) = \sum_{k=1}^{n} \psi_k(t) \frac{\partial}{\partial q_k} \in \Pi T_{\gamma(t)} M.$$

Now let ε be an odd real element, and for every $(\gamma, \boldsymbol{\psi}) \in \Pi T \Omega_I(M)$ consider the supersymmetry transformation — the vector fields along γ, defined in local coordinates by

(5.5)

$$\delta_\varepsilon \mathbf{q}(t) = i\varepsilon \boldsymbol{\psi}(t) \in \Pi T_{\gamma(t)} M, \quad \delta_\varepsilon \boldsymbol{\psi}(t) = -m\varepsilon \dot{\mathbf{q}}(t) \in \Pi T_{\gamma(t)} M, \quad t \in I.$$

LEMMA 5.1. *Supersymmetry transformation* (5.5) *is well-defined, i.e., does not depend on the choice of local coordinates.*

PROOF. Let $\tilde{\mathbf{q}}$ be another coordinate system, $\tilde{q}_k = f_k(q_1, \dots, q_n)$, $k = 1, \dots, n$. Along the path γ,

$$\dot{\tilde{q}}_k(t) = \sum_{l=1}^{n} \frac{\partial f_k}{\partial q_l}(\gamma(t)) \dot{q}_l(t),$$

and

$$\boldsymbol{\psi}(t) = \sum_{k=1}^{n} \tilde{\psi}_k(t) \frac{\partial}{\partial \tilde{q}_k},$$

where

$$\tilde{\psi}_k(t) = \sum_{l=1}^{n} \frac{\partial f_k}{\partial q_l}(\gamma(t)) \psi_l(t).$$

We have

$$\delta_\varepsilon \tilde{q}_k(t) = \sum_{l=1}^{n} \frac{\partial f_k}{\partial q_l}(\gamma(t)) \delta_\varepsilon q_l(t) = i \sum_{l=1}^{n} \frac{\partial f_k}{\partial q_l}(\gamma(t)) \varepsilon \psi_l(t) = i\varepsilon \tilde{\psi}_k(t),$$

and

$$\begin{aligned}
\delta_\varepsilon\tilde{\psi}_k(t) &= \delta_\varepsilon\left(\sum_{l=1}^{n}\frac{\partial f_k}{\partial q_l}(\gamma(t))\psi_l(t))\right)\\
&= \sum_{l=1}^{n}\frac{\partial f_k}{\partial q_l}(\gamma(t))\delta_\varepsilon\psi_l(t) + \sum_{j,l=1}^{n}\frac{\partial^2 f_k}{\partial q_j\partial q_l}(\gamma(t))\delta_\varepsilon q_j(t)\psi_l(t)\\
&= -m\varepsilon\sum_{l=1}^{n}\frac{\partial f_k}{\partial q_l}(\gamma(t))\dot{q}_l(t) + i\varepsilon\sum_{j,l=1}^{n}\frac{\partial^2 f_k}{\partial q_j\partial q_l}(\gamma(t))\psi_j(t)\psi_l(t)\\
&= -m\varepsilon\dot{\tilde{q}}_k(t),
\end{aligned}$$

since ψ_k anticommute. $\square$

For a $\gamma \in \Omega_I(M)$ let $\boldsymbol{\psi} \in \Pi T_\gamma\Omega_I(M)$ and along the path γ set

$$Q(t) = i\langle\dot{q}(t), \boldsymbol{\psi}(t)\rangle,$$

and denote by $\nabla_{\dot{\gamma}}$ the covariant derivative in the tangent bundles TM and ΠTM along γ, given by Levi-Civita connection.

PROPOSITION 5.1. *Along $\gamma \in \Omega_I(M)$,*

$$\delta_\varepsilon Q = -2i\varepsilon L,$$

where

$$L = \frac{m}{2}\langle\dot{\mathbf{q}}, \dot{\mathbf{q}}\rangle + \frac{i}{2}\langle\boldsymbol{\psi}, \nabla_{\dot{\gamma}}\boldsymbol{\psi}\rangle$$

is a supersymmetric Lagrangian for a spin $\frac{1}{2}$ particle on a Riemannian manifold M,

$$\delta_\varepsilon L = \frac{\varepsilon}{2}\frac{dQ}{dt}.$$