MAT 561 Mathematical Physics II. Quantum Theory

Leon A. Takhtajan

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

E-mail address: `leontak@math.stonybrook.edu`

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Part 1

Quantum Mechanics

LECTURE 1

Observables and states in classical mechanics

1.1. Measurement in classical mechanics

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

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

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

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

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

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

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

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

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

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

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

S4. If $f_1 = \varphi \circ f_2$ with smooth $\varphi : \mathbb{R} \to \mathbb{R}$, then for every Borel subset $E \subseteq \mathbb{R}$,
$$\mu_{f_1}(E) = \mu_{f_2}(\varphi^{-1}(E)).$$

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

$$\mathsf{E}_\mu(\varphi(f)) = \int_{-\infty}^{\infty} \varphi(\lambda) d\mu_f(\lambda). \tag{1.1}$$

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

Assuming that the functional E_μ extends to the space of bounded, piecewise continuous functions on $\mathscr{M}$, and satisfies (1.1) for measurable functions φ, one can recover the distribution function from the expectation values by the formula

$$\mu_f(\lambda) = \mathsf{E}_\mu\left(\theta(\lambda - f)\right), \tag{1.2}$$

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

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

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

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

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

$$E_\mu(f) = \int_{-\infty}^{\infty} \lambda d\mu_f(\lambda) = \int_{\mathscr{M}} f d\mu. \tag{1.3}$$

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

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

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*[2]. All other states are called *mixed states*. A process of measurement in classical mechanics is the correspondence

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

which to every observable $f \in \mathcal{A}$ and state $\mu \in \mathcal{S}$ assigns a probability measure μ_f on $\mathbb{R}$ — a push-forward of the measure $d\mu$ on $\mathscr{M}$ by f. For every Borel subset $E \subseteq \mathbb{R}$ the quantity $0 \leq \mu_f(E) \leq 1$ is the probability that for a system in the state μ the result of a measurement of the observable f is in the set E. The expectation value of an observable f in a state μ is given by (1.3).

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

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

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

Lemma 1.1. *Pure states are the only states in which every observable has zero variance.*

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

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

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

Pure states are used for systems consisting of few interacting particles (say, a motion of planets in celestial mechanics), when it is possible to

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

measure all coordinates and momenta. Mixed states necessarily appear for *macroscopic* systems, when it is impossible to measure all coordinates and momenta[3].

REMARK. As a topological space, the space of states $\mathscr{M}$ can be reconstructed from the commutative algebra $\mathcal{A}$ of classical observables (equipped with the $\mathbb{C}^*$-algebra structure) by using the Gelfand-Naimark theorem. Namely, commutativity of the algebra of observables $\mathcal{A}$ results in its realization as an algebra of functions on the topological space.

1.2. Hamilton's and Liouville's dynamical pictures

There are two equivalent ways of describing the dynamics — the time evolution of a Hamiltonian system $((\mathscr{M}, \{\ ,\ \}), H)$ with the algebra of observables $\mathcal{A} = C^\infty(\mathscr{M})$ and the set of states $\mathcal{S} = \mathscr{P}(\mathscr{M})$. Here we assume that the Hamiltonian phase flow g_t exists for all times, and that the phase space $\mathscr{M}$ carries a volume form dx invariant under the phase flow[4].

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.

LIOUVILLE'S DESCRIPTION OF DYNAMICS. The observables do not depend on time

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

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

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

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

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

Here the Radon-Nikodim derivative $\rho(x) = \dfrac{d\mu}{dx}$ and the 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

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

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

PROBLEM 1.1. Prove formula (1.2).

PROBLEM 1.2. Prove Lemma 1.1.

LECTURE 2

Observables and states in quantum mechanics

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

Still, it is quite remarkable that we can formulate quantum mechanics using the general notions of states, observables, and time evolution, described in Lecture 1! Since commutativity of the algebra of observables $\mathcal{A}$ brings us to the realm of classical mechanics, in order to get a different realization of observables and states we must assume that the $\mathbb{C}^*$-algebra associated with the quantum observables is no longer commutative. A 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!

2.1. Dirac–von Neumann axioms

The following axioms constitute the basis of quantum mechanics.

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

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

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

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

A4. A process of measurement is the correspondence

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

where P_A is a projection-valued measure on $\mathbb{R}$ associated with the self-adjoint operator A. In particular, when $M = P_\psi$ and $\psi \in D(A)$,

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

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.

From the Hilbert-Schmidt decomposition (2.1) we get

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

so that indeed $0 \leq \mu_A(E) \leq 1$.

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

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

[3] Actually a complete lattice.

Of course, for bounded operators this condition is equivalent to

$$AB = BA.$$

Slightly abusing notation[4], we will often write $[A, B] = AB - BA = 0$ for commuting self-adjoint operators A and B. It follows from the spectral theorem that commutativity of self-adjoint operators A and B is equivalent to the commutativity of the unitary operators e^{iuA} and e^{ivB} for all $u, v \in \mathbb{R}$, or to the commutativity of the resolvents

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

for all $\lambda, \mu \in \mathbb{C}$, $\operatorname{Im}\lambda, \operatorname{Im}\mu \neq 0$.

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

$$\mu_{\boldsymbol{A}}(\boldsymbol{E}) = \operatorname{Tr}(\mathsf{P}_{A_1}(E_1) \dots \mathsf{P}_{A_n}(E_n) M), \quad \boldsymbol{E} = E_1 \times \dots \times E_n \in \mathscr{B}(\mathbb{R}^n). \tag{2.3}$$

However, formula (2.3) 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 $\mathsf{P}_{\boldsymbol{A}}(\boldsymbol{E}) = \mathsf{P}_{A_1}(E_1) \dots \mathsf{P}_{A_n}(E_n)$ 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 $0 \leq \mu_{\boldsymbol{A}}(\boldsymbol{E}) \leq 1$ is the probability that for a quantum system in the state M the result of simultaneous measurement of observables $A_1, \dots, A_n$ belongs to $\boldsymbol{E}$.

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

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

2.2. Heisenberg's uncertainty relations

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

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

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

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

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

Proof. It follows from the spectral theorem that

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

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

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

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

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

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

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

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

it is sufficient to prove the inequality

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

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

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

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

The same argument works for the mixed states. $\square$

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

2.3. Dynamics

The set $\mathscr{A}$ of quantum observables does not form an algebra with respect to an operator product[5]. 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 is the *Heisenberg picture* in quantum mechanics, where the states do not depend on time

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

and bounded observables satisfy the *Heisenberg equation of motion*

$$\frac{dA}{dt} = \{H, A\}_\hbar, \quad A \in \mathscr{A}_0, \tag{2.4}$$

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

where

$$\{\ ,\ \}_\hbar = \frac{i}{\hbar}[\ ,\ ] \tag{2.5}$$

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[6].

The Heisenberg equation (2.4) is well defined when $H \in \mathscr{A}_0$. Indeed, let $U(t)$ be a strongly continuous one-parameter group of unitary operators associated with a bounded self-adjoint operator $H/\hbar$,

$$U(t) = e^{-\frac{i}{\hbar}tH}, \quad t \in \mathbb{R}. \tag{2.6}$$

It satisfies the differential equation

$$i\hbar\frac{dU(t)}{dt} = HU(t) = U(t)H, \tag{2.7}$$

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

$$A(t) = U(t)^{-1}AU(t). \tag{2.8}$$

In general, a strongly one-parameter group of unitary operators (2.6), associated with a self-adjoint operator H by the spectral theorem, satisfies differential equation (2.7) only on $D(H)$ in a strong sense, that is, applied to $\varphi \in D(H)$. The quantum dynamics is defined by the same formula (2.8), and in this sense all quantum observables satisfy the Heisenberg equation of motion (2.4). 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.

By Stone's theorem, every strongly-continuous one-parameter group of unitary operators[7] $U(t)$ is of the form (2.6), where

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

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

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

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

We summarize these arguments as the following axiom.

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

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

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

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

Infinitesimally, the evolution of quantum observables is described by the Heisenberg equation of motion (2.4), where the Hamiltonian operator H is the infinitesimal generator of $U(t)$.

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

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

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

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

$$\mathscr{S} \ni M \mapsto M(t) = U_{-t}(M) = U(t)MU(t)^{-1} \in \mathscr{S}. \tag{2.9}$$

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

$$\frac{dM}{dt} = -\{H, M\}_h, \quad M \in \mathscr{S}, \tag{2.10}$$

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

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

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

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

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

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

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

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

i.e., A commutes with $U(t)$. Thus $A \in \mathscr{A}$ is an integral of motion if and only if it commutes with the Hamiltonian H, so that, in agreement with (2.4),

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

This is a quantum analog of the Poisson commutativity property.

It follows from (2.10) that the time evolution of a pure state $M = P_\psi$ is given by $M(t) = P_{\psi(t)}$, where $\psi(t) = U(t)\psi$. Suppose that $\psi \in D(H)$. Since $D(H)$ is invariant under $U(t)$, the vector $\psi(t) = U(t)\psi$ satisfies the *time-dependent Schrödinger equation*

$$i\hbar\frac{d\psi}{dt} = H\psi \tag{2.11}$$

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

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

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

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

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

in agreement with (2.10). The following simple result is fundamental.

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

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

and in this case

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

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

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

PROBLEM 2.1. Prove Lemma 2.1.

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

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

PROBLEM 2.4. Show that if an observable A is such that for every state M the expectation value $\langle A|M(t)\rangle$ does not depend on t, then A is a quantum integral of motion. (This is the definition of integrals of motion in the Schrödinger picture.)

PROBLEM 2.5. Prove Heisenberg uncertainty relation

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

for mixed states.

PROBLEM 2.6. Show that a solution of the initial value problem for the time-dependent Schrödinger equation (2.11) is given by

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

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

PROBLEM 2.7. 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 $H\psi_f = \frac{\hbar}{i}\psi_{f'}$.)

Lecture 3. Quantization

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

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

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

and

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

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

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

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

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

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

3.1. Heisenberg commutation relations

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

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

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

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

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

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

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

Property **CR2** is called the *Heisenberg commutation relation* for one degree of freedom. In terms of the quantum bracket (2.5) it takes the form

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

which is exactly the same as the Poisson bracket (3.1)! 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.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Indeed, it follows from (3.5) that $[\boldsymbol{u}X, \boldsymbol{v}Y] = -\boldsymbol{u}\boldsymbol{v}c$ is a central element, so that using the Baker-Campbell-Hausdorff formula we obtain

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

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

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

It follows from Stone theorem that

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

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

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

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

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

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

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

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

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

3.2. Coordinate and momentum representations

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Physically, this is interpreted that in the state P_ψ with the "wave function" $\psi(q)$, the probability of finding a quantum particle between q and $q + dq$ is $|\psi(q)|^2 dq$. In other words, the modulus square of a wave function is the probability distribution for the coordinate of a quantum particle.

The corresponding momentum operator P is given by a differential operator

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

with $D(P) = W^{1,2}(\mathbb{R})$ — the Sobolev space of absolutely continuous functions f on $\mathbb{R}$ such that f and its derivative f' (defined a.e.) are in $L^2(\mathbb{R})$.

The operator P is self-adjoint and it is straightforward to verify that on $D = C_c^\infty(\mathbb{R})$, the space of smooth functions on $\mathbb{R}$ with compact support,

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

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

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

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

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

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

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

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

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

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

and satisfy the Heisenberg commutation relation. As the coordinate representation, the momentum representation is an irreducible, unitary, integrable representation of the Heisenberg algebra. In the momentum representation, the modulus square of the wave function $\psi(p)$ of a pure state

$M = P_\psi$, $\|\psi\| = 1$, is the probability distribution for the momentum of the quantum particle, i.e., the probability that a quantum particle has momentum between p and $p + dp$ is $|\psi(p)|^2 dp$.

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

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

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

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

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

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

and

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

REMARK. 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 anti-linear isomorphism) by a *bra vector* $\langle\varphi|$, and their inner product by $\langle\varphi|\psi\rangle$. In standard mathematics notation,

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

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

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

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

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

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

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

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

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

LECTURE 4

Schrödinger equation

4.1. Examples of quantum systems

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

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

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

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

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

and in the coordinate representation is

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

where

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

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

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

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

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

The Hamiltonian operator of a Newtonian particle is

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

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

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

have the same form as Hamilton's equations.

In coordinate representation the Hamiltonian is the *Schrödinger operator*

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

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

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

Example 4.3 (Interacting quantum particles). In Hamiltonian formalism a closed classical system of N interacting particles on $\mathbb{R}^3$ is described by the canonical coordinates $\boldsymbol{r} = (\boldsymbol{r}_1, \dots, \boldsymbol{r}_N)$, the canonical momenta $\boldsymbol{p} = (\boldsymbol{p}_1, \dots, \boldsymbol{p}_N)$, $\boldsymbol{r}_a, \boldsymbol{p}_a \in \mathbb{R}^3$, and by the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{r}) = \sum_{a=1}^{N} \frac{\boldsymbol{p}_a^2}{2m_a} + V(\boldsymbol{r}), \tag{4.3}$$

where m_a is the mass of the a-th particle, $a = 1, \dots, N$. The corresponding Hamiltonian operator H in the coordinate representation has the form

$$H = -\sum_{a=1}^{N} \frac{\hbar^2}{2m_a}\Delta_a + V(\boldsymbol{r}). \tag{4.4}$$

In particular, when

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

[2]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.

the Schrödinger operator (4.4) 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 (4.3)

$$H_{\mathrm{c}}(\boldsymbol{P}, \boldsymbol{p}, \boldsymbol{R}, \boldsymbol{r}) = \frac{\boldsymbol{P}^2}{2M} + \sum_{a=1}^{N} \frac{\boldsymbol{p}_a^2}{2m} - \sum_{a=1}^{N} \frac{Ne^2}{|\boldsymbol{R} - \boldsymbol{r}_a|} + \sum_{1 \le a < b \le N} \frac{e^2}{|\boldsymbol{r}_a - \boldsymbol{r}_b|},$$

where $\boldsymbol{P}$ is the canonical momentum of the nucleus. The corresponding Schrödinger operator H in the coordinate representation has the form[3]

$$H = -\frac{\hbar^2}{2M}\Delta - \sum_{a=1}^{N} \frac{\hbar^2}{2m}\Delta_a - \sum_{a=1}^{N} \frac{Ne^2}{|\boldsymbol{R} - \boldsymbol{r}_a|} + \sum_{1 \le a < b \le N} \frac{e^2}{|\boldsymbol{r}_a - \boldsymbol{r}_b|}.$$

In the simplest case of the hydrogen atom, when $N = 1$ and the nucleus consists of a single proton[4], 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

$$H = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|\boldsymbol{r}|}. \tag{4.5}$$

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

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

[3] Ignoring the fact that electron has spin.

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

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

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

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

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

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

The Hamiltonian operator of a quantum particle is

$$H = \frac{1}{2m}\left(\boldsymbol{P} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\varphi(\boldsymbol{r}) \tag{4.6}$$

— 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:

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

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

4.2. Free quantum particle

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

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

is a positive operator with absolutely continuous spectrum $[0, \infty)$ of multiplicity two. Indeed, let $\mathfrak{H}_0 = L^2(\mathbb{R}_{>0}, \mathbb{C}^2; d\sigma)$ be the Hilbert space of $\mathbb{C}^2$-valued measurable functions Ψ on the semi-line $\mathbb{R}_{>0} = (0, \infty)$, which are square-integrable with respect to the measure $d\sigma(\lambda) = \sqrt{\frac{m}{2\lambda}}\, d\lambda$,

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

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

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

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

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

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

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

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

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

The Cauchy problem

$$i\hbar\frac{d\psi(t)}{dt} = H_0\psi(t), \quad \psi(0) = \psi, \tag{4.7}$$

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

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

so that

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

In the coordinate representation, the solution of (4.7) is given by

$$\psi(q,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}pq}\hat{\psi}(p,t)dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\chi(p,q,t)t}\hat{\psi}(p)dp, \tag{4.8}$$

where

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

Formula (4.8) describes the motion of a quantum particle, and admits the following physical interpretation. Let initial condition ψ in (4.7) be such that its Fourier transform $\hat{\psi} = \mathcal{F}_\hbar(\psi)$ is a smooth function supported in a neighborhood U_0 of $p_0 \in \mathbb{R} \setminus \{0\}$, $0 \notin U_0$, and

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

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

$$\lim_{|t|\to\infty} \int_E |\psi(q,t)|^2 dq = 0. \tag{4.9}$$

Since

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

for all t, it follows from (4.9) that the particle leaves every compact subset of $\mathbb{R}$ as $|t| \to \infty$ and the quantum motion is infinite. To prove (4.9), observe that the function $\chi(p,q,t)$ — the "phase" in integral representation (4.8) — has the property that $|\frac{\partial\chi}{\partial p}| > C > 0$ for all $p \in U_0$, $q \in E$ and large enough $|t|$. Integrating by parts we get

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

so that uniformly on E,

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

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

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

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

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

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

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

as $N \to \infty$.

Applying the stationary phase method to the integral representation (4.8) (and setting $N = t$), we find that the critical point of $\chi(p, q, t)$ is $p_0 = \frac{mq}{t}$ with $\chi''(p_0) = -\frac{1}{m} \neq 0$, and

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

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

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

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

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

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

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

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

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

Let $\mathfrak{H}_0^{(n)} = L^2(\mathbb{R}_{>0}, \mathfrak{h}; d\sigma_n)$ be the Hilbert space of $\mathfrak{h}$-valued measurable functions[5] 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

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

is solved by the Fourier transform

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

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

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

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

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

LECTURE 5

Quantum harmonic oscillator

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

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

Hamilton's equations

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

with the initial conditions p_0, q_0 are readily solved,

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

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

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

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

We have

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

so that Hamilton's equations decouple,

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

and are trivially solved,

$$z(t) = e^{-i\omega t} z_0, \quad \bar{z} = e^{i\omega t} \bar{z}_0. \tag{5.6}$$

Here

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

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[1] algebraic and analytic properties.

5.1. Exact solution

Temporarily set $m = 1$ and consider the operators

$$a = \frac{1}{\sqrt{2\omega\hbar}}(\omega Q + iP), \quad a^* = \frac{1}{\sqrt{2\omega\hbar}}(\omega Q - iP), \tag{5.7}$$

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

$$[a, a^*] = I \tag{5.8}$$

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

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

[1] 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.

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 (5.8) 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[2] that the Hamiltonian operator H is self-adjoint.

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

$$[N, a] = -a, \quad [N, a^*] = a^*, \quad [a, a^*] = I. \tag{5.9}$$

Commutation relations (5.9) allow to solve explicitly the Heisenberg equations of motion for the harmonic oscillator. Namely, we have

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

so that

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

Comparing with (5.6) we see that solutions of classical and quantum equations of motion for the harmonic oscillator have the same form!

Next, using commutation relations (5.9) 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 5.1. *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.

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

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

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

(ii) *The vectors*

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

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

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

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

Proof. Rewriting commutation relations (5.9) as

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

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

$$Na^n\psi = (\mu - n)a^n\psi \quad \text{and} \quad N(a^*)^n\psi = (\mu + n)(a^*)^n\psi. \tag{5.10}$$

Since $N \geq 0$ on $D(N)$, it follows from the first equation in (5.10) that there exists $n_0 \geq 0$ such that $a^{n_0}\psi \neq 0$ but $a^{n_0+1}\psi = 0$. Setting $\psi_0 = \dfrac{a^{n_0}\psi}{\|a^{n_0}\psi\|} \in \mathscr{H}$ we get

$$a\psi_0 = 0 \quad \text{and} \quad N\psi_0 = 0. \tag{5.11}$$

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

$$[a, (a^*)^n] = n(a^*)^{n-1}, \tag{5.12}$$

which follow from (5.8) and the Leibniz rule. Using (5.11)-(5.12), we get

$$a^*\psi_n = \sqrt{n+1}\,\psi_{n+1}, \quad a\psi_n = \sqrt{n}\,\psi_{n-1}, \tag{5.13}$$

so that

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

From the second equation in (5.10) it follows that $N\psi_n = n\psi_n$, so ψ_n are normalized eigenvectors of H with the eigenvalues $\hbar\omega(n+\frac{1}{2})$. The eigenvectors ψ_n are orthogonal since the corresponding eigenvalues are distinct and the operator H is symmetric. Finally, part (iii) immediately follows from the fact that, according to part (ii), the subspaces Im $(H \pm iI)|_{\mathscr{H}_0}$ are dense in $\mathscr{H}_0$, which is the criterion of essential self-adjointness. $\square$

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

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

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

so that

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

and

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

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

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

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

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

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

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

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

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

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 5.1. *The Hamiltonian*

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

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

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

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*

$$\psi_n(q) = \sqrt[4]{\frac{m\omega}{\pi\hbar}} \frac{1}{\sqrt{2^n n!}} e^{-\frac{m\omega}{2\hbar}q^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, q\right), \tag{5.14}$$

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

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

5.2. Holomorphic representation

Let

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

be the Hilbert ℓ^2-space. The choice of an orthonormal basis $\{\psi_n\}_{n=0}^{\infty}$ for $L^2(\mathbb{R}, dq)$, given by the eigenfunctions (5.14) of the Schrödinger operator for the harmonic oscillator, establishes the Hilbert space isomorphism $L^2(\mathbb{R}, dq) \simeq \ell^2$,

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

where

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

since the functions ψ_n are real-valued. Using (5.13) we get

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

and

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

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

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

As a result,

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

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

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

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

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

$$(f, g) = \frac{1}{\pi} \int_{\mathbb{C}} f(z)\overline{g(z)} e^{-|z|^2} d^2z, \tag{5.15}$$

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

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

The correspondence

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

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

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

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

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

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

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

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

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

with the kernel

$$U(z,q) = \sum_{n=0}^{\infty} \psi_n(q)f_n(z) = \sqrt[4]{\frac{m\omega}{\pi\hbar}}\, e^{\frac{m\omega}{2\hbar}q^2 - \left(\sqrt{\frac{m\omega}{\hbar}}q - \frac{1}{\sqrt{2}}z\right)^2}. \tag{5.16}$$

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

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

given by

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

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

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

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

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

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

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

and satisfy the commutation relations

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

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

Problem 5.2. Let $q(t) = A\cos(\omega t + \alpha)$ be the classical trajectory of the harmonic oscillator with $m = 1$ and the energy $E = \frac{1}{2}\omega^2 A^2$, 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 5.3. Show that when $n \to \infty$ and $\hbar \to 0$ such that $\hbar\omega(n + \frac{1}{2}) = \frac{1}{2}\omega^2 A^2$ remains fixed, the envelope of the distribution function $|\psi_n(q)|^2$ on the interval $|q| \leq A$ coincides with the classical distribution function $\mu(q)$ from the previous problem. (*Hint:* Prove the integral representation

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

and derive the asymptotic formula

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

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

Problem 5.4. Complete the proof of Theorem 5.1.

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

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