Quantum Mechanics for Mathematicians

Leon A. Takhtajan

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

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

To my teacher Ludwig Dmitrievich Faddeev with admiration and gratitude.

Contents

Preface

This book is based on graduate courses taught by the author over the last fourteen years in the mathematics department of Stony Brook University. The goal of these courses was to introduce second year graduate students with no prior knowledge of physics to the basic concepts and methods of quantum mechanics. For the last 50 years quantum physics has been a driving force behind many dramatic achievements in mathematics, similar to the role played by classical physics in the seventeenth to nineteenth centuries. Classical physics, especially classical mechanics, was an integral part of mathematical education up to the early twentieth century, with lecture courses given by Hilbert and Poincaré. Surprisingly, quantum physics, especially quantum mechanics, with its intrinsic beauty and connections with many branches of mathematics, has never been a part of a graduate mathematics curriculum. This course was developed to partially fill this gap and to make quantum mechanics accessible to graduate students and research mathematicians.

L.D. Faddeev was the first to develop a course in quantum mechanics for undergraduate students specializing in mathematics. From 1968 to 1973 he regularly lectured in the mathematics department of St. Petersburg State University in St. Petersburg, Russia[1], and the author enjoyed the opportunity to take his course. The notes for this book emerged from an attempt to create a similar course for graduate students, which uses more sophisticated mathematics and covers a larger variety of topics, including the Feynman path integral approach to quantum mechanics.

[1] At that time in Leningrad, Soviet Union.

There are many excellent physics textbooks on quantum mechanics, starting with the classic texts by P.A.M. Dirac [**Dir47**], L.D. Landau and E.M. Lifshitz [**LL58**], and V.A. Fock [**Foc78**], to the encyclopedic treatise by A. Messiah [**Mes99**], the recent popular textbook by J.J. Sakurai [**Sak94**], and many others. From a mathematics perspective, there are classic monographs by J. von Neumann [**vN96**] and by H. Weyl [**Wey50**], as well as a more recent book by G.W. Mackey [**Mac04**], which deal with the basic mathematical formalism and logical foundations of the theory. There is also a monumental project [**DEF$^+$99**], created with the purpose of introducing graduate students and research mathematicians to the realm of quantum fields and strings, both from a mathematics and a physics perspective. Though it contains a very detailed exposition of classical mechanics, classical field theory, and supersymmetry, oriented at the mathematical audience, quantum mechanics is discussed only briefly (with the exception of L.D. Faddeev's elegant introduction to quantum mechanics in [**Fad99**]). Excellent lecture notes for undergraduate students by L.D. Faddeev and O.A. Yakubovskiĭ [**FY80**] seems to be the only book on quantum mechanics completely accessible to mathematicians[2]. Recent books by S.J. Gustafson and I.M. Sigal [**GS03**] and by F. Strocchi [**Str05**] are also oriented at mathematicians. The latter is a short introductory course, while the former is more an intermediate level monograph on quantum theory rather than a textbook on quantum mechanics. There are also many specialized books on different parts of quantum mechanics, like scattering theory, the Schrödinger operator, $\mathbb{C}^*$-algebras and foundations, etc.

The present book gives a comprehensive treatment of quantum mechanics from a mathematics perspective and covers such topics as mathematical foundations, quantization, the Schrödinger equation, the Feynman path integral and functional methods, and supersymmetry. It can be used as a one-year graduate course, or as two one-semester courses: the introductory course based on the material in Part 1, and a more advanced course based on Part 2. Part 1 of the book, which consists of Chapters 1-4, can be considered as an expanded version of [**FY80**]. It uses more advanced mathematics than [**FY80**], and contains rigorous proofs of all main results, including the celebrated Stone-von Neumann theorem. It should be accessible to a second-year graduate student. As in [**FY80**], we adopt the approach, which goes back to Dirac and was further developed by Faddeev, that classical mechanics and quantum mechanics are just two different realizations of the fundamental mathematical structure of a physical theory that uses the notions of observables, states, measurement, and the time evolution — dynamics. Part 2, which consists of Chapters 5-8, deals with functional methods in quantum

[2]The English translation will appear in the AMS "The Student Mathematical Library" series.

mechanics, and goes beyond the material in [**FY80**]. Exposition there is less detailed and requires certain mathematical sophistication.

Though our presentation freely uses all the necessary tools of modern mathematics, it follows the spirit and tradition of the classical texts and monographs mentioned above. In this sense it can be considered "neoclassical" (as compared with a more abstract approach in [**DF99a**]). Each chapter in the book concludes with a special *Notes and references* section, which provides references to the necessary mathematics background and physics sources. A courageous reader can actually learn the relevant mathematics by studying the main text and consulting these references, and with enough sophistication, could "translate" corresponding parts in physics textbooks into the mathematics language. For the physics students, the book presents an opportunity to become familiar with the mathematical foundations and methods of quantum mechanics on a "case by case" basis. It is worth mentioning that development of many mathematics disciplines has been stimulated by quantum mechanics.

There are several ways to study the material in this book. A casual reader can study the main text in a cursory manner, and ignore numerous remarks and problems, located at the end of the sections. This would be sufficient to obtain basic minimal knowledge of quantum mechanics. A determined reader is supposed to fill in the details of the computations in the main text (a pencil and paper are required), which is the only way to master the material, and to attempt to solve the basic problems[3]. Finally, a truly devoted reader should try to solve all the problems (probably consulting the corresponding references at the end of each section) and to follow up on the remarks, which may often be linked to other topics not covered in the main text.

The author would like to thank the students in his courses for their comments on the draft of the lecture notes. He is especially grateful to his colleagues Peter Kulish and Lee-Peng Teo for the careful reading of the manuscript. The work on the book was partially supported by the NSF grants DMS-0204628 and DMS-0705263. Any opinions, findings, and conclusions or recommendations expressed in this book are those of the author and do not necessarily reflect the views of the National Science Foundation.

[3]We leave it to the reader to decide which problems are basic and which are advanced.

Part 1

Foundations

Chapter 1

Classical Mechanics

We assume that the reader is familiar with the basic notions from the theory of smooth (that is, C^∞) manifolds and recall here the standard notation. Unless it is stated explicitly otherwise, all maps are assumed to be smooth and all functions are assumed to be smooth and real-valued. Local coordinates $\boldsymbol{q} = (q^1, \dots, q^n)$ on a smooth n-dimensional manifold M at a point $q \in M$ are Cartesian coordinates on $\varphi(U) \subset \mathbb{R}^n$, where (U, φ) is a coordinate chart on M centered at $q \in U$. For $f : U \to \mathbb{R}^n$ we denote $(f \circ \varphi^{-1})(q^1, \dots, q^n)$ by $f(\boldsymbol{q})$, and we let

$$\frac{\partial f}{\partial \boldsymbol{q}} = \left(\frac{\partial f}{\partial q^1}, \dots, \frac{\partial f}{\partial q^n} \right)$$

stand for the gradient of a function f at a point $\boldsymbol{q} \in \mathbb{R}^n$ with Cartesian coordinates $(q^1, \dots, q^n)$. We denote by

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

the graded algebra of smooth differential forms on M with respect to the wedge product, and by d the de Rham differential — a graded derivation of $\mathcal{A}^\bullet(M)$ of degree 1 such that df is a differential of a function $f \in \mathcal{A}^0(M) = C^\infty(M)$. Let $\mathrm{Vect}(M)$ be the Lie algebra of smooth vector fields on M with the Lie bracket $[\ ,\ ]$, given by a commutator of vector fields. For $X \in \mathrm{Vect}(M)$ we denote by $\mathcal{L}_X$ and i_X, respectively, the Lie derivative along X and the inner product with X. The Lie derivative is a degree 0 derivation of $\mathcal{A}^\bullet(M)$ which commutes with d and satisfies $\mathcal{L}_X(f) = X(f)$ for $f \in \mathcal{A}^0(M)$, and the inner product is a degree -1 derivation of $\mathcal{A}^\bullet(M)$ satisfying $i_X(f) = 0$

and $i_X(df) = X(f)$ for $f \in \mathcal{A}^0(M)$. They satisfy Cartan formulas

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

For a smooth mapping of manifolds $f : M \to N$ we denote by $f_* : TM \to TN$ and $f^* : T^*N \to T^*M$, 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. Lagrangian Mechanics

1.1. Generalized coordinates. Classical mechanics describes systems of finitely many interacting *particles*[1]. A system is called *closed* if its particles do not interact with the outside material bodies. The position of a system in space 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*[2].

The *state* of a system at any instant 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 the *Newton-Laplace determinacy principle* which asserts that a state of a system at a given instant completely determines its motion at all times t (in the future and in the past). The motion is described by the *classical trajectory* — a path $\gamma(t)$ in the configuration space M. In generalized coordinates $\gamma(t) = (q^1(t), \dots, q^n(t))$, and corresponding derivatives $\dot{q}^i = \dfrac{dq^i}{dt}$ are called *generalized velocities*. The Newton-Laplace principle is a fundamental experimental fact confirmed by our perception of everyday experiences. It implies that *generalized accelerations* $\ddot{q}^i = \dfrac{d^2q^i}{dt^2}$ are uniquely defined by generalized coordinates q^i and generalized velocities $\dot{q}^i$, so that classical trajectories satisfy a system of second order ordinary differential equations, called *equations of motion*. In the next section we formulate the most general principle governing the motion of mechanical systems.

1.2. The principle of the least action. A *Lagrangian system* on a configuration space M is defined by a smooth, real-valued function L on $TM \times \mathbb{R}$ — the direct product of a tangent bundle TM of M and the time axis[3] — called the *Lagrangian function* (or simply, *Lagrangian*). The motion of a

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

[2] Systems with infinitely many degrees of freedom are described by classical field theory.

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

Lagrangian system (M, L) is described by the *principle of the least action in the configuration space* (or *Hamilton's principle*), formulated as follows.

Let

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

be the space of smooth parametrized paths in M connecting points q_0 and q_1. The path space $P(M) = P(M)_{q_0,t_0}^{q_1,t_1}$ is an infinite-dimensional real Fréchet manifold, and the tangent space $T_\gamma P(M)$ to $P(M)$ at $\gamma \in P(M)$ consists of all smooth vector fields along the path γ in M which vanish at the endpoints q_0 and q_1. A smooth path Γ in $P(M)$, passing through $\gamma \in P(M)$, is called a *variation with fixed ends* of the path $\gamma(t)$ in M. A variation Γ is a family $\gamma_\varepsilon(t) = \Gamma(t, \varepsilon)$ of paths in M given by a smooth map

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

such that $\Gamma(t, 0) = \gamma(t)$ for $t_0 \le t \le t_1$ and $\Gamma(t_0, \varepsilon) = q_0, \Gamma(t_1, \varepsilon) = q_1$ for $-\varepsilon_0 \le \varepsilon \le \varepsilon_0$. The tangent vector

$$\delta\gamma = \left.\frac{\partial \Gamma}{\partial \varepsilon}\right|_{\varepsilon=0} \in T_\gamma P(M)$$

corresponding to a variation $\gamma_\varepsilon(t)$ is traditionally called an *infinitesimal variation*. Explicitly,

$$\delta\gamma(t) = \Gamma_*(\tfrac{\partial}{\partial \varepsilon})(t, 0) \in T_{\gamma(t)}M,\ \ t_0 \le t \le t_1,$$

where $\frac{\partial}{\partial \varepsilon}$ is a tangent vector to the interval $[-\varepsilon_0, \varepsilon_0]$ at 0. Finally, a tangential lift of a path $\gamma : [t_0, t_1] \to M$ is the path $\gamma' : [t_0, t_1] \to TM$ defined by $\gamma'(t) = \gamma_*(\frac{\partial}{\partial t}) \in T_{\gamma(t)}M,\ t_0 \le t \le t_1$, where $\frac{\partial}{\partial t}$ is a tangent vector to $[t_0, t_1]$ at t. In other words, $\gamma'(t)$ is the velocity vector of a path $\gamma(t)$ at time t.

Definition. The *action functional* $S : P(M) \to \mathbb{R}$ of a Lagrangian system (M, L) is defined by

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

Principle of the Least Action (Hamilton's principle)**.** A path $\gamma \in PM$ describes the motion of a Lagrangian 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 of the action functional S,

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

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

The critical points of the action functional are called *extremals* and the principle of the least action states that a Lagrangian system (M, L)

moves along the extremals[4]. The extremals are characterized by equations of motion — a system of second order differential equations in local coordinates on TM. The equations of motion have the most elegant form for the following choice of local coordinates on TM.

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

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

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

Standard coordinates are Cartesian coordinates on $\varphi_*(TU) \subset T\mathbb{R}^n \simeq \mathbb{R}^n \times \mathbb{R}^n$ and have the property that for $(q, v) \in TU$ and $f \in C^\infty(U)$,

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

Let (U, φ) and (U', φ') be coordinate charts on M with the transition functions $F = (F^1, \dots, F^n) = \varphi' \circ \varphi^{-1} : \varphi(U \cap U') \to \varphi'(U \cap U')$, and let $(\boldsymbol{q}, \boldsymbol{v})$ and $(\boldsymbol{q}', \boldsymbol{v}')$, respectively, be the standard coordinates on TU and TU'. We have $\boldsymbol{q}' = F(\boldsymbol{q})$ and $\boldsymbol{v}' = F_*(\boldsymbol{q})\boldsymbol{v}$, where $F_*(\boldsymbol{q}) = \left\{ \dfrac{\partial F^i}{\partial q^j}(\boldsymbol{q}) \right\}_{i,j=1}^{n}$ is a matrix-valued function on $\varphi(U \cap U')$. Thus "vertical" coordinates $\boldsymbol{v} = (v^1, \dots, v^n)$ in the fibers of $TM \to M$ transform like components of a tangent vector on M under the change of coordinates on M.

The tangential lift $\gamma'(t)$ of a path $\gamma(t)$ in M in standard coordinates on TU is $(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t)) = (q^1(t), \dots, q^n(t), \dot{q}^1(t), \dots, \dot{q}^n(t))$, where the dot stands for the time derivative, so that

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

Following a centuries long tradition[5], we will usually denote standard coordinates by

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

where the dot *does not* stand for the time derivative. Since we only consider paths in TM that are tangential lifts of paths in M, there will be no confusion[6].

---

[4] The principle of the least action does not state that an extremal connecting points q_0 and q_1 is a minimum of S, nor that such an extremal is unique. It also does not state that any two points can be connected by an extremal.

[5] Used in all texts on classical mechanics and theoretical physics.

[6] We reserve the notation $(\boldsymbol{q}(t), \boldsymbol{v}(t))$ for general paths in TM.

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

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

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

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

The second sum in the last line vanishes due to the property $\delta q^i(t_0) = \delta q^i(t_1) = 0,\ i = 1, \ldots, n$. The first sum is zero for arbitrary smooth functions δq^i on the interval $[t_0, t_1]$ which vanish at the endpoints. This implies that for each term in the sum the integrand is identically zero,

$$\frac{\partial L}{\partial q^i}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t)\right) = 0, \quad i = 1, \ldots, n.$$

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

Remark. In calculus of variations, the directional derivative of a functional S with respect to a tangent vector $V \in T_\gamma P(M)$ — the *Gato derivative* — is defined by

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

where γ_ε is a path in $P(M)$ with a tangent vector V at $\gamma_0 = \gamma$. The result of the above computation (when γ lies in a coordinate chart $U \subset M$) can be written as

$$\begin{aligned} \delta_V S &= \int_{t_0}^{t_1} \sum_{i=1}^{n} \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right) (\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t) v^i(t) dt \\ &= \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial \boldsymbol{q}} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\boldsymbol{q}}}\right) (\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t) \boldsymbol{v}(t) dt. \end{aligned} \tag{1.1}$$

Here $V(t) = \sum_{i=1}^{n} v^i(t) \frac{\partial}{\partial q^i}$ is a vector field along the path γ in M. Formula (1.1) is called the formula for the *first variation of the action with fixed ends*. The principle of the least action is a statement that $\delta_V S(\gamma) = 0$ for all $V \in T_\gamma P(M)$.

Remark. It is also convenient to consider a space $\widehat{P(M)} = \{\gamma : [t_0, t_1] \to M\}$ of all smooth parametrized paths in M. The tangent space $T_\gamma \widehat{P(M)}$ to $\widehat{P(M)}$ at $\gamma \in \widehat{P(M)}$ is the space of all smooth vector fields along the path γ in M (no condition at the endpoints). The computation in the proof of Theorem 1.1 yields the following formula for the *first variation of the action with free ends*:

$$\delta_V S = \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial \boldsymbol{q}} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \right) \boldsymbol{v}\, dt + \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \boldsymbol{v} \Big|_{t_0}^{t_1}. \tag{1.2}$$

Problem 1.1. Show that the action functional is given by the evaluation of the 1-form Ldt on $TM \times \mathbb{R}$ over the 1-chain $\tilde{\gamma}$ on $TM \times \mathbb{R}$,

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

where $\tilde{\gamma} = \{(\gamma'(t), t); t_0 \le t \le t_1\}$ and $Ldt\left(w, c\frac{\partial}{\partial t}\right) = cL(q, v)$, $w \in T_{(q,v)}TM$, $c \in \mathbb{R}$.

Problem 1.2. Let $f \in C^\infty(M)$. Show that Lagrangian systems (M, L) and $(M, L+df)$ (where df is a fibre-wise linear function on TM) have the same equations of motion.

Problem 1.3. Give examples of Lagrangian systems such that an extremal connecting two given points (i) is not a local minimum; (ii) is not unique; (iii) does not exist.

Problem 1.4. For γ an extremal of the action functional S, the *second variation* of S is defined by

$$\delta^2_{V_1 V_2} S = \left. \frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \right|_{\varepsilon_1 = \varepsilon_2 = 0} S(\gamma_{\varepsilon_1, \varepsilon_2}),$$

where $\gamma_{\varepsilon_1,\varepsilon_2}$ is a smooth two-parameter family of paths in M such that the paths $\gamma_{\varepsilon_1,0}$ and γ_{0,ε_2} in $P(M)$ at the point $\gamma_{0,0} = \gamma \in P(M)$ have tangent vectors V_1 and V_2, respectively. For a Lagrangian system (M, L) find the second variation of S and verify that for given V_1 and V_2 it does not depend on the choice of $\gamma_{\varepsilon_1,\varepsilon_2}$.

1.3. Examples of Lagrangian systems. To describe a mechanical phenomena it is necessary to choose a *frame of reference*. The properties of the *space-time* where the motion takes place depend on this choice. The space-time is characterized by the following postulates[7].

[7]Strictly speaking, these postulates are valid only in the non-relativistic limit of special relativity, when the speed of light in the vacuum is assumed to be infinite.

Newtonian Space-Time. The space is a three-dimensional affine Euclidean space E^3. A choice of the *origin* $0 \in E^3$ — a *reference point* — establishes the isomorphism $E^3 \simeq \mathbb{R}^3$, where the vector space $\mathbb{R}^3$ carries the Euclidean inner product and has a fixed orientation. The time is one-dimensional — a time axis $\mathbb{R}$ — and the space-time is a direct product $E^3 \times \mathbb{R}$. An *inertial* reference frame is a coordinate system with respect to the origin $0 \in E^3$, initial time t_0, and an orthonormal basis in $\mathbb{R}^3$. In an inertial frame the space is *homogeneous* and *isotropic* and the time is *homogeneous*. The laws of motion are invariant with respect to the transformations

$$\boldsymbol{r} \mapsto g \cdot \boldsymbol{r} + \boldsymbol{r}_0, \quad t \mapsto t + t_0,$$

where $\boldsymbol{r}, \boldsymbol{r}_0 \in \mathbb{R}^3$ and g is an orthogonal linear transformation in $\mathbb{R}^3$. The time in classical mechanics is *absolute*.

The Galilean group is the group of all affine transformations of $E^3 \times \mathbb{R}$ which preserve time intervals and which for every $t \in \mathbb{R}$ are isometries in E^3. Every Galilean transformation is a composition of rotation, space-time translation, and a transformation

$$\boldsymbol{r} \mapsto \boldsymbol{r} + \boldsymbol{v}t, \quad t \mapsto t,$$

where $\boldsymbol{v} \in \mathbb{R}^3$. Any two inertial frames are related by a Galilean transformation.

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

These postulates impose restrictions on Lagrangians of mechanical systems. Thus it follows from the first postulate that the Lagrangian L of a closed system does not explicitly depend on time. Physical systems are described by special Lagrangians, in agreement with the experimental facts about the motion of material bodies.

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

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

Here $m > 0$[8] is the mass of a particle and $\dot{\boldsymbol{r}}^2 = |\dot{\boldsymbol{r}}|^2$ is the length square of the velocity vector $\dot{\boldsymbol{r}} \in T_{\boldsymbol{r}}\mathbb{R}^3 \simeq \mathbb{R}^3$. Euler-Lagrange equations give *Newton's law of inertia*,

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

[8] Otherwise the action functional is not bounded from below.

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

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

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

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

where

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

is called *kinetic energy* of a system and $V(\boldsymbol{r})$ is *potential energy*. The Euler-Lagrange equations give *Newton's equations*

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

where

$$\boldsymbol{F}_a = -\frac{\partial V}{\partial \boldsymbol{r}_a}$$

is the *force* on the a-th particle, $a = 1, \dots, N$. Forces of this form are called *conservative*. It follows from homogeneity of space that potential energy $V(\boldsymbol{r})$ of a closed system of N interacting particles with conservative forces depends only on relative positions of the particles, which leads to the equation

$$\sum_{a=1}^{N} \boldsymbol{F}_a = 0.$$

In particular, for a closed system of two particles $\boldsymbol{F}_1 + \boldsymbol{F}_2 = 0$, which is the equality of action and reaction forces, also called *Newton's third law*.

The potential energy of a closed system with only pair-wise interaction between the particles has the form

$$V(\boldsymbol{r}) = \sum_{1 \le a < b \le N} V_{ab}(\boldsymbol{r}_a - \boldsymbol{r}_b).$$

It follows from the isotropy of space that $V(\boldsymbol{r})$ depends only on relative distances between the particles, so that the Lagrangian of a closed system of N particles with pair-wise interaction has the form

$$L = \sum_{a=1}^{N} \tfrac{1}{2} m_a \dot{\boldsymbol{r}}_a^2 \; - \sum_{1 \le a < b \le N} V_{ab}(|\boldsymbol{r}_a - \boldsymbol{r}_b|).$$

If the potential energy $V(\boldsymbol{r})$ is a homogeneous function of degree ρ, $V(\lambda\boldsymbol{r}) = \lambda^\rho V(\boldsymbol{r})$, then the average values $\overline{T}$ and $\overline{V}$ of kinetic energy and potential energy over a closed trajectory are related by the *virial theorem*

$$2\overline{T} = \rho\overline{V}. \tag{1.3}$$

Indeed, let $\boldsymbol{r}(t)$ be a periodic trajectory with period $\tau > 0$, i.e., $\boldsymbol{r}(0) = \boldsymbol{r}(\tau)$, $\dot{\boldsymbol{r}}(0) = \dot{\boldsymbol{r}}(\tau)$. Using integration by parts, Newton's equations, and Euler's homogeneous function theorem, we get

$$\begin{aligned} 2\overline{T} &= \frac{1}{\tau}\int_0^\tau \sum_{a=1}^N m_a \dot{\boldsymbol{r}}_a^2 dt = -\frac{1}{\tau}\int_0^\tau \sum_{a=1}^N m_a \boldsymbol{r}_a \ddot{\boldsymbol{r}}_a dt \\ &= \frac{1}{\tau}\int_0^\tau \sum_{a=1}^N \boldsymbol{r}_a \frac{\partial V}{\partial \boldsymbol{r}_a} dt = \rho\overline{V}. \end{aligned}$$

Example 1.3 (Universal gravitation)**.** According to *Newton's law of gravitation*, the potential energy of the gravitational force between two particles with masses m_a and m_b is

$$V(\boldsymbol{r}_a - \boldsymbol{r}_b) = -G\frac{m_a m_b}{|\boldsymbol{r}_a - \boldsymbol{r}_b|},$$

where G is the gravitational constant. The configuration space of N particles with gravitational interaction is

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

Example 1.4 (Particle in an external potential field)**.** Here $M = \mathbb{R}^3$ and

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

where potential energy can explicitly depend on time. Equations of motion are Newton's equations

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

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

Example 1.5 (Charged particle in electromagnetic field[9])**.** Consider a particle of charge e and mass m in $\mathbb{R}^3$ moving in a time-independent electromagnetic field with scalar and vector potentials $\varphi(\boldsymbol{r})$ and $\boldsymbol{A}(\boldsymbol{r}) = (A_1(\boldsymbol{r}), A_2(\boldsymbol{r}), A_3(\boldsymbol{r}))$. The Lagrangian has the form

$$L = \frac{m\dot{\boldsymbol{r}}^2}{2} + e\left(\frac{\dot{\boldsymbol{r}}\,\boldsymbol{A}}{c} - \varphi\right),$$

[9]This is a non-relativistic limit of an example in classical electrodynamics.

where c is the speed of light. The Euler-Lagrange equations give Newton's equations with the *Lorentz force*,

$$m\ddot{\boldsymbol{r}} = e\left(\boldsymbol{E} + \frac{\dot{\boldsymbol{r}}}{c} \times \boldsymbol{B}\right),$$

where $\times$ is the cross-product of vectors in $\mathbb{R}^3$, and

$$\boldsymbol{E} = -\frac{\partial \varphi}{\partial \boldsymbol{r}} \quad \text{and} \quad \boldsymbol{B} = \operatorname{curl} \boldsymbol{A}$$

are electric and magnetic[10] fields, respectively.

Example 1.6 (Small oscillations)**.** Consider a particle of mass m with n degrees of freedom moving in a potential field $V(\boldsymbol{q})$, and suppose that potential energy U has a minimum at $\boldsymbol{q} = 0$. Expanding $V(\boldsymbol{q})$ in Taylor series around 0 and keeping only quadratic terms, one obtains a Lagrangian system which describes small oscillations from equilibrium. Explicitly,

$$L = \tfrac{1}{2} m\dot{\boldsymbol{q}}^2 - V_0(\boldsymbol{q}),$$

where V_0 is a positive-definite quadratic form on $\mathbb{R}^n$ given by

$$V_0(\boldsymbol{q}) = \tfrac{1}{2} \sum_{i,j=1}^{n} \frac{\partial^2 V}{\partial q^i \partial q^j}(0) q^i q^j.$$

Since every quadratic form can be diagonalized by an orthogonal transformation, we can assume from the very beginning that coordinates $\boldsymbol{q} = (q^1, \dots, q^n)$ are chosen so that $V_0(\boldsymbol{q})$ is diagonal and

$$L = \tfrac{1}{2} m\big(\dot{\boldsymbol{q}}^2 - \sum_{i=1}^{n} \omega_i^2 (q^i)^2\big), \tag{1.4}$$

where $\omega_1, \dots, \omega_n > 0$. Such coordinates $\boldsymbol{q}$ are called *normal coordinates*. In normal coordinates Euler-Lagrange equations take the form

$$\ddot{q}^i + \omega_i^2 q^i = 0, \quad i = 1, \dots, n,$$

and describe n decoupled (i.e., non-interacting) *harmonic oscillators* with *frequencies* $\omega_1, \dots, \omega_n$.

Example 1.7 (Free particle on a Riemannian manifold)**.** Let (M, ds^2) be a Riemannian manifold with the Riemannian metric ds^2. In local coordinates $x^1, \dots, x^n$ on M,

$$ds^2 = g_{\mu\nu}(x) dx^\mu dx^\nu,$$

where following tradition we assume the summation over repeated indices. The Lagrangian of a free particle on M is

$$L(v) = \tfrac{1}{2}\langle v, v\rangle = \tfrac{1}{2}\|v\|^2, \; v \in TM,$$

[10] Notation $\boldsymbol{B} = \operatorname{rot} \boldsymbol{A}$ is also used.

where $\langle\ ,\ \rangle$ stands for the inner product in fibers of TM given by the Riemannian metric. The corresponding functional

$$S(\gamma) = \tfrac{1}{2}\int_{t_0}^{t_1} \|\gamma'(t)\|^2 dt = \tfrac{1}{2}\int_{t_0}^{t_1} g_{\mu\nu}(x)\dot{x}^\mu \dot{x}^\nu dt$$

is called the action functional in Riemannian geometry. The Euler-Lagrange equations are

$$g_{\mu\nu}\ddot{x}^\mu + \frac{\partial g_{\mu\nu}}{\partial x^\lambda}\dot{x}^\mu\dot{x}^\lambda = \frac{1}{2}\frac{\partial g_{\mu\lambda}}{\partial x^\nu}\dot{x}^\mu\dot{x}^\lambda,$$

and after multiplying by the inverse metric tensor $g^{\sigma\nu}$ and summation over ν they take the form

$$\ddot{x}^\sigma + \Gamma^\sigma_{\mu\nu}\dot{x}^\mu\dot{x}^\nu = 0, \quad \sigma = 1,\dots,n,$$

where

$$\Gamma^\sigma_{\mu\nu} = \frac{1}{2}g^{\sigma\lambda}\left(\frac{\partial g_{\mu\lambda}}{\partial x^\nu} + \frac{\partial g_{\nu\lambda}}{\partial x^\mu} - \frac{\partial g_{\mu\nu}}{\partial x^\lambda}\right)$$

are Christoffel's symbols. The Euler-Lagrange equations of a free particle moving on a Riemannian manifold are geodesic equations.

Let ∇ be the Levi-Civita connection — the metric connection in the tangent bundle TM — and let ∇_ξ be a covariant derivative with respect to the vector field $\xi \in \mathrm{Vect}(M)$. Explicitly,

$$(\nabla_\xi\,\eta)^\mu = \left(\frac{\partial\eta^\mu}{\partial x^\nu} + \Gamma^\mu_{\nu\lambda}\eta^\lambda\right)\xi^\nu, \quad \text{where} \quad \xi = \xi^\mu(x)\frac{\partial}{\partial x^\mu},\ \eta = \eta^\mu(x)\frac{\partial}{\partial x^\mu}.$$

For a path $\gamma(t) = (x^\mu(t))$ denote by $\nabla_{\dot\gamma}$ a covariant derivative along γ,

$$(\nabla_{\dot\gamma}\eta)^\mu(t) = \frac{d\eta^\mu(t)}{dt} + \Gamma^\mu_{\nu\lambda}(\gamma(t))\dot{x}^\nu(t)\eta^\lambda(t), \quad \text{where} \quad \eta = \eta^\mu(t)\frac{\partial}{\partial x^\mu}$$

is a vector field along γ. Formula (1.1) can now be written in an invariant form

$$\delta S = -\int_{t_0}^{t_1}\langle\nabla_{\dot\gamma}\dot\gamma, \delta\gamma\rangle dt,$$

which is known as the formula for the first variation of the action in Riemannian geometry.

Example 1.8 (The rigid body)**.** The configuration space of a rigid body in $\mathbb{R}^3$ with a fixed point is a Lie group $G = \mathrm{SO}(3)$ of orientation preserving orthogonal linear transformations in $\mathbb{R}^3$. Every left-invariant Riemannian metric $\langle\ ,\ \rangle$ on G defines a Lagrangian $L : TG \to \mathbb{R}$ by

$$L(v) = \tfrac{1}{2}\langle v, v\rangle, \quad v \in TG.$$

According to the previous example, equations of motion of a rigid body are geodesic equations on G with respect to the Riemannian metric $\langle\ ,\ \rangle$. Let $\mathfrak{g} = \mathfrak{so}(3)$ be the Lie algebra of G. A velocity vector $\dot g \in T_gG$ defines the *angular velocity of the body* by $\Omega = (L_{g^{-1}})_*\dot g \in \mathfrak{g}$, where $L_g : G \to G$ are

left translations on G. In terms of angular velocity, the Lagrangian takes the form

$$L = \tfrac{1}{2}\langle \Omega, \Omega \rangle_e,$$

where $\langle\ ,\ \rangle_e$ is an inner product on $\mathfrak{g} = T_eG$ given by the Riemannian metric $\langle\ ,\ \rangle$. The Lie algebra $\mathfrak{g}$ — the Lie algebra of 3×3 skew-symmetric matrices — has the invariant inner product $\langle u, v\rangle_0 = -\frac{1}{2}\operatorname{Tr} uv$ (the Killing form), so that $\langle \Omega, \Omega\rangle_e = \langle \boldsymbol{A}\cdot\Omega, \Omega\rangle_0$ for some symmetric linear operator $\boldsymbol{A} : \mathfrak{g} \to \mathfrak{g}$ which is positive-definite with respect to the Killing form. Such a linear operator $\boldsymbol{A}$ is called the *inertia tensor* of the body. The *principal axes of inertia* of the body are orthonormal eigenvectors e_1, e_2, e_3 of $\boldsymbol{A}$; corresponding eigenvalues I_1, I_2, I_3 are called the *principal moments of inertia*. Setting $\Omega = \Omega_1 e_1 + \Omega_2 e_2 + \Omega_3 e_3$[11], we get

$$L = \tfrac{1}{2}(I_1\Omega_1^2 + I_2\Omega_2^2 + I_3\Omega_3^2).$$

In this parametrization, the Euler-Lagrange equations become *Euler's equations*

$$\begin{aligned} I_1\dot{\Omega}_1 &= (I_2 - I_3)\Omega_2\Omega_3,\\ I_2\dot{\Omega}_2 &= (I_3 - I_1)\Omega_1\Omega_3,\\ I_3\dot{\Omega}_3 &= (I_1 - I_2)\Omega_1\Omega_2. \end{aligned}$$

Euler's equations describe the rotation of a free rigid body around a fixed point. In the system of coordinates with axes which are the principal axes of inertia, principal moments of inertia of the body are I_1, I_2, I_3.

Problem 1.5. Determine the motion of a charged particle in a constant uniform magnetic field. Show that if the initial velocity $v_3 = 0$ in the z-axis (taken in the direction of the field, $\boldsymbol{B} = (0, 0, B)$), the trajectories are circles of radii $r = \dfrac{cmv_t}{eB}$ in a plane perpendicular to the field (the xy-plane), where $v_t = \sqrt{v_1^2 + v_2^2}$ is the initial velocity in the xy-plane. The centers (x_0, y_0) of circles are given by

$$x_0 = \frac{cmv_1}{eB} + x, \quad y_0 = -\frac{cmv_2}{eB} + y,$$

where (x, y) are points on a circle of radius r.

Problem 1.6. Show that the Euler-Lagrange equations for the Lagrangian $L(v) = \|v\|$, $v \in TM$, coincide with the geodesic equations written with respect to a constant multiple of the natural parameter.

Problem 1.7. Prove that for a particle in a potential field, discussed in Example 1.4, the second variation of the action functional, defined in Problem 1.4, is given by

$$\delta^2 S = \int_{t_0}^{t_1} \mathcal{J}(\delta_1 \boldsymbol{r})\delta_2 \boldsymbol{r}\, dt,$$

[11] This establishes the Lie algebra isomorphism $\mathfrak{g} \simeq \mathbb{R}^3$, where the Lie bracket in $\mathbb{R}^3$ is given by the cross-product.

where $\delta_1 \boldsymbol{r}, \delta_2 \boldsymbol{r} \in T_\gamma P\mathbb{R}^3$, $\gamma = \boldsymbol{r}(t)$ is the classical trajectory, $\mathcal{J} = -m\dfrac{d^2}{dt^2}I - \dfrac{\partial^2 V}{\partial \boldsymbol{r}^2}(t)$, I is the 3×3 identity matrix, and $\dfrac{\partial^2 V}{\partial \boldsymbol{r}^2}(t) = \left\{\dfrac{\partial^2 V}{\partial \boldsymbol{r}_a \partial \boldsymbol{r}_b}(\boldsymbol{r}(t))\right\}_{a,b=1}^{3}$. A second-order linear differential operator $\mathcal{J}$, acting on vector fields along γ, is called the *Jacobi operator*.

Problem 1.8. Find normal coordinates and frequencies for the Lagrangian system considered in Example 1.6 with $V_0(\boldsymbol{q}) = \frac{1}{2}a^2\sum_{i=1}^{n}(q^{i+1}-q^i)^2$, where $q^{n+1} = q^1$.

Problem 1.9. Prove that the second variation of the action functional in Riemannian geometry is given by

$$\delta^2 S = \int_{t_0}^{t_1} \langle \mathcal{J}(\delta_1\gamma), \delta_2\gamma\rangle dt.$$

Here $\delta_1\gamma, \delta_2\gamma \in T_\gamma PM$, $\mathcal{J} = -\nabla^2_{\dot\gamma} - R(\dot\gamma, \cdot)\dot\gamma$ is the Jacobi operator, and R is a curvature operator — a fibre-wise linear mapping $R : TM \otimes TM \to \mathrm{End}(TM)$ of vector bundles, defined by $R(\xi,\eta) = \nabla_\eta\nabla_\xi - \nabla_\xi\nabla_\eta + \nabla_{[\xi,\eta]} : TM \to TM$, where $\xi, \eta \in \mathrm{Vect}(M)$.

Problem 1.10. Choosing the principal axes of inertia as a basis in $\mathbb{R}^3$, show that the Lie algebra isomorphism $\mathfrak{g} \simeq \mathbb{R}^3$ is given by $\mathfrak{g} \ni \begin{pmatrix} 0 & -\Omega_3 & \Omega_2 \\ \Omega_3 & 0 & -\Omega_1 \\ -\Omega_2 & \Omega_1 & 0 \end{pmatrix} \mapsto (\Omega_1, \Omega_2, \Omega_3) \in \mathbb{R}^3$.

Problem 1.11. Show that for every symmetric $\boldsymbol{A} \in \mathrm{End}\ \mathfrak{g}$ there exists a symmetric 3×3 matrix A such that $\boldsymbol{A}\cdot\Omega = A\Omega + \Omega A$, and find A for diagonal $\boldsymbol{A}$.

Problem 1.12. Derive Euler's equations for a rigid body. (*Hint:* Use that $L = -\frac{1}{2}\,\mathrm{Tr}\, A\Omega^2$, where $\Omega = g^{-1}\dot g$ and $\delta\Omega = -g^{-1}\delta g\,\Omega + g^{-1}\delta\dot g$, and obtain the Euler-Lagrange equations in the matrix form $A\dot\Omega + \dot\Omega A = A\Omega^2 - \Omega^2 A$.)

1.4. Symmetries and Noether's theorem. To describe the motion of a mechanical system one needs to solve the corresponding Euler-Lagrange equations — a system of second order ordinary differential equations for the generalized coordinates. This could be a very difficult problem. Therefore of particular interest are those functions of generalized coordinates and velocities which remain constant during the motion.

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

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

for all extremals γ of the action functional.

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

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

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

Proof. Let (U, φ) and (U', φ') be coordinate charts on M with the transition functions $F = (F^1, \dots, F^n) = \varphi' \circ \varphi^{-1} : \varphi(U \cap U') \to \varphi'(U \cap U')$. Corresponding standard coordinates $(\boldsymbol{q}, \dot{\boldsymbol{q}})$ and $(\boldsymbol{q}', \dot{\boldsymbol{q}}')$ are related by $\boldsymbol{q}' = F(\boldsymbol{q})$ and $\dot{\boldsymbol{q}}' = F_*(\boldsymbol{q})\dot{\boldsymbol{q}}$ (see Section 1.2). We have $d\boldsymbol{q}' = F_*(\boldsymbol{q})d\boldsymbol{q}$ and $d\dot{\boldsymbol{q}}' = G(\boldsymbol{q}, \dot{\boldsymbol{q}})d\boldsymbol{q} + F_*(\boldsymbol{q})d\dot{\boldsymbol{q}}$ (for some matrix-valued function $G(\boldsymbol{q}, \dot{\boldsymbol{q}})$), so that

$$\begin{aligned} dL &= \frac{\partial L}{\partial \boldsymbol{q}'} d\boldsymbol{q}' + \frac{\partial L}{\partial \dot{\boldsymbol{q}}'} d\dot{\boldsymbol{q}}' + \frac{\partial L}{\partial t} dt \\ &= \left(\frac{\partial L}{\partial \boldsymbol{q}'} F_*(\boldsymbol{q}) + \frac{\partial L}{\partial \dot{\boldsymbol{q}}'} G(\boldsymbol{q}, \dot{\boldsymbol{q}}) \right) d\boldsymbol{q} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}'} F_*(\boldsymbol{q}) d\dot{\boldsymbol{q}} + \frac{\partial L}{\partial t} dt \\ &= \frac{\partial L}{\partial \boldsymbol{q}} d\boldsymbol{q} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}} d\dot{\boldsymbol{q}} + \frac{\partial L}{\partial t} dt. \end{aligned}$$

Thus under a change of coordinates

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

so that E is a well-defined function on TM. □

Corollary 1.2. *Under a change of local coordinates on* M*, components of* $\dfrac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = \left(\dfrac{\partial L}{\partial \dot{q}^1}, \dots, \dfrac{\partial L}{\partial \dot{q}^n} \right)$ *transform like components of a* 1*-form 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,

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

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

Conservation of energy for a closed mechanical system is a fundamental law of physics which follows from the homogeneity of time. For a general closed system of N interacting particles considered in Example 1.2,

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

In other words, the total energy $E = T + V$ is a sum of the kinetic energy and the potential energy.

Definition. A Lagrangian $L : TM \to \mathbb{R}$ is invariant with respect to the diffeomorphism $g : M \to M$ if $L(g_*(v)) = L(v)$ for all $v \in TM$. The diffeomorphism g is called the *symmetry* of a closed Lagrangian system (M, L). A Lie group G is the *symmetry group* of (M, L) (group of *continuous symmetries*) if there is a left G-action on M such that for every $g \in G$ the mapping $M \ni x \mapsto g \cdot x \in M$ is a symmetry.

Continuous symmetries give rise to conservation laws.

Theorem 1.3 (Noether)**.** *Suppose that a Lagrangian $L : TM \to \mathbb{R}$ is invariant under a one-parameter group $\{g_s\}_{s\in\mathbb{R}}$ of diffeomorphisms of M. Then the Lagrangian system (M, L) admits an integral of motion I, given in standard coordinates on TM by*

$$I(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}^i}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \left(\frac{dg_s^i(\boldsymbol{q})}{ds}\bigg|_{s=0} \right) = \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \boldsymbol{a},$$

where $X = \sum_{i=1}^{n} a^i(\boldsymbol{q}) \dfrac{\partial}{\partial q^i}$ is the vector field on M associated with the flow g_s. The integral of motion I is called the Noether integral.

Proof. It follows from Corollary 1.2 that I is a well-defined function on TM. Now differentiating $L((g_s)_*(\gamma'(t))) = L(\gamma'(t))$ with respect to s at $s = 0$ and using the Euler-Lagrange equations we get

$$0 = \frac{\partial L}{\partial \boldsymbol{q}} \boldsymbol{a} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \dot{\boldsymbol{a}} = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}} \right) \boldsymbol{a} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \frac{d\boldsymbol{a}}{dt} = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}} \boldsymbol{a} \right),$$

where $\boldsymbol{a}(t) = \big(a^1(\gamma(t)), \dots, a^n(\gamma(t))\big)$. □

Remark. A vector field X on M is called an *infinitesimal symmetry* if the corresponding local flow g_s of X (defined for each $s \in \mathbb{R}$ on some $U_s \subseteq M$) is a symmetry: $L \circ (g_s)_* = L$ on U_s. Every vector field X on M lifts to a vector field X' on TM, defined by a local flow on TM induced from the corresponding local flow on M. In standard coordinates on TM,

$$X = \sum_{i=1}^{n} a^i(\boldsymbol{q}) \frac{\partial}{\partial q^i} \quad \text{and} \quad X' = \sum_{i=1}^{n} a^i(\boldsymbol{q}) \frac{\partial}{\partial q^i} + \sum_{i,j=1}^{n} \dot{q}^j \frac{\partial a^i}{\partial q^j}(\boldsymbol{q}) \frac{\partial}{\partial \dot{q}^i}. \tag{1.5}$$

It is easy to verify that X is an infinitesimal symmetry if and only if $dL(X') = 0$ on TM, which in standard coordinates has the form

$$\sum_{i=1}^{n} a^i(\boldsymbol{q}) \frac{\partial L}{\partial q^i} + \sum_{i,j=1}^{n} \dot{q}^j \frac{\partial a^i}{\partial q^j}(\boldsymbol{q}) \frac{\partial L}{\partial \dot{q}^i} = 0. \tag{1.6}$$

Remark. Noether's theorem generalizes to time-dependent Lagrangians $L : TM \times \mathbb{R} \to \mathbb{R}$. Namely, on the *extended configuration space* $M_1 = M \times \mathbb{R}$ define a time-independent Lagrangian L_1 by

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

where $(\boldsymbol{q}, \tau)$ are local coordinates on M_1 and $(\boldsymbol{q}, \tau, \dot{\boldsymbol{q}}, \dot{\tau})$ are standard coordinates on TM_1. The Noether integral I_1 for a closed system (M_1, L_1) defines an integral of motion I for a system (M, L) by the formula

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

When the Lagrangian L does not depend on time, L_1 is invariant with respect to the one-parameter group of translations $\tau \mapsto \tau + s$, and the Noether integral $I_1 = \dfrac{\partial L_1}{\partial \dot{\tau}}$ gives $I = -E$.

Noether's theorem can be generalized as follows.

Proposition 1.2. *Suppose that for the Lagrangian $L : TM \to \mathbb{R}$ there exist a vector field X on M and a function K on TM such that for every path γ in M,*

$$dL(X')(\gamma(t)) = \frac{d}{dt}K(\gamma'(t)).$$

Then

$$I = \sum_{i=1}^{n} a^i(\boldsymbol{q})\,\frac{\partial L}{\partial \dot{q}^i}(\boldsymbol{q}, \dot{\boldsymbol{q}}) - K(\boldsymbol{q}, \dot{\boldsymbol{q}})$$

is an integral of motion for the Lagrangian system (M, L).

Proof. Using Euler-Lagrange equations, we have along the extremal γ,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}\boldsymbol{a}\right) = \frac{\partial L}{\partial \boldsymbol{q}}\boldsymbol{a} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}}\dot{\boldsymbol{a}} = \frac{dK}{dt}. \qquad \square$$

Example 1.9 (Conservation of momentum)**.** Let $M = V$ be a vector space, and suppose that a Lagrangian L is invariant with respect to a one-parameter group $g_s(q) = q + sv$, $v \in V$. According to Noether's theorem,

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

is an integral of motion. Now let (M, L) be a closed Lagrangian system of N interacting particles considered in Example 1.2. We have $M = V = \mathbb{R}^{3N}$, and the Lagrangian L is invariant under simultaneous translation of

coordinates $\boldsymbol{r}_a = (r_a^1, r_a^2, r_a^3)$ of all particles by the same vector $\boldsymbol{c} \in \mathbb{R}^3$. Thus $v = (\boldsymbol{c}, \dots, \boldsymbol{c}) \in \mathbb{R}^{3N}$ and for every $\boldsymbol{c} = (c^1, c^2, c^3) \in \mathbb{R}^3$,

$$I = \sum_{a=1}^{N} \left(c^1 \frac{\partial L}{\partial \dot{r}_a^1} + c^2 \frac{\partial L}{\partial \dot{r}_a^2} + c^3 \frac{\partial L}{\partial \dot{r}_a^3} \right) = c^1 P_1 + c^2 P_2 + c^3 P_3$$

is an integral of motion. The integrals of motion P_1, P_2, P_3 define the vector

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

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

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

so that the total momentum of a closed system is the sum of momenta of individual particles. Conservation of momentum is a fundamental physical law which reflects the homogeneity of space.

Traditionally, $p_i = \dfrac{\partial L}{\partial \dot{q}^i}$ are called *generalized momenta* corresponding to generalized coordinates q^i, and $F_i = \dfrac{\partial L}{\partial q^i}$ are called *generalized forces*. In these notations, the Euler-Lagrange equations have the same form

$$\dot{\boldsymbol{p}} = \boldsymbol{F}$$

as Newton's equations in Cartesian coordinates. Conservation of momentum implies Newton's third law.

Example 1.10 (Conservation of angular momentum)**.** Let $M = V$ be a vector space with Euclidean inner product. Let $G = \mathrm{SO}(V)$ be the connected Lie group of automorphisms of V preserving the inner product, and let $\mathfrak{g} = \mathfrak{so}(V)$ be the Lie algebra of G. Suppose that a Lagrangian L is invariant with respect to the action of a one-parameter subgroup $g_s(q) = e^{sx} \cdot q$ of G on V, where $x \in \mathfrak{g}$ and e^x is the exponential map. According to Noether's theorem,

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

is an integral of motion. Now let (M, L) be a closed Lagrangian system of N interacting particles considered in Example 1.2. We have $M = V = \mathbb{R}^{3N}$, and the Lagrangian L is invariant under a simultaneous rotation of coordinates $\boldsymbol{r}_a$ of all particles by the same orthogonal transformation in $\mathbb{R}^3$.

Thus $x = (u, \dots, u) \in \underbrace{\mathfrak{so}(3) \oplus \cdots \oplus \mathfrak{so}(3)}_{N}$, and for every $u \in \mathfrak{so}(3)$,

$$I = \sum_{a=1}^{N} \left((u \cdot \boldsymbol{r}_a)^1 \frac{\partial L}{\partial \dot{r}_a^1} + (u \cdot \boldsymbol{r}_a)^2 \frac{\partial L}{\partial \dot{r}_a^2} + (u \cdot \boldsymbol{r}_a)^3 \frac{\partial L}{\partial \dot{r}_a^3} \right)$$

is an integral of motion. Let $u = u^1 X_1 + u^2 X_2 + u^3 X_3$, where $X_1 = \left(\begin{smallmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{smallmatrix}\right), X_2 = \left(\begin{smallmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{smallmatrix}\right), X_3 = \left(\begin{smallmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{smallmatrix}\right)$ is the basis in $\mathfrak{so}(3) \simeq \mathbb{R}^3$ corresponding to the rotations about the vectors e_1, e_2, e_3 of the standard orthonormal basis in $\mathbb{R}^3$ (see Problem 1.10). We get

$$I = u^1 M_1 + u^2 M_2 + u^3 M_3,$$

where $\boldsymbol{M} = (M_1, M_2, M_3) \in \mathbb{R}^3$ (or rather a vector in the dual space to $\mathfrak{so}(3)$) is given by

$$\boldsymbol{M} = \sum_{a=1}^{N} \boldsymbol{r}_a \times \frac{\partial L}{\partial \dot{\boldsymbol{r}}_a}.$$

The vector $\boldsymbol{M}$ is called the *angular momentum* of the system. Explicitly,

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

so that the total angular momentum of a closed system is the sum of angular momenta of individual particles. Conservation of angular momentum is a fundamental physical law which reflects the isotropy of space.

Problem 1.13. Find how total momentum and total angular momentum transform under the Galilean transformations.

1.5. One-dimensional motion. The motion of systems with one degree of freedom is called one-dimensional. In terms of a Cartesian coordinate x on $M = \mathbb{R}$ the Lagrangian takes the form

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

The conservation of energy

$$E = \frac{1}{2} m \dot{x}^2 + V(x)$$

allows us to solve the equation of motion in a closed form by separation of variables. We have

$$\frac{dx}{dt} = \sqrt{\frac{2}{m}(E - V(x))},$$

so that

$$t = \sqrt{\frac{m}{2}} \int \frac{dx}{\sqrt{E - V(x)}}.$$

The inverse function $x(t)$ is a general solution of Newton's equation

$$m\ddot{x} = -\frac{dV}{dx},$$

with two arbitrary constants, the energy E and the constant of integration.

Since kinetic energy is non-negative, for a given value of E the actual motion takes place in the region of $\mathbb{R}$ where $V(x) \leq E$. The points where $V(x) = E$ are called *turning points*. The motion which is confined between two turning points is called *finite*. The finite motion is periodic — the particle oscillates between the turning points x_1 and x_2 with the period

$$T(E) = \sqrt{2m} \int_{x_1}^{x_2} \frac{dx}{\sqrt{E - V(x)}}.$$

If the region $V(x) \leq E$ is unbounded, then the motion is called *infinite* and the particle eventually goes to infinity. The regions where $V(x) > E$ are forbidden.

On the phase plane with coordinates (x, y) Newton's equation reduces to the first order system

$$m\dot{x} = y, \quad \dot{y} = -\frac{dV}{dx}.$$

Trajectories correspond to the phase curves $(x(t), y(t))$, which lie on the level sets

$$\frac{y^2}{2m} + V(x) = E$$

of the energy function. The points $(x_0, 0)$, where x_0 is a critical point of the potential energy $V(x)$, correspond to the equilibrium solutions. The local minima correspond to the stable solutions and local maxima correspond to the unstable solutions. For the values of E which do not correspond to the equilibrium solutions the level sets are smooth curves. These curves are closed if the motion is finite.

The simplest non-trivial one-dimensional system, besides the free particle, is the harmonic oscillator with $V(x) = \frac{1}{2}kx^2$ $(k > 0)$, considered in Example 1.6. The general solution of the equation of motion is

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

where A is the *amplitude*, $\omega = \sqrt{\dfrac{k}{m}}$ is the *frequency*, and α is the *phase* of a simple harmonic motion with the period $T = \dfrac{2\pi}{\omega}$. The energy is $E = \frac{1}{2}m\omega^2 A^2$ and the motion is finite with the same period T for $E > 0$.

Problem 1.14. Show that for $V(x) = -x^4$ there are phase curves which do not exist for all times. Prove that if $V(x) \geq 0$ for all x, then all phase curves exist for all times.

Problem 1.15. The simple pendulum is a Lagrangian system with $M = S^1 = \mathbb{R}/2\pi\mathbb{Z}$ and $L = \frac{1}{2}\dot{\theta}^2 + \cos\theta$. Find the period T of the pendulum as a function of the amplitude of the oscillations.

Problem 1.16. Suppose that the potential energy $V(x)$ is even, $V(0) = 0$, and $V(x)$ is a one-to-one monotonically increasing function for $x \geq 0$. Prove that the inverse function $x(V)$ and the period $T(E)$ are related by the Abel transform

$$T(E) = 2\sqrt{2m}\int_0^E \frac{dx}{dV}\frac{dV}{\sqrt{E-V}} \quad \text{and} \quad x(V) = \frac{1}{2\pi\sqrt{2m}}\int_0^V \frac{T(E)dE}{\sqrt{V-E}}.$$

1.6. The motion in a central field and the Kepler problem. The motion of a system of two interacting particles — the *two-body problem* — can also be solved completely. Namely, in this case (see Example 1.2) $M = \mathbb{R}^6$ and

$$L = \frac{m_1\dot{\boldsymbol{r}}_1^2}{2} + \frac{m_2\dot{\boldsymbol{r}}_2^2}{2} - V(|\boldsymbol{r}_1 - \boldsymbol{r}_2|).$$

Introducing on $\mathbb{R}^6$ new coordinates

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2 \quad \text{and} \quad \boldsymbol{R} = \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2}{m_1 + m_2},$$

we get

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

where $m = m_1 + m_2$ is the *total mass* and $\mu = \dfrac{m_1 m_2}{m_1 + m_2}$ is the *reduced mass* of a two-body system. The Lagrangian L depends only on the velocity $\dot{\boldsymbol{R}}$ of the center of mass and not on its position $\boldsymbol{R}$. A generalized coordinate with this property is called *cyclic*. It follows from the Euler-Lagrange equations that generalized momentum corresponding to the cyclic coordinate is conserved. In our case it is a total momentum of the system,

$$\boldsymbol{P} = \frac{\partial L}{\partial \dot{\boldsymbol{R}}} = m\dot{\boldsymbol{R}},$$

so that the center of mass $\boldsymbol{R}$ moves uniformly. Thus in the frame of reference where $\boldsymbol{R} = 0$, the two-body problem reduces to the problem of a single particle of mass μ in the external central field $V(|\boldsymbol{r}|)$. In spherical coordinates in $\mathbb{R}^3$,

$$x = r\sin\vartheta\cos\varphi,\ y = r\sin\vartheta\sin\varphi,\ z = r\cos\vartheta,$$

where $0 \leq \vartheta < \pi$, $0 \leq \varphi < 2\pi$, its Lagrangian takes the form

$$L = \tfrac{1}{2}\mu(\dot{r}^2 + r^2\dot{\vartheta}^2 + r^2\sin^2\vartheta\,\dot{\varphi}^2) - V(r).$$

It follows from the conservation of angular momentum $\boldsymbol{M} = \mu\boldsymbol{r}\times\dot{\boldsymbol{r}}$ that during motion the position vector $\boldsymbol{r}$ lies in the plane P orthogonal to $\boldsymbol{M}$ in $\mathbb{R}^3$. Introducing polar coordinates (r, χ) in the plane P we get $\dot{\chi}^2 = \dot{\vartheta}^2 + \sin^2\vartheta\,\dot{\varphi}^2$, so that

$$L = \tfrac{1}{2}\mu(\dot{r}^2 + r^2\dot{\chi}^2) - V(r).$$

The coordinate χ is cyclic and its generalized momentum $\mu r^2\dot\chi$ coincides with $|\boldsymbol{M}|$ if $\dot\chi > 0$ and with $-|\boldsymbol{M}|$ if $\dot\chi < 0$. Denoting this quantity by M, we get the equation

$$\mu r^2\dot\chi = M, \tag{1.7}$$

which is equivalent to *Kepler's second law*[12]. Using (1.7) we get for the total energy

$$E = \tfrac{1}{2}\mu(\dot r^2 + r^2\dot\chi^2) + V(r) = \tfrac{1}{2}\mu\dot r^2 + V(r) + \frac{M^2}{2\mu r^2}. \tag{1.8}$$

Thus the radial motion reduces to a one-dimensional motion on the half-line $r > 0$ with the effective potential energy

$$V_{eff}(r) = V(r) + \frac{M^2}{2\mu r^2},$$

where the second term is called the *centrifugal energy*. As in the previous section, the solution is given by

$$t = \sqrt{\frac{\mu}{2}}\int \frac{dr}{\sqrt{E - V_{eff}(r)}}. \tag{1.9}$$

It follows from (1.7) that the angle χ is a monotonic function of t, given by another quadrature

$$\chi = \frac{M}{\sqrt{2\mu}}\int \frac{dr}{r^2\sqrt{E - V_{eff}(r)}}, \tag{1.10}$$

yielding an equation of the trajectory in polar coordinates.

The set $V_{eff}(r) \le E$ is a union of annuli $0 \le r_{min} \le r \le r_{max} \le \infty$, and the motion is finite if $0 < r_{min} \le r \le r_{max} < \infty$. Though for a finite motion $r(t)$ oscillates between r_{min} and r_{max}, corresponding trajectories are not necessarily closed. The necessary and sufficient condition for a finite motion to have a closed trajectory is that the angle

$$\Delta\chi = \frac{M}{\sqrt{2\mu}}\int_{r_{min}}^{r_{max}} \frac{dr}{r^2\sqrt{E - V_{eff}(r)}}$$

is commensurable with 2π, i.e., $\Delta\chi = 2\pi\dfrac{m}{n}$ for some $m, n \in \mathbb{Z}$. If the angle $\Delta\chi$ is not commensurable with 2π, the orbit is everywhere dense in the annulus $r_{min} \le r \le r_{max}$. If

$$\lim_{r\to\infty} V_{eff}(r) = \lim_{r\to\infty} V(r) = V < \infty,$$

the motion is infinite for $E > V$ — the particle goes to ∞ with finite velocity $\sqrt{\frac{2}{\mu}(E - V)}$.

[12]It is the statement that *sectorial velocity* of a particle in a central field is constant.

A very important special case is when

$$V(r) = -\frac{\alpha}{r}.$$

It describes Newton's gravitational attraction ($\alpha > 0$) and Coulomb electrostatic interaction (either attractive or repulsive). First consider the case when $\alpha > 0$ — Kepler's problem. The effective potential energy is

$$V_{eff}(r) = -\frac{\alpha}{r} + \frac{M^2}{2\mu r^2}$$

and has the global minimum

$$V_0 = -\frac{\alpha^2 \mu}{2M^2}$$

at $r_0 = \dfrac{M^2}{\alpha\mu}$. The motion is infinite for $E \geq 0$ and is finite for $V_0 \leq E < 0$. The explicit form of trajectories can be determined by an elementary integration in (1.10), which gives

$$\chi = \cos^{-1} \frac{\dfrac{M}{r} - \dfrac{M}{r_0}}{\sqrt{2\mu(E - V_0)}} + C.$$

Choosing a constant of integration $C = 0$ and introducing notation

$$p = r_0 \quad \text{and} \quad e = \sqrt{1 - \frac{E}{V_0}},$$

we get the equation of the orbit (trajectory)

$$\frac{p}{r} = 1 + e\cos\chi. \tag{1.11}$$

This is the equation of a conic section with one focus at the origin. Quantity $2p$ is called the *latus rectum* of the orbit, and e is called the *eccentricity*. The choice $C = 0$ is such that the point with $\chi = 0$ is the point nearest to the origin (called the *perihelion*). When $V_0 \leq E < 0$, the eccentricity $e < 1$ so that the orbit is the ellipse[13] with the major and minor semi-axes

$$a = \frac{p}{1 - e^2} = \frac{\alpha}{2|E|}, \quad b = \frac{p}{\sqrt{1 - e^2}} = \frac{|M|}{\sqrt{2\mu|E|}}. \tag{1.12}$$

Correspondingly, $r_{min} = \dfrac{p}{1 + e}$, $r_{max} = \dfrac{p}{1 - e}$, and the period T of elliptic orbit is given by

$$T = \pi\alpha\sqrt{\frac{\mu}{2|E|^3}}.$$

The last formula is *Kepler's third law*. When $E > 0$, the eccentricity $e > 1$ and the motion is infinite — the orbit is a hyperbola with the origin as

[13] The statement that planets have elliptic orbits with a focus at the Sun is *Kepler's first law*.

internal focus. When $E = 0$, the eccentricity $e = 1$ — the particle starts from rest at ∞ and the orbit is a parabola.

For the repulsive case $\alpha < 0$ the effective potential energy $V_{eff}(r)$ is always positive and decreases monotonically from ∞ to 0. The motion is always infinite and the trajectories are hyperbolas (parabola if $E = 0$)

$$\frac{p}{r} = -1 + e\cos\chi$$

with

$$p = \frac{M^2}{\alpha\mu} \quad \text{and} \quad e = \sqrt{1 + \frac{2EM^2}{\mu\alpha^2}}.$$

Kepler's problem is very special: for every $\alpha \in \mathbb{R}$ the Lagrangian system on $\mathbb{R}^3$ with

$$L = \tfrac{1}{2}\mu\dot{\boldsymbol{r}}^2 + \frac{\alpha}{r} \tag{1.13}$$

has three extra integrals of motion W_1, W_2, W_3 in addition to the components of the angular momentum $\boldsymbol{M}$. The corresponding vector $\boldsymbol{W} = (W_1, W_2, W_3)$, called the *Laplace-Runge-Lenz vector*, is given by

$$\boldsymbol{W} = \dot{\boldsymbol{r}} \times \boldsymbol{M} - \frac{\alpha \boldsymbol{r}}{r}. \tag{1.14}$$

Indeed, using equations of motion $\mu\ddot{\boldsymbol{r}} = -\dfrac{\alpha\boldsymbol{r}}{r^3}$ and conservation of the angular momentum $\boldsymbol{M} = \mu\boldsymbol{r} \times \dot{\boldsymbol{r}}$, we get

$$\begin{aligned}
\dot{\boldsymbol{W}} &= \mu\ddot{\boldsymbol{r}} \times (\boldsymbol{r} \times \dot{\boldsymbol{r}}) - \frac{\alpha\dot{\boldsymbol{r}}}{r} + \frac{\alpha(\dot{\boldsymbol{r}} \cdot \boldsymbol{r})\boldsymbol{r}}{r^3} \\
&= (\mu\ddot{\boldsymbol{r}} \cdot \dot{\boldsymbol{r}})\boldsymbol{r} - (\mu\ddot{\boldsymbol{r}} \cdot \boldsymbol{r})\dot{\boldsymbol{r}} - \frac{\alpha\dot{\boldsymbol{r}}}{r} + \frac{\alpha(\dot{\boldsymbol{r}} \cdot \boldsymbol{r})\boldsymbol{r}}{r^3} \\
&= 0.
\end{aligned}$$

Using $\mu(\dot{\boldsymbol{r}} \times \boldsymbol{M}) \cdot \boldsymbol{r} = \boldsymbol{M}^2$ and the identity $(\boldsymbol{a} \times \boldsymbol{b})^2 = \boldsymbol{a}^2\,\boldsymbol{b}^2 - (\boldsymbol{a} \cdot \boldsymbol{b})^2$, we get

$$\boldsymbol{W}^2 = \alpha^2 + \frac{2\boldsymbol{M}^2 E}{\mu} \tag{1.15}$$

where

$$E = \frac{\boldsymbol{p}^2}{2\mu} - \frac{\alpha}{r}$$

is the energy corresponding to the Lagrangian (1.13). The fact that all orbits are conic sections follows from this extra symmetry of Kepler's problem.

Problem 1.17. Prove all the statements made in this section.

Problem 1.18. Show that if

$$\lim_{r\to 0} V_{eff}(r) = -\infty,$$

then there are orbits with $r_{min} = 0$ — "fall" of the particle to the center.

Problem 1.19. Prove that all finite trajectories in the central field are closed only when

$$V(r) = kr^2,\ k > 0, \quad \text{and} \quad V(r) = -\frac{\alpha}{r},\ \alpha > 0.$$

Problem 1.20. Find parametric equations for orbits in Kepler's problem.

Problem 1.21. Prove that the Laplace-Runge-Lenz vector $\boldsymbol{W}$ points in the direction of the major axis of the orbit and that $|\boldsymbol{W}| = \alpha e$, where e is the eccentricity of the orbit.

Problem 1.22. Using the conservation of the Laplace-Runge-Lenz vector, prove that trajectories in Kepler's problem with $E < 0$ are ellipses. (*Hint:* Evaluate $\boldsymbol{W} \cdot \boldsymbol{r}$ and use the result of the previous problem.)

1.7. Legendre transform. The equations of motion of a Lagrangian system (M, L) in standard coordinates associated with a coordinate chart $U \subset M$ are the Euler-Lagrange equations. In expanded form, they are given by the following system of second order ordinary differential equations:

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

In order for this system to be solvable for the highest derivatives for all initial conditions in TU, the symmetric $n \times n$ matrix

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

should be invertible on TU.

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

Remark. Note that the $n \times n$ matrix H_L is a Hessian of the Lagrangian function L for vertical directions on TM. Under the change of standard coordinates $\boldsymbol{q}' = F(\boldsymbol{q})$ and $\boldsymbol{q}' = F_*(\boldsymbol{q})\boldsymbol{v}$ (see Section 1.2) it has the transformation law

$$H_L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = F_*(\boldsymbol{q})^T H_L(\boldsymbol{q}', \dot{\boldsymbol{q}}') F_*(\boldsymbol{q}),$$

where $F_*(\boldsymbol{q})^T$ is the transposed matrix, so that the condition $\det H_L \neq 0$ does not depend on the choice of standard coordinates.

For an invariant formulation, consider the 1-form θ_L, defined in standard coordinates associated with a coordinate chart $U \subset M$ by

$$\theta_L = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}^i} dq^i = \frac{\partial L}{\partial \dot{\boldsymbol{q}}} d\boldsymbol{q}.$$

It follows from Corollary 1.2 that θ_L is a well-defined 1-form on TM.

Lemma 1.2. *A Lagrangian 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,

$$d\theta_L = \sum_{i,j=1}^{n} \left(\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} d\dot{q}^j \wedge dq^i + \frac{\partial^2 L}{\partial \dot{q}^i \partial q^j} dq^j \wedge dq^i \right),$$

and it is easy to see, by considering the $2n$-form $d\theta_L^n = \underbrace{d\theta_L \wedge \cdots \wedge d\theta_L}_{n}$, that the 2-form $d\theta_L$ is non-degenerate if and only if the matrix H_L is non-degenerate. □

Remark. Using the 1-form θ_L, the Noether integral I in Theorem 1.3 can be written as

$$I = i_{X'}(\theta_L), \tag{1.16}$$

where X' is a lift to TM of a vector field X on M given by (1.5). It also immediately follows from (1.6) that if X is an infinitesimal symmetry, then

$$\mathcal{L}_{X'}(\theta_L) = 0. \tag{1.17}$$

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

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

on the chart $T^*U \simeq \mathbb{R}^n \times U$ on the cotangent bundle T^*M are called *standard coordinates*[14] if for $(p, q) \in T^*U$ and $f \in C^\infty(U)$

$$p_i(df) = \frac{\partial f}{\partial q^i}, \quad i = 1, \ldots, n.$$

Equivalently, standard coordinates on T^*U are uniquely characterized by the condition that $\boldsymbol{p} = (p_1, \ldots, p_n)$ are coordinates in the fiber corresponding to the basis $dq^1, \ldots, dq^n$ for T_q^*M, dual to the basis $\dfrac{\partial}{\partial q^1}, \ldots, \dfrac{\partial}{\partial q^n}$ for T_qM.

[14]Following tradition, the first n coordinates parametrize the fiber of T^*U and the last n coordinates parametrize the base.

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

$$\theta = \sum_{i=1}^{n} p_i dq^i = \boldsymbol{p} d\boldsymbol{q},$$

is called *Liouville's canonical* 1*-form.*

Corollary 1.2 shows that θ is a well-defined 1-form on T^*M. Clearly, the 1-form θ also admits an invariant definition

$$\theta(u) = p(\pi_*(u)), \quad \text{where} \quad u \in T_{(p,q)}T^*M,$$

and $\pi : T^*M \to M$ is the canonical projection.

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

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

In standard coordinates the Legendre transform is given by

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

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

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

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

In standard coordinates,

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

where $\dot{\boldsymbol{q}}$ is a function of $\boldsymbol{p}$ and $\boldsymbol{q}$ defined by the equation $\boldsymbol{p} = \dfrac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}, \dot{\boldsymbol{q}})$ through the implicit function theorem. The cotangent bundle T^*M is called the *phase space* of the Lagrangian system (M, L). It turns out that on the phase space the equations of motion take a very simple and symmetric form.

Theorem 1.4. *Suppose that the Legendre transform $\tau_L : TM \to T^*M$ is a diffeomorphism. Then the Euler-Lagrange equations in standard coordinates on TM,*

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = 0, \quad i = 1, \ldots, n,$$

are equivalent to the following system of first order differential equations in standard coordinates on T^*M:

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

Proof. We have

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

Thus under the Legendre transform,

$$\dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}} \quad \text{and} \quad \dot{\boldsymbol{p}} = \frac{d}{dt} \frac{\partial L}{\partial \dot{\boldsymbol{q}}} = \frac{\partial L}{\partial \boldsymbol{q}} = -\frac{\partial H}{\partial \boldsymbol{q}}. \qquad \square$$

Corresponding first order differential equations on T^*M are called *Hamilton's equations* (*canonical equations*).

Corollary 1.5. *The Hamiltonian H is constant on the solutions of Hamilton's equations.*

Proof. For $H(t) = H(\boldsymbol{p}(t), \boldsymbol{q}(t))$ we have

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

For the Lagrangian

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

of a particle of mass m in a potential field $V(\boldsymbol{r})$, considered in Example 1.4, we have

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

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

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

Hamilton's equations

$$\dot{\boldsymbol{r}} = \frac{\partial H}{\partial \boldsymbol{p}} = \frac{\boldsymbol{p}}{m},$$
$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{r}} = -\frac{\partial V}{\partial \boldsymbol{r}}$$

are equivalent to Newton's equations with the force $\boldsymbol{F} = -\dfrac{\partial V}{\partial \boldsymbol{r}}$.

For the Lagrangian system describing small oscillators, considered in Example 1.6, we have $\boldsymbol{p} = m\dot{\boldsymbol{q}}$, and using normal coordinates we get

$$H(\boldsymbol{p},\boldsymbol{q}) = (\boldsymbol{p}\dot{\boldsymbol{q}} - L(\boldsymbol{q},\dot{\boldsymbol{q}}))|_{\dot{\boldsymbol{q}}=\frac{\boldsymbol{p}}{m}} = \frac{\boldsymbol{p}^2}{2m} + V_0(\boldsymbol{q}) = \frac{1}{2m}\big(\boldsymbol{p}^2 + m^2\sum_{i=1}^{n}\omega_i^2(q^i)^2\big).$$

Similarly, for the system of N interacting particles, considered in Example 1.2, we have $\boldsymbol{p} = (\boldsymbol{p}_1,\dots,\boldsymbol{p}_N)$, where

$$\boldsymbol{p}_a = \frac{\partial L}{\partial \dot{\boldsymbol{r}}_a} = m_a\dot{\boldsymbol{r}}_a, \quad a = 1,\dots,N.$$

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

$$H(\boldsymbol{p},\boldsymbol{r}) = (\boldsymbol{p}\dot{\boldsymbol{r}} - L)|_{\dot{\boldsymbol{r}}=\frac{\boldsymbol{p}}{m}} = \sum_{a=1}^{N}\frac{\boldsymbol{p}_a^2}{2m_a} + V(\boldsymbol{r}) = T + V.$$

In particular, for a closed system with pair-wise interaction,

$$H(\boldsymbol{p},\boldsymbol{r}) = \sum_{a=1}^{N}\frac{\boldsymbol{p}_a^2}{2m_a} + \sum_{1\le a<b\le N} V_{ab}(\boldsymbol{r}_a - \boldsymbol{r}_b).$$

In general, consider the Lagrangian

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

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

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

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

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

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

Problem 1.23 (Second tangent bundle)**.** Let $\pi : TM \to M$ be the canonical projection and let $T_{\mathrm{V}}(TM)$ be the *vertical tangent bundle* of TM along the fibers of π — the kernel of the bundle mapping $\pi_* : T(TM) \to TM$. Prove that there is a natural bundle isomorphism $i : TM \simeq T_{\mathrm{V}}(TM)$.

Problem 1.24 (Invariant definition of the 1-form θ_L)**.** Show that $\theta_L(v) = dL((i \circ \pi_*)v)$, where $v \in T(TM)$.

Problem 1.25. Give an invariant proof of (1.17).

Problem 1.26. Prove that the path $\gamma(t)$ in M is a trajectory for the Lagrangian system (M, L) if and only if

$$i_{\dot\gamma'(t)}(d\theta_L) + dE_L(\gamma'(t)) = 0,$$

where $\dot\gamma'(t)$ is the velocity vector of the path $\gamma'(t)$ in TM.

Problem 1.27. Show that for a charged particle in an electromagnetic field, considered in Example 1.5,

$$\boldsymbol{p} = m\dot{\boldsymbol{r}} + \frac{e}{c}\boldsymbol{A} \quad \text{and} \quad H(\boldsymbol{p}, \boldsymbol{r}) = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\varphi(\boldsymbol{r}).$$

Problem 1.28. Suppose that for a Lagrangian system $(\mathbb{R}^n, L)$ the Legendre transform τ_L is a diffeomorphism and let H be the corresponding Hamiltonian. Prove that for fixed $\boldsymbol{q}$ and $\dot{\boldsymbol{q}}$ the function $\boldsymbol{p}\dot{\boldsymbol{q}} - H(\boldsymbol{p}, \boldsymbol{q})$ has a single critical point at $\boldsymbol{p} = \dfrac{\partial L}{\partial \dot{\boldsymbol{q}}}$.

Problem 1.29. Give an example of a non-degenerate Lagrangian system (M, L) such that the Legendre transform $\tau_L : TM \to T^*M$ is one-to-one but not onto.

2. Hamiltonian Mechanics

2.1. Hamilton's equations. With every function $H : T^*M \to \mathbb{R}$ on the phase space T^*M there are associated Hamilton's equations — a first-order system of ordinary differential equations, which in the standard coordinates on T^*U has the form

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{q}}, \quad \dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}}. \tag{2.1}$$

The corresponding vector field X_H on T^*U,

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

gives rise to a well-defined vector field X_H on T^*M, called the *Hamiltonian vector field*. Suppose now that the vector field X_H on T^*M is complete, i.e., its integral curves exist for all times. The corresponding one-parameter group $\{g_t\}_{t\in\mathbb{R}}$ of diffeomorphisms of T^*M generated by X_H is called the *Hamiltonian phase flow*. It is defined by $g_t(p, q) = (p(t), q(t))$, where $p(t)$, $q(t)$ is a solution of Hamilton's equations satisfying $p(0) = p$, $q(0) = q$.

Liouville's canonical 1-form θ on T^*M defines a 2-form $\omega = d\theta$. In standard coordinates on T^*M it is given by

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

and is a non-degenerate 2-form. The form ω is called the *canonical symplectic form* on T^*M. The symplectic form ω defines an isomorphism $J : T^*(T^*M) \to T(T^*M)$ between tangent and cotangent bundles to T^*M. For every $(p,q) \in T^*M$ the linear mapping $J^{-1} : T_{(p,q)}T^*M \to T^*_{(p,q)}T^*M$ is given by

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

The mapping J induces the isomorphism between the infinite-dimensional vector spaces $\mathcal{A}^1(T^*M)$ and $\mathrm{Vect}(T^*M)$, which is linear over $C^\infty(T^*M)$. If ϑ is a 1-form on T^*M, then the corresponding vector field $J(\vartheta)$ on T^*M satisfies

$$\omega(X, J(\vartheta)) = \vartheta(X), \quad X \in \mathrm{Vect}(T^*M),$$

and $J^{-1}(X) = -i_X\omega$. In particular, in standard coordinates,

$$J(d\boldsymbol{p}) = \frac{\partial}{\partial \boldsymbol{q}} \quad \text{and} \quad J(d\boldsymbol{q}) = -\frac{\partial}{\partial \boldsymbol{p}},$$

so that $X_H = J(dH)$.

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

Proof. We need to prove that $(g_t)^*\omega = \omega$. Since g_t is a one-parameter group of diffeomorphisms, it is sufficient to show that

$$\frac{d}{dt}(g_t)^*\omega\Big|_{t=0} = \mathcal{L}_{X_H}\omega = 0,$$

where $\mathcal{L}_{X_H}$ is the Lie derivative along the vector field X_H. Since for every vector field X,

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

we compute

$$\mathcal{L}_{X_H}(dp_i) = -d\left(\frac{\partial H}{\partial q^i}\right) \quad \text{and} \quad \mathcal{L}_{X_H}(dq^i) = d\left(\frac{\partial H}{\partial p_i}\right),$$

so that

$$\begin{aligned}\mathcal{L}_{X_H}\omega &= \sum_{i=1}^{n} \left(\mathcal{L}_{X_H}(dp_i) \wedge dq^i + dp_i \wedge \mathcal{L}_{X_H}(dq^i)\right) \\ &= \sum_{i=1}^{n} \left(-d\left(\frac{\partial H}{\partial q^i}\right) \wedge dq^i + dp_i \wedge d\left(\frac{\partial H}{\partial p_i}\right)\right) = -d(dH) = 0. \quad \square\end{aligned}$$

Corollary 2.2. $\mathcal{L}_{X_H}(\theta) = d(-H + \theta(X_H))$, *where* θ *is Liouville's canonical* 1*-form.*

The canonical symplectic form ω on T^*M defines the volume form $\dfrac{\omega^n}{n!} = \dfrac{1}{n!}\underbrace{\omega \wedge \cdots \wedge \omega}_{n}$ on T^*M, called *Liouville's volume form.*

Corollary 2.3 (Liouville's theorem)**.** *The Hamiltonian phase flow on* T^*M *preserves Liouville's volume form.*

The restriction of the symplectic form ω on T^*M to the configuration space M is 0. Generalizing this property, we get the following notion.

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

It follows from Theorem 2.1 that the image of a Lagrangian submanifold under the Hamiltonian phase flow is a Lagrangian submanifold.

Problem 2.1. Verify that X_H is a well-defined vector field on T^*M.

Problem 2.2. Show that if all level sets of the Hamiltonian H are compact submanifolds of T^*M, then the Hamiltonian vector field X_H is complete.

Problem 2.3. Let $\pi : T^*M \to M$ be the canonical projection, and let $\mathscr{L}$ be a Lagrangian submanifold. Show that if the mapping $\pi|_{\mathscr{L}} : \mathscr{L} \to M$ is a diffeomorphism, then $\mathscr{L}$ is a graph of a smooth function on M. Give examples when for some $t > 0$ the corresponding projection of $g_t(\mathscr{L})$ onto M is no longer a diffeomorphism.

2.2. The action functional in the phase space. With every function H on the phase space T^*M there is an associated 1-form

$$\theta - H dt = \boldsymbol{p} d\boldsymbol{q} - H dt$$

on the *extended phase space* $T^*M \times \mathbb{R}$, called the *Poincaré-Cartan form.* Let $\gamma : [t_0, t_1] \to T^*M$ be a smooth parametrized path in T^*M such that $\pi(\gamma(t_0)) = q_0$ and $\pi(\gamma(t_1)) = q_1$, where $\pi : T^*M \to M$ is the canonical projection. By definition, the lift of a path γ to the extended phase space $T^*M \times \mathbb{R}$ is a path $\sigma : [t_0, t_1] \to T^*M \times \mathbb{R}$ given by $\sigma(t) = (\gamma(t), t)$, and a path σ in $T^*M \times \mathbb{R}$ is called an *admissible* path if it is a lift of a path γ in T^*M. The space of admissible paths in $T^*M \times \mathbb{R}$ is denoted by $\tilde{P}(T^*M)_{q_0,t_0}^{q_1,t_1}$. A variation of an admissible path σ is a smooth family of admissible paths σ_ε, where $\varepsilon \in [-\varepsilon_0, \varepsilon_0]$ and $\sigma_0 = \sigma$, and the corresponding infinitesimal variation is

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

(cf. Section 1.2). The principle of the least action in the phase space is the following statement.

Theorem 2.4 (Poincaré)**.** *The admissible path σ in $T^*M \times \mathbb{R}$ is an extremal for the action functional*

$$S(\sigma) = \int_\sigma (\boldsymbol{p}d\boldsymbol{q} - Hdt) = \int_{t_0}^{t_1} (\boldsymbol{p}\dot{\boldsymbol{q}} - H)dt$$

if and only if it is a lift of a path $\gamma(t) = (\boldsymbol{p}(t), \boldsymbol{q}(t))$ in T^*M, where $\boldsymbol{p}(t)$ and $\boldsymbol{q}(t)$ satisfy canonical Hamilton's equations

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

Proof. As in the proof of Theorem 1.1, for an admissible family $\sigma_\varepsilon(t) = (\boldsymbol{p}(t,\varepsilon), \boldsymbol{q}(t,\varepsilon), t)$ we compute using integration by parts,

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

Since $\delta\boldsymbol{q}(t_0) = \delta\boldsymbol{q}(t_1) = 0$, the path σ is critical if and only if $\boldsymbol{p}(t)$ and $\boldsymbol{q}(t)$ satisfy canonical Hamilton's equations (2.1). □

Remark. For a Lagrangian system (M, L), every path $\gamma(t) = (\boldsymbol{q}(t))$ in the configuration space M connecting points q_0 and q_1 defines an admissible path $\hat{\gamma}(t) = (\boldsymbol{p}(t), \boldsymbol{q}(t), t)$ in the phase space T^*M by setting $\boldsymbol{p} = \dfrac{\partial L}{\partial \dot{\boldsymbol{q}}}$. If the Legendre transform $\tau_L : TM \to T^*M$ is a diffeomorphism, then

$$S(\hat{\gamma}) = \int_{t_0}^{t_1} (\boldsymbol{p}\dot{\boldsymbol{q}} - H)dt = \int_{t_0}^{t_1} L(\gamma'(t), t)dt.$$

Thus the principle of the least action in a configuration space — Hamilton's principle — follows from the principle of the least action in a phase space. In fact, in this case the two principles are equivalent (see Problem 1.28).

From Corollary 1.5 we immediately get the following result.

Corollary 2.5. *Solutions of canonical Hamilton's equations lying on the hypersurface $H(\boldsymbol{p}, \boldsymbol{q}) = E$ are extremals of the functional $\int_\sigma \boldsymbol{p}d\boldsymbol{q}$ in the class of admissible paths σ lying on this hypersurface.*

Corollary 2.6 (Maupertuis' principle)**.** *The trajectory $\gamma = (\boldsymbol{q}(\tau))$ of a closed Lagrangian system (M, L) connecting points q_0 and q_1 and having energy E is the extremal of the functional*

$$\int_\gamma \boldsymbol{p}d\boldsymbol{q} = \int_\gamma \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(\tau), \dot{\boldsymbol{q}}(\tau))\dot{\boldsymbol{q}}(\tau)d\tau$$

on the space of all paths in the configuration space M connecting points q_0 and q_1 and parametrized such that $H(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\tau), \boldsymbol{q}(\tau)) = E$.

The functional

$$S_0(\gamma) = \int_\gamma \boldsymbol{p} d\boldsymbol{q}$$

is called the *abbreviated action*[15].

Proof. Every path $\gamma = \boldsymbol{q}(\tau)$, parametrized such that $H(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}, \boldsymbol{q}) = E$, lifts to an admissible path $\sigma = (\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\tau), \boldsymbol{q}(\tau), \tau)$, $a \le \tau \le b$, lying on the hypersurface $H(\boldsymbol{p}, \boldsymbol{q}) = E$. □

Problem 2.4 (Jacobi)**.** On a Riemannian manifold (M, ds^2) consider a Lagrangian system with $L(q, v) = \frac{1}{2}\|v\|^2 - V(q)$. Let $E > V(q)$ for all $q \in M$. Show that the trajectories of a closed Lagrangian system (M, L) with total energy E are geodesics for the Riemannian metric $d\hat{s}^2 = (E - V(q))ds^2$ on M.

2.3. The action as a function of coordinates. Consider a non-degenerate Lagrangian system (M, L) and denote by $\gamma(t; q_0, v_0)$ the solution of Euler-Lagrange equations

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

with the initial conditions $\gamma(t_0) = q_0 \in M$ and $\dot{\gamma}(t_0) = v_0 \in T_{q_0}M$. Suppose that there exist a neighborhood $V_0 \subset T_{v_0}M$ of v_0 and $t_1 > t_0$ such that for all $v \in V_0$ the extremals $\gamma(t; q_0, v)$, which start at time t_0 at q_0, do not intersect in the extended configuration space $M \times \mathbb{R}$ for times $t_0 < t < t_1$. Such extremals are said to form a *central field* which includes the extremal $\gamma_0(t) = \gamma(t; q_0, v_0)$. The existence of the central field of extremals is equivalent to the condition that for every $t_0 < t < t_1$ there is a neighborhood $U_t \subset M$ of $\gamma_0(t) \in M$ such that the mapping

$$V_0 \ni v \mapsto q(t) = \gamma(t; q_0, v) \in U_t \tag{2.2}$$

is a diffeomorphism. Basic theorems in the theory of ordinary differential equations guarantee that for t_1 sufficiently close to t_0 every extremal $\gamma(t)$ for $t_0 < t < t_1$ can be included into the central field. In standard coordinates the mapping (2.2) is given by $\dot{\boldsymbol{q}} \mapsto \boldsymbol{q}(t) = \gamma(t; \boldsymbol{q}_0, \dot{\boldsymbol{q}})$.

For the central field of extremals $\gamma(t; \boldsymbol{q}_0, \dot{\boldsymbol{q}})$, $t_0 < t < t_1$, we define the *action as a function of coordinates and time* (or, *classical action*) by

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

[15]The accurate formulation of Maupertuis' principle is due to Euler and Lagrange.

where $\gamma(\tau)$ is the extremal from the central field that connects $\boldsymbol{q}_0$ and $\boldsymbol{q}$. For given $\boldsymbol{q}_0$ and t_0, the classical action is defined for $t \in (t_0, t_1)$ and $\boldsymbol{q} \in \bigcup_{t_0<t<t_1} U_t$. For a fixed energy E,

$$S(\boldsymbol{q}, t; \boldsymbol{q}_0, t_0) = S_0(\boldsymbol{q}, t; \boldsymbol{q}_0, t_0) - E(t - t_0), \tag{2.3}$$

where S_0 is the abbreviated action from the previous section.

Theorem 2.7. *The differential of the classical action $S(\boldsymbol{q}, t)$ with fixed initial point is given by*

$$dS = \boldsymbol{p}d\boldsymbol{q} - Hdt,$$

where $\boldsymbol{p} = \dfrac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}, \dot{\boldsymbol{q}})$ and $H = \boldsymbol{p}\dot{\boldsymbol{q}} - L(\boldsymbol{q}, \dot{\boldsymbol{q}})$ are determined by the velocity $\dot{\boldsymbol{q}}$ of the extremal $\gamma(\tau)$ at time t.

Proof. Let $\boldsymbol{q}_\varepsilon$ be a path in M passing through $\boldsymbol{q}$ at $\varepsilon = 0$ with the tangent vector $\boldsymbol{v} \in T_{\boldsymbol{q}}M \simeq \mathbb{R}^n$, and for ε small enough let $\gamma_\varepsilon(\tau)$ be the family of extremals from the central field satisfying $\gamma_\varepsilon(t_0) = \boldsymbol{q}_0$ and $\gamma_\varepsilon(t) = \boldsymbol{q}_\varepsilon$. For the infinitesimal variation $\delta\gamma$ we have $\delta\gamma(t_0) = 0$ and $\delta\gamma(t) = \boldsymbol{v}$, and for fixed t we get from the formula for variation with the free ends (1.2) that

$$dS(\boldsymbol{v}) = \frac{\partial L}{\partial \dot{\boldsymbol{q}}}\boldsymbol{v}.$$

This shows that $\dfrac{\partial S}{\partial \boldsymbol{q}} = \boldsymbol{p}$. Setting $\boldsymbol{q}(t) = \gamma(t)$, we obtain

$$\frac{d}{dt}S(\boldsymbol{q}(t), t) = \frac{\partial S}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}} + \frac{\partial S}{\partial t} = L,$$

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

Corollary 2.8. *The classical action satisfies the following nonlinear partial differential equation*

$$\frac{\partial S}{\partial t} + H\left(\frac{\partial S}{\partial \boldsymbol{q}}, \boldsymbol{q}\right) = 0. \tag{2.4}$$

This equation is called the *Hamilton-Jacobi equation*. Hamilton's equations (2.1) can be used for solving the Cauchy problem

$$S(\boldsymbol{q}, t)|_{t=0} = s(\boldsymbol{q}), \quad s \in C^\infty(M), \tag{2.5}$$

for Hamilton-Jacobi equation (2.4) by the method of characteristics. Namely, assume the existence of the Hamiltonian phase flow g_t on T^*M and consider the Lagrangian submanifold

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

a graph of the 1-form ds on M — a section of the cotangent bundle $\pi : T^*M \to M$. The mapping $\pi|_{\mathscr{L}}$ is one-to-one and for sufficiently small t the restriction of the projection π to the Lagrangian submanifold $\mathscr{L}_t = g_t(\mathscr{L})$ remains to be one-to-one. In other words, there is $t_1 > 0$ such that for all $0 \le t < t_1$ the mapping $\pi_t = \pi \circ g_t \circ (\pi|_{\mathscr{L}})^{-1} : M \to M$ is a diffeomorphism, and the extremals $\gamma(\tau, \boldsymbol{q}_0, \dot{\boldsymbol{q}}_0)$ in the extended configuration space $M \times \mathbb{R}$, where $\dot{\boldsymbol{q}}_0 = \dfrac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{p}_0, \boldsymbol{q}_0)$ and $(\boldsymbol{p}_0, \boldsymbol{q}_0) \in \mathscr{L}$, do not intersect. Such extremals are called the *characteristics* of the Hamilton-Jacobi equation.

Proposition 2.1. *For $0 \le t < t_1$ the solution $S(\boldsymbol{q}, t)$ to the Cauchy problem* (2.4)–(2.5) *is given by*

$$S(\boldsymbol{q}, t) = s(\boldsymbol{q}_0) + \int_0^t L(\gamma'(\tau))d\tau.$$

Here $\gamma(\tau)$ is the characteristic with $\gamma(t) = \boldsymbol{q}$ and with the starting point $\boldsymbol{q}_0 = \gamma(0)$ which is uniquely determined by $\boldsymbol{q}$.

Proof. As in the proof of Theorem 2.7 we use formula (1.2), where now $\boldsymbol{q}_0$ depends on $\boldsymbol{q}$, and obtain

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

since $\dfrac{\partial s}{\partial \boldsymbol{q}_0}(\boldsymbol{q}_0) = \boldsymbol{p}_0 = \dfrac{\partial L}{\partial \dot{\boldsymbol{q}}_0}(\boldsymbol{q}_0, \dot{\boldsymbol{q}}_0)$. Setting $\boldsymbol{q}(t) = \gamma(t)$ we get

$$\frac{d}{dt}S(\boldsymbol{q}(t), t) = \frac{\partial S}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}} + \frac{\partial S}{\partial t} = L(\boldsymbol{q}, \dot{\boldsymbol{q}}),$$

so that

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

and S satisfies the Hamilton-Jacobi equation. □

We can also consider the action $S(\boldsymbol{q}, t; \boldsymbol{q}_0, t_0)$ as a function of both variables $\boldsymbol{q}$ and $\boldsymbol{q}_0$. The analog of Theorem 2.7 is the following statement.

Proposition 2.2. *The differential of the classical action as a function of initial and final points is given by*

$$dS = \boldsymbol{p}d\boldsymbol{q} - \boldsymbol{p}_0 d\boldsymbol{q}_0 - H(\boldsymbol{p}, \boldsymbol{q})dt + H(\boldsymbol{p}_0, \boldsymbol{q}_0)dt_0.$$

Problem 2.5. Prove that the solution to the Cauchy problem for the Hamilton-Jacobi equation is unique.

2.4. Classical observables and Poisson bracket. Smooth real-valued functions on the phase space T^*M are called *classical observables*. The vector space $C^\infty(T^*M)$ is an $\mathbb{R}$-algebra — an associative algebra over $\mathbb{R}$ with a unit given by the constant function 1, and with a multiplication given by the point-wise product of functions. The commutative algebra $C^\infty(T^*M)$ is called the *algebra of classical observables*. Assuming that the Hamiltonian phase flow g_t exists for all times, the time evolution of every observable $f \in C^\infty(T^*M)$ is given by

$$f_t(p,q) = f(g_t(p,q)) = f(p(t),q(t)), \quad (p,q) \in TM.$$

Equivalently, the time evolution is described by the differential equation

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

called Hamilton's equation for classical observables. Setting

$$\{f,g\} = X_f(g) = \frac{\partial f}{\partial \boldsymbol{p}}\frac{\partial g}{\partial \boldsymbol{q}} - \frac{\partial f}{\partial \boldsymbol{q}}\frac{\partial g}{\partial \boldsymbol{p}}, \quad f,g \in C^\infty(T^*M), \tag{2.6}$$

we can rewrite Hamilton's equation in the concise form

$$\frac{df}{dt} = \{H,f\}, \tag{2.7}$$

where it is understood that (2.7) is a differential equation for a family of functions f_t on T^*M with the initial condition $f_t(p,q)|_{t=0} = f(p,q)$. The properties of the bilinear mapping

$$\{\ ,\ \} : C^\infty(T^*M) \times C^\infty(T^*M) \to C^\infty(T^*M)$$

are summarized below.

Theorem 2.9. *The mapping* $\{\ ,\ \}$ *satisfies the following properties.*

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

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

(ii) *(Skew-symmetry)*

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

(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 ω and J in Section 2.1. Properties (ii)-(iii) are obvious. The Jacobi identity could be verified by a direct computation using (2.6), or by the following elegant argument. Observe that $\{f, g\}$ is a bilinear form in the first partial derivatives of f and g, and every term in the left-hand side of the Jacobi identity is a linear homogenous function of second partial derivatives of f, g, and h. Now the only terms in the Jacobi identity which could actually contain second partial derivatives of a function h are the following:

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

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

The observable $\{f, g\}$ is called the *canonical Poisson bracket* of the observables f and g. The Poisson bracket map $\{\ ,\ \} : C^\infty(T^*M) \times C^\infty(T^*M) \to C^\infty(T^*M)$ turns the algebra of classical observables $C^\infty(T^*M)$ into a Lie algebra with a Lie bracket given by the Poisson bracket. It has an important property that the Lie bracket is a bi-derivation with respect to the multiplication in $C^\infty(T^*M)$. The algebra of classical observables $C^\infty(T^*M)$ is an example of the *Poisson algebra* — a commutative algebra over $\mathbb{R}$ carrying a structure of a Lie algebra with the property that the Lie bracket is a derivation with respect to the algebra product.

In Lagrangian mechanics, a function I on TM is an integral of motion for the Lagrangian system (M, L) if it is constant along the trajectories. In Hamiltonian mechanics, an observable I — a function on the phase space T^*M — is called an integral of motion (first integral) for Hamilton's equations (2.1) if it is constant along the Hamiltonian phase flow. According to (2.7), this is equivalent to the condition

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

It is said that the observables H and I are *in involution* (*Poisson commute*).

2.5. Canonical transformations and generating functions.

Definition. A diffeomorphism g of the phase space T^*M is called a *canonical transformation*, if it preserves the canonical symplectic form ω on T^*M, i.e., $g^*(\omega) = \omega$. By Theorem 2.1, the Hamiltonian phase flow g_t is a one-parameter group of canonical transformations.

Proposition 2.3. *Canonical transformations preserve Hamilton's equations.*

Proof. From $g^*(\omega) = \omega$ it follows that the mapping $J : T^*(T^*M) \to T(T^*M)$ satisfies

$$g_* \circ J \circ g^* = J. \tag{2.8}$$

Indeed, for all $X, Y \in \mathrm{Vect}(M)$ we have[16]

$$\omega(X,Y) = g^*(\omega)(X,Y) = \omega(g_*(X), g_*(Y)) \circ g,$$

so that for every 1-form ϑ on M,

$$\omega(X, J(g^*(\vartheta))) = g^*(\vartheta)(X) = \vartheta(g_*(X)) \circ g = \omega(g_*(X), J(\vartheta)) \circ g,$$

which gives $g_*(J(g^*(\vartheta))) = J(\vartheta)$. Using (2.8), we get

$$g_*(X_H) = g_*(J(dH)) = J((g^*)^{-1}(dH)) = X_K,$$

where $K = H \circ g^{-1}$. Thus the canonical transformation g maps trajectories of the Hamiltonian vector field X_H into the trajectories of the Hamiltonian vector field X_K. □

Remark. In classical terms, Proposition 2.3 means that canonical Hamilton's equations

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{p}, \boldsymbol{q}), \quad \dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{p}, \boldsymbol{q})$$

in new coordinates $(\boldsymbol{P}, \boldsymbol{Q}) = g(\boldsymbol{p}, \boldsymbol{q})$ continue to have the canonical form

$$\dot{\boldsymbol{P}} = -\frac{\partial K}{\partial \boldsymbol{Q}}(\boldsymbol{P}, \boldsymbol{Q}), \quad \dot{\boldsymbol{Q}} = \frac{\partial K}{\partial \boldsymbol{P}}(\boldsymbol{P}, \boldsymbol{Q})$$

with the old Hamiltonian function $K(\boldsymbol{P}, \boldsymbol{Q}) = H(\boldsymbol{p}, \boldsymbol{q})$.

Consider now the classical case $M = \mathbb{R}^n$. For a canonical transformation $(\boldsymbol{P}, \boldsymbol{Q}) = g(\boldsymbol{p}, \boldsymbol{q})$ set $\boldsymbol{P} = \boldsymbol{P}(\boldsymbol{p}, \boldsymbol{q})$ and $\boldsymbol{Q} = \boldsymbol{Q}(\boldsymbol{p}, \boldsymbol{q})$. Since $d\boldsymbol{P} \wedge d\boldsymbol{Q} = d\boldsymbol{p} \wedge d\boldsymbol{q}$ on $T^*M \simeq \mathbb{R}^{2n}$, the 1-form $\boldsymbol{p}d\boldsymbol{q} - \boldsymbol{P}d\boldsymbol{Q}$ — the difference between the canonical Liouville 1-form and its pullback by the mapping g — is closed. From the Poincaré lemma it follows that there exists a function $F(\boldsymbol{p}, \boldsymbol{q})$ on $\mathbb{R}^{2n}$ such that

$$\boldsymbol{p}d\boldsymbol{q} - \boldsymbol{P}d\boldsymbol{Q} = dF(\boldsymbol{p}, \boldsymbol{q}). \tag{2.9}$$

Now assume that at some point $(\boldsymbol{p}_0, \boldsymbol{q}_0)$ the $n \times n$ matrix $\dfrac{\partial \boldsymbol{P}}{\partial \boldsymbol{p}} = \left\{ \dfrac{\partial P_i}{\partial p_j} \right\}_{i,j=1}^{n}$ is non-degenerate. By the inverse function theorem, there exists a neighborhood U of $(\boldsymbol{p}_0, \boldsymbol{q}_0)$ in $\mathbb{R}^{2n}$ for which the functions $\boldsymbol{P}, \boldsymbol{q}$ are coordinate functions. The function

$$S(\boldsymbol{P}, \boldsymbol{q}) = F(\boldsymbol{p}, \boldsymbol{q}) + \boldsymbol{P}\boldsymbol{Q}$$

[16] Since g is a diffeomorphism, g_*X is a well-defined vector field on M.

is called a *generating function* of the canonical transformation g in U. It follows from (2.9) that in new coordinates $\boldsymbol{P}, \boldsymbol{q}$ on U,

$$\boldsymbol{p} = \frac{\partial S}{\partial \boldsymbol{q}}(\boldsymbol{P}, \boldsymbol{q}) \quad \text{and} \quad \boldsymbol{Q} = \frac{\partial S}{\partial \boldsymbol{P}}(\boldsymbol{P}, \boldsymbol{q}).$$

The converse statement below easily follows from the implicit function theorem.

Proposition 2.4. *Let $S(\boldsymbol{P}, \boldsymbol{q})$ be a function in some neighborhood U of a point $(\boldsymbol{P}_0, \boldsymbol{q}_0) \in \mathbb{R}^{2n}$ such that the $n \times n$ matrix*

$$\frac{\partial^2 S}{\partial \boldsymbol{P} \partial \boldsymbol{q}}(\boldsymbol{P}_0, \boldsymbol{q}_0) = \left\{ \frac{\partial^2 S}{\partial P_i \partial q^j}(\boldsymbol{P}_0, \boldsymbol{q}_0) \right\}_{i,j=1}^{n}$$

is non-degenerate. Then S is a generating function of a local (i.e., defined in some neighborhood of $(\boldsymbol{P}_0, \boldsymbol{q}_0)$ in $\mathbb{R}^{2n}$) canonical transformation.

Suppose there is a canonical transformation $(\boldsymbol{P}, \boldsymbol{Q}) = g(\boldsymbol{p}, \boldsymbol{q})$ such that $H(\boldsymbol{p}, \boldsymbol{q}) = K(\boldsymbol{P})$ for some function K. Then in the new coordinates Hamilton's equations take the form

$$\dot{\boldsymbol{P}} = 0, \quad \dot{\boldsymbol{Q}} = \frac{\partial K}{\partial \boldsymbol{P}}, \tag{2.10}$$

and are trivially integrated:

$$\boldsymbol{P}(t) = \boldsymbol{P}(0), \quad \boldsymbol{Q}(t) = \boldsymbol{Q}(0) + t \frac{\partial K}{\partial \boldsymbol{P}}(\boldsymbol{P}(0)).$$

Assuming that the matrix $\dfrac{\partial \boldsymbol{P}}{\partial \boldsymbol{p}}$ is non-degenerate, the generating function $S(\boldsymbol{P}, \boldsymbol{q})$ satisfies the differential equation

$$H\Big(\frac{\partial S}{\partial \boldsymbol{q}}(\boldsymbol{P}, \boldsymbol{q}), \boldsymbol{q}\Big) = K(\boldsymbol{P}), \tag{2.11}$$

where after the differentiation one should substitute $\boldsymbol{q} = \boldsymbol{q}(\boldsymbol{P}, \boldsymbol{Q})$, defined by the canonical transformation g^{-1}. The differential equation (2.11) for fixed $\boldsymbol{P}$, as it follows from (2.3), coincides with the Hamilton-Jacobi equation for the abbreviated action $S_0 = S - Et$ where $E = K(\boldsymbol{P})$,

$$H\Big(\frac{\partial S_0}{\partial \boldsymbol{q}}(\boldsymbol{P}, \boldsymbol{q}), \boldsymbol{q}\Big) = E.$$

Theorem 2.10 (Jacobi)**.** *Suppose that there is a function $S(\boldsymbol{P}, \boldsymbol{q})$ which depends on n parameters $\boldsymbol{P} = (P_1, \dots, P_n)$, satisfies the Hamilton-Jacobi equation* (2.11) *for some function $K(\boldsymbol{P})$, and has the property that the $n \times n$ matrix $\dfrac{\partial^2 S}{\partial \boldsymbol{P} \partial \boldsymbol{q}}$ is non-degenerate. Then Hamilton's equations*

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{q}}, \quad \dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}}$$

can be solved explicitly, and the functions $\boldsymbol{P}(\boldsymbol{p},\boldsymbol{q}) = (P_1(\boldsymbol{p},\boldsymbol{q}),\dots,P_n(\boldsymbol{p},\boldsymbol{q}))$, *defined by the equations* $\boldsymbol{p} = \dfrac{\partial S}{\partial \boldsymbol{q}}(\boldsymbol{P},\boldsymbol{q})$, *are integrals of motion in involution.*

Proof. Set $\boldsymbol{p} = \dfrac{\partial S}{\partial \boldsymbol{q}}(\boldsymbol{P},\boldsymbol{q})$ and $\boldsymbol{Q} = \dfrac{\partial S}{\partial \boldsymbol{P}}(\boldsymbol{P},\boldsymbol{q})$. By the inverse function theorem, $g(\boldsymbol{p},\boldsymbol{q}) = (\boldsymbol{P},\boldsymbol{Q})$ is a local canonical transformation with the generating function S. It follows from (2.11) that $H(\boldsymbol{p}(\boldsymbol{P},\boldsymbol{Q}),\boldsymbol{q}(\boldsymbol{P},\boldsymbol{Q})) = K(\boldsymbol{P})$, so that Hamilton's equations take the form (2.10). Since $\omega = d\boldsymbol{P} \wedge d\boldsymbol{Q}$, integrals of motion $P_1(\boldsymbol{p},\boldsymbol{q}),\dots,P_n(\boldsymbol{p},\boldsymbol{q})$ are in involution. □

The solution of the Hamilton-Jacobi equation satisfying conditions in Theorem 2.10 is called the *complete integral*. At first glance it seems that solving the Hamilton-Jacobi equation, which is a nonlinear partial differential equation, is a more difficult problem then solving Hamilton's equations, which is a system of ordinary differential equations. It is quite remarkable that for many problems of classical mechanics one can find the complete integral of the Hamilton-Jacobi equation by the method of separation of variables. By Theorem 2.10, this solves the corresponding Hamilton's equations.

Problem 2.6. Find the generating function for the identity transformation $\boldsymbol{P} = \boldsymbol{p}, \boldsymbol{Q} = \boldsymbol{q}$.

Problem 2.7. Prove Proposition 2.4.

Problem 2.8. Suppose that the canonical transformation $g(\boldsymbol{p},\boldsymbol{q}) = (\boldsymbol{P},\boldsymbol{Q})$ is such that locally $(\boldsymbol{Q},\boldsymbol{q})$ can be considered as new coordinates (canonical transformations with this property are called *free*). Prove that $S_1(\boldsymbol{Q},\boldsymbol{q}) = F(\boldsymbol{p},\boldsymbol{q})$, also called a generating function, satisfies

$$\boldsymbol{p} = \frac{\partial S_1}{\partial \boldsymbol{q}} \quad \text{and} \quad \boldsymbol{P} = -\frac{\partial S_1}{\partial \boldsymbol{Q}}.$$

Problem 2.9. Find the complete integral for the case of a particle in $\mathbb{R}^3$ moving in a central field.

2.6. Symplectic manifolds. The notion of a symplectic manifold is a generalization of the example of a cotangent bundle T^*M.

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

Since a symplectic form ω is non-degenerate, a symplectic manifold $\mathscr{M}$ is necessarily even-dimensional, $\dim \mathscr{M} = 2n$. The nowhere vanishing $2n$-form ω^n defines a canonical orientation on $\mathscr{M}$, and as in the case $\mathscr{M} = T^*M$, $\dfrac{\omega^n}{n!}$ is called Liouville's volume form. We also have the general notion of a Lagrangian submanifold.

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

Symplectic manifolds form a category. A morphism between $(\mathscr{M}_1, \omega_1)$ and $(\mathscr{M}_2, \omega_2)$, also called a *symplectomorphism*, is a mapping $f : \mathscr{M}_1 \to \mathscr{M}_2$ such that $\omega_1 = f^*(\omega_2)$. When $\mathscr{M}_1 = \mathscr{M}_2$ and $\omega_1 = \omega_2$, the notion of a symplectomorphism generalizes the notion of a canonical transformation. 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 in the Cartesian product.

Besides cotangent bundles, another important class of symplectic manifolds is given by Kähler manifolds[17]. Recall that a complex manifold $\mathscr{M}$ is a Kähler manifold if it carries the Hermitian metric whose imaginary part is a closed $(1,1)$-form. In local complex coordinates $\boldsymbol{z} = (z^1, \ldots, z^n)$ on $\mathscr{M}$ the Hermitian metric is written as

$$h = \sum_{\alpha,\beta=1}^{n} h_{\alpha\bar{\beta}}(\boldsymbol{z}, \bar{\boldsymbol{z}}) dz^\alpha \otimes d\bar{z}^\beta.$$

Correspondingly,

$$g = \operatorname{Re} h = \frac{1}{2} \sum_{\alpha,\beta=1}^{n} h_{\alpha\bar{\beta}}(\boldsymbol{z}, \bar{\boldsymbol{z}})(dz^\alpha \otimes d\bar{z}^\beta + d\bar{z}^\beta \otimes dz^\alpha)$$

is the Riemannian metric on $\mathscr{M}$ and

$$\omega = -\operatorname{Im} h = \frac{i}{2} \sum_{\alpha,\beta=1}^{n} h_{\alpha\bar{\beta}}(\boldsymbol{z}, \bar{\boldsymbol{z}}) dz^\alpha \wedge d\bar{z}^\beta$$

is the symplectic form on $\mathscr{M}$ (considered as a $2n$-dimensional real manifold).

The simplest compact Kähler manifold is $\mathbb{C}P^1 \simeq S^2$ with the symplectic form given by the area 2-form of the Hermitian metric of Gaussian curvature 1 — the round metric on the 2-sphere. In terms of the local coordinate z associated with the stereographic projection $\mathbb{C}P^1 \simeq \mathbb{C} \cup \{\infty\}$,

$$\omega = 2i \, \frac{dz \wedge d\bar{z}}{(1 + |z|^2)^2}.$$

Similarly, the natural symplectic form on the complex projective space $\mathbb{C}P^n$ is the symplectic form of the Fubini-Study metric. By pull-back, it defines symplectic forms on complex projective varieties.

[17] Needless to say, not every symplectic manifold admits a complex structure, not to mention a Kähler structure.

The simplest non-compact Kähler manifold is the n-dimensional complex vector space $\mathbb{C}^n$ with the standard Hermitian metric. In complex coordinates $\boldsymbol{z} = (z^1, \dots, z^n)$ on $\mathbb{C}^n$ it is given by

$$h = d\boldsymbol{z} \otimes d\bar{\boldsymbol{z}} = \sum_{\alpha=1}^{n} dz^\alpha \otimes d\bar{z}^\alpha.$$

In terms of real coordinates $(\boldsymbol{x}, \boldsymbol{y}) = (x^1, \dots, x^n, y^1, \dots, y^n)$ on $\mathbb{R}^{2n} \simeq \mathbb{C}^n$, where $\boldsymbol{z} = \boldsymbol{x} + i\boldsymbol{y}$, the corresponding symplectic form $\omega = -\operatorname{Im} h$ has the canonical form

$$\omega = \frac{i}{2} d\boldsymbol{z} \wedge d\bar{\boldsymbol{z}} = \sum_{\alpha=1}^{n} dx^\alpha \wedge dy^\alpha = d\boldsymbol{x} \wedge d\boldsymbol{y}.$$

This example naturally leads to the following definition.

Definition. A *symplectic vector space* is a pair (V, ω), where V is a vector space over $\mathbb{R}$ and ω is a non-degenerate, skew-symmetric bilinear form on V.

It follows from basic linear algebra that every symplectic vector space V has a *symplectic basis* — a basis $e^1, \dots, e^n, f_1, \dots, f_n$ of V, where $2n = \dim V$, such that

$$\omega(e^i, e^j) = \omega(f_i, f_j) = 0 \quad \text{and} \quad \omega(e^i, f_j) = \delta^i_j, \quad i, j = 1, \dots, n.$$

In coordinates $(\boldsymbol{p}, \boldsymbol{q}) = (p_1, \dots, p_n, q^1, \dots, q^n)$ corresponding to this basis, $V \simeq \mathbb{R}^{2n}$ and

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

Thus every symplectic vector space is isomorphic to a direct product of the phase planes $\mathbb{R}^2$ with the canonical symplectic form $dp \wedge dq$. Introducing complex coordinates $\boldsymbol{z} = \boldsymbol{p} + i\boldsymbol{q}$, we get the isomorphism $V \simeq \mathbb{C}^n$, so that every symplectic vector space admits a Kähler structure.

It is a basic fact of symplectic geometry that every symplectic manifold is locally isomorphic to a symplectic vector space.

Theorem 2.11 (Darboux' theorem)**.** *Let $(\mathscr{M}, \omega)$ be a $2n$-dimensional symplectic manifold. For every point $x \in \mathscr{M}$ there is a neighborhood U of x with local coordinates $(\boldsymbol{p}, \boldsymbol{q}) = (p_1, \dots, p_n, q^1, \dots, q^n)$ such that on U*

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

Coordinates $\boldsymbol{p}, \boldsymbol{q}$ are called *canonical coordinates* (*Darboux coordinates*). The proof proceeds by induction on n with the two main steps stated as Problems 2.13 and 2.14.

A non-degenerate 2-form ω for every $x \in \mathscr{M}$ defines an isomorphism $J : T_x^*\mathscr{M} \to T_x\mathscr{M}$ by

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

Explicitly, for every $X \in \mathrm{Vect}(\mathscr{M})$ and $\vartheta \in \mathcal{A}^1(\mathscr{M})$ we have

$$\omega(X, J(\vartheta)) = \vartheta(X) \quad \text{and} \quad J^{-1}(X) = -i_X(\omega)$$

(cf. Section 2.1). In local coordinates $\boldsymbol{x} = (x^1, \ldots, x^{2n})$ for the coordinate chart (U, φ) on $\mathscr{M}$, the 2-form ω is given by

$$\omega = \tfrac{1}{2} \sum_{i,j=1}^{2n} \omega_{ij}(\boldsymbol{x})\, dx^i \wedge dx^j,$$

where $\{\omega_{ij}(\boldsymbol{x})\}_{i,j=1}^{2n}$ is a non-degenerate, skew-symmetric matrix-valued function on $\varphi(U)$. Denoting the inverse matrix by $\{\omega^{ij}(\boldsymbol{x})\}_{i,j=1}^{2n}$, we have

$$J(dx^i) = -\sum_{j=1}^{2n} \omega^{ij}(\boldsymbol{x}) \frac{\partial}{\partial x^j}, \quad i = 1, \ldots, 2n.$$

Definition. A *Hamiltonian system* is a pair consisting of a symplectic manifold $(\mathscr{M}, \omega)$, called a *phase space*, and a smooth real-valued function H on $\mathscr{M}$, called a *Hamiltonian*. The motion of points on the phase space is described by the vector field

$$X_H = J(dH),$$

called a *Hamiltonian vector field*.

The trajectories of a Hamiltonian system $((\mathscr{M}, \omega), H)$ are the integral curves of a Hamiltonian vector field X_H on $\mathscr{M}$. In canonical coordinates $(\boldsymbol{p}, \boldsymbol{q})$ they are described by the canonical Hamilton's equations (2.1),

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

Suppose now that the Hamiltonian vector field X_H on $\mathscr{M}$ is complete. The *Hamiltonian 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 2.12. *The Hamiltonian phase flow preserves the symplectic form.*

Proof. It is sufficient to show that $\mathcal{L}_{X_H}\omega = 0$. Using Cartan's formula

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

and $d\omega = 0$, we get for every $X \in \mathrm{Vect}(\mathscr{M})$,

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

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

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

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

Corollary 2.13. *A vector field X on $\mathscr{M}$ is a Hamiltonian vector field if and only if the 1-form $i_X(\omega)$ is exact.*

Definition. A vector field X on a symplectic manifold $(\mathscr{M}, \omega)$ is called a *symplectic vector field* if the 1-form $i_X(\omega)$ is closed, which is equivalent to $\mathscr{L}_X\omega = 0$.

The commutative algebra $C^\infty(\mathscr{M})$, with a multiplication given by the point-wise product of functions, is called the *algebra of classical observables*. Assuming that the Hamiltonian phase flow g_t exists for all times, the time evolution of every observable $f \in C^\infty(\mathscr{M})$ is given by

$$f_t(x) = f(g_t(x)), \quad x \in \mathscr{M},$$

and is described by the differential equation

$$\frac{df_t}{dt} = X_H(f_t)$$

— Hamilton's equation for classical observables. Hamilton's equations for observables on $\mathscr{M}$ have the same form as Hamilton's equations on $\mathscr{M} = T^*M$, considered in Section 2.3. Since

$$X_H(f) = df(X_H) = \omega(X_H, J(df)) = \omega(X_H, X_f),$$

we have the following.

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

$$\{f, g\} = \omega(X_f, X_g), \quad f, g \in C^\infty(\mathscr{M}).$$

Now Hamilton's equation takes the concise form

$$\frac{df}{dt} = \{H, f\}, \tag{2.12}$$

understood as a differential equation for a family of functions f_t on $\mathscr{M}$ with the initial condition $f_t|_{t=0} = f$. In local coordinates $\boldsymbol{x} = (x^1, \dots, x^{2n})$ on $\mathscr{M}$,

$$\{f, g\}(\boldsymbol{x}) = -\sum_{i,j=1}^{2n} \omega^{ij}(\boldsymbol{x}) \frac{\partial f(\boldsymbol{x})}{\partial x^i} \frac{\partial g(\boldsymbol{x})}{\partial x^j}.$$

Theorem 2.14. *The Poisson bracket $\{\ ,\ \}$ on a symplectic manifold $(\mathscr{M}, \omega)$ is skew-symmetric and satisfies Leibniz rule and the Jacobi identity.*

Proof. The first two properties are obvious. It follows from the definition of a Poisson bracket and the formula

$$[X_f, X_g](h) = (X_g X_f - X_f X_g)(h) = \{g, \{f, h\}\} - \{f, \{g, h\}\}$$

that the Jacobi identity is equivalent to the property

$$[X_f, X_g] = X_{\{f,g\}}. \tag{2.13}$$

Let X and Y be symplectic vector fields. Using Cartan's formulas we get

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

where Z is a Hamiltonian vector field corresponding to $\omega(X, Y) \in C^\infty(\mathscr{M})$. Since the 2-form ω is non-degenerate, this implies $[X, Y] = Z$, so that setting $X = X_f, Y = X_g$ and using $\{f, g\} = \omega(X_f, X_g)$, we get (2.13). □

From (2.13) we immediately get the following result.

Corollary 2.15. *The subspace* $\mathrm{Ham}(\mathscr{M})$ *of Hamiltonian vector fields on* $\mathscr{M}$ *is a Lie subalgebra of* $\mathrm{Vect}(\mathscr{M})$. *The mapping* $C^\infty(\mathscr{M}) \to \mathrm{Ham}(\mathscr{M})$, *given by* $f \mapsto X_f$, *is a Lie algebra homomorphism with the kernel consisting of locally constant functions on* $\mathscr{M}$.

As in the case $\mathscr{M} = T^*M$ (see Section 2.4), an observable I — a function on the phase space $\mathscr{M}$ — is called an integral of motion (first integral) for the Hamiltonian system $((\mathscr{M}, \omega), H)$ if it is constant along the Hamiltonian phase flow. According to (2.12), this is equivalent to the condition

$$\{H, I\} = 0. \tag{2.14}$$

It is said that the observables H and I are *in involution* (*Poisson commute*). From the Jacobi identity for the Poisson bracket we get the following result.

Corollary 2.16 (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

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

It follows from Poisson's theorem that integrals of motion form a Lie algebra and, by (2.13), corresponding Hamiltonian vector fields form a Lie subalgebra in $\mathrm{Vect}(\mathscr{M})$. Since $\{I, H\} = dH(X_I) = 0$, the vector fields X_I are tangent to submanifolds $\mathscr{M}_E = \{x \in \mathscr{M} : H(x) = E\}$ — the level sets of the Hamiltonian H. This defines a Lie algebra of integrals of motion for the Hamiltonian system $((\mathscr{M}, \omega), H)$ at the level set $\mathscr{M}_E$.

Let G be a finite-dimensional Lie group that acts on a connected symplectic manifold $(\mathscr{M},\omega)$ by symplectomorphisms. The Lie algebra $\mathfrak{g}$ of G acts on $\mathscr{M}$ by vector fields

$$X_\xi(f)(x) = \frac{d}{ds}\Big|_{s=0} f(e^{-s\xi}\cdot x),$$

and the linear mapping $\mathfrak{g}\ni\xi\mapsto X_\xi\in\mathrm{Vect}(\mathscr{M})$ is a homomorphism of Lie algebras,

$$[X_\xi, X_\eta] = X_{[\xi,\eta]},\quad \xi,\eta\in\mathfrak{g}.$$

The G-action is called a *Hamiltonian action* if X_ξ are Hamiltonian vector fields, i.e., for every $\xi\in\mathfrak{g}$ there is $\Phi_\xi\in C^\infty(\mathscr{M})$, defined up to an additive constant, such that $X_\xi = X_{\Phi_\xi} = J(d\Phi_\xi)$. It is called a *Poisson action* if there is a choice of functions Φ_ξ such that the linear mapping $\Phi:\mathfrak{g}\to C^\infty(\mathscr{M})$ is a homomorphism of Lie algebras,

$$\{\Phi_\xi,\Phi_\eta\} = \Phi_{[\xi,\eta]},\quad \xi,\eta\in\mathfrak{g}. \tag{2.15}$$

Definition. A Lie group G is a *symmetry group* of the Hamiltonian system $((\mathscr{M},\omega),H)$ if there is a Hamiltonian action of G on $\mathscr{M}$ such that

$$H(g\cdot x) = H(x),\quad g\in G,\ x\in\mathscr{M}.$$

Theorem 2.17 (Noether theorem with symmetries)**.** *If G is a symmetry group of the Hamiltonian system $((\mathscr{M},\omega),H)$, then the functions Φ_ξ, $\xi\in\mathfrak{g}$, are the integrals of motion. If the action of G is Poisson, the integrals of motion satisfy* (2.15).

Proof. By definition of the Hamiltonian action, for every $\xi\in\mathfrak{g}$,

$$0 = X_\xi(H) = X_{\Phi_\xi}(H) = \{\Phi_\xi, H\}. \qquad \square$$

Corollary 2.18. *Let (M,L) be a Lagrangian system such that the Legendre transform $\tau_L: TM\to T^*M$ is a diffeomorphism. Then if a Lie group G is a symmetry of (M,L), then G is a symmetry group of the corresponding Hamiltonian system $((T^*M,\omega), H = E_L\circ\tau_L^{-1})$, and the corresponding G-action on T^*M is Poisson. In particular, $\Phi_\xi = -I_\xi\circ\tau_L^{-1}$, where I_ξ are Noether integrals of motion for the one-parameter subgroups of G generated by $\xi\in\mathfrak{g}$.*

Proof. Let X be the vector field associated with the one-parameter subgroup $\{e^{s\xi}\}_{s\in\mathbb{R}}$ of diffeomorphisms of M, used in Theorem 1.3, and let X' be its lift to TM. We have[18]

$$X_\xi = -(\tau_L)_*(X'), \tag{2.16}$$

[18]The negative sign reflects the difference in definitions of X and X_ξ.

and it follows from (1.16) that $\Phi_\xi = i_{X_\xi}(\theta) = \theta(X_\xi)$, where θ is the canonical Liouville 1-form on T^*M. From Cartan's formula and (1.17) we get

$$d\Phi_\xi = d(i_{X_\xi}(\theta)) = -i_{X_\xi}(d\theta) + \mathcal{L}_{X_\xi}(\theta) = -i_{X_\xi}(\omega),$$

so that

$$J(d\Phi_\xi) = -J(i_{X_\xi}(\omega)) = X_\xi,$$

and the G-action is Hamiltonian. Using (1.17) and another Cartan's formula, we obtain

$$\begin{aligned}\Phi_{[\xi,\eta]} &= i_{[X_\xi,X_\eta]}(\theta) = \mathcal{L}_{X_\xi}(i_{X_\eta}(\theta)) + i_{X_\eta}(\mathcal{L}_{X_\xi}(\theta)) \\ &= X_\xi(\Phi_\eta) = \{\Phi_\xi, \Phi_\eta\}.\end{aligned}$$

□

Example 2.1. The Lagrangian

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

for a particle in $\mathbb{R}^3$ moving in a central field (see Section 1.6) is invariant with respect to the action of the group SO(3) of orthogonal transformations of the Euclidean space $\mathbb{R}^3$. Let u_1, u_2, u_3 be a basis for the Lie algebra $\mathfrak{so}(3)$ corresponding to the rotations with the axes given by the vectors of the standard basis e_1, e_2, e_3 for $\mathbb{R}^3$ (see Example 1.10 in Section 1.4). These generators satisfy the commutation relations

$$[u_i, u_j] = \varepsilon_{ijk}u_k,$$

where $i, j, k = 1, 2, 3$, and ε_{ijk} is a totally anti-symmetric tensor, $\varepsilon_{123} = 1$. Corresponding Noether integrals of motion are given by $\Phi_{u_i} = -M_i$, where

$$\begin{aligned}M_1 &= (\boldsymbol{r} \times \boldsymbol{p})_1 = r_2p_3 - r_3p_2, \\ M_2 &= (\boldsymbol{r} \times \boldsymbol{p})_2 = r_3p_1 - r_1p_3, \\ M_3 &= (\boldsymbol{r} \times \boldsymbol{p})_3 = r_1p_2 - r_2p_1\end{aligned}$$

are components of the angular momentum vector $\boldsymbol{M} = \boldsymbol{r} \times \boldsymbol{p}$. (Here it is convenient to lower the indices of the coordinates r_i by the Euclidean metric on $\mathbb{R}^3$.) For the Hamiltonian

$$H = \frac{\boldsymbol{p}^2}{2m} + V(r)$$

we have

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

According to Theorem 2.17 and Corollary 2.18, Poisson brackets of the components of the angular momentum satisfy

$$\{M_i, M_j\} = -\varepsilon_{ijk}M_k,$$

which is also easy to verify directly using (2.6),

$$\{f, g\}(\boldsymbol{p}, \boldsymbol{r}) = \frac{\partial f}{\partial \boldsymbol{p}}\frac{\partial g}{\partial \boldsymbol{r}} - \frac{\partial f}{\partial \boldsymbol{r}}\frac{\partial g}{\partial \boldsymbol{p}}.$$

Example 2.2 (Kepler's problem)**.** For every $\alpha \in \mathbb{R}$ the Lagrangian system on $\mathbb{R}^3$ with

$$L = \tfrac{1}{2} m \dot{\boldsymbol{r}}^2 + \frac{\alpha}{r}$$

has three extra integrals of motion — the components W_1, W_2, W_3 of the Laplace-Runge-Lenz vector, given by

$$\boldsymbol{W} = \frac{\boldsymbol{p}}{m} \times \boldsymbol{M} - \frac{\alpha \boldsymbol{r}}{r}$$

(see Section 1.6). Using Poisson brackets from the previous example, together with $\{r_i, M_j\} = -\varepsilon_{ijk} r_k$ and $\{p_i, M_j\} = -\varepsilon_{ijk} p_k$, we get by a straightforward computation,

$$\{W_i, M_j\} = -\varepsilon_{ijk} W_k \quad \text{and} \quad \{W_i, W_j\} = \frac{2H}{m} \varepsilon_{ijk} M_k,$$

where $H = \dfrac{\boldsymbol{p}^2}{2m} - \dfrac{\alpha}{r}$ is the Hamiltonian of Kepler's problem.

The Hamiltonian system $((\mathscr{M}, \omega), H)$, $\dim \mathscr{M} = 2n$, is called *completely integrable* if it has n independent integrals of motion $F_1 = H, \dots, F_n$ in involution. The former condition means that $dF_1(x), \dots, dF_n(x) \in T_x^* \mathscr{M}$ are linearly independent for almost all $x \in \mathscr{M}$. Hamiltonian systems with one degree of freedom such that dH has only finitely many zeros are completely integrable. Complete separation of variables in the Hamilton-Jacobi equation (see Section 2.5) provides other examples of completely integrable Hamiltonian systems.

Let $((\mathscr{M}, \omega), H)$ be a completely integrable Hamiltonian system. Suppose that the level set $\mathscr{M}_f = \{x \in \mathscr{M} : F_1(x) = f_1, \dots, F_n(x) = f_n\}$ is compact and tangent vectors $J dF_1, \dots, J dF_n$ are linearly independent for all $x \in \mathscr{M}_f$. Then by the Liouville-Arnold theorem, in a neighborhood of $\mathscr{M}_f$ there exist so-called *action-angle variables*: coordinates $\boldsymbol{I} = (I_1, \dots, I_n) \in \mathbb{R}^n_+ = (\mathbb{R}_{>0})^n$ and $\boldsymbol{\varphi} = (\varphi_1, \dots, \varphi_n) \in T^n = (\mathbb{R}/2\pi\mathbb{Z})^n$ such that $\omega = d\boldsymbol{I} \wedge d\boldsymbol{\varphi}$ and $H = H(I_1, \dots, I_n)$. According to Hamilton's equations,

$$\dot{I}_i = 0 \quad \text{and} \quad \dot{\varphi}_i = \omega_i = \frac{\partial H}{\partial I_i}, \quad i = 1, \dots, n,$$

so that action variables are constants, and angle variables change uniformly, $\varphi_i(t) = \varphi_i(0) + \omega_i t$, $i = 1, \dots, n$. The classical motion is almost-periodic with the frequencies $\omega_1, \dots, \omega_n$.

Problem 2.10. Show that a symplectic manifold $(\mathscr{M}, \omega)$ admits an *almost complex structure*: a bundle map $\mathscr{J} : T\mathscr{M} \to T\mathscr{M}$ such that $\mathscr{J}^2 = -\mathrm{id}$.

Problem 2.11. Give an example of a symplectic manifold which admits a complex structure but not a Kähler structure.

Problem 2.12 (Coadjont orbits)**.** Let G be a finite-dimensional Lie group, let $\mathfrak{g}$ be its Lie algebra, and let $\mathfrak{g}^*$ be the dual vector space to $\mathfrak{g}$. For $u \in \mathfrak{g}^*$ let $\mathscr{M} = \mathcal{O}_u$ be the orbit of u under the coadjoint action of G on $\mathfrak{g}^*$. Show that the formula

$$\omega(u_1, u_2) = u([x_1, x_2]),$$

where $u_1 = \mathrm{ad}^* x_1(u), u_2 = \mathrm{ad}^* x_2(u) \in \mathcal{O}_u$, and ad^* stands for the coadjoint action of a Lie algebra $\mathfrak{g}$ on $\mathfrak{g}^*$, gives rise to a well-defined 2-form on $\mathscr{M}$, which is closed and non-degenerate. (The 2-form ω is called the *Kirillov-Kostant* symplectic form.)

Problem 2.13. Let $(\mathscr{M}, \omega)$ be a symplectic manifold. For $x \in \mathscr{M}$ choose a function q^1 on $\mathscr{M}$ such that $q^1(x) = 0$ and dq^1 does not vanish at x, and set $X = -X_{q^1}$. Show that there is a neighborhood U of $x \in \mathscr{M}$ and a function p_1 on U such that $X(q^1) = 1$ on U, and there exist coordinates $p_1, q^1, z^1, \dots, z^{2n-2}$ on U such that

$$X = \frac{\partial}{\partial p_1} \quad \text{and} \quad Y = X_{p_1} = \frac{\partial}{\partial q^1}.$$

Problem 2.14. Continuing Problem 2.13, show that the 2-form $\omega - dp_1 \wedge dq^1$ on U depends only on coordinates $z^1, \dots, z^{2n-2}$ and is non-degenerate.

Problem 2.15. Do the computation in Example 2.2 and show that the Lie algebra of the integrals $M_1, M_2, M_3, W_1, W_2, W_3$ in Kepler's problem at $H(\boldsymbol{p}, \boldsymbol{r}) = E$ is isomorphic to the Lie algebra $\mathfrak{so}(4)$, if $E < 0$, to the Euclidean Lie algebra $\mathfrak{e}(3)$, if $E = 0$, and to the Lie algebra $\mathfrak{so}(1,3)$, if $E > 0$.

Problem 2.16. Find the action-angle variables for a particle with one degree of freedom, when the potential $V(x)$ is a convex function on $\mathbb{R}$ satisfying $\lim_{|x|\to\infty} V(x) = \infty$. (*Hint:* Define $I = \oint p dx$, where integration goes over the closed orbit with $H(p, x) = E$.)

Problem 2.17. Show that a Hamiltonian system describing a particle in $\mathbb{R}^3$ moving in a central field is completely integrable, and find the action-angle variables.

Problem 2.18 (Symplectic quotients)**.** For a Poisson action of a Lie group G on a symplectic manifold $(\mathscr{M}, \omega)$, define the *moment map* $P : \mathscr{M} \to \mathfrak{g}^*$ by

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

where $\mathfrak{g}$ is the Lie algebra of G. For every $p \in \mathfrak{g}^*$ such that a stabilizer G_p of p acts freely and properly on $\mathscr{M}_p = P^{-1}(p)$ (such p is called *the regular value* of the moment map), the quotient $M_p = G_p \backslash \mathscr{M}_p$ is called a *reduced phase space*. Show that M_p is a symplectic manifold with the symplectic form 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.

2.7. Poisson manifolds. The notion of a Poisson manifold generalizes the notion of a symplectic manifold.

Definition. A *Poisson manifold* is a manifold $\mathscr{M}$ equipped with a *Poisson structure* — a skew-symmetric bilinear mapping

$$\{\ ,\ \} : C^\infty(\mathscr{M}) \times C^\infty(\mathscr{M}) \to C^\infty(\mathscr{M})$$

which satisfies the Leibniz rule and Jacobi identity.

Equivalently, $\mathscr{M}$ is a Poisson manifold if the algebra $\mathcal{A} = C^\infty(\mathscr{M})$ of classical observables is a Poisson algebra — a Lie algebra such that the Lie bracket is a bi-derivation with respect to the multiplication in $\mathcal{A}$ (a pointwise product of functions). It follows from the derivation property that in local coordinates $\boldsymbol{x} = (x^1, \dots, x^N)$ on $\mathscr{M}$, the Poisson bracket has the form

$$\{f, g\}(\boldsymbol{x}) = \sum_{i,j=1}^{N} \eta^{ij}(\boldsymbol{x}) \frac{\partial f(\boldsymbol{x})}{\partial x^i} \frac{\partial g(\boldsymbol{x})}{\partial x^j}.$$

The 2-tensor $\eta^{ij}(\boldsymbol{x})$, called a *Poisson tensor*, defines a global section η of the vector bundle $T\mathscr{M} \wedge T\mathscr{M}$ over $\mathscr{M}$.

The evolution of classical observables on a Poisson manifold is given by Hamilton's equations, which have the same form as (2.12),

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

The phase flow g_t for a complete Hamiltonian vector field $X_H = \{H, \cdot\}$ defines the *evolution operator* $U_t : \mathcal{A} \to \mathcal{A}$ by

$$U_t(f)(x) = f(g_t(x)), \ f \in \mathcal{A}.$$

Theorem 2.19. *Suppose that every Hamiltonian vector field on a Poisson manifold $(\mathscr{M}, \{\ ,\ \})$ is complete. Then for every $H \in \mathcal{A}$, the corresponding evolution operator U_t is an automorphism of the Poisson algebra $\mathcal{A}$, i.e.,*

$$U_t(\{f, g\}) = \{U_t(f), U_t(g)\} \quad \textit{for all} \quad f, g \in \mathcal{A}. \tag{2.17}$$

Conversely, if a skew-symmetric bilinear mapping $\{\ ,\ \} : C^\infty(\mathscr{M}) \times C^\infty(\mathscr{M}) \to C^\infty(\mathscr{M})$ is such that $X_H = \{H, \cdot\}$ are complete vector fields for all $H \in \mathcal{A}$, and corresponding evolution operators U_t satisfy (2.17)*, then $(\mathscr{M}, \{\ ,\ \})$ is a Poisson manifold.*

Proof. Let $f_t = U_t(f)$, $g_t = U_t(g)$, and[19] $h_t = U_t(\{f, g\})$. By definition,

$$\frac{d}{dt}\{f_t, g_t\} = \{\{H, f_t\}, g_t\} + \{f_t, \{H, g_t\}\} \quad \text{and} \quad \frac{dh_t}{dt} = \{H, h_t\}.$$

If $(\mathscr{M}, \{\ ,\ \})$ is a Poisson manifold, then it follows from the Jacobi identity that

$$\{\{H, f_t\}, g_t\} + \{f_t, \{H, g_t\}\} = \{H, \{f_t, g_t\}\},$$

so that h_t and $\{f_t, g_t\}$ satisfy the same differential equation (2.12). Since these functions coincide at $t = 0$, (2.17) follows from the uniqueness theorem for the ordinary differential equations.

Conversely, we get the Jacobi identity for the functions f, g, and H by differentiating (2.17) with respect to t at $t = 0$. □

[19] Here g_t is not the phase flow!

Corollary 2.20. *A global section η of $T\mathscr{M} \wedge T\mathscr{M}$ is a Poisson tensor if and only if*

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

Definition. The *center* of a Poisson algebra $\mathcal{A}$ is

$$\mathcal{Z}(\mathcal{A}) = \{f \in \mathcal{A} : \{f, g\} = 0 \quad \text{for all} \quad g \in \mathcal{A}\}.$$

A Poisson manifold $(\mathscr{M}, \{\ ,\ \})$ is called *non-degenerate* if the center of a Poisson algebra of classical observables $\mathcal{A} = C^\infty(\mathscr{M})$ consists only of locally constant functions ($\mathcal{Z}(\mathcal{A}) = \mathbb{R}$ for connected $\mathscr{M}$).

Equivalently, a Poisson manifold $(\mathscr{M}, \{\ ,\ \})$ is non-degenerate if the Poisson tensor η is non-degenerate everywhere on $\mathscr{M}$, so that $\mathscr{M}$ is necessarily an even-dimensional manifold. A non-degenerate Poisson tensor for every $x \in \mathscr{M}$ defines an isomorphism $J : T_x^*\mathscr{M} \to T_x\mathscr{M}$ by

$$\eta(u_1, u_2) = u_2(J(u_1)),\ u_1, u_2 \in T_x^*\mathscr{M}.$$

In local coordinates $\boldsymbol{x} = (x^1, \ldots, x^N)$ for the coordinate chart (U, φ) on $\mathscr{M}$, we have

$$J(dx^i) = \sum_{j=1}^{N} \eta^{ij}(\boldsymbol{x}) \frac{\partial}{\partial x^j}, \quad i = 1, \ldots, N.$$

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

$$\{f \circ \varphi, g \circ \varphi\}_1 = \{f, g\}_2 \circ \varphi \quad \text{for all} \quad f, g \in C^\infty(\mathscr{M}_2).$$

A direct product of Poisson manifolds $(\mathscr{M}_1, \{\ ,\ \}_1)$ and $(\mathscr{M}_2, \{\ ,\ \}_2)$ is a Poisson manifold $(\mathscr{M}_1 \times \mathscr{M}_2, \{\ ,\ \})$ defined by the property that natural projection 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. For $f \in C^\infty(\mathscr{M}_1 \times \mathscr{M}_2)$ and $(x_1, x_2) \in \mathscr{M}_1 \times \mathscr{M}_2$ denote, respectively, by $f^{(1)}_{x_2}$ and $f^{(2)}_{x_1}$ restrictions of f to $\mathscr{M} \times \{x_2\}$ and $\{x_1\} \times \mathscr{M}_2$. Then for $f, g \in C^\infty(\mathscr{M}_1 \times \mathscr{M}_2)$,

$$\{f, g\}(x_1, x_2) = \{f^{(1)}_{x_2}, g^{(1)}_{x_2}\}_1(x_1) + \{f^{(2)}_{x_1}, g^{(2)}_{x_1}\}_2(x_2).$$

Non-degenerate Poisson manifolds form a subcategory of the category of Poisson manifolds.

Theorem 2.21. *The category of symplectic manifolds is (anti-) isomorphic to the category of non-degenerate Poisson manifolds.*

Proof. According to Theorem 2.14, every symplectic manifold carries a Poisson structure. Its non-degeneracy follows from the non-degeneracy of a symplectic form. Conversely, let $(\mathscr{M}, \{\ ,\ \})$ be a non-degenerate Poisson manifold. Define the 2-form ω on $\mathscr{M}$ by

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

where the isomorphism $J : T^*\mathscr{M} \to T\mathscr{M}$ is defined by the Poisson tensor η. In local coordinates $\boldsymbol{x} = (x^1, \dots, x^N)$ on $\mathscr{M}$,

$$\omega = -\sum_{1 \le i < j \le N} \eta_{ij}(\boldsymbol{x})\, dx^i \wedge dx^j,$$

where $\{\eta_{ij}(\boldsymbol{x})\}_{i,j=1}^N$ is the inverse matrix to $\{\eta^{ij}(\boldsymbol{x})\}_{i,j=1}^N$. The 2-form ω is skew-symmetric and non-degenerate. For every $f \in \mathcal{A}$ let $X_f = \{f, \cdot\}$ be the corresponding vector field on $\mathscr{M}$. The Jacobi identity for the Poisson bracket $\{\ ,\ \}$ is equivalent to $\mathcal{L}_{X_f}\eta = 0$ for every $f \in \mathcal{A}$, so that

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

Since $X_f = Jdf$, we have $\omega(X, Jdf) = df(X)$ for every $X \in \mathrm{Vect}(\mathscr{M})$, so that

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

By Cartan's formula,

$$\begin{aligned} d\omega(X,Y,Z) = \tfrac{1}{3}\,(&\mathcal{L}_X\omega(Y,Z) - \mathcal{L}_Y\omega(X,Z) + \mathcal{L}_Z\omega(X,Y) \\ &-\omega([X,Y],Z) + \omega([X,Z],Y) - \omega([Y,Z],X))\,, \end{aligned}$$

where $X, Y, Z \in \mathrm{Vect}(\mathscr{M})$. Now setting $X = X_f, Y = X_g, Z = X_h$, we get

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

The exact 1-forms df, $f \in \mathcal{A}$, generate the vector space of 1-forms $\mathcal{A}^1(\mathscr{M})$ as a module over $\mathcal{A}$, so that Hamiltonian vector fields $X_f = Jdf$ generate the vector space $\mathrm{Vect}(\mathscr{M})$ as a module over $\mathcal{A}$. Thus $d\omega = 0$ and $(\mathscr{M}, \omega)$ is a symplectic manifold associated with the Poisson manifold $(\mathscr{M}, \{\ ,\ \})$. It follows from the definitions that Poisson mappings of non-degenerate Poisson manifolds correspond to symplectomorphisms of associated symplectic manifolds. □

Remark. One can also prove this theorem by a straightforward computation in local coordinates $\boldsymbol{x} = (x^1, \dots, x^N)$ on $\mathscr{M}$. Just observe that the condition

$$\frac{\partial \eta_{ij}(\boldsymbol{x})}{\partial x^l} + \frac{\partial \eta_{jl}(\boldsymbol{x})}{\partial x^i} + \frac{\partial \eta_{li}(\boldsymbol{x})}{\partial x^j} = 0, \quad i,j,l = 1, \dots, N,$$

which is a coordinate form of $d\omega = 0$, follows from the condition

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

which is a coordinate form of the Jacobi identity, by multiplying it three times by the inverse matrix $\eta_{ij}(\boldsymbol{x})$ using

$$\sum_{p=1}^{N}\left(\eta^{ip}(\boldsymbol{x})\frac{\partial\eta_{pk}(\boldsymbol{x})}{\partial x^j}+\frac{\partial\eta^{ip}(\boldsymbol{x})}{\partial x^j}\eta_{pk}(\boldsymbol{x})\right)=0.$$

Remark. Let $\mathscr{M}=T^*\mathbb{R}^n$ with the Poisson bracket $\{\ ,\ \}$ given by the canonical symplectic form $\omega=d\boldsymbol{p}\wedge d\boldsymbol{q}$, where $(\boldsymbol{p},\boldsymbol{q})=(p_1,\dots,p_n,q^1,\dots,q^n)$ are coordinate functions on $T^*\mathbb{R}^n$. The non-degeneracy of the Poisson manifold $(T^*\mathbb{R}^n,\{\ ,\ \})$ can be formulated as the property that the only observable $f\in C^\infty(T^*\mathbb{R}^n)$ satisfying

$$\{f,p_1\}=\dots=\{f,p_n\}=0,\quad \{f,q^1\}=\dots=\{f,q^n\}=0$$

is $f(\boldsymbol{p},\boldsymbol{q})=\text{const}$.

Problem 2.19 (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. For $f,g\in C^\infty(\mathfrak{g}^*)$ define

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

where $u\in\mathfrak{g}^*$ and $T^*_u\mathfrak{g}^*\simeq\mathfrak{g}$. Prove that $\{\ ,\ \}$ is a Poisson bracket. (It was introduced by Sophus Lie and is called a *linear*, or *Lie-Poisson* bracket.) Show that this bracket is degenerate and determine the center of $\mathcal{A}=C^\infty(\mathfrak{g}^*)$.

Problem 2.20. A Poisson bracket $\{\ ,\ \}$ on $\mathscr{M}$ restricts to a Poisson bracket $\{\ ,\ \}_0$ on a submanifold $\mathscr{N}$ if the inclusion $\imath:\mathscr{N}\to\mathscr{M}$ is a Poisson mapping. Show that the Lie-Poisson bracket on $\mathfrak{g}^*$ restricts to a non-degenerate Poisson bracket on a coadjoint orbit, associated with the Kirillov-Kostant symplectic form.

Problem 2.21 (Lie-Poisson groups)**.** A finite-dimensional Lie group 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, where $G\times G$ is a direct product of Poisson manifolds. Using a basis $\partial_1,\dots,\partial_n$ of left-invariant vector fields on G corresponding to a basis $x_1,\dots,x_n$ of the Lie algebra $\mathfrak{g}$, the Poisson bracket $\{\ ,\ \}$ can be written as

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

where the 2-tensor $\eta^{ij}(g)$ defines a mapping $\eta:G\to\Lambda^2\mathfrak{g}$ by $\eta(g)=\sum_{i,j=1}^n\eta^{ij}(g)x_i\otimes x_j$. Show that the bracket $\{\ ,\ \}$ equips G with a Lie-Poisson structure if and only if the following conditions are satisfied: (i) for all $g\in G$,

$$\xi^{ijk}(g)=\sum_{l=1}^{n}\left(\eta^{il}(g)\partial_l\eta^{jk}(g)+\eta^{jl}(g)\partial_l\eta^{ki}(g)+\eta^{kl}(g)\partial_l\eta^{ij}(g)\right)$$
$$+\sum_{l,p=1}^{n}\left(c^i_{lp}\eta^{pj}(g)\eta^{kl}(g)+c^j_{lp}\eta^{pk}(g)\eta^{il}(g)+c^k_{lp}\eta^{pi}(g)\eta^{jl}(g)\right)=0,$$

where $[x_i,x_j]=\sum_{k=1}^n c^k_{ij}x_k$; (ii) the mapping η is a group 1-cocycle with the adjoint action on $\Lambda^2\mathfrak{g}$, i.e., $\eta(g_1g_2)=\mathrm{Ad}^{-1}g_2\cdot\eta(g_1)+\eta(g_2),\ g_1,g_2\in G$.

Problem 2.22. Show that the second condition in the previous problem trivially holds when η is a coboundary, $\eta(g) = -r + \mathrm{Ad}^{-1}g \cdot r$ for some $r = \sum_{i,j=1}^{n} r^{ij} x_i \otimes x_j \in \Lambda^2\mathfrak{g}$, and then the first condition is satisfied if and only if the element

$$\xi(r) = [r_{12}, r_{13} + r_{23}] + [r_{13}, r_{23}] \in \Lambda^3\mathfrak{g}$$

is invariant under the adjoint action of $\mathfrak{g}$ on $\Lambda^3\mathfrak{g}$. Here $r_{12} = \sum_{i,j=1}^{n} r^{ij} x_i \otimes x_j \otimes 1$, $r_{13} = \sum_{i,j=1}^{n} r^{ij} x_i \otimes 1 \otimes x_j$, and $r_{23} = \sum_{i,j=1}^{n} r^{ij} 1 \otimes x_i \otimes x_j$ are corresponding elements in the universal enveloping algebra $U\mathfrak{g}$ of a Lie algebra $\mathfrak{g}$. In particular, G is a Lie-Poisson group if $\xi(r) = 0$, which is called the *classical Yang-Baxter equation*.

Problem 2.23. Suppose that $r = \sum_{i,j=1}^{n} r^{ij} x_i \otimes x_j \in \Lambda^2\mathfrak{g}$ is such that the matrix $\{r^{ij}\}$ is non-degenerate, and let $\{r_{ij}\}$ be the inverse matrix. Show that r satisfies the classical Yang-Baxter equation if and only if the map $c : \Lambda^2\mathfrak{g} \to \mathbb{C}$, defined by $c(x, y) = \sum_{i,j=1}^{n} r_{ij} u^i v^j$, where $x = \sum_{i=1}^{n} u^i x_i$, $y = \sum_{i=1}^{n} v^i x_i$, is a non-degenerate Lie algebra 2-cocycle, i.e., it satisfies

$$c(x, [y, z]) + c(z, [x, y]) + c(y, [z, x]) = 0, \quad x, y, z \in \mathfrak{g}.$$

2.8. Hamilton's and Liouville's representations. To complete the formulation of classical mechanics, we need to describe the process of *measurement*. In physics, by a measurement of a classical system one understands the result of a physical experiment which gives numerical values for classical observables. 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 $\mathcal{A} = C^\infty(\mathscr{M})$ of classical observables on the phase space $\mathscr{M}$ is the assignment

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

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

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

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

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

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

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

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

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

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

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

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

$$\mathsf{E}_\mu(\varphi(f)) = \int_{-\infty}^{\infty} \varphi(\lambda) d\mu_f(\lambda). \tag{2.18}$$

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

Assuming that the functional E_μ extends to the space of bounded, piecewise continuous functions on $\mathscr{M}$, and satisfies (2.18) for measurable functions φ, one can recover the distribution function from the expectation values by the formula

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

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

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

Indeed, let χ be the characteristic function of the interval $(-\infty, \lambda) \subset \mathbb{R}$. Using (2.18) and the definition of the Lebesgue-Stieltjes integral we get

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

Every probability measure $d\mu$ on $\mathscr{M}$ defines the state on $\mathcal{A}$ by assigning[20] to every observable f a probability measure $\mu_f = f_*(\mu)$ on $\mathbb{R}$ — a push-forward of the measure $d\mu$ on $\mathscr{M}$ by the mapping $f : \mathscr{M} \to \mathbb{R}$. It is defined by $\mu_f(E) = \mu(f^{-1}(E))$ for every Borel subset $E \subseteq \mathbb{R}$, and has the distribution function

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

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

$$E_\mu(f) = \int_{-\infty}^{\infty} \lambda d\mu_f(\lambda) = \int_{\mathscr{M}} f d\mu. \tag{2.19}$$

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

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

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

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

Definition. The set of states $\mathcal{S}$ for a Hamiltonian system with the phase space $\mathscr{M}$ is the convex set $\mathscr{P}(\mathscr{M})$ of all probability measures on $\mathscr{M}$. The states corresponding to Dirac measures $d\mu_x$ supported at points $x \in \mathscr{M}$ are called *pure states*, and the phase space $\mathscr{M}$ is also called the *space of states*[21]. All other states are called *mixed states*. A process of measurement in classical mechanics is the correspondence

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

which to every observable $f \in \mathcal{A}$ and state $\mu \in \mathcal{S}$ assigns a probability measure μ_f on $\mathbb{R}$ — a push-forward of the measure $d\mu$ on $\mathscr{M}$ by f. For every Borel subset $E \subseteq \mathbb{R}$ the quantity $0 \leq \mu_f(E) \leq 1$ is the probability that for a system in the state μ the result of a measurement of the observable f is in the set E. The expectation value of an observable f in a state μ is given by (2.19).

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

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

be the *variance* of the observable f in the state μ.

Lemma 2.1. *Pure states are the only states in which every observable has zero variance.*

Proof. It follows from the Cauchy-Bunyakovski-Schwarz inequality that $\sigma_\mu^2(f) = 0$ if only if f is constant on the support of a probability measure $d\mu$. □

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

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

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

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

For a system consisting of few interacting particles (say, a motion of planets in celestial 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[22].

Remark. As a topological space, the space of states $\mathscr{M}$ can be reconstructed from the algebra $\mathcal{A}$ of classical observables. Namely, suppose for simplicity that $\mathscr{M}$ is compact. Then the $\mathbb{C}$-algebra $\mathcal{C} = C(\mathscr{M})$ of complex-valued continuous functions on $\mathscr{M}$ — the completion of the complexification of the $\mathbb{R}$-algebra $\mathcal{A}$ of classical observables with respect to the sup-norm — is a commutative $\mathbb{C}^*$-algebra. This means that $C(\mathscr{M})$ is a Banach space with respect to the norm $\|f\| = \sup_{x\in\mathscr{M}} |f(x)|$, has a $\mathbb{C}$-algebra structure (associative algebra over $\mathbb{C}$ with a unit) given by the point-wise product of functions such that $\|f \cdot g\| \le \|f\|\|g\|$, and has a complex anti-linear anti-involution: a map $^* : \mathcal{C} \to \mathcal{C}$ given by the complex conjugation $f^*(x) = \overline{f(x)}$ and satisfying $\|f \cdot f^*\| = \|f\|^2$. Then the Gelfand-Naimark theorem asserts that every commutative $\mathbb{C}^*$-algebra $\mathcal{C}$ is isomorphic to the algebra $C(\mathscr{M})$ of continuous functions on its spectrum — the set of maximal ideals of $\mathcal{C}$ — a compact topological space with the topology induced by the weak topology on $\mathcal{C}^*$, the dual space of $\mathcal{C}$.

We conclude our exposition of classical mechanics by presenting two equivalent ways of describing the dynamics — the time evolution of a Hamiltonian system $((\mathscr{M}, \{\,,\,\}), H)$ with the algebra of observables $\mathcal{A} = C^\infty(\mathscr{M})$ and the set of states $\mathcal{S} = \mathscr{P}(\mathscr{M})$. In addition, we assume that the Hamiltonian phase flow g_t exists for all times, and that the phase space $\mathscr{M}$ carries a volume form dx invariant under the phase flow[23].

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

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

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

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

where $\rho(x) = \dfrac{d\mu}{dx}$ is the Radon-Nikodim derivative. In particular, the expectation value of f in the pure state $d\mu_x$ corresponding to the point $x \in \mathscr{M}$ is $f(g_t(x))$. Hamilton's picture is commonly used for mechanical systems consisting of few interacting particles.

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

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

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

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

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

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

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

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

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

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

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

3. Notes and references

Classical references are the textbooks [**Arn89**] and [**LL76**], which are written, respectively, from mathematics and physics perspectives. The elegance of [**LL76**] is supplemented by the attention to detail in [**Gol80**], another physics classic. A brief overview of Hamiltonian formalism necessary for quantum mechanics can be found in [**FY80**]. The treatise [**AM78**] and the encyclopaedia surveys [**AG90**], [**AKN97**] provide a comprehensive exposition of classical mechanics, including the history of the subject, and the references to classical works and recent contributions. The textbook [**Ste83**], monographs [**DFN84**], [**DFN85**], and lecture notes [**Bry95**] contain all the necessary material from differential geometry and the theory of Lie groups, as well as references to other sources. In addition, the lectures [**God69**] also provide an introduction to differential geometry and classical mechanics. In particular, [**God69**] and [**Bry95**] discuss the role the second tangent bundle plays in Lagrangian mechanics (see also the monograph [**YI73**] and [**Cra83**]). For a brief review of integration theory, including the Riesz-Markov theorem, see [**RS80**]; for the proof of the Gelfand-Naimark theorem and more details on $\mathbb{C}^*$-algebras, see [**Str05**] and references therein.

Our exposition follows the traditional outline in [**LL76**] and [**Arn89**], which starts with the Lagrangian formalism and introduces Hamiltonian formalism through

the Legendre transform. As in [**Arn89**], we made special emphasis on precise mathematical formulations. Having graduate students and research mathematicians as a main audience, we have the advantage to use freely the calculus of differential forms and vector fields on smooth manifolds. This differs from the presentation in [**Arn89**], which is oriented at undergraduate students and needs to introduce this material in the main text. Since the goal of this chapter was to present only those basics of classical mechanics which are fundamental for the formulation of quantum mechanics, we have omitted many important topics, including mechanical–geometrical optics analogy, theory of oscillations, rotation of a rigid body, perturbation theory, etc. The interested reader can find this material in [**LL76**] and [**Arn89**] and in the above-mentioned monographs. Completely integrable Hamiltonian systems were also only briefly mentioned at the end of Section 2.6. We refer the reader to [**AKN97**] and references therein for a comprehensive exposition, and to the monograph [**FT07**] for the so-called Lax pair method in the theory of integrable systems, especially for the case of infinitely many degrees of freedom.

In Section 2.7, following [**FY80**], [**DFN84**], [**DFN85**], we discussed Poisson manifolds and Poisson algebras. These notions, usually not emphasized in standard exposition of classical mechanics, are fundamental for understanding the meaning of quantization — a passage from classical mechanics to quantum mechanics. We also have included in Sections 1.6 and 2.7 the treatment of the Laplace-Runge-Lenz vector, whose components are extra integrals of motions for the Kepler problem[24]. Though briefly mentioned in [**LL76**], the Laplace-Runge-Lenz vector does not actually appear in many textbooks, with the exception of [**Gol80**] and [**DFN84**]. In Section 2.7, following [**FY80**], we also included Theorem 2.19, which clarifies the meaning of the Jacobi identity, and presented Hamilton's and Liouville's descriptions of the dynamics.

Most of the problems in this chapter are fairly standard and are taken from various sources, mainly from [**Arn89**], [**LL76**], [**Bry95**], [**DFN84**], and [**DFN85**]. Other problems indicate interesting relations with representation theory and symplectic geometry. Thus Problems 2.12 and 2.20 introduce the reader to the orbit method [**Kir04**], and Problem 2.18 — to the method of symplectic reduction (see [**Arn89**], [**Bry95**] and references therein). Problems 2.21 – 2.23 introduce the reader to the theory of Lie-Poisson groups (see [**Dri86**], [**Dri87**], [**STS85**], and [**Tak90**] for an elementary exposition).

[24]We will see in Chapter 3 that these extra integrals are responsible for the hidden SO(4) symmetry of the hydrogen atom.

Chapter 2

Basic Principles of Quantum Mechanics

We recall the standard notation 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 $(\ ,\ )$, which is complex-linear with respect to the first argument, and let A be a linear operator in $\mathscr{H}$ with the domain $D(A) \subseteq \mathscr{H}$ — a linear subset of $\mathscr{H}$. An operator A is called *closed* if its graph $\Gamma(A) = \{(\varphi, A\varphi) \in \mathscr{H} \times \mathscr{H} : \varphi \in D(A)\}$ is a closed subspace in $\mathscr{H} \times \mathscr{H}$. If the domain of A is dense[1] in $\mathscr{H}$, i.e., $\overline{D(A)} = \mathscr{H}$, the domain $D(A^*)$ of the *adjoint operator* A^* consists of $\varphi \in \mathscr{H}$ such that there is $\eta \in \mathscr{H}$ with the property that

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

and the operator A^* is defined by $A^*\varphi = \eta$. An operator A is called *symmetric* if

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

By definition, the *regular set* of a closed operator A with a dense domain $D(A)$ is the set

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

and for $\lambda \in \rho(A)$, the bounded operator $R_\lambda(A) = (A - \lambda I)^{-1}$ is called the *resolvent* of A at λ. The regular set $\rho(A) \subset \mathbb{C}$ is open and its complement $\sigma(A) = \mathbb{C} \setminus \rho(A)$ is the *spectrum* of A. The subset $\sigma_p(A)$ of $\sigma(A)$ consisting of eigenvalues of A of finite multiplicity is called the *point spectrum*.

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

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

An operator A is *self-adjoint* (or *Hermitian*) if $A = A^*$. Equivalently, 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-adjoint. For a symmetric operator A the following conditions are equivalent:

(i) A is essentially self-adjoint.

(ii) $\mathrm{Ker}(A^* + iI) = \mathrm{Ker}(A^* - iI) = \{0\}$.

(iii) $\overline{\mathrm{Im}(A + iI)} = \overline{\mathrm{Im}(A - iI)} = \mathscr{H}$.

A symmetric operator A with $D(A) = \mathscr{H}$ is bounded and self-adjoint. An operator A is positive[3] if $(A\varphi, \varphi) \geq 0$ for all $\phi \in D(A)$, which we denote by $A \geq 0$. Positive operators satisfy the Cauchy-Bunyakovski-Schwarz inequality

$$|(A\varphi, \psi)|^2 \leq (A\varphi, \varphi)(A\psi, \psi) \quad \text{for all} \quad \varphi, \psi \in D(A). \tag{0.1}$$

In particular, $(A\varphi, \varphi) = 0$ implies that $A\varphi = 0$. Every bounded positive operator is self-adjoint[4]. We denote by $\mathscr{L}(\mathscr{H})$ the $\mathbb{C}^*$-algebra of bounded linear operators on $\mathscr{H}$ with the operator norm $\| \cdot \|$ and with the anti-involution * given by the operator adjoint. Operator $A \in \mathscr{L}(\mathscr{H})$ is called *compact* if it maps bounded sets in $\mathscr{H}$ into pre-compact sets[5]. The vector space $\mathscr{C}(\mathscr{H})$ of compact operators on $\mathscr{H}$ is a closed two-sided ideal[6] of the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$.

An operator $A \in \mathscr{C}(\mathscr{H})$ is of *trace class* if

$$\|A\|_1 = \sum_{n=1}^{\infty} \mu_n(A) < \infty,$$

where $\mu_n(A)$ are singular values of A: $\mu_n(A) = \sqrt{\lambda_n(A)} \geq 0$, where $\lambda_n(A)$ are eigenvalues of A^*A. Equivalently, an operator $A \in \mathscr{L}(\mathscr{H})$ is of trace class if and only if for every orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$

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

Since a permutation of an orthonormal basis is again an orthonormal basis, this condition can be replaced by

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

[3] Non-negative, to be precise.

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

[5] The sets with compact closure.

[6] Ideal $\mathscr{C}(\mathscr{H})$ is the only closed two-sided ideal of $\mathscr{L}(\mathscr{H})$.

for every orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$. The *trace* of a trace class operator A is defined by

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

and does not depend on the choice of an orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$. A positive operator $A \in \mathscr{L}(\mathscr{H})$ is of trace class if

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

for some orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$. The space $\mathscr{S}_1$ of trace class operators in $\mathscr{H}$ is a Banach algebra with the norm $\|A\|_1 = \operatorname{Tr}\sqrt{A^*A}$, and is a two-sided ideal (von Neumann-Schatten ideal) in the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$.

The property

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

is called the cyclic property of the trace. If $A \in \mathscr{S}_1$, the mapping $l_A(B) = \operatorname{Tr} AB$, $B \in \mathscr{L}(\mathscr{H})$, is a continuous linear functional on $\mathscr{L}(\mathscr{H})$, so that $\mathscr{S}_1 \subset \mathscr{L}(\mathscr{H})^*$ — the dual Banach space to $\mathscr{L}(\mathscr{H})$. However, $\mathscr{S}_1 \neq \mathscr{L}(\mathscr{H})^*$, but rather $\mathscr{S}_1 = \mathscr{C}(\mathscr{H})^*$, and the mapping $A \mapsto l_A$ is an isomorphism of Banach spaces. Similarly, the mapping $B \mapsto l_B$ gives an isomorphism $\mathscr{L}(\mathscr{H}) = \mathscr{S}_1^*$.

An operator $A \in \mathscr{L}(\mathscr{H})$ is called a *Hilbert-Schmidt operator* if $AA^* \in \mathscr{S}_1$. Equivalently, an operator $A \in \mathscr{L}(\mathscr{H})$ is a Hilbert-Schmidt operator if and only if for some orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$

$$\sum_{n=1}^{\infty} \|Ae_n\|^2 < \infty.$$

The vector space $\mathscr{S}_2$ of Hilbert-Schmidt operators in $\mathscr{H}$ is a Hilbert space with the inner product $(A, B)_2 = \operatorname{Tr} AB^*$. The Hilbert-Schmidt space $\mathscr{S}_2$ is also a two-sided ideal in the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$.

1. Observables, states, and dynamics

Quantum mechanics studies the microworld — the physical laws at an atomic scale — that cannot be adequately described by classical mechanics. The properties of the microworld are so different from our everyday experiences that it is no surprise that its laws seem to contradict the common sense. Thus classical mechanics and classical electrodynamics cannot explain the stability of atoms and molecules. Neither can these theories reconcile different properties of light, its wave-like behavior in interference and diffraction phenomena, and its particle-like behavior in photo-electric emission and scattering by free photons. The fundamental difference between

the microworld and the perceived 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 cannot be measured simultaneously.

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, described in Section 2.8 in Chapter 1. There we have seen that commutativity of the algebra of observables $\mathcal{A}$ results in its realization as an algebra of functions on the topological space — the space of states — and thus brings us to the realm of classical mechanics. Therefore in order to get a realization of observables and states which is different from classical mechanics, we must assume that the $\mathbb{C}^*$-algebra associated with observables is no longer commutative. A fundamental example of a non-commutative $\mathbb{C}^*$-algebra is given by the algebra of all bounded operators on a complex Hilbert space, and it turns out that it is this algebra which plays a fundamental role in quantum mechanics!

Here we formulate the basic principles of quantum mechanics using precise mathematical language. At this point it should be noted that one can not verify directly the principles lying at the foundation of quantum mechanics. Nevertheless, the validity of quantum mechanics, whenever it is applicable, is continuously being confirmed by numerous experimental facts which perfectly agree with the predictions of the theory[7].

1.1. Mathematical formulation. The following axioms constitute the basis of quantum mechanics.

A1. With every *quantum system* there is associated an infinite-dimensional separable complex Hilbert space $\mathscr{H}$, in physics terminology called the *space of states*[8]. The Hilbert space of a *composite quantum system* is a tensor product of Hilbert spaces of component systems.

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

A3. The set of *states* $\mathscr{S}$ of a quantum system with a Hilbert space $\mathscr{H}$ consists of all positive (and hence self-adjoint) trace class operators M with

[7]This refers to non-relativistic phenomena at the atomic scale.

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

$\operatorname{Tr} M = 1$. *Pure states* are projection operators onto one-dimensional subspaces of $\mathscr{H}$. For $\psi \in \mathscr{H}$, $\|\psi\| = 1$, the corresponding projection onto $\mathbb{C}\psi$ is denoted by P_ψ. All other states are called *mixed states*[9].

A4. A process of measurement is the correspondence

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

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

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

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

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

$$M = \sum_{n=1}^{N} \alpha_n P_{\psi_n} \quad \text{and} \quad \operatorname{Tr} M = \sum_{n=1}^{N} \alpha_n = 1, \tag{1.1}$$

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

Lemma 1.1. *A state $M \in \mathscr{S}$ is a pure state if and only if it cannot be represented as a non-trivial convex linear combination in $\mathscr{S}$.*

Proof. Suppose that

$$P_\psi = aM_1 + (1-a)M_2, \quad 0 < a < 1,$$

and 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

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

so that $(M_1\varphi, \varphi) = 0$ for all $\varphi \in \mathscr{H}_1$ and by (0.1) we get $M_1|_{\mathscr{H}_1} = 0$. Since M_1 is self-adjoint, it leaves the complementary subspace $\mathbb{C}\psi$ invariant, and from $\operatorname{Tr} M_1 = 1$ it follows that $M_1 = P_\psi$. Therefore, $M_1 = M_2 = P_\psi$. □

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

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

Definition. A *projection-valued measure* on $\mathbb{R}$ is 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 algebra of bounded operators on $\mathscr{H}$, satisfying the following properties.

PM1. For every Borel subset $E \subseteq \mathbb{R}$, $\mathsf{P}(E)$ is an orthogonal projection, i.e., $\mathsf{P}(E) = \mathsf{P}(E)^2$ and $\mathsf{P}(E) = \mathsf{P}(E)^*$.

PM2. $\mathsf{P}(\emptyset) = 0,\ \mathsf{P}(\mathbb{R}) = I$, the identity operator on $\mathscr{H}$.

PM3. For every disjoint union of Borel subsets,

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

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

Remark. Similarly, a projection-valued measure on $\mathbb{R}^n$ is a mapping $\mathsf{P} : \mathscr{B}(\mathbb{R}^n) \to \mathscr{L}(\mathscr{H})$, satisfying the same properties **PM1**-**PM3**.

It follows from **PM1**-**PM3** that

$$\mathsf{P}(E_1)\mathsf{P}(E_2) = \mathsf{P}(E_1 \cap E_2) \quad \text{for all } E_1, E_2 \in \mathscr{B}(\mathbb{R}). \tag{1.2}$$

With every projection-valued measure P on $\mathbb{R}$ we associate a projection-valued function

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

called the *projection-valued resolution of the identity*. It is characterized by the following properties.

PD1.

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

PD2.

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

PD3.

$$\lim_{\substack{\mu\to\lambda \\ \mu<\lambda}} \mathsf{P}(\mu) = \mathsf{P}(\lambda).$$

For every $\varphi \in \mathscr{H}$ the resolution of the identity $\mathsf{P}(\lambda)$ 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 on $\mathbb{R}$ — a complex linear combination of measures.

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

The next statement is the celebrated general spectral theorem of von Neumann.

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

(i)
$$D(A)=\left\{\varphi\in\mathscr{H}:\int_{-\infty}^{\infty}\lambda^2 d(\mathsf{P}(\lambda)\varphi,\varphi)<\infty\right\},$$
and for every $\varphi\in D(A)$
$$A\varphi=\int_{-\infty}^{\infty}\lambda\, d\mathsf{P}(\lambda)\varphi,$$
defined as a limit of Riemann-Stieltjes sums in the strong topology on $\mathscr{H}$. The support of the corresponding projection-valued measure P coincides with the spectrum of the operator A: $\lambda\in\sigma(A)$ if and only if $\mathsf{P}_A((\lambda-\varepsilon,\lambda+\varepsilon))\neq 0$ for all $\varepsilon>0$.

(ii) *For every continuous function f on $\mathbb{R}$, $f(A)$ is a linear operator on $\mathscr{H}$ with a dense domain*
$$D(f(A))=\left\{\varphi\in\mathscr{H}:\int_{-\infty}^{\infty}|f(\lambda)|^2 d(\mathsf{P}(\lambda)\varphi,\varphi)<\infty\right\},$$
defined for $\varphi\in D(f(A))$ as
$$f(A)\varphi=\int_{-\infty}^{\infty}f(\lambda)d\mathsf{P}(\lambda)\varphi,$$
and understood as in part (i)*. The operator $f(A)$ satisfies*
$$f(A)^*=\bar f(A),$$
where $\bar f$ is the complex conjugate function to f, and the operator $f(A)$ is bounded if and only if the function f is bounded on $\sigma(A)$. For bounded on $\sigma(A)$ continuous functions f and g,
$$f(A)g(A)\varphi=\int_{-\infty}^{\infty}f(\lambda)g(\lambda)d\mathsf{P}(\lambda)\varphi,\quad \varphi\in\mathscr{H}.$$

(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 $\mathscr{H}$ defined as in* (ii)*, where the integral for $f(A)\varphi$ is now understood in the weak sense: for $\varphi \in D(f(A))$ and every $\psi \in \mathscr{H}$,*

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

— a Lebesgue-Stieltjes integral with respect to a complex measure. The correspondence $f \mapsto f(A)$ satisfies the same properties as in (ii)*, where the integrals are understood in the weak sense.*

(iv) *A bounded operator B commutes with A, that is, $B(D(A)) \subset D(A)$ and $AB = BA$ on $D(A)$, if and only if it commutes with $\mathsf{P}(\lambda)$ for all λ and, therefore, B commutes with every operator $f(A)$.*

(v) *For every projection-valued resolution of identity $\mathsf{P}(\lambda)$ the operator A on $\mathscr{H}$, defined as in part* (i)*, is self-adjoint.*

Using the spectral theorem, the correspondence $(A, M) \mapsto \mu_A$, postulated in **A4**, can be explicitly described as follows.

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

$$\mu_A(E) = \operatorname{Tr} \mathsf{P}_A(E) M, \quad E \in \mathscr{B}(\mathbb{R}), \tag{1.3}$$

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

Remark. The probability measure μ_A on $\mathbb{R}$ can be considered as a "quantum push-forward" of the state M by the observable A (cf. the discussion in Section 2.8 in Chapter 1).

From the Hilbert-Schmidt decomposition (1.1) we get

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

so that indeed $0 \le \mu_A(E) \le 1$. Denote by $\mu_A(\lambda)$ the distribution function of the probability measure μ_A, $\mu_A(\lambda) = (\mathsf{P}_A(\lambda)\psi, \psi)$ for $M = P_\psi$.

Proposition 1.1. *Suppose that an observable $A \in \mathscr{A}$ and a state $M \in \mathscr{S}$ are such that $\langle A|M\rangle < \infty$ and $\operatorname{Im} M \subseteq D(A)$. Then $AM \in \mathscr{S}_1$ and*

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

In particular, if $M = P_\psi$ and $\psi \in D(A)$, then

$$\langle A|M\rangle = (A\psi, \psi) \quad \text{and} \quad \langle A^2|M\rangle = \|A\psi\|^2.$$

Proof. Let $\{e_n\}_{n=1}^{\infty}$ be an orthonormal basis for $\mathscr{H}$. Since

$$\mu_A(E) = \operatorname{Tr} \mathsf{P}_A(E)M = \sum_{n=1}^{\infty} (\mathsf{P}_A(E)Me_n, e_n),$$

we get for every $E \in \mathscr{B}(\mathbb{R})$,

$$\mu_A(E) = \sum_{n=1}^{\infty} \mu_n(E),$$

where μ_n are finite measures on $\mathbb{R}$ defined by $\mu_n(E) = (\mathsf{P}_A(E)Me_n, e_n)$. Since

$$\int_{\mathbb{R}} f d\mu_A = \sum_{n=1}^{\infty} \int_{\mathbb{R}} f d\mu_n$$

for every function f integrable with respect to the measure μ_A, it follows from the spectral theorem that

$$\sum_{n=1}^{\infty} (AMe_n, e_n) = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \lambda d\mu_n(\lambda) = \int_{-\infty}^{\infty} \lambda d\mu_A(\lambda) < \infty.$$

Thus $AM \in \mathscr{S}_1$ and $\langle A|M\rangle = \operatorname{Tr} AM$. In particular, when $M = P_\psi$ and $\psi \in D(A)$,

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

Finally, from the spectral theorem and the change of variables formula we get

$$\|A\psi\|^2 = \int_{-\infty}^{\infty} \lambda^2 d(\mathsf{P}_A(\lambda)\psi, \psi) = \int_0^{\infty} \lambda d(\mathsf{P}_{A^2}(\lambda)\psi, \psi) = \langle A^2|M\rangle. \qquad \square$$

Corollary 1.2. *If $\langle A|M\rangle, \langle A^2|M\rangle < \infty$, then $AM \in \mathscr{S}_1$ and $\langle A|M\rangle = \operatorname{Tr} AM$.*

Proof. Since

$$\int_{-\infty}^{\infty} \lambda^2 d\mu_n(\lambda) \le \int_{-\infty}^{\infty} \lambda^2 d\mu_A(\lambda) = \langle A^2|M\rangle < \infty,$$

we get that $e_n \in D(AM)$, and the result follows from the proof of Proposition 1.1. $\square$

Remark. It is convenient to approximate an unbounded self-adjoint operator A by bounded operators $A_n = f_n(A)$, where $f_n = \chi_{[-n,n]}$ — a characteristic function of the interval $[-n, n]$. Assuming that $\langle A|M\rangle$ exists, we have

$$\langle A|M\rangle = \int_{-\infty}^{\infty} \lambda d\mu_A(\lambda) = \lim_{n\to\infty} \int_{-n}^{n} \lambda d\mu_A(\lambda) = \lim_{n\to\infty} \langle A_n|M\rangle.$$

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

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

The following results, which follow from the spectral theorem, are very useful in applications.

Proposition 1.2. *The following statements are equivalent.*

(i) *Self-adjoint operators A and B commute.*

(ii) *For all $\lambda, \mu \in \mathbb{C}$, $\operatorname{Im}\lambda, \operatorname{Im}\mu \neq 0$,*

$$R_\lambda(A)R_\mu(B) = R_\mu(B)R_\lambda(A).$$

(iii) *For all $u, v \in \mathbb{R}$,*

$$e^{iuA}e^{ivB} = e^{ivB}e^{iuA}.$$

(iv) *For all $u \in \mathbb{R}$, the operators e^{iuA} and B commute.*

Slightly abusing notation[10], we will often write $[A, B] = AB - BA = 0$ for commuting self-adjoint operators A and B.

Proposition 1.3. *Let $\boldsymbol{A} = \{A_1, \ldots, A_n\}$ be a finite set of self-adjoint, pairwise commuting operators on $\mathscr{H}$. There exists a unique projection-valued measure $\mathsf{P}_{\boldsymbol{A}}$ on the Borel subsets of $\mathbb{R}^n$ having the following properties.*

(i) *For every $\boldsymbol{E} = E_1 \times \cdots \times E_n \in \mathscr{B}(\mathbb{R}^n)$,*

$$\mathsf{P}_{\boldsymbol{A}}(\boldsymbol{E}) = \mathsf{P}_{A_1}(E_1) \ldots \mathsf{P}_{A_n}(E_n).$$

(ii) *In the strong operator topology,*

$$A_k = \int_{\mathbb{R}^n} \lambda_k d\mathsf{P}_{\boldsymbol{A}}, \quad k = 1, \ldots, n,$$

where λ_k is the k-th coordinate function on $\mathbb{R}^n$, $\lambda_k(x_1, \ldots, x_n) = x_k$.

(iii) *For every measurable function f on $\mathbb{R}^n$, finite a.e. with respect to the projection-valued measure $\mathsf{P}_{\boldsymbol{A}}$, $f(A_1, \ldots, A_n)$ is a linear operator on $\mathscr{H}$ defined by*

$$f(A_1, \ldots, A_n) = \int_{\mathbb{R}^n} f d\mathsf{P}_{\boldsymbol{A}},$$

where the integral is understood in the weak operator topology. The correspondence $f \mapsto f(A_1, \ldots, A_n)$ satisfies the same properties as in part (ii) *of the spectral theorem.*

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

The support of the projection-valued measure $\mathsf{P}_{\boldsymbol{A}}$ *on* $\mathbb{R}^n$ *is called the joint spectrum of the commutative family* $\boldsymbol{A} = \{A_1, \dots, A_n\}$.

Remark. According to von Neumann's theorem on a generating operator, for every commutative family $\boldsymbol{A}$ of self-adjoint operators (not necessarily finite) on a separable Hilbert space $\mathscr{H}$ there is a generating operator — a self-adjoint operator R on $\mathscr{H}$ such that all operators in $\boldsymbol{A}$ are functions of R.

It seems natural that simultaneous measurement of a finite set of observables $\boldsymbol{A} = \{A_1, \dots, A_n\}$ in the state $M \in \mathscr{S}$ should be described by the probability measure $\mu_{\boldsymbol{A}}$ on $\mathbb{R}^n$ given by the following generalization of the Born-von Neumann formula:

$$\mu_{\boldsymbol{A}}(\boldsymbol{E}) = \operatorname{Tr}(\mathsf{P}_{A_1}(E_1) \dots \mathsf{P}_{A_n}(E_n) M), \quad \boldsymbol{E} = E_1 \times \dots \times E_n \in \mathscr{B}(\mathbb{R}^n). \tag{1.4}$$

However, formula (1.4) defines a probability measure on $\mathbb{R}^n$ if and only if $\mathsf{P}_{A_1}(E_1) \dots \mathsf{P}_{A_n}(E_n)$ defines a projection-valued measure on $\mathbb{R}^n$. Since a product of orthogonal projections is an orthogonal projection only when the projection operators commute, we conclude that the operators $A_1, \dots, A_n$ should form a commutative family. This agrees with the requirement that simultaneous measurement of several observables should be independent of the order of the measurements of individual observables. We summarize these arguments as the following axiom.

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

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

where $\mathsf{P}_{\boldsymbol{A}}$ is the projection-valued measure from Proposition 1.3. Explicitly, $\mathsf{P}_{\boldsymbol{A}}(\boldsymbol{E}) = \mathsf{P}_{A_1}(E_1) \dots \mathsf{P}_{A_n}(E_n)$ for $\boldsymbol{E} = E_1 \times \dots \times E_n \in \mathscr{B}(\mathbb{R}^n)$. For every Borel subset $\boldsymbol{E} \subseteq \mathbb{R}^n$ the quantity $0 \le \mu_{\boldsymbol{A}}(\boldsymbol{E}) \le 1$ is the probability that for a quantum system in the state M the result of the simultaneous measurement of observables $A_1, \dots, A_n$ belongs to $\boldsymbol{E}$.

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

Problem 1.1. Prove property (1.2).

Problem 1.2. Prove that the state M is a pure state if and only if $\operatorname{Tr} M^2 = 1$.

Problem 1.3. Prove that the Born-von Neumann formula (1.3) defines a probability measure on $\mathbb{R}$, i.e., μ_A is a σ-additive function on $\mathscr{B}(\mathbb{R})$.

Problem 1.4. Prove all the remaining statements in this section.

1.2. Heisenberg's uncertainty relations. The variance of the observable A in the state M, which measures the mean deviation of A from its expectation value, is defined by

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

provided the expectation values $\langle A^2|M\rangle$ and $\langle A|M\rangle$ exist. It follows from Proposition 1.1 that for $M = P_\psi$, where $\psi \in D(A)$,

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

Lemma 1.2. *For $A \in \mathscr{A}$ and $M \in \mathscr{S}$ the variance $\sigma_M(A) = 0$ if and only if $\operatorname{Im} M$ is an eigenspace for the operator A with the eigenvalue $a = \langle A|M\rangle$. In particular, if $M = P_\psi$, then ψ is an eigenvector of A, $A\psi = a\psi$.*

Proof. It follows from the spectral theorem that

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

so that $\sigma_M(A) = 0$ if and only if the probability measure μ_A is supported at the point $a \in \mathbb{R}$, i.e., $\mu_A(\{a\}) = 1$. Since $\mu_A(\{a\}) = \operatorname{Tr} P_A(\{a\})M$ and $\operatorname{Tr} M = 1$, we conclude that this is equivalent to $\operatorname{Im} M$ being an invariant subspace for $P_A(\{a\})$, and it follows from the spectral theorem that $\operatorname{Im} M$ is an eigenspace for A with the eigenvalue a. □

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

Proposition 1.4 (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 $\alpha \in \mathbb{R}$,

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

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

The same argument works for the mixed states. Since

$$\sigma_M^2(A)\sigma_M^2(B) = \lim_{n\to\infty} \sigma_M^2(A_n)\sigma_M^2(B_n)$$

(see the remark in the previous section), it is sufficient to prove the inequality for bounded A and B. Then using the cyclic property of the trace we have for all $\alpha \in \mathbb{R}$,

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

so that $4 \operatorname{Tr} A^2M \operatorname{Tr} B^2M \ge \operatorname{Tr}(i[A,B]M)^2$. □

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

1.3. Dynamics. The set $\mathscr{A}$ of quantum observables does not form an algebra with respect to an operator product[11]. Nevertheless, a real vector space $\mathscr{A}_0$ of bounded observables has a Lie algebra structure with the Lie bracket

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

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

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

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

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

Specifically, the analog of Hamilton's picture in classical mechanics (see Section 2.8 in Chapter 1) is the *Heisenberg picture* in quantum mechanics, where the states do not depend on time

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

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

and bounded observables satisfy the *Heisenberg equation of motion*

$$\frac{dA}{dt} = \{H, A\}_\hbar, \quad A \in \mathscr{A}_0, \tag{1.5}$$

where

$$\{\ ,\ \}_\hbar = \frac{i}{\hbar}[\ ,\ ] \tag{1.6}$$

is the *quantum bracket* — the $\hbar$-dependent Lie bracket on $\mathscr{A}_0$. The positive number $\hbar$, called the *Planck constant*, is one of the fundamental constants in physics[12].

The Heisenberg equation (1.5) is well defined when $H \in \mathscr{A}_0$. Indeed, let $U(t)$ be a strongly continuous one-parameter group of unitary operators associated with a bounded self-adjoint operator H,

$$U(t) = e^{-\frac{i}{\hbar}tH}, \quad t \in \mathbb{R}. \tag{1.7}$$

It satisfies the differential equation

$$i\hbar\frac{dU(t)}{dt} = HU(t) = U(t)H, \tag{1.8}$$

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

$$A(t) = U(t)^{-1}AU(t). \tag{1.9}$$

In general, a strongly one-parameter group of unitary operators (1.7), associated with a self-adjoint operator H, satisfies differential equation (1.8) only on $D(H)$ in a strong sense, that is, applied to $\varphi \in D(H)$. The quantum dynamics is defined by the same formula (1.9), and in this sense all quantum observables satisfy the Heisenberg equation of motion (1.5). The *evolution operator* $U_t : \mathscr{A} \to \mathscr{A}$ is defined by $U_t(A) = A(t) = U(t)^{-1}AU(t)$, and is an automorphism of the Lie algebra $\mathscr{A}_0$ of bounded observables. This is a quantum analog of the statement that the evolution operator in classical mechanics is an automorphism of the Poisson algebra of classical observables (see Theorem 2.19 in Section 2.7 of Chapter 1).

By Stone's theorem, every strongly-continuous one-parameter group of unitary operators[13] $U(t)$ is of the form (1.7), where

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

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

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

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

We summarize the presented arguments as the following axiom.

A7 (Heisenberg's Picture). The dynamics of a quantum system is described by the strongly continuous one-parameter group $U(t)$ of unitary operators. Quantum states do not depend on time, $\mathscr{S} \ni M \mapsto M(t) = M \in \mathscr{S}$, and time dependence of quantum observables is given by the evolution operator U_t,

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

Infinitesimally, the evolution of quantum observables is described by the Heisenberg equation of motion (1.5), where the Hamiltonian operator H is the infinitesimal generator of $U(t)$.

The analog of Liouville's picture in classical mechanics (see Section 2.8 in Chapter 1) is *Schrödinger's picture* in quantum mechanics, defined as follows.

A8 (Schrödinger's Picture). The dynamics of a quantum system is described by the strongly continuous one-parameter group $U(t)$ of unitary operators. Quantum observables do not depend on time, $\mathscr{A} \ni A \mapsto A(t) = A \in \mathscr{A}$, and time dependence of states is given by the inverse of the evolution operator $U_t^{-1} = U_{-t}$,

$$\mathscr{S} \ni M \mapsto M(t) = U_{-t}(M) = U(t) M U(t)^{-1} \in \mathscr{S}. \tag{1.10}$$

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

$$\frac{dM}{dt} = -\{H, M\}_h, \quad M \in \mathscr{S}, \tag{1.11}$$

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

Proposition 1.5. *Heisenberg and Schrödinger descriptions of dynamics are equivalent.*

Proof. Let $\mu_{A(t)}$ and $(\mu_t)_A$ be, respectively, probability measures on $\mathbb{R}$ associated with $(A(t), M) \in \mathscr{A} \times \mathscr{S}$ and $(A, M(t)) \in \mathscr{A} \times \mathscr{S}$ according to **A3**-**A4**, where $A(t) = U_t(A)$ and $M(t) = U_{-t}(M)$. We need to show that $\mu_{A(t)} = (\mu_t)_A$. It follows from the spectral theorem that $\mathsf{P}_{A(t)} = U(t)^{-1} \mathsf{P}_A U(t)$, so that using the Born-von Neumann formula (1.3) and the cyclic property of the trace, we get for $E \in \mathscr{B}(\mathbb{R})$,

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

Corollary 1.3. $\langle A(t) | M \rangle = \langle A | M(t) \rangle$.

In analogy with classical mechanics (see Section 1.4 of Chapter 1), we have the following definition.

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

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

It follows from Proposition 1.2 that $A \in \mathscr{A}$ is an integral of motion if and only if it commutes with the Hamiltonian H, so that, in agreement with (1.5),

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

This is a quantum analog of the Poisson commutativity property, given by formula (2.14) in Section 2.6 of Chapter 1.

It follows from (1.11) that the time evolution of a pure state $M = P_\psi$ is given by $M(t) = P_{\psi(t)}$, where $\psi(t) = U(t)\psi$. Since $D(H)$ is invariant under $U(t)$, the vector $\psi(t) = U(t)\psi$ satisfies the *time-dependent Schrödinger equation*

$$i\hbar\frac{d\psi}{dt} = H\psi \tag{1.12}$$

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

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

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

The state M is stationary if and only if $[M, U(t)] = 0$ for all t, and by Proposition 1.2 this is equivalent to

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

in agreement with (1.11). The following simple result is fundamental.

Lemma 1.3. *The pure state $M = P_\psi$ is stationary if and only if ψ is an eigenvector for H,*

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

and in this case

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

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

In physics terminology, the eigenvectors of H are called *bound states*. The corresponding eigenvalues are called *energy levels* and are usually denoted by E. The eigenvalue equation $H\psi = E\psi$ is called the *stationary Schrödinger equation*.

Problem 1.5. Show that if an observable A is such that for every state M the expectation value $\langle A|M(t)\rangle$ does not depend on t, then A is a quantum integral of motion. (This is the definition of integrals of motion in the Schrödinger picture.)

Problem 1.6. Show that a solution of the initial value problem for the time-dependent Schrödinger equation (1.12) is given by

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

where $\mathsf{P}(\lambda)$ is the resolution of identity for the Hamiltonian H.

Problem 1.7. Let D be a linear subspace of $\mathscr{H}$, consisting of *Gårding vectors*

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

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

2. Quantization

To study the quantum system one needs to describe its Hilbert space of states $\mathscr{H}$ and the Hamiltonian H — a self-adjoint operator in $\mathscr{H}$ which defines the evolution of a system. When the quantum system has a classical analog, the procedure of constructing the corresponding Hilbert space $\mathscr{H}$ and the Hamiltonian H is called *quantization*.

Definition. Quantization of a classical system $((\mathscr{M}, \{\ ,\ \}), H_{\mathrm{c}})$ with the Hamiltonian function[14] H_{c} is a one-to-one mapping $\mathrm{Q}_\hbar : \mathcal{A} \to \mathscr{A}$ from the set of classical observables $\mathcal{A} = C^\infty(\mathscr{M})$ to the set $\mathscr{A}$ of quantum observables — the set of self-adjoint operators on a Hilbert space $\mathscr{H}$. The map $\mathrm{Q}_\hbar$ depends on the parameter $\hbar > 0$, and its restriction to the subspace of bounded classical observables $\mathcal{A}_0$ is a linear mapping to the subspace $\mathscr{A}_0$ of bounded quantum observables, which satisfies the properties

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

and

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

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

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

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

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

Quantum mechanics is different from classical mechanics, so that the correspondence $f \mapsto \mathrm{Q}_\hbar(f)$ cannot be an isomorphism between the Lie algebras of bounded classical and quantum observables with respect to classical and quantum brackets. It becomes an isomorphism only in the limit $\hbar \to 0$ when, according to the correspondence principle, quantum mechanics turns into classical mechanics. Since quantum mechanics provides a more accurate and refined description than classical mechanics, quantization of a classical system may not be unique.

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

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

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

$$\{p, q\} = 1. \tag{2.1}$$

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

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

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

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

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

Property **CR2** is called the *Heisenberg commutation relation* for one degree of freedom. In terms of the quantum bracket (1.6) it takes the form

$$\{P, Q\}_\hbar = I, \tag{2.2}$$

which is exactly the same as the Poisson bracket (2.1). Property **CR3** is a quantum analog of the classical property that the Poisson manifold $(\mathbb{R}^2, \{\ ,\ \})$ is non-degenerate: every function which Poisson commutes with p and q is a constant (see the last remark in Section 2.7 of Chapter 1).

The operators P and Q are called, respectively, the *momentum operator* and the *coordinate operator*. The correspondence $p \mapsto P$, $q \mapsto Q$ with P and Q satisfying **CR1-CR3** is the cornerstone for the quantization of classical systems. The validity of (2.2), as well as of quantum mechanics as a whole, is confirmed by the agreement of the theory with numerous experiments.

Remark. It is tempting to extend the correspondence $p \mapsto P$, $q \mapsto Q$ to all observables by defining the mapping $f(p, q) \mapsto f(P, Q)$. However, this approach to quantization is rather naive: operators P and Q satisfy (2.2) and do not commute, so that one needs to understand how $f(P, Q)$ — a "function of non-commuting variables" — is actually defined. We will address this problem of the ordering of non-commuting operators P and Q in Section 3.3.

It follows from Heisenberg's uncertainty relations (see Proposition 1.4), that for any pure state $M = P_\psi$ with $\psi \in D$,

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

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

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

$$\{p_k, p_l\} = 0, \quad \{q^k, q^l\} = 0, \quad \{p_k, q^l\} = \delta_k^l, \quad k, l = 1, \dots, n. \tag{2.3}$$

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

$$\{P_k, P_l\}_\hbar = 0, \quad \{Q^k, Q^l\}_\hbar = 0, \quad \{P_k, Q^l\}_\hbar = \delta_k^l I, \quad k, l = 1, \dots, n. \tag{2.4}$$

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

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

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

$$[e^k, c] = 0, \quad [f_k, c] = 0, \quad [e^k, f_l] = \delta_l^k c, \quad k, l = 1, \dots, n. \tag{2.5}$$

The invariant definition is the following. Let (V, ω) be a $2n$-dimensional symplectic vector space considered as an abelian Lie algebra, and let $\mathfrak{g}$ be a one-dimensional central extension of V by a Lie algebra 2-cocycle given by the bilinear form ω. This means that there is an exact sequence of vector spaces

$$0 \to \mathbb{R} \to \mathfrak{g} \to V \to 0, \tag{2.6}$$

and the Lie bracket in $\mathfrak{g}$ is defined by

$$[x, y] = \omega(\bar{x}, \bar{y})c, \tag{2.7}$$

where $\bar{x}, \bar{y}$ are the images in V of elements $x, y \in \mathfrak{g}$, and c is the image of 1 under the embedding $\mathbb{R} \hookrightarrow \mathfrak{g}$, called the central element of $\mathfrak{g}$. A choice of a symplectic basis $e^1, \dots, e^n, f_1, \dots, f_n$ for V (see Section 2.6 of Chapter 1) establishes the isomorphism $\mathfrak{g} \simeq \mathfrak{h}_n$, and relations (2.5) are obtained from the Lie bracket (2.7).

By Ado's theorem, the Heisenberg algebra $\mathfrak{h}_n$ is isomorphic to a Lie subalgebra of a matrix algebra over $\mathbb{R}$. Explicitly, it is realized as a nilpotent subalgebra of the Lie algebra $\mathfrak{gl}_{n+2}$ of $(n+2) \times (n+2)$ matrices with the elements

$$\sum_{k=1}^{n} (u^k f_k + v_k e^k) + \alpha c = \begin{pmatrix} 0 & u^1 & u^2 & \dots & u^n & \alpha \\ 0 & 0 & 0 & \cdots & 0 & v_1 \\ 0 & 0 & 0 & \cdots & 0 & v_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & v_n \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}. \tag{2.8}$$

Remark. The faithful representation $\mathfrak{h}_n \to \mathfrak{gl}_{n+2}$, given by (2.8), is clearly reducible: the subspace $V = \{\boldsymbol{x} = (x_1, \dots, x_{n+2}) \in \mathbb{R}^{n+2} : x_{n+2} = 0\}$ is an invariant subspace for $\mathfrak{h}_n$ with the central element c acting by zero. However, this representation is not decomposable: the vector space $\mathbb{R}^{n+2}$ cannot be written as a direct sum of V and a one-dimensional invariant subspace for $\mathfrak{h}_n$. This explains why the central element c is not represented by a diagonal matrix with the first $n+1$ zeros, but rather has a special form given by (2.8).

Analytically, Heisenberg commutation relations (2.5) correspond to an irreducible unitary representation of the Heisenberg Lie algebra $\mathfrak{h}_n$. Recall that a unitary representation ρ of $\mathfrak{h}_n$ in the Hilbert space $\mathscr{H}$ is the linear mapping $\rho : \mathfrak{h}_n \to i\mathscr{A}$ — the space of skew-Hermitian operators in $\mathscr{H}$ — such that all self-adjoint operators $i\rho(x)$, $x \in \mathfrak{h}_n$, have a common invariant dense linear subset $D \subset \mathscr{H}$ and satisfy

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

Formally applying Schur's lemma we say that the representation ρ is irreducible if every bounded operator which commutes with all operators $i\rho(x)$ is a multiple of the identity operator I. Then Heisenberg commutation relations (2.5) define an irreducible unitary representation ρ of the Heisenberg Lie algebra $\mathfrak{h}_n$ in the Hilbert space $\mathscr{H}$ by setting

$$\rho(f_k) = -iP_k, \quad \rho(e^k) = -iQ^k, \quad k = 1, \dots, n, \quad \rho(c) = -i\hbar I. \tag{2.9}$$

Since the operators P^k and Q_k are necessarily unbounded (see Problem 2.1), the condition

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

does not necessarily imply (see Problem 2.2) that self-adjoint operators P_k and P_l commute in the sense of the definition in Section 1.1. To avoid such "pathological" representations, we will assume that ρ is an *integrable* representation, i.e., it can be integrated (in a precise sense specified below) to an irreducible unitary representation of the *Heisenberg group* $\mathbf{H}_n$ — a connected, simply-connected Lie group with the Lie algebra $\mathfrak{h}_n$.

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

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

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

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

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

$$\exp \boldsymbol{u}X \exp \boldsymbol{v}Y = \exp(-\boldsymbol{u}\boldsymbol{v}c) \exp \boldsymbol{v}Y \exp \boldsymbol{u}X, \quad \boldsymbol{u}\boldsymbol{v} = \sum_{k=0}^{n} u^k v_k. \tag{2.10}$$

Indeed, it follows from (2.5) that $[\boldsymbol{u}X, \boldsymbol{v}Y] = -\boldsymbol{u}\boldsymbol{v}c$ is a central element, so that using the Baker-Campbell-Hausdorff formula we obtain

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

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

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

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

Then it follows from (2.10) that unitary operators $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$ satisfy commutation relations

$$U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar\boldsymbol{u}\boldsymbol{v}} V(\boldsymbol{v})U(\boldsymbol{u}), \tag{2.11}$$

called *Weyl relations*. Let $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ be, respectively, infinitesimal generators of the subgroups $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$, given by the Stone theorem,

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

Taking the second partial derivatives of Weyl relations (2.11) at the origin $\boldsymbol{u} = \boldsymbol{v} = 0$ and using the solution of Problem 1.7 in the previous section, we easily obtain the following result.

Lemma 2.1. *Let $R : \mathbf{H}_n \to \mathscr{U}(\mathscr{H})$ be an irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ in $\mathscr{H}$ such that $R(e^{\alpha c}) = e^{-i\hbar\alpha} I$, and let $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ be, respectively, infinitesimal generators of the strongly continuous n-parameter abelian subgroups $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$.*

Then formulas (2.9) *define an irreducible unitary representation* ρ *of the Heisenberg algebra* $\mathfrak{h}_n$ *in* $\mathscr{H}$.

The representation ρ in Lemma 2.1 is called the differential of a representation R, and is denoted by dR. The irreducible unitary representation ρ of $\mathfrak{h}_n$ is called *integrable* if $\rho = dR$ for some irreducible unitary representation R of $\mathbf{H}_n$.

Remark. Not every irreducible unitary representation of the Heisenberg algebra is integrable, so that Weyl relations cannot be obtained from the Heisenberg commutation relations. However, the following heuristic argument (which ignores the subtleties of dealing with unbounded operators) is commonly used in physics textbooks. Consider the case of one degree of freedom and start with

$$\{P, Q\}_\hbar = I.$$

Since the quantum bracket satisfies the Leibniz rule we have, for a "suitable" function f,

$$\{f(P), Q\}_h = f'(P).$$

In particular, choosing $f(P) = e^{-iuP} = U(u)$, we obtain

$$U(u)Q - QU(u) = \hbar u U(u) \quad \text{or} \quad U(u)QU(u)^{-1} = Q + \hbar u I.$$

This implies, for a "suitable" function g,

$$U(u)g(Q) = g(Q + \hbar u I)U(u),$$

and setting $g(Q) = e^{-ivQ} = V(v)$, we get the Weyl relation.

We will prove in Section 3.1 that all integrable irreducible unitary representations of the Heisenberg algebra $\mathfrak{h}_n$ with the same action of the central element c are unitarily equivalent. This justifies the following mathematical formulation of the Heisenberg commutation relations for n degrees of freedom.

A9 (Heisenberg's Commutation Relations). Momenta and coordinate operators $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ for a quantum particle with n degrees of freedom are defined by formulas (2.9), where ρ is an integrable irreducible unitary representation of the Heisenberg algebra $\mathfrak{h}_n$ with the property $\rho(c) = -i\hbar I$.

Problem 2.1. Prove that there are no bounded operators on the Hilbert space $\mathscr{H}$ satisfying $[A, B] = I$.

Problem 2.2. Give an example of self-adjoint operators A and B which have a common invariant dense linear subset $D \subset \mathscr{H}$ such that $AB\varphi = BA\varphi$ for all $\varphi \in D$, but e^{iA} and e^{iB} do not commute.

Problem 2.3. Prove Lemma 2.1. (*Hint:* As in Problem 1.7, let D be the linear set of Gårding vectors

$$\psi_f = \int_{\mathbb{R}^{2n}} f(\boldsymbol{u},\boldsymbol{v})U(\boldsymbol{u})V(\boldsymbol{v})\psi\, d^n\boldsymbol{u}d^n\boldsymbol{v}, \quad f \in \mathscr{S}(\mathbb{R}^{2n}),\ \psi \in \mathscr{H},$$

where $\mathscr{S}(\mathbb{R}^{2n})$ is the Schwartz space of rapidly decreasing functions on $\mathbb{R}^{2n}$.)

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

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

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

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

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

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

$$(\mathsf{P}(E)\varphi)(q) = \chi_E(q)\varphi(q), \tag{2.12}$$

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

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

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

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

Lemma 2.2. *The coordinate operator Q has an absolutely continuous spectrum $\mathbb{R}$, and every bounded operator B which commutes with Q is a function of Q, $B = f(Q)$ with $f \in L^\infty(\mathbb{R})$.*

Proof. It follows from (2.12) that $\nu_\psi(E) = \int_E |\psi(q)|^2 dq$, which proves the first statement. Now a bounded operator B on $\mathscr{H}$ commutes with Q if and only if $B\mathsf{P}(E) = \mathsf{P}(E)B$ for all $E \in \mathscr{B}(\mathbb{R})$, and using (2.12) we get

$$B(\chi_E\varphi) = \chi_E B(\varphi). \tag{2.13}$$

Choosing in (2.13) $E = E_1$ and $\varphi = \chi_{E_2}$, where E_1 and E_2 have finite Lebesgue measure, we obtain

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

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

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

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

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

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

Remark. By the Schwartz kernel theorem, the operator B can be represented by an integral operator with a distributional kernel $K(q, q')$. Then the commutativity $BQ = QB$ implies that, in the distributional sense,

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

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

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

with some $f \in L^\infty(\mathbb{R})$. This argument is usually given in the physics textbooks.

Remark. The operator Q has no eigenvectors — the eigenvalue equation

$$Q\varphi = \lambda\,\varphi$$

has no solutions in $L^2(\mathbb{R})$. However, in the distributional sense, this equation for every $\lambda \in \mathbb{R}$ has a unique (up to a constant factor) solution $\varphi_\lambda(q) = \delta(q - \lambda)$, and these "generalized eigenfunctions", also called eigenfunctions of the continuous spectrum, combine to a Schwarz kernel of the identity operator I on $L^2(\mathbb{R})$. This reflects the fact that operator Q is diagonal in the coordinate representation.

Remark. Normalization of the eigenfunctions of the continuous spectrum $\varphi_\lambda(q)$ can be also determined by the condition that for every $\lambda \in \mathbb{R}$ the function

$$\Phi_\lambda(q) = \int_{\lambda_0}^{\lambda} \varphi_\mu(q)d\mu, \quad \Phi_\lambda \in L^2(\mathbb{R}),$$

satisfies

$$\lim_{\Delta\to 0} \frac{1}{\Delta} \|\Phi_{\lambda+\Delta} - \Phi_\lambda\|^2 = 1. \tag{2.14}$$

Here $\lambda_0 \in \mathbb{R}$ is fixed and does not enter (2.14). Indeed, in our case $\Phi_\lambda = \chi_{(\lambda_0,\lambda)}$ — the characteristic function of the interval (λ_0, λ) — so that $\|\Phi_{\lambda+\Delta} - \Phi_\lambda\|^2 = \Delta$.

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

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

Physically, this is interpreted that in the state P_ψ with the "wave function" $\psi(q)$, the probability of finding a quantum particle between q and $q + dq$ is $|\psi(q)|^2 dq$. In other words, the modulus square of a wave function is the probability distribution for the coordinate of a quantum particle.

The corresponding momentum operator P is given by a differential operator

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

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

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

Remark. The operator P on $\mathscr{H}$ has no eigenvectors — the eigenvalue equation

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

has a solution

$$\varphi(q) = \text{const} \times e^{\frac{i}{\hbar}pq}$$

which does not belong to $L^2(\mathbb{R})$. We will see later that the family of normalized eigenfunctions of the continuous spectrum

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

combines to a Schwartz kernel of the inverse $\hbar$-dependent Fourier transform operator, which diagonalizes the momentum operator P. In the distributional sense,

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

Remark. As for the case of the coordinate operator, the normalization of the eigenfunctions of the continuous spectrum $\varphi_p(q)$ of the momentum operator can be determined from the condition (2.14). Indeed,

$$\Phi_p(q) = \int_{p_0}^{p} ce^{\frac{i}{\hbar}kq}dk = \frac{c\hbar}{iq}\left(e^{\frac{i}{\hbar}pq} - e^{\frac{i}{\hbar}p_0 q}\right),$$

so that

$$\Phi_{p+\Delta}(q) - \Phi_p(q) = \frac{2c\hbar}{q} e^{\frac{i}{\hbar}(p+\frac{1}{2}\Delta)q} \sin\frac{\Delta q}{2\hbar}.$$

Using the elementary integral, we obtain

$$\frac{1}{\Delta}\|\Phi_{p+\Delta}(q) - \Phi_p(q)\|^2 = 2c^2\hbar \int_{-\infty}^{\infty} \frac{\sin^2 q}{q^2}\, dq = 2\pi c^2\hbar,$$

so that $c = \frac{1}{\sqrt{2\pi\hbar}}$.

Proposition 2.1. *The coordinate representation defines an irreducible, unitary, integrable representation of the Heisenberg algebra.*

Proof. To show that the coordinate representation is integrable, let $U(u) = e^{-iuP}$ and $V(v) = e^{-ivQ}$ be the corresponding one-parameter groups of unitary operators. Clearly, $(V(v)\varphi)\psi(q) = e^{-ivq}\varphi(q)$ and it easily follows from the Stone theorem (or by the definition of a derivative) that $(U(u)\varphi)(q) = \varphi(q - \hbar u)$, so that unitary operators $U(u)$ and $V(v)$ satisfy the Weyl relation (2.11). Such a realization of the Weyl relation is called the *Schrödinger representation.*

To prove that the coordinate representation is irreducible, let B be a bounded operator commuting with P and Q. By Lemma 2.2, $T = f(Q)$ for some $f \in L^\infty(\mathbb{R})$. Now commutativity between T and P implies that

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

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

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

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

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

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

and satisfy the Heisenberg commutation relation. As the coordinate representation, the momentum representation is an irreducible, unitary, integrable representation of the Heisenberg algebra. In the momentum representation, the modulus square of the wave function $\psi(p)$ of a pure state $M = P_\psi$,

$\|\psi\| = 1$, is the probability distribution for the momentum of the quantum particle, i.e., the probability that a quantum particle has momentum between p and $p + dp$ is $|\psi(p)|^2 dp$.

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

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

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

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

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

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

and

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

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

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

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

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

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

where $E \in \mathscr{B}(\mathbb{R})$ and $\lambda_k : \mathbb{R}^n \to \mathbb{R}$ is a canonical projection onto the k-th component, $k = 1, \dots, n$. Correspondingly, the projection-valued measure P for the commutative family $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ (see Proposition 1.3) is defined on the Borel subsets $\boldsymbol{E} \subseteq \mathbb{R}^n$ by

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

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

Coordinate operators $Q^1, \dots, Q^n$ form a *complete system of commuting observables*. This means, by definition, that none of these operators is a function of the other operators, and that every bounded operator commuting with $Q^1, \dots, Q^n$ is a function of $Q^1, \dots, Q^n$, i.e., is a multiplication by $f(\boldsymbol{q})$

operator for some $f \in L^\infty(\mathbb{R}^n)$. The proof repeats verbatim the proof of Lemma 2.2. For a pure state $M = P_\psi$, $\|\psi\| = 1$, the modulus square $|\psi(\boldsymbol{q})|^2$ of the wave function is the density of a joint distribution function $\mu_{\boldsymbol{Q}}$ for the commutative family $\boldsymbol{Q}$, i.e., the probability of finding a quantum particle in a Borel subset $\boldsymbol{E} \subseteq \mathbb{R}^n$ is given by

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

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

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

and satisfy Weyl relations (2.11). The same argument as in the proof of Proposition 2.1 shows that this representation of the Heisenberg group $\mathbf{H}_n$, called the *Schrödinger representation for n degrees of freedom*, is irreducible.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

as well as $\langle \boldsymbol{q}|\boldsymbol{q}'\rangle = \delta(\boldsymbol{q}-\boldsymbol{q}')$, $\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}')$. Though in our exposition we are not using Dirac's notation, these formulas would help the interested reader "translate" the notation used in physics textbooks to standard mathematics notation.

Remark. We will show in Section 3.2 that every Lagrangian subspace of the symplectic vector space $\mathbb{R}^{2n}$ with the canonical symplectic form $\omega = d\boldsymbol{p}\wedge d\boldsymbol{q}$ gives rise to an integrable, unitary, irreducible representation of the Heisenberg algebra $\mathfrak{h}_n$. This is the simplest example of the *real polarization*, which for a given symplectic manifold $(\mathscr{M},\omega)$ is defined as an integrable distribution $\{\mathscr{L}_x\}_{x\in\mathscr{M}}$ of Lagrangian subspaces $\mathscr{L}_x$ of tangent spaces $T_x\mathscr{M}$. The notion of a polarization plays a fundamental role in *geometric quantization*: it allows us to construct (under certain conditions) the Hilbert space of states $\mathscr{H}$ associated with the classical phase space $(\mathscr{M},\omega)$. In the linear case $\mathscr{M} = \mathbb{R}^{2n}$ every Lagrangian subspace $\mathscr{L}$ in $\mathbb{R}^{2n}$ gives rise to a real polarization by using the identification $T_x\mathbb{R}^{2n} \simeq \mathbb{R}^{2n}$. In particular, for the coordinate representation, $\mathscr{L}$ is given by the equation $\boldsymbol{q} = 0$, and for the momentum representation — by the equation $\boldsymbol{p} = 0$. The corresponding Hilbert $\mathscr{H}$ space consists of functions on $\mathbb{R}^{2n}$ which are constant along the fibers of the polarization.

Problem 2.4. Give an example of a non-integrable representation of the Heisenberg algebra.

Problem 2.5. Prove that there exists $\varphi \in \mathscr{H} = L^2(\mathbb{R}, dq)$ such that the vectors $\mathsf{P}(E)\varphi$, $E \in \mathscr{B}(\mathbb{R})$, where P is a projection-valued measure for the coordinate operator Q, are dense in $\mathscr{H}$.

Problem 2.6. Find the generating operator for the commutative family $\boldsymbol{Q} = (Q^1,\dots,Q^n)$. Does it have a physical interpretation?

Problem 2.7. Find the projection-valued measure for the commutative family $\boldsymbol{P} = (P_1,\dots,P_n)$ in the coordinate representation.

2.3. Free quantum particle. A free classical particle with one degree of freedom is described by the phase space $\mathbb{R}^2$ with coordinates p, q and the Poisson bracket (2.1), and by the Hamiltonian function

$$H_{\rm c}(p,q) = \frac{p^2}{2m}. \tag{2.15}$$

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

$$H_0 = \frac{P^2}{2m},$$

and in coordinate representation is given by

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

It is a self-adjoint operator on $\mathscr{H} = L^2(\mathbb{R}, dq)$ with $D(H_0) = W^{2,2}(\mathbb{R})$ — the Sobolev space of functions in $L^2(\mathbb{R})$, whose generalized first and second derivatives are in $L^2(\mathbb{R})$.

The operator H_0 is positive with absolutely continuous spectrum $[0,\infty)$ of multiplicity two. Indeed, let $\mathfrak{H}_0 = L^2(\mathbb{R}_{>0}, \mathbb{C}^2; d\sigma)$ be the Hilbert space of $\mathbb{C}^2$-valued measurable functions Ψ on the semi-line $\mathbb{R}_{>0} = (0,\infty)$, which are square-integrable with respect to the measure $d\sigma(\lambda) = \sqrt{\frac{m}{2\lambda}}\, d\lambda$,

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

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

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

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

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

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

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

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

In the distributional sense, these eigenfunctions of the continuous spectrum combine to a Schwartz kernel of the unitary operator $\mathscr{U}_0$, which establishes

the isomorphism between $\mathscr{H} = L^2(\mathbb{R}, dq)$ and the Hilbert space $\mathfrak{H}_0$, where H_0 acts as a multiplication by λ operator. The normalization of the eigenfunctions of the continuous spectrum is also determined by the condition (2.14):

$$\lim_{\Delta\to 0}\frac{1}{\Delta}\left\|\Psi^{(\pm)}_{k+\Delta}-\Psi^{(\pm)}_{k}\right\|^2=1,\quad \lim_{\Delta\to 0}\frac{1}{\Delta}\left(\Psi^{(+)}_{k+\Delta}-\Psi^{(+)}_{k},\Psi^{(-)}_{k+\Delta}-\Psi^{(-)}_{k}\right)=0,$$

where $\Psi^{(\pm)}_k(q)=\int_{k_0}^{k}\psi^{(\pm)}_p(q)dp$.

The Cauchy problem for the Schrödinger equation for a free particle,

$$i\hbar\frac{d\psi(t)}{dt}=H_0\psi(t),\quad \psi(0)=\psi, \tag{2.16}$$

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

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

so that

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

In the coordinate representation, the solution of (2.16) is given by

$$\psi(q,t)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}pq}\hat\psi(p,t)dp=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}\chi(p,q,t)t}\hat\psi(p)dp, \tag{2.17}$$

where

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

Formula (2.17) describes the motion of a quantum particle, and admits the following physical interpretation. Let initial condition ψ in (2.16) be such that its Fourier transform $\hat\psi=\mathcal{F}_\hbar(\psi)$ is a smooth function supported in a neighborhood U_0 of $p_0\in\mathbb{R}\setminus\{0\}$, $0\notin U_0$, and

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

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

$$\lim_{|t|\to\infty}\int_E|\psi(q,t)|^2dq=0. \tag{2.18}$$

Since

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

for all t, it follows from (2.18) that the particle leaves every compact subset of $\mathbb{R}$ as $|t|\to\infty$ and the quantum motion is infinite. To prove (2.18), observe that the function $\chi(p,q,t)$ — the "phase" in integral representation (2.17)

— has the property that $|\frac{\partial\chi}{\partial p}| > C > 0$ for all $p \in U_0$, $q \in E$ and large enough $|t|$. Integrating by parts we get

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

so that uniformly on E,

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

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

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

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

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

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

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

as $N \to \infty$.

Applying the stationary phase method to the integral representation (2.17) (and setting $N = t$), we find that the critical point of $\chi(p,q,t)$ is $p_0 = \frac{mq}{t}$ with $\chi''(p_0) = -\frac{1}{m} \neq 0$, and

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

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

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

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

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

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

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

A free classical particle with n degrees of freedom is described by the phase space $\mathbb{R}^{2n}$ with coordinates $\boldsymbol{p} = (p_1, \dots, p_n)$ and $\boldsymbol{q} = (q^1, \dots, q^n)$, the Poisson bracket (2.3), and the Hamiltonian function

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

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

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

and in the coordinate representation is

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

where

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

is the Laplace operator[15] in the Cartesian coordinates on $\mathbb{R}^n$. The Hamiltonian H_0 is a self-adjoint operator on $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ with $D(H_0) = W^{2,2}(\mathbb{R}^n)$ — the Sobolev space on $\mathbb{R}^n$. In the momentum representation,

$$H_0 = \frac{\boldsymbol{p}^2}{2m}$$

— a multiplication by a function operator on $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{p})$.

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

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

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

Let $\mathfrak{H}_0^{(n)} = L^2(\mathbb{R}_{>0}, \mathfrak{h}; d\sigma_n)$ be the Hilbert space of $\mathfrak{h}$-valued measurable functions[16] Ψ on $\mathbb{R}_{>0} = (0, \infty)$, square-integrable on $\mathbb{R}_{>0}$ with respect to the measure $d\sigma_n(\lambda) = (2m\lambda)^{\frac{n}{2}} \frac{d\lambda}{2\lambda}$,

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

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

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

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

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

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

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

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

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

As in the case $n = 1$, the Schrödinger equation for free particle,

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

is solved by the Fourier transform

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

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

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

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

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

Problem 2.8. Find the asymptotic wave function for a free quantum particle with n degrees of freedom.

2.4. Examples of quantum systems. Here we describe quantum systems that correspond to the classical Lagrangian systems introduced in Section 1.3 of Chapter 1. In Hamiltonian formulation, the phase space of these systems, except for the last example, is a symplectic vector space $\mathbb{R}^{2n}$ with canonical coordinates $\boldsymbol{p}, \boldsymbol{q}$ and symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$.

Example 2.1 (Newtonian particle)**.** According to Section 1.7 in Chapter 1, a classical particle in $\mathbb{R}^n$ moving in a potential field $V(\boldsymbol{q})$ is described by the Hamiltonian function

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

Assume that the Hamiltonian operator for the quantum system is given by

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

with some operator V, so that coordinate and momenta operators satisfy Heisenberg equations of motion

$$\dot{\boldsymbol{P}} = \{H, \boldsymbol{P}\}_\hbar, \ \dot{\boldsymbol{Q}} = \{H, \boldsymbol{Q}\}_\hbar. \tag{2.19}$$

To determine V, we require that the classical relation $\dot{\boldsymbol{q}} = \dfrac{\boldsymbol{p}}{m}$ between the velocity and the momentum of a particle is preserved under the quantization, i.e.,

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

Since $\{\boldsymbol{P}^2, \boldsymbol{Q}\}_\hbar = 2\boldsymbol{P}$, it follows from (2.19) that this condition is equivalent to

$$[V, Q_k] = 0, \quad k = 1, \dots, n.$$

It follows from Section 2.2 that V is a function of commuting operators $Q_1, \dots, Q_n$, and the natural choice[17] is $V = V(\boldsymbol{Q})$. Thus the Hamiltonian operator of a Newtonian particle is

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

[17]Confirmed by the agreement of the theory with the experiments.

in agreement with $H = H_{\mathrm{c}}(\boldsymbol{P}, \boldsymbol{Q})$[18]. In coordinate representation the Hamiltonian is the *Schrödinger operator*

$$H = -\frac{\hbar^2}{2m}\Delta + V(\boldsymbol{q}) \tag{2.20}$$

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

Remark. The sum of two unbounded, self-adjoint operators is not necessarily self-adjoint, and one needs to describe admissible potentials $V(\boldsymbol{q})$ for which H is a self-adjoint operator on $L^2(\mathbb{R}^n, d^n\boldsymbol{q})$. If the potential $V(\boldsymbol{q})$ is a real-valued, locally integrable function on $\mathbb{R}^n$, then the differential operator (2.20) defines a symmetric operator H with the domain $C_0^2(\mathbb{R}^n)$ — twice continuously differentiable functions on $\mathbb{R}^n$ with compact support. Potentials for which the symmetric operator H has no self-adjoint extensions are obviously non-physical. It may also happen that H has several self-adjoint extensions[19]. These extensions are specified by some boundary conditions at infinity and there are no physical principles distinguishing between them. The only physical case is when the symmetric operator H admits a unique self-adjoint extension, that is, when H is essentially self-adjoint. In Chapter 3 we present necessary conditions for the essential self-adjointness. Here we only mention the von Neumann criterion that if A is a closed operator and $\overline{D(A)} = \mathscr{H}$, then $H = A^*A$ is a positive self-adjoint operator.

Example 2.2 (Interacting quantum particles)**.** In Lagrangian formalism, a closed classical system of N interacting particles on $\mathbb{R}^3$ was described in Example 1.2 in Section 1.3 of Chapter 1. In Hamiltonian formalism, it is described by the canonical coordinates $\boldsymbol{r} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$, the canonical momenta $\boldsymbol{p} = (\boldsymbol{p}_1, \ldots, \boldsymbol{p}_N)$, $\boldsymbol{r}_a, \boldsymbol{p}_a \in \mathbb{R}^3$, and by the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{r}) = \sum_{a=1}^{N} \frac{\boldsymbol{p}_a^2}{2m_a} + V(\boldsymbol{r}), \tag{2.21}$$

where m_a is the mass of the a-th particle, $a = 1, \ldots, N$ (see Section 1.7 in Chapter 1). The corresponding Hamiltonian operator H in the coordinate representation has the form

$$H = -\sum_{a=1}^{N} \frac{\hbar^2}{2m_a}\Delta_a + V(\boldsymbol{r}). \tag{2.22}$$

In particular, when

$$V(\boldsymbol{r}) = \sum_{1 \le a < b \le N} V(\boldsymbol{r}_a - \boldsymbol{r}_b),$$

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

[19] This is the case when the defect indices of H are equal and are non-zero.

the Schrödinger operator (2.22) describes the N-body problem in quantum mechanics. The fundamental quantum system is the complex atom, formed by a nucleus of charge Ne and mass M, and by N electrons of charge $-e$ and mass m. Denoting by $\boldsymbol{R} \in \mathbb{R}^3$ the position of the nucleus, and by $\boldsymbol{r}_1, \dots, \boldsymbol{r}_N$ the positions of the electrons and assuming that the interaction is given by the Coulomb attraction, we get for the Hamiltonian function (2.21)

$$H_{\mathrm{c}}(\boldsymbol{P}, \boldsymbol{p}, \boldsymbol{R}, \boldsymbol{r}) = \frac{\boldsymbol{P}^2}{2M} + \sum_{a=1}^{N} \frac{\boldsymbol{p}_a^2}{2m} - \sum_{a=1}^{N} \frac{Ne^2}{|\boldsymbol{R} - \boldsymbol{r}_a|} + \sum_{1 \le a < b \le N} \frac{e^2}{|\boldsymbol{r}_a - \boldsymbol{r}_b|},$$

where $\boldsymbol{P}$ is the canonical momentum of the nucleus. The corresponding Schrödinger operator H in the coordinate representation has the form[20]

$$H = -\frac{\hbar^2}{2M}\Delta - \sum_{a=1}^{N} \frac{\hbar^2}{2m}\Delta_a - \sum_{a=1}^{N} \frac{Ne^2}{|\boldsymbol{R} - \boldsymbol{r}_a|} + \sum_{1 \le a < b \le N} \frac{e^2}{|\boldsymbol{r}_a - \boldsymbol{r}_b|}.$$

In the simplest case of the hydrogen atom, when $N = 1$ and the nucleus consists of a single proton[21], the Hamiltonian is

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

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

$$H = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|\boldsymbol{r}|}. \tag{2.23}$$

We will solve the Schrödinger equation with this Hamiltonian H and determine its energy levels in Section 5.1 of Chapter 3.

Example 2.3 (Charged particle in an electromagnetic field)**.** A classical particle of charge e and mass m moving in the time-independent electromagnetic field with scalar and vector potentials $\varphi(\boldsymbol{r})$ and $\boldsymbol{A}(\boldsymbol{r})$, $\boldsymbol{r} \in \mathbb{R}^3$, is described by the Hamiltonian function

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

(see Problem 1.27 in Section 1.7 of Chapter 1). The corresponding classical velocity vector $\boldsymbol{v} = \{H_{\mathrm{c}}, \boldsymbol{r}\}$ is given by

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

[20] Ignoring the fact that electron has spin, see Chapter **??**.

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

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

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

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

The Hamiltonian operator of a quantum particle is

$$H = \frac{1}{2m} \left(\boldsymbol{P} - \frac{e}{c} \boldsymbol{A} \right)^2 + e\varphi(\boldsymbol{r}) \tag{2.24}$$

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

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

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

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

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

Example 2.4 (Free quantum particle on a Riemannian manifold)**.** The phase space of a classical particle of mass $m = 1$ moving on a Riemannian manifold (M, g) is the cotangent bundle T^*M, and the corresponding Hamiltonian function is given by

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{x}) = \tfrac{1}{2} g^{\mu\nu}(\boldsymbol{x}) p_\mu p_\nu,$$

where $g^{\mu\nu}(\boldsymbol{x})$ is the inverse of the metric tensor $g_{\mu\nu}(\boldsymbol{x})$, and

$$(\boldsymbol{p}, \boldsymbol{x}) = (p_1, \ldots, p_n, x^1, \ldots, x^n)$$

are standard coordinates on T^*M (see Section 1.7 of Chapter 1). The Hilbert space of the quantum system is $\mathscr{H} = L^2(M, d\mu)$, where $d\mu = \sqrt{g(\boldsymbol{x})} d^n \boldsymbol{x}$, $g(\boldsymbol{x}) = \det(g_{\mu\nu}(\boldsymbol{x}))$, is the measure associated with the density of the Riemannian metric (Riemannian volume form if M is oriented). When canonical coordinates $(\boldsymbol{p}, \boldsymbol{x})$ are only locally defined on T^*M, it is not possible to construct corresponding operators $\boldsymbol{P}$ and $\boldsymbol{Q}$. Still, one can always define the Hamiltonian operator by

$$H = \frac{\hbar^2}{2} \Delta_g, \quad \text{where} \quad \Delta_g = -\frac{1}{\sqrt{g(\boldsymbol{x})}} \frac{\partial}{\partial x^\mu} \left(\sqrt{g(\boldsymbol{x})}\, g^{\mu\nu} \frac{\partial}{\partial x^\nu} \right) \tag{2.25}$$

is the Laplace-Beltrami operator of the Riemannian metric g on M. Note that in this case there is a non-trivial problem of the ordering of non-commuting operators in the quantization of $H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{x})$, which arises if in a

coordinate chart on M one replaces canonical coordinates $\boldsymbol{p}$ and $\boldsymbol{x}$ by $\boldsymbol{P}$ and $\boldsymbol{Q}$. The formula

$$\Delta_g = -g^{\mu\nu}(\boldsymbol{x})\frac{\partial^2}{\partial x^\mu \partial x^\nu} + g^{\mu\sigma}(\boldsymbol{x})\Gamma^\nu_{\mu\sigma}(\boldsymbol{x})\frac{\partial}{\partial x^\nu}$$

shows that local expressions defined by

$$H_{\rm c}(\boldsymbol{P},\boldsymbol{Q}) = \tfrac{1}{2}\big(g^{\mu\nu}(\boldsymbol{Q})P_\mu P_\nu + i\hbar g^{\mu\sigma}(\boldsymbol{Q})\Gamma^\nu_{\mu\sigma}(\boldsymbol{Q})P_\nu\big) \tag{2.26}$$

combine to a well-defined self-adjoint operator H on $\mathscr{H}$ given by (2.25). Thus even when $M = \mathbb{R}^n$ and canonical coordinates $(\boldsymbol{p},\boldsymbol{x})$ are globally defined on $T^*\mathbb{R}^n$, the correct formula for $H_{\rm c}(\boldsymbol{P},\boldsymbol{Q})$ — the one which extends to general Riemannian manifolds — is given by (2.26), where the second term represents the "quantum correction" to the naive expression $g^{\mu\nu}(\boldsymbol{Q})P_\mu P_\nu$.

2.5. Old quantum mechanics. The formulation of quantum mechanics presented here goes back to 1925-1927, and is due to Heisenberg, Schrödinger, Born, Jordan, and Dirac. It replaced the old quantum theory, proposed in 1913 by Bohr, which was based on Rutherford's planetary model of the atom. In the old theory, the energy levels of a one-dimensional quantum system correspond to the closed orbits of the associated classical Hamiltonian system which satisfy the *Bohr-Wilson-Sommerfeld quantization rule* (BWS rule)

$$\oint p\,dq = 2\pi\hbar(n+\tfrac{1}{2}),$$

where n is a non-negative integer, and integration goes over the closed orbit in the phase space $\mathbb{R}^2$. Bohr-Wilson-Sommerfeld quantization rules also apply to completely integrable Hamiltonian systems with several degrees of freedom (see Section 2.6 of Chapter 1). Namely, let $F_1 = H_{\rm c}, \dots, F_N$ be N independent integrals of motion in involution. The BWS quantization rules are

$$\oint_\gamma \boldsymbol{p}\,d\boldsymbol{q} = 2\pi\hbar(n_\gamma + \tfrac{1}{4}\operatorname{ind}\gamma),$$

where integration goes over all 1-cycles γ in the Lagrangian submanifold $\Lambda = \{(\boldsymbol{p},\boldsymbol{q}) \in \mathbb{R}^{2N} : H_{\rm c}(\boldsymbol{p},\boldsymbol{q}) = E, F_2(\boldsymbol{p},\boldsymbol{q}) = E_2, \dots, F_N(\boldsymbol{p},\boldsymbol{q}) = E_N\}$, and $\operatorname{ind}\gamma \in \mathbb{Z}$ is the so-called *Maslov index* of a cycle γ in Λ. In the one-dimensional case the closed orbit is topologically a circle and its Maslov index is 2. It will be shown in Section 6.3 of Chapter 3 that, in general, Bohr-Wilson-Sommerfeld quantization rules only give asymptotics of the energy levels as $\hbar \to 0$. However, for integrable systems with extra symmetry, such as the harmonic oscillator and the Kepler problem, the BWS quantization rules determine the energy levels exactly. We will show this in the next section for the harmonic oscillator, and in Section 5.1 of Chapter 3 — for the Kepler problem.

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

$$H_{\mathrm{c}}(p,q) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} \tag{2.27}$$

(see Sections 1.5 and 1.7 in Chapter 1). Hamilton's equations

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

with the initial conditions p_0, q_0 are readily solved,

$$p(t) = p_0 \cos\omega t - m\omega q_0 \sin\omega t, \tag{2.28}$$

$$q(t) = q_0 \cos\omega t + \frac{1}{m\omega} p_0 \sin\omega t, \tag{2.29}$$

and describe the harmonic motion. As in Section 2.6 of Chapter 1, it is convenient to introduce complex coordinates on the phase space on $\mathbb{R}^2 \simeq \mathbb{C}$,

$$z = \frac{1}{\sqrt{2\omega}} \left(\omega q + ip\right), \quad \bar{z} = \frac{1}{\sqrt{2\omega}} \left(\omega q - ip\right). \tag{2.30}$$

We have

$$\{z, \bar{z}\} = \frac{i}{m}, \quad H_{\mathrm{c}}(z,\bar{z}) = m\omega|z|^2, \tag{2.31}$$

so that Hamilton's equations decouple,

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

and are trivially solved,

$$z(t) = e^{-i\omega t} z_0, \quad \bar{z} = e^{i\omega t}\bar{z}_0. \tag{2.32}$$

Here

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

For the quantum system, the corresponding Hamiltonian operator is

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

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

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

The quantum harmonic oscillator is the simplest non-trivial quantum system, besides the free particle, whose Schrödinger equation can be solved explicitly. It appears in all problems involving quantized oscillations, namely in molecular and crystalline vibrations. The exact solution of the harmonic

oscillator, described below, has remarkable[22] algebraic and analytic properties.

Temporarily set $m = 1$ and consider the operators

$$a = \frac{1}{\sqrt{2\omega\hbar}}\left(\omega Q + iP\right), \quad a^* = \frac{1}{\sqrt{2\omega\hbar}}\left(\omega Q - iP\right), \tag{2.33}$$

which are quantum analogs of complex coordinates (2.30). The operators a and a^* are defined on $W^{1,2}(\mathbb{R}) \cap \widehat{W}^{1,2}(\mathbb{R})$, where $\widehat{W}^{1,2}(\mathbb{R}) = \mathscr{F}(W^{1,2}(\mathbb{R}))$, and it is easy to show that a^* is the adjoint operator to a and $a^{**} = a$, so that a is a closed operator. From the Heisenberg commutation relation (2.2) we get the *canonical commutation relation*

$$[a, a^*] = I \tag{2.34}$$

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

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

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 (2.34) holds on $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$, where $\widehat{W}^{2,2}(\mathbb{R}) = \mathscr{F}(W^{2,2}(\mathbb{R}))$, and

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

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

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

$$[N, a] = -a, \quad [N, a^*] = a^*, \quad [a, a^*] = I. \tag{2.35}$$

These commutation relations correspond to the irreducible unitary representation of a four-dimensional solvable Lie algebra $\tilde{\mathfrak{h}}$ associated with the Heisenberg algebra $\mathfrak{h} = \mathfrak{h}_1$, introduced in Section 2.1. Namely, $\tilde{\mathfrak{h}}$ is a Lie algebra with the generators e, f, h, and c, where e, f, c satisfy the relations of the Heisenberg algebra $\mathfrak{h}$, and

$$[h, e] = -f, \quad [h, f] = \omega^2 e, \quad [h, c] = 0.$$

The irreducible integrable representation ρ of the Heisenberg algebra $\mathfrak{h}$ (see (2.9) in Section 2.1) extends to a unitary representation of the Lie algebra

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

$\tilde{\mathfrak{h}}$ by setting

$$\rho(h) = -i\omega N = \frac{P^2 + \omega^2 Q^2}{2i\hbar} + \frac{i\omega}{2} I.$$

Remark. In invariant terms, the Lie algebra $\tilde{\mathfrak{h}}$ is a one-dimensional right extension of the Heisenberg algebra $\mathfrak{h}$,

$$0 \to \mathfrak{h} \to \tilde{\mathfrak{h}} \to \mathbb{R} \to 0.$$

It is defined by the $\mathfrak{h}$-valued Lie algebra 1-cocycle $r \in Z^1(\mathfrak{h}, \mathfrak{h})$ — a derivation of $\mathfrak{h}$, given on generators by

$$r(e) = f, \quad r(f) = -\omega^2 e, \quad r(c) = 0.$$

Explicitly, if $h \in \tilde{\mathfrak{h}}$ is such that $\bar{h} = 1 \in \mathbb{R}$ under the projection $\tilde{\mathfrak{h}} \to \mathbb{R}$, then identifying elements in $\mathfrak{h}$ with their images under the embedding $\mathfrak{h} \hookrightarrow \tilde{\mathfrak{h}}$, we have

$$[x + \alpha h, y + \beta h] = [x, y] - \alpha r(y) + \beta r(y), \quad x, y \in \mathfrak{h}.$$

It is due to this Lie-algebraic structure of commutation relations (2.35) that Heisenberg equations of motion for the harmonic oscillator can be solved exactly. Namely, we have

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

so that

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

Comparing with (2.32) we see that solutions of classical and quantum equations of motion for the harmonic oscillator have the same form!

Next, using commutation relations (2.35) and positivity of the operator N, we will solve the eigenvalue problem for the Hamiltonian H of the harmonic oscillator explicitly by finding its energy levels and corresponding eigenvectors. We will prove that the eigenvectors form a complete system of vectors in $\mathscr{H}$, so that the spectrum of the Hamiltonian H is the point spectrum. This is a quantum mechanical analog of the fact that classical motion of the harmonic oscillator is always finite.

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

Proposition 2.2. *Suppose that there exists a non-zero $\psi \in D(a^n) \cap D((a^*)^n)$, $n = 1, 2, \ldots$, such that*

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

Then the following statements hold.

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

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

(ii) *The vectors*

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

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

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

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

Proof. Rewriting commutation relations (2.35) as

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

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

$$Na^n\psi = (\mu - n)a^n\psi \quad \text{and} \quad N(a^*)^n\psi = (\mu + n)(a^*)^n\psi. \tag{2.36}$$

Since $N \geq 0$ on $D(N)$, it follows from the first equation in (2.36) that there exists $n_0 \geq 0$ such that $a^{n_0}\psi \neq 0$ but $a^{n_0+1}\psi = 0$. Setting $\psi_0 = \dfrac{a^{n_0}\psi}{\|a^{n_0}\psi\|} \in \mathscr{H}$ we get

$$a\psi_0 = 0 \quad \text{and} \quad N\psi_0 = 0. \tag{2.37}$$

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

$$[a, (a^*)^n] = n(a^*)^{n-1}, \tag{2.38}$$

which follow from (2.34) and the Leibniz rule. Using (2.37)-(2.38), we get

$$a^*\psi_n = \sqrt{n+1}\,\psi_{n+1}, \quad a\psi_n = \sqrt{n}\,\psi_{n-1}, \tag{2.39}$$

so that

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

From the second equation in (2.36) it follows that $N\psi_n = n\psi_n$, so ψ_n are normalized eigenvectors of H with the eigenvalues $\hbar\omega(n + \frac{1}{2})$. The eigenvectors ψ_n are orthogonal since the corresponding eigenvalues are distinct and the operator H is symmetric. Finally, part (iii) immediately follows from the fact that, according to part (ii), the subspaces $\operatorname{Im}(H \pm iI)|_{\mathscr{H}_0}$ are dense in $\mathscr{H}_0$, which is the criterion of essential self-adjointness. □

Remark. Since the coordinate representation of the Heisenberg commutation relations is irreducible, it is tempting to conclude, using Proposition 2.2, that $\mathscr{H}_0 = \mathscr{H}$. Namely, it follows from the construction that the linear span of vectors ψ_n — a dense subspace of $\mathscr{H}_0$ — is invariant for the operators P and Q. However, this does not immediately imply that the projection

operator Π_0 onto the subspace $\mathscr{H}_0$ commutes with self-adjoint operators P and Q in the sense of the definition in Section 1.1.

Using the coordinate representation, we can immediately show the existence of the vector ψ_0 in Proposition 2.2, and prove that $\mathscr{H}_0 = \mathscr{H}$. Indeed, equation $a\psi_0 = 0$ becomes a first order linear differential equation

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

so that

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

and

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

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

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

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

Lemma 2.3. *The functions $q^n e^{-q^2}$, $n = 0, 1, 2, \ldots$, are complete in $L^2(\mathbb{R}, dq)$.*

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

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

The integral

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

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

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

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

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

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

Namely, using the identity

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

we obtain

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

We summarize the obtained results as follows.

Theorem 2.1. *The Hamiltonian*

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

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

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

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

$$\psi_n(q) = \sqrt[4]{\frac{m\omega}{\pi\hbar}} \frac{1}{\sqrt{2^n n!}} e^{-\frac{m\omega}{2\hbar} q^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, q\right), \tag{2.40}$$

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

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

Remark. The energy levels of the harmonic oscillator can be also obtained from the Bohr-Wilson-Sommerfeld quantization rule. Indeed, the corresponding classical orbit with the energy E is an ellipse in the phase plane

given by the equations $q(t) = A\cos(\omega t+\alpha)$, $p(t) = -m\omega A\sin(\omega t+\alpha)$, where $E = \frac{1}{2}m\omega^2A^2$ (see Section 1.5 in Chapter 1). Thus

$$\oint pdq = \iint dp\wedge dq = \pi m\omega A^2 = \frac{2\pi}{\omega}E,$$

and the BWS quantization rule gives the energy levels $E_n = \hbar\omega(n+\frac{1}{2})$.

Remark. Since the energy levels of the Hamiltonian H are equidistant by $\hbar\omega$, the quantum harmonic oscillator describes the system of identical "quanta" with the energy $\hbar\omega$. The ground state $|0\rangle = \psi_0$, in Dirac's notation, is the *vacuum state* with no quanta present and with the vacuum energy $\frac{1}{2}\hbar\omega$, and the states $|n\rangle = \psi_n$ consist of n quanta with the energy $\hbar\omega(n+\frac{1}{2})$. According to (2.39), the operator a^* adds one quantum to the state $|n\rangle$ and is called a *creation operator*, and the operator a destroys one quantum in the state $|n\rangle$ and is called an *annihilation operator*.

An example of the harmonic oscillator illustrates the dramatic difference between the motion in quantum mechanics and in classical mechanics. The classical motion in the potential field $V(q) = \frac{1}{2}m\omega^2q^2$ is finite: a particle with energy E moves in the region $|\omega q| \le \sqrt{\frac{2E}{m}}$, whereas there is always a non-zero probability of finding a quantum particle outside the classical region. Thus for the ground state energy $E = \frac{1}{2}\hbar\omega$ this probability is

$$\int_{|q|\ge\sqrt{\frac{\hbar}{m\omega}}} |\psi_0(q)|^2dq = \frac{2}{\sqrt{\pi}}\int_1^\infty e^{-x^2}dx \simeq 0.1572992070.$$

The classical harmonic oscillator with n degrees of freedom is described by the phase space $\mathbb{R}^{2n}$ with the canonical coordinates $\boldsymbol{p}, \boldsymbol{q}$, and the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{q}) = \frac{\boldsymbol{p}^2}{2m} + \sum_{j=1}^n \frac{m\omega_j^2q_j^2}{2},$$

where $\omega_1,\dots,\omega_n > 0$ (see Sections 1.3 and 1.7 in Chapter 1).

The corresponding Hamiltonian operator is

$$H = \frac{\boldsymbol{P}^2}{2m} + \sum_{j=1}^n \frac{m\omega_j^2Q_j^2}{2}$$

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

$$H = -\frac{\hbar^2}{2m}\Delta + \sum_{j=1}^n \frac{m\omega_j^2q_j^2}{2}.$$

The Hamiltonian H is a self-adjoint operator with $D(H) = W^{2,2}(\mathbb{R}^n) \cap \widehat{W}^{2,2}(\mathbb{R}^n)$ and a pure point spectrum. The corresponding eigenfunctions

$$\psi_{\boldsymbol{k}}(\boldsymbol{q}) = \psi_{k_1}(q_1) \dots \psi_{k_n}(q_n),$$

where $\boldsymbol{k} = (k_1, \dots, k_n)$ and $\psi_{k_j}(q_j)$ are eigenfunctions (2.40) with $\omega = \omega_j$, form an orthonormal basis for $L^2(\mathbb{R}^n, d^n\boldsymbol{q})$. The corresponding energy levels are given by

$$\lambda_{\boldsymbol{k}} = \hbar\omega_1(k_1 + \tfrac{1}{2}) + \dots + \hbar\omega_n(k_n + \tfrac{1}{2}).$$

The spectrum of H is simple if and only if $\hbar\omega_1, \dots, \hbar\omega_n$ are linearly independent over $\mathbb{Z}$. The highest degeneracy case is $\omega_1 = \dots = \omega_n = \omega$, when the multiplicity of the eigenvalue

$$\lambda_{\boldsymbol{k}} = \hbar\omega \sum_{j=1}^{n} (k_j + \tfrac{1}{2})$$

is the partition function $p_n(|\boldsymbol{k}|)$ — the number of representations of the integer $|\boldsymbol{k}| = k_1 + \dots + k_n$ as a sum of n non-negative integers. Setting $m = 1$ and introducing the operators[23]

$$a_j = \frac{1}{\sqrt{2\omega\hbar}} \left(\omega Q_j + iP_j\right), \quad a_j^* = \frac{1}{\sqrt{2\omega\hbar}} \left(\omega Q_j - iP_j\right), \quad j = 1, \dots, n, \tag{2.41}$$

we get canonical commutation relations for creation and annihilation operators for n degrees of freedom,

$$[a_j, a_l] = 0, \quad [a_j^*, a_l^*] = 0, \quad [a_j, a_l^*] = \delta_{jl} I, \quad j, l = 1, \dots, n, \tag{2.42}$$

which generalize relation (2.34) for the one degree of freedom. The operators a_j, a_j^* and $N_j = a_j^* a_j$, $j = 1, \dots, n$, satisfy commutation relations

$$[N_j, a_l] = -\delta_{jl} a_l, \quad [N_j, a_l^*] = \delta_{jl} a_l^*, \quad j, l = 1, \dots, n. \tag{2.43}$$

In particular, the operator

$$N = \sum_{j=1}^{n} N_j = \sum_{j=1}^{n} a_j^* a_j$$

satisfies

$$[N, a_j] = -a_j, \quad [N, a_j^*] = a_j^*, \quad j = 1, \dots, n,$$

and $H = \hbar\omega(N + \frac{n}{2} I)$.

Commutation relations (2.42) and (2.43) correspond to the irreducible unitary representation of the solvable Lie algebra $\tilde{\mathfrak{h}}_n$ with $3n + 1$ generators e_j, f_j, h_j, and c, where e_j, f_j, c satisfy the relations in the Heisenberg algebra $\mathfrak{h}_n$, and

$$[h_j, e_l] = -\delta_{jl} f_l, \quad [h_j, f_l] = \delta_{jl} \omega_l^2 e_l, \quad [h_j, c] = 0, \quad j, l = 1, \dots, n.$$

[23] Here, using the standard Euclidean metric on $\mathbb{R}^n$, we lowered the indices for Q^j.

Problem 2.9. Show that $\langle H|M\rangle \geq \frac{1}{2}\hbar\omega$ for every $M \in \mathscr{S}$, where H is the Hamiltonian of the harmonic oscillator with one degree of freedom.

Problem 2.10. Let $q(t) = A\cos(\omega t + \alpha)$ be the classical trajectory of the harmonic oscillator with $m = 1$ and the energy $E = \frac{1}{2}\omega^2 A^2$, and let μ_α be the probability measure on $\mathbb{R}$ supported at the point $q(t)$. Show that the convex linear combination of the measures μ_α, $0 \leq \alpha \leq 2\pi$, is the probability measure on $\mathbb{R}$ with the distribution function $\mu(q) = \frac{\theta(A^2-q^2)}{\pi\sqrt{A^2-q^2}}$, where $\theta(q)$ is the Heavyside step function.

Problem 2.11. Show that when $n \to \infty$ and $\hbar \to 0$ such that $\hbar\omega(n+\frac{1}{2}) = \frac{1}{2}\omega^2 A^2$ remains fixed, the envelope of the distribution function $|\psi_n(q)|^2$ on the interval $|q| \leq A$ coincides with the classical distribution function $\mu(q)$ from the previous problem. (*Hint:* Prove the integral representation

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

and derive the asymptotic formula

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

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

Problem 2.12. Complete the proof of Theorem 2.1.

Problem 2.13 (The N-representation theorem)**.** Let $\psi \in \mathscr{S}(\mathbb{R})$. Show that the L^2-convergent expansion $\psi = \sum_{n=0}^\infty c_n\psi_n$, where $c_n = (\psi, \psi_n)$, converges in $\mathscr{S}(\mathbb{R})$. (*Hint*: Use $N\psi_n = n\psi_n$.)

Problem 2.14. Show that the operators $E_{ij} = a_i^* a_j$, $i, j = 1, \ldots, n$, satisfy the commutation relations of the Lie algebra $\mathrm{sl}(n, \mathbb{C})$.

2.7. Holomorphic representation and Wick symbols. Let

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

be the Hilbert ℓ^2-space. The choice of an orthonormal basis $\{\psi_n\}_{n=0}^\infty$ for $L^2(\mathbb{R}, dq)$, given by the eigenfunctions (2.40) of the Schrödinger operator for the harmonic oscillator, establishes the Hilbert space isomorphism $L^2(\mathbb{R}, dq) \simeq \ell^2$,

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

where

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

since the functions ψ_n are real-valued. Using (2.39) we get

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

and

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

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

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

As a result,

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

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

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

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

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

$$(f, g) = \frac{1}{\pi}\int_{\mathbb{C}} f(z)\overline{g(z)}e^{-|z|^2} d^2z, \tag{2.44}$$

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

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

The correspondence

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

establishes the Hilbert space isomorphism $\ell^2 \simeq \mathscr{D}$. The realization of a Hilbert space $\mathscr{H}$ as the Hilbert space $\mathscr{D}$ of entire functions is called a *holomorphic representation*. In the holomorphic representation,

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

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

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

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

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

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

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

with the kernel

$$U(z,q) = \sum_{n=0}^{\infty} \psi_n(q)f_n(z) = \sqrt[4]{\frac{m\omega}{\pi\hbar}}\, e^{\frac{m\omega}{2\hbar}q^2 - \left(\sqrt{\frac{m\omega}{\hbar}}q - \frac{1}{\sqrt{2}}z\right)^2}. \tag{2.45}$$

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

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

given by

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

Remark. Holomorphic and anti-holomorphic representations correspond to different choices of a *complex polarization* of the symplectic manifold $\mathbb{R}^2$. By definition, a complex polarization of a symplectic manifold $(\mathscr{M},\omega)$ is an integrable distribution on $\mathscr{M}$ of complex Lagrangian subspaces of the complexified vector spaces $T_x\mathscr{M} \otimes_{\mathbb{R}} \mathbb{C}$. As the notion of real polarization, the notion of complex polarization plays a fundamental role in geometric quantization. In particular, holomorphic representation corresponds to the complex Lagrangian subspace in $T_x\mathbb{R}^2 \otimes_{\mathbb{R}} \mathbb{C} \simeq \mathbb{C}^2$ given by the equation $z = 0$, where z and $\bar{z}$ are complex coordinates on $\mathbb{C}^2$. (Note that here $\bar{z}$ is not a complex conjugate to z!) The equation $\bar{z} = 0$ defines a complex Lagrangian subspace which corresponds to the anti-holomorphic representation.

The anti-holomorphic representation is used to introduce the so-called *Wick symbols* of the operators. Namely, let A be an operator in $\bar{\mathscr{D}}$ which is a polynomial with constant coefficients in creation and annihilation operators a^* and a. Using the commutation relation (2.34), we can move all operators a^* to the left of the operators a, and represent A in the *Wick normal form* as follows:

$$A = \sum_{l,m} A_{lm} (a^*)^l a^m. \tag{2.46}$$

By definition, the Wick symbol $A(\bar{z}, z)$ of the operator A is

$$A(\bar{z}, z) = \sum_{l,m} A_{lm} \bar{z}^l z^m. \tag{2.47}$$

It is a restriction of a polynomial $A(v, z)$ in variables v and z to $v = \bar{z}$.

In order to define Wick symbols of bounded operators in $\bar{\mathscr{D}}$, we consider the family of *coherent states* (or *Poisson vectors*) $\Phi_v \in \bar{\mathscr{D}}$, $v \in \mathbb{C}$, defined by

$$\Phi_v(\bar{z}) = e^{v\bar{z}}, \quad z \in \mathbb{C}.$$

They satisfy the properties

$$a\Phi_v = v\Phi_v \quad \text{and} \quad f(\bar{v}) = (f, \Phi_v), \quad f \in \bar{\mathscr{D}},\ v \in \mathbb{C}. \tag{2.48}$$

Indeed, the first property is trivial, whereas the "reproducing property" immediately follows from the formula

$$\Phi_v(\bar{z}) = \sum_{n=0}^{\infty} f_n(v) \bar{f}_n(\bar{z}), \tag{2.49}$$

where $\bar{f}_n(\bar{z}) = \overline{f_n(z)}$, $n = 0, 1, 2, \ldots$, is the orthonormal basis for $\bar{\mathscr{D}}$.

We also have

$$(f, g) = \frac{1}{\pi} \int_{\mathbb{C}} (f, \Phi_v) \overline{(g, \Phi_v)} e^{-|v|^2} d^2 v. \tag{2.50}$$

Now for the operator A in the Wick normal form (2.46) we get, using the first property in (2.48),

$$\begin{aligned} (A\Phi_z, \Phi_{\bar{v}}) &= \sum_{l,m} A_{lm} ((a^*)^l a^m \Phi_z, \Phi_{\bar{v}}) = \sum_{l,m} A_{lm} (a^m \Phi_z, a^l \Phi_{\bar{v}}) \\ &= A(v, z)(\Phi_z, \Phi_{\bar{v}}). \end{aligned}$$

Therefore,

$$A(v, z) = \frac{(A\Phi_z, \Phi_{\bar{v}})}{(\Phi_z, \Phi_{\bar{v}})} = e^{-vz} (A\Phi_z, \Phi_{\bar{v}}),$$

since by the reproducing property, $(\Phi_z, \Phi_{\bar{v}}) = \Phi_z(v) = e^{vz}$.

Definition. The Wick symbol $A(\bar{z}, z)$ of a bounded operator A in the Hilbert space $\bar{\mathscr{D}}$ is a restriction to $v = \bar{z}$ of an entire function $A(v, z)$ in variables v and z, defined by

$$A(v, z) = e^{-vz}(A\Phi_z, \Phi_{\bar{v}}).$$

In the next theorem, we summarize the properties of the Wick symbols.

Theorem 2.2. *Wick symbols of the bounded operators on $\bar{\mathscr{D}}$ have the following properties.*

(i) *If $A(\bar{z}, z)$ is the Wick symbol of an operator A, then for the Wick symbol of the operator A^* we have $A^*(\bar{z}, z) = \overline{A(\bar{z}, z)}$ and*

$$A^*(v, z) = \overline{A(\bar{z}, \bar{v})}.$$

(ii) *For $f \in \bar{\mathscr{D}}$,*

$$(Af)(\bar{z}) = \frac{1}{\pi} \int_{\mathbb{C}} A(\bar{z}, v) f(\bar{v}) e^{-v(\bar{v}-\bar{z})} d^2v.$$

(iii) *A real-analytic function $A(\bar{z}, z)$ is a Wick symbol of a bounded operator A in $\bar{\mathscr{D}}$ if and only if it is a restriction to $v = \bar{z}$ of an entire function $A(v, z)$ in variables v and z with the property that for every $f \in \bar{\mathscr{D}}$ the integral in part* (ii) *is absolutely convergent and defines a function in $\bar{\mathscr{D}}$.*

(iv) *If $A_1(\bar{z}, z)$ and $A_2(\bar{z}, z)$ are the Wick symbols of operators A_1 and A_2, then the Wick symbol of the operator $A = A_1A_2$ is given by*

$$A(\bar{z}, z) = \frac{1}{\pi} \int_{\mathbb{C}} A_1(\bar{z}, v) A_2(\bar{v}, z) e^{-(v-z)(\bar{v}-\bar{z})} d^2v.$$

Proof. We have

$$A^*(v, z) = e^{-vz}(A^*\Phi_z, \Phi_{\bar{v}}) = e^{-vz}(\Phi_z, A\Phi_{\bar{v}}) = e^{-vz}\overline{(A\Phi_{\bar{v}}, \Phi_z)} = \overline{A(\bar{z}, \bar{v})},$$

which proves (i). To prove (ii), we use the reproducing property to get

$$(Af)(\bar{z}) = (Af, \Phi_z) = (f, A^*\Phi_z) = \frac{1}{\pi} \int_{\mathbb{C}} f(\bar{v}) \overline{(A^*\Phi_z)(\bar{v})} e^{-|v|^2} d^2v.$$

Using the reproducing property once again we have

$$(A^*\Phi_z)(\bar{v}) = (A^*\Phi_z, \Phi_v) = A^*(\bar{v}, z)(\Phi_z, \Phi_v) = \overline{e^{v\bar{z}} A(\bar{z}, v)},$$

which proves (ii). Property (iii) follows from the definition and the uniform boundness principle, which is needed to show that the operator A on $\bar{\mathscr{D}}$,

defined by the integral in (ii), is bounded. We leave the standard details to the reader. To prove (iv), by using (2.50) and (i) we get

$$\begin{aligned} A(\bar{z},z) &= e^{-|z|^2}(A_1A_2\Phi_z,\Phi_z) = e^{-|z|^2}(A_2\Phi_z,A_1^*\Phi_z) \\ &= \frac{1}{\pi}\int_{\mathbb{C}}(A_2\Phi_z,\Phi_v)\overline{(A_1^*\Phi_z,\Phi_v)}e^{-(|v|^2+|z|^2)}d^2v \\ &= \frac{1}{\pi}\int_{\mathbb{C}}A_1(\bar{z},v)A_2(\bar{v},z)e^{-(v-z)(\bar{v}-\bar{z})}d^2v. \end{aligned}$$ □

Remark. Properties (i) and (iv) remain valid for the polynomials in a^* and a — operators of the form (2.46).

A *matrix symbol* $\tilde{A}(\bar{z},z)$ of a bounded operator A in the Hilbert space $\bar{\mathscr{D}}$ is a restriction to $v=\bar{z}$ of an entire function $\tilde{A}(v,z)$ in variables v and z, defined by the following absolutely convergent series:

$$\tilde{A}(v,z) = \sum_{m,n=0}^{\infty}(A\bar{f}_m,\bar{f}_n)f_n(v)f_m(z). \tag{2.51}$$

The matrix and Wick symbols are related as follows.

Lemma 2.4. *For a bounded operator A in the Hilbert space $\bar{\mathscr{D}}$,*

$$\tilde{A}(v,z) = e^{vz}A(v,z).$$

Proof. Using (2.49) we get

$$\begin{aligned} \tilde{A}(v,z) &= \frac{1}{\pi}\sum_{m,n=0}^{\infty}f_n(v)f_m(z)\int_{\mathbb{C}}(A\bar{f}_m)(\bar{u})f_n(u)e^{-|u|^2}d^2u \\ &= \frac{1}{\pi}\int_{\mathbb{C}}(A\Phi_z)(\bar{u})\overline{\Phi_{\bar{v}}(\bar{u})}e^{-|u|^2}d^2u = (A\Phi_z,\Phi_{\bar{v}}) = e^{vz}A(v,z). \end{aligned}$$

Changing the order of summation and integration is justified by the absolute convergence. □

Corollary 2.3. *If $\tilde{A}_1(\bar{z},z)$ and $\tilde{A}_2(\bar{z},z)$ are matrix symbols of operators A_1 and A_2, then the matrix symbol of the operator $A=A_1A_2$ is given by*

$$\tilde{A}(\bar{z},z) = \frac{1}{\pi}\int_{\mathbb{C}}\tilde{A}_1(\bar{z},v)\tilde{A}_2(\bar{v},z)e^{-|v|^2}d^2v.$$

Proof. The proof immediately follows from part (iv) of Theorem 2.2 and Lemma 2.4. □

It is straightforward to generalize these constructions to n degrees of freedom. The Hilbert space $\mathscr{D}_n$ defining the holomorphic representation is

the space of entire functions $f(\boldsymbol{z})$ of n complex variables $\boldsymbol{z} = (z_1, \dots, z_n)$ with the inner product

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

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

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

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

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

The Hilbert space $\bar{\mathscr{D}}_n$ of anti-holomorphic functions $f(\bar{\boldsymbol{z}})$ on $\mathbb{C}^n$ is defined by the inner product

$$(f, g) = \frac{1}{\pi^n} \int_{\mathbb{C}^n} f(\bar{\boldsymbol{z}}) \overline{g(\bar{\boldsymbol{z}})} e^{-|\boldsymbol{z}|^2} d^{2n}\boldsymbol{z} < \infty, \tag{2.52}$$

and the creation and annihilation operators are given by

$$a_j^* = \bar{z}_j, \quad a_j = \frac{\partial}{\partial \bar{z}_j}, \quad j = 1, \dots, n.$$

The coherent states are $\Phi_{\boldsymbol{v}}(\bar{\boldsymbol{z}}) = e^{\boldsymbol{v}\bar{\boldsymbol{z}}}$, where $\boldsymbol{v}\bar{\boldsymbol{z}} = v_1\bar{z}_1 + \cdots + v_n z_n$, and satisfy the reproducing property

$$f(\bar{\boldsymbol{v}}) = (f, \Phi_{\boldsymbol{v}}), \quad f \in \bar{\mathscr{D}}_n, \quad \boldsymbol{v} \in \mathbb{C}^n.$$

The Wick symbol $A(\bar{\boldsymbol{z}}, \boldsymbol{z})$ of a bounded operator A on $\bar{\mathscr{D}}_n$ is defined as a restriction to $\boldsymbol{v} = \bar{\boldsymbol{z}}$ of an entire function $A(\boldsymbol{v}, \boldsymbol{z})$ of $2n$ variables $\boldsymbol{v} = (v_1, \dots, v_n)$ and $\boldsymbol{z} = (z_1, \dots, z_n)$, given by

$$A(\boldsymbol{v}, \boldsymbol{z}) = e^{-\boldsymbol{v}\boldsymbol{z}} (A\Phi_{\boldsymbol{z}}, \Phi_{\bar{\boldsymbol{v}}}).$$

We have

$$(Af)(\bar{\boldsymbol{z}}) = \frac{1}{\pi^n} \int_{\mathbb{C}^n} A(\bar{\boldsymbol{z}}, \boldsymbol{v}) f(\bar{\boldsymbol{v}}) e^{-\boldsymbol{v}(\bar{\boldsymbol{v}} - \bar{\boldsymbol{z}})} d^{2n}\boldsymbol{v}, \quad f \in \bar{\mathscr{D}}_n,$$

and the Wick symbol $A(\bar{\boldsymbol{z}}, \boldsymbol{z})$ of the operator $A = A_1 A_2$ is given by

$$A(\bar{\boldsymbol{z}}, \boldsymbol{z}) = \frac{1}{\pi^n} \int_{\mathbb{C}^n} A_1(\bar{\boldsymbol{z}}, \boldsymbol{v}) A_2(\bar{\boldsymbol{v}}, \boldsymbol{z}) e^{-(\boldsymbol{v} - \boldsymbol{z})(\bar{\boldsymbol{v}} - \bar{\boldsymbol{z}})} d^{2n}\boldsymbol{v},$$

where $A_1(\bar{\boldsymbol{z}}, \boldsymbol{z})$ and $A_2(\bar{\boldsymbol{z}}, \boldsymbol{z})$ are the Wick symbols of the operators A_1 and A_2.

The matrix symbol $\tilde{A}(\bar{\boldsymbol{z}}, \boldsymbol{z})$ of a bounded operator A on $\bar{\mathscr{D}}_n$ is defined as a restriction to $\boldsymbol{v} = \bar{\boldsymbol{z}}$ of an entire function $\tilde{A}(\boldsymbol{v}, \boldsymbol{z})$ of $2n$ variables $\boldsymbol{v} = (v_1, \dots, v_n)$ and $\boldsymbol{z} = (z_1, \dots, z_n)$, given by the absolutely convergent series

$$\tilde{A}(\boldsymbol{v}, \boldsymbol{z}) = \sum_{\boldsymbol{k},\boldsymbol{m}=0}^{\infty} (A\bar{f}_{\boldsymbol{k}}, \bar{f}_{\boldsymbol{m}}) f_{\boldsymbol{m}}(\boldsymbol{v}) f_{\boldsymbol{k}}(\boldsymbol{z}),$$

where $\boldsymbol{k} = (k_1, \dots, k_n)$, $\boldsymbol{m} = (m_1, \dots, m_n)$ are multi-indices, and $\bar{f}_{\boldsymbol{m}}(\bar{\boldsymbol{z}}) = \overline{f_{\boldsymbol{m}}(\boldsymbol{z})}$. The matrix and Wick symbols of a bounded operator A are related by

$$\tilde{A}(\boldsymbol{v}, \boldsymbol{z}) = e^{\boldsymbol{v}\boldsymbol{z}} A(\boldsymbol{v}, \boldsymbol{z}).$$

Remark. The anti-holomorphic representation is very useful in quantum mechanics and especially in quantum field theory, where it is called holomorphic representation (with respect to the variables $\bar{\boldsymbol{z}}$). Slightly abusing terminology, in Part 2 we will also call it holomorphic representation.

Problem 2.15. Find an explicit formula for the unitary operator establishing the Hilbert space isomorphism $\bar{\mathscr{D}}_n \simeq L^2(\mathbb{R}^n, d^n\boldsymbol{q})$.

Problem 2.16. Prove that for the bounded operator A the functions $A(\boldsymbol{v}, \boldsymbol{z})$ and $\tilde{A}(\boldsymbol{v}, \boldsymbol{z})$ are entire functions of $2n$ variables.

Problem 2.17. Let A be a trace class operator on $\bar{\mathscr{D}}_n$ with the Wick symbol $A(\bar{\boldsymbol{z}}, \boldsymbol{z})$. Prove that

$$\operatorname{Tr} A = \frac{1}{\pi^n} \int_{\mathbb{C}^n} A(\bar{\boldsymbol{z}}, \boldsymbol{z}) e^{-|\boldsymbol{z}|^2} d^{2n}\boldsymbol{z}.$$

Problem 2.18. Show that the Wick symbol $A(\bar{z}, z)$ of the product $A = A_l \dots A_1$ is given by

$$A(\bar{z}, z) = \frac{1}{\pi^l} \int_{\mathbb{C}^l} A_l(\bar{z}, z_{l-1}) \dots A_1(\bar{z}_1, z) \exp\Big\{ \sum_{k=1}^{l} \bar{z}_k (z_{k-1} - z_k) \Big\} d^2 z_1 \dots d^2 z_{l-1},$$

where $z_0 = z_l = z$, $\bar{z}_l = \bar{z}$, and $A_k(\bar{z}, z)$ are the Wick symbols of the operators A_k.

3. Weyl relations

Let R be an irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ in Hilbert space $\mathscr{H}$. It follows from Schur's lemma that $R(e^{\alpha c}) = e^{i\hbar\alpha} I$ for some $\hbar \in \mathbb{R}$, where I is the identity operator on $\mathscr{H}$. If $\hbar = 0$, the n-parameter abelian groups of unitary operators $U(\boldsymbol{u}) = R(e^{\boldsymbol{u}X})$ and $V(\boldsymbol{v}) = R(e^{\boldsymbol{v}Y})$ commute, so using Schur's lemma once again we conclude that there exist $\boldsymbol{p}, \boldsymbol{q} \in \mathbb{R}^n$ such that $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{p}} I$ and $V(\boldsymbol{v}) = e^{-i\boldsymbol{v}\boldsymbol{q}} I$. Therefore, in this case the irreducible representation R is one-dimensional and is parametrized by a vector $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n}$. When $\hbar \neq 0$, unitary operators $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$ satisfy the Weyl relations

$$U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar\boldsymbol{u}\boldsymbol{v}} V(\boldsymbol{v})U(\boldsymbol{u}), \tag{3.1}$$

which admit the Schrödinger representation, introduced in Section 2.2. It turns out that every unitary irreducible representation of the Heisenberg group $\mathbf{H}_n$ is unitarily equivalent either to a one-dimensional representation with parameters $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n}$, or to the Schrödinger representation with some $\hbar \neq 0$. The physically meaningful case corresponds to $\hbar > 0$, and representation with $-\hbar$ is given by the operators $U^{-1}(\boldsymbol{u}) = U(-\boldsymbol{u})$ and $V(\boldsymbol{v})$.

3.1. Stone-von Neumann theorem. Here we prove the following fundamental result.

Theorem 3.1 (Stone-von Neumann theorem)**.** *Every irreducible unitary representation of the Weyl relations for n degrees of freedom,*

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

is unitarily equivalent to the Schrödinger representation.

Proof. It is sufficient to consider $n = 1$, the general case $n > 1$ is treated similarly. Set

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

The unitary operator $S(u, v)$ satisfies

$$S(u, v)^* = S(-u, -v), \tag{3.2}$$

and it follows from the Weyl relation that

$$S(u_1, v_1)S(u_2, v_2) = e^{\frac{i\hbar}{2}(u_1 v_2 - u_2 v_1)} S(u_1 + u_2, v_1 + v_2). \tag{3.3}$$

Define a linear map $W : L^1(\mathbb{R}^2) \to \mathscr{L}(\mathscr{H})$, called the *Weyl transform*, by

$$W(f) = \frac{1}{2\pi} \int_{\mathbb{R}^2} f(u, v)S(u, v)dudv.$$

Here the integral is understood in the weak sense: for every $\psi_1, \psi_2 \in \mathscr{H}$,

$$(W(f)\psi_1, \psi_2) = \frac{1}{2\pi} \int_{\mathbb{R}^2} f(u, v)(S(u, v)\psi_1, \psi_2)dudv.$$

The integral is absolutely convergent for all $\psi_1, \psi_2 \in \mathscr{H}$, and defines a bounded operator $W(f)$ satisfying

$$\|W(f)\| \leq \frac{1}{2\pi} \|f\|_{L^1}.$$

The Weyl transform has the following properties.

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

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

where

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

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

$$S(u_1, v_1)W(f)S(u_2, v_2) = W(\tilde{f}),$$

where

$$\tilde{f}(u, v) = e^{\frac{i\hbar}{2}\{(u_1-u_2)v-(v_1-v_2)u+u_1v_2-u_2v_1\}} f(u - u_1 - u_2, v - v_1 - v_2).$$

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

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

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

where

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

The first two properties follow from the definition and (3.2) and (3.3). To prove **WT3**, suppose that $W(f) = 0$. Then for every $\psi_1, \psi_2 \in \mathscr{H}$ and all $u', v' \in \mathbb{R}$ we have

$$\begin{aligned} 0 &= (W(f)S(u', v')\psi_1, S(u', v')\psi_2) \\ &= \frac{1}{2\pi} \int_{\mathbb{R}^2} e^{i\hbar(uv'-u'v)} f(u, v)(S(u, v)\psi_1, \psi_2) dudv. \end{aligned}$$

Therefore $f(u, v)(S(u, v)\psi_1, \psi_2) = 0$ a.e. on $\mathbb{R}^2$, so that $f = 0$.

To prove **WT4**, we compute

$$\begin{aligned} (W(f_1)W(f_2)\psi_1, \psi_2) &= (W(f_2)\psi_1, W(f_1)^*\psi_2) \\ &= \frac{1}{2\pi} \int_{\mathbb{R}^2} f_2(u_2, v_2)(S(u_2, v_2)\psi_1, W(f_1)^*\psi_2) du_2dv_2 \\ &= \frac{1}{2\pi} \int_{\mathbb{R}^2} f_2(u_2, v_2)(W(f_1)S(u_2, v_2)\psi_1, \psi_2) du_2dv_2 \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} f_1(u_1 - u_2, v_1 - v_2) f_2(u_2, v_2) \cdot \\ &\quad \cdot e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1)} (S(u_1, v_1)\psi_1, \psi_2) du_1dv_1du_2dv_2 \\ &= \frac{1}{2\pi} \int_{\mathbb{R}^2} (f_1 *_\hbar f_2)(u, v)(S(u, v)\psi_1, \psi_2) dudv. \end{aligned}$$

We have $f_1 *_\hbar f_2 \in L^1(\mathbb{R}^2)$, and it follows from the associativity of the operator product and property **WT3** that the linear mapping

$$*_\hbar : L^1(\mathbb{R}^2) \times L^1(\mathbb{R}^2) \to L^1(\mathbb{R}^2)$$

defines a new associative product on $L^1(\mathbb{R}^2)$,

$$f_1 *_\hbar (f_2 *_\hbar f_3) = (f_1 *_\hbar f_2) *_\hbar f_3 \quad \text{for all} \quad f_1, f_2, f_3 \in L^1(\mathbb{R}^2).$$

When $\hbar = 0$, the product $*_\hbar$ becomes the usual convolution product on $L^1(\mathbb{R}^2)$.

For every non-zero $\psi \in \mathscr{H}$ 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 invariant for all operators $U(u)$ and $V(v)$. Since the representation of the Weyl relation is irreducible, $\mathscr{H}_\psi = \mathscr{H}$.

There is a vector $\psi_0 \in \mathscr{H}$ for which all inner products of the generating vectors $S(u,v)\psi_0$ of $\mathscr{H}_{\psi_0}$ can be explicitly computed. Namely, let

$$f_0(u,v) = \hbar\, e^{-\frac{\hbar}{4}(u^2+v^2)}$$

and set

$$W_0 = W(f_0).$$

Then $W_0^* = W_0$ and

$$W_0 S(u,v) W_0 = e^{-\frac{\hbar}{4}(u^2+v^2)} W_0.$$

In particular, $W_0^2 = W_0$, so that W_0 is an orthogonal projection. Indeed, using **WT4**, we have

$$W_0 S(u,v) W_0 = W(f_0 *_\hbar \tilde{f}_0),$$

where

$$\tilde{f}_0(u',v') = e^{\frac{i\hbar}{2}(uv'-u'v)} f_0(u'-u, v'-v).$$

By "completing the square" we obtain

$$(f_0 *_\hbar \tilde{f}_0)(u',v') = \hbar e^{-\frac{\hbar}{4}(u^2+v^2+u'^2+v'^2)} I(u',v'),$$

where

$$I(u',v') = \frac{\hbar}{2\pi} \int_{\mathbb{R}^2} e^{-\frac{\hbar}{2}\{(u''-u-u'+iv+iv')^2+(v''-v-v'-iu-iu')^2\}} du'' dv''.$$

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

$$I(u',v') = \frac{\hbar}{2\pi} \int_{\mathbb{R}^2} e^{-\frac{\hbar}{2}(\xi^2+\eta^2)} d\xi d\eta = 1.$$

Now let $\mathscr{H}_0 = \operatorname{Im} W_0$ — a non-zero closed subspace of $\mathscr{H}$ by property **WT3**. 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

$$\begin{aligned}
(S(u_1,v_1)\psi_1, S(u_2,v_2)\psi_2) &= (S(u_1,v_1)W_0\psi_1, S(u_2,v_2)W_0\psi_2) \\
&= (W_0 S(-u_2,-v_2) S(u_1,v_1) W_0\psi_1, \psi_2) \\
&= e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1)} (W_0 S(u_1-u_2, v_1-v_2) W_0\psi_1, \psi_2) \\
&= e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1) - \frac{\hbar}{4}\{(u_1-u_2)^2+(v_1-v_2)^2\}} (W_0\psi_1, \psi_2) \\
&= e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1) - \frac{\hbar}{4}\{(u_1-u_2)^2+(v_1-v_2)^2\}} (\psi_1, \psi_2).
\end{aligned}$$

This implies that the subspace $\mathscr{H}_0$ is one-dimensional. Indeed, for every $\psi_1, \psi_2 \in \mathscr{H}_0$ such that $(\psi_1, \psi_2) = 0$, we have that the corresponding subspaces $\mathscr{H}_{\psi_1}$ and $\mathscr{H}_{\psi_2}$ are orthogonal. Since $\mathscr{H}_\psi = \mathscr{H}$ for every non-zero ψ, 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

$$S(u,v)\psi_{\alpha,\beta} = e^{\frac{i\hbar}{2}(u\beta-v\alpha)}\psi_{\alpha+u,\beta+v}.$$

Next we consider the Schrödinger representation of the Weyl relation in $L^2(\mathbb{R}, dq)$:

$$\begin{aligned}(\mathsf{U}(u)\varphi)(q) &= \varphi(q-\hbar u),\\ (\mathsf{V}(v)\varphi)(q) &= e^{-ivq}\varphi(q),\\ (\mathsf{S}(u,v)\varphi)(q) &= e^{\frac{i\hbar}{2}uv-ivq}\varphi(q-\hbar u).\end{aligned}$$

For the corresponding operator W_0 we have

$$\begin{aligned}(\mathsf{W}_0\varphi)(q) &= \frac{\hbar}{2\pi}\int_{\mathbb{R}^2} e^{-\frac{\hbar}{4}(u^2+v^2)}e^{\frac{i\hbar}{2}uv-ivq}\varphi(q-\hbar u)\,du\,dv\\ &= \sqrt{\frac{\hbar}{\pi}}\int_{-\infty}^{\infty} e^{-\frac{\hbar}{4}\{u^2+(u-\frac{2}{\hbar}q)^2\}}\varphi(q-\hbar u)\,du\\ &= \frac{1}{\sqrt{\hbar\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2\hbar}(q^2+q'^2)}\varphi(q')\,dq',\end{aligned}$$

so that W_0 is a projection onto the one-dimensional subspace of $L^2(\mathbb{R}, dq)$ spanned by the Gaussian exponential $\varphi_0(q) = \frac{1}{\sqrt[4]{\pi\hbar}}e^{-\frac{1}{2\hbar}q^2}$, $\|\varphi_0\| = 1$. Let

$$\varphi_{\alpha,\beta} = \mathsf{S}(\alpha,\beta)\varphi_0.$$

Since the Schrödinger representation is irreducible, the closed subspace spanned by the functions $\varphi_{\alpha,\beta}$ for all $\alpha, \beta \in \mathbb{R}$ is the whole Hilbert space $L^2(\mathbb{R}, dq)$. (This also follows from the completeness of Hermite-Tchebyscheff functions, since $\varphi_{\alpha,\beta}(q) = \frac{1}{\sqrt[4]{\pi\hbar}}e^{\frac{i\hbar}{2}\alpha\beta-i\beta q-\frac{1}{2\hbar}(q-\hbar\alpha)^2}$.) 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

$$\mathscr{U}(\psi) = \sum_{i=1}^n c_i \varphi_{\alpha_i,\beta_i} \in L^2(\mathbb{R}, dq).$$

Since inner products between the vectors $\psi_{\alpha,\beta}$ coincide with the inner products between the vectors $\varphi_{\alpha,\beta}$, we have

$$\|\mathscr{U}(\psi)\|^2_{L^2} = \|\psi\|^2_{\mathscr{H}},$$

so that $\mathscr{U}$ is a well-defined unitary operator between the subspaces spanned by the 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 $\mathscr{U} : \mathscr{H} \to L^2(\mathbb{R}, dq)$ and

$$\mathscr{U} S(\alpha,\beta) = \mathsf{S}(\alpha,\beta)\mathscr{U} \quad \text{for all} \quad \alpha,\beta \in \mathbb{R}. \qquad \square$$

Lemma 2.1 in Section 2.1 is now an easy corollary of the Stone-von Neumann theorem.

Corollary 3.2. *The self-adjoint generators $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ of the n-parameter abelian groups of unitary operators $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$ satisfy Heisenberg commutation relations.*

Proof. It follows from the Stone theorem that in the Schrödinger representation the generators $\boldsymbol{P}$ and $\boldsymbol{Q}$ are momenta and coordinate operators. $\square$

Remark. For n degrees of freedom

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

and formally using the Baker-Campbell-Hausdorff formula, we get

$$S(\boldsymbol{u},\boldsymbol{v}) = e^{-i(\boldsymbol{u}\boldsymbol{P}+\boldsymbol{v}\boldsymbol{Q})}. \tag{3.4}$$

Thus the Weyl transform

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

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

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

Remark. The Stone-von Neumann theorem is a very strong result. In particular, it implies that creation and annihilation operators for n degrees of freedom,

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

where $\boldsymbol{P}$ and $\boldsymbol{Q}$ are the corresponding generators[24] satisfying Heisenberg commutation relations, are unitarily equivalent to the corresponding operators in the Schrödinger representation. Thus there always exists a ground state — a vector $\psi_0 \in \mathscr{H}$, annihilated by the operators $\boldsymbol{a} = (a_1, \dots, a_n)$. The corresponding statement no longer holds for quantum systems with infinitely many degrees of freedom, described by quantum field theory, where one needs to postulate the existence of the ground state (the "physical vacuum").

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

$$(S(\boldsymbol{u},\boldsymbol{v})\psi)(\boldsymbol{q}) = e^{\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v} - i\boldsymbol{v}\boldsymbol{q}}\psi(\boldsymbol{q}-\hbar\boldsymbol{u}), \quad \psi \in L^2(\mathbb{R}^n, d^n\boldsymbol{q}), \tag{3.5}$$

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

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

where

$$K(\boldsymbol{q},\boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} f(\tfrac{\boldsymbol{q}-\boldsymbol{q}'}{\hbar}, \boldsymbol{v})e^{-\frac{i}{2}(\boldsymbol{q}+\boldsymbol{q}')\boldsymbol{v}}d^n\boldsymbol{v}. \tag{3.6}$$

The interchange of the order of integrations is justified by the Fubini theorem. Thus $W(f)$ is an integral operator with the integral kernel $K(\boldsymbol{q},\boldsymbol{q}')$,

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

By the Plancherel theorem,

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

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

[24] Here it is convenient to lower the indices by the Euclidean metric on $\mathbb{R}^n$ and use $\boldsymbol{Q} = (Q_1, \dots, Q_n)$.

Lemma 3.1. *The Weyl transform W defines the isomorphism $L^2(\mathbb{R}^{2n}) \simeq \mathscr{S}_2$.*

Problem 3.1. Let $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q_1, \dots, Q_n)$ be self-adjoint operators[25] on $\mathscr{H}$ satisfying Heisenberg commutation relations (2.4) on some dense domain D in $\mathscr{H}$, and such that the symmetric operator $H = \sum_{k=1}^n (P_k^2 + Q_k^2)$, defined on D, is essentially self-adjoint. Also suppose that every bounded operator which commutes with $\boldsymbol{P}$ and $\boldsymbol{Q}$ is a multiple of the identity operator in $\mathscr{H}$. Prove that $\boldsymbol{P}$ and $\boldsymbol{Q}$ are unitarily equivalent to momenta and coordinate operators in the Schrödinger representation. (*Hint:* By the Stone-von Neumann theorem, it is sufficient to show that $\boldsymbol{P}$ and $\boldsymbol{Q}$ define an integrable representation of the Heisenberg algebra. One can also prove this result directly by using commutation relations between the operators H, $\boldsymbol{a}^*$, $\boldsymbol{a}$ and the arguments in Section 2.6. This would give another proof of the Stone-von Neumann theorem.)

Problem 3.2. Prove formula (3.4).

3.2. Invariant formulation. Here we present a coordinate-free description of the Schrödinger representation. Let (V, ω) be a finite-dimensional symplectic vector space, $\dim V = 2n$. Recall that (see Section 2.1) the Heisenberg algebra $\mathfrak{g} = \mathfrak{g}(V)$ is a one-dimensional central extension of the abelian Lie algebra V by the skew-symmetric bilinear form ω. As a vector space,

$$\mathfrak{g} = V \oplus \mathbb{R}c,$$

with the Lie bracket

$$[u + \alpha c, v + \beta c] = \omega(u, v)c, \quad u, v \in V, \ \ \alpha, \beta \in \mathbb{R}.$$

Every Lagrangian subspace ℓ of V defines an abelian subalgebra $\ell \oplus \mathbb{R}c$ of $\mathfrak{g}$. A Lagrangian subspace ℓ' is complementary to ℓ in V if $\ell \oplus \ell' = V$. A choice of the complementary Lagrangian subspace ℓ' to ℓ establishes the isomorphism

$$\mathfrak{g}/(\ell \oplus \mathbb{R}c) \simeq \ell'.$$

The Heisenberg group $G = G(V)$ is a connected and simply-connected Lie group with the Lie algebra $\mathfrak{g}$. By the exponential map, $G \simeq V \oplus \mathbb{R}c$ as a manifold, with the group law

$$\exp(v_1 + \alpha_1 c) \exp(v_2 + \alpha_2 c) = \exp(v_1 + v_2 + (\alpha_1 + \alpha_2 + \tfrac{1}{2}\omega(v_1, v_2))c),$$

where $v_1, v_2 \in V$, $\alpha_1, \alpha_2 \in \mathbb{R}$. A choice of the symplectic basis for V establishes the isomorphism $G(V) \simeq \mathbf{H}_n$ with the matrix Heisenberg group defined in Section 2.1. The volume form $d^{2n}\boldsymbol{v} \wedge dc$, where $d^{2n}\boldsymbol{v} \in \Lambda^{2n} V^*$ is a volume form on V and V^* is the dual vector space to V, defines a bi-invariant Haar measure on G. Every Lagrangian subspace ℓ defines an

[25] See previous footnote.

abelian subgroup $L = \exp(\ell \oplus \mathbb{R}c)$ of G, and a choice of the complementary Lagrangian subspace ℓ' establishes the isomorphism

$$G/L \simeq \ell'. \tag{3.7}$$

The isomorphism $\Lambda^{2n}V^* \simeq \Lambda^n\ell^* \wedge \Lambda^n\ell'^*$ gives rise to the volume form $d^n\boldsymbol{v}'$ on ℓ' and defines a measure dg on the homogeneous space G/L. The measure dg is invariant under the left G-action and does not depend on the choice of ℓ'.

For a given $\hbar \in \mathbb{R}$, the function $\chi : L \to \mathbb{C}$,

$$\chi(\exp(v + \alpha c)) = e^{i\hbar\alpha}, \quad v \in V,\ \alpha \in \mathbb{R},$$

defines a one-dimensional unitary character of L,

$$\chi(l_1 l_2) = \chi(l_1)\chi(l_2), \quad l_1, l_2 \in L.$$

Definition. The Schrödinger representation S_ℓ of the Heisenberg group $G(V)$, associated with a Lagrangian subspace ℓ of V, is a representation of G induced by the one-dimensional representation χ of the corresponding abelian Lie group L,

$$S_\ell = \mathrm{Ind}_L^G \chi.$$

By definition of the induced representation, the Hilbert space $\mathscr{H}_\ell$ of the representation S_ℓ consists of measurable functions $f : G \to \mathbb{C}$ satisfying the property

$$f(gl) = \chi(l)^{-1} f(g), \quad g \in G,\ l \in L,$$

and such that

$$\|f\|^2 = \int_{G/L} |f(g)|^2 dg < \infty.$$

Corresponding unitary operators $S_\ell(g)$, $g \in G$, are defined by the left translations,

$$(S_\ell(g)f)(g') = f(g^{-1}g'), \quad f \in \mathscr{H}_\ell,\ g \in G.$$

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 $\mathscr{H}_\ell$.

For every Lagrangian subspace ℓ of V, the representation S_ℓ is unitarily equivalent to the Schrödinger representation. This can be explicitly shown as follows. By (3.7), a choice of a complementary Lagrangian subspace ℓ' gives rise to the unique decomposition $g = \exp v' \exp(v + \alpha c)$, and for $f \in \mathscr{H}_\ell$ we get

$$f(g) = f(\exp v' \exp(v + \alpha c)) = e^{-i\hbar\alpha} f(\exp v'), \quad v \in \ell,\ v' \in \ell',\ \alpha \in \mathbb{R}.$$

Thus every $f \in \mathscr{H}_\ell$ is completely determined by its restriction to $\exp \ell' \simeq \ell'$, and the mapping $\mathscr{U}_\ell : \mathscr{H}_\ell \to L^2(\ell', d^n\boldsymbol{v}')$, defined by

$$\mathscr{U}_\ell(f)(v') = f(\exp \tfrac{1}{\hbar} v'), \quad v' \in \ell',$$

is the isomorphism of Hilbert spaces. For the corresponding representation $\mathsf{S}_\ell = \mathscr{U}_\ell S_\ell \mathscr{U}_\ell^{-1}$ in $L^2(\ell', d^n\boldsymbol{v}')$ we have

$$(\mathsf{S}_\ell(\exp v)\psi)(v') = e^{i\omega(v,v')}\psi(v'), \quad v \in \ell,\ v' \in \ell',$$
$$(\mathsf{S}_\ell(\exp u')\psi)(v') = \psi(v' - \hbar u'), \quad u',\ v' \in \ell'.$$

Let $e^1, \dots, e^n, f_1, \dots, f_n$ be the symplectic basis for V such that

$$\ell = \mathbb{R}e^1 \oplus \cdots \oplus \mathbb{R}e^n \quad \text{and} \quad \ell' = \mathbb{R}f_1 \oplus \cdots \oplus \mathbb{R}f_n,$$

and let $(\boldsymbol{p}, \boldsymbol{q}) = (p_1, \dots, p_n, q^1, \dots, q^n)$ be the corresponding coordinates in V (see Section 2.6 in Chapter 1). Then $L^2(\ell', d^n\boldsymbol{v}') \simeq L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ and

$$\mathsf{S}_\ell(\exp \boldsymbol{u}X) = U(\boldsymbol{u}) \quad \text{and} \quad \mathsf{S}_\ell(\exp \boldsymbol{v}Y) = V(\boldsymbol{v}),$$

where $\boldsymbol{u}X = \sum_{k=1}^n u^k f_k$, $\boldsymbol{v}Y = \sum_{k=1}^n v_k e^k$, and $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{P}}$, $V(\boldsymbol{v}) = e^{-i\boldsymbol{v}\boldsymbol{Q}}$ are, respectively, n-parameter groups of unitary operators corresponding to momenta and coordinate operators $\boldsymbol{P}$ and $\boldsymbol{Q}$.

The mapping $*_h$ — the new associative product on $L^1(\mathbb{R}^{2n})$ introduced in the last section — can also be described in invariant terms. Let $B_\hbar = G/\Gamma_\hbar$ be the quotient group, where $\Gamma_\hbar = \{\exp(\frac{2\pi n}{\hbar} c) \in G \mid n \in \mathbb{Z}\}$ is a discrete central subgroup in G, and let $db = d^{2n}\boldsymbol{v} \wedge d^*\alpha$ be the left-invariant Haar measure on $B_\hbar$, where $d^*\alpha$ is the normalized Haar measure on the circle $\mathbb{R}/\frac{2\pi}{\hbar}\mathbb{Z}$. The Banach space $L^1(B_\hbar, db)$ has an algebra structure with respect to the convolution:

$$(\varphi_1 *_{B_\hbar} \varphi_2)(b) = \int_{B_\hbar} \varphi_1(b_1)\varphi_2(b_1^{-1}b)db_1, \quad \varphi_1, \varphi_2 \in L^1(B_\hbar, db).$$

The correspondence

$$L^1(V, d^{2n}\boldsymbol{v}) \ni f(v) \mapsto \varphi(\exp(v + \alpha c)) = e^{-i\hbar\alpha} f(v) \in L^1(B_\hbar, db)$$

defines the inclusion map $L^1(V, d^{2n}\boldsymbol{v}) \hookrightarrow L^1(B_\hbar, db)$, and the image of $L^1(V, d^{2n}\boldsymbol{v})$ is a subalgebra of $L^1(B_\hbar, db)$ under the convolution. We have for $f_1, f_2 \in L^1(V, d^{2n}\boldsymbol{v})$,

$$\begin{aligned}
(\varphi_1 *_{B_\hbar} \varphi_2)(\exp v) &= \int_{B_\hbar} \varphi_1(\exp(u + \alpha c))\varphi_2(\exp(-u - \alpha c)\exp v)d^{2n}\boldsymbol{v}d^*\alpha \\
&= \int_V \varphi_1(\exp u)\varphi_2(\exp(v - u)\exp(-\tfrac{1}{2}\omega(u, v)c))d^{2n}\boldsymbol{v} \\
&= \int_V f_1(u) f_2(v - u) e^{\frac{i\hbar}{2}\omega(u,v)} d^{2n}\boldsymbol{v} \\
&= (f_1 *_\hbar f_2)(v), \quad v \in V.
\end{aligned}$$

Problem 3.3. Prove that the Weyl transform is the restriction to $L^1(V, d^{2n}\boldsymbol{v})$ of the mapping

$$L^1(B_\hbar, db) \ni \varphi \mapsto \int_{B_\hbar} \varphi(b) S_\ell(b) db \in \mathscr{L}(\mathscr{H}_\ell).$$

Problem 3.4. Let ℓ_1, ℓ_2, ℓ_3 be Lagrangian subspaces of V. Define the *triple Maslov index* $\tau(\ell_1, \ell_2, \ell_3)$ as a signature of the quadratic form Q on $\ell_1 \oplus \ell_2 \oplus \ell_3$, defined by

$$Q(x_1, x_2, x_3) = \omega(x_1, x_2) + \omega(x_2, x_3) + \omega(x_3, x_1).$$

For Lagrangian subspaces ℓ_1, ℓ_2 of V let $\mathscr{F}_{\ell_2,\ell_1}$ be the unitary operator establishing the Hilbert space isomorphism $\mathscr{H}_{\ell_1} \simeq \mathscr{H}_{\ell_2}$ and intertwining representations S_{ℓ_1} and S_{ℓ_2},

$$\mathscr{F}_{\ell_2,\ell_1} S_{\ell_1}(g) = S_{\ell_2}(g) \mathscr{F}_{\ell_2,\ell_1}, \quad g \in G.$$

Prove that $\mathscr{F}_{\ell_1,\ell_3} \mathscr{F}_{\ell_3,\ell_2} \mathscr{F}_{\ell_2,\ell_1} = e^{-\pi i \tau(\ell_1,\ell_2,\ell_3)} I_1$, where I_1 is the identity operator in $\mathscr{H}_{\ell_1}$.

Problem 3.5. Let $\mathrm{Sp}(V)$ be the symplectic group of (V, ω) — the subgroup of $\mathrm{GL}(V)$, preserving the symplectic form ω. The group $\mathrm{Sp}(V)$ acts as a group of automorphisms of the Heisenberg group G by the formula $h \cdot \exp(v + \alpha c) = \exp(h \cdot v + \alpha c)$, $h \in \mathrm{Sp}(V)$, $v \in V$. Let R be an irreducible unitary representation of G in the Hilbert space $\mathscr{H}$. Show that there exist unitary operators $U(h)$, defined up to multiplication by complex numbers of modulus 1, such that

$$U(h) R(g) U(h)^{-1} = R(h \cdot g), \quad h \in \mathrm{Sp}(V), \ g \in G,$$

and that U defines a projective unitary representation of $\mathrm{Sp}(V)$ in $\mathscr{H}$, called the *Shale-Weil representation*. Find a realization of the Hilbert space $\mathscr{H}$ such that the 2-cocycle of the Shale-Weil representation is explicitly computed in terms of the Maslov index.

3.3. Weyl quantization. The Weyl transform, introduced in Section 3.1, defines a quantization of classical systems associated with the phase space $\mathbb{R}^{2n}$ with coordinates $\boldsymbol{p} = (p_1, \dots, p_n)$, $\boldsymbol{q} = (q^1, \dots, q^n)$, and the Poisson bracket $\{\ ,\ \}$ associated with the canonical symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$. Let

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

where W is the Weyl transform and $\mathscr{F}^{-1}$ is the inverse Fourier transform, be the linear mapping of the Schwartz space $\mathscr{S}(\mathbb{R}^{2n})$ of complex-valued functions of rapid decay on $\mathbb{R}^{2n}$ into the Banach space of bounded operators $\mathscr{L}(\mathscr{H})$ on $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$. It is given explicitly by the integral

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

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

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

and $S(\boldsymbol{u},\boldsymbol{v}) = e^{-\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v}}U(\boldsymbol{u})V(\boldsymbol{v})$. It follows from (3.6) that $\Phi(f)$ is an integral operator: for every $\psi \in L^2(\mathbb{R}^n, d^n\boldsymbol{q})$,

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

where

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

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

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

so that classical observables — real-valued functions on $\mathbb{R}^{2n}$, correspond to quantum observables — self-adjoint operators in $\mathscr{H}$. It follows from the property **WT3** in Section 3.1 that the mapping Φ is injective; its image $\operatorname{Im}\Phi$ and the inverse mapping Φ^{-1} are explicitly described as follows.

Proposition 3.1. *The subspace* $\operatorname{Im}\Phi \subset \mathscr{L}(\mathscr{H})$ *consists of operators* $B \in \mathscr{S}_1$ *such that corresponding functions* $g(\boldsymbol{u},\boldsymbol{v}) = \hbar^n \operatorname{Tr}(B\,S(\boldsymbol{u},\boldsymbol{v})^{-1})$ *belong to the Schwartz class* $\mathscr{S}(\mathbb{R}^{2n})$*; in this case* $W(g) = B$*. The inverse mapping* $\Phi^{-1} = \mathscr{F}\circ W^{-1}$ *is given by the Weyl's inversion formula*

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

Proof. 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 $\omega = 1$. According to Theorem 2.1, the operator H has a complete orthonormal system of real-valued eigenfunctions $\psi_n(q)$, given by Hermite-Tchebyscheff functions, with the eigenvalues $\hbar(n+\frac{1}{2})$, so that the inverse operator $H^{-1} \in \mathscr{S}_2$. The operator $H\Phi(f)$ is an integral operator with the kernel $\frac{1}{2}(-\hbar^2\frac{\partial^2}{\partial q^2} + q^2)K(q,q')$, which is a Schwartz class function on $\mathbb{R}^2$, so that $H\Phi(f) \in \mathscr{S}_2$. The operator

$$\Phi(f) = H^{-1}H\Phi(f)$$

is a product of Hilbert-Schmidt operators and, therefore, is of trace class. Using the orthonormal basis $\{\psi_n(q)\}_{n=0}^{\infty}$ for $\mathscr{H} = L^2(\mathbb{R})$, we get

$$K(q,q') = \sum_{m,n=0}^{\infty} c_{mn}\psi_n(q)\psi_m(q'), \tag{3.8}$$

where

$$c_{mn} = \int_{\mathbb{R}^2} K(q,q')\psi_n(q)\psi_m(q')dqdq',$$

and the series (3.8) converges in $L^2(\mathbb{R}^2)$. Since $K \in \mathscr{S}(\mathbb{R}^2)$, it follows from the N-representation theorem (see Problem 2.13) that this series is also convergent in the $\mathscr{S}(\mathbb{R}^2)$ topology. It is this fact which allows us to set $q' = q$ in (3.8) and to get the expansion

$$K(q,q) = \sum_{m,n=0}^{\infty} c_{mn}\psi_n(q)\psi_m(q),$$

which converges in $\mathscr{S}(\mathbb{R})$. Thus we obtain

$$\operatorname{Tr}\Phi(f) = \sum_{n=0}^{\infty}(\Phi(f)\psi_n,\psi_n) = \sum_{n=0}^{\infty} c_{nn} = \int_{-\infty}^{\infty} K(q,q)dq,$$

where the interchange of orders of summation and integration is legitimate.

The general case $n > 1$ is similar. We consider the operator

$$H = \frac{\boldsymbol{P}^2 + \boldsymbol{Q}^2}{2}$$

and use the fact that operators $H^n\Phi(f)$ and H^{-n} are Hilbert-Schmidt. To prove the formula

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

we expand the kernel $K(\boldsymbol{q},\boldsymbol{q}')$ using the orthonormal basis $\{\psi_{\boldsymbol{k}}(\boldsymbol{q})\}_{\boldsymbol{k},=0}^{\infty}$ for $L^2(\mathbb{R}^n)$, where

$$\psi_{\boldsymbol{k}}(\boldsymbol{q}) = \psi_{k_1}(q_1)\cdots\psi_{k_n}(q_n), \quad \boldsymbol{k} = (k_1,\dots,k_n).$$

From the explicit form of the kernel K we get

$$\operatorname{Tr}\Phi(f) = \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \check{f}(0,\boldsymbol{v})e^{-i\boldsymbol{v}\boldsymbol{q}}d^n\boldsymbol{v}\,d^n\boldsymbol{q} = \hbar^{-n}\check{f}(0,0), \tag{3.9}$$

which gives the inversion formula for $\boldsymbol{u} = \boldsymbol{v} = 0$. To get the inversion formula for all $\boldsymbol{u},\boldsymbol{v} \in \mathbb{R}^n$, it is sufficient to apply (3.9) to the function $f_{\boldsymbol{u}\boldsymbol{v}} = \mathscr{F}(\check{f}_{\boldsymbol{u},\boldsymbol{v}})$, where

$$\check{f}_{\boldsymbol{u},\boldsymbol{v}}(\boldsymbol{u}',\boldsymbol{v}') = \check{f}(\boldsymbol{u}+\boldsymbol{u}',\boldsymbol{v}+\boldsymbol{v}')e^{\frac{i\hbar}{2}(\boldsymbol{v}'\boldsymbol{u}-\boldsymbol{u}'\boldsymbol{v})},$$

and to use $S(\boldsymbol{u},\boldsymbol{v})^{-1} = S(\boldsymbol{u},\boldsymbol{v})^* = S(-\boldsymbol{u},-\boldsymbol{v})$ and the property **WT2** in Section 3.1,

$$W(\check{f})S(-\boldsymbol{u},-\boldsymbol{v}) = W(\check{f}_{\boldsymbol{u},\boldsymbol{v}}).$$

To complete the proof, we need to show that $\operatorname{Im}\Phi$ consists of all $B \in \mathscr{S}_1$ with the property that the function $g(\boldsymbol{u},\boldsymbol{v}) = \hbar^n \operatorname{Tr}(B\,S(\boldsymbol{u},\boldsymbol{v})^{-1})$ belongs to the Schwartz class. By the inversion formula,

$$g(\boldsymbol{u},\boldsymbol{v}) = \hbar^n \operatorname{Tr}(\Phi(f)\,S(\boldsymbol{u},\boldsymbol{v})^{-1}),$$

where $f = \mathscr{F}(g)$, so it is sufficient to prove that if

$$\operatorname{Tr}(B\, S(\boldsymbol{u}, \boldsymbol{v})^{-1}) = 0$$

for all $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n$, then $B = 0$. Indeed, multiplying by $\overline{f(\boldsymbol{u}, \boldsymbol{v})}$ and integrating, we get

$$\operatorname{Tr} BW(f)^* = 0$$

for all $f \in \mathscr{S}(\mathbb{R}^{2n})$. Since Schwartz class functions are dense in $L^2(\mathbb{R}^{2n})$, by Lemma 3.1 we get $\operatorname{Tr} BB^* = 0$ and, therefore, $B = 0$. □

Corollary 3.3.

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

Remark. By the Schwartz kernel theorem, the operator $S(\boldsymbol{u}, \boldsymbol{v})$ is an integral operator with the distributional kernel

$$e^{\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v} - i\boldsymbol{v}\boldsymbol{q}}\, \delta(\boldsymbol{q} - \boldsymbol{q}' - \hbar\boldsymbol{u}),$$

so that

$$\operatorname{Tr} S(\boldsymbol{u}, \boldsymbol{v}) = \left(\frac{2\pi}{\hbar}\right)^n \delta(\boldsymbol{u})\delta(\boldsymbol{v}).$$

Thus, as is customary in physics texts,

$$\operatorname{Tr} \Phi(f) = \hbar^{-n} \int_{\mathbb{R}^n} \check{f}(\boldsymbol{u}, \boldsymbol{v})\delta(\boldsymbol{u})\delta(\boldsymbol{v}) d^n\boldsymbol{u}\, d^n\boldsymbol{v} = \hbar^{-n} \check{f}(0, 0).$$

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

Proposition 3.2. *The mapping $\mathcal{A}_0 \ni f \mapsto \Phi(f) \in \mathscr{A}_0$ is a quantization, i.e., it satisfies*

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

and the correspondence principle

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

where

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

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

Proof. In terms of the product $*_\hbar$ introduced in Section 3.1 we have

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

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

$$\Phi^{-1}(\Phi(f_1)\Phi(f_2))(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{(2\pi)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}} \check{f}_1(\boldsymbol{u}_1,\boldsymbol{v}_1)\check{f}_2(\boldsymbol{u}_2,\boldsymbol{v}_2)\cdot \tag{3.10}$$
$$\cdot\, e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1)-i(\boldsymbol{u}_1+\boldsymbol{u}_2)\boldsymbol{p}-i(\boldsymbol{v}_1+\boldsymbol{v}_2)\boldsymbol{q}} d^n\boldsymbol{u}_1 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_1 d^n\boldsymbol{v}_2.$$

Using the expansion

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

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

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

we get from (3.10) that as $\hbar\to 0$,

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

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

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

$$K(\boldsymbol{q},\boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} f(\boldsymbol{p},\tfrac{\boldsymbol{q}+\boldsymbol{q}'}{2})e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')}d^n\boldsymbol{p}, \tag{3.11}$$

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

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

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

$$f(\boldsymbol{p},\boldsymbol{q}) = \int_{\mathbb{R}^n} K(\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v},\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v})e^{\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{v}}d^n\boldsymbol{v}. \tag{3.12}$$

The distribution $f(\boldsymbol{p},\boldsymbol{q})$ defined by (3.12) is called the *Weyl symbol* of the operator in $L^2(\mathbb{R}^n,d^n\boldsymbol{q})$ with the Schwartz kernel $K(\boldsymbol{q},\boldsymbol{q}')$.

Examples below describe classes of distributions f such that the operators $\Phi(f)$ are essentially self-adjoint unbounded operators on the domain $\mathscr{S}(\mathbb{R}^n)\subset L^2(\mathbb{R}^n,d^n\boldsymbol{q})$.

Example 3.1. Let $f = f(\boldsymbol{q}) \in L^p(\mathbb{R}^n)$ for some $1 \le p \le \infty$, or let f be a polynomially bounded function as $|\boldsymbol{q}| \to \infty$. In the distributional sense,

$$\check{f}(\boldsymbol{u}, \boldsymbol{v}) = (2\pi)^{n/2} \delta(\boldsymbol{u}) \check{f}(\boldsymbol{v})$$

so that

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

Thus the operator $\Phi(f)$ is a multiplication by $f(\boldsymbol{q})$ operator on $L^2(\mathbb{R}^n)$. In particular, coordinates $\boldsymbol{q}$ in classical mechanics correspond to coordinate operators $\boldsymbol{Q}$ in quantum mechanics. Similarly, if $f = f(\boldsymbol{p})$, then $\Phi(f) = f(\boldsymbol{P})$. In particular, momenta $\boldsymbol{p}$ in classical mechanics correspond to the momenta operators $\boldsymbol{P}$ in quantum mechanics.

Example 3.2. Let

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

be the Hamiltonian function in classical mechanics. Then $H = \Phi(H_{\mathrm{c}})$ is the corresponding Hamiltonian operator in quantum mechanics,

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

In Chapter 3 we give necessary conditions for the operator H to be essentially self-adjoint.

Example 3.3. Here we find $f \in \mathscr{S}(\mathbb{R}^{2n})'$ such that

$$\Phi(f) = P_\psi$$

— a pure state P_ψ, where $\psi \in L^2(\mathbb{R}^n)$, $\|\psi\| = 1$. The projection P_ψ is an integral operator with the kernel $\psi(\boldsymbol{q})\overline{\psi(\boldsymbol{q}')}$, and we get from (3.11),

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

Introducing $\boldsymbol{q}_+ = \frac{1}{2}(\boldsymbol{q}+\boldsymbol{q}'), \boldsymbol{q}_- = \frac{1}{2}(\boldsymbol{q}-\boldsymbol{q}')$, we obtain

$$\check{f}(\tfrac{2\boldsymbol{q}_-}{\hbar}, \boldsymbol{v}) = \hbar^n \int_{\mathbb{R}^n} \psi(\boldsymbol{q}_- + \boldsymbol{q}_+)\overline{\psi(\boldsymbol{q}_+ - \boldsymbol{q}_-)} e^{i\boldsymbol{v}\boldsymbol{q}_+} d^n\boldsymbol{q}_+,$$

or

$$\check{f}(\boldsymbol{u}, \boldsymbol{v}) = \hbar^n \int_{\mathbb{R}^n} \psi(\boldsymbol{q} + \tfrac{1}{2}\hbar\boldsymbol{u})\overline{\psi(\boldsymbol{q} - \tfrac{1}{2}\hbar\boldsymbol{u})} e^{i\boldsymbol{v}\boldsymbol{q}} d^n\boldsymbol{q}.$$

Assuming that ψ does not depend on $\hbar$, we get in accordance with Corollary 3.3,

$$\check{\rho}(\boldsymbol{u}, \boldsymbol{v}) = \lim_{\hbar\to 0} \frac{1}{(2\pi\hbar)^n} \check{f}(\boldsymbol{u}, \boldsymbol{v}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} |\psi(\boldsymbol{q})|^2 e^{i\boldsymbol{v}\boldsymbol{q}} d^n\boldsymbol{v}.$$

Thus in the classical limit $\hbar \to 0$ the pure state P_ψ in quantum mechanics becomes a mixed state in classical mechanics, given by a probability measure $d\mu = \rho(\boldsymbol{p}, \boldsymbol{q}) d^n\boldsymbol{p}\, d^n\boldsymbol{q}$ on $\mathbb{R}^{2n}$ with the density

$$\rho(\boldsymbol{p}, \boldsymbol{q}) = \delta(\boldsymbol{p})|\psi(\boldsymbol{q})|^2.$$

It describes a classical particle at rest ($\boldsymbol{p} = 0$) with the distribution of coordinates given by the probability measure $|\psi(\boldsymbol{q})|^2 d^n\boldsymbol{q}$ on $\mathbb{R}^n$. When $\psi(\boldsymbol{q}) = e^{\frac{i}{\hbar}\boldsymbol{p}_0\boldsymbol{q}}\varphi(\boldsymbol{q})$, where $\varphi(\boldsymbol{q})$ does not depend on $\hbar$, the corresponding density is $\rho(\boldsymbol{p}, \boldsymbol{q}) = \delta(\boldsymbol{p} - \boldsymbol{p}_0)|\varphi(\boldsymbol{q})|^2$.

Remark. The Weyl quantization can be considered as a way of defining a function $f(\boldsymbol{P}, \boldsymbol{Q})$ of non-commuting operators $\boldsymbol{P} = (P_1, \dots, P_n)$ and $\boldsymbol{Q} = (Q^1, \dots, Q^n)$ by setting

$$f(\boldsymbol{P}, \boldsymbol{Q}) = \Phi(f).$$

In particular, if $f(\boldsymbol{p}, \boldsymbol{q}) = g(\boldsymbol{p}) + h(\boldsymbol{q})$, then

$$f(\boldsymbol{P}, \boldsymbol{Q}) = g(\boldsymbol{P}) + h(\boldsymbol{Q}).$$

For $f(\boldsymbol{p}, \boldsymbol{q}) = \boldsymbol{p}\boldsymbol{q} = p_1 q^1 + \dots + p_n q^n$ we get, using (3.11),

$$f(\boldsymbol{P}, \boldsymbol{Q}) = \frac{\boldsymbol{P}\boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{P}}{2}.$$

This shows that the Weyl quantization symmetrizes products of the non-commuting factors $\boldsymbol{P}$ and $\boldsymbol{Q}$. In general, let f be a polynomial function,

$$f(\boldsymbol{p}, \boldsymbol{q}) = \sum_{|\alpha|, |\beta| \le N} c_{\alpha\beta}\, \boldsymbol{p}^\alpha \boldsymbol{q}^\beta, \tag{3.13}$$

where for the multi-indices $\alpha = (\alpha_1, \dots, \alpha_n)$ and $\beta = (\beta_1, \dots, \beta_n)$,

$$\boldsymbol{p}^\alpha = p_1^{\alpha_1} \dots p_n^{\alpha_n}, \quad \boldsymbol{q}^\beta = (q^1)^{\beta_1} \dots (q^n)^{\beta_n},$$

and $|\alpha| = \alpha_1 + \dots + \alpha_n, \quad |\beta| = \beta_1 + \dots + \beta_n$. Using (3.11), we get the following formula

$$\Phi(f) = \sum_{|\alpha|, |\beta| \le N} c_{\alpha\beta}\, \mathrm{Sym}(\boldsymbol{P}^\alpha \boldsymbol{Q}^\beta). \tag{3.14}$$

Here $\mathrm{Sym}(\boldsymbol{P}^\alpha \boldsymbol{Q}^\beta)$ is a symmetric product, defined by

$$(\boldsymbol{u}\boldsymbol{P} + \boldsymbol{v}\boldsymbol{Q})^k = \sum_{|\alpha| + |\beta| = k} \frac{k!}{\alpha!\beta!} \boldsymbol{u}^\alpha \boldsymbol{v}^\beta\, \mathrm{Sym}(\boldsymbol{P}^\alpha \boldsymbol{Q}^\beta), \tag{3.15}$$

where $\boldsymbol{u}\boldsymbol{P} + \boldsymbol{v}\boldsymbol{Q} = u^1 P_1 + \dots + u^n P_n + v_1 Q^1 + \dots + v_n Q^n$ and

$$\alpha! = \alpha_1! \dots \alpha_n!, \quad \beta! = \beta_1! \dots \beta_n!.$$

Remark. In addition to the Weyl quantization Φ, consider also the mappings $\Phi_1 : \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H})$ and $\Phi_2 : \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H})$, defined by

$$\Phi_1(f) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \check{f}(\boldsymbol{u}, \boldsymbol{v}) e^{\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v}} S(\boldsymbol{u}, \boldsymbol{v}) d^n\boldsymbol{u}\, d^n\boldsymbol{v}$$

and

$$\Phi_2(f) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \check{f}(\boldsymbol{u}, \boldsymbol{v}) e^{-\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v}} S(\boldsymbol{u}, \boldsymbol{v}) d^n\boldsymbol{u}\, d^n\boldsymbol{v},$$

where $\check{f} = \mathscr{F}^{-1}(f)$ is the inverse Fourier transform. Though Φ_1 and Φ_2 no longer map $\mathcal{A}_0$ into the real vector space $\mathscr{A}_0$ of bounded quantum observables, they satisfy all the properties in Proposition 3.2. It follows from (3.5) that for $f \in \mathscr{S}(\mathbb{R}^{2n})$ the operators $\Phi_1(f)$ and $\Phi_2(f)$ are integral operators with the integral kernels

$$K_1(\boldsymbol{q}, \boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} f(\boldsymbol{p}, \boldsymbol{q}') e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')} d^n\boldsymbol{p}$$

and

$$K_2(\boldsymbol{q}, \boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} f(\boldsymbol{p}, \boldsymbol{q}) e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')} d^n\boldsymbol{p},$$

respectively. As in the case of the Weyl quantization, these formulas extend the mappings $f \mapsto \Phi_1(f)$ and $f \mapsto \Phi_2(f)$ of the space $\mathscr{S}(\mathbb{R}^{2n})'$ of tempered distributions on $\mathbb{R}^{2n}$. In particular, if $f(\boldsymbol{p}, \boldsymbol{q})$ is a polynomial function (3.13), then

$$\Phi_1(f) = \sum_{|\alpha|,|\beta|\le N} c_{\alpha\beta}\, \boldsymbol{P}^\alpha \boldsymbol{Q}^\beta \tag{3.16}$$

and

$$\Phi_2(f) = \sum_{|\alpha|,|\beta|\le N} c_{\alpha\beta}\, \boldsymbol{Q}^\beta \boldsymbol{P}^\alpha. \tag{3.17}$$

Therefore the mapping $f \mapsto \Phi_1(f)$ is called the ***pq**-quantization*, and the mapping $f \mapsto \Phi_2(f)$ — the ***qp**-quantization*. Corresponding inversion formulas are

$$f(\boldsymbol{p}, \boldsymbol{q}) = \int_{\mathbb{R}^n} K_1(\boldsymbol{q} - \boldsymbol{v}, \boldsymbol{q}) e^{\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{v}} d^n\boldsymbol{v} \tag{3.18}$$

and

$$f(\boldsymbol{p}, \boldsymbol{q}) = \int_{\mathbb{R}^n} K_2(\boldsymbol{q}, \boldsymbol{q} + \boldsymbol{v}) e^{\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{v}} d^n\boldsymbol{v}. \tag{3.19}$$

The distribution $f(\boldsymbol{p}, \boldsymbol{q})$ defined by (3.18) is called the ***pq**-symbol* of an operator with the Schwartz kernel $K_1(\boldsymbol{q}, \boldsymbol{q}')$, and the distribution $f(\boldsymbol{p}, \boldsymbol{q})$ defined by (3.19) — the ***qp**-symbol* of an operator with the Schwartz kernel $K_2(\boldsymbol{q}, \boldsymbol{q}')$. The ***qp***-symbols are commonly used in the theory of pseudodifferential operators. It follows from (3.18) and (3.19) that if $f(\boldsymbol{p}, \boldsymbol{q})$ is a ***pq***-symbol of the operator $\Phi_1(f)$, then $\overline{f(\boldsymbol{p}, \boldsymbol{q})}$ is a ***qp***-symbol of the adjoint operator $\Phi_1(f)^*$.

Problem 3.6. Prove formula (3.14).

Problem 3.7. Prove formulas (3.16)-(3.17).

Problem 3.8. Prove that Weyl, $\boldsymbol{pq}$, and $\boldsymbol{qp}$-quantizations are equivalent. (*Hint:* Find the relations between Weyl, $\boldsymbol{pq}$, and $\boldsymbol{qp}$-symbols of a given operator.)

3.4. The $\star$-product. The Weyl quantization $\Phi : \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H})$, studied in the previous section, defines a new bilinear operation

$$\star_\hbar : \mathscr{S}(\mathbb{R}^{2n}) \times \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{S}(\mathbb{R}^{2n})$$

on $\mathscr{S}(\mathbb{R}^{2n})$ by the formula

$$f_1 \star_\hbar f_2 = \Phi^{-1}(\Phi(f_1)\Phi(f_2)).$$

This operation is called the $\star$-product[26]. According to (3.10),

$$(f_1 \star_\hbar f_2)(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{(2\pi)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} \check{f}_1(\boldsymbol{u}_1,\boldsymbol{v}_1)\check{f}_2(\boldsymbol{u}_2,\boldsymbol{v}_2) \cdot \tag{3.20}$$
$$\cdot\, e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1)-i(\boldsymbol{u}_1+\boldsymbol{u}_2)\boldsymbol{p}-i(\boldsymbol{v}_1+\boldsymbol{v}_2)\boldsymbol{q}} d^n\boldsymbol{u}_1 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_1 d^n\boldsymbol{v}_2.$$

The $\star$-product on $\mathscr{S}(\mathbb{R}^{2n})$ has the following properties.

1. Associativity:

$$f_1 \star_\hbar (f_2 \star_\hbar f_3) = (f_1 \star_\hbar f_2) \star_\hbar f_3.$$

2. Semi-classical limit:

$$(f_1 \star_\hbar f_2)(\boldsymbol{p},\boldsymbol{q}) = (f_1 f_2)(\boldsymbol{p},\boldsymbol{q}) - \tfrac{i\hbar}{2}\{f_1,f_2\}(\boldsymbol{p},\boldsymbol{q}) + O(\hbar^2) \text{ as } \hbar \to 0.$$

3. Property of the unit:

$$f \star_\hbar \mathbf{1} = \mathbf{1} \star_\hbar f,$$

where $\mathbf{1}$ is a function which identically equals 1 on $\mathbb{R}^{2n}$.

4. The cyclic trace property:

$$\tau(f_1 \star_\hbar f_2) = \tau(f_2 \star_\hbar f_1),$$

where the $\mathbb{C}$-linear map $\tau : \mathscr{S}(\mathbb{R}^{2n}) \to \mathbb{C}$ is defined by

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

Property **1** follows from the corresponding property for the product $*_\hbar$ (see Section 3.1), property **2** follows from Proposition 3.2, and properties **3** and **4** directly follow from the definition (3.20). The complex vector space $\mathscr{S}(\mathbb{R}^{2n}) \oplus \mathbb{C}\,\mathbf{1}$ with the bilinear operation $\star_\hbar$ is an associative algebra over $\mathbb{C}$ with unit $\mathbf{1}$ and the cyclic trace τ, satisfying the correspondence principle,

$$\lim_{\hbar\to 0} \tfrac{i}{\hbar}(f_1 \star_\hbar f_2 - f_2 \star_\hbar f_1) = \{f_1,f_2\}.$$

[26] Also called *Moyal product* in physics.

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 define the unitary operator $\boldsymbol{U}_1$ on $L^2(\mathbb{R}^{2n}) \otimes L^2(\mathbb{R}^{2n})$ by

$$\boldsymbol{U}_1 = e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial \boldsymbol{p}} \otimes \frac{\partial}{\partial \boldsymbol{q}}\right)},$$

where

$$\frac{\partial}{\partial \boldsymbol{p}} \otimes \frac{\partial}{\partial \boldsymbol{q}} = \sum_{k=1}^{n} \frac{\partial}{\partial p_k} \otimes \frac{\partial}{\partial q^k}.$$

It follows from the theory of Fourier transform that for $f_1, f_2 \in \mathscr{S}(\mathbb{R}^{2n})$,

$$\left(\boldsymbol{U}_1(f_1 \otimes f_2)\right)(\boldsymbol{p}_1, \boldsymbol{q}_1, \boldsymbol{p}_2, \boldsymbol{q}_2) = \frac{1}{(2\pi)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} \check{f}_1(\boldsymbol{u}_1, \boldsymbol{v}_1) \check{f}_2(\boldsymbol{u}_2, \boldsymbol{v}_2) \cdot$$
$$\cdot\, e^{\frac{i\hbar}{2}\boldsymbol{u}_1\boldsymbol{v}_2 - i\boldsymbol{u}_1\boldsymbol{p}_1 - i\boldsymbol{u}_2\boldsymbol{p}_2 - i\boldsymbol{v}_1\boldsymbol{q}_1 - i\boldsymbol{v}_2\boldsymbol{q}_2} d^n\boldsymbol{u}_1 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_1 d^n\boldsymbol{v}_2.$$

Similarly, defining the unitary operator $\boldsymbol{U}_2$ on $L^2(\mathbb{R}^{2n}) \otimes L^2(\mathbb{R}^{2n})$ by

$$\boldsymbol{U}_2 = e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial \boldsymbol{q}} \otimes \frac{\partial}{\partial \boldsymbol{p}}\right)},$$

we get

$$\left(\boldsymbol{U}_2(f_1 \otimes f_2)\right)(\boldsymbol{p}_1, \boldsymbol{q}_1, \boldsymbol{p}_2, \boldsymbol{q}_2) = \frac{1}{(2\pi)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} \check{f}_1(\boldsymbol{u}_1, \boldsymbol{v}_1) \check{f}_2(\boldsymbol{u}_2, \boldsymbol{v}_2) \cdot$$
$$\cdot\, e^{\frac{i\hbar}{2}\boldsymbol{u}_2\boldsymbol{v}_1 - i\boldsymbol{u}_1\boldsymbol{p}_1 - i\boldsymbol{u}_2\boldsymbol{p}_2 - i\boldsymbol{v}_1\boldsymbol{q}_1 - \boldsymbol{v}_2\boldsymbol{q}_2} d^n\boldsymbol{u}_1 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_1 d^n\boldsymbol{v}_2.$$

Finally, define the unitary operator $\boldsymbol{U}_\hbar$ on $L^2(\mathbb{R}^{2n}) \otimes L^2(\mathbb{R}^{2n})$ by

$$\boldsymbol{U}_\hbar = \boldsymbol{U}_1 \boldsymbol{U}_2^{-1} = e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial \boldsymbol{p}} \otimes \frac{\partial}{\partial \boldsymbol{q}} - \frac{\partial}{\partial \boldsymbol{q}} \otimes \frac{\partial}{\partial \boldsymbol{p}}\right)},$$

and denote by $m : \mathscr{S}(\mathbb{R}^{2n}) \otimes \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{S}(\mathbb{R}^{2n})$ the point-wise product of functions, $(m(f_1 \otimes f_2))(\boldsymbol{p}, \boldsymbol{q}) = f_1(\boldsymbol{p}, \boldsymbol{q}) f_2(\boldsymbol{p}, \boldsymbol{q})$. Then the $\star$-product can be written in the following concise form:

$$f_1 \star_\hbar f_2 = (m \circ \boldsymbol{U}_\hbar)\,(f_1 \otimes f_2). \tag{3.21}$$

In analogy with the Poisson bracket $\{\ ,\ \}$ on $\mathbb{R}^{2n}$ associated with the canonical symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$,

$$\{f_1, f_2\} = \frac{\partial f_1}{\partial \boldsymbol{p}} \frac{\partial f_2}{\partial \boldsymbol{q}} - \frac{\partial f_1}{\partial \boldsymbol{q}} \frac{\partial f_2}{\partial \boldsymbol{p}},$$

we introduce the notation

$$\{\ \overset{\otimes}{,}\ \} = \frac{\partial}{\partial \boldsymbol{p}} \otimes \frac{\partial}{\partial \boldsymbol{q}} - \frac{\partial}{\partial \boldsymbol{q}} \otimes \frac{\partial}{\partial \boldsymbol{p}} = \frac{\partial^2}{\partial \boldsymbol{p}_1 \partial \boldsymbol{q}_2} - \frac{\partial^2}{\partial \boldsymbol{q}_1 \partial \boldsymbol{p}_2}.$$

Then it follows from the theory of Fourier transform that formula (3.21) for the $\star$-product can be rewritten as

$$(f_1 \star_\hbar f_2)(\boldsymbol{p}, \boldsymbol{q}) = \left(e^{-\frac{i\hbar}{2}\{\ \overset{\otimes}{,}\ \}} f_1(\boldsymbol{p}_1, \boldsymbol{q}_1) f_2(\boldsymbol{p}_2, \boldsymbol{q}_2)\right) \Big|_{\substack{\boldsymbol{p}_1 = \boldsymbol{p}_2 = \boldsymbol{p} \\ \boldsymbol{q}_1 = \boldsymbol{q}_2 = \boldsymbol{q}}}. \tag{3.22}$$

Thus we have shown that on $\mathscr{S}(\mathbb{R}^{2n})$ the $\star$-product can be equivalently defined by (3.20), or by (3.21) and (3.22). The latter representation has the advantage that the formal expansion of the exponential $e^{-\frac{i\hbar}{2}\{\overset{\otimes}{,}\}}$ into the power series gives the asymptotic expansion of the $\star$-product as $\hbar \to 0$. Namely, define the bidifferential operators

$$B_k : \mathscr{S}(\mathbb{R}^{2n}) \otimes \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{S}(\mathbb{R}^{2n})$$

by $B_k = m \circ \{\overset{\otimes}{,}\}^k$ for $k \geq 1$ and $B_0 = m$.

Lemma 3.2. *For every $f_1, f_2 \in \mathscr{S}(\mathbb{R}^{2n})$ and $l \in \mathbb{N}$ there is $C > 0$ such that for all $\boldsymbol{p}, \boldsymbol{q} \in \mathbb{R}^{2n}$*

$$\left| (f_1 \star_\hbar f_2)(\boldsymbol{p}, \boldsymbol{q}) - \sum_{k=0}^{l} \frac{(-i\hbar)^k}{2^k k!} B_k(f_1, f_2)(\boldsymbol{p}, \boldsymbol{q}) \right| \leq C\hbar^{l+1} \quad \textit{as} \quad \hbar \to 0.$$

Succinctly,

$$(f_1 \star_\hbar f_2)(\boldsymbol{p}, \boldsymbol{q}) = \sum_{k=0}^{\infty} \frac{(-i\hbar)^k}{2^k k!} B_k(f_1, f_2)(\boldsymbol{p}, \boldsymbol{q}) + O(\hbar^\infty). \tag{3.23}$$

Proof. Expanding the exponential function $e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2 - \boldsymbol{u}_2\boldsymbol{v}_1)}$ into the power series and repeating the proof of Proposition 3.2 gives the result. □

Finally, we get another integral representation for the $\star$-product. Applying the Fourier inversion formula to the integral over $d^n\boldsymbol{u}_1 d^n\boldsymbol{v}_1$ in (3.20), we get

$$\begin{aligned}(f_1 \star_\hbar f_2)(\boldsymbol{p}, \boldsymbol{q}) &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f_1(\boldsymbol{p} - \tfrac{\hbar}{2}\boldsymbol{v}_2, \boldsymbol{q} + \tfrac{\hbar}{2}\boldsymbol{u}_2) \check{f}_2(\boldsymbol{u}_2, \boldsymbol{v}_2) \cdot \\ &\qquad \cdot e^{-i\boldsymbol{u}_2\boldsymbol{p} - i\boldsymbol{v}_2\boldsymbol{q}} d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_2 \\ &= \frac{1}{(2\pi)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} f_1(\boldsymbol{p} - \tfrac{\hbar}{2}\boldsymbol{v}_2, \boldsymbol{q} + \tfrac{\hbar}{2}\boldsymbol{u}_2) f_2(\boldsymbol{p}_2, \boldsymbol{q}_2) \cdot \\ &\qquad \cdot e^{-i\boldsymbol{u}_2\boldsymbol{p} - i\boldsymbol{v}_2\boldsymbol{q} + i\boldsymbol{u}_2\boldsymbol{p}_2 + i\boldsymbol{v}_2\boldsymbol{q}_2} d^n\boldsymbol{p}_2 d^n\boldsymbol{q}_2 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_2,\end{aligned}$$

and changing variables $\boldsymbol{p}_1 = \boldsymbol{p} - \frac{\hbar}{2}\boldsymbol{v}_2$, $\boldsymbol{q}_1 = \boldsymbol{q} + \frac{\hbar}{2}\boldsymbol{u}_2$, we obtain

$$\begin{aligned}(f_1 \star_\hbar f_2)(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{(\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} f_1(\boldsymbol{p}_1, \boldsymbol{q}_1) f_2(\boldsymbol{p}_2, \boldsymbol{q}_2) \cdot \\ \cdot e^{\frac{2i}{\hbar}(\boldsymbol{p}_1\boldsymbol{q} - \boldsymbol{p}\boldsymbol{q}_1 + \boldsymbol{q}_1\boldsymbol{p}_2 - \boldsymbol{q}_2\boldsymbol{p}_1 + \boldsymbol{p}\boldsymbol{q}_2 - \boldsymbol{p}_2\boldsymbol{q})} d^n\boldsymbol{p}_1 d^n\boldsymbol{q}_1 d^n\boldsymbol{p}_2 d^n\boldsymbol{q}_2.\end{aligned}$$

Let $\triangle$ be a Euclidean triangle (a 2-simplex) in the phase space $\mathbb{R}^{2n}$ with the vertices $(\boldsymbol{p}, \boldsymbol{q})$, $(\boldsymbol{p}_1, \boldsymbol{q}_1)$, and $(\boldsymbol{p}_2, \boldsymbol{q}_2)$. It is easy to see that

$$\boldsymbol{p}_1\boldsymbol{q} - \boldsymbol{p}\boldsymbol{q}_1 + \boldsymbol{q}_1\boldsymbol{p}_2 - \boldsymbol{q}_2\boldsymbol{p}_1 + \boldsymbol{p}\boldsymbol{q}_2 - \boldsymbol{p}_2\boldsymbol{q} = 2\int_{\triangle} \omega,$$

which is twice the symplectic area of $\triangle$ — the sum of oriented areas of the projections of $\triangle$ onto two-dimensional planes $(p_1, q^1), \ldots, (p_n, q^n)$. Thus we have the final formula

$$(f_1 \star_\hbar f_2)(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{(\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} f_1(\boldsymbol{p}_1, \boldsymbol{q}_1) f_2(\boldsymbol{p}_2, \boldsymbol{q}_2) \cdot \cdot e^{\frac{4i}{\hbar} \int_\triangle \omega} d^n\boldsymbol{p}_1 d^n\boldsymbol{q}_1 d^n\boldsymbol{p}_2 d^n\boldsymbol{q}_2, \tag{3.24}$$

which is a composition formula for the Weyl symbols.

Remark. It is instructive to compare formulas (3.23) and (3.24). The latter formula represents the $\star$-product on $\mathscr{S}(\mathbb{R}^{2n})$ as an absolutely convergent integral, and is equivalent to the Weyl quantization. The former formula is an asymptotic expansion of the $\star$-product as $\hbar \to 0$, and does not capture all properties of the Weyl quantization. In general, the power series in (3.23) diverges; for polynomial functions this series becomes a finite sum and gives a formula for the $\star$-product of polynomials.

Problem 3.9 (Composition formula for $\boldsymbol{pq}$-symbols)**.** Let $f_1(\boldsymbol{p}, \boldsymbol{q})$ and $f_2(\boldsymbol{p}, \boldsymbol{q})$ be, respectively, the $\boldsymbol{pq}$-symbols of the operators $\Phi_1(f_1)$ and $\Phi_1(f_2)$. Show that the $\boldsymbol{pq}$-symbol of the operator $\Phi_1(f_1)\Phi_1(f_2)$ is given by

$$f(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} f_1(\boldsymbol{p}, \boldsymbol{q}_1) f_2(\boldsymbol{p}_1, \boldsymbol{q}) e^{\frac{i}{\hbar}(\boldsymbol{p}-\boldsymbol{p}_1)(\boldsymbol{q}-\boldsymbol{q}_1)} d^n\boldsymbol{p}_1 d^n\boldsymbol{q}_1.$$

(*Hint:* Use the formula for $\left(m \circ \boldsymbol{U}_1^2\right)(f_1 \otimes f_2)$.)

Problem 3.10 (Composition formula for $\boldsymbol{qp}$-symbols)**.** Let $f_1(\boldsymbol{p}, \boldsymbol{q})$ and $f_2(\boldsymbol{p}, \boldsymbol{q})$ be, respectively, the $\boldsymbol{qp}$-symbols of the operators $\Phi_2(f_1)$ and $\Phi_2(f_2)$. Show that the $\boldsymbol{qp}$-symbol of the operator $\Phi_2(f_1)\Phi_2(f_2)$ is given by

$$f(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} f_1(\boldsymbol{p}_1, \boldsymbol{q}) f_2(\boldsymbol{p}, \boldsymbol{q}_1) e^{-\frac{i}{\hbar}(\boldsymbol{p}-\boldsymbol{p}_1)(\boldsymbol{q}-\boldsymbol{q}_1)} d^n\boldsymbol{p}_1 d^n\boldsymbol{q}_1.$$

(*Hint:* Use the formula for $\left(m \circ \boldsymbol{U}_2^{-2}\right)(f_1 \otimes f_2)$.)

Problem 3.11. Using (3.24) prove that the $\star$-product is associative.

Problem 3.12. For classical observable $f(\boldsymbol{p}, \boldsymbol{q})$ define the $\star$-exponential (the analog of the evolution operator) by

$$\exp_\star f = \sum_{n=0}^{\infty} \frac{\hbar^{-n}}{n!} \underbrace{f \star_\hbar f \star_\hbar \cdots \star_\hbar f}_{n}.$$

Compute $\exp_\star(-itH_{\mathrm{c}})$, where $H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{q})$ is the Hamiltonian function (2.27) of the harmonic oscillator.

3.5. Deformation quantization. Here we consider the quantization procedure from a formal algebraic point of view as the deformation theory of associative algebras. Let $\mathcal{A}$ be a $\mathbb{C}$-algebra (or an associative algebra with unit over a field k of characteristic zero) with a bilinear multiplication map

$m_0 : \mathcal{A} \otimes_{\mathbb{C}} \mathcal{A} \to \mathcal{A}$, which we will abbreviate as $a \cdot b = m_0(a, b)$. Denote by $\mathbb{C}[[t]]$ the ring of formal power series in t with coefficients in $\mathbb{C}$,

$$\mathbb{C}[[t]] = \left\{ \sum_{n=0}^{\infty} a_n t^n : a_n \in \mathbb{C} \right\},$$

and let

$$\mathcal{A}_t = \mathbb{C}[[t]] \otimes_{\mathbb{C}} \mathcal{A}$$

be the $\mathbb{C}[[t]]$-algebra of formal power series in t with coefficients in $\mathcal{A}$. The multiplication in $\mathcal{A}_t$ is a $\mathbb{C}[[t]]$-bilinear extension of the multiplication in $\mathcal{A}$, which we continue to denote by m_0. 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 $A_m \cdot A_m \subset A_{m+n}$.

Definition. A *formal deformation* of a $\mathbb{C}$-algebra $\mathcal{A}$ with a multiplication m_0 is an associative algebra $\mathcal{A}_t$ over the ring $\mathbb{C}[[t]]$ with a $\mathbb{C}[[t]]$-bilinear multiplication map $m_t : \mathcal{A}_t \otimes_{\mathbb{C}[[t]]} \mathcal{A}_t \to \mathcal{A}_t$ such that

$$m_t(a, b) = a \cdot b + \sum_{n=1}^{\infty} t^n m_n(a, b)$$

for all $a, b \in \mathcal{A}$, where $m_n : \mathcal{A} \otimes_{\mathbb{C}} \mathcal{A} \to \mathcal{A}$ are bilinear mappings.

It follows from $\mathbb{C}[[t]]$-bilinearity of m_t that the associativity condition is equivalent to

$$m_t(m_t(a, b), c) = m_t(a, m_t(b, c)) \tag{3.25}$$

for all $a, b, c \in \mathcal{A}$.

Definition. Two formal deformations m_t and $\tilde{m}_t$ of a $\mathbb{C}$-algebra $\mathcal{A}$ are equivalent if there is a $\mathbb{C}[[t]]$-linear mapping $F_t : \mathcal{A}_t \to \mathcal{A}_t$ such that

(i) for every $a \in \mathcal{A}$,

$$F_t(a) = a + \sum_{n=1}^{\infty} t^n f_n(a),$$

where $f_n : \mathcal{A} \to \mathcal{A}$ are linear mappings;

(ii) for all $a, b \in \mathcal{A}$,

$$F_t(\tilde{m}_t(a, b)) = m_t(F_t(a), F_t(b)).$$

The bilinear maps m_n satisfy infinitely many relations which are obtained by expanding (3.25) into formal power series in t. The first two of them, arising from comparing the coefficients at t and t^2, are

$$a \cdot m_1(b, c) - m_1(a \cdot b, c) + m_1(a, b \cdot c) - m_1(a, b) \cdot c = 0,$$

and

$$a \cdot m_2(b,c) - m_2(a \cdot b, c) + m_2(a, b \cdot c) - m_2(a,b) \cdot c \\ = m_1(m_1(a,b),c) - m_1(a, m_1(b,c)).$$

In general

$$a \cdot m_n(b,c) - m_n(a \cdot b, c) + m_n(a, b \cdot c) - m_n(a,b) \cdot c \\ = \sum_{j=1}^{n-1} (m_j(m_{n-j}(a,b),c) - m_j(a, m_{n-j}(b,c))).$$

The main tool for understanding these equations and studying the deformation theory of associative algebras is the *Hochschild cohomology*. Namely, let M be an $\mathcal{A}$-bimodule, i.e., a left and right module for the $\mathbb{C}$-algebra $\mathcal{A}$.

Definition. The Hochschild cochain complex $\mathsf{C}^\bullet(\mathcal{A}, M)$ of a $\mathbb{C}$-algebra $\mathcal{A}$ with coefficients in $\mathcal{A}$-bimodule M is defined by the cochains

$$\mathsf{C}^n(\mathcal{A}, M) = \mathrm{Hom}_{\mathbb{C}}(\mathcal{A}^{\otimes n}, M),$$

i.e., n-linear maps $f(a_1, \ldots, a_n)$ on $\mathcal{A}$ with values in M, and the differential $d_n : \mathsf{C}^n(\mathcal{A}, M) \to \mathsf{C}^{n+1}(\mathcal{A}, M)$,

$$\begin{aligned}(d_n f)(a_1, a_2, \ldots, a_{n+1}) = {} & a_1 \cdot f(a_2, \ldots, a_{n+1}) \\ & + \sum_{j=1}^{n} (-1)^j f(a_1, \ldots, a_{j-1}, a_j \cdot a_{j+1}, a_{j+2} \ldots, a_{n+1}) \\ & + (-1)^{n+1} f(a_1, \ldots, a_n) \cdot a_{n+1}.\end{aligned}$$

We have $d^2 = 0$, i.e., $d_{n+1} \circ d_n = 0$, and the cohomology $H^\bullet(\mathcal{A}, M)$ of the complex $(\mathsf{C}^\bullet(\mathcal{A}, M), d)$,

$$H^n(\mathcal{A}, M) = \ker d_n / \operatorname{Im} d_{n-1},$$

is called the Hochschild cohomology of the algebra $\mathcal{A}$ with coefficients in the $\mathcal{A}$-bimodule M.

In the deformation theory of associative algebras we have the simplest non-trivial case $M = \mathcal{A}$ with the left and right $\mathcal{A}$-actions given by the multiplication map. The associativity equation (3.25) can be written as

$$(d_2 m_1)(a,b,c) = 0,$$

$$(d_2 m_n)(a,b,c) = \sum_{j=1}^{n-1} \left(m_j(m_{n-j}(a,b),c) - m_j(a, m_{n-j}(b,c))\right), \quad a,b,c \in \mathcal{A}.$$

It is quite remarkable that the Hochschild cochain complex $\mathsf{C}^\bullet(\mathcal{A}, \mathcal{A})$ carries an additional structure of a graded Lie algebra, which plays a fundamental

role in studying the associativity equation (3.25). Namely, for $f \in \mathsf{C}^m(\mathcal{A},\mathcal{A})$ and $g \in \mathsf{C}^n(\mathcal{A},\mathcal{A})$ let

$$(f \circ g)(a_1,\dots,a_{m+n-1})$$
$$= \sum_{j=0}^{m-1} (-1)^j f(a_1,\dots,a_j, g(a_{j+1},\dots,a_{j+n}), a_{j+n+1},\dots,a_{m+n-1}),$$

and define

$$[f,g]_G = f\circ g - (-1)^{(m-1)(n-1)} g\circ f.$$

The linear mapping $[\ ,\ ]_G : \mathsf{C}^m(\mathcal{A},\mathcal{A}) \times \mathsf{C}^n(\mathcal{A},\mathcal{A}) \to \mathbb{C}^{m+n-1}(\mathcal{A},\mathcal{A})$ satisfies $[f,g]_G = -(-1)^{(m-1)(n-1)}[g,f]_G$, and is called the *Gerstenhaber bracket*[27]. Considering the restriction of a multiplication m_t to $\mathcal{A}\otimes_{\mathbb{C}}\mathcal{A}$ as formal power series in t with coefficients in $\mathsf{C}^\bullet(\mathcal{A},\mathcal{A})$ and using the Gerstenhaber bracket, we can rewrite (3.25) in the succinct form:

$$[m_t, m_t]_G = 0. \tag{3.26}$$

Let $\mathcal{A}$ be a commutative $\mathbb{C}$-algebra, and let $\mathcal{A}_t$ be a formal deformation of $\mathcal{A}$. Define the bilinear map $\{\ ,\ \} : \mathcal{A}\otimes_{\mathbb{C}}\mathcal{A} \to \mathcal{A}$ by

$$\{a,b\} = m_1(a,b) - m_1(b,a), \quad a,b\in\mathcal{A}. \tag{3.27}$$

Lemma 3.3. *A formal deformation $\mathcal{A}_t$ of a commutative $\mathbb{C}$-algebra $\mathcal{A}$ equips $\mathcal{A}$ with a Poisson algebra structure with the bracket $\{\ ,\ \}$.*

Proof. 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 $\mathcal{A}$, we obtain

$$\{a\cdot b, c\} - \{a, b\cdot c\} = a\cdot\{b,c\} - c\cdot\{a,b\}.$$

Interchanging b and c, we get

$$\{a\cdot c, b\} - \{a, b\cdot c\} = a\cdot\{c,b\} - b\cdot\{a,c\},$$

and interchanging further a and c, we obtain

$$\{a\cdot c, b\} - \{c, a\cdot b\} = c\cdot\{a,b\} - b\cdot\{c,a\}.$$

Adding the first and third equations and subtracting the second equation gives

$$\{a\cdot b, c\} = a\cdot\{a,c\} + b\cdot\{a,c\},$$

so that the skew-symmetric cochain $\{\ ,\ \} \in \mathsf{C}^2(\mathcal{A},\mathcal{A})$ satisfies the Leibniz rule. To prove the Jacobi identity, observe that

$$\{a,b\} = \frac{m_t(a,b) - m_t(b,a)}{t} \bmod t\mathcal{A}_t. \tag{3.28}$$

[27] Together with the cup product of cochains, the Gerstenhaber bracket equips $\mathsf{C}^\bullet(\mathcal{A},\mathcal{A})$ with the structure of a *Gerstenhaber algebra*.

Using associativity condition (3.25) (associativity modulo $t^2\mathcal{A}_t$ is sufficient) we get

$$\begin{aligned}\{\{a,b\},c\}+\{\{c,a\},b\}+\{\{b,c\},a\} = \frac{1}{t^2}((m_t(m_t(a,b)-m_t(b,a)),c)\\ -m_t(c,m_t(a,b)-m_t(b,a))+m_t(m_t(c,a)-m_t(a,c),b)\\ -m_t(b,m_t(c,a)-m_t(a,c))+m_t(m_t(b,c)-m_t(c,b),a)\\ -m_t(a,m_t(b,c)-m_t(c,b)))\bmod t\mathcal{A}_t = 0.\end{aligned}$$ □

This result motivates the following definition.

Definition. A *deformation quantization* of a Poisson algebra $(\mathcal{A},\{\ ,\ \})$ with the commutative product $m_0 : \mathcal{A}\otimes_{\mathbb{C}}\mathcal{A}\to\mathcal{A}$ is a formal deformation $\mathcal{A}_t$ of an algebra $\mathcal{A}$ such that the multiplication map m_t satisfies (3.28).

By Lemma 3.3, every formal deformation $\mathcal{A}_t$ of a commutative algebra $\mathcal{A}$ is a deformation quantization of the Poisson algebra $(\mathcal{A},\{\ ,\ \})$ with the Poisson bracket given by (3.27).

According to Lemma 3.2, a deformation quantization of the Poisson algebra $(\mathscr{S}(\mathbb{R}^{2n}),\{\ ,\ \})$, where the Poisson bracket is associated with the canonical symplectic form $\omega = d\boldsymbol{p}\wedge d\boldsymbol{q}$, is the algebra $\mathscr{S}(\mathbb{R}^{2n})[[t]]$, where $t=-i\hbar$ and $\hbar$ is considered as a formal parameter, and the multiplication map is given by the $\star$-product. The following statement is a formal algebraic analog of the representation (3.22) for the $\star$-product.

Theorem 3.4 (Universal deformation)**.** *Let $\mathcal{A}$ be a commutative $\mathbb{C}$-algebra with the multiplication map m_0, and let φ_1 and φ_2 be two commuting derivations of $\mathcal{A}$, i.e., linear maps $\varphi_1,\varphi_2:\mathcal{A}\to\mathcal{A}$ satisfying Leibniz rule and*

$$\varphi_1\circ\varphi_2=\varphi_2\circ\varphi_1.$$

Then

$$\{a,b\}=\varphi_1(a)\cdot\varphi_2(b)-\varphi_2(a)\cdot\varphi_1(b),\quad a,b\in\mathcal{A},$$

defines a Poisson bracket on $\mathcal{A}$, and the formula

$$m_t = m_0\circ e^{t\Phi},\quad \Phi=\varphi_1\otimes\varphi_2,$$

called the universal deformation formula, gives a deformation quantization of the Poisson algebra $(\mathcal{A},\{\ ,\ \})$.

Proof. The Jacobi identity for the bracket $\{\ ,\ \}$ follows from the commutativity of the derivations φ_1 and φ_2. To show that $\mathcal{A}_t$ is a deformation quantization of the Poisson algebra $(\mathcal{A},\{\ ,\ \})$, we need to verify the associativity condition (3.25) for the map m_t. Let $\Delta:\mathcal{A}\to\mathcal{A}\otimes_{\mathbb{C}}\mathcal{A}$ be the coproduct map,

$$\Delta(a)=a\otimes 1+1\otimes a,\quad a\in\mathcal{A}.$$

It extends to a $\mathbb{C}$-linear mapping from $\mathrm{Hom}_{\mathbb{C}}(\mathcal{A},\mathcal{A})$ to $\mathrm{Hom}_{\mathbb{C}}(\mathcal{A}^{\otimes 2},\mathcal{A}^{\otimes 2})$, which we continue to denote by Δ, and

$$\Delta(\varphi) = \varphi\otimes\mathrm{id} + \mathrm{id}\otimes\varphi, \quad \varphi\in\mathrm{Hom}_{\mathbb{C}}(\mathcal{A},\mathcal{A}).$$

To prove (3.25), we observe that the Leibniz rule and the binomial formula yield the following identity for a derivation φ of $\mathcal{A}$:

$$e^{t\varphi}\circ m_0 = m_0\circ e^{t\Delta(\varphi)}.$$

Using commutativity of φ_1 and φ_2, we obtain

$$\begin{aligned} m_t(a,m_t(b,c)) &= m_0(e^{t\Phi}(a\otimes m_0(e^{t\Phi}(b\otimes c)))) \\ &= (m_0\circ(\mathrm{id}\otimes m_0))(e^{t(\mathrm{id}\otimes\Delta)(\Phi)}e^{t\,\mathrm{id}\otimes\Phi}(a\otimes b\otimes c)) \\ &= (m_0\circ(\mathrm{id}\otimes m_0))(e^{t(\mathrm{id}\otimes\Delta)(\Phi)+t\,\mathrm{id}\otimes\Phi}(a\otimes b\otimes c)), \end{aligned}$$

where $(\mathrm{id}\otimes\Delta)(\Phi) = \varphi_1\otimes\Delta(\varphi_2)\in\mathcal{A}^{\otimes 3}$. Similarly,

$$m_t(m_t(a,b),c) = (m_0\circ(m_0\otimes\mathrm{id}))(e^{t(\Delta\otimes\mathrm{id})(\Phi)+t\Phi\otimes\mathrm{id}}(a\otimes b\otimes c)),$$

where $(\Delta\otimes\mathrm{id})(\Phi) = \Delta(\varphi_1)\otimes\varphi_2\in\mathcal{A}^{\otimes 3}$. Since $m_0\circ(\mathrm{id}\otimes m_0) = m_0\circ(m_0\otimes\mathrm{id})$, the associativity of the multiplication m_t is equivalent to

$$(\Delta\otimes\mathrm{id})(\Phi) + \Phi\otimes\mathrm{id} = (\mathrm{id}\otimes\Delta)(\Phi) + \mathrm{id}\otimes\Phi,$$

which is obviously satisfied since $\Phi = \varphi_1\otimes\varphi_2$. □

In general, $2n$ pair-wise commuting derivations φ_i on a commutative algebra $\mathcal{A}$ define a Poisson bracket on $\mathcal{A}$,

$$\{a,b\} = \sum_{i=1}^{n}(\varphi_i(a)\cdot\varphi_{i+n}(b) - \varphi_{i+n}(a)\cdot\varphi_i(b)),$$

and deformation quantization of the corresponding Poisson algebra $(\mathcal{A},\{\ ,\ \})$ is given by the universal deformation formula

$$m_t = m_0\circ e^{t\sum_{i=1}^{n}(\varphi_i\otimes\varphi_{i+n}-\varphi_{i+n}\otimes\varphi_i)}.$$

A deformation quantization of a Poisson manifold $(\mathscr{M},\{\ ,\ \})$ (see Section 2.7 in Chapter 1) is, by definition, a deformation quantization of the corresponding Poisson algebra of classical observables $(C^\infty(\mathscr{M}),\{\ ,\ \})$ with the property that the linear maps m_n, $n\geq 1$, are bidifferential operators[28]. The formal power series expansion (3.22) of the $\star$-product is a deformation quantization of the Poisson manifold $(\mathbb{R}^{2n},\{\ ,\ \})$, where the Poisson bracket corresponding to the canonical symplectic form $\omega = d\boldsymbol{p}\wedge d\boldsymbol{q}$.

[28]This property ensures that the unit in Poisson algebra is preserved under the deformation.

Problem 3.13. Show that $C^\bullet(\mathcal{A},\mathcal{A})$ is a *graded Lie algebra* with respect to the Gerstenhaber bracket, i.e., that $[\ ,\ ]_G$ satisfies the *graded Jacobi identity*

$$(-1)^{(m-1)(p-1)}[f,[g,h]]+(-1)^{(n-1)(p-1)}[h,[f,g]]+(-1)^{(m-1)(n-1)}[g,[h,f]]=0$$

for all $f\in C^m(\mathcal{A},\mathcal{A}), g\in C^n(\mathcal{A},\mathcal{A}), h\in C^p(\mathcal{A},\mathcal{A})$.

Problem 3.14. Verify that $d_nf=[f,m_0]_G$, where $f\in \mathsf{C}^n(\mathcal{A},\mathcal{A})$ and d_n is the Hochschild differential.

Problem 3.15. Show that deformation quantizations associated with Weyl, ***pq***, and ***qp***-quantizations are equivalent. (In fact, all deformation quantizations of the canonical Poisson manifold $(\mathbb{R}^{2n},\{\ ,\ \})$ are equivalent.)

Problem 3.16. Let $\mathfrak{g}$ be a finite-dimensional Lie algebra with a basis $x_1,\dots,x_n$, and let $\mathfrak{g}^*$ be its dual space equipped with the Lie-Poisson bracket $\{\ ,\ \}$ (see Problem 2.20 in Section 2.7 of Chapter 1). For $u\in\mathfrak{g}^*$ and $x=\sum_{i=1}^n\xi^ix_i, y=\sum_{i=1}^n\eta^ix_i\in\mathfrak{g}$ let

$$e^{u(\frac{1}{t}\log e^{tx}e^{ty}-x-y)}=\sum_{\alpha,\beta}a_{\alpha\beta}(u,t)\xi^\alpha\eta^\beta,$$

where $\xi^\alpha=(\xi^1)^{\alpha_1}\dots(\xi^n)^{\alpha_n}$, $\eta^\beta=(\eta^1)^{\beta_1}\dots(\eta^n)^{\beta_n}$, be the formal group law — the "Baker-Campbell-Hausdorff series". Show that the product

$$m_t(f_1,f_2)=\sum_{\alpha,\beta}a_{\alpha\beta}(u,t)D^\alpha f_1(u)D^\beta f_2(u),\quad f_1,f_2\in C^\infty(\mathfrak{g}^*),$$

where for a multi-index $\alpha=(\alpha_1,\dots,\alpha_n)$ and $f\in C^\infty(\mathfrak{g}^*)$, $D^\alpha f=\frac{\partial^{\alpha_1+\dots+\alpha_n}f}{\partial u_1^{\alpha_1}\dots\partial u_n^{\alpha_n}}$, gives a deformation quantization of the Poisson manifold $(\mathfrak{g}^*,\{\ ,\ \})$.

Problem 3.17. Let $(G,\{\ ,\ \})$ be a Lie-Poisson group, where $\eta(g)=-r+\mathrm{Ad}^{-1}g\cdot r$ and non-degenerate r satisfies the classical Yang-Baxter equation (see Problems 2.21 – 2.23 in Section 2.7 of Chapter 1). Using Baker-Campbell-Hausdorff series for the Lie algebra $\tilde{\mathfrak{g}}$ — the one-dimensional central extension of $\mathfrak{g}$ by the 2-cocycle c (see Problem 2.23 in Section 2.7 of Chapter 1), show that there exists an element $F\in(U\mathfrak{g}\otimes U\mathfrak{g})[[t]]$ of the form $F=1-\frac{1}{2}tr+O(t^2)$, satisfying

$$(\Delta\otimes\mathrm{id})(F)(F\otimes 1)=(\mathrm{id}\otimes\Delta)(F)(1\otimes F),$$

where Δ is the standard coproduct in $U\mathfrak{g}$.

Problem 3.18. Let F_L and F_R be the images of F and F^{-1} under the identifications of the universal enveloping algebra $U\mathfrak{g}$ with the algebras of left and right-invariant differential operators on G (see Problem 2.21 in Section 2.7 of Chapter 1), and let $\mathscr{F}=F_L\circ F_R$. Show that the product $m_t=m_0\circ\mathscr{F}$ gives a deformation quantization of the Poisson-Lie group $(G,\{\ ,\ \})$ such that

$$\Delta\circ m_t=(m_t\otimes m_t)\circ\Delta,$$

where Δ is the standard coproduct on functions on G, $\Delta(f)(g_1,g_2)=f(g_1g_2), f\in C^\infty(G)$. The *Hopf algebra* $(C^\infty(G),m_t,\Delta,S)$, where S is the standard antipode on G, $S(f)(g)=f(g^{-1})$, is called the *quantum group* corresponding to the Poisson-Lie group G, and is denoted by G_q, $q=e^t$.

Problem 3.19. Let $R = \sigma(F^{-1})F \in (U\mathfrak{g} \otimes U\mathfrak{g})[[t]]$, where σ is a permutation — an involution of $U\mathfrak{g} \otimes U\mathfrak{g}$, defined by $\sigma(a \otimes b) = b \otimes a$, $a, b \in U\mathfrak{g}$. Show that $R = 1 - tr + O(t^2)$ and satisfies the *quantum Yang-Baxter equation*

$$R_{12}R_{13}R_{23} = R_{23}R_{13}R_{12}$$

(see Problem 2.22 in Section 2.7 in Chapter 1 for notation).

4. Notes and references

Dirac's classical monograph [**Dir47**] is the fundamental text. Other classical references are physics textbooks [**Foc78**] and [**LL58**]. The monograph [**Sak94**] is a popular text for graduate courses in physics departments. Another useful physics reference is the encyclopedic treatise [**Mes99**], which discusses at length the origin of quantum theory and the development of its mathematical formalism. An elementary textbook [**PW35**] provides an introduction to the old quantum theory, including Bohr-Wilson-Sommerfeld quantization rules, and applications of quantum mechanics to chemistry. We refer the interested reader to these sources for physical formulation and the origin of quantum mechanics, including a discussion of basic experimental facts: the double-slit experiment and particle-wave duality. Quantum mechanics does not account for single measurement outcomes in a deterministic way, and the quantum process of measurement admits different interpretations. The accepted one is the so-called Copenhagen interpretation, in which a measurement causes an instantaneous "collapse" of the wave function describing the quantum system.

Monographs [**Rud87, BS87, AG93**], as well as [**RS80, RS75**], contain all the necessary material from the theory of operators in Hilbert spaces; the latter treatise also covers the theory of distributions, Fourier transform, and self-adjointness. The book [**Kir76**] introduces the reader to various methods in the representation theory, and the monograph [**BR86**], written for theoretical physicists, contains all the necessary information on the representation theory of Lie groups and Lie algebras. A succinct introduction to the method of stationary phase and other asymptotic methods is given in the classical text [**Erd56**] and in [**Olv97**]; see also Appendix B in [**BW97**]. Properties of Hermite-Tchebyscheff polynomials[29] can be found in the classical monograph [**Sze75**], as well as in many other reference books on special functions and orthogonal polynomials.

Our exposition in Section 1.1 follows a traditional approach to the mathematical foundation of quantum mechanics based on Dirac-von Neumann axioms. These axioms go back to von Neumann's classical monograph [**vN96**], with more detailed discussion in [**Mac04**]; see also [**BS91**], notes to Chapter VIII of [**RS80**], and references therein. Another mathematical description of quantum mechanics is based

[29] Following V.A. Fock [**Foc78**], in Section 2.6 we used the more appropriate name Hermite-Tchebyscheff polynomials instead of the customary Hermite polynomials (see [**Ger50**] for the relevant historic arguments).

on $\mathbb{C}^*$-algebras and the Gelfand-Naimark-Segal reconstruction theorem, and can be found in [**Str05**] and references therein.

Our exposition in Section 2 follows the outline in [**FY80**]; see [**Ber74**] for the general mathematical formulation of the quantization problem and the recent survey [**AE05**]. Having in mind a more advanced audience than for [**FY80**], in Sections 2.1 and 2.2 we included a complete mathematical treatment of Heisenberg commutation relations and coordinate and momentum representations. In Sections 2.2 and 2.3 we use the same normalization of the eigenfunctions of continuous spectrum as in [**Foc78**]; it corresponds to the orthogonality relation in Section 2.2 of Chapter 3. In our exposition in Section 2.6, which is otherwise standard, we include a proof of the completeness of the eigenfunctions $\psi_n(q)$, which is usually only mentioned in the physics textbooks. Holomorphic representation in quantum mechanics was introduced by V.A. Fock in 1932 [**Foc32**], where the scalar product in $\mathscr{D}_n$ was given in terms of the orthonormal basis of monomials $f_{\boldsymbol{m}}(\boldsymbol{z})$. In terms of the integral (2.52) this scalar product was defined by V. Bargmann [**Bar61**]; holomorphic representation is also called *Fock-Bargmann representation*. Discussion of Wick symbols of operators in Section 2.7 essentially follows [**BS91**]; more details can be found in the original paper [**Ber71b**]. The method of geometric quantization is only briefly mentioned in remarks in Sections 2.2 and 2.7; the interested reader is referred to monographs [**GS77, Woo92**], lecture notes [**SW76, BW97**] and the survey [**Kir90**].

Our proof of the celebrated Stone-von Neumann theorem in Section 3.1 essentially follows the original paper of von Neumann [**vN31**]. The main instrument of the proof — the Weyl transform — was introduced by Weyl in the classical monograph [**Wey50**] (see [**Ros04**] for the history and generalizations of the Stone-von Neumann theorem). Invariant formulation of the Stone-von Neumann theorem, discussed in Section 3.2, as well as the relation with the triple Maslov index, methaplectic group, Shale-Weil representation, and applications to number theory, can be found in [**LV80**]. We refer to [**BS91**] for the extended discussion of $\boldsymbol{pq}$ and $\boldsymbol{qp}$-quantizations as their relations with the Weyl quantization, as well as for more details on the $\star$-product, introduced in Section 3.4. The beautiful formula (3.24) for the $\star$-product — composition of the Weyl symbols — belongs to Berezin [**Ber71a**].

The notion of the deformation quantization was introduced in [**BFF$^+$78a, BFF$^+$78b**], where the solution of Problem 3.12 can be found. The fundamental theorem that every Poisson manifold admits a deformation quantization was proved by Kontsevich in [**Kon03**]. More on Hochschild cohomology and the deformation theory of associative algebras can be found in the survey [**Vor05**] and references therein. The deformation theory point of view on the evolution of physical theories, like a passage from classical mechanics to quantum mechanics emphasized in Faddeev's lectures [**FY80**], can be found in [**Fla82**] and [**Fad98**].

Most of the problems in this chapter are rather standard and are mainly taken from the references [**RS80, BS91**]. Other require more sophistication and are aimed at introducing the reader to a new topic. Thus the asymptotic expansion in Problem 2.11, which can be found in monograph [**Sze75**], is an example of semi-classical asymptotics, and Problem 3.1, taken from [**Nel59**], gives a criterion when the irreducible unitary representation of the Heisenberg algebra is integrable. Problems 3.17–3.19 introduce the reader to the theory of quantum groups (see [**Jim85, Dri86, Dri87, RTF89**]) and are taken from [**Dri83**] (see also [**Tak90**]). The fundamental result that every Lie-Poisson group admits a deformation quantization described in Problem 3.18 has been proved in [**EK96**] (see also [**Enr01**]).

Chapter 3

Schrödinger Equation

1. General properties

Here we describe the general properties of the Schrödinger operator for a quantum particle in $\mathbb{R}^n$ moving in a potential field. To simplify the notation, in this chapter we set $\hbar = 1$ and $m = \frac{1}{2}$, and use $\boldsymbol{x} = (x_1, \dots, x_n)$ for Cartesian coordinates on $\mathbb{R}^n$. Recall (see Section 2.4 in Chapter 2) that the corresponding Schrödinger operator is given by the formal differential expression

$$H = -\Delta + V(\boldsymbol{x}),$$

where $V(\boldsymbol{x})$ is a real-valued, measurable function on $\mathbb{R}^n$. Denote by

$$H_0 = -\Delta = -\left(\frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2}\right)$$

the Schrödinger operator of a free quantum particle of mass $m = \frac{1}{2}$ on $\mathbb{R}^n$, also called the *kinetic energy operator*, and by V — the multiplication by $V(\boldsymbol{x})$ operator, also called the *potential energy operator*, so that

$$H = H_0 + V. \tag{1.1}$$

According to Section 2.3 of Chapter 2, the operator H_0 is self-adjoint and unbounded on $\mathscr{H} = L^2(\mathbb{R}^n)$, with the domain $D(H_0) = W^{2,2}(\mathbb{R}^n)$ and absolutely continuous spectrum $[0, \infty)$, and the operator V is self-adjoint and is bounded if and only if $V(\boldsymbol{x}) \in L^\infty(\mathbb{R}^n)$, when $\|V\| = \|V\|_\infty$. The sum $H_0 + V$ is not necessarily self-adjoint, and the first major mathematical problem of quantum mechanics is to characterize potentials $V(\boldsymbol{x})$ for which the formal differential expression (1.1) uniquely defines a self-adjoint operator H on $\mathscr{H}$. We start by presenting some useful criteria for the self-adjointness.

1.1. Self-adjointness. The main result here is the Kato-Rellich theorem on perturbation of self-adjoint operators.

Definition. Let A and B be densely defined operators in $\mathscr{H}$. The operator B is smaller than A in the sense of Kato if $D(A) \subseteq D(B)$ and there exist $a, b \in \mathbb{R}$ with $a < 1$ such that for all $\psi \in D(A)$,

$$\|B\psi\| \le a\|A\psi\| + b\|\psi\|. \tag{1.2}$$

Equivalently, the operator B is smaller than A in the sense of Kato, if there exist $\alpha, \beta \in \mathbb{R}$ with $\alpha < 1$ such that for all $\psi \in D(A)$,

$$\|B\psi\|^2 \le \alpha\|A\psi\|^2 + \beta\|\psi\|^2. \tag{1.3}$$

Theorem 1.1 (Kato-Rellich)**.** *If A is a self-adjoint operator with domain $D(A)$ and B is a symmetric operator smaller than A in the sense of Kato, then $H = A + B$ with $D(H) = D(A)$ is a self-adjoint operator.*

Proof. Recall that the operator H is self-adjoint if and only if $\operatorname{Im}(H+\lambda I) = \operatorname{Im}(H - \lambda I) = \mathscr{H}$ for some $\lambda \in i\,\mathbb{R}$, and hence for all $\lambda \in \mathbb{C} \setminus \sigma(H)$. Since $A = A^*$, for every $\lambda \in i\,\mathbb{R}$ we have $R_\lambda = (A - \lambda I)^{-1} \in \mathscr{L}(\mathscr{H})$ and $\operatorname{Im} R_\lambda = D(A)$. Now

$$H - \lambda I = (I + BR_\lambda)(A - \lambda I),$$

and in order to prove that $\operatorname{Im}(H - \lambda I) = \mathscr{H}$ it is sufficient to show that for $|\lambda|$ large enough $\|BR_\lambda\| < 1$, since then by Neumann series $I + BR_\lambda$ is an invertible bounded operator and $\operatorname{Im}(I + BR_\lambda) = \mathscr{H}$. Indeed, for all $\varphi \in \mathscr{H}$ we have the inequalities

$$\|R_\lambda\varphi\| \le \tfrac{1}{|\lambda|}\|\varphi\| \quad \text{and} \quad \|AR_\lambda\varphi\| \le \|\varphi\|,$$

which follow from the equation $\|(A-\lambda I)\psi\|^2 = \|A\psi\|^2 + |\lambda|^2\|\psi\|^2$ by setting $\varphi = (A - \lambda I)\psi$. Now using (1.2) with $\psi = R_\lambda\varphi$, we get

$$\|BR_\lambda\varphi\| \le a\|AR_\lambda\varphi\| + b\|R_\lambda\varphi\| \le (a + \tfrac{b}{|\lambda|})\|\varphi\|,$$

so that $\|BR_\lambda\| < 1$ for large enough $|\lambda|$. □

We use the Kato-Rellich criterion for the physically important case when $A = H_0$ — the Schrödinger operator of a free particle in $\mathbb{R}^3$ — and $B = V$ — the multiplication by $V(\boldsymbol{x})$ operator.

Theorem 1.2. *Let $V = V_1 + V_2$, where $V_1(\boldsymbol{x}) \in L^2(\mathbb{R}^3)$ and $V_2(\boldsymbol{x}) \in L^\infty(\mathbb{R}^3)$. Then $H = H_0 + V$ is a self-adjoint operator and $D(H) = W^{2,2}(\mathbb{R}^3)$.*

Proof. It is sufficient to show that V is smaller than H_0 in the sense of Kato on $C_0^\infty(\mathbb{R}^3) \subset W^{2,2}(\mathbb{R}^3)$. Denoting by $\|\cdot\|_\infty$ the norm in $L^\infty(\mathbb{R}^3)$, for $\varphi \in C_0^\infty(\mathbb{R}^3)$ we have

$$\|V\varphi\| \le \|V_1\|\,\|\varphi\|_\infty + \|V_2\|_\infty\,\|\varphi\|.$$

Let $h(\boldsymbol{p}) = \boldsymbol{p}^2$. Denoting by $\|\cdot\|_1$ the norm in $L^1(\mathbb{R}^3)$ and using the Fourier transform and the Cauchy-Bunyakovski-Schwarz inequality, we get

$$\begin{aligned}(2\pi)^{3/2}\|\varphi\|_\infty &= \sup_{\boldsymbol{x}\in\mathbb{R}^3}\left|\int_{\mathbb{R}^3} e^{i\boldsymbol{p}\boldsymbol{x}}\check{\varphi}(\boldsymbol{p})d^3\boldsymbol{p}\right| \le \|\check{\varphi}\|_1 \\ &\le \|(h+1)^{-1}\|\,\|(h+1)\check{\varphi}\| \le C(\|h\check{\varphi}\| + \|\check{\varphi}\|) \\ &= C(\|H_0\varphi\| + \|\varphi\|).\end{aligned}$$

Now replace $\check{\varphi}(\boldsymbol{p})$ by $\check{\varphi}_r(\boldsymbol{p}) = r^3\check{\varphi}(r\boldsymbol{p})$, $r > 0$. Since $\|\check{\varphi}_r\|_\infty = \|\check{\varphi}\|_\infty$, $\|\check{\varphi}_r\|_1 = \|\check{\varphi}\|_1$, $\|\check{\varphi}_r\| = r^{3/2}\|\check{\varphi}\|$, and $\|h\check{\varphi}_r\| = r^{-1/2}\|h\check{\varphi}\|$, we get

$$(2\pi)^{3/2}\|\varphi\|_\infty \le r^{-1/2}C(\|H_0\varphi\| + r^2\|\varphi\|),$$

where $r > 0$ is arbitrary. Choosing r such that $a = r^{-1/2}(2\pi)^{-3/2}C\|V_1\| < 1$ completes the proof. □

Corollary 1.3. *The Schrödinger operator of a complex atom, considered in Example* 2.2 *in Section* 2.4 *of Chapter* 2*, is essentially self-adjoint on* $C_0^\infty(\mathbb{R}^{3(N+1)})$.

Proof. We consider only the special case of the Hamiltonian of the hydrogen atom,

$$H = -\Delta - \frac{e^2}{r}, \quad r = |\boldsymbol{x}|.$$

Writing $V = \chi_1 V + (1-\chi_1)V = V_1 + V_2$, where χ_1 is the characteristic function of the unit ball $B_1 = \{x \in \mathbb{R}^3 : |x| \le 1\}$, we have $V_1(\boldsymbol{x}) \in L^2(\mathbb{R}^3)$ and $V_2(\boldsymbol{x}) \in L^\infty(\mathbb{R}^3)$. □

Another useful criterion applies to real-valued potentials $V(\boldsymbol{x}) \in L^\infty_{\mathrm{loc}}(\mathbb{R}^n)$, the space of locally bounded a.e. functions on $\mathbb{R}^n$. In this case the operator H, defined by the formal differential expression (1.1), is symmetric on $C_0^\infty(\mathbb{R}^n)$ and we have the following result.

Theorem 1.4. *If* $V(\boldsymbol{x}) \in L^\infty_{\mathrm{loc}}(\mathbb{R}^n)$ *is bounded from below,* $V(\boldsymbol{x}) \ge C$ *a.e. on* $\mathbb{R}^n$*, then the Schrödinger operator* $H = H_0 + V$ *is essentially self-adjoint on* $C_0^\infty(\mathbb{R}^n)$.

In fact, a much more general statement holds.

Theorem 1.5 (Sears)**.** *Suppose that the potential* $V(\boldsymbol{x}) \in L^\infty_{\mathrm{loc}}(\mathbb{R}^n)$ *for all* $\boldsymbol{x} \in \mathbb{R}^n$ *satisfies the condition*

$$V(\boldsymbol{x}) \ge -Q(|\boldsymbol{x}|),$$

where $Q(r)$ *is an increasing continuous positive function on* $[0,\infty)$ *such that*

$$\int_0^\infty \frac{dr}{\sqrt{Q(r)}} = \infty.$$

Then the Schrödinger operator $H = H_0 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Problem 1.1. Prove the general case of Corollary 1.3 (*Hint*: Derive the estimate (1.3) for each term in the corresponding potential energy operator.)

Problem 1.2 (Kato's inequality)**.** Let $\psi \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$ be such that $\Delta\psi$, defined in the distributional sense, is represented by a function in $L^1_{\mathrm{loc}}(\mathbb{R}^n)$. Prove that in the distributional sense, $\Delta|u| \geq \mathrm{Re}\left(\frac{\bar{u}}{u}\Delta u\right)$, where it is assumed that $\frac{\overline{u(\boldsymbol{x})}}{u(\boldsymbol{x})} = 0$ if $u(\boldsymbol{x}) = 0$. (The distribution $T \in \mathscr{S}(\mathbb{R}^n)'$ is non-negative if $T(\varphi) \geq 0$ for all non-negative $\varphi \in \mathscr{S}(\mathbb{R}^n)$.)

Problem 1.3. Prove Theorem 1.4 using Kato's inequality. (*Hint*: Show that if $\psi \in L^2(\mathbb{R}^n)$ in the distributional sense satisfies $(-\Delta + V(\boldsymbol{x}) + C + 1)\psi = 0$, then $\psi = 0$.)

Problem 1.4. Prove that one-dimensional Schrödinger operators with unbounded below potentials $V(x) = x$ and $V(x) = -x^2$ are essentially self-adjoint on $C_0^\infty(\mathbb{R})$.

1.2. Characterization of the spectrum. The second major mathematical problem in quantum mechanics is to describe the spectral properties of the Schrödinger operator H. Here we present some general results characterizing the spectrum of H. The first basic result is the following.

Theorem 1.6. *Suppose that $V(\boldsymbol{x}) \in L^\infty_{\mathrm{loc}}(\mathbb{R}^n)$ satisfies*

$$\lim_{|\boldsymbol{x}|\to\infty} V(\boldsymbol{x}) = \infty.$$

Then the operator H has a pure point spectrum: there exists an orthonormal basis $\{\psi_n\}_{n\in\mathbb{N}}$ for $\mathscr{H}$ consisting of eigenfunctions of H with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \leq \cdots$ of finite multiplicity,

$$H\psi_n = \lambda_n\psi_n,$$

and $\lim\limits_{n\to\infty} \lambda_n = \infty$.

Recall that the essential spectrum $\sigma_{\mathrm{ess}}(A)$ of a self-adjoint operator A consists of all non-isolated points of $\sigma(A)$ and of eigenvalues of infinite multiplicity. The following result gives a sufficient condition for the essential spectrum of the Schrödinger operator to fill $[0, \infty)$.

Theorem 1.7. *Suppose that $V = V_1 + V_2$, where $V_1(\boldsymbol{x}) \in L^q(\mathbb{R}^n)$, $2q \geq n$ for $n > 4$ and $q \geq 2$ for $n \leq 4$[1], and $V_2(\boldsymbol{x}) \in L^\infty(\mathbb{R}^n)$ satisfies*

$$\lim_{|\boldsymbol{x}|\to\infty} V_2(\boldsymbol{x}) = 0.$$

Then $\sigma_{\mathrm{ess}}(H) = [0, \infty)$, so that $\sigma(H) \cap (-\infty, 0)$ consists of isolated eigenvalues of H of finite multiplicity.

[1] In the special case $n = 4$ one has $q > 2$.

The next result gives a sufficient condition for the Schrödinger operator with decaying potential to have only negative eigenvalues.

Theorem 1.8 (Kato). *Suppose that* $V(\boldsymbol{x}) \in L^\infty(\mathbb{R}^n)$ *and*

$$\lim_{|\boldsymbol{x}|\to\infty} |\boldsymbol{x}|V(\boldsymbol{x}) = 0.$$

Then the Schrödinger operator $H = H_0 + V$ *has no positive eigenvalues.*

Recall that the absolutely continuous spectrum and the singular spectrum of a self-adjoint operator A on $\mathscr{H}$ are defined, respectively, by $\sigma_{\mathrm{ac}}(A) = \sigma(A|_{\mathscr{H}_{\mathrm{ac}}})$ and $\sigma_{\mathrm{sc}}(A) = \sigma(A|_{\mathscr{H}_{\mathrm{sc}}})$, where $\mathscr{H}_{\mathrm{ac}}$ and $\mathscr{H}_{\mathrm{sc}}$ are closed subspaces for A defined as follows. Let P_A be the projection-valued measure for the self-adjoint operator A and let $\nu_\psi = (\mathsf{P}_A\psi, \psi)$ be the finite Borel measure on $\mathbb{R}$ corresponding to $\psi \in \mathscr{H}$, $\psi \neq 0$. Then $\mathscr{H}_{\mathrm{ac}}$ consists of 0 and all $\psi \in \mathscr{H}$ such that the measure ν_ψ is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$, and $\mathscr{H}_{\mathrm{sc}}$ consists of 0 and all $\psi \in \mathscr{H}$ such that the measure ν_ψ is continuous singular with respect to the Lebesgue measure on $\mathbb{R}$.

Theorem 1.9. *Suppose that the potential* $V(\boldsymbol{x}) \in L^\infty(\mathbb{R}^n)$ *for some* $\varepsilon > 0$ *satisfies*

$$V(\boldsymbol{x}) = O(|\boldsymbol{x}|^{-1-\varepsilon}) \quad \textit{as} \quad |\boldsymbol{x}| \to \infty.$$

Then the Schrödinger operator $H = H_0 + V$ *has no singular spectrum and* $\sigma_{\mathrm{ac}}(H) = [0, \infty)$. *Moreover,* $\sigma(H) \cap (-\infty, 0)$ *consists of eigenvalues of* H *of finite multiplicity with the only possible accumulation point at* 0.

Finally, for the physically important case $n = 3$ there is a useful estimate for the number of eigenvalues of the Schrödinger operator.

Theorem 1.10 (Birman-Schwinger). *Suppose that* $V(\boldsymbol{x}) \in L^\infty(\mathbb{R}^3)$ *and*

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|V(\boldsymbol{x})V(\boldsymbol{y})|}{|\boldsymbol{x}-\boldsymbol{y}|^2} d^3\boldsymbol{x}\, d^3\boldsymbol{y} < \infty.$$

Then for the total number N *of eigenvalues of the Schrödinger operator* $H = H_0 + V$, *counted with multiplicities, we have*

$$N \le \frac{1}{16\pi^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|V(\boldsymbol{x})V(\boldsymbol{y})|}{|\boldsymbol{x}-\boldsymbol{y}|^2} d^3\boldsymbol{x}\, d^3\boldsymbol{y}.$$

Problem 1.5. Prove all results stated in this section. (*Hint*: See the list of references to this chapter.)

1.3. The virial theorem. Let $H = H_0 + V$ be the Schrödinger operator whose potential is a homogeneous function on $\mathbb{R}^n$ of degree ρ, i.e., $V(a\boldsymbol{x}) = a^\rho V(\boldsymbol{x})$. The *virial theorem* in quantum mechanics is the relation between the expectation values of the kinetic and potential energy operators H_0 and V in the stationary state.

Theorem 1.11 (The virial theorem)**.** *Let $\psi \in \mathscr{H}$, $\|\psi\| = 1$, be the eigenfunction of the Schrödinger operator with the homogeneous potential of degree ρ, and let $T_0 = (H_0\psi, \psi)$ and $V_0 = (V\psi, \psi)$ be the corresponding expectation values of kinetic and potential energy operators. Then*

$$2T_0 = \rho V_0.$$

Proof. It follows from the Schrödinger equation

$$-\Delta\psi + V(\boldsymbol{x})\psi = \lambda\psi$$

that

$$T_0 + V_0 = -(\Delta\psi, \psi) + (V\psi, \psi) = \lambda.$$

For every $a > 0$ the function $\psi_a(\boldsymbol{x}) = \psi(a\boldsymbol{x})$ satisfies

$$-\Delta\psi_a + a^{\rho+2}V(\boldsymbol{x})\psi_a = a^2\lambda\psi_a,$$

so that by differentiating this equation with respect to a at $a = 1$ and using Euler's homogenous function theorem, we get

$$-\Delta\dot{\psi} + V(\boldsymbol{x})\dot{\psi} = \lambda\dot{\psi} + (2\lambda - (\rho+2)V(\boldsymbol{x}))\psi. \tag{1.4}$$

Since $\dot{\psi} \in D(H)$ and H is self-adjoint,

$$((H - \lambda I)\dot{\psi}, \psi) = (\dot{\psi}, (H - \lambda I)\psi) = 0,$$

and we obtain from (1.4) that

$$2\lambda = (\rho + 2)V_0,$$

which completes the proof. □

Remark. Since energy levels of quantum systems are related to the closed orbits of corresponding classical systems, Theorem 1.11 is the quantum analog of the classical virial theorem (see Example 1.2 in Section 1.3 of Chapter 1).

Problem 1.6 (The Raleigh-Ritz principle)**.** Prove that λ is an eigenvalue of a self-adjoint operator H with the eigenfunction ψ if and only if ψ is a critical point of the functional $F(\varphi) = ((H - \lambda I)\varphi, \varphi)$ on $D(H)$.

Problem 1.7. Derive the virial theorem from the Raleigh-Ritz principle.

2. One-dimensional Schrödinger equation

The Schrödinger operator on the real line — the one-dimensional Schrödinger operator — has the form

$$H = -\frac{d^2}{dx^2} + V(x),$$

where the real-valued potential $V(x) \in L^1_{\mathrm{loc}}(\mathbb{R})$, the space of locally integrable functions on $\mathbb{R}$. The corresponding eigenvalue problem

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

reduces to the second order ordinary differential equation

$$-y'' + V(x)y = k^2 y, \quad -\infty < x < \infty, \tag{2.1}$$

where it is convenient to set $\lambda = k^2$. In this section, we will study in detail the one-dimensional Schrödinger equation (2.1) for the case when

$$\int_{-\infty}^{\infty} (1 + |x|)|V(x)|dx < \infty. \tag{2.2}$$

Condition (2.2) is a mathematical formulation of the physical statement that the potential $V(x)$ decays as $|x| \to \infty$. It allows us to compare solutions $y(x,k)$ of the Schrödinger equation (2.1) with the solutions $e^{\pm ikx}$ of the Schrödinger equation for the free quantum particle, which corresponds to the case $V = 0$ in (2.1). All results in this section hold for the real-valued potential $V(x) \in L^1_{\mathrm{loc}}(\mathbb{R})$ satisfying (2.2); to simplify the presentation we will additionally assume that the potential $V(x)$ in (2.2) is continuous on $\mathbb{R}$.

2.1. Jost functions and transition coefficients. Let

$$\sigma(x) = \int_x^{\infty} |V(s)|ds \quad \text{and} \quad \sigma_1(x) = \int_x^{\infty} \sigma(s)ds.$$

Since $V \in L^1(\mathbb{R})$, we have $\lim_{x\to\infty} \sigma(x) = 0$, and using condition (2.2) and the Fubini theorem we get

$$\sigma_1(x) = \int_x^{\infty}\int_s^{\infty} |V(t)|dtds = \int_x^{\infty}\int_x^{t} |V(t)|dsdt = \int_x^{\infty} (t-x)|V(t)|dt < \infty,$$

so that $\sigma \in L^1(x,\infty)$ for all $x \in \mathbb{R}$ and $\lim_{x\to\infty} \sigma_1(x) = 0$. Similarly, the functions

$$\tilde{\sigma}(x) = \int_{-\infty}^{x} |V(s)|ds \quad \text{and} \quad \tilde{\sigma}_1(x) = \int_{-\infty}^{x} \tilde{\sigma}(s)ds$$

satisfy $\lim_{x\to-\infty} \tilde{\sigma}(x) = \lim_{x\to-\infty} \tilde{\sigma}_1(x) = 0$. Condition (2.2) ensures that for real k the differential equation (2.1) has solutions $f_1(x,k)$ and $f_2(x,k)$,

uniquely defined by the following asymptotics:

$$f_1(x,k) = e^{ikx} + o(1) \quad \text{as} \quad x \to \infty,$$
$$f_2(x,k) = e^{-ikx} + o(1) \quad \text{as} \quad x \to -\infty.$$

They are called *Jost solutions* and play a fundamental role in the theory of a one-dimensional Schrödinger equation.

Theorem 2.1. *For real k the differential equation* (2.1) *has solutions $f_1(x,k)$ and $f_2(x,k)$ satisfying the following properties.*

(i) *Estimates for $k \in \mathbb{R}$:*

$$|e^{-ikx} f_1(x,k) - 1| \le \big(\sigma_1(x) - \sigma_1(x + \tfrac{1}{|k|})\big) e^{\sigma_1(x)},$$
$$|e^{ikx} f_2(x,k) - 1| \le \big(\tilde\sigma_1(x) - \tilde\sigma_1(x - \tfrac{1}{|k|})\big) e^{\tilde\sigma_1(x)}.$$

(ii) *Asymptotics as $|x| \to \infty$:*

$$\lim_{x\to\infty} e^{-ikx} f_1(x,k) = 1, \quad \lim_{x\to\infty} e^{-ikx} f_1'(x,k) = ik,$$
$$\lim_{x\to-\infty} e^{ikx} f_2(x,k) = 1, \quad \lim_{x\to-\infty} e^{ikx} f_1'(x,k) = -ik.$$

.

(iii) *Analyticity: $f_1(x,k)$ and $f_2(x,k)$ admit analytic continuation to the upper half-plane $\operatorname{Im} k > 0$, and are continuous functions on $\operatorname{Im} k \ge 0$, uniformly in x on compact subsets of $\mathbb{R}$.*

(iv) *The conjugation property:*

$$\overline{f_1(x,k)} = f_1(x,-\bar k), \quad \overline{f_2(x,k)} = f_2(x,-\bar k), \quad \operatorname{Im} k \ge 0.$$

(v) *Estimates in part* (i) *hold for $\operatorname{Im} k \ge 0$. For $k \ne 0$,*

$$|f_1(x,k) - e^{ikx}| \le \frac{e^{-\operatorname{Im} kx}}{|k|} \sigma(x) e^{\frac{1}{|k|}\sigma(x)},$$
$$|f_2(x,k) - e^{-ikx}| \le \frac{e^{\operatorname{Im} kx}}{|k|} \tilde\sigma(x) e^{\frac{1}{|k|}\tilde\sigma(x)}.$$

(vi) *Asymptotics as $|k| \to \infty$, $\operatorname{Im} k \ge 0$:*

$$e^{-ikx} f_1(x,k) = 1 + O(|k|^{-1}), \quad e^{ikx} f_2(x,k) = 1 + O(|k|^{-1}).$$

Proof. It follows from the method of variation of parameters that differential equation (2.1) with the boundary condition $\lim_{x\to\infty} e^{-ikx} f_1(x,k) = 1$ is equivalent to the integral equation

$$f_1(x,k) = e^{ikx} - \int_x^\infty \frac{\sin k(x-t)}{k} V(t) f_1(t,k)\, dt. \tag{2.3}$$

Setting $\varphi(x,k) = e^{-ikx} f_1(x,k)$, we get

$$\varphi(x,k) = 1 - \int_x^\infty \frac{1 - e^{-2ik(x-t)}}{2ik} V(t)\varphi(t,k)dt. \tag{2.4}$$

For $\operatorname{Im} k \geq 0$ the integral equation (2.4) is of Volterra type and can be solved by the method of successive approximations. Namely, we look for the solution in the form

$$\varphi(x,k) = \sum_{n=0}^{\infty} \varphi_n(x,k), \tag{2.5}$$

where $\varphi_0(x,k) = 1$ and

$$\begin{aligned}\varphi_{n+1}(x,k) &= -\int_x^\infty \frac{1 - e^{-2ik(x-t)}}{2ik} V(t)\varphi_n(t,k)dt \\ &= \int_x^\infty \left(\int_x^t e^{-2ik(x-s)} V(t)\varphi_n(t,k)ds \right) dt.\end{aligned}$$

From here we conclude that for $\operatorname{Im} k \geq 0$

$$|\varphi_n(x,k)| \leq \frac{\sigma_1(x)^n}{n!}. \tag{2.6}$$

Indeed, this estimate is true for $n = 0$, and using the Fubini theorem and the induction hypothesis we get

$$\begin{aligned}|\varphi_{n+1}(x,k)| &\leq \frac{1}{n!} \int_x^\infty \left(\int_x^t |V(t)|\sigma_1(t)^n ds \right) dt \\ &= \frac{1}{n!} \int_x^\infty \left(\int_s^\infty |V(t)|\sigma_1(t)^n dt \right) ds \\ &\leq \frac{1}{n!} \int_x^\infty \sigma(s)\sigma_1(s)^n ds = \frac{\sigma_1(x)^{n+1}}{(n+1)!}.\end{aligned}$$

Thus

$$|\varphi(x,k)| \leq e^{\sigma_1(x)}. \tag{2.7}$$

By the Weierstrass M-test the function $\varphi(x,k)$, defined by convergent series (2.5), is analytic for $\operatorname{Im} k > 0$. It is also continuous up to $\operatorname{Im} k = 0$ uniformly in x on compact subsets of $\mathbb{R}$.

The first estimate in part (i) now follows from (2.4) and (2.7). Namely, using $|V(t)| = -\sigma'(t)$ and integration by parts, we obtain

$$\begin{aligned}
|\varphi(x,k)-1| &\le \int_x^\infty \left|\frac{1-e^{-2ik(x-t)}}{2ik}\right| |V(t)||\varphi(t,k)|dt \\
&\le e^{\sigma_1(x)}\left(\int_x^{x+\frac{1}{|k|}} (t-x)|V(t)|dt + \frac{1}{|k|}\int_{x+\frac{1}{|k|}}^\infty |V(t)|dt\right) \\
&= e^{\sigma_1(x)}\left(-(t-x)\sigma(t)\Big|_x^{x+\frac{1}{|k|}} + \int_x^{x+\frac{1}{|k|}} \sigma(t)dt + \frac{1}{|k|}\int_{x+\frac{1}{|k|}}^\infty |V(t)|dt\right) \\
&= e^{\sigma_1(x)}\big(\sigma_1(x) - \sigma_1(x+\tfrac{1}{|k|})\big).
\end{aligned}$$

For $k=0$ this estimate should be understood as $|\varphi(x,0)-1| \le \sigma_1(x)e^{\sigma_1(x)}$. The function $f_1(x,k) = e^{ikx}\varphi(x,k)$ satisfies the integral equation (2.3), and (2.7) allows us to differentiate under the integral sign in (2.3). This proves that $f_1(x,k)$ satisfies the differential equation (2.1) and the first estimate in part (i). In particular, $\lim_{x\to\infty} e^{-ikx} f_1(x,k) = 1$ for $\operatorname{Im} k \ge 0$. Differentiating (2.3) and using $e^{-\operatorname{Im} k(t-x)}|\cos k(x-t)| \le 1$ for $t \ge x$ and $\operatorname{Im} k \ge 0$, we obtain

$$|e^{-ikx} f_1'(x,k) - ik| \le \int_x^\infty |V(t)||\varphi(t,k)|dt \le \sigma(x)e^{\sigma_1(x)}, \tag{2.8}$$

so that $\lim_{x\to\infty} e^{-ikx} f_1'(x,k) = ik$ for $\operatorname{Im} k \ge 0$.

The conjugation property follows from the uniqueness of the solution $f_1(x,k)$ satisfying the estimate in part (i). To prove the uniqueness, denote by $\chi(x,k)$ the homogeneous solution of the integral equation (2.4) with the property that $\alpha(x) = \sup_{x\le t<\infty} |\chi(t,k)| < \infty$ for all $x \in \mathbb{R}$. Consider the inequality

$$|\chi(x,k)| \le \int_x^\infty \left(\int_x^t |V(t)||\chi(t,k)|ds\right) dt,$$

which follows from the homogeneous form of equation (2.4). Repeating the proof of the estimate (2.6), we get $|\chi(x,k)| \le \alpha(x)\dfrac{\sigma_1(x)^n}{n!}$, and passing to the limit $n \to \infty$ gives $\chi(x,k) = 0$.

To prove the first estimate in part (v), consider the inequality

$$|\varphi(x,k)-1| \le \frac{\sigma(x)}{|k|} - \frac{1}{|k|}\int_x^\infty \sigma'(t)|\varphi(t,k)-1|dt \tag{2.9}$$

which follows from (2.4) for $k \ne 0$. Iterating (2.9) we get

$$|\varphi(x,k)-1| \le \frac{\sigma(x)}{|k|} e^{\frac{1}{|k|}\sigma(x)}.$$

The asymptotic in part (vi) follows from the estimate in part (v), which completes the proof for the solution $f_1(x,k)$. The existence and analytic properties of the solution $f_2(x,k)$ are proved similarly by considering the integral equation

$$f_2(x,k) = e^{-ikx} + \int_{-\infty}^{x} \frac{\sin k(x-t)}{k} V(t) f_2(t,k)\,dt. \tag{2.10}$$ □

Corollary 2.2. *For* $\operatorname{Im} k \geq 0$ *and* $k \neq 0$,

$$\lim_{x\to\infty} e^{-ikx}(\dot{f}_1(x,k) - ixf_1(x,k)) = 0, \quad \lim_{x\to-\infty} e^{ikx}(\dot{f}_2(x,k) + ixf_2(x,k)) = 0,$$

where the dot stands for the partial derivative with respect to k.

Proof. Differentiating (2.4) with respect to k we obtain the following integral equation for $\dot{\varphi}(x,k) = e^{-ikx}(\dot{f}_1(x,k) - ixf_1(x,k))$:

$$\dot{\varphi}(x,k) = g(x,k) - \int_x^{\infty} \frac{1 - e^{-2ik(x-t)}}{2ik} V(t)\dot{\varphi}(t,k)\,dt,$$

where

$$g(x,k) = \frac{1}{k}\int_x^{\infty} (t-x)e^{-2ik(x-t)} V(t)\varphi(t,k)\,dt + \frac{1}{k}(1 - \varphi(x,k)).$$

It follows the estimate in part (i) of Theorem 2.1 and (2.7) that $|g(x,k)| \leq \frac{2}{|k|}\sigma_1(x)e^{\sigma_1(x)}$, and repeating the proof of the estimate (2.7), we obtain that $|\dot{\varphi}(x,k)| \leq \frac{2}{|k|}\sigma_1(x)e^{2\sigma_1(x)}$. Since $\lim_{x\to\infty}\sigma_1(x) = 0$, this proves the statement for $f_1(x,k)$. The corresponding result for $f_2(x,k)$ is proved similarly. □

For real $k \neq 0$ the pairs $f_1(x,k)$, $f_1(x,-k) = \overline{f_1(x,k)}$ and $f_2(x,k)$, $f_2(x,-k) = \overline{f_2(x,k)}$ are fundamental solutions of the differential equation (2.1). Indeed, the Wronskian $W(y_1,y_2) = y_1'y_2 - y_1y_2'$ of two solutions of (2.1) does not depend on x, and we get from part (ii) that

$$W(f_1(x,k), f_1(x,-k)) = \lim_{x\to\infty} W(f_1(x,k), f_1(x,-k)) = 2ik,$$
$$W(f_2(x,k), f_2(x,-k)) = \lim_{x\to-\infty} W(f_2(x,k), f_2(x,-k)) = -2ik.$$

Therefore for such k we have

$$f_2(x,k) = a(k)f_1(x,-k) + b(k)f_1(x,k), \tag{2.11}$$

where the *transition coefficients* $a(k)$ and $b(k)$ are given by

$$a(k) = \frac{1}{2ik}W(f_1(x,k), f_2(x,k)), \quad b(k) = \frac{1}{2ik}W(f_2(x,k), f_1(x,-k)), \tag{2.12}$$

and satisfy $\overline{a(k)} = a(-k)$, $\overline{b(k)} = b(-k)$. Similarly we find that

$$f_1(x,k) = a(k)f_2(x,-k) - b(-k)f_2(x,k). \tag{2.13}$$

Back substituting (2.13) for $f_1(x,k)$ and $f_1(x,-k)$ into (2.11), for real $k \neq 0$ we find the so-called *normalization condition*,

$$|a(k)|^2 = 1 + |b(k)|^2. \tag{2.14}$$

It follows from parts (iii) and (vi) of Theorem 2.1 that coefficient $a(k)$ admits analytic continuation to $\operatorname{Im} k > 0$ and

$$a(k) = 1 + O(|k|^{-1}) \quad \text{as} \quad |k| \to \infty. \tag{2.15}$$

Moreover, the function $ka(k)$ is continuous in $\operatorname{Im} k \geq 0$.

Normalization condition (2.14) implies that all zeros of $a(k)$ are in the upper half-plane $\operatorname{Im} k > 0$. Let k_0 be such a zero, $a(k_0) = 0$. It follows from the first equation in (2.12) that $W(f_1(x,k_0), f_2(x,k_0)) = 0$, so that the Jost solutions $f_1(x,k_0)$, $f_2(x,k_0)$ are linearly dependent,

$$f_1(x,k_0) = c_0 f_2(x,k_0),$$

for some $c_0 \neq 0$. It follows from part (i) of Theorem 2.1 that for $\operatorname{Im} k > 0$ the solution $f_1(x,k)$ is exponentially decaying as $x \to \infty$, and the solution $f_2(x,k)$ is exponentially decaying as $x \to -\infty$. Therefore $f_1(\,\cdot\,,k_0) \in L^2(\mathbb{R})$ is an eigenfunction of the Schrödinger operator H with the eigenvalue $\lambda_0 = k_0^2$. Since H is symmetric, its eigenvalues are real:

$$\lambda_0 \|f_1(\,\cdot\,,k_0)\|^2 = \int_{-\infty}^{\infty} \big(-f_1''(x,k_0) + V(x) f_1(x,k_0)\big)\overline{f_1(x,k_0)}\,dx$$
$$= \int_{-\infty}^{\infty} f_1(x,k_0)\big(-\overline{f_1''(x,k_0)} + V(x)\overline{f_1(x,k_0)}\big)\,dx = \bar{\lambda}_0 \|f_1(\,\cdot\,,k_0)\|^2,$$

as is easily seen by integrating by parts twice; due to part (i) of Theorem 2.1 and estimate (2.8) the boundary terms vanish as $|x| \to \infty$. Thus $k_0 = i\varkappa_0$ is pure imaginary with $\varkappa_0 > 0$ so that $\lambda_0 = -\varkappa_0^2 < 0$, and the corresponding eigenfunction $f_1(x, i\varkappa_0)$ is real-valued.

Proposition 2.1. *The function $a(k)$ in the upper half-plane $\operatorname{Im} k > 0$ has only finitely many pure imaginary simple zeros $k_l = i\varkappa_l$, and*

$$\dot{a}(i\varkappa_l) = -ic_l \|f_2(\,\cdot\,, i\varkappa_l)\|^2, \quad l = 1, \dots, n,$$

where the dot stands for the derivative and $f_1(x, i\varkappa_l) = c_l f_2(x, i\varkappa_l)$. The function $1/a(k)$ is bounded in some neighborhood of $k = 0$ in $\operatorname{Im} k \geq 0$.

Proof. It follows from (2.14) and (2.15) that $k = 0$ is the only possible accumulation point of zeros of $a(k)$ in $\operatorname{Im} k \geq 0$. First suppose that functions $f_1(x,k)$ and $f_2(x,k)$ are linearly independent for $k = 0$. Then the continuous in $\operatorname{Im} k > 0$ function $ka(k)$ satisfies $\lim_{k\to 0} ka(k) = W(f_1(x,0), f_2(x,0)) \neq 0$. Therefore $a(k) \neq 0$ in some neighborhood of 0, and $a(k)$ has only finitely many zeros in $\operatorname{Im} k > 0$.

The case when $f_1(x,0) = cf_2(x,0)$, $c \neq 0$, is more subtle. Suppose that there is a converging to 0 subsequence $k_n = i\varkappa_n$ of zeros of $a(k)$ in $\operatorname{Im} k > 0$. It follows from part (i) of Theorem 2.1 that there exists $A > 0$ such that for all $\varkappa \geq 0$ we have $f_1(x, i\varkappa) > \frac{1}{2}e^{-\varkappa x}$ for $x \geq A$ and $f_2(x, i\varkappa) > \frac{1}{2}e^{\varkappa x}$ for $x \leq A$, so that

$$\int_A^\infty f_1(x, i\varkappa_n) f_1(x,0)dx, \ \int_{-\infty}^{-A} f_2(x, i\varkappa_n) f_2(x,0)dx \geq \frac{1}{4\varkappa} e^{-\varkappa A}.$$

Using integration by parts, we get, as before,

$$\begin{aligned}\varkappa_n^2 \int_{-\infty}^\infty f_1(x, i\varkappa_n) f_1(x,0)dx &= \int_{-\infty}^\infty \big(f_1''(x, i\varkappa_n) - V(x) f_1(x, i\varkappa_n)\big) f_1(x,0)dx \\ &= \int_{-\infty}^\infty f_1(x, i\varkappa_n)\big(f_1''(x,0) - V(x) f_1(x,0)\big)dx = 0.\end{aligned}$$

On other hand, we have

$$\begin{aligned}0 = \int_A^\infty f_1(x, i\varkappa_n) f_1(x,0)dx + \int_{-A}^A f_1(x, i\varkappa_n) f_1(x,0)dx \\ + c \cdot c_n \int_{-\infty}^{-A} f_2(x, i\varkappa_n) f_2(x,0)dx.\end{aligned} \tag{2.16}$$

Since $f_1(x,k)$ is continuous on $\operatorname{Im} k \geq 0$, uniformly in x on the compact subsets of $\mathbb{R}$, we have

$$\lim_{n\to\infty} \int_{-A}^A f_1(x, i\varkappa_n) f_1(x,0)dx = \int_{-A}^A f_1(x,0)^2 dx \geq 0.$$

Using

$$\lim_{n\to\infty} c \cdot c_n = c \lim_{n\to\infty} \frac{f_1(x, i\varkappa_n)}{f_2(x, i\varkappa_n)} = c\,\frac{f_1(x,0)}{f_2(x,0)} = c^2 > 0,$$

we obtain from (2.16) that for large enough n,

$$0 > \frac{1}{4\varkappa_n} e^{-\varkappa_n A}.$$

This is clearly a contradiction, so $a(k)$ has only finitely many zeros. The proof of local boundness of $1/a(k)$ in this case is left to the reader.

Next, consider the differential equation (2.1) together with the equation obtained from it by differentiating with respect to k:

$$-y'' + V(x)y = k^2 y, \tag{2.17}$$

$$-\dot{y}'' + V(x)\dot{y} = k^2\dot{y} + 2ky. \tag{2.18}$$

Set $y = f_1(x,k)$ in equation (2.17), $y = f_2(x,k)$ in equation (2.18), and multiply (2.17) by $\dot{f}_2(x,k)$ and (2.18) by $f_1(x,k)$. Subtracting the resulting equations, we obtain

$$W(f_1(x,k), \dot{f}_2(x,k))' = 2k f_1(x,k) f_2(x,k).$$

Similarly, setting $y = f_2(x,k)$ in (2.17), $y = f_1(x,k)$ in (2.18), cross multiplying and subtracting, we obtain

$$-W(\dot f_1(x,k), f_2(x,k))' = 2k f_1(x,k) f_2(x,k).$$

Therefore

$$W(f_1(x,k), \dot f_2(x,k))\Big|_{-A}^{x} = 2k\int_{-A}^{x} f_1(x,k) f_2(x,k)dx, \tag{2.19}$$

$$-W(\dot f_1(x,k), f_2(x,k))\Big|_{x}^{A} = 2k\int_{x}^{A} f_1(x,k) f_2(x,k)dx. \tag{2.20}$$

Now suppose that $a(k_0) = 0$. We have

$$W(f_1(x,k), f_2(x,k)) = 2ika(k),$$

so that differentiating with respect to k and setting $k = k_0$ gives

$$W(\dot f_1(x,k_0), f_2(x,k_0)) + W(f_1(x,k_0), \dot f_2(x,k_0)) = 2ik_0\dot a(k_0).$$

Since $f_1(x,k_0) = c_0 f_2(x,k_0)$, it follows from Theorem 2.1 and Corollary 2.2 that boundary terms in (2.19)–(2.20) vanish as $A \to \infty$, and we obtain, using that $f(x,k_0)$ is real-valued:

$$\dot a(k_0) = -i\int_{-\infty}^{\infty} f_1(x,k_0) f_2(x,k_0)dx = -ic_0\|f_2(\,\cdot\,,k_0)\|^2. \qquad \square$$

The eigenvalues of the Schrödinger operator H are simple. Indeed, the function $f_1(x,i\varkappa)$ is a solution of the differential equation (2.1) for $\lambda = -\varkappa^2 < 0$, which decays exponentially as $x \to \infty$. Since the Wronskian of any two solutions of (2.1) is constant, the second solution of (2.1), linearly independent with $f_1(x,i\varkappa)$, is exponentially increasing as $x \to \infty$. Thus every exponentially decaying as $x \to \infty$ solution of (2.1) for $\lambda = -\varkappa^2$ is a constant multiple of $f_1(x,i\varkappa)$. In particular, this proves that the point spectrum of H is simple. This result also follows from the simplicity of zeros of the function $a(k)$ and the eigenfunction expansion theorem, proved in the next section.

Problem 2.1 (The oscillation theorem)**.** Let $\lambda_1 = -\varkappa_1^2 < \cdots < \lambda_n = \varkappa_n^2 < 0$ be the eigenvalues of the one-dimensional Schrödinger operator H. Prove that corresponding eigenfunctions $f_1(x,i\varkappa_l)$ have exactly $l-1$ simple zeros, $l = 1,\dots,n$.

Problem 2.2. Prove that for $\operatorname{Im} k \ge 0$ the Jost solution $f_1(x,k)$ admits the representation

$$f_1(x,k) = e^{ikx} + \int_x^{\infty} K_1(x,t)e^{ikt}dt,$$

where

$$K(x,x) = \tfrac{1}{2}\int_x^{\infty} V(t)dt \quad \text{and} \quad |K_1(x,t)| \le \tfrac{1}{2}\sigma(\tfrac{x+t}{2})e^{\sigma_1(x)-\sigma_1(\frac{x+t}{2})}.$$

Moreover, the kernel $K_1(x,t)$ is differentiable and

$$|\tfrac{\partial K_1}{\partial x}(x,t)+\tfrac{1}{4}V(\tfrac{x+t}{2})|\le\tfrac{1}{2}\sigma_1(x)\sigma(\tfrac{x+t}{2})e^{\sigma_1(x)},$$

with the similar inequality for $\frac{\partial K_1}{\partial t}(x,t)$. Correspondingly, for $\operatorname{Im} k\le 0$ the Jost solution $f_2(x,k)$ admits the integral representation

$$f_2(x,k)=e^{-ikx}+\int_{-\infty}^{x}K_2(x,t)e^{-ikt}dt,$$

where the kernel $K_2(x,t)$ satisfies similar estimates. (*Hint:* Show that (2.3) is equivalent to the integral equation

$$K_1(x,t)=\tfrac{1}{2}\int_{\frac{x+t}{2}}^{\infty}V(s)ds+\tfrac{1}{2}\int_{x}^{\infty}V(s)\int_{t-(s-x)}^{t+(s-x)}K_1(s,u)duds$$

with the condition $K_1(x,t)=0$ for $t<x$, which is solved by the method of successive approximations.)

Problem 2.3. Show that transition coefficients $a(k)$ and $b(k)$ have the representations

$$a(k)=1-\frac{1}{2ik}\int_{-\infty}^{\infty}V(x)dx-\frac{1}{2ik}\int_{0}^{\infty}A(t)e^{ikt}dt,\quad b(k)=\frac{1}{2ik}\int_{-\infty}^{\infty}B(t)e^{-ikt}dt,$$

where $A(t)\in L^1(0,\infty)$ and $B(t)\in L^1(-\infty,\infty)$.

Problem 2.4. Show that for $\operatorname{Im} k>0$ the transition coefficient $a(k)$ satisfies the *dispersion relation*

$$a(k)=\exp\left\{\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{\log(1+|b(p)|^2)}{p-k}dp\right\}\prod_{l=1}^{n}\frac{k-i\varkappa_l}{k+i\varkappa_l}.$$

2.2. Eigenfunction expansion. Here we explicitly construct the resolvent kernel for the one-dimensional Schrödinger operator H, and show that it is self-adjoint with the domain consisting of functions $\psi\in L^2(\mathbb{R})$, which are twice differentiable on $\mathbb{R}$, and such that $-\psi''+V(x)\psi\in L^2(\mathbb{R})$. Using the method of complex integration we derive the eigenfunction expansion theorem for the operator H, which generalizes the corresponding result for the operator H_0 of a free quantum particle, considered in Section 2.3 of Chapter 2.

For $\lambda\in\mathbb{C}\setminus[0,\infty)$ let

$$R_\lambda(x,y)=\begin{cases}-\dfrac{f_1(x,k)f_2(y,k)}{2ika(k)} & \text{if } x\ge y,\\[2ex] -\dfrac{f_1(y,k)f_2(x,k)}{2ika(k)} & \text{if } x\le y,\end{cases}\tag{2.21}$$

where the branch of the function $k=\sqrt{\lambda}$ on $\mathbb{C}\setminus[0,\infty)$ is defined by the condition that $\operatorname{Im} k>0$. For fixed x and y the function $R_\lambda(x,y)$ is meromorphic on $\mathbb{C}\setminus[0,\infty)$ with simple poles at $\lambda_l=-\varkappa_l^2$, $l=1,\dots,n$. For fixed

$\lambda \neq \lambda_l$ the function $R_\lambda(x,y) = R_\lambda(y,x)$ is continuous in x and y, and it follows from part (v) of Theorem 2.1 and (2.15) that

$$|R_\lambda(x,y)| \leq C\,\frac{e^{-\operatorname{Im} k|x-y|}}{|k|}, \quad C>0. \tag{2.22}$$

The kernel $R_\lambda(x,y)$ for $\lambda \neq \lambda_l$ defines a bounded integral operator R_λ in $L^2(\mathbb{R})$ by the formula

$$(R_\lambda \psi)(x) = \int_{-\infty}^{\infty} R_\lambda(x,y)\psi(y)dy.$$

Indeed, it follows from (2.22) that for $\psi \in L^2(\mathbb{R})$,

$$|k|^2\,\|R_\lambda\psi\|^2 \leq C^2 \int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} e^{-\operatorname{Im} k|x-y|}|\psi(y)|dy\right)^2 dx$$
$$= C^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\operatorname{Im} k(|y_1|+|y_2|)} \int_{-\infty}^{\infty} |\psi(x+y_1)\psi(x+y_2)|dx dy_1 dy_2$$
$$\leq 4C^2(\operatorname{Im} k)^{-2}\|\psi\|^2.$$

In particular,

$$\|R_\lambda\| \leq \frac{2C}{|k|\operatorname{Im} k}.$$

Lemma 2.1. *The operator H is self-adjoint and $R_\lambda = (H-\lambda I)^{-1}$ for $\lambda \in \mathbb{C} \setminus \big\{[0,\infty) \cup \{\lambda_1,\dots,\lambda_n\}\big\}$, where I is the identity operator in $L^2(\mathbb{R})$.*

Proof. Let $g \in L^2(\mathbb{R})$. As in the variation of parameters method, it follows from (2.21) that for $\lambda \in \mathbb{C} \setminus \big\{[0,\infty) \cup \{\lambda_1,\dots,\lambda_n\}\big\}$ the function $y = R_\lambda g \in L^2(\mathbb{R})$ is twice differentiable a.e. on $\mathbb{R}$ and satisfies the differential equation

$$-y'' + V(x)y = \lambda y + g(x).$$

Thus $(H-\lambda I)R_\lambda = I$ and, in particular, $\operatorname{Im}(H \pm iI) = L^2(\mathbb{R})$, so that H is self-adjoint. □

Let $\mathfrak{H}_0$ be the Hilbert space of $\mathbb{C}^2$-valued functions $\Phi(\lambda) = \begin{pmatrix}\varphi_1(\lambda)\\ \varphi_2(\lambda)\end{pmatrix}$ on $[0,\infty)$ with the norm

$$\|\Phi\|_0^2 = \int_0^\infty (|\varphi_1(\lambda)|^2 + |\varphi_2(\lambda)|^2)d\sigma(\lambda),$$

where $d\sigma(\lambda) = \frac{1}{2\sqrt{\lambda}}d\lambda$ and $\sqrt{\lambda} \geq 0$ for $\lambda \geq 0$ (see Section 2.3 of Chapter 2, where one should put $\hbar = 1$ and $m = \frac{1}{2}$). For $\lambda \geq 0$ set

$$u_j(x,\sqrt{\lambda}) = \frac{1}{a(\sqrt{\lambda})} f_j(x,\sqrt{\lambda}), \quad j=1,2, \tag{2.23}$$

and for $\psi \in C_0^2(\mathbb{R})$ define the $\mathbb{C}^2$-valued function $\mathscr{U}\psi$ on $[0,\infty)$ with components $(\mathscr{U}\psi)_1$ and $(\mathscr{U}\psi)_2$ by

$$(\mathscr{U}\psi)_j(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\overline{u_j(x,\sqrt{\lambda})}dx, \quad j = 1, 2. \tag{2.24}$$

By Proposition 2.1 the function $\mathscr{U}\psi$ is bounded at $\lambda = 0$, and for large λ using differential equation (2.1) and integration by parts we get

$$(\mathscr{U}\psi)_j(\lambda) = \frac{1}{\lambda\sqrt{2\pi}} \int_{-\infty}^{\infty} \big(-\psi''(x) + V(x)\psi(x)\big)\overline{u_j(x,\sqrt{\lambda})}dx,$$

which shows that $\mathscr{U}\psi \in \mathfrak{H}_0$.

Let P be the orthogonal projection on the subspace of $\mathscr{H} = L^2(\mathbb{R})$ spanned by the eigenfunctions $\psi_l(x) = f_1(x, i\varkappa_l)$, $l = 1, \dots, n$. The functions ψ_l are real-valued and orthogonal, so that for $\psi \in \mathscr{H}$

$$(P\psi)(x) = \sum_{l=1}^{n} \frac{1}{\|\psi_l\|^2}\psi_l(x) \int_{-\infty}^{\infty} \psi(y)\psi_l(y)dy.$$

Theorem 2.3. *The operator $\mathscr{U}$ extends to a partial isometry operator $\mathscr{U} : \mathscr{H} \to \mathfrak{H}_0$,*

$$\mathscr{U}^*\mathscr{U} = I - P \quad \text{and} \quad \mathscr{U}\mathscr{U}^* = I_0,$$

and establishes the isomorphism $(I-P)\mathscr{H} \simeq \mathfrak{H}_0$. Here I and I_0 are, respectively, identity operators in $\mathscr{H}$ and $\mathfrak{H}_0$. For the spectrum of the corresponding Schrödinger operator H we have $\sigma(H) = \{-\varkappa_1^2, \dots, -\varkappa_n^2\} \cup [0,\infty)$, and

$$\mathscr{H} = \mathscr{H}_{\rm pp} \oplus \mathscr{H}_{\rm ac},$$

where $\mathscr{H}_{\rm pp} = P\mathscr{H}$ and $\mathscr{H}_{\rm ac} = (I-P)\mathscr{H}$ are, respectively, invariant subspaces associated with pure point and absolutely continuous spectra of H. The operator $\mathscr{U}H\mathscr{U}^*$ is a multiplication by λ operator in $\mathfrak{H}_0$, so that the absolutely continuous spectrum $[0,\infty)$ of H has multiplicity two, and the operator $\mathscr{U}$ "diagonalizes" the restriction of H to the subspace $\mathscr{H}_{\rm ac}$.

Proof. To proof the relation $\mathscr{U}^*\mathscr{U} = I - P$ — the so-called *completeness relation* — it is sufficient to establish the following classical eigenfunction expansion formula for $\psi \in C_0^2(\mathbb{R})$:

$$\psi(x) = \frac{1}{2\pi}\int_0^{\infty}\bigg(u_1(x,k)\int_{-\infty}^{\infty}\psi(y)\overline{u_1(y,k)}dy + u_2(x,k)\int_{-\infty}^{\infty}\psi(y)\overline{u_2(y,k)}dy\bigg)dk$$
$$+\sum_{l=1}^{n}\frac{1}{\|\psi_l\|^2}\psi_l(x)\int_{-\infty}^{\infty}\psi(y)\psi_l(y)dy, \tag{2.25}$$

where all integrals are absolutely convergent, and we put $\sqrt{\lambda} = k$, $d\sigma(\lambda) = dk$. Indeed, assuming that (2.25) holds, we get for $\psi, \varphi \in C_0^2(\mathbb{R})$

$$\begin{aligned}(\psi,\varphi) &= \int_{-\infty}^{\infty}\psi(x)\overline{\varphi(x)}dx = \frac{1}{2\pi}\int_{-\infty}^{\infty}\overline{\varphi(x)}\bigg(\int_0^{\infty}\bigg(u_1(x,k)\int_{-\infty}^{\infty}\psi(y)\overline{u_1(y,k)}dy\\ &\quad + u_2(x,k)\int_{-\infty}^{\infty}\psi(y)\overline{u_2(y,k)}dy\bigg)dk\bigg)dx + \sum_{l=1}^{n}\frac{1}{\|\psi_l\|^2}(\psi,\psi_l)(\psi_l,\varphi)\\ &= (\mathscr{U}\psi,\mathscr{U}\varphi)_0 + \sum_{l=1}^{n}\frac{1}{\|\psi_l\|^2}(\psi,\psi_l)(\psi_l,\varphi),\end{aligned}$$

where $(\ ,\ )_0$ is the inner product in $\mathfrak{H}_0$, and the interchange of integrals over x and k is justified by the Fubini theorem. Thus

$$(\mathscr{U}\psi,\mathscr{U}\varphi)_0 = ((I-P)\psi,\varphi) \tag{2.26}$$

for $\psi, \varphi \in C_0^2(\mathbb{R})$, and we conclude that $\mathscr{U}$ extends to a bounded operator from $\mathscr{H}$ and $\mathfrak{H}_0$ satisfying (2.26) for all $\psi, \varphi \in \mathscr{H}$.

To prove the eigenfunction expansion formula (2.25), for $\lambda \in \mathbb{C} \setminus [0,\infty)$ set $g(x,\lambda) = (R_\lambda\psi)(x)$. The function $g(x,\lambda)$ for fixed x is meromorphic in $\lambda \in \mathbb{C} \setminus [0,\infty)$ with simple poles at $\lambda = \lambda_l$, $l = 1,\dots,n$. It follows from (2.21) and Proposition 2.1 that

$$\operatorname{Res}_{\lambda=\lambda_l} g(x,\lambda) = \frac{ic_l}{\dot{a}(i\varkappa_l)}f_2(x,i\varkappa_l)\int_{-\infty}^{\infty}f_2(y,i\varkappa_l)\psi(y)dy = -\frac{(\psi,\psi_l)}{\|\psi_l\|^2}\psi_l(x).$$

Since $HR_\lambda = R_\lambda H = I + \lambda R_\lambda$, we have

$$-g''(x,\lambda) + V(x)g(x,\lambda) = \psi(x) + \lambda g(x,\lambda),$$

so that

$$g(x,\lambda) = -\frac{1}{\lambda}\psi(x) + \frac{1}{\lambda}(R_\lambda\varphi)(x),$$

where $\varphi = -\psi'' + V(x)\psi \in C_0(\mathbb{R})$. From (2.22) we get

$$|(R_\lambda\varphi)(x)| \le \frac{C}{|\sqrt{\lambda}|} \quad \text{as} \quad |\lambda| \to \infty,$$

so that

$$g(x,\lambda) = -\frac{1}{\lambda}\psi(x) + O(|\lambda|^{-3/2}) \quad \text{as} \quad |\lambda| \to \infty. \tag{2.27}$$

It follows from Proposition 2.1 and (2.21) that

$$g(x,\lambda) = O(|\lambda|^{-1/2}) \quad \text{as} \quad \lambda \to 0. \tag{2.28}$$

For $0 < \varepsilon < 1 < N$ let $\mathcal{C} = \mathcal{C}_{\varepsilon,N}$ be the contour consisting of the following parts: (i) the arc $\mathcal{C}_\varepsilon$ of a circle $\lambda = \varepsilon e^{i\theta}$, $\varepsilon \le |\arg\theta| \le \pi$, oriented clockwise; (ii) the arc $\mathcal{C}_N$ of a circle $\lambda = Ne^{i\theta}$, $\varepsilon_N \le |\arg\theta| \le \pi$, oriented anti-clockwise, where $N\sin\varepsilon_N = \varepsilon\sin\varepsilon$; (iii) the segments $\mathcal{I}_\pm$ of the straight

lines $\operatorname{Im}\lambda = \pm\varepsilon \sin\varepsilon$ which connect the boundaries of the arcs. Choose ε and N such that all poles λ_l of $g(x,\lambda)$ are inside $\mathcal{C}$, and consider the integral

$$I = \frac{1}{2\pi i}\int_{\mathcal{C}} g(x,\lambda)d\lambda.$$

On one hand, by the Cauchy residue theorem

$$I = \sum_{l=1}^{n} \operatorname{Res}_{\lambda=\lambda_l} g(x,\lambda) = -\sum_{l=1}^{n} \frac{(\psi,\psi_l)}{\|\psi_l\|^2}\psi_l(x).$$

On the other hand, it follows from (2.27) and (2.28) that

$$\lim_{N\to\infty}\frac{1}{2\pi i}\int_{\mathcal{C}_N} g(x,\lambda)d\lambda = -\psi(x) \quad \text{and} \quad \lim_{\varepsilon\to 0}\frac{1}{2\pi i}\int_{\mathcal{C}_\varepsilon} g(x,\lambda)d\lambda = 0.$$

Thus we obtain

$$\psi(x) - \sum_{l=1}^{n}\frac{1}{\|\psi_l\|^2}(\psi,\psi_l)\psi_l(x) = \lim_{\varepsilon\to 0}\lim_{N\to\infty}\frac{1}{2\pi i}\left(\int_{\mathcal{I}_+} g(x,\lambda)d\lambda - \int_{\mathcal{I}_-} g(x,\lambda)d\lambda\right)$$

$$= \frac{1}{2\pi i}\int_0^\infty \left(\int_{-\infty}^{\infty}(R_{\lambda+i0}(x,y) - R_{\lambda-i0}(x,y))\psi(y)dy\right)d\lambda, \tag{2.29}$$

where

$$R_{\lambda\pm i0}(x,y) = \lim_{\varepsilon\to 0} R_{\lambda\pm i\varepsilon}(x,y).$$

To compute the difference $R_{\lambda+i0}(x,y) - R_{\lambda-i0}(x,y)$, observe that on the cut $\lambda \geq 0$ we have $\sqrt{\lambda+i0} = k \geq 0$ and $\sqrt{\lambda-i0} = -k \leq 0$. It follows from (2.21) that for $x \geq y$

$$R_{\lambda+i0}(x,y) - R_{\lambda-i0}(x,y) = -\frac{1}{2ik}\left(\frac{f_1(x,k)f_2(y,k)}{a(k)} + \frac{f_1(x,-k)f_2(y,-k)}{a(-k)}\right),$$

and using the equations

$$f_1(x,k) = \frac{1}{a(-k)}f_2(x,-k) - \frac{b(-k)}{a(-k)}f_1(x,-k),$$
$$f_2(y,-k) = \frac{1}{a(k)}f_1(y,k) + \frac{b(-k)}{a(k)}f_2(y,k),$$

which follow from (2.11) and (2.13), we obtain

$$R_{\lambda+i0}(x,y) - R_{\lambda-i0}(x,y) = \frac{i}{2k|a(k)|^2}(f_1(x,k)\overline{f_1(y,k)} + f_2(x,k)\overline{f_2(y,k)})$$
$$= \frac{i}{2k}(u_1(x,k)\overline{u_1(y,k)} + u_2(x,k)\overline{u_2(y,k)}),$$

where $\lambda = k^2$. Substituting this into (2.29) and using the symmetry $R_\lambda(x,y) = R_\lambda(y,x)$ of the resolvent kernel, we get the eigenfunction expansion (2.25).

Let $\mathscr{U}_{\text{ac}}$ be the restriction of the operator $\mathscr{U}$ to the subspace $\mathscr{H}_{\text{ac}} = (I-P)\mathscr{H}$. It follows from the completeness relation that the operator $\mathscr{U}_{\text{ac}}$

is an isometry, so that $\operatorname{Im}\mathscr{U} = \operatorname{Im}\mathscr{U}_{\rm ac}$ is a closed subspace of $\mathfrak{H}_0$. Thus to verify the *orthogonality relation* $\mathscr{U}\mathscr{U}^* = I_0$, it is sufficient to show that $\operatorname{Im}\mathscr{U} = \mathfrak{H}_0$. Using integration by parts we easily get that a self-adjoint operator $\mathscr{U}_{\rm ac} H \mathscr{U}_{\rm ac}^{-1}$ is a multiplication by λ operator in $\operatorname{Im}\mathscr{U}$ with the domain $\mathscr{U}D(H)$. Moreover,

$$\mathscr{U}R_\mu = R_\mu^{(0)}\mathscr{U}, \quad \mu \in \mathbb{C}\setminus[0,\infty),$$

where $R_\mu^{(0)}$ is the resolvent of the multiplication by λ operator in $\mathfrak{H}_0$, so that $\operatorname{Im}\mathscr{U}$ is an invariant subspace for $R_\mu^{(0)}$. Now it follows from Lemma 2.2 in Section 2.2 of Chapter 2 that there are Borel subsets $E_1, E_2 \subseteq [0,\infty)$ such that

$$\operatorname{Im}\mathscr{U} = \left\{ \tilde{\Phi} = \begin{pmatrix} \chi_{E_1}\varphi_1 \\ \chi_{E_2}\varphi_2 \end{pmatrix}, \quad \Phi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \in \mathfrak{H}_0 \right\}.$$

If, say, $E_1^{\rm c} = [0,\infty)\setminus E_1$ has positive Lebesgue measure, then for $\lambda = k^2 \in E_1^{\rm c}$ we have

$$\int_{-\infty}^{\infty} \overline{u_1(x,k)}\psi(x)dx = 0 \quad \text{for all} \quad \psi \in C_0^2(\mathbb{R}),$$

so that $u(x,k) = 0$ for all $x \in \mathbb{R}$ — a contradiction. Therefore, $\operatorname{Im}\mathscr{U} = \mathfrak{H}_0$. □

Let $\mathscr{U}_0 : \mathscr{H} \to \mathfrak{H}_0$ be the corresponding unitary operator for the Schrödinger operator H_0 of a free particle, constructed in Section 2.3 of Chapter 2 (with $\hbar = 1$ and $m = \frac{1}{2}$), and set $U = \mathscr{U}^*\mathscr{U}_0 : \mathscr{H} \to \mathscr{H}_{\rm ac}$.

Corollary 2.4. *The restriction of H to the absolutely continuous subspace $\mathscr{H}_{\rm ac}$ is unitarily equivalent to H_0,*

$$H|_{\mathscr{H}_{\rm ac}} = UH_0U^{-1}.$$

Remark. In physics literature, completeness and orthogonality relations, understood in the distributional sense, are usually written as

$$\frac{1}{2\pi}\int_0^\infty (u_1(x,k)\overline{u_1(y,k)} + u_2(x,k)\overline{u_2(y,k)})dk + \sum_{l=1}^n \frac{\psi_l(x)\psi_l(y)}{\|\psi_l\|^2} = \delta(x-y)$$

and

$$\frac{1}{2\pi}\int_{-\infty}^\infty u_j(x,k)\overline{u_k(x,p)}dx = \delta_{jk}\delta(k-p),$$

where $i,k = 1,2$ and $k,p > 0$. When transition coefficients $a(k)$ and $b(k)$ are differentiable for $k \neq 0$[2], the orthogonality relation can be derived from the identity

$$\frac{d}{dx}W(u_j(x,k), \overline{u_k(x,p)}) = (k^2-p^2)u_j(x,k)\overline{u_k(x,p)}, \tag{2.30}$$

[2]This is the case when $V(x)$ satisfies $\int_{-\infty}^{\infty}(1+|x|^2)|V(x)|dx < \infty$.

which immediately follows from the differential equation (2.1). Namely, consider the case $j = k = 1$ and integrate (2.30) over $[-N, N]$. Using (2.13) and asymptotics of Jost solutions, we get

$$\int_{-N}^{N} u_1(x,k)\overline{u_1(x,p)}dx = \frac{1}{(k^2-p^2)a(k)\overline{a(p)}} W(f_1(x,k), \overline{f_1(x,p)})\Big|_{-N}^{N}$$
$$= \frac{i}{a(k)\overline{a(p)}} \left(\frac{e^{i(k-p)N} - a(k)\overline{a(p)}e^{-i(k-p)N} + \overline{b(k)}b(p)e^{i(k-p)N}}{k-p} \right.$$
$$\left. + \frac{a(k)b(p)e^{-i(k+p)N} - \overline{b(k)a(p)}e^{i(k+p)N}}{k+p} \right) + o(1) \quad \text{as} \quad N \to \infty.$$

Since $k, p > 0$, by the Riemann-Lebesgue lemma the distributional limit as $N \to \infty$ of the terms in the third line is zero. Since $a(k)$ and $b(k)$ are assumed differentiable, in the second line we can replace $\overline{a(p)}$ and $b(p)$ by $\overline{a(k)}$ and $b(k)$, respectively, since the difference goes to zero as $N \to \infty$ by the Riemann-Lebesgue lemma. Finally, using (2.14) we obtain

$$\lim_{N\to\infty} \int_{-N}^{N} u_1(x,k)\overline{u_1(x,p)}dx = 2 \lim_{N\to\infty} \frac{\sin(k-p)N}{k-p} = 2\pi\delta(k-p),$$

where the last equality is the distributional form of the orthogonality relation for the Fourier transform.

Remark. The eigenfunctions of the continuous spectrum $u_j(x,\lambda)$ also satisfy the normalization condition (2.14) in Section 2.2 of Chapter 2:

$$\lim_{\Delta\to 0} \frac{1}{\Delta} (U_{j,k+\Delta} - U_{j,k}, U_{l,k+\Delta} - U_{l,k}) = \delta_{jl}, \quad j,l = 1,2,$$

where

$$U_{j,k}(x) = \int_{k_0^2}^{k^2} u_j(x,\sqrt{\lambda}) \frac{d\lambda}{2\sqrt{\lambda}} = \int_{k_0}^{k} \frac{f_j(x,p)}{a(p)} dp, \quad j = 1,2.$$

Remark. The qualitative structure of the spectrum of the Schrödinger operator H is determined by the structure of the level sets $H_c(p,x) = \lambda$ of the classical Hamiltonian function $H_c(p,x) = p^2 + V(x)$. Namely, condition $\lim_{|x|\to\infty} V(x) = 0$ implies that the level sets for $\lambda > 0$ are non-compact and the classical motion is unbounded in both directions, and these values of λ fill the absolutely continuous spectrum $[0,\infty)$ of H of multiplicity two. For $\lambda < 0$ the level sets are compact and classical motion is periodic. According to BWS quantization rules (see Section 2.5 in Chapter 2), the energy levels — eigenvalues of H — correspond to the closed orbits, and condition (2.2) guarantees that H has only finitely many eigenvalues.

Problem 2.5. Find the energy levels for the potential

$$V(x) = -\frac{V_0}{\cosh^2 \varkappa x}, \quad V_0 > 0.$$

In particular, show that when $V_0 = 2\varkappa^2$ there is only one eigenvalue $E = -\varkappa^2$.

Problem 2.6. Show that the operator $R_\lambda - R_\lambda^{(0)}$, where $R_\lambda^{(0)} = (H_0 - \lambda I)^{-1}$ and $\lambda \in \mathbb{C} \setminus [0, \infty)$, is of the trace class, and

$$\operatorname{Tr}(R_\lambda - R_\lambda^{(0)}) = -\frac{d}{d\lambda} \log a(\sqrt{\lambda}).$$

(*Hint:* Use Wronskian identities (2.19)-(2.20) from the previous section.)

2.3. S-matrix and scattering theory. It was shown in the previous section that for potentials $V(x)$ satisfying (2.2) the operators $H = H_0 + V$ and H_0 have the same absolutely continuous spectrum. Among many partial isometry operators in $\mathscr{H}$ which establish the unitary equivalence between $H|_{\mathscr{H}_{\mathrm{ac}}}$ and H_0, there are two operators $W_\pm$ of fundamental physical significance. They are defined as

$$W_\pm = \lim_{t \to \pm\infty} e^{iHt} e^{-itH_0}, \tag{2.31}$$

where the limit is understood in the strong operator topology, and are called *wave operators* (or *Möller operators*). In general, the wave operators exist for a Schrödinger operator $H = H_0 + V$ on $\mathbb{R}^n$ with the potential $V(\boldsymbol{q})$ decaying sufficiently fast as $|\boldsymbol{q}| \to \infty$. In this section, we will show that for potentials $V(x)$ satisfying (2.2) the limits (2.31) exist.

The wave operators satisfy the partial isometry relation

$$W_\pm^* W_\pm = I. \tag{2.32}$$

Indeed, strong limits of unitary operators preserve the inner products, so that $(W_\pm \psi, W_\pm \varphi) = (\psi, \varphi)$ for all $\psi, \varphi \in \mathscr{H}$. Convergence $A_n \to A$ as $n \to \infty$ in the strong operator topology does not necessarily imply that $A_n^* \to A^*$, so that we cannot conclude that $W_\pm W_\pm^* = I$. Thus in general the wave operators are not unitary. In fact, it can be shown that $\operatorname{Im} W_\pm = \mathscr{H}_{\mathrm{ac}} = (I - P)\mathscr{H}$ or, equivalently,

$$W_\pm W_\pm^* = I - P, \tag{2.33}$$

where P is the orthogonal projection on the subspace $\mathscr{H}_{\mathrm{pp}}$. Though the proof of (2.33) is rather non-trivial, it is easy to show that $\operatorname{Im} W_\pm \subseteq (I - P)\mathscr{H}$. Indeed, let $\psi \in \mathscr{H}$ be a bound state — an eigenvector for H,

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

Then for every $\varphi \in \mathscr{H}$ we have

$$(W_\pm \varphi, \psi) = \lim_{t \to \pm\infty} e^{i\lambda t} (e^{-itH_0}\varphi, \psi) = 0$$

by the Riemann-Lebesgue lemma, as we have seen in Section 2.3 of Chapter 2.

Assuming that wave operators exist and satisfy (2.33), it is easy to prove that

$$f(H)W_\pm = W_\pm f(H_0) \tag{2.34}$$

for any measurable function f on $\mathbb{R}$. Indeed, according to the spectral theorem, it is sufficient to prove this property for the functions $f(\lambda) = e^{i\tau\lambda}$ for all $\tau \in \mathbb{R}$. In this case, (2.34) immediately follows from the identity

$$e^{i\tau H} e^{i(t-\tau)H} e^{-i(t-\tau)H_0} = e^{itH} e^{-itH_0} e^{i\tau H_0}$$

by passing to the limits $t \to \pm\infty$. Using (2.34) and (2.32) we conclude

$$W_\pm^* H W_\pm = H_0,$$

so that restrictions of the wave operators to the subspace $\mathscr{H}_{\mathrm{ac}}$ establish the unitary equivalence between $H|_{\mathscr{H}_{\mathrm{ac}}}$ and H_0.

Remark. The physical meaning of the wave operators is the following. The one-parameter group $U(t) = e^{-itH}$ of unitary operators describes the evolution of the quantum particle moving in a short-ranged potential field. For large $|t|$ the particle with positive energy moves far away from the center and as $|t| \to \infty$ its evolution is described by the one-parameter group $U_0(t) = e^{-itH_0}$ which corresponds to the free motion. Mathematically this is expressed by the fact that for every $\varphi_- \in \mathscr{H}$ there exists a vector $\psi \in \mathscr{H}$ such that

$$\lim_{t\to-\infty} \|e^{-itH}\psi - e^{-itH_0}\varphi_-\| = 0,$$

and such a vector is given by $\psi = W_-\varphi_-$. Similarly, for every $\varphi_+ \in \mathscr{H}$ the vector $\psi = W_+\varphi_+$ satisfies

$$\lim_{t\to\infty} \|e^{-itH}\psi - e^{-itH_0}\varphi_+\| = 0.$$

As a physical interpretation, orthogonality of $\operatorname{Im} W_\pm$ to the subspace $\mathscr{H}_{\mathrm{pp}}$ is explained by the fact that for all times t bound states are localized near the potential center, whereas the free quantum particle goes to infinity as $|t| \to \infty$.

The wave operators are used to describe the scattering of the quantum particle by the potential center. Namely, given $\varphi_- \in \mathscr{H}$, there is $\psi = W_-\varphi_- \in \mathscr{H}$ such that the solution $\psi(t) = U(t)\psi$ of the non-stationary Schrödinger equation with Hamiltonian H and initial condition $\psi(0) = \psi$ as $t \to -\infty$ approaches the solution $\varphi_-(t) = U_0(t)\varphi_-$ of the non-stationary Schrödinger equation with free Hamiltonian H_0 and initial condition $\varphi_-(0) = \varphi_-$. Since $\operatorname{Im} W_- = \operatorname{Im} W_+$, there is $\varphi_+ \in \mathscr{H}$ such that $\psi = W_+\varphi_+$ and

the solution $\psi(t)$ of the non-stationary Schrödinger equation with Hamiltonian H and initial condition $\psi(0) = \psi$ as $t \to \infty$ approaches the solution $\varphi_+(t) = U_0(t)\varphi_+$ of the non-stationary Schrödinger equation with free Hamiltonian H_0 and initial condition $\varphi_+(0) = \varphi_+$. The passage from the solution $\varphi_-(t)$ of the free Schrödinger equation describing the motion of quantum particle at $t = -\infty$ to the solution $\varphi_+(t)$ describing its motion at $t = \infty$ is the result of scattering of the quantum particle by a potential center. All information about the scattering is contained in the *scattering operator* S (also called *S-matrix* in physics), which relates initial and final conditions φ_- and φ_+:

$$\varphi_+ = S\varphi_-.$$

From (2.32) and $\psi = W_-\varphi_- = W_+\varphi_+$ we immediately get that

$$S = W_+^* W_-, \tag{2.35}$$

and from (2.32)–(2.34) we obtain that the scattering operator S is a unitary operator in $\mathscr{H}$ and commutes with the free Hamiltonian H_0:

$$S^*S = SS^* = I \quad \text{and} \quad SH_0 = H_0S.$$

This is the outline of a *non-stationary approach* to scattering theory.

In the *stationary approach* to scattering theory, the wave operators $W_\pm$ and the scattering operator S are constructed as integral operators in the coordinate representation with integral kernels expressed through special solutions of the stationary Schrödinger equation. Here we present this construction for the one-dimensional Schrödinger operator considered in the previous section.

Namely, let $u_1(x,k)$ and $u_2(x,k)$ be solutions of the one-dimensional Schrödinger equation (2.1) given by (2.23), where $\sqrt{\lambda} = k > 0$. It follows from Theorem 2.1 and (2.11), (2.13) that these solutions have the following asymptotics:

$$u_1(x,k) = s_{11}(k)e^{ikx} + o(1) \qquad \text{as} \quad x \to \infty, \tag{2.36}$$

$$u_1(x,k) = e^{ikx} + s_{21}(k)e^{-ikx} + o(1) \quad \text{as} \quad x \to -\infty, \tag{2.37}$$

and

$$u_2(x,k) = e^{-ikx} + s_{12}(k)e^{ikx} + o(1) \quad \text{as} \quad x \to \infty, \tag{2.38}$$

$$u_2(x,k) = s_{22}(k)e^{-ikx} + o(1) \qquad \text{as} \quad x \to -\infty, \tag{2.39}$$

where

$$s_{11}(k) = s_{22}(k) = \frac{1}{a(k)}, \quad s_{12}(k) = \frac{b(k)}{a(k)}, \quad s_{21}(k) = -\frac{\overline{b(k)}}{a(k)}. \tag{2.40}$$

Solutions $u_1(x,k)$ and $u_2(x,k)$ are called *scattering solutions*, the function $s_{11}(k)$ is called the *complex transmission coefficient*, and functions $s_{12}(k)$ and

$s_{21}(k)$, respectively, are called *right* and *left complex reflection coefficients*. Correspondingly, $T = |s_{11}(k)|^2$ is called the *transmission coefficient* and $R = |s_{12}(k)|^2 = |s_{21}(k)|^2$ — the *reflection coefficient*. The 2×2 matrix

$$S(k) = \begin{pmatrix} s_{11}(k) & s_{12}(k) \\ s_{21}(k) & s_{22}(k) \end{pmatrix}$$

is called the *scattering matrix*. It follows from (2.14) that the scattering matrix is unitary, $S^*(k)S(k) = I$, where I is the 2×2 identity matrix, and satisfies $\overline{S(k)} = S(-k)$. In particular, unitarity of the scattering matrix implies that $T + R = 1$, which is called *conservation of probability*.

The physical interpretation of the solutions $u_1(x,k)$ and $u_2(x,k)$ is the following. For simplicity, suppose that the potential $V(x)$ is smooth and vanishes for $|x| > A$, so that asymptotics (2.36) and (2.38) become equalities for $x > A$, and asymptotics (2.37) and (2.39) become equalities for $x < -A$. In this case elements $s_{ij}(k)$ of the scattering matrix are smooth functions for $k \neq 0$. As in Section 2.3 of Chapter 2, let $\varphi_1(k)$ and $\varphi_2(k)$ be the wave packets: smooth functions on $(0, \infty)$ supported in some neighborhood U_0 of $k_0 > 0$. The functions, called *scattering waves*,

$$\psi_j(x,t) = \int_0^\infty \varphi_j(k) u_j(x,k) e^{-ik^2 t} dk, \quad j = 1, 2,$$

are solutions of the time-dependent Schrödinger equation

$$i\frac{\partial \psi}{\partial t} = H\psi.$$

In the region $|x| > A$ the solution $\psi_1(x,t)$ can be simplified as follows:

$$\psi_1(x,t) = \int_0^\infty \varphi_1(k) s_{11}(k) e^{ikx - ik^2 t} dk, \qquad \text{when} \quad x > A,$$

$$\psi_1(x,t) = \int_0^\infty \varphi_1(k) (e^{ikx - ik^2 t} + s_{21}(k) e^{-ikx - ik^2 t}) dk, \quad \text{when} \quad x < -A.$$

Using the method of stationary phase (see Section 2.3 in Chapter 2) we get as $t \to -\infty$,

$$\psi_1(x,t) = O(|t|^{-1}), \qquad \text{when} \quad x > A,$$

$$\psi_1(x,t) = \frac{1}{\sqrt{|t|}} \varphi_1\left(\frac{x}{2t}\right) e^{\frac{ix^2}{4t} + \frac{i\pi}{4}} + O(|t|^{-1}), \qquad \text{when} \quad x < -A,$$

and as $t \to \infty$,

$$\psi_1(x,t) = \frac{1}{\sqrt{t}} \varphi_1\left(\frac{x}{2t}\right) s_{11}\left(\frac{x}{2t}\right) e^{\frac{ix^2}{4t} - \frac{i\pi}{4}} + O(t^{-1}), \qquad \text{when} \quad x > A,$$

$$\psi_1(x,t) = \frac{1}{\sqrt{t}} \varphi_1\left(-\frac{x}{2t}\right) s_{21}\left(-\frac{x}{2t}\right) e^{\frac{ix^2}{4t} - \frac{i\pi}{4}} + O(t^{-1}), \quad \text{when} \quad x < -A.$$

Assuming that the neighborhood U_0 is "sufficiently small", we see as in Section 2.3 of Chapter 2 that as $t \to -\infty$ the solution $\psi_1(x,t)$ represents a plane wave with amplitude $|\varphi_1(k_0)|$ moving from $x = -\infty$ to the right, toward the potential center, with velocity $v = 2k_0$. When $t \to \infty$, the solution $\psi_1(x,t)$ is a superposition of two plane waves: the transmitted wave with amplitude $|s_{11}(k_0)|$ times the original amplitude, located to the right of the potential center and moving toward ∞ with velocity v, and the reflected wave with amplitude factor $|s_{21}(k_0)|$, located to the left of the potential center and moving toward $-\infty$ with velocity $-v$. Corresponding transmission and reflection coefficients are $T = |s_{11}(k_0)|^2$ and $R = |s_{21}(k_0)|^2$.

Analogously, we have as $t \to -\infty$,

$$\psi_2(x,t) = \frac{1}{\sqrt{|t|}}\,\varphi_2\left(-\frac{x}{2t}\right) e^{\frac{ix^2}{4t} - \frac{i\pi}{4}} + O(|t|^{-1}), \qquad \text{when} \quad x > A,$$

$$\psi_2(x,t) = O(|t|^{-1}), \qquad \text{when} \quad x < -A,$$

and as $t \to \infty$,

$$\psi_2(x,t) = \frac{1}{\sqrt{t}}\,\varphi_2\left(\frac{x}{2t}\right) s_{12}\left(\frac{x}{2t}\right) e^{\frac{ix^2}{4t} - \frac{i\pi}{4}} + O(t^{-1}), \qquad \text{when} \quad x > A,$$

$$\psi_2(x,t) = \frac{1}{\sqrt{t}}\,\varphi_2\left(-\frac{x}{2t}\right) s_{22}\left(-\frac{x}{2t}\right) e^{\frac{ix^2}{4t} - \frac{i\pi}{4}} + O(t^{-1}), \quad \text{when} \quad x < -A.$$

As $t \to -\infty$, the solution $\psi_2(x,t)$ is a plane wave with amplitude $|\varphi_2(k_0)|$ moving from $x = \infty$ to the left, toward the potential center, with velocity $-v$. When $t \to \infty$, the solution $\psi_2(x,t)$ is a superposition of two plane waves: the transmitted wave with the same amplitude factor $|s_{22}(k_0)|$, located to the left of the potential center and moving toward $-\infty$ with velocity $-v$, and the reflected wave with amplitude factor $|s_{12}(k_0)|$, located to the right of the potential center and moving toward ∞ with velocity v. Formulas (2.40) show that transmission and reflection coefficients for the solution $\psi_2(x,t)$ are the same as for the solution $\psi_1(x,t)$, and are independent of the direction of travel. This is the so-called *reciprocity property of the transmission coefficient*.

The solutions $u_1(x,k)$ and $u_2(x,k)$ of the stationary Schrödinger equation have the property that corresponding solutions $\psi_1(x,t)$ and $\psi_2(x,t)$ of the time-dependent Schrödinger equation become the plane waves as $t \to -\infty$. In accordance with this interpretation, we denote them, respectively, by $u_1^{(-)}(x,k)$ and $u_2^{(-)}(x,k)$. Solutions of the stationary Schrödinger equation,

$$u_1^{(+)}(x,k) = \overline{u_2(x,k)} = u_2(x,-k) \quad \text{and} \quad u_2^{(+)}(x,k) = \overline{u_1(x,k)} = u_1(x,-k),$$

admit a similar interpretation: they correspond to the solutions of the time-dependent Schrödinger equation which become the plane waves as $t \to \infty$.

Introducing

$$U_+(x,k)=\begin{pmatrix}u_1^{(+)}(x,k)\\ u_2^{(+)}(x,k)\end{pmatrix}\quad\text{and}\quad U_-(x,k)=\begin{pmatrix}u_1^{(-)}(x,k)\\ u_2^{(-)}(x,k)\end{pmatrix}$$

we get by a straightforward computation using (2.11) and (2.13) that

$$U_+(x,k)=\overline{S(k)}U_-(x,k). \tag{2.41}$$

The following result establishes equivalence between stationary and non-stationary approaches to scattering theory.

Theorem 2.5. *For the one-dimensional Schrödinger operator $H=H_0+V$ with potential $V(x)$ satisfying condition* (2.2) *the wave operators exist and are given explicitly by*

$$W_\pm=\mathscr{U}_\pm^*\mathscr{U}_0.$$

Here $\mathscr{U}_\pm:\mathscr{H}\to\mathfrak{H}_0$ are the integral operators given by

$$\mathscr{U}_\pm(\psi)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x)\overline{U_\pm(x,\sqrt{\lambda})}dx,$$

and $\mathscr{U}_0:\mathscr{H}\to\mathfrak{H}_0$ establishes the unitary equivalence between the operator H_0 in $\mathscr{H}$ and the multiplication by λ operator in $\mathfrak{H}_0$,

$$\mathscr{U}_0(\psi)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x)\begin{pmatrix}e^{-i\sqrt{\lambda}x}\\ e^{i\sqrt{\lambda}x}\end{pmatrix}dx.$$

The scattering operator S in $\mathscr{H}$ and the multiplication by the scattering matrix $S(\sqrt{\lambda})$ operator in $\mathfrak{H}_0$ are unitarily equivalent:

$$S=\mathscr{U}_0^*S(\sqrt{\lambda})\mathscr{U}_0.$$

Proof. The formula for the scattering operator immediately follows from the definition of the operators $\mathscr{U}_\pm$, formula (2.41), and orthogonality relation $\mathscr{U}_-\mathscr{U}_-^*=I_0$ (see Theorem 2.3). To prove that $W_\pm=\mathscr{U}_\pm^*\mathscr{U}_0$, it is sufficient to show that for all $\Phi=\begin{pmatrix}\varphi_1\\ \varphi_2\end{pmatrix}\in\mathfrak{H}_0$, where $\varphi_1(k)$ and $\varphi_2(k)$ are smooth functions on $(0,\infty)$ with compact support,

$$\lim_{t\to\pm\infty}\|(e^{-itH}\mathscr{U}_\pm^*-e^{-itH_0}\mathscr{U}_0^*)\Phi\|_{\mathscr{H}}=0.$$

Indeed, setting $\chi^{(\pm)}(t)=(e^{-itH}\mathscr{U}_\pm^*-e^{-itH_0}\mathscr{U}_0^*)\Phi$, we have

$$\chi^{(\pm)}(x,t)=\frac{1}{\sqrt{2\pi}}\int_0^\infty\big((u_1^{(\pm)}(x,k)-e^{ikx})\varphi_1(k)$$
$$+(u_2^{(\pm)}(x,k)-e^{-ikx})\varphi_2(k)\big)e^{-ik^2t}dk,$$

and it is not difficult to estimate the integral

$$\|\chi^{(\pm)}(t)\|^2 = \int_{-\infty}^{\infty} |\chi^{(\pm)}(x,t)|^2 dx \tag{2.42}$$

as $t \to \pm\infty$. Namely, it follows from the Riemann-Lebesgue lemma that for any fixed $A > 0$ the contribution to (2.42) from the interval $[-A, A]$ goes to 0 as $t \to \pm\infty$. In integrals over $-\infty \le x \le -A$ and $A \le x \le \infty$ we replace $u_{1,2}^{(\pm)}(x,k)$ by their asymptotics (2.36)–(2.39). Using estimates in Theorem 2.1, part (v), it is easy to show that for sufficiently large A the difference can be made arbitrarily small uniformly in t. To finish the proof it remains to show that for every continuous function $\varphi(k)$ on $(0,\infty)$ with compact support the integrals

$$J_1^{(\pm)}(t) = \frac{1}{2}\int_A^{\infty} \left| \int_0^{\infty} \varphi(k) e^{\mp ikx - ik^2 t} dk \right|^2 dx$$

and

$$J_2^{(\pm)}(t) = \frac{1}{2}\int_{-\infty}^{A} \left| \int_0^{\infty} \varphi(k) e^{\pm ikx - ik^2 t} dk \right|^2 dx$$

vanish as $t \to \pm\infty$. Consider, for instance, the integral $J_1^{(+)}(t)$. Given $\varepsilon > 0$, there exists a smooth function $\eta(k)$ on $(0,\infty)$ with compact support $[\alpha, \beta]$ such that

$$\|\varphi - \eta\|_{\mathscr{H}_0}^2 < \frac{\varepsilon}{4\pi}.$$

We have by the Plancherel theorem,

$$J_1^{(+)}(t) = \frac{1}{2}\int_A^{\infty} \left| \int_0^{\infty} ((\varphi(k) - \eta(k)) + \eta(k)) e^{-ikx - ik^2 t} dk \right|^2 dx$$

$$\le \int_A^{\infty} \left| \int_0^{\infty} (\varphi(k) - \eta(k)) e^{-ikx - ik^2 t} dk \right|^2 dx + \int_A^{\infty} \left| \int_0^{\infty} \eta(k) e^{-ikx - ik^2 t} dk \right|^2 dx$$

$$\le \int_{-\infty}^{\infty} \left| \int_0^{\infty} (\varphi(k) - \eta(k)) e^{-ikx - ik^2 t} dk \right|^2 dx + \int_A^{\infty} \left| \int_0^{\infty} \eta(k) e^{-ikx - ik^2 t} dk \right|^2 dx$$

$$\le \frac{\varepsilon}{2} + \int_A^{\infty} \left| \int_0^{\infty} \eta(k) e^{-ikx - ik^2 t} dk \right|^2 dx.$$

To estimate the remaining integral we use integration by parts to obtain

$$\int_0^{\infty} \eta(k) e^{-i(kx + k^2 t)} dk = \int_0^{\infty} \frac{\eta'(k)}{i(x + 2kt)} e^{-i(kx + k^2 t)} dk,$$

and since $\dfrac{|\eta'(k)|}{x + 2kt} \le \dfrac{C}{x + 2\alpha t}$ for $x, t > 0$, we have

$$\int_A^{\infty} \left| \int_0^{\infty} \eta(k) e^{-i(kx + k^2 t)} dk \right|^2 dx \le C^2 \int_A^{\infty} \frac{dx}{(x + 2\alpha t)^2} = \frac{C^2}{A + 2\alpha t}.$$

Choosing $t > \dfrac{2C^2}{\alpha\varepsilon}$, we obtain $J_1^{(+)}(t) < \varepsilon$. Other integrals are treated similarly. □

Corollary 2.6. *The wave operators satisfy orthogonality and completeness relations* $W_\pm^* W_\pm = I$ *and* $W_\pm W_\pm^* = I - P$.

Proof. The result of Theorem 2.3, proved for the operator $\mathscr{U} = \mathscr{U}_-$, obviously holds for the operator $\mathscr{U}_+$. Thus relations (2.32) and (2.33) follow from the corresponding orthogonality and completeness relations for the operators $\mathscr{U}_\pm$. □

Remark. The orthogonality relation (2.32) is trivial once the existence of the wave operators is established. Thus Theorem 2.5 gives another proof of the orthogonality relation in Theorem 2.3.

Problem 2.7 (The Cook's criterion)**.** In abstract scattering theory, prove that the wave operators $W_\pm$ exist if for all $\varphi \in \mathscr{H}$,

$$\int_0^\infty \|Ve^{-itH_0}\varphi\| dt < \infty.$$

Problem 2.8. Find the scattering matrix $S(k)$ for the potential $V(x)$ from Problem 2.5 and show that when $V_0 = 2\varkappa^2$, the scattering matrix is diagonal.

Problem 2.9 (Quantum tunneling)**.** Find the scattering matrix $S(k)$ for the rectangular potential barrier: $V(x) = 0$ for $x < 0$ and $x > 2a$, and $V(x) = V_0 > 0$ for $0 \le x \le 2a$. Show that when E varies from 0 to V_0, T increases from 0 to $(1 + V_0 a^2)^{-1}$ — the penetration of a potential barrier by a quantum particle.

2.4. Other boundary conditions. Here we consider two examples of the Schrödinger operator

$$H = -\frac{d^2}{dx^2} + V(x)$$

with the potential $V(x)$ having different asymptotics as $x \to \pm\infty$.

Example 2.1. Suppose that the potential $V(x)$ satisfies

$$\int_{-\infty}^0 (1 + |x|)|V(x) - c^2| dx < \infty \quad \text{and} \quad \int_0^\infty (1 + |x|)|V(x)| dx < \infty$$

for some $c > 0$. The Schrödinger operator H has negative discrete spectrum, consisting of finitely many simple eigenvalues $\lambda_1 < \cdots < \lambda_n < 0$, and absolutely continuous spectrum $[0, \infty)$, which is simple for $0 < \lambda < c^2$ and is of multiplicity two for $\lambda > c^2$. This qualitative structure of the spectrum is determined by the structure of the level sets $H_{\mathrm{c}}(p, x) = \lambda$ of the classical Hamiltonian function $H_{\mathrm{c}}(p, x) = p^2 + V(x)$: the eigenvalues could only appear for compact level sets, when the classical motion is periodic, while the values of λ with non-compact level sets, where the classical motion is

infinite, belong to the absolutely continuous spectrum. The absolutely continuous spectrum has multiplicity one or two depending on whether the corresponding classical motion is unbounded in one or in both directions, i.e., when $0 < \lambda < c^2$ or $\lambda > c^2$.

These results can be proved using methods in Section 2.1. Namely, set $\lambda = k^2$ and define the function $k_1 = \sqrt{k^2 - c^2}$ by the condition that $\operatorname{Im} k_1 \geq 0$ for $\operatorname{Im} k \geq 0$. In particular, $\operatorname{sgn} k_1 = \operatorname{sgn} k$ for k real, $|k| > c$. The differential equation

$$-y'' + V(x)y = k^2 y \tag{2.43}$$

for real k has two linear independent solutions $f_1(x,k), f_1(x,-k) = \overline{f_1(x,k)}$, where $f_1(x,k)$ has the asymptotics

$$f_1(x,k) = e^{ikx} + o(1) \quad \text{as} \quad x \to \infty.$$

For real k, $|k| > c$, equation (2.43) also has two linear independent solutions $f_2(x,k), f_2(x,-k) = \overline{f_2(x,-k)}$, where $f_2(x,k)$ has the asymptotics

$$f_2(x,k) = e^{-ik_1 x} + o(1) \quad \text{as} \quad x \to -\infty.$$

(Actually, these solutions satisfy estimates similar to that in Theorem 2.1.) As in Section 2.1, for real k, $|k| > c$, we have

$$f_2(x,k) = a(k) f_1(x,-k) + b(k) f_1(x,k),$$

where

$$a(k) = \frac{1}{2ik} W(f_1(x,k), f_2(x,k)), \quad b(k) = \frac{1}{2ik} W(f_2(x,k), f_1(x,-k)), \tag{2.44}$$

and $a(-k) = \overline{a(k)}$, $b(-k) = \overline{b(k)}$. However, $W(f_2(x,k), f_2(x,-k)) = -2ik_1$, so that for real k, $|k| > c$, we have

$$f_1(x,k) = \frac{k}{k_1} a(k) f_2(x,-k) - \frac{k}{k_1} b(-k) f_2(x,k).$$

From here we obtain the normalization condition

$$|a(k)|^2 - |b(k)|^2 = \frac{k_1}{k}, \quad |k| > c.$$

For fixed x solutions $f_1(x,k)$ and $f_2(x,k)$ can be analytically continued to the upper half-plane $\operatorname{Im} k > 0$. For $-c < k < c$ solution $f_2(x,k)$ is real-valued and satisfies

$$f_2(x,k) = a(k) f_1(x,-k) + \overline{a(k) f_1(x,-k)},$$

where $a(k)$ is still given by the same formula (2.44). The function $a(k)$ does not vanish for real k and admits meromorphic continuation to the upper half-plane $\operatorname{Im} k > 0$ where it has finitely many pure imaginary simple zeros $i\varkappa_1, \dots, i\varkappa_n$ which correspond to the eigenvalues $\lambda_1 = -\varkappa_1^2, \dots, \lambda_n = -\varkappa_n^2$.

The absolutely continuous spectrum of the Schrödinger operator H fills $[0,\infty)$. For $0<\lambda=k^2<c^2$ the spectrum is simple and

$$u(x,\lambda)=\frac{1}{a(k)}f_2(x,k),\quad 0<k<c,$$

are the corresponding normalized eigenfunctions of the continuous spectrum. For $\lambda=k^2>c^2$ the spectrum has multiplicity two and

$$u_1(x,\lambda)=\frac{1}{a(k)}f_2(x,k),\quad u_2(x,k)=\frac{k_1}{ka(k)}f_1(x,k),\quad k>c,$$

are the corresponding normalized eigenfunctions of the continuous spectrum. Denoting by $\psi_l(x)$ the normalized eigenfunctions of H corresponding to the eigenvalues λ_l, we get the eigenfunction expansion theorem: for $\psi\in L^2(\mathbb{R})$,

$$\psi(x)=\sum_{l=1}^{n}C_l\psi_l(x)+\int_0^c C(k)u(x,k)dk$$
$$+\int_c^\infty (C_1(k)u_1(x,k)+C_2(k)u_2(x,k))dk,$$

where $C_l=(\psi,\psi_l)$, $l=1,\dots,n$, and

$$C(k)=\int_{-\infty}^{\infty}\psi(x)\overline{u(x,k)}dx,\quad C_j(k)=\int_{-\infty}^{\infty}\psi(x)\overline{u_j(x,k)}dx,\quad j=1,2.$$

Example 2.2. Suppose that the potential $V(x)$ grows as $x\to-\infty$ and decays as $x\to\infty$:

$$\int_a^\infty (1+|x|)|V(x)|dx<\infty\quad\text{for all}\quad a,$$

and there exists $x_0\in\mathbb{R}$ such that the spectrum of the Sturm-Liouville problem

$$-y''+V(x)y=\lambda y,\quad -\infty<x\le x_0,\quad\text{and}\quad y'(x_0)=0$$

is bounded below and discrete. The latter condition is a quantitative formulation of the property $\lim_{x\to-\infty}V(x)=\infty$.

Then for every real k there exists a solution $f(x,k)$ of the differential equation (2.43) with the asymptotics

$$f(x,k)=e^{ikx}+o(1)\quad\text{as}\quad x\to\infty,$$

and there is a function $s(k)$ such that

$$u(x,k)=f(x,-k)+s(k)f(x,k)$$

is square integrable over $(-\infty, a)$ for any real a. The Schrödinger operator H has simple absolutely continuous spectrum $[0, \infty)$ and discrete spectrum consisting of finitely many negative eigenvalues. Functions $u(x, k)$ are normalized eigenfunctions of the continuous spectrum and the corresponding eigenfunction expansion theorem has the following form: for every $\psi \in L^2(\mathbb{R})$,

$$\psi(x) = \sum_{l=1}^{n} C_l \psi_l(x) + \int_0^\infty C(k) u(x, k) dk,$$

where $C_l = (\psi, \psi_l)$, $l = 1, \dots, n$, and

$$C(k) = \int_{-\infty}^{\infty} \psi(x) \overline{u(x, k)} dx.$$

Problem 2.10. Give an explicit form of the eigenfunction expansion theorem for the potential $V(x) = e^x$.

Problem 2.11. Find energy levels for the *Morse potential* $V(x) = e^{-2\alpha x} - 2e^{-\alpha x}$, $\alpha > 0$.

Problem 2.12. Give an explicit form of the eigenfunction expansion theorem for the potential $V(x) = Fx$, describing the motion of a quantum particle in a homogeneous field; according to Problem 1.4, the corresponding Schrödinger operator is self-adjoint. (*Hint:* Solve the Schrödinger equation explicitly in the momentum representation, and express normalized eigenfunctions of the continuous spectrum in the coordinate representation in terms of Airy-Fock functions, defined in Section 6.2.)

Problem 2.13. Give an explicit form of the eigenfunction expansion theorem for the potential $V(x) = -\frac{1}{2}kx^2$, where $k > 0$ (according to Problem 1.4, the corresponding Schrödinger operator is self-adjoint).

3. Angular momentum and SO(3)

3.1. Angular momentum operators. In Chapter 1 (see Example 1.10 in Section 1.4) for a classical particle in $\mathbb{R}^3$ we introduced the angular momentum vector $\boldsymbol{M}_{\mathrm{c}} = \boldsymbol{x} \times \boldsymbol{p}$ with components

$$M_{\mathrm{c}1} = x_2 p_3 - x_3 p_2, \quad M_{\mathrm{c}2} = x_3 p_1 - x_1 p_3, \quad M_{\mathrm{c}3} = x_1 p_2 - x_2 p_1.$$

According to Example 2.1 in Section 2.6 of Chapter 1, they have the following Poisson brackets with respect to the canonical Poisson structure on $T^*\mathbb{R}^3$:

$$\{M_{\mathrm{c}1}, M_{\mathrm{c}2}\} = -M_{\mathrm{c}3}, \quad \{M_{\mathrm{c}2}, M_{\mathrm{c}3}\} = -M_{\mathrm{c}1}, \quad \{M_{\mathrm{c}3}, M_{\mathrm{c}1}\} = -M_{\mathrm{c}2}. \tag{3.1}$$

The square of the angular momentum $\boldsymbol{M}_{\mathrm{c}}^2 = M_{\mathrm{c}1}^2 + M_{\mathrm{c}2}^2 + M_{\mathrm{c}3}^2$ satisfies

$$\{\boldsymbol{M}_{\mathrm{c}}^2, M_{\mathrm{c}1}\} = \{\boldsymbol{M}_{\mathrm{c}}^2, M_{\mathrm{c}2}\} = \{\boldsymbol{M}_{\mathrm{c}}^2, M_{\mathrm{c}3}\} = 0.$$

If the Hamiltonian function

$$H_{\rm c}(\boldsymbol{p},\boldsymbol{x}) = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{x})$$

is invariant under rotations, $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$, then components of the angular momentum are the integrals of motion

$$\{H_{\rm c}, M_{\rm c1}\} = \{H_{\rm c}, M_{\rm c2}\} = \{H_{\rm c}, M_{\rm c3}\} = 0 \quad \text{and} \quad \{H_{\rm c}, \boldsymbol{M}_{\rm c}^2\} = 0.$$

This can also be verified directly using Poisson brackets

$$\{M_{{\rm c}j}, p_k\} = -\varepsilon_{jkl} p_l \quad \text{and} \quad \{M_{{\rm c}j}, x_k\} = -\varepsilon_{jkl} x_l, \quad i,j,k = 1,2,3, \tag{3.2}$$

where ε_{jkl} is a totally anti-symmetric tensor, $\varepsilon_{123} = 1$.

Correspondingly, in quantum mechanics the components of the angular momentum operator $\boldsymbol{M} = \boldsymbol{Q} \times \boldsymbol{P}$ are defined by

$$M_1 = Q_2P_3 - Q_3P_2, \quad M_2 = Q_3P_1 - Q_1P_3, \quad M_3 = Q_2P_3 - Q_3P_2,$$

where $\boldsymbol{Q} = (Q_1, Q_2, Q_3)$ and $\boldsymbol{P} = (P_1, P_2, P_3)$ are, respectively, coordinate and momentum operators. Since operators Q_i and P_k commute for $i \neq k$, there is no ordering problem when defining quantum angular momentum operators. It follows from Heisenberg commutation relations that their quantum brackets are the same as the corresponding Poisson brackets (3.1):

$$\{M_1, M_2\}_\hbar = -M_3, \quad \{M_2, M_3\}_\hbar = -M_1, \quad \{M_3, M_1\}_\hbar = -M_2. \tag{3.3}$$

Equivalently,

$$[M_1, M_2] = i\hbar M_3, \quad [M_2, M_3] = i\hbar M_1, \quad [M_3, M_1] = i\hbar M_2. \tag{3.4}$$

The operator of the square of the total angular momentum $\boldsymbol{M}^2 = M_1^2 + M_2^2 + M_3^2$ satisfies

$$[\boldsymbol{M}^2, M_1] = [\boldsymbol{M}^2, M_2] = [\boldsymbol{M}^2, M_3] = 0.$$

Correspondingly, for the Hamiltonian operator

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

with spherically symmetric potential $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$ operators M_1, M_2, M_3 and, therefore, $\boldsymbol{M}^2$, are quantum integrals of motion:

$$[H, M_1] = [H, M_2] = [H, M_3] = 0 \quad \text{and} \quad [H, \boldsymbol{M}^2] = 0.$$

This can be verified directly by using quantum brackets

$$\{M_j, P_k\}_\hbar = -\varepsilon_{jkl} P_l, \quad \{M_j, Q_k\}_\hbar = -\varepsilon_{jkl} Q_l, \quad j,k,l = 1,2,3, \tag{3.5}$$

which are the same as Poisson brackets (3.2), and follow from Heisenberg commutation relations.

In the coordinate representation $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$ the operators of angular momentum are given by the following first order self-adjoint differential operators:

$$M_1 = i\hbar\left(x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3}\right), \tag{3.6}$$

$$M_2 = i\hbar\left(x_1\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_1}\right), \tag{3.7}$$

$$M_3 = i\hbar\left(x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2}\right). \tag{3.8}$$

They have the property that

$$M_1\psi = M_2\psi = M_3\psi = 0$$

for any spherically symmetric smooth function $\psi(\boldsymbol{x}) = \psi(|\boldsymbol{x}|)$. In other words, angular momentum operators act only on the angle coordinates in $\mathbb{R}^3$. Namely, let

$$x_1 = r\sin\vartheta\cos\varphi, \quad x_2 = r\sin\vartheta\sin\varphi, \quad x_3 = r\cos\vartheta,$$

where $0 \le \vartheta < \pi$, $0 \le \varphi < 2\pi$, be the spherical coordinates in $\mathbb{R}^3$. Explicit computation gives

$$\begin{aligned} M_1 &= i\hbar\left(\sin\varphi\frac{\partial}{\partial\vartheta} + \cot\vartheta\cos\varphi\frac{\partial}{\partial\varphi}\right),\\ M_2 &= -i\hbar\left(\cos\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\sin\varphi\frac{\partial}{\partial\varphi}\right),\\ M_3 &= -i\hbar\frac{\partial}{\partial\varphi}. \end{aligned}$$

Thus

$$\boldsymbol{M}^2 = -\hbar^2\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right),$$

so that the operator $-\dfrac{1}{\hbar^2}\boldsymbol{M}^2$ is the spherical part of the Laplace operator in $\mathbb{R}^3$,

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\boldsymbol{M}^2. \tag{3.9}$$

3.2. Representation theory of SO(3)**.** Quantum operators of angular momentum are related with the representation theory of the rotation group SO(3) — the group of 3×3 orthogonal matrices with determinant 1. SO(3) is a compact Lie group, isomorphic to the real projective space $\mathbb{RP}^3$ as a smooth manifold. There is a Lie group isomorphism $\mathrm{SO}(3) \simeq \mathrm{SU}(2)/\{\pm I\}$, where SU(2) is a Lie group of 2×2 unitary matrices with determinant 1.

The Lie algebra $\mathfrak{so}(3)$ of SO(3) is a three-dimensional Lie algebra of 3×3 skew-symmetric matrices, with the basis

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The matrices X_1, X_2, X_3 correspond, respectively, to the one-parameter subgroups of SO(3) consisting of rotations about coordinate axes in $\mathbb{R}^3$. They satisfy commutation relations

$$[X_1, X_2] = X_3, \quad [X_2, X_3] = X_1, \quad [X_3, X_1] = X_2,$$

which are similar to (3.4). To establish the connection between quantum angular momentum operators and representation theory of SO(3), consider the regular representation R of SO(3) in $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$, defined by

$$(R(g)\psi)(\boldsymbol{x}) = \psi(g^{-1}\boldsymbol{x}), \quad g \in \mathrm{SO}(3), \ \psi \in \mathscr{H}.$$

Lemma 3.1. *We have*

$$R(e^{u_1X_1+u_2X_2+u_3X_3}) = e^{-\frac{i}{\hbar}(u_1M_1+u_2M_2+u_3M_3)}.$$

Proof. Put $\boldsymbol{uX} = u_1X_1 + u_2X_2 + u_3X_3$ and $\boldsymbol{uM} = u_1M_1 + u_2M_2 + u_3M_3$. It follows from the Stone theorem and direct computation that

$$i\hbar \left.\frac{\partial}{\partial u_j}\right|_{\boldsymbol{u}=0} R(e^{\boldsymbol{uX}}) = M_j, \quad j = 1, 2, 3,$$

where self-adjoint operators M_1, M_2, M_3 are given by (3.6)-(3.8). Next, for fixed u_1, u_2, u_3, consider the following one-parameter group $U(t) = R(e^{t\boldsymbol{uX}})$ of unitary operators in $\mathscr{H}$. By the Stone theorem, $U(t) = e^{-itA}$, where

$$A = i \left.\frac{d}{dt}\right|_{t=0} U(t) = \frac{1}{\hbar}\boldsymbol{uM}. \qquad \square$$

Remark. We have $M_j = i\hbar\rho(X_j)$, where $\rho = dR$ is the corresponding regular representation of the Lie algebra $\mathfrak{so}(3)$ in $\mathscr{H}$.

All irreducible unitary representations R_l of the Lie group SO(3) are finite-dimensional and are parametrized by non-negative integers $l \geq 0$. The corresponding irreducible representation $\rho_l = dR_l$ of the Lie algebra $\mathfrak{so}(3)$ in $2l + 1$-dimensional complex vector space V_l can be explicitly described as follows. Introduce Hermitian operators $T_j = i\rho_l(X_j)$, $j = 1, 2, 3$, which satisfy commutation relations

$$[T_1, T_2] = iT_3, \quad [T_3, T_1] = iT_2, \quad [T_2, T_3] = iT_1.$$

The vector space V_l has an orthonormal basis $\{e_{lm}\}_{m=-l}^{m=l}$ such that

$$(T_1 - iT_2)e_{lm} = -\sqrt{(l+m)(l-m+1)}e_{lm-1}, \tag{3.10}$$

$$(T_1 + iT_2)e_{lm} = -\sqrt{(l-m)(l+m+1)}e_{lm+1}, \tag{3.11}$$

$$T_3 e_{lm} = m e_{lm}. \tag{3.12}$$

In particular, $(T_1 + iT_2)e_{ll} = 0$, so that V_l is the highest weight module. The representation ρ_l is irreducible, and we have by Schur's lemma

$$\boldsymbol{T}^2 = l(l+1)I_l,$$

where I_l is the identity operator in V_l. This can also be verified directly by using (3.10)–(3.12).

Remark. When l is a half-integer, i.e., $l \in \frac{1}{2} + \mathbb{Z}_{\geq 0}$, and $m = -l, -l+1, \ldots, l-1, l$, formulas (3.10)–(3.12) still define an irreducible highest weight representation ρ_l of the Lie algebra $\mathfrak{so}(3)$ of dimension $2l+1$, and every irreducible n-dimensional representation of $\mathfrak{so}(3)$ is isomorphic to the representation ρ_l with $l = \frac{n-1}{2}$. For half-integer l, representations ρ_l are not integrable: they give rise to two-valued representations of SO(3), the so-called *spinor representations*. However, considered as representations of the Lie algebra $\mathfrak{su}(2) \simeq \mathfrak{so}(3)$, ρ_l correspond to the irreducible unitary representations of the Lie group SU(2). It follows from the representation theory of SU(2) that for $l, l' \in \frac{1}{2}\mathbb{Z}_{\geq 0}$,

$$V_l \otimes V_{l'} = \bigoplus_{j=|l-l'|}^{l+l'} V_j, \tag{3.13}$$

the so-called *Clebsch-Gordan decomposition*. In physics, it corresponds to the *addition of angular momenta*.

The regular representation R of SO(3) in $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$ is not irreducible. We have

$$\mathscr{H} = L^2(S^2, d\boldsymbol{n}) \otimes L^2(\mathbb{R}_{>0}, r^2 dr), \tag{3.14}$$

where $d\boldsymbol{n}$ is the measure on S^2 induced by the Lebesgue measure on $\mathbb{R}^3$. The group SO(3) acts by rotations in the first factor of the tensor product (3.14), whereas in the second factor it acts as the identity operator. Thus the problem of decomposing the regular representation R reduces to finding SO(3) invariant subspaces of the Hilbert space $L^2(S^2, d\boldsymbol{n})$. The result is the orthogonal sum decomposition

$$L^2(S^2, d\boldsymbol{n}) = \bigoplus_{l=0}^{\infty} \mathscr{D}_l, \tag{3.15}$$

where $\mathscr{D}_l \simeq V_l$. Under this isomorphism, the orthonormal basis Y_{lm} in $\mathscr{D}_l$ which corresponds to the basis e_{lm} in V_l is given by the normalized spherical functions

$$Y_{lm}(\vartheta,\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} P_l^m(\cos\vartheta), \quad m = -l,\dots,l,$$

where $P_l^m(x)$ are normalized associated Legendre polynomials,

$$P_l^m(x) = (-1)^m \sqrt{\frac{(l+m)!}{(l-m)!}} \sqrt{\frac{2l+1}{2}} \frac{1}{2^l l!} (1-x^2)^{-\frac{m}{2}} \frac{d^{l-m}}{dx^{l-m}} (x^2-1)^l, \quad |x| < 1.$$

The self-adjoint operator $\boldsymbol{M}^2$ in the Hilbert space $L^2(S^2, d\boldsymbol{n})$ has pure point spectrum consisting of eigenvalues $\hbar^2 l(l+1)$ of multiplicities $2l+1$, $l = 0,1,2,\dots$, and the decomposition (3.15) gives its eigenfunction expansion: for every $\psi \in L^2(S^2, d\boldsymbol{n})$,

$$\psi = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_{lm} Y_{lm}, \quad \text{where} \quad C_{lm} = \int_0^{2\pi} \int_0^{\pi} \psi(\vartheta,\varphi) \overline{Y_{lm}(\vartheta,\varphi)} \sin\vartheta \, d\vartheta d\varphi.$$

Problem 3.1. Prove all results in this section. (*Hint*: See the list of references to this chapter.)

4. Two-body problem

4.1. Separation of the center of mass. Consider the Schrödinger operator for the two-body problem (see Example 2.2 in Section 2.4 in Chapter 2)

$$H = -\frac{\hbar^2}{2m_1}\Delta_1 - \frac{\hbar^2}{2m_2}\Delta_2 + V(\boldsymbol{x}_1 - \boldsymbol{x}_2).$$

Introducing

$$\boldsymbol{X} = \frac{m_1\boldsymbol{x}_1 + m_2\boldsymbol{x}_2}{m_1+m_2} \quad \text{and} \quad \boldsymbol{x} = \boldsymbol{x}_1 - \boldsymbol{x}_2,$$

the coordinate of the center of mass and the relative coordinate, we get

$$H = -\frac{\hbar^2}{2M}\Delta_{\boldsymbol{X}} - \frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{x}} + V(\boldsymbol{x}),$$

where $M = m_1 + m_2$ is the total mass and $\mu = \dfrac{m_1 m_2}{m_1+m_2}$ is the reduced mass. The Hamiltonian operator H can be diagonalized by the method of separation of variables. Namely, consider the following decomposition of the two-body Hilbert space $\mathscr{H} = L^2(\mathbb{R}^6)$ into the tensor product of Hilbert spaces:

$$\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{X}) \otimes L^2(\mathbb{R}^3, d^3\boldsymbol{x}). \tag{4.1}$$

The operator

$$H_{\boldsymbol{X}} = -\frac{\hbar^2}{2M}\Delta_{\boldsymbol{X}} \tag{4.2}$$

acts as the identity operator in the second factor of (4.1), and the operator

$$H_{\boldsymbol{x}} = -\frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{x}} + V(\boldsymbol{x}) \tag{4.3}$$

acts as the identity operator in the first factor of (4.1). For the solutions of the eigenvalue problem

$$H\psi = E\psi \tag{4.4}$$

in the product form

$$\psi(\boldsymbol{X}, \boldsymbol{x}) = \Psi(\boldsymbol{X})\psi(\boldsymbol{x}),$$

the variables are separated:

$$H_{\boldsymbol{X}}\Psi(\boldsymbol{X}) = E_1\Psi(\boldsymbol{X}) \quad \text{and} \quad H_{\boldsymbol{x}}\psi(\boldsymbol{x}) = E_2\psi(\boldsymbol{x}),$$

where $E = E_1 + E_2$. Since

$$\Psi(\boldsymbol{X}) = \left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\boldsymbol{k}\boldsymbol{X}}, \quad \boldsymbol{k}^2 = 2ME_1,$$

the quantum two-body problem reduces to the problem of a quantum particle moving in the potential field, and is described by the Hamiltonian operator (4.3) in the Hilbert space $L^2(\mathbb{R}^3, d^3\boldsymbol{x})$.

4.2. Three-dimensional scattering theory. Here we outline the scattering theory for the Schrödinger operator $H = -\Delta + V(\boldsymbol{x})$ (where we put $\hbar = 1$ and $\mu = \frac{1}{2}$) with rapidly decreasing potential. Specifically, assume that the bounded, real-valued function $V(\boldsymbol{x})$ on $\mathbb{R}^3$ satisfies

$$V(\boldsymbol{x}) = O(|\boldsymbol{x}|^{-3-\varepsilon}) \quad \text{as} \quad |\boldsymbol{x}| \to \infty \tag{4.5}$$

for some $\varepsilon > 0$. Then for every $\boldsymbol{k} \in \mathbb{R}^3$ the Schrödinger equation

$$-\Delta\psi(\boldsymbol{x}) + V(\boldsymbol{x})\psi(\boldsymbol{x}) = k^2\psi(\boldsymbol{x}), \quad k = |\boldsymbol{k}|, \tag{4.6}$$

has two solutions $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ satisfying the following asymptotics as $|\boldsymbol{x}| \to \infty$:

$$u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k}) = e^{i\boldsymbol{k}\boldsymbol{x}} + f^{(\pm)}(k, \boldsymbol{\omega}, \boldsymbol{n})\frac{e^{\pm ikr}}{r} + o\left(\frac{1}{r}\right), \tag{4.7}$$

where $\boldsymbol{k} = k\boldsymbol{\omega}$, $\boldsymbol{x} = r\boldsymbol{n}$. Asymptotics (4.7) are called *Sommerfeld's radiation conditions*. To prove the existence of solutions $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$, one should consider the following integral equations:

$$u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k}) = e^{i\boldsymbol{k}\boldsymbol{x}} + \int_{\mathbb{R}^3} G^{(\pm)}(\boldsymbol{x} - \boldsymbol{y}, k)V(\boldsymbol{y})u^{(\pm)}(\boldsymbol{y}, \boldsymbol{k})d^3\boldsymbol{y}, \tag{4.8}$$

where

$$G^{(\pm)}(\boldsymbol{x},k)=-\frac{1}{4\pi}\frac{e^{\pm ikr}}{r}.$$

Integral equations (4.8) are equivalent to the Schrödinger equation (4.6) with Sommerfeld's radiation conditions (4.7), and are called *Lippman-Schwinger equations*. Their analysis uses Fredholm theory and Kato's Theorem 1.8.

Solutions $u^{(\pm)}(\boldsymbol{x},\boldsymbol{k})$ are called *stationary scattering waves*. They are analogous to the solutions $u_j^{(\pm)}(x,k)$ for the one-dimensional case, where the vector $\boldsymbol{\omega}\in S^2$ replaces the index $j=1,2$. The absolutely continuous spectrum of H fills $[0,\infty)$ and has a uniform infinite multiplicity, parametrized by the two-dimensional sphere S^2. Solutions $u^{(\pm)}(\boldsymbol{x},\boldsymbol{k})$ are normalized eigenfunctions of the continuous spectrum. In general, the operator H has finitely many negative eigenvalues $\lambda_l<0$ of finite multiplicities m_l, $l=1,\dots,n$.

In terms of the operators $\mathscr{U}_\pm:\mathscr{H}\to\mathscr{H}$ given by

$$\mathscr{U}_\pm(\psi)(\boldsymbol{k})=(2\pi)^{-\frac{3}{2}}\int_{\mathbb{R}^3}\psi(\boldsymbol{x})u^{(\pm)}(\boldsymbol{x},\boldsymbol{k})d^3\boldsymbol{x},$$

completeness and orthogonality relations take the form

$$\mathscr{U}_\pm^*\mathscr{U}_\pm=I-P,\quad \mathscr{U}_\pm\mathscr{U}_\pm^*=I,$$

where P is the orthogonal projection on the invariant subspace for the operator H associated with the pure point spectrum. Now let

$$W_\pm=\mathscr{U}_\pm^*\mathscr{U}_0,$$

where $\mathscr{U}_0=\mathscr{F}^{-1}$ is the inverse Fourier transform. As in Section 2.3, one can prove the following result.

Theorem 4.1. *The operators $W_\pm$ are wave operators for the Schrödinger operator H. The corresponding scattering operator $S=W_+^*W_-$ has the form*

$$S=\mathscr{F}\hat{S}\mathscr{F}^{-1},$$

where $\hat{S}$ is the integral operator,

$$(\hat{S}\psi)(k,\boldsymbol{\omega})=\psi(k,\boldsymbol{\omega})+\frac{ik}{2\pi}\int_{S^2}f(k,\boldsymbol{\omega},\boldsymbol{\omega}')\psi(k,\boldsymbol{\omega}')d\boldsymbol{\omega}',$$

and $f(k,\boldsymbol{\omega},\boldsymbol{\omega}')=f^{(+)}(k,\boldsymbol{\omega},\boldsymbol{\omega}')$.

The function $f(k,\boldsymbol{\omega},\boldsymbol{\omega}')$ is called the *scattering amplitude*.

Problem 4.1. Prove that if

$$\sup_{\boldsymbol{x}\in\mathbb{R}^3}\int_{\mathbb{R}^3}|V(\boldsymbol{y})|\frac{1}{|\boldsymbol{x}-\boldsymbol{y}|}d^3\boldsymbol{y}<4\pi,$$

then the Lippman-Schwinger integral equations can be solved by Neumann series and for fixed $\boldsymbol{x}$ and $\boldsymbol{\omega}$ solutions $u^{(\pm)}(\boldsymbol{x},\boldsymbol{k})$, $\boldsymbol{k}=k\boldsymbol{\omega}$, admit analytic continuation to

the upper half-plane $\operatorname{Im} k > 0$. Show also that in this case the Schrödinger operator H has no eigenvalues.

Problem 4.2 (Born's approximation)**.** Show that $u^{(+)}(\boldsymbol{x}, \boldsymbol{k}) = e^{i\boldsymbol{k}\boldsymbol{x}} + o(1)$ as $k \to \infty$, and deduce from this that

$$f(k, \boldsymbol{n}, \boldsymbol{\omega}) + \frac{1}{4\pi} \int_{\mathbb{R}^3} e^{ik(\boldsymbol{n}-\boldsymbol{\omega})\boldsymbol{x}} V(\boldsymbol{x}) d^3\boldsymbol{x} = o(1) \quad \text{as} \quad k \to \infty,$$

uniformly on $\boldsymbol{n}, \boldsymbol{\omega} \in S^2$.

Problem 4.3. Prove unitarity of the operator $\hat{S}$ using Schrödinger equation (4.6), radiation conditions (4.7), and the Green's formula.

Problem 4.4 (The optical theorem)**.** Show that

$$\int_{S^2} |f(k, \boldsymbol{n}, \boldsymbol{\omega})|^2 d\boldsymbol{n} = \frac{4\pi}{k} \operatorname{Im} f(k, \boldsymbol{\omega}, \boldsymbol{\omega}).$$

(Here the left-hand side is the *total cross-section* in direction $\boldsymbol{\omega}$ at the energy $E = k^2$.)

Problem 4.5. Let $\lambda_l = -\varkappa_l^2 < 0$ be the eigenvalues of H with multiplicities m_l, $l = 1, \dots, n$. Prove that for fixed $\boldsymbol{x}$ and $\boldsymbol{\omega}$ solutions $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ admit a meromorphic continuation to the upper half-plane $\operatorname{Im} k > 0$ with poles of orders m_l at $i\varkappa_l$, $l = 1, \dots, n$.

Problem 4.6. Prove that the wave operators $W_\pm$ exist using the non-stationary approach. (*Hint*: Show that when $V(\boldsymbol{x})$ satisfies (4.5), Cook's criterion, formulated in Problem 2.7, is applicable.)

4.3. Particle in a central potential. The eigenvalue problem for the Schrödinger operator

$$H = -\frac{\hbar^2}{2\mu}\Delta + V(\boldsymbol{x})$$

simplifies, when H commutes with the SO(3)-action in $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$:

$$[H, T(g)] = 0 \quad \text{for all} \quad g \in \mathrm{SO}(3).$$

This reduces to the conditions

$$[H, M_i] = 0, \quad i = 1, 2, 3, \tag{4.9}$$

and is equivalent to the property that the potential V is spherically symmetric, $V(\boldsymbol{x}) = V(r)$, $r = |\boldsymbol{x}|$. In particular

$$[H, M_3] = [H, \boldsymbol{M}^2] = 0,$$

where $\boldsymbol{M}^2 = M_1^2 + M_2^2 + M_3^2$, and operators M_3 and $\boldsymbol{M}^2$ are commuting quantum integrals of motion for the Hamiltonian H. As follows from results in Section 3.2, one can look for the solutions of the eigenvalue problem

$$H\psi = E\psi$$

satisfying

$$M_3\psi = m\psi \quad \text{and} \quad \boldsymbol{M}^2\psi = \hbar^2 l(l+1)\psi, \;\; m = -l, \dots, l.$$

Using (3.9), we get

$$H = -\frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\boldsymbol{M}^2}{\mu r^2} + V(r),$$

so that in accordance with the decompositions (3.14) and (3.15), we look for the solutions in the form

$$\psi(\boldsymbol{x}) = R_l(r)Y_{lm}(\boldsymbol{n}), \quad \boldsymbol{x} = r\boldsymbol{n},$$

where Y_{lm} are normalized spherical functions. Separating the variables, one gets the following ordinary differential equation for the function $R_l(r)$:

$$\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) + \frac{\hbar^2 l(l+1)}{\mu r^2}R_l + V(r)R_l = ER_l.$$

Introducing

$$f_l(r) = rR_l(r),$$

we obtain the so-called *radial Schrödinger equation*

$$-\frac{\hbar^2}{2\mu}\frac{d^2 f_l}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2}f_l + V(r)f_l = Ef_l. \tag{4.10}$$

Since for the continuous potential $V(\boldsymbol{x})$ the solution $\psi(\boldsymbol{x})$ is also continuous, equation (4.10) should be supplemented by the boundary condition $f_l(0) = 0$.

The radial Schrödinger equation looks similar to the Schrödinger equation for a one-dimensional particle, if one introduces the so-called *effective potential*

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2},$$

where the second term is called the centrifugal energy. However, since f_l is defined only for $r > 0$, equation (4.10) is equivalent to equation (2.1) with the potential satisfying $V(x) = \infty$ for $x < 0$, which describes the infinite potential barrier at $x = 0$.

Since the radial Schrödinger operators

$$H_l = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

are obtained from the three-dimensional Schrödinger operator

$$H = -\frac{\hbar^2}{2\mu}\Delta + V(r)$$

by separation of variables, the operators H_l with boundary condition $f_l(0) = 0$ are self-adjoint in $L^2(0,\infty)$ whenever H is a self-adjoint operator in $L^2(\mathbb{R}^3)$.

In particular, it follows from Theorem 1.9 in Section 1.2 that when the bounded potential V satisfies

$$V(r) = O(r^{-1-\varepsilon}) \quad \text{as} \quad r \to \infty$$

for some $\varepsilon > 0$, then H_l are self-adjoint operators with simple absolutely continuous spectrum filling $[0, \infty)$, and negative eigenvalues with possible accumulation point at 0. If

$$V(r) = O(r^{-2-\varepsilon}) \quad \text{as} \quad r \to \infty,$$

then the operators H_l have only finitely many negative eigenvalues, and for l large enough have no eigenvalues at all. The same conclusion holds if

$$\int_0^\infty r|V(r)|dr < \infty. \tag{4.11}$$

Such potentials $V(r)$ are called *short-range potentials*. Decaying at infinity potentials which do not satisfy (4.11) are called *long-range potentials*.

For a short-range potential $V(r)$ the differential equation (4.10) for $E \neq 0$ has two linearly independent solutions $f_l^{\pm}(r)$ satisfying the following asymptotics as $r \to \infty$:

$$f_l^{\pm}(r) = e^{\pm \varkappa r}(1 + o(1)), \tag{4.12}$$

where $\varkappa = \sqrt{-2\mu E}$ is pure imaginary, $\operatorname{Im} \varkappa > 0$ for $E > 0$, and $\varkappa > 0$ for $E < 0$. When $r \to 0$, the most singular term in the radial Schrödinger equation is given by the centrifugal energy. Since the elementary differential equation

$$f'' = \frac{l(l+1)}{r^2} f$$

has two linearly independent solutions r^{-l} and r^{l+1}, the solution $f_l(r)$ satisfying the boundary condition $f_l(0) = 0$ has the asymptotics

$$f_l(r) = Cr^{l+1} + o(1) \quad \text{as} \quad r \to 0, \tag{4.13}$$

and is uniquely determined (up to a constant). Since

$$f_l(r) = C_1 f_l^+(r) + C_2 f_l^-(r),$$

for some constants C_1 and C_2 depending on E, the differential equation (4.10) has no square-integrable solutions for $E > 0$. The corresponding solution $f_l(r)$ is bounded on $[0, \infty)$, and is an eigenfunction of the continuous spectrum. This agrees with the description in Section 1.6 of Chapter 1, since for $E > 0$ the classical particle in the central potential $V_{\text{eff}}(r)$ goes to infinity with finite velocity. For $E < 0$ the equation $C_1(E) = 0$ determines the eigenvalues of H_l, which are simple. This also agrees with the classical picture, since classical motion is finite for $E < 0$. For a short range potential the equation $C_1(E) = 0$ has only finitely many solutions. When

$V_{\text{eff}}(r) > 0$ for $r > 0$ — the case of repulsive potential — the operator H_l has no eigenvalues.

Remark. When $V(r) = 0$, the radial Schrödinger operator H_l has only simple absolutely continuous spectrum filling $[0, \infty)$. The substitution

$$f_l(r) = \sqrt{\xi}\, J(\xi), \quad \xi = \frac{kr}{\hbar} \quad \text{and} \quad k = |\varkappa| = \sqrt{2\mu E} > 0,$$

reduces differential equation (4.10) to the Bessel equation

$$\xi^2 \frac{d^2 J}{d\xi^2} + \xi \frac{dJ}{d\xi} + (\xi^2 - \nu^2) J = 0$$

of the half-integer order $\nu = l + \frac{1}{2}$. The corresponding solution regular at 0 — the Bessel function of the first kind $J_{l+\frac{1}{2}}(\xi)$ — is given explicitly by

$$J_{l+\frac{1}{2}}(\xi) = (-1)^l \sqrt{\frac{2}{\pi\xi}}\, \xi^{l+1} \left(\frac{1}{\xi} \frac{d}{d\xi} \right)^l \frac{\sin \xi}{\xi}$$

and

$$J_{l+\frac{1}{2}}(\xi) = \sqrt{\frac{2}{\pi\xi}} \sin\left(\xi - \frac{l\pi}{2} \right) \quad \text{as} \quad \xi \to \infty. \tag{4.14}$$

It can be shown that

$$f_{El}(r) = \sqrt{\frac{kr}{\hbar}} J_{l+\frac{1}{2}} \left(\frac{kr}{\hbar} \right)$$

satisfy the normalization condition (2.14) in Section 2.2 of Chapter 2:

$$\lim_{\Delta \to 0} \frac{1}{\Delta} \int_0^\infty \left(\int_k^{k+\Delta} f_{El}(r) d\sigma(E) \right)^2 dr = 1, \tag{4.15}$$

where $k = \sqrt{2\mu E}$ and $d\sigma(E) = \sqrt{\frac{\mu}{2E}}\, dE = dk$. The corresponding eigenfunction expansion theorem is the special case of the classical Fourier-Bessel transform for integer l, which generalizes the Fourier sine transform: for every $f \in L^2(0, \infty)$,

$$f(r) = \int_0^\infty c_l(E) f_{El}(r) d\sigma(E), \quad c_l(E) = \int_0^\infty f(r) f_{El}(r) dr.$$

In general, for every $l = 0, 1, \ldots$, denote by $f_{El}(r)$ the solution of the radial Schrödinger equation (4.10) with the following asymptotics:

$$f_{El}(r) = \sqrt{\frac{2}{\pi\hbar}} \sin\left(\frac{kr}{\hbar} - \frac{l\pi}{2} + \delta_l \right) + o(1) \quad \text{as} \quad r \to \infty. \tag{4.16}$$

The function $\delta_l(k)$, $k = \sqrt{2\mu E}$, is called the *phase shift*. It follows from (4.14) that for the free case $\delta_l(k) = 0$. The eigenfunctions of the continuous spectrum $f_{El}(r)$ satisfy the same normalization condition (4.15) as the

eigenfunctions for the free case. The function $S_l(k) = e^{2i\delta_l(k)}$ plays the role of the scattering matrix for the radial Schrödinger operator H_l. It admits a meromorphic continuation to the upper half-plane $\operatorname{Im} k > 0$ with simple poles $k = i\varkappa_{kl} = i\sqrt{-2\mu E_{kl}}$, where E_{kl} are the eigenvalues of H_l.

Let $E_{0l} < E_{2l} < \cdots < E_{N_l-1l} < 0$ be the eigenvalues of H_l, and let $f_{jl}(r)$, $j = 0, \ldots, N_l - 1$, be the corresponding normalized eigenfunctions. By the oscillation theorem, the eigenfunctions $f_{jl}(r)$ have j simple zeros in $(0, \infty)$. The functions

$$\psi_{jlm}(\boldsymbol{x}) = \frac{f_{jl}(r)}{r} Y_{lm}(\boldsymbol{n}), \quad m = -l, \ldots, l,$$

are normalized eigenfunctions of the Schrödinger operator H with eigenvalues E_{jl}, and the functions

$$\psi_{Elm}(\boldsymbol{x}) = \frac{f_{El}(r)}{r} Y_{lm}(\boldsymbol{n}), \quad m = -l, \ldots, l,$$

are normalized eigenfunctions of the continuous spectrum. The corresponding eigenfunction expansion theorem for the Schrödinger operator H with spherically symmetric potential states that for every $\psi \in L^2(\mathbb{R}^3, d^3\boldsymbol{x})$,

$$\psi(\boldsymbol{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^{\infty} c_{lm}(E) \psi_{Elm}(\boldsymbol{x}) d\sigma(E) + \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{j=0}^{N_l-1} c_{jlm} \psi_{jlm}(\boldsymbol{x}),$$

where

$$c_{lm}(E) = \int_{\mathbb{R}^3} \psi(\boldsymbol{x}) \overline{\psi_{Elm}(\boldsymbol{x})} d^3\boldsymbol{x}, \quad c_{jlm} = \int_{\mathbb{R}^3} \psi(\boldsymbol{x}) \overline{\psi_{jlm}(\boldsymbol{x})} d^3\boldsymbol{x}.$$

Remark. In physics, it is traditional to call the parameter j in the eigenfunction $\psi_{jlm}(\boldsymbol{x})$ the *radial quantum number* and denote it by n_r. The parameter l is called the *azimuthal quantum number*, and the parameter m — the *magnetic quantum number*. This terminology originated from the old quantum theory, where to each value E_{kl} there corresponds a classical orbit. The parameter $n = n_r + l + 1$ is called the *principal quantum number*, so that $n_r = n - l - 1$ is always the number of zeros of the corresponding radial eigenfunction $f_{jl}(r)$.

Remark. In general, the eigenvalues E_{jl} of a Schrödinger operator H with spherically symmetric potential have multiplicity $2l + 1$. For special potentials, due to the extra symmetry of a problem, there may be "accidental degeneracy" with respect to the azimuthal quantum number l. This is the case for the Schrödinger operator of the hydrogen atom, considered in the next section.

Problem 4.7. Prove all results stated in this section. (*Hint*: See the list of references to this chapter.)

Problem 4.8. Find the energy levels of a particle with angular momentum $l = 0$ in the centrally symmetric potential well $V(r) = -V_0 < 0$ when $0 < r < a$ and $V(r) = 0$ when $r > a$.

Problem 4.9. Find the spectrum of the Schrödinger operator with the potential $V(r) = ar^{-2} + br^2$, $a, b > 0$.

Problem 4.10. Prove that the scattering wave $u(\boldsymbol{x}, \boldsymbol{k}) = u^{(+)}(\boldsymbol{x}, \boldsymbol{k})$ in the central potential is given by

$$u(\boldsymbol{x}, \boldsymbol{k}) = \frac{1}{kr}\sqrt{\frac{\pi}{2}} \sum_{l=0}^{\infty}(2l+1)i^l e^{i\delta_l(k)} f_{El}(r)P_l(\cos\vartheta),$$

where $\boldsymbol{x} \cdot \boldsymbol{k} = kr\cos\vartheta$ and, as in Section 4.2, $\hbar = 1$ and $\mu = \frac{1}{2}$.

Problem 4.11. Using the result of the previous problem, show that

$$f(k, \boldsymbol{n}, \boldsymbol{\omega}) = f(k, \cos\vartheta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(S_l(k) - 1)P_l(\cos\vartheta)$$

— the *partial wave decomposition* of the scattering amplitude — and get the following formula for the total cross-section

$$\sigma_{\text{tot}}(k) = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l(k).$$

5. Hydrogen atom and SO(4)

The hydrogen atom is described by the long-range potential

$$V(\boldsymbol{r}) = -\frac{\alpha}{r}$$

— the *Coulomb potential*, where $\alpha > 0$[3]. The corresponding eigenvalue problem for the Schrödinger operator with Coulomb potential is called the *Coulomb problem*. Here we present its exact solution using the so-called *Coulomb units* $\hbar = 1$, $\mu = 1$, and $\alpha = 1$[4] .

5.1. Discrete spectrum. To determine the discrete spectrum, it is convenient to put $2E = -\varkappa^2 < 0$, so that the eigenvalue equation (4.10) becomes

$$f_l'' + \left(\frac{2}{r} - \frac{l(l+1)}{r^2} - \varkappa^2\right) f_l = 0. \tag{5.1}$$

Asymptotics (4.12)–(4.13) for the short-range potentials suggest that for the long-range Coulomb potential one can look for a square-integrable solution in the following form:

$$f_l(r) = r^{l+1}e^{-\varkappa r}\Lambda(r).$$

[3]For the hydrogen atom $\alpha = e^2$, where e is the electron charge. The case $\alpha = Ze^2$, where $Z = 2, 3, \ldots$, corresponds to the hydrogen ions.

[4]When $\alpha = e^2$, Coulomb units coincide with *atomic units*.

Substituting it into (5.1), we get the equation

$$\Lambda_l'' + \left(\frac{2(l+1)}{r} - 2\varkappa\right)\Lambda_l' + \left(\frac{2}{r} - \frac{2\varkappa(l+1)}{r}\right)\Lambda_l = 0, \tag{5.2}$$

which can be solved by the power series

$$\Lambda_l(r) = \sum_{k=0}^{\infty} a_k r^k. \tag{5.3}$$

Substituting these power series into (5.2) yields the following recurrence relation for the coefficients a_k:

$$a_{k+1} = \frac{2\varkappa(k+l+1) - 2}{(k+1)(k+2l+2)} a_k, \quad k = 1, 2, \ldots,$$

where $a_0 \neq 0$. The power series (5.3) converges for all $r > 0$ by the ratio test. When $\varkappa > 0$ is such that $a_k \neq 0$ for all k, we have

$$\lim_{k\to\infty} \frac{(k+1)a_{k+1}}{a_k} = 2\varkappa.$$

Thus for every $\varepsilon > 0$ there is N such that for $k > N$ all a_k are of the same sign, say $a_k > 0$, and

$$\frac{a_{k+1}}{a_k} \geq \frac{2\varkappa - \varepsilon}{k+1}.$$

Then for $k > N$ we get

$$a_k \geq C\frac{(2\varkappa - \varepsilon)^k}{k!}$$

with some constant $C > 0$ (depending on ε), and since for fixed N the sum of the first N terms in (5.3) grows like r^N as $r \to \infty$, for r large enough we obtain[5]

$$\Lambda_l(r) \geq Ce^{(2\varkappa-\varepsilon)r} - C_1 r^N > C_2 e^{(2\varkappa-\varepsilon)r}.$$

This proves that for such values of $\varkappa$ the function $f_l(r)$ is not square-integrable on $(0, \infty)$. However, for the special values

$$\varkappa = \varkappa_{kl} = \frac{1}{k+l+1}$$

the power series (5.3) terminates: $\Lambda_l(r)$ becomes a polynomial $\Lambda_{kl}(r)$ of order k and $f_{kl}(r) = r^{l+1}e^{-\varkappa_{kl}r}\Lambda_{kl}(r) \in L^2(0,\infty)$. Setting $n = k+l+1$, we get an explicit formula for the eigenvalues

$$E_n = -\frac{1}{2n^2}, \quad n = 1, 2, \ldots.$$

[5]It can be shown that $\Lambda_l(r) = Ce^{2\varkappa r}(1 + o(1))$ as $r \to \infty$.

For fixed n the integer l varies from 0 to $n-1$, and for each l there are $2l+1$ orthogonal eigenfunctions $\dfrac{f_{kl}(r)}{r}Y_{lm}(\boldsymbol{n})$ with the eigenvalue E_n. Thus the overall multiplicity of the eigenvalue E_n is

$$\sum_{l=0}^{n-1}(2l+1)=n^2.$$

The eigenfunctions $f_{kl}(r)$ of the radial Schrödinger equation (5.1) corresponding to the eigenvalue E_n can be expressed in terms of classical Laguerre polynomials. Namely, for $\varkappa=\dfrac{1}{n}$ the substitution $x=\dfrac{2r}{n}$ reduces the differential equation (5.2) to

$$xQ''+(p+1-x)Q'+kQ=0,$$

where $p=2l+1$ and $Q(x)=\Lambda_l(r)$. This is the differential equation satisfied by the associated Laguerre polynomials $Q_k^p(x)$, defined by[6]

$$Q_k^p(x)=e^x x^{-p}\frac{d^k}{dx^k}(e^{-x}x^{k+p}),$$

which are polynomials of order k with leading coefficient $(-1)^k$, having k zeros in $(0,\infty)$. For every p the associated Laguerre polynomials $\{Q_k^p(x)\}_{k=0}^{\infty}$ are orthogonal polynomials on $(0,\infty)$ with respect to the measure $e^{-x}x^p dx$, and have the property

$$\int_0^\infty e^{-x}x^{p+1}Q_k^p(x)^2dx=k!(k+p)!(2k+p+1).$$

The orthonormal eigenfunctions of the Schrödinger operator H for the hydrogen atom corresponding to the eigenvalue E_n have the form

$$\psi_{klm}(\boldsymbol{q})=\frac{2}{n^2}\frac{1}{\sqrt{k!(n+l)!}}\left(\frac{2r}{n}\right)^l e^{-\frac{r}{n}}Q_k^{2l+1}\left(\frac{2r}{n}\right)Y_{lm}(\boldsymbol{n}), \tag{5.4}$$

where $n=k+l+1$, $l=0,\dots,n-1$, and $m=-l,\dots,l$.

Remark. Returning to the physical units $\alpha=e^2$, where e is the electron charge, we get for the energy levels of the hydrogen atom

$$E_n=-\frac{\mu e^4}{2n^2\hbar^2},$$

where μ is the reduced mass of the electron and the nucleus. In particular, the ground state energy is $E_1=-13.6$ eV; its absolute value is the *ionization energy* — the energy required to remove the electron from the hydrogen atom. Using Bohr's formula for the frequencies of the spectral lines

$$\hbar\omega_{mn}=E_n-E_m,$$

[6]Polynomials $L_n^m(x)=(-1)^m\frac{n!}{(n-m)!}Q_{n-m}^m(x)$ are also being used.

we get for the hydrogen atom

$$\omega_{mn} = \frac{\mu e^4}{2\hbar^3}\left(\frac{1}{n^2} - \frac{1}{m^2}\right), \quad m < n.$$

When $n = 1$ and $m = 2, 3, \ldots$, we get classical Lyman series, $n = 2$ and $m = 3, 4, \ldots$ give Balmer series, and $n = 3$ and $m = 4, 5, \ldots$ give Paschen series. These series of spectral lines were discovered experimentally long before the formulation of quantum mechanics.

Remark. The energy levels of the hydrogen atom can also be determined from Bohr-Wilson-Sommerfeld quantization rules. Namely, in spherical coordinates (r, ϑ, φ) in $\mathbb{R}^3$ the Lagrangian of Kepler's problem takes the form (see Section 1.6 in Chapter 1)

$$L = \tfrac{1}{2}\mu(\dot r^2 + r^2\dot\vartheta^2 + r^2\sin^2\vartheta\,\dot\varphi^2) + \frac{\alpha}{r},$$

and the corresponding generalized momenta are

$$p_r = \mu\dot r, \;\; p_\vartheta = \mu r^2\dot\vartheta, \;\; p_\varphi = \mu r^2\sin^2\vartheta\,\dot\varphi.$$

The BWS quantization conditions

$$\oint p_r dr = 2\pi\hbar(k + \tfrac{1}{2}), \tag{5.5}$$

$$\oint p_\vartheta d\vartheta = 2\pi(l - m + \tfrac{1}{2}), \tag{5.6}$$

$$\oint p_\varphi d\varphi = 2\pi\hbar m, \tag{5.7}$$

where integration goes over the closed orbit of the Kepler problem with the energy $E < 0$, exactly determine the energy levels E_n, $n = k + l + 1$.

Indeed, we have $p_\varphi = M_{c3}$, where $\boldsymbol{M}_c = (M_{c1}, M_{c2}, M_{c3})$ is the classical angular momentum. It is constant along the orbit, so that (5.7) determines the eigenvalues of operator M_3 (see Section 3.2). To evaluate $\oint p_\vartheta d\vartheta$, we use polar coordinates (r, χ) in the orbit plane P (see Section 1.6 in Chapter 1). Since $\dot\chi^2 = \dot\vartheta^2 + \sin^2\vartheta\,\dot\varphi^2$, along the orbit we get $p_\chi d\chi = p_\vartheta d\vartheta + p_\varphi d\varphi$, where $p_\chi = \mu r^2\dot\chi = |\boldsymbol{M}_c|$. Condition (5.6) now follows from

$$\oint p_\chi d\chi = 2\pi|\boldsymbol{M}_c| = 2\pi\hbar(l + \tfrac{1}{2}), \tag{5.8}$$

which is the quantization rule for the square of total angular momentum[7]. Finally, to evaluate $\oint p_r dr$, we use equations (1.7) and (1.11) in Section 1.6

[7]It gives the quantized values $\hbar^2(l + \frac{1}{2})^2$, which for large l agree well with the eigenvalues $\hbar^2 l(l+1)$ of the operator $\boldsymbol{M}^2$.

of Chapter 1 and get

$$p_r dr = \mu \dot{r} dr = \mu \frac{dr}{d\chi} \dot{\chi}\, dr = \frac{|\boldsymbol{M}_c|}{r^2} \left(\frac{dr}{d\chi}\right)^2 d\chi = p_\chi \frac{e^2 \sin^2 \chi}{(1 + e\cos\chi)^2} d\chi,$$

where $0 < e < 1$ is the eccentricity of the orbit. We have

$$\oint p_r dr = p_\chi \int_0^{2\pi} \frac{e^2 \sin^2 \chi}{(1 + e\cos\chi)^2} d\chi = 2\pi p_\chi \left(\frac{1}{\sqrt{1-e^2}} - 1\right),$$

as can be shown by using the substitution $z = e^{i\chi}$ and the Cauchy residue theorem[8]. It follows from equation (1.12) in Section 1.6 of Chapter 1 that

$$\sqrt{1-e^2} = \frac{|\boldsymbol{M}_c|\sqrt{2|E|}}{\alpha\sqrt{\mu}},$$

and we obtain from (5.5) and (5.8),

$$|E| = -E_n = \frac{\mu\alpha^2}{2n^2\hbar^2}, \quad n = k + l + 1.$$

5.2. Continuous spectrum. Set $2E = k^2$, where $k > 0$, and consider the equation

$$f_l'' + \left(\frac{2}{r} - \frac{l(l+1)}{r^2} + k^2\right) f_l = 0. \tag{5.9}$$

Substitution

$$f_l(r) = r^{l+1} e^{-ikr} F_l(r)$$

reduces (5.9) to

$$F_l'' + \left(\frac{2(l+1)}{r} - 2ik\right) F_l' + \left(\frac{2}{r} - \frac{2ik(l+1)}{r}\right) F_l = 0. \tag{5.10}$$

The solution of equation (5.10) satisfying $F_l(0) = 1$ can be explicitly written as

$$F_l(r) = F\left(l + 1 + i\lambda, 2l + 2, 2ikr\right), \quad \lambda = \frac{1}{k},$$

where $F(\alpha, \gamma, z)$ is a confluent hypergeometric function, defined by the absolutely convergent series

$$F(\alpha, \gamma, z) = \sum_{n=0}^{\infty} \frac{\Gamma(\alpha + n)\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma + n)} \frac{z^n}{n!}$$

for all α and $\gamma \neq 0, -1, -2, \ldots$. The confluent hypergeometric function is an entire function of the variable z and satisfies the differential equation

$$zF'' + (\gamma - z)F' - \alpha F = 0.$$

[8]This integral was evaluated by Sommerfeld in 1916.

For $\alpha = -k$ and $\gamma = p+1$, where $k, p = 0, 1, 2, \dots$, the confluent hypergeometric function reduces to associated Laguerre polynomials

$$Q_k^p(x) = \frac{(k+p)!}{p!} F(-k, p+1, x),$$

considered in the previous section. For $\operatorname{Re}\gamma > \operatorname{Re}\alpha > 0$ the function $F(\alpha, \gamma, z)$ admits the integral representation

$$F(\alpha, \gamma, z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma-\alpha)} \int_0^1 t^{\alpha-1}(1-t)^{\gamma-\alpha-1} e^{zt} dt, \tag{5.11}$$

obtained by the Laplace method. The confluent hypergeometric function satisfies the functional equation

$$F(\alpha, \gamma, z) = e^z F(\gamma-\alpha, \gamma, -z) \tag{5.12}$$

and has the following asymptotics as $z \to \infty$:

$$\begin{aligned} F(\alpha, \gamma, z) = \frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)} (-z)^{-\alpha} \big(1 + O(z^{-1})\big) \\ + \frac{\Gamma(\gamma)}{\Gamma(\alpha)} e^z z^{\alpha-\gamma} \big(1 + O(z^{-1})\big). \end{aligned} \tag{5.13}$$

It follows from (5.12) that $f_l(r) = r^{l+1} e^{-ikr} F(l+1+i\lambda, 2l+2, 2ikr)$ is real-valued and it follows from (5.13) that the function

$$f_{El}(r) = \frac{(2k)^{l+1}}{\sqrt{2\pi}(2l+1)!} e^{\frac{\pi}{2k}} |\Gamma(l+1-i\lambda)| f_l(r) \tag{5.14}$$

has the following asymptotics as $r \to \infty$:

$$f_{El}(r) = \sqrt{\frac{2}{\pi}} \sin\Big(kr + \lambda \log 2kr - \frac{l\pi}{2} + \delta_l\Big), \tag{5.15}$$

where

$$\delta_l(k) = \arg\Gamma(l+1-i\lambda), \quad \lambda = \frac{1}{k} = \frac{1}{\sqrt{2E}}, \tag{5.16}$$

is the phase shift. The partial S-matrix for the Coulomb problem is

$$S_l(k) = e^{2i\delta_l(k)} = \frac{\Gamma(l+1-i\lambda)}{\Gamma(l+1+i\lambda)}.$$

It admits meromorphic continuation to the upper half-plane $\operatorname{Im} k > 0$ and has simple poles at $k = i\varkappa_{jl}$, which correspond to the eigenvalues E_{kl} of the radial Schrödinger operator H_l. The radial eigenfunctions of the continuous spectrum (5.14) satisfy normalization condition (4.15).

Remark. It is instructive to compare asymptotics (5.15) for the Coulomb potential, which is long-range, with the corresponding formula (4.16) for the general short-range potential. The long range nature of the Coulomb interaction manifests itself by the extra logarithmic term $\lambda \log 2kr$ in (5.15).

The eigenfunction expansion theorem for the Schrödinger operator H of the hydrogen atom has the same form as in Section 4.3: the eigenfunctions $\psi_{klm}(\boldsymbol{x})$ are given by (5.4) where $k = 0, 1, \ldots, N_l = \infty$, and the eigenfunctions of the continuous spectrum are given by

$$\psi_{Elm}(\boldsymbol{x}) = \frac{f_{El}(r)}{r} Y_{lm}(\boldsymbol{n}), \quad l = 0, 1, \ldots, \quad m = -l, \ldots, l.$$

5.3. Hidden SO(4) **symmetry.** As we have seen in Section 1.6 of Chapter 1, classical system with the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{x}) = \frac{\boldsymbol{p}^2}{2m} - \frac{\alpha}{r},$$

in addition to the angular momentum $\boldsymbol{M}_{\mathrm{c}}$, has three extra integrals of motion given by the Laplace-Runge-Lenz vector

$$\boldsymbol{W}_{\mathrm{c}} = \frac{\boldsymbol{p}}{m} \times \boldsymbol{M}_{\mathrm{c}} - \frac{\alpha \boldsymbol{x}}{r}.$$

According to Example 2.2 in Section 2.6 of Chapter 1, the integrals $\boldsymbol{M}_{\mathrm{c}}$ and $\boldsymbol{W}_{\mathrm{c}}$ for the Kepler problem have the Poisson brackets

$$\{M_{\mathrm{c}j}, M_{\mathrm{c}k}\} = -\varepsilon_{jkl} M_{\mathrm{c}l}, \quad \{W_{\mathrm{c}j}, M_{\mathrm{c}k}\} = -\varepsilon_{jkl} W_{\mathrm{c}l},$$
$$\{W_{\mathrm{c}j}, W_{\mathrm{c}k}\} = 2H_{\mathrm{c}} \varepsilon_{jkl} M_{\mathrm{c}l},$$

where $j, k, l = 1, 2, 3$ and $\varepsilon_{123} = 1$.

The quantum Kepler problem is the Coulomb problem. In the coordinate representation $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$, its Hamiltonian is

$$H = \frac{\boldsymbol{P}^2}{2} - \frac{\alpha}{r},$$

where $r = |\boldsymbol{x}|$ and we put $m = 1$. The quantum Laplace-Runge-Lenz vector — the Laplace-Runge-Lenz operator $\boldsymbol{W}$ — is defined by

$$\boldsymbol{W} = \frac{1}{2}(\boldsymbol{P} \times \boldsymbol{M} - \boldsymbol{M} \times \boldsymbol{P}) - \frac{\alpha \boldsymbol{Q}}{r},$$

or in components

$$W_j = \frac{1}{2} \varepsilon_{jkl} (P_k M_l + M_l P_k) - \frac{\alpha Q_j}{r}, \quad j = 1, 2, 3.$$

Here Q_i are multiplication by x_i operators, and it is always understood that there is a summation over repeated indices $1, 2, 3$. Using commutation relations (3.5), we also have

$$\boldsymbol{W} = \boldsymbol{P} \times \boldsymbol{M} - \frac{\alpha \boldsymbol{Q}}{r} - i\hbar \boldsymbol{P} = -\boldsymbol{M} \times \boldsymbol{P} - \frac{\alpha \boldsymbol{Q}}{r} + i\hbar \boldsymbol{P}, \tag{5.17}$$

where the term $i\hbar \boldsymbol{P}$ plays the role of a "quantum correction". The following result reveals the hidden symmetry of the Coulomb problem.

Proposition 5.1. *The Schrödinger operator H of the hydrogen atom has quantum integrals of motion $\boldsymbol{M}$ and $\boldsymbol{W}$,*

$$[H, M_i] = [H, W_i] = 0, \quad i = 1, 2, 3,$$

satisfying $\boldsymbol{W} \cdot \boldsymbol{M} = \boldsymbol{M} \cdot \boldsymbol{W} = 0$ and

$$\boldsymbol{W}^2 = \alpha^2 + 2H\boldsymbol{M}^2 + 2\hbar^2 H. \tag{5.18}$$

Moreover, self-adjoint operators $\boldsymbol{M}$ and $\boldsymbol{W}$ have the following commutation relations:

$$[M_j, M_k] = i\hbar\varepsilon_{jkl}M_l, \quad [W_j, M_k] = i\hbar\varepsilon_{jkl}W_l, \quad [W_j, W_k] = -2i\hbar\varepsilon_{jkl}M_l H.$$

Proof. We know that $[H, M_j] = 0$. To prove that W_j are quantum integrals of motion, we first compute $\left[\boldsymbol{P}^2, \dfrac{Q_j}{r}\right]$. It follows from Heisenberg's commutation relations that

$$\left[P_j, \frac{1}{r}\right] = i\hbar\frac{Q_j}{r^3}, \tag{5.19}$$

so that using Leibniz rule and relations $r^2 = x_1^2 + x_2^3 + x_3^2$, $[M_l, r] = 0$, and $Q_j P_k - Q_k P_j = \varepsilon_{jkl}M_l$, we obtain

$$\left[\boldsymbol{P}^2, \frac{Q_j}{r}\right] = 2i\hbar\frac{Q_j}{r^3} + 2i\hbar\varepsilon_{jkl}\frac{Q_k}{r^3}M_l.$$

Now using the first equation in (5.17) and (5.19), we get

$$\begin{aligned}[H, W_j] &= \left[\frac{\boldsymbol{P}^2}{2} - \frac{\alpha}{r}, \varepsilon_{jkl}P_k M_l - \frac{\alpha Q_j}{r} - i\hbar P_j\right] \\ &= -i\alpha\hbar\frac{Q_j}{r^3} - i\alpha\hbar\varepsilon_{jkl}\frac{Q_k}{r^3}M_l + i\alpha\hbar\varepsilon_{jkl}\frac{Q_k}{r^3}M_l + i\alpha\hbar\frac{Q_j}{q^3} = 0.\end{aligned}$$

It is easy to prove the relation $\boldsymbol{W} \cdot \boldsymbol{M} = W_1M_1 + W_2M_2 + W_3M_3 = 0$. Indeed, it follows from the definition of $\boldsymbol{M}$ and commutativity of P_k and Q_l for $k \neq l$ that

$$\boldsymbol{M} \cdot \boldsymbol{P} = \boldsymbol{P} \cdot \boldsymbol{M} = \boldsymbol{M} \cdot \boldsymbol{Q} = \boldsymbol{Q} \cdot \boldsymbol{M} = 0,$$

and using the first equation in (5.17) and commutation relations for the components of the angular momentum, we immediately get $\boldsymbol{W} \cdot \boldsymbol{M} = 0$. To prove that $\boldsymbol{M} \cdot \boldsymbol{W} = 0$, one should use the second equation in (5.17).

Verification of (5.18) is more involved. We have

$$\begin{aligned}\boldsymbol{W}^2 = W_jW_j &= \left(\varepsilon_{jkl}M_lP_k - \frac{\alpha Q_j}{r} + i\hbar P_j\right)\left(\varepsilon_{jmn}P_mM_n - \frac{\alpha Q_j}{r} - i\hbar P_j\right)\\ &= \varepsilon_{jkl}(\varepsilon_{jmn}M_lP_kP_mM_n - \alpha M_lP_k\frac{Q_j}{r} - i\hbar M_lP_kP_j) - \alpha\varepsilon_{jmn}\frac{Q_j}{q}P_mM_n\\ &+ \alpha^2\frac{Q_jQ_j}{r^2} + i\alpha\hbar\frac{Q_j}{r}P_j + i\hbar\varepsilon_{jmn}P_jP_mM_n - i\alpha\hbar P_j\frac{Q_j}{r} + \hbar^2P_jP_j\\ &= \alpha^2I + \hbar^2\boldsymbol{P}^2 + \varepsilon_{jkl}\varepsilon_{jmn}M_lP_kP_mM_n - \alpha\varepsilon_{jkl}\left(M_lP_k\frac{Q_j}{q} + \frac{Q_j}{r}P_kM_l\right)\\ &- i\alpha\hbar\left[P_j, \frac{Q_j}{r}\right].\end{aligned}$$

Since operators M_j and P_j commute, the identity $(\boldsymbol{a}\times\boldsymbol{b})^2 = \boldsymbol{a}^2\,\boldsymbol{b}^2 - (\boldsymbol{a}\cdot\boldsymbol{b})^2$ is still applicable and we get

$$\varepsilon_{jkl}\varepsilon_{jmn}M_lP_kP_mM_n = -(\boldsymbol{M}\times\boldsymbol{P})\cdot(\boldsymbol{P}\times\boldsymbol{M}) = \boldsymbol{M}^2\boldsymbol{P}^2 - (\boldsymbol{M}\cdot\boldsymbol{P})^2 = \boldsymbol{M}^2\boldsymbol{P}^2.$$

Using (5.19) we easily obtain (summation over repeated indices)

$$\left[P_j, \frac{Q_j}{r}\right] = i\hbar\left(-\frac{3}{r} + \frac{r^2}{r^3}\right) = -\frac{2i\hbar}{r}.$$

Since $[\boldsymbol{M}^2, r] = 0$ it follows from $\boldsymbol{M} = \boldsymbol{Q}\times\boldsymbol{P}$ that

$$\varepsilon_{jkl}\left(M_lP_k\frac{Q_j}{r} + \frac{Q_j}{r}P_kM_l\right) = \boldsymbol{M}^2\frac{1}{r} + \frac{1}{r}\boldsymbol{M}^2 = \frac{2\boldsymbol{M}^2}{r}.$$

Putting everything together, we get (5.18).

It is also not difficult to establish commutation relations between M_j and W_k. Using (3.5) and properties of ε_{jkl}, we get

$$\begin{aligned}[M_j, W_k] &= \left[M_j, \varepsilon_{kmn}P_mM_n - \frac{\alpha Q_k}{r} - i\hbar P_k\right]\\ &= i\hbar(\varepsilon_{jmp}\varepsilon_{kmn}P_pM_n + \varepsilon_{jnp}\varepsilon_{kmn}P_mM_p) - i\hbar\varepsilon_{jkl}\left(\frac{\alpha Q_l}{r} + i\hbar P_l\right)\\ &= i\hbar(P_jM_k - M_kP_j) - i\hbar\varepsilon_{jkl}\left(\frac{\alpha r_l}{r} + i\hbar P_l\right) = i\hbar\varepsilon_{jkl}W_l.\end{aligned}$$

Finally, to establish commutation relations between components of $\boldsymbol{W}$, we use the representations

$$\boldsymbol{W} = \boldsymbol{Q}\,\boldsymbol{P}^2 - \boldsymbol{P}(\boldsymbol{Q}\cdot\boldsymbol{P}) - \frac{\alpha\boldsymbol{Q}}{r} = \boldsymbol{P}^2\boldsymbol{Q} - (\boldsymbol{P}\cdot\boldsymbol{Q})\boldsymbol{P} - \frac{\alpha\boldsymbol{Q}}{r}. \tag{5.20}$$

The first formula in (5.20) follows from the first formula in (5.17) by using

$$\begin{aligned}\varepsilon_{jkl}P_kM_l &= \varepsilon_{jkl}\varepsilon_{lmn}P_kQ_mP_l = \varepsilon_{jkl}(\varepsilon_{ljk}P_kQ_jP_k + \varepsilon_{lkj}P_kQ_kP_j)\\ &= P_k(P_kQ_j - P_jQ_k) = Q_j\boldsymbol{P}^2 - P_j(\boldsymbol{P}\cdot\boldsymbol{Q}) - 2i\hbar P_j,\end{aligned}$$

and relation $\boldsymbol{P}\cdot\boldsymbol{Q}=\boldsymbol{Q}\cdot\boldsymbol{P}-3i\hbar I$. The second formula in (5.20) follows from the first by using Heisenberg's commutation relations. Now we have

$$\begin{aligned}\varepsilon_{jkl}[W_k,W_l]&=2\varepsilon_{jmn}W_mW_n\\ =2\varepsilon_{jmn}&\left(\boldsymbol{P}^2Q_m-(\boldsymbol{P}\cdot\boldsymbol{Q})P_m-\frac{\alpha Q_m}{r}\right)\left(Q_n\boldsymbol{P}^2-P_n(\boldsymbol{Q}\cdot\boldsymbol{P})-\frac{\alpha Q_n}{r}\right)\\ &=2M_j\left(-\boldsymbol{P}^2(\boldsymbol{Q}\cdot\boldsymbol{P})+(\boldsymbol{P}\cdot\boldsymbol{Q})\boldsymbol{P}^2+\frac{\alpha}{r}(\boldsymbol{Q}\cdot\boldsymbol{P})-(\boldsymbol{P}\cdot\boldsymbol{Q})\frac{\alpha}{r}\right)\\ &=-2i\hbar M_j\left(\boldsymbol{P}^2-\frac{2\alpha}{r}\right)=-4i\hbar M_jH,\end{aligned}$$

where we have used $[\boldsymbol{M},\boldsymbol{P}\cdot\boldsymbol{Q}]=0$ and $\left[\boldsymbol{P}\cdot\boldsymbol{Q},\dfrac{1}{r}\right]=\dfrac{i\hbar}{r}$. This proves that $[W_k,W_l]=-2i\hbar\varepsilon_{jkl}M_jH$. □

Let $\mathscr{H}_0=\mathsf{P}_H(-\infty,0)\mathscr{H}$, where P_H is the projection-valued measure for the Schrödinger operator H. Since self-adjoint operators $\boldsymbol{M}$ and $\boldsymbol{W}$ commute with H, the subspace $\mathscr{H}_0$ is an invariant subspace for these operators. The Schrödinger operator H is non-negative on $\mathscr{H}_0$, so that on this subspace the operator $(-2H)^{-1/2}$ is well defined. Now on $\mathscr{H}_0$ we set

$$\boldsymbol{J}^{(\pm)}=\frac{1}{2}(\boldsymbol{M}\pm(-2H)^{-1/2}\boldsymbol{W}).$$

It follows from Proposition 5.1 that self-adjoint operators $J_j^{(\pm)}$ on $\mathscr{H}_0$ satisfy the commutation relations

$$\left[J_j^{(\pm)},J_k^{(\pm)}\right]=i\hbar\varepsilon_{jkl}J_l^{(\pm)},\quad \left[J_j^{(+)},J_k^{(-)}\right]=0 \tag{5.21}$$

and

$$(\boldsymbol{J}^{(+)})^2=(\boldsymbol{J}^{(-)})^2=-\frac{1}{4}\left(\hbar^2I+\frac{\alpha^2}{2H}\right). \tag{5.22}$$

Equations (5.21) are commutation relations for the generators of the Lie algebra $\mathfrak{so}(4)$, which correspond to the Lie isomorphism $\mathfrak{so}(4)\simeq\mathfrak{so}(3)\oplus\mathfrak{so}(3)$, and exhibit the hidden SO(4) symmetry of the Coulomb problem! Together with (5.22), they allow us to find the energy levels pure algebraically.

Namely, the eigenvalues of the operators $(\boldsymbol{J}^{(+)})^2$ and $(\boldsymbol{J}^{(-)})^2$ are, respectively, $\hbar^2l_1(l_1+1)$ and $\hbar^2l_2(l_2+1)$, and it follows from (5.22) that $l_1=l_2=l$ so that the corresponding eigenvalue of H is

$$E_n=-\frac{\alpha^2}{2\hbar^2n^2},\quad n=2l+1.$$

Assuming that

$$\mathscr{H}_0\simeq\bigoplus_{l\in\frac{1}{2}\mathbb{Z}_{\geq0}}V_l\otimes V_l, \tag{5.23}$$

where summation goes over all non-negative integer and half-integer values of l, we get from the Clebsch-Gordan decomposition (3.13) that the multiplicity of the eigenvalue E_n is

$$\dim V_l \otimes V_l = \sum_{j=0}^{2l}(2j+1) = (2l+1)^2 = n^2.$$

To prove the orthogonal sum decomposition (5.23), one should consider the Schrödinger equation for the hydrogen atom in the momentum representation. Using spherical coordinates in $\mathbb{R}^3$ and the elementary integral

$$\int_0^\infty \frac{\sin r}{r} dr = \frac{\pi}{2},$$

it is easy to show that for every $\psi \in \mathscr{S}(\mathbb{R}^3)$

$$\frac{1}{2\pi^2\hbar}\int_{\mathbb{R}^3} \frac{\hat{\psi}(\boldsymbol{q})}{|\boldsymbol{p}-\boldsymbol{q}|^2} d^3\boldsymbol{q} = \frac{1}{(\sqrt{2\pi\hbar})^3}\int_{\mathbb{R}^3} \frac{1}{r}\psi(\boldsymbol{x}) e^{-\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{x}} d^3\boldsymbol{x}, \tag{5.24}$$

where $\hat{\psi} = \mathscr{F}_\hbar(\psi)$ is the $\hbar$-dependent Fourier transform[9]. Let ψ be the eigenfunction of H with the the eigenvalue $E < 0$. It follows from (5.24) that in the momentum representation the corresponding Schrödinger equation — the eigenvalue equation $H\psi = E\psi$ — takes the form

$$(\boldsymbol{p}^2 + p_0^2)\hat{\psi}(\boldsymbol{p}) = \lambda \int_{\mathbb{R}^3} \frac{\hat{\psi}(\boldsymbol{q})}{|\boldsymbol{p}-\boldsymbol{q}|^2} d^3\boldsymbol{q}, \tag{5.25}$$

where $p_0 = \sqrt{-2\mu E}$ and $\lambda = \dfrac{\alpha\mu}{p_0\hbar}$. Next, consider the homogeneous coordinates $\dfrac{\boldsymbol{p}}{p_0}$ in $\mathbb{R}^3$ as coordinates of the stereographic projection of the unit sphere S^3 in $\mathbb{R}^4$. Namely, denoting by $\boldsymbol{n}$ the unit vector from the origin to the north pole of S^3, we get for the point $\boldsymbol{u} \in S^3$ corresponding to $\dfrac{\boldsymbol{p}}{p_0} \in \mathbb{R}^3$:

$$\boldsymbol{u} = \frac{\boldsymbol{p}^2 - p_0^2}{\boldsymbol{p}^2 + p_0^2}\,\boldsymbol{n} + \frac{2p_0}{\boldsymbol{p}^2 + p_0^2}\,\boldsymbol{p}.$$

For the volume form on S^3 we have

$$d\Omega = \frac{(2p_0)^3}{(\boldsymbol{p}^2 + p_0^2)^3} d^3\boldsymbol{p}, \quad \int_{S^3} d\Omega = 2\pi^2.$$

Using

$$|\boldsymbol{p}-\boldsymbol{q}|^2 = \frac{(\boldsymbol{p}^2 + p_0^2)(\boldsymbol{q}^2 + p_0^2)}{(2p_0)^2}|\boldsymbol{u}-\boldsymbol{v}|^2,$$

[9]Since $\boldsymbol{x}$ is the variable in the coordinate representation, here $\boldsymbol{q}$ is another variable in the momentum representation.

where $\boldsymbol{v} \in S^3$ corresponds to $\dfrac{\boldsymbol{q}}{p_0} \in \mathbb{R}^3$, and introducing

$$\Psi(\boldsymbol{u}) = \frac{1}{\sqrt{p_0}} \frac{(\boldsymbol{p}^2 + p_0^2)^2}{(2p_0)^2} \hat{\psi}(\boldsymbol{p}),$$

we can rewrite equation (5.25) as

$$\Psi(\boldsymbol{u}) = \frac{\lambda}{2\pi^2} \int_{S^3} \frac{\Psi(\boldsymbol{v})}{|\boldsymbol{u} - \boldsymbol{v}|^2} d\Omega_{\boldsymbol{v}}. \tag{5.26}$$

We also have

$$\int_{S^3} |\Psi(\boldsymbol{u})|^2 d\Omega_{\boldsymbol{u}} = \int_{\mathbb{R}^3} \frac{\boldsymbol{p}^2 + p_0^2}{2p_0^2} |\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p} = \int_{\mathbb{R}^3} |\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p}. \tag{5.27}$$

Indeed, it follows from the Schrödinger equation that

$$\frac{1}{2\mu} \int_{\mathbb{R}^3} \boldsymbol{p}^2 |\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p} = \frac{1}{2\mu} \int_{\mathbb{R}^3} \left| \frac{\partial \psi(\boldsymbol{x})}{\partial \boldsymbol{x}} \right|^2 d^3\boldsymbol{x} = \int_{\mathbb{R}^3} (E - V(r)) |\psi(\boldsymbol{x})|^2 d^3\boldsymbol{x},$$

and by the virial theorem (see Section 1.3) we get

$$\frac{1}{2\mu} \int_{\mathbb{R}^3} \left| \frac{\partial \psi(\boldsymbol{x})}{\partial \boldsymbol{x}} \right|^2 d^3\boldsymbol{x} = -\frac{1}{2\mu} \int_{\mathbb{R}^3} \Delta\psi(\boldsymbol{x}) \overline{\psi(\boldsymbol{x})} d^3\boldsymbol{x} = -\frac{1}{2} \int_{\mathbb{R}^3} V(r) |\psi(\boldsymbol{x})|^2 d^3\boldsymbol{x},$$

where $V(r) = -\dfrac{\alpha}{r}$, so that

$$\int_{\mathbb{R}^3} V(r) |\psi(\boldsymbol{x})|^2 d^3\boldsymbol{x} = 2E \int_{\mathbb{R}^3} |\psi(\boldsymbol{x})|^2 d^3\boldsymbol{x} = 2E \int_{\mathbb{R}^3} |\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p}.$$

This shows that the eigenvalue problem for the Schrödinger equation is equivalent to the eigenvalue problem for the integral equation (5.26) in $L^2(S^3, d\Omega)$. The latter is a classical problem in the theory of spherical harmonics. Namely, the function $G(\boldsymbol{u}) = -\dfrac{1}{4\pi^2 u^2}$, where $u = |\boldsymbol{u}|$, $\boldsymbol{u} \in \mathbb{R}^4$, is the fundamental solution for the Laplace operator Δ in $\mathbb{R}^4$,

$$\Delta = \frac{\partial^2}{\partial u_1^2} + \frac{\partial^2}{\partial u_2^2} + \frac{\partial^2}{\partial u_3^2} + \frac{\partial^2}{\partial u_4^2},$$

and equation (5.26) is the equation satisfied by the spherical harmonics on S^3: the eigenfunctions of the spherical part Δ_0 of the Laplace operator on $\mathbb{R}^4$, defined by

$$\Delta = \frac{1}{u^3} \frac{\partial}{\partial u} \left(u^3 \frac{\partial}{\partial u} \right) + \frac{1}{u^2} \Delta_0.$$

It is well known from the representation theory of the Lie group SO(4) that spherical harmonics are restrictions to S^3 of homogeneous harmonic polynomials in $\mathbb{R}^4$ of degree $n-1$, $n \in \mathbb{N}$. Correspondingly, equation (5.26) is obtained as a limit $|\boldsymbol{u}| \to 1$ of the Green's formula for the homogeneous harmonic function of degree $n-1$ in the unit ball in $\mathbb{R}^4$, by using the

property of a double layer potential. This gives $\lambda = n$, which once again establishes the exact formula for the energy levels of the hydrogen atom. The isomorphism $\mathscr{H}_0 \simeq L^2(S^3, d\Omega)$ follows from (5.27), and (5.23) — from the decomposition

$$L^2(S^3, d\Omega) \simeq \bigoplus_{l \in \frac{1}{2}\mathbb{Z}_{\geq 0}} V_l \otimes V_l$$

of the regular representation of SO(4) into the direct sum of irreducible components. One can also obtain the explicit form (5.4) of the eigenfunctions by using the representation theory of SO(4). We leave all these details to the interested reader.

Remark. For $E > 0$ one should consider the subspace $\mathscr{H}_1 = \mathsf{P}_H(0, \infty)\mathscr{H}$ and define $\boldsymbol{J}^{(\pm)} = \frac{1}{2}(\boldsymbol{M} \pm (2H)^{-1/2}\boldsymbol{W})$. Instead of (5.21), these operators satisfy commutation relations of the Lie algebra $\mathfrak{so}(3,1)$ of the Lorentz group SO(3, 1). The problem of finding eigenfunctions of the continuous spectrum for the Coulomb problem can be solved by using harmonic analysis on the three-dimensional Lobachevsky space.

Problem 5.1. Show that components of angular momentum $\boldsymbol{M}$ are generators of $\mathfrak{so}(4)$ that correspond to the infinitesimal rotations in the subspace of $\mathbb{R}^4$ with coordinates $(0, \boldsymbol{p})$, and components of the Laplace-Runge-Lenz vector $\boldsymbol{W}$ correspond to the infinitesimal rotations in the $(p_0 p_1)$, (p_0, p_2), and $(p_0 p_3)$ planes in $\mathbb{R}^4$.

6. Semi-classical asymptotics – I

Here we describe the relation between classical and quantum mechanics by considering the behavior of the wave function $\psi(\boldsymbol{q}, t)$ — the solution of the time dependent Schrödinger equation[10]

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V(\boldsymbol{q})\psi \tag{6.1}$$

as $\hbar \to 0$. The substitution

$$\psi(\boldsymbol{q}, t) = e^{-\frac{i}{\hbar}S(\boldsymbol{q}, t; \hbar)} \tag{6.2}$$

reduces (6.1) to the following non-linear partial differential equation:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial \boldsymbol{q}}\right)^2 + V(\boldsymbol{q}) = \frac{i\hbar}{2m}\Delta S. \tag{6.3}$$

It is remarkable that (6.3) differs from the Hamilton-Jacobi equation (2.4) for the Hamiltonian function $H_c(\boldsymbol{p}, \boldsymbol{q}) = \dfrac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$, considered in Section 2.3 of Chapter 1, only by the term in the right-hand side which is proportional to $\hbar$. Thus as $\hbar \to 0$, equations of motion in quantum mechanics turn into classical equations of motion.

[10] Here it is convenient to denote Cartesian coordinates on $\mathbb{R}^n$ by $\boldsymbol{q} = (q_1, \ldots, q_n)$.

For the stationary state $\psi(\boldsymbol{q},t)=\psi(\boldsymbol{q})e^{-\frac{i}{\hbar}Et}$ the substitution (6.2) becomes

$$\psi(\boldsymbol{q},t)=e^{-\frac{i}{\hbar}(\sigma(\boldsymbol{q};\hbar)-Et)}. \tag{6.4}$$

The corresponding non-linear partial differential equation

$$\frac{1}{2m}\left(\frac{\partial\sigma}{\partial\boldsymbol{q}}\right)^2+V(\boldsymbol{q})=E+\frac{i\hbar}{2m}\Delta\sigma \tag{6.5}$$

differs from the corresponding Hamilton-Jacobi equation for the abbreviated action, considered in Section 2.5 of Chapter 1, by the term proportional to $\hbar$ in the right-hand side.

In this section we consider *semi-classical asymptotics*: asymptotics of the partial differential equations (6.3) and (6.5) as $\hbar\to 0$. They describe the precise relation between quantum mechanics and classical mechanics, and provide a quantitative form of the correspondence principle, discussed in Section 2 of Chapter 2. In particular, using semi-classical asymptotics for the stationary Schrödinger equation, we derive Bohr-Wilson-Sommerfeld quantization rules, postulated in Section 2.5 of Chapter 2.

6.1. Time-dependent asymptotics. Here we consider the problem of finding *short-wave asymptotics* — asymptotics as $\hbar\to 0$ of the solution $\psi_\hbar(q,t)$ of the Cauchy problem for the Schrödinger equation (6.1) in one dimension,

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\,\frac{\partial^2\psi}{\partial q^2}+V(q)\psi,$$

with the initial condition

$$\psi_\hbar(q,t)|_{t=0}=\varphi(q)e^{\frac{i}{\hbar}s(q)}.$$

It is assumed that the real-valued functions $\varphi(q)$ and $s(q)$ are smooth, $s(q),\varphi(q)\in C^\infty(\mathbb{R})$, and that the "amplitude" $\varphi(q)$ has compact support. The substitution (6.2) is $\psi_\hbar(q,t)=e^{\frac{i}{\hbar}S(q,t,\hbar)}$, and differential equation (6.3) takes the form

$$\frac{\partial S}{\partial t}+\frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2+V(q)=\frac{i\hbar}{2m}\,\frac{\partial^2 S}{\partial q^2}. \tag{6.6}$$

To determine the asymptotic behavior of $S(q,t,\hbar)$ as $\hbar\to 0$, we assume that as $\hbar\to 0$

$$S(q,t,\hbar)=\sum_{n=0}^{\infty}(-i\hbar)^n S_n(q,t),$$

and substitute this expansion into (6.6). Comparing terms with the same powers of $\hbar$ we obtain that $S_0(q,t)$ satisfies the initial value problem

$$\frac{\partial S_0}{\partial t} + \frac{1}{2m}\left(\frac{\partial S_0}{\partial q}\right)^2 + V(q) = 0, \tag{6.7}$$

and

$$S_0(q,t)|_{t=0} = s(q), \tag{6.8}$$

whereas $S_1(q,t)$ satisfies the differential equation

$$\frac{\partial S_1}{\partial t} + \frac{1}{m}\frac{\partial S_0}{\partial q}\frac{\partial S_1}{\partial q} = -\frac{1}{2m}\frac{\partial^2 S_0}{\partial q^2}, \tag{6.9}$$

the so-called *transport equation*, and

$$S_1(q,t)|_{t=0} = \varphi(q). \tag{6.10}$$

The functions $S_n(q,t)$ for $n > 1$ satisfy non-homogeneous differential equations similar to (6.9).

The initial value problem (6.7)–(6.8) is the Cauchy problem for the Hamilton-Jacobi equation with the Hamiltonian function

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

considered in Section 2.3 of Chapter 1. According to Proposition 2.1 in Section 2.3 of Chapter 1, the solution of (6.7)–(6.8) is given by the method of characteristics,

$$S_0(q,t) = s(q_0) + \int_0^t L(\gamma'(\tau))d\tau. \tag{6.11}$$

Here $L(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q)$ is the Lagrangian function, and $\gamma(\tau)$ is the characteristic — the classical trajectory which starts at q_0 at time $\tau = 0$ with the momentum $p_0 = \dfrac{\partial s}{\partial q}(q_0)$, and ends at q at time $\tau = t$, where q_0 is uniquely determined by q. (We are assuming that the Hamiltonian phase flow g_t satisfies the assumptions made in Section 2.3 of Chapter 1.) It follows from Theorem 2.7 in Section 2.3 of Chapter 1 that along the characteristic,

$$\frac{\partial S_0}{\partial q}(q,t) = m\frac{d\gamma}{dt}(t),$$

so that

$$\left(\frac{\partial}{\partial t} + \frac{\partial S_0}{\partial q}\right) S_1(\gamma(t),t) = \frac{d}{dt}S_1(\gamma(t),t). \tag{6.12}$$

Now we can solve the Cauchy problem (6.9)–(6.10) for the transport equation explicitly. Consider the flow $\pi_t : \mathbb{R} \to \mathbb{R}$, defined in Section 2.3 of

Chapter 1, and denote[11] by $\gamma(Q,q;\tau)$ the characteristic connecting points q at $\tau=0$ and $Q=\pi^t(q)$ at $\tau=t$ (under our assumptions the flow π_t is a diffeomorphism and the mapping $q\mapsto Q$ is one to one). 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 (6.9) can be rewritten as

$$\frac{d}{dt}S_1(Q,t)=-\frac{1}{2}\frac{d}{dt}\log\frac{\partial Q}{\partial q},$$

and using (6.10) we obtain

$$S_1(Q,t)=\varphi(q)\left|\frac{\partial Q}{\partial q}(q)\right|^{-\frac{1}{2}}.$$

Therefore,

$$\psi_\hbar(Q,t)=\varphi(q)\left|\frac{\partial Q}{\partial q}(q)\right|^{-\frac{1}{2}}e^{\frac{i}{\hbar}(S(Q,q;t)+s(q))}(1+O(\hbar)), \tag{6.13}$$

where $S(Q,q;t)$ is the classical action along the characteristic that starts at q at time $\tau=0$ and ends at Q at time $\tau=t$.

The rigorous proof that (6.13) is an asymptotic expansion as $\hbar\to 0$ uses the assumptions made in Section 2.3 of Chapter 1, and is left to the interested reader. Here we just mention that asymptotics (6.13) is consistent with the *conservation of probability*: for any Borel subset $E\subset\mathbb{R}$,

$$\int_{E_t}|\psi_\hbar(Q,t)|^2dQ=\int_E|\varphi(q)|^2dq+O(\hbar)$$

as $\hbar\to 0$, where $E_t=\pi_t(E)$.

Remark. When assumptions in Section 2.3 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,

$$\psi_\hbar(Q,t)=\sum_j\varphi(q_j)\left|\frac{\partial Q}{\partial q}(q_j)\right|^{-\frac{1}{2}}e^{\frac{i}{\hbar}(S(Q,q_j;t)+s(q_j))-\frac{\pi i}{2}\mu_j}(1+O(\hbar)),$$

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 initial data

[11] There should not be any confusion with the quantum coordinate operator Q.

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.

The case of n degrees of freedom is considered similarly. Under the assumptions in Section 2.3 of Chapter 1, the solution $\psi_\hbar(\boldsymbol{q}, t)$ of the Schrödinger equation (6.1) with the initial condition

$$\psi_\hbar(\boldsymbol{q}, t)|_{t=0} = \varphi(\boldsymbol{q}) e^{\frac{i}{\hbar} s(\boldsymbol{q})},$$

where real-valued functions $s(\boldsymbol{q})$ and $\varphi(\boldsymbol{q})$ are smooth and $\varphi(\boldsymbol{q})$ is compactly supported, has the following asymptotics as $\hbar \to 0$:

$$\psi_\hbar(\boldsymbol{Q}, t) = \varphi(\boldsymbol{q}) \left| \det \left(\frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{q}}(\boldsymbol{q}) \right) \right|^{-\frac{1}{2}} e^{\frac{i}{\hbar}(S(\boldsymbol{Q},\boldsymbol{q};t)+s(\boldsymbol{q}))}(1 + O(\hbar)). \tag{6.14}$$

6.2. Time independent asymptotics. Here we consider semi-classical asymptotics for the one-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi. \tag{6.15}$$

This asymptotic method is also known as the *WKB method* (after G. Wentzel, H. Kramers, and L. Brillouin). The substitution (6.4) is $\psi_\hbar(x) = e^{\frac{i}{\hbar}\sigma(x;\hbar)}$ and equation (6.5) takes the form

$$\frac{1}{2m} \left(\frac{d\sigma}{dx} \right)^2 + V(x) = E + \frac{i\hbar}{2m} \frac{d^2\sigma}{dx^2}.$$

As in the previous section, we use the expansion

$$\sigma(x, \hbar) = \sum_{n=0}^{\infty} (-i\hbar)^n \sigma_n(x),$$

and for the first two terms obtain

$$\frac{1}{2m}\sigma_0'^2 = E - V(x) \quad \text{and} \quad \sigma_0'\sigma_1' = -\tfrac{1}{2}\sigma_0''. \tag{6.16}$$

Let $p(x) = \sqrt{2m(E - V(x))}$ be the classical momentum of a particle moving in a potential $V(x)$ with the energy E. The solution of the first equation in (6.16) is given by

$$\sigma_0 = \pm \int p(x)dx,$$

and from the second equation in (6.16) we get

$$\sigma_1 = -\tfrac{1}{2} \log p.$$

The wave function in the WKB approximation has the form

$$\psi_\hbar(x) = \tfrac{1}{\sqrt{|p(x)|}}(C_1 e^{\frac{i}{\hbar}\int p(x)dx} + C_2 e^{-\frac{i}{\hbar}\int p(x)dx})(1 + O(\hbar)), \tag{6.17}$$

where $p(x)$ is real in the classical region $V(x) < E$, and is pure imaginary in the classically forbidden region $V(x) > E$ (see Section 1.5 of Chapter 1).

Note that the asymptotic (6.17) is valid only if $\sigma'^2 \ll \hbar\sigma''$, which in the first approximation gives

$$\left| \frac{d}{dx}\left(\frac{\hbar}{p(x)}\right)\right| \ll 1.$$

Introducing the classical force $F = -\dfrac{dV}{dx}$, this condition can be written as

$$\frac{m\hbar F}{p^3} \ll 1. \tag{6.18}$$

Thus the WKB approximation does not work when the classical momentum $p(x)$ is small. In particular, it is not applicable near the turning points where $E = V(x)$ and, therefore, $p(x) = 0$. Let $x = a$ be a turning point. If $F_0 = F(a) \neq 0$, using the approximation $E - V(x) \simeq F_0(x-a)$ near $x = a$, one can replace (6.15) by

$$\frac{\hbar^2}{2m}\,\psi'' = F_0(x-a)\psi.$$

This differential equation can be explicitly solved by the Laplace method. Its bounded solution is

$$\psi(x) = \Phi(\xi), \quad \xi = \left(\frac{2mF_0}{\hbar^2}\right)^{\frac{1}{3}}(a-x),$$

where $\Phi(\xi)$ is the Airy-Fock function, defined by the improper integral

$$\Phi(\xi) = \frac{1}{\sqrt{\pi}}\int_0^\infty \cos\left(\tfrac{1}{3}t^3 + \xi t\right) dt.$$

The large ξ asymptotics of the Airy-Fock function, obtained by the steepest descent method, are the following:

$$\Phi(\xi) = \frac{1}{2\sqrt[4]{\xi}} e^{-\frac{2}{3}\xi^{\frac{3}{2}}}\left(1 + O\left(\xi^{-\frac{3}{2}}\right)\right) \quad \text{as} \quad \xi \to \infty, \tag{6.19}$$

$$\Phi(\xi) = \frac{1}{\sqrt[4]{|\xi|}} \sin\left(\tfrac{2}{3}|\xi|^{\frac{3}{2}} + \tfrac{\pi}{4}\right)\left(1 + O\left(|\xi|^{-\frac{3}{2}}\right)\right) \quad \text{as} \quad \xi \to -\infty. \tag{6.20}$$

Using asymptotics (6.19)–(6.20) one can obtain connection formulas relating WKB approximations for classical and forbidden regions. The rigorous justification of this approach is technically rather involved and we will not present it here. Instead we highlight the simplest case when there is only one turning point $x = a$ with $F_0 > 0$, so that $x < a$ is a classically forbidden region. From (6.17) we obtain that the WKB wave function in the forbidden region $x < a$ is exponentially decaying,

$$\psi_{\text{WKB}}(x) = \frac{A}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int_a^x |p(s)|ds},$$

whereas in the classical region $x < a$ it is oscillating,

$$\psi_{\text{WKB}}(x) = \frac{1}{\sqrt{p(x)}}(C_1 e^{\frac{i}{\hbar}\int_a^x p(s)ds} + C_2 e^{-\frac{i}{\hbar}\int_a^x p(s)ds}) = \frac{B}{\sqrt{p(x)}}\sin(\tfrac{1}{\hbar}\textstyle\int_a^x p(s)ds + \alpha).$$

As follows from (6.18), the WKB approximation near the turning point $x = a$ remains valid whenever $|x - a| \gg \frac{1}{2}\left(\frac{\hbar^2}{mF_0}\right)^{\frac{1}{3}}$, which is equivalent to the condition $|\xi| \gg 1$. On the other hand, when $|x - a| \ll 1$ the wave function has the asymptotic

$$\psi_\hbar(x) = C\Phi(\xi)(1 + O(\hbar)).$$

To determine the unknown phase α and to find the relation between coefficients A, B, and C, we consider the domain $\frac{1}{2}\left(\frac{\hbar^2}{mF_0}\right)^{\frac{1}{3}} \ll |x - a| \ll 1$ and compare the WKB approximation for the wave function with the large ξ asymptotics of the Airy-Fock function. Namely, for $x < a$ we have $\xi \gg 1$ and

$$\frac{2}{3}\xi^{\frac{3}{2}} = \frac{2}{3\hbar}\sqrt{2mF_0}(a - x)^{\frac{3}{2}} \simeq \frac{1}{\hbar}\int_x^a |p(s)|ds, \quad \sqrt[4]{\xi} = \frac{\sqrt{|p(x)|}}{\sqrt[6]{2m\hbar F_0}}.$$

Comparing (6.19) with the WKB wave function for $x < a$ we obtain that $2A = \sqrt[6]{2m\hbar F_0}C$. For $x > a$ we have $\xi \ll -1$ and

$$\frac{2}{3}|\xi|^{\frac{3}{2}} = \frac{2}{3\hbar}\sqrt{2mF_0}(x - a)^{\frac{3}{2}} \simeq \frac{1}{\hbar}\int_a^x p(s)ds, \quad \sqrt[4]{|\xi|} = \frac{\sqrt{p(x)}}{\sqrt[6]{2m\hbar F_0}}.$$

Comparing (6.20) with the WKB wave function for $x < a$ we obtain that $\alpha = \frac{\pi}{4}$ and $B = \sqrt[6]{2m\hbar F_0}C$, so that $B = 2A$. Thus for this example the WKB wave function is

$$\psi_{\text{WKB}}(x) = \begin{cases} \frac{A}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int_a^x |p(s)|ds} & \text{when } x < a, \\ \frac{2A}{\sqrt{p(x)}}\sin(\frac{1}{\hbar}\int_a^x p(s)ds + \frac{\pi}{4}) & \text{when } x > a. \end{cases} \tag{6.21}$$

The case when there is only one turning point $x = b$ with $F_0 < 0$, so that $x > b$ is a classically forbidden region, reduces to the previous example by reversing the orientation $x \mapsto -x$. As the result, we obtain

$$\psi_{\text{WKB}}(x) = \begin{cases} \frac{2B}{\sqrt{p(x)}}\sin(\frac{1}{\hbar}\int_x^b p(s)ds + \frac{\pi}{4}) & \text{when } x < b, \\ \frac{B}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_b^x |p(s)|ds} & \text{when } x > b. \end{cases} \tag{6.22}$$

Problem 6.1 (Penetration through a potential barrier)**.** Consider a potential barrier for a given energy E — a potential $V(x)$ such that $\{x \in \mathbb{R} : V(x) > E\} = (a, b)$. Show that

$$T_{\text{WKB}} = e^{-\frac{2}{\hbar}\int_a^b |p(x)|dx}.$$

Verify directly that transmission coefficient for the potential in Problem 2.9 in the semi-classical approximation is given by this formula.

Problem 6.2 (Above barrier reflection)**.** Suppose that a potential $V(x)$ admits analytic continuation into the upper half-plane, and let E be the energy such that $E > V(x)$ for all real x. Suppose that there is only one complex x_0 such that $V(x_0) = E$. Show that in the semi-classical approximation

$$R_{\text{WKB}} = e^{-\frac{4}{\hbar}\operatorname{Im}\int_a^{x_0} p(x)dx},$$

where $p(x) = \sqrt{2m(E - V(x))}$ and $a \in \mathbb{R}$ (the choice of a does not change the imaginary part of the integral in the exponent). Verify directly that the reflection coefficient for the potential in Problem 2.9 in the semi-classical approximation is given by this formula.

Problem 6.3. Find transmission and reflection coefficients for the parabolic barrier — a potential $V(x) = -\frac{1}{2}kx^2$, where $k > 0$ — and verify directly that in the semi-classical approximation they satisfy, for $E < 0$ and $E > 0$, respectively, formulas in Problems 6.1 and 6.2.

6.3. Bohr-Wilson-Sommerfeld quantization rules. The WKB method allows us to determine energy levels in the semi-classical approximation. Consider, for simplicity, the finite motion of a one-dimensional particle in a potential well: in a potential $V(x)$ at the energy E such that there are two turning points a and b. The classical region is $a \le x \le b$, and the motion is periodic with the period

$$T = 2\int_a^b \frac{dx}{\dot{x}} = 2m\int_a^b \frac{dx}{p} = \sqrt{2m}\int_a^b \frac{dx}{\sqrt{E - V(x)}}.$$

The regions $x < a$ and $x > b$ are forbidden (see Section 1.5 of Chapter 1).

It follows from (6.21)–(6.22) that the WKB wave function exponentially decays in the forbidden regions $x < a$ and $x > b$. Using (6.21) we see that in the classical region the WKB wave function has the form

$$\psi_{\text{WKB}}(x) = \tfrac{2A}{\sqrt{p(x)}}\sin\left(\tfrac{1}{\hbar}\int_a^x p(s)ds + \tfrac{\pi}{4}\right),$$

while using (6.22) we obtain

$$\begin{aligned}\psi_{\text{WKB}}(x) &= \tfrac{2B}{\sqrt{p(x)}}\sin\left(\tfrac{1}{\hbar}\int_x^b p(s)ds + \tfrac{\pi}{4}\right)\\ &= \tfrac{2B}{\sqrt{p(x)}}\sin\left(\tfrac{1}{\hbar}\int_a^b p(s)ds + \tfrac{\pi}{2} - \left(\tfrac{1}{\hbar}\int_a^x p(s)ds + \tfrac{\pi}{4}\right)\right).\end{aligned}$$

These two expressions define the same function in $a \le x \le b$ if and only if there is a positive integer n such that

$$\tfrac{1}{\hbar}\int_a^b p(x)dx + \frac{\pi}{2} = (n+1)\pi, \tag{6.23}$$

in which case $A = (-1)^{n+1}B$. Equation (6.23), written in the form

$$\int_a^b \sqrt{2m(E - V(x))}\, dx = \pi\hbar(n + \tfrac{1}{2}),$$

determines the semi-classical energy levels. It follows from (6.21)–(6.22) that the integer n is equal to the number of zeros of the WKB wave function. In accordance with the oscillation theorem, the case $n = 0$ corresponds to the ground state, case $n = 1$ — to the next energy level state, etc.

Denoting, as in Chapters 1 and 2, coordinate x by q, we can rewrite (6.23) as

$$\oint p dq = 2\pi\hbar(n + \tfrac{1}{2}), \tag{6.24}$$

where integration goes over the closed classical orbit in the phase plane $\mathbb{R}^2$ with canonical coordinates p, q. Condition (6.24) is the famous Bohr-Wilson-Sommerfeld quantization rule for the case of one degree of freedom (see Section 2.5 of Chapter 2). We emphasize that, in general, the BWS quantization rule is applicable only for large n and gives the semi-classical asymptotic of energy levels E_n. However, as was shown in Section 2.6 of Chapter 2, the energy levels of the harmonic oscillator obtained by the BWS quantization rule are exact. The BWS rules are also exact for the energy levels of the hydrogen atom (see Section 5.1).

This semi-classical analysis can be generalized for quantum systems with n degrees of freedom which correspond to completely integrable classical Hamiltonian systems (see Section 2.6 of Chapter 1). Bohr-Wilson-Sommerfeld quantization rules take the form

$$\oint_\gamma \boldsymbol{p} d\boldsymbol{q} = 2\pi\hbar(n_\gamma + \tfrac{1}{4}\operatorname{ind}\gamma). \tag{6.25}$$

Here integration goes over all 1-cycles γ in the Lagrangian submanifold $\Lambda = \{(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n} : H_c(\boldsymbol{p}, \boldsymbol{q}) = E, F_2(\boldsymbol{p}, \boldsymbol{q}) = E_2, \dots, F_n(\boldsymbol{p}, \boldsymbol{q}) = E_n\}$, and $\operatorname{ind}\gamma$ is the Maslov index of a cycle γ in Λ. For the action-angle variables $(\boldsymbol{I}, \boldsymbol{\varphi})$ the integration in (6.25) goes over the basic 1-cycles on the n-torus T^n, and we obtain quantization conditions $I_i = (n_i + \frac{1}{2})\hbar$, $i = 1, \dots, n$.

7. Notes and references

The classical text [**LL58**] is the source of many basic facts on the Schrödinger equation, written from the physics perspective. The textbook [**Foc78**], another classic, shows meticulous attention to detail. There are numerous mathematics papers and monographs devoted to the different aspects of the Schrödinger equation, and here we mention only the sources being used. For the self-adjointness criteria in Section 1.1 we refer the reader to the encyclopaedia survey [**RSS94**] and to the treatise

[**RS75**], and references therein; in particular, in [**RS75**] one can find the proof that the Schrödinger operator for a complex atom is essentially self-adjoint. For the proof of Sears theorem, see [**BS91**]. Theorems 1.6 and 1.7 (the latter in the special case $V_1 = 0$) in Section 1.2 are proved in [**BS91**] and [**RSS94**]; see [**RS78**] for the proof of Theorem 1.7 in the general case, and for other generalizations. The proof of the Kato theorem can be found in [**RS78**]; see also [**RSS94**]. For the proof of the Birman-Schwinger bound, see [**RS78**]. The monograph [**HS96**], besides the introduction to spectral theory, contains the proofs of many results in Sections 1.1-1.2; see also the monograph [**CFKS08**] for these and other results.

Section 2 is based on the fundamental paper [**Fad64**], classical surveys [**Fad59, Fad74**], and the monograph [**Mar86**], devoted to the inverse scattering problems. For more information and details on the material in Section 2.1 and Problems 2.2, 2.3, 2.4, see [**Fad64**] and [**Mar86**]. The complex integration of the resolvent kernel is a powerful method for proving the eigenfunction expansion theorem, especially in the presence of the absolutely continuous spectrum, and in Section 2.2 we followed the elegant approach from [**Fad59**]; Problem 2.6 is taken from [**Fad74**]. Section 2.3 is based on [**Fad59, Fad64, Fad74**]; see also the monograph [**New02**] for a comprehensive exposition of the scattering theory from the physics perspective, and the recent book [**Yaf92**] for its abstract mathematical formulation. We refer the reader to [**Fad74**] and references therein for more details on the material in Section 2.4.

Section 3 is fairly standard; from a physics point of view, its material can be found in almost any textbook on quantum mechanics; see [**LL58, Foc78**] for a clear exposition. It was H. Weyl who introduced Lie groups into quantum mechanics [**Wey50**], and nowadays representation theory of Lie groups is a part of the theoretical physics curriculum; see, e.g., [**BR86**]. There are also many mathematics textbooks and monographs on representation theory of compact Lie groups; see, e.g., [**Kir76, FH91**], as well as [**Vil68**]. Section 4 contains the standard material presented in any textbook on quantum mechanics; see [**LL58, Foc78, Mes99**] for the physics presentation. Our goal here was precise mathematical formulation of the basic facts; for the proofs of all results in this section (and of the problems as well), and for their generalizations, we refer the reader to the treatise [**RS79**].

The solution of the eigenvalue problem for the hydrogen atom, given by E. Schrödinger in 1926, was the major triumph of quantum mechanics. Before that, the energy levels of the hydrogen atom were obtained by N. Bohr in 1913 using the Bohr model (later replaced by the Bohr-Sommerfeld model and the BWS quantization rules), and in 1926 by W. Pauli by using the quantum Laplace-Runge-Lenz vector. Sections 5.1 and 5.2 are standard and our exposition follows [**LL58, Foc78**]. We started Section 5.3 by presenting Pauli's approach (see [**BR86**] for more details on representation theory). The hidden SO(4) symmetry of the hydrogen atom was discovered by V.A. Fock, and the end of Section 5.3 is based on [**Foc78**] (see

[**BI66a, BI66b**] for more details and for the treatment of the absolutely continuous spectrum).

There exists an extensive literature on semi-classical asymptotics and the WKB method, which we just barely touched on in Section 6. We refer to [**LL58**] and [**Dav76**] for a physics discussion and to [**GS77, BW97**] for a mathematical introduction. Detailed exposition of the one-dimensional WKB method can be found in [**Olv97**] — a reference book on special functions used in this chapter. We refer to the monographs [**MF81**] and [**Ler81**] for the detailed exposition of the much more complicated multi-dimensional WKB method.

Bibliography

[AM78] R. Abraham and J.E. Marsden, *Foundations of mechanics*, Benjamin/Cummings Publishing Co. Inc., Reading, MA, 1978.

[AG93] N.I. Akhiezer and I.M. Glazman, *Theory of linear operators in Hilbert space*, Dover Publications Inc., New York, 1993.

[AHK76] S.A. Albeverio and R.J. Høegh-Krohn, *Mathematical theory of Feynman path integrals*, Lecture Notes in Mathematics, vol. 523, Springer-Verlag, Berlin, 1976.

[AE05] S.T. Ali and M. Engliš, *Quantization methods: a guide for physicists and analysts*, Rev. Math. Phys. **17** (2005), no. 4, 391–490.

[AG83] L. Alvarez-Gaumé, *Supersymmetry and the Atiyah-Singer index theorem*, Comm. Math. Phys. **90** (1983), no. 2, 161–173.

[ASW90] O. Alvarez, I.M. Singer, and P. Windey, *Quantum mechanics and the geometry of the Weyl character formula*, Nuclear Phys. B **337** (1990), no. 2, 467–486.

[Alv95] O. Alvarez, *Lectures on quantum mechanics and the index theorem*, Geometry and quantum field theory (Park City, UT, 1991), IAS/Park City Math. Ser., vol. 1, Amer. Math. Soc., Providence, RI, 1995, pp. 271–322.

[Apo76] T.M. Apostol, *Introduction to analytic number theory*, Undergraduate Texts in Mathematics, Springer-Verlag, New York, 1976.

[Arn89] V.I. Arnol′d, *Mathematical methods of classical mechanics*, Graduate Texts in Mathematics, vol. 60, Springer-Verlag, New York, 1989.

[AG90] V.I. Arnol′d and A.B. Givental′, *Symplectic geometry*, Dynamical systems IV, Encyclopaedia of Mathematical Sciences, vol. 4, Springer-Verlag, Berlin, 1990, pp. 1–136.

[AKN97] V.I. Arnol′d, V.V. Kozlov, and A.I. Neishtadt, *Mathematical aspects of classical and celestial mechanics*, Encyclopaedia of Mathematical Sciences, vol. 3, Springer-Verlag, Berlin, 1997.

[Ati85] M.F. Atiyah, *Circular symmetry and stationary-phase approximation*, Astérisque (1985), no. 131, 43–59, Colloquium in honor of Laurent Schwartz, Vol. 1 (Palaiseau, 1983).

[BI66a] M. Bander and C. Itzykson, *Group theory and the hydrogen atom. Part I*, Rev. Mod. Phys. **38** (1966), 330–345.

[BI66b] ———, *Group theory and the hydrogen atom. Part II*, Rev. Mod. Phys. **38** (1966), 346–358.

[Bar61] V. Bargmann, *On a Hilbert space of analytic functions*, Comm. Pure Appl. Math. **3** (1961), 215–228.

[BR86] A.O. Barut and R. Rączka, *Theory of group representations and applications*, second ed., World Scientific Publishing Co., Singapore, 1986.

[BW97] S. Bates and A. Weinstein, *Lectures on the geometry of quantization*, Berkeley Mathematics Lecture Notes, vol. 8, Amer. Math. Soc., Providence, RI, 1997.

[BFF$^+$78a] F. Bayen, M. Flato, C. Fronsdal, A. Lichnerowicz, and D. Sternheimer, *Deformation theory and quantization. I. Deformations of symplectic structures*, Ann. Physics **111** (1978), no. 1, 61–110.

[BFF$^+$78b] ———, *Deformation theory and quantization. II. Physical applications*, Ann. Physics **111** (1978), no. 1, 111–151.

[Bel87] J.S. Bell, *Speakable and unspeakable in quantum mechanics*, Collected papers on quantum philosophy, Cambridge University Press, Cambridge, 1987.

[Ber61] F.A. Berezin, *Canonical operator transformation in representation of secondary quantization*, Soviet Physics Dokl. **6** (1961), 212–215 (in Russian).

[Ber66] ———, *The method of second quantization*, Pure and Applied Physics, vol. 24, Academic Press, New York, 1966.

[Ber71a] ———, *Non-Wiener path integrals*, Teoret. Mat. Fiz. **6** (1971), no. 2, 194–212 (in Russian), English translation in Theoret. and Math. Phys. **6** (1971), 141–155.

[Ber71b] ———, *Wick and anti-Wick symbols of operators*, Mat. Sb. (N.S.) **86(128)** (1971), 578–610 (in Russian), English translation in Math. USSR Sb. **15** (1971), 577–606.

[Ber74] ———, *Quantization*, Izv. Akad. Nauk SSSR Ser. Mat. **38** (1974), 1116–1175 (in Russian), English translation in Math. USSR-Izv. **78** (1974), 1109–1165.

[Ber87] ———, *Introduction to superanalysis*, Mathematical Physics and Applied Mathematics, vol. 9, D. Reidel Publishing Co., Dordrecht, 1987.

[BS91] F.A. Berezin and M.A. Shubin, *The Schrödinger equation*, Mathematics and its Applications (Soviet Series), vol. 66, Kluwer Academic Publishers Group, Dordrecht, 1991.

[BGV04] N. Berline, E. Getzler, and M. Vergne, *Heat kernels and Dirac operators*, Corrected reprint of the 1992 original, Grundlehren Text Editions, Springer-Verlag, Berlin, 2004.

[BS87] M.Sh. Birman and M.Z. Solomjak, *Spectral theory of selfadjoint operators in Hilbert space*, Mathematics and its Applications (Soviet Series), D. Reidel Publishing Co., Dordrecht, 1987.

[Bis84a] J.-M. Bismut, *The Atiyah-Singer theorems: a probabilistic approach. I. The index theorem*, J. Funct. Anal. **57** (1984), no. 1, 56–99.

[Bis84b] ———, *The Atiyah-Singer theorems: a probabilistic approach. II. The Lefschetz fixed point formulas*, J. Funct. Anal. **57** (1984), no. 3, 329–348.

[Bis85] ———, *Index theorem and equivariant cohomology on the loop space*, Comm. Math. Phys. **98** (1985), no. 2, 213–237.

[BT95] M. Blau and G. Thompson, *Localization and diagonalization: a review of functional integral techniques for low-dimensional gauge theories and topological field theories*, J. Math. Phys. **36** (1995), no. 5, 2192–2236.

[Bry95] R.L. Bryant, *An introduction to Lie groups and symplectic geometry*, Geometry and quantum field theory (Park City, UT, 1991), IAS/Park City Math. Ser., vol. 1, Amer. Math. Soc., Providence, RI, 1995, pp. 5–181.

[BFK91] D. Burghelea, L. Friedlander, and T. Kappeler, *On the determinant of elliptic differential and finite difference operators in vector bundles over S^1*, Comm. Math. Phys. **138** (1991), no. 1, 1–18.

[BFK95] ———, *On the determinant of elliptic boundary value problems on a line segment*, Proc. Amer. Math. Soc. **123** (1995), no. 10, 3027–3038.

[BF60] V.S. Buslaev and L.D. Faddeev, *Formulas for traces for a singular Sturm-Liouville differential operator*, Dokl. Akad. Nauk. SSSR **132** (1960), 13–16 (in Russian), English translation in Soviet Math. Dokl. **1** (1960), 451–454.

[Cam63] R.H. Cameron, *The Ilstow and Feynman integrals*, J. Analyse Math. **10** (1962/1963), 287–361.

[Cra83] M. Crampin, *Tangent bundle geometry for Lagrangian dynamics*, J. Phys. A **16** (1983), no. 16, 3755–3772.

[CFKS08] H.L. Cycon, R.G. Froese, W. Kirsch, and B. Simon, *Schrödinger operators with application to quantum mechanics and global geometry*, Corrected and extended 2nd printing, Texts and Monographs in Physics, Springer-Verlag, Berlin, 2008.

[Dav76] A.S. Davydov, *Quantum mechanics*, International Series in Natural Philosophy, vol. 1, Pergamon Press, Oxford, 1976.

[DEF+99] P. Deligne, P. Etingof, D.S. Freed, L.C. Jeffrey, D. Kazhdan, J.W. Morgan, D.R. Morrison, and E. Witten (eds.), *Quantum fields and strings: a course for mathematicians. Vol. 1, 2*, Amer. Math. Soc., Providence, RI, 1999, Material from the Special Year on Quantum Field Theory held at the Institute for Advanced Study, Princeton, NJ, 1996–1997.

[DF99a] P. Deligne and D.S. Freed, *Classical field theory*, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 137–225.

[DF99b] ———, *Supersolutions*, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 227–355.

[DM99] P. Deligne and J.W. Morgan, *Notes on supersymmetry (following J. Bernstein)*, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 41–97.

[Dik58] L.A. Dikiĭ, *Trace formulas for Sturm-Liouville differential operators*, Uspekhi Mat. Nauk (N.S.) **13** (1958), no. 3(81), 111–143 (in Russian), English translation in Amer. Math. Soc. Transl. (2) **18** (1961), 81–115.

[Dir47] P.A.M. Dirac, *The principles of quantum mechanics*, Clarendon Press, Oxford, 1947.

[DR01] W. Dittrich and M. Reuter, *Classical and quantum dynamics. From classical paths to path integrals*, third ed., Advanced Texts in Physics, Springer-Verlag, Berlin, 2001.

[Dri83] V.G. Drinfel′d, *Constant quasiclassical solutions of the Yang-Baxter quantum equation*, Dokl. Akad. Nauk SSSR **273** (1983), no. 3, 531–535 (in Russian), English translation in Soviet Math. Dokl. **28** (1983), 667–671.

[Dri86] ———, *Quantum groups*, Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI) **155** (1986), 18–49 (in Russian), English translation in J. Soviet Math. **41** (1988), no. 2, 898–915.

[Dri87] ———, *Quantum groups*, Proceedings of the International Congress of Mathematicians, Vol. 1, 2 (Berkeley, Calif., 1986) (Providence, RI), Amer. Math. Soc., 1987, pp. 798–820.

[DFN84] B.A. Dubrovin, A.T. Fomenko, and S.P. Novikov, *Modern geometry — methods and applications. Part I*, Graduate Texts in Mathematics, vol. 93, Springer-Verlag, New York, 1984.

[DFN85] ———, *Modern geometry — methods and applications. Part II*, Graduate Texts in Mathematics, vol. 104, Springer-Verlag, New York, 1985.

[Dyn98] A. Dynin, *A rigorous path integral construction in any dimension*, Lett. Math. Phys. **44** (1998), no. 4, 317–329.

[Enr01] B. Enriquez, *Quantization of Lie bialgebras and shuffle algebras of Lie algebras*, Selecta Math. (N.S.) **7** (2001), no. 3, 321–407.

[Erd56] A. Erdélyi, *Asymptotic expansions*, Dover Publications Inc., New York, 1956.

[EK96] P. Etingof and D. Kazhdan, *Quantization of Lie bialgebras. I*, Selecta Math. (N.S.) **2** (1996), no. 1, 1–41.

[Fad57] L.D. Faddeev, *An expression for the trace of the difference between two singular differential operators of the Sturm-Liouville type*, Dokl. Akad. Nauk SSSR (N.S.) **115** (1957), 878–881 (in Russian).

[Fad59] ———, *The inverse problem in the quantum theory of scattering*, Uspekhi Mat. Nauk **14** (1959), no. 4 (88), 57–119 (in Russian), English translation in J. Math. Phys. **4** (1963), 72–104.

[Fad64] ———, *Properties of the S-matrix of the one-dimensional Schrödinger equation*, Trudy Mat. Inst. Steklov. **73** (1964), 314–336 (in Russian), English translation in Amer. Math. Soc. Transl. (2), Vol. 65: Nine papers on partial differential equations and functional analysis (1967), 139–166.

[Fad74] ———, *The inverse problem in the quantum theory of scattering. II*, Current problems in mathematics, Vol. 3, Akad. Nauk SSSR Vsesojuz. Inst. Naučn. i Tehn. Informacii, Moscow, 1974, pp. 93–180 (in Russian), English translation in J. Soviet Math. **5** (1976), no. 3, 334–396.

[Fad76] ———, *Course 1. Introduction to functional methods*, Méthodes en théorie des champs/Methods in field theory (École d'Été Phys. Théor., Session XXVIII, Les Houches, 1975), North-Holland, Amsterdam, 1976, pp. 1–40.

[Fad98] ———, *A mathematician's view of the development of physics*, Les relations entre les mathématiques et la physique théorique, Inst. Hautes Études Sci., Bures, 1998, pp. 73–79.

[Fad99] ———, *Elementary introduction to quantum field theory*, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 513–550.

[FY80] L.D. Faddeev and O.A. Yakubovskiĭ, *Lectures on quantum mechanics for mathematics students*, Leningrad University Publishers, Leningrad, 1980 (in Russian).

[FS91] L.D. Faddeev and A.A. Slavnov, *Gauge fields. Introduction to quantum theory*, Frontiers in Physics, vol. 83, Addison-Wesley Publishing Company, Redwood City, CA, 1991.

[FT07] L.D. Faddeev and L.A. Takhtajan, *Hamiltonian methods in the theory of solitons*, Reprint of 1987 English edition, Classics in Mathematics, Springer-Verlag, New York, 2007.

[Fey48] R.P. Feynman, *Space-time approach to non-relativistic quantum mechanics*, Rev. Modern Physics **20** (1948), 367–387.

[Fey51] ———, *An operator calculus having applications in quantum electrodynamics*, Physical Rev. (2) **84** (1951), 108–128.

[FH65] R.P. Feynman and A.R. Hibbs, *Quantum mechanics and path integrals*, McGraw Hill, New York, 1965.

[Fla82] M. Flato, *Deformation view of physical theories*, Czechoslovak J. Phys. **B32** (1982), 472–475.

[Foc32] V.A. Fock, *Konfigurationsraum und zweite Quantelung*, Z. Phys. **75** (1932), no. 9-10, 622–647.

[Foc78] ———, *Fundamentals of quantum mechanics*, Mir Publishers, Moscow, 1978.

[Fre99] D.S. Freed, *Five lectures on supersymmetry*, Amer. Math. Soc., Providence, RI, 1999.

[Fuj80] D. Fujiwara, *Remarks on convergence of the Feynman path integrals*, Duke Math. J. **47** (1980), no. 3, 559–600.

[FH91] W. Fulton and J. Harris, *Representation theory*, Graduate Texts in Mathematics, vol. 129, Springer-Verlag, New York, 1991.

[GL53] I.M. Gel′fand and B.M. Levitan, *On a simple identity for the characteristic values of a differential operator of the second order*, Dokl. Akad. Nauk SSSR (N.S.) **88** (1953), 593–596 (in Russian).

[GY56] I.M. Gel′fand and A.M. Yaglom, *Integration in function spaces and its application to quantum physics*, Uspekhi Mat. Nauk (N.S.) **11** (1956), no. 1(67), 77–114, English translation in J. Math. Phys. **1** (1960), 48–69.

[Ger50] Ya.L. Geronimus, *Teoriya ortogonal′nyh mnogočlenov*, Gosudarstv. Izdat. Tehn.-Teor. Lit., Moscow-Leningrad, 1950 (in Russian).

[Gil95] P.B. Gilkey, *Invariance theory, the heat equation, and the Atiyah-Singer index theorem*, second ed., CRC Press, Boca Raton, FL, 1995.

[God69] C. Godbillon, *Géometrie differéntielle et mécanique analytique*, Hermann, Paris, 1969.

[GK69] I.C. Gohberg and M.G. Kreĭn, *Introduction to the theory of linear nonselfadjoint operators*, Translations of Mathematical Monographs, Vol. 18, Amer. Math. Soc., Providence, RI, 1969.

[Gol80] H. Goldstein, *Classical mechanics*, Addison Wesley, 1980.

[GW98] R. Goodman and N.R. Wallach, *Representations and invariants of the classical groups*, Encyclopedia of Mathematics and its Applications, vol. 68, Cambridge University Press, Cambridge, 1998.

[GS77] V. Guillemin and S. Sternberg, *Geometric asymptotics*, Mathematical Surveys, No. 14, Amer. Math. Soc., Providence, RI, 1977.

[GS03] S.J. Gustafson and I.M. Sigal, *Mathematical concepts of quantum mechanics*, Universitext, Springer-Verlag, Berlin, 2003.

[HS96] P.D. Hislop and I.M. Sigal, *Introduction to spectral theory: With applications to Schrödinger operators*, Applied Mathematical Sciences, vol. 113, Springer-Verlag, New York, 1996.

[IM74] K. Itô and H.P. McKean, Jr., *Diffusion processes and their sample paths*, Second printing, corrected, Die Grundlehren der mathematischen Wissenschaften, Band 125, Springer-Verlag, Berlin, 1974.

[IZ80] C. Itzykson and J.B. Zuber, *Quantum field theory*, International Series in Pure and Applied Physics, McGraw-Hill International Book Co., New York, 1980.

[Jim85] M. Jimbo, *A q-difference analogue of $U(\mathfrak{g})$ and the Yang-Baxter equation*, Lett. Math. Phys. **10** (1985), no. 1, 63–69.

[JW28] P. Jordan and E. Wigner, *Über das Paulische Aquivalenzverbot*, Z. Phys. **47** (1928), 631–658.

[Kac59] M. Kac, *Probability and related topics in physical sciences*, Lectures in Applied Mathematics. Proceedings of the Summer Seminar, Boulder, CO, 1957, vol. 1, Interscience Publishers, London-New York, 1959.

[Kac80] ———, *Integration in function spaces and some of its applications*, Lezioni Fermiane, Accademia Nazionale dei Lincei, Pisa, 1980.

[Kaz99] D. Kazhdan, *Introduction to QFT*, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 377–418.

[Kho07] D. Khoshnevisan, *Probability*, Graduate Studies in Mathematics, vol. 80, Amer. Math. Soc., Providence, RI, 2007.

[Kir76] A.A. Kirillov, *Elements of the theory of representations*, Grundlehren der Mathematischen Wissenschaften, Band 220, Springer-Verlag, Berlin, 1976.

[Kir90] ———, *Geometric quantization*, Dynamical systems IV, Encyclopaedia of Mathematical Sciences, vol. 4, Springer-Verlag, Berlin, 1990, pp. 137–172.

[Kir04] ———, *Lectures on the orbit method*, Graduate Studies in Mathematics, vol. 64, Amer. Math. Soc., Providence, RI, 2004.

[KSV02] A.Yu. Kitaev, A.H. Shen, and M.N. Vyalyi, *Classical and quantum computation*, Graduate Studies in Mathematics, vol. 47, Amer. Math. Soc., Providence, RI, 2002.

[Kon03] M. Kontsevich, *Deformation quantization of Poisson manifolds*, Lett. Math. Phys. **66** (2003), no. 3, 157–216.

[Kos77] B. Kostant, *Graded manifolds, graded Lie theory, and prequantization*, Differential geometrical methods in mathematical physics (Proc. Sympos., Univ. Bonn, Bonn, 1975), Lecture Notes in Math., vol. 570, Springer-Verlag, Berlin, 1977.

[Kre62] M.G. Kreĭn, *On perturbation determinants and a trace formula for unitary and self-adjoint operators*, Dokl. Akad. Nauk SSSR **144** (1962), 268–271 (in Russian), English translation in Soviet Math. Dokl. **3** (1962), 707–710.

[LL58] L.D. Landau and E.M. Lifshitz, *Quantum mechanics: non-relativistic theory. Course of Theoretical Physics, Vol. 3*, Pergamon Press Ltd., London-Paris, 1958.

[LL76] L.D. Landau and E.M. Lifshitz, *Mechanics. Course of theoretical physics. Vol. 1*, Pergamon Press, Oxford, 1976.

[Lan87] S. Lang, *Elliptic functions*, second ed., Springer-Verlag, New York, 1987.

[Ler81] J. Leray, *Lagrangian analysis and quantum mechanics*, A mathematical structure related to asymptotic expansions and the Maslov index, MIT Press, Cambridge, MA, 1981.

[LS91] B.M. Levitan and I.S. Sargsjan, *Sturm-Liouville and Dirac operators*, Mathematics and its Applications (Soviet Series), vol. 59, Kluwer Academic Publishers Group, Dordrecht, 1991.

[LV80] G. Lion and M. Vergne, *The Weil representation, Maslov index and theta series*, Progress in Mathematics, vol. 6, Birkhäuser, Boston, MA, 1980.

[Loè77] M. Loève, *Probability theory. I*, fourth ed., Graduate Texts in Mathematics, vol. 45, Springer-Verlag, New York, 1977.

[Loè78] ———, *Probability theory. II*, fourth ed., Graduate Texts in Mathematics, vol. 46, Springer-Verlag, New York, 1978.

[Mac04] G.W. Mackey, *Mathematical foundations of quantum mechanics*, Reprint of the 1963 original, Dover Publications Inc., Mineola, NY, 2004.

[Man97] Y.I. Manin, *Gauge field theory and complex geometry*, second ed., Grundlehren der Mathematischen Wissenschaften, vol. 289, Springer-Verlag, Berlin, 1997.

[Mar86] V.A. Marchenko, *Sturm-Liouville operators and applications*, Operator Theory: Advances and Applications, vol. 22, Birkhäuser Verlag, Basel, 1986.

[Mar59a] J.L. Martin, *The Feynman principle for a Fermi system*, Proc. Roy. Soc. Ser. A **251** (1959), no. 1267, 543–549.

[Mar59b] ———, *Generalized classical dynamics, and the 'classical analogue' of a Fermi oscillator*, Proc. Roy. Soc. Ser. A **251** (1959), no. 1267, 536–542.

[MF81] V.P. Maslov and M.V. Fedoriuk, *Semiclassical approximation in quantum mechanics*, Mathematical Physics and Applied Mathematics, vol. 7, D. Reidel Publishing Co., Dordrecht, 1981.

[Mes99] A. Messiah, *Quantum mechanics*, Dover Publications Inc., Mineola, NY, 1999.

[MP49] S. Minakshisundaram and Å. Pleijel, *Some properties of the eigenfunctions of the Laplace-operator on Riemannian manifolds*, Canadian J. Math. **1** (1949), 242–256.

[Mon52] E.W. Montroll, *Markoff chains, Wiener integrals, and quantum theory*, Comm. Pure Appl. Math. **5** (1952), 415–453.

[Nel59] E. Nelson, *Analytic vectors*, Ann. of Math. (2) **70** (1959), 572–615.

[Nel64] ———, *Feynman integrals and the Schrödinger equation*, J. Math. Phys. **5** (1964), 332–343.

[New02] R.G. Newton, *Scattering theory of waves and particles*, Reprint of the 1982 second edition, with list of errata prepared by the author, Dover Publications Inc., Mineola, NY, 2002.

[Olv97] F.W.J. Olver, *Asymptotics and special functions*, Reprint of the 1974 original, AKP Classics, A K Peters Ltd., Wellesley, MA, 1997.

[PW35] L. Pauling and E.B. Wilson, *Introduction to quantum mechanics. With applications to chemistry*, McGraw-Hill Book Company, New York and London, 1935.

[Rab95] J.M. Rabin, *Introduction to quantum field theory for mathematicians*, Geometry and quantum field theory (Park City, UT, 1991), IAS/Park City Math. Ser., vol. 1, Amer. Math. Soc., Providence, RI, 1995, pp. 183–269.

[RS71] D.B. Ray and I.M. Singer, *R-torsion and the Laplacian on Riemannian manifolds*, Advances in Math. **7** (1971), 145–210.

[RS80] M. Reed and B. Simon, *Methods of modern mathematical physics. I*, Academic Press, New York, 1980.

[RS75] ———, *Methods of modern mathematical physics. II. Fourier analysis, self-adjointness*, Academic Press, New York, 1975.

[RS79] ———, *Methods of modern mathematical physics. III. Scattering theory*, Academic Press, New York, 1979.

[RS78] ———, *Methods of modern mathematical physics. IV. Analysis of operators*, Academic Press, New York, 1978.

[RTF89] N.Yu. Reshetikhin, L.A. Takhtadzhyan, and L.D. Faddeev, *Quantization of Lie groups and Lie algebras*, Algebra i Analiz **1** (1989), no. 1, 178–206 (in Russian), English translation in Leningrad Math. J. **1** (1990), 193–225.

[Ros04] J. Rosenberg, *A selective history of the Stone-von Neumann theorem*, Operator algebras, quantization, and noncommutative geometry, Contemp. Math., vol. 365, Amer. Math. Soc., Providence, RI, 2004, pp. 331–353.

[RSS94] G.V. Rozenblyum, M.Z. Solomyak, and M.A. Shubin, *Spectral theory of differential operators*, Partial differential equations. VII, Encyclopaedia of Mathematical Sciences, vol. 64, Springer-Verlag, Berlin, 1994.

[Rud87] W. Rudin, *Real and complex analysis*, third ed., McGraw-Hill Book Co., New York, 1987.

[Sak94] J.J. Sakurai, *Modern quantum mechanics*, Addison-Wesley Publishing Company, 1994.

[See67] R.T. Seeley, *Complex powers of an elliptic operator*, Singular Integrals (Proc. Sympos. Pure Math., Chicago, IL, 1966), Amer. Math. Soc., Providence, RI, 1967, pp. 288–307.

[STS85] M.A. Semenov-Tian-Shansky, *Dressing transformations and Poisson group actions*, Publ. Res. Inst. Math. Sci. **21** (1985), no. 6, 1237–1260.

[SW76] D.J. Simms and N.M.J. Woodhouse, *Lectures in geometric quantization*, Lecture Notes in Physics, 53, Springer-Verlag, Berlin, 1976.

[Ste83] S. Sternberg, *Lectures on differential geometry*, second ed., Chelsea Publishing Co., New York, 1983.

[Str05] F. Strocchi, *An introduction to the mathematical structure of quantum mechanics. A short course for mathematicians*, Advanced Series in Mathematical Physics, vol. 27, World Sci. Publishing, London-Singapore, 2005.

[Sza00] R.J. Szabo, *Equivariant cohomology and localization of path integrals*, Lecture Notes in Physics. New Series: Monographs, vol. 63, Springer-Verlag, Berlin, 2000.

[Sze75] G. Szegő, *Orthogonal polynomials*, Amer. Math. Soc., Providence, RI, 1975.

[Tak90] L. A. Takhtajan, *Lectures on quantum groups*, Introduction to quantum group and integrable massive models of quantum field theory (Nankai, 1989), Nankai Lectures Math. Phys., World Sci. Publishing, River Edge, NJ, 1990, pp. 69–197.

[Tob56] W. Tobocman, *Transition amplitudes as sums over histories*, Nuovo Cimento (10) **3** (1956), 1213–1229.

[Var04] V.S. Varadarajan, *Supersymmetry for mathematicians: an introduction*, Courant Lecture Notes in Mathematics, vol. 11, New York University Courant Institute of Mathematical Sciences, New York, 2004.

[Vil68] N.Ja. Vilenkin, *Special functions and the theory of group representations*, Translations of Mathematical Monographs, Vol. 22, Amer. Math. Soc., Providence, RI, 1968.

[vN31] J. von Neumann, *Die Eindeutigkeit der Schrödingershen Operatoren*, Mathematische Annalen **104** (1931), 570–578.

[vN96] ———, *Mathematical foundations of quantum mechanics*, Princeton Landmarks in Mathematics, Princeton University Press, Princeton, NJ, 1996.

[Vor05] A.A. Voronov, *Notes on universal algebra*, Graphs and patterns in mathematics and theoretical physics (Stony Brook, NY, 2001), Proc. Sympos. Pure Math., vol. 73, Amer. Math. Soc., Providence, RI, 2005, pp. 81–103.

[Wey50] H. Weyl, *Theory of groups and quantum mechanics*, Dover Publications, New York, 1950.

[Wig59] E.P. Wigner, *Group theory: And its application to the quantum mechanics of atomic spectra*, Pure and Applied Physics, Vol. 5, Academic Press, New York, 1959.

[Wit82a] E. Witten, *Constraints on supersymmetry breaking*, Nuclear Phys. B **202** (1982), no. 2, 253–316.

[Wit82b] ———, *Supersymmetry and Morse theory*, J. Differential Geom. **17** (1982), no. 4, 661–692 (1983).

[Wit99a] ———, *Homework*, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 609–717.

[Wit99b] ———, *Index of Dirac operators*, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 475–511.

[Woo92] N.M.J. Woodhouse, *Geometric quantization*, second ed., Oxford Mathematical Monographs, The Clarendon Press Oxford University Press, New York, 1992.

[Yaf92] D.R. Yafaev, *Mathematical scattering theory. General theory*, Translations of Mathematical Monographs, vol. 105, Amer. Math. Soc., Providence, RI, 1992.

[YI73] K. Yano and S. Ishihara, *Tangent and cotangent bundles: differential geometry*, Pure and Applied Mathematics, No. 16, Marcel Dekker Inc., New York, 1973.

Index