Talking about algebra we always have in mind unital (having unit element) associative algebra over complex numbers with involution denoted by *. (An involution is an antilinear map $A \to A^*$ obeying $A^{**} = A$, $(AB)^* = B^*A^*$.) We assume that the algebra is a topological space and all operations are continuous, but for many of our statements these requirements are not sufficient (one should assume that we have a Banach algebra or C^* -algebra or impose some other conditions). In our terminology an automorphism preserves not only operations in the algebra, but also the involution.

We are saying that h is a derivation of the algebra \mathcal{A} if h(AB) = h(A)B + Ah(B); we assume also that the derivation is compatible with involution. We say that a derivation is an infinitesimal automorphism if the equation $i\frac{dA}{dt} = h(A(t))$ has a solution for all initial data A(0); then a map $A(0) \to A(t)$ specifies an automorphism α_t . It is easy to check that $\alpha_{t+s} = \alpha_t \alpha_s$ (an infinitesimal automorphism generates a one-parameter group of automorphisms). One can consider infinitesimal automorphisms as elements of the Lie algebra of the group of automorphisms. (This Lie algebra should be defined on the vector space of tangent vectors to one-parameter families of automorphisms at the unit element of the group. In infinite-dimensional case it is not clear whether such a vector can be considered also as a tangent vector to a one-parameter group of automorphisms. In what follows we disregard these subtleties.)

0.1 Hamiltonian formalism

The equations of motion of a three-dimensional non-relativistic particle in potential field $U(\vec{x})$ have the form

$$\frac{d\vec{p}}{dt} = -\nabla U$$

where $\vec{p}=m\frac{\vec{dx}}{dt}$ stands for the momentum of the particle. To solve these equations (to find the trajectory of the particle) we should know the initial data: the coordinates and the momenta at some moment of time. One says that the coordinates and the momenta specify the state of our particle at the given moment and that the equations of motion allow us to find the state of the particle at any moment if we know it at one of moments. The equations of motion can be written in the form

$$\frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{x}},$$

$$\frac{\vec{dx}}{dt} = \frac{\partial H}{\partial \vec{p}},$$

where $H = \frac{p^2}{m} + U(\vec{x})$ is called Hamiltonian function (one can say the Hamiltonian function is the energy expressed in terms of momenta and coordinates). Similar equations are valid for any mechanical system, but the number of degrees of freedom (the number of coordinates and momenta) and the Hamiltonian function can be arbitrary. This gives so

called Hamiltonian formalism of mechanics. (In Lagrangian formalism the state is specified by coordinates and velocities).

In Hamiltonian formalism the (pure) state of classical mechanical system (at the time t) is characterized by 2n numbers: $p = (p_1, ..., p_n)$ (generalized momenta) and $q = (q^1, ..., q^n)$ (generalized coordinates). (Together these numbers specify a point of 2n-dimensional space called the phase space of the system).

More generally we can define a state as a probability distribution on the phase space. The set \mathcal{D} of probability distributions is a convex set, the pure states can be identified with extreme points of this set. Every state can be considered as a mixture of pure states. (The mixture of states $\omega_1, ..., \omega_n$ with probabilities $p_1, ..., p_n$ is the state $p_1\omega_1 + ... + p_n\omega_n$. If states are labelled by continuous parameter $\lambda \in \Lambda$ one defines the mixture of the states as an integral $\int \omega(\lambda)\rho(\lambda)d\lambda$ where $\rho(\lambda)$ stands for the density of the probability distribution on Λ . Notice that the definition of mixture can be used for any convex set.)

The evolution of a pure state is governed by Hamiltonian equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \frac{dp}{dt} = -\frac{\partial H}{\partial q},\tag{1}$$

where the function H(p, q, t) is called the Hamiltonian.

$$\frac{d}{dt}\rho(p,q,t) = \{H, \rho(p,q,t)\}. \tag{2}$$

governing the evolution of state (Liouville equation). If U(t) denotes the evolution operator (the operator transforming the state at the moment 0 into the state at the moment t) we can write (2) in the form

$$\frac{d}{dt}U(t) = LU(t)$$

where $L\rho = \{H, \rho\}$. Notice that ρ is in general a generalized function on phase space. To verify (2) it is sufficient to check that for pure states (represented by δ -functions) it is equivalent to (17).

A physical quantity (an observable) can be considered as a real function f(p,q) on the phase space. It follows from the chain rule that

$$\frac{d}{dt}f(p(t),q(t)) = -\frac{\partial f}{\partial p}\frac{\partial H}{\partial a} + \frac{\partial f}{\partial a}\frac{\partial H}{\partial p}.$$
 (3)

One can rewrite (3) in the form

$$\frac{d}{dt}f(p(t),q(t)) = \{f,H\}. \tag{4}$$

It follows that in the case $\{f, H\} = 0$ the expression f(p(t), q(t)) does not depend on time (in other words f is an integral of motion). In particular, if H does not depend on time

the function H(p,q) is an integral of motion. It can be identified with the energy of the system.

Let us denote by \mathcal{A} the set of all complex continuous functions on the phase space considered as an algebra with respect to the conventional addition and multiplication of functions. The formula (4) gives an equation for the evolution in the algebra \mathcal{A} .

Notice that every state ω (considered as a measure on the phase space) specifies a linear functional on \mathcal{A} by the formula $\omega(f) = \int f\omega$. This functional obeys the positivity condition: $\omega(f) \geq 0$ if $f \geq 0$. The evolution of states and the evolution in \mathcal{A} are related by the formula $(\omega(t))(f) = \omega(f(t))$.

0.2 Quantum mechanics. Algebraic approach

The picture of the preceding section can be modified to describe quantum mechanics. The main idea is to allow non-commuting physical quantities.

The starting point is a unital associative algebra \mathcal{A} over complex numbers equipped with an antilinear involution $A \to A^*$ (generalizing complex conjugation in the algebra \mathcal{A} of preceding section).

States are identified with positive linear functionals on \mathcal{A} (linear functional ω is positive if $\omega(A^*A) \geq 0$). We assume that states are normalized, i.e. $\omega(1) = 1$. The set D of normalized states is convex. The extreme points of this set are called pure states. Every state is a mixture of pure states.

Let us denote by Aut the group of automorphisms of the algebra \mathcal{A} commuting with involution. This group naturally acts on states. In quantum system the state depends on time and this dependence can be described by the evolution operator U(t) transforming $\omega(0)$ into $\omega(t)$. This is so called Schrödinger picture; it is equivalent to Heisenberg picture where the elements of \mathcal{A} depend of time, but the states do not depend: $\omega(t)(A) = \omega(A(t))$.

The evolution operator satisfies the equation

$$i\frac{dU}{dt} = H(t)U(t); (5)$$

this equation is equivalent to the equation of motion $i\frac{d\omega}{dt} = H(t)\omega(t)$. Here H(t) stands for an element of Lie algebra of the group Aut (for infinitesimal automorphism). It plays the role of the Hamiltonian of the quantum system. If H does not depend on t the evolution operators obey $U(t+\tau) = U(t)U(\tau)$ (constitute a one-parameter subgroup).

To specify a quantum system we should fix an algebra with involution A and an infinitesimal automorphism H (or a family of infinitesimal automorphisms H(t)). Then the evolution is governed by (5).

In what follows we assume that H does not depend on t unless the dependence on t is explicitly mentioned.

Notice that an infinitesimal automorphism can be considered as a derivation of the algebra \mathcal{A} . However, a derivation specifies a quantum system only if it can be integrated to a one-parameter group of automorphisms.

The textbook form of quantum mechanics corresponds to the case when \mathcal{A} is the algebra of bounded linear operators in Hilbert space \mathcal{E} with involution defined as Hermitian conjugation. The states are specified by density matrices (positive operators with unit trace) by the formula $\omega_K(A) = TrKA$. Pure states correspond to vectors $\Psi \in \mathcal{E}$; proportional vectors specify the same state. If the vector Ψ is normalized the corresponding state is the functional $\langle A\Psi, \Psi \rangle$.

Every unitary operator W determines an automorphism of the algebra with involution \mathcal{A} by the formula $A \to W^{-1}AW$. This correspondence allows us to identify the group Aut with the group of unitary operators and infinitesimal automorphisms with self-adjoint operators. The equation of motion for the density matrix has the form $i\frac{dK}{dt} = HK$ where H is an operator on the space \mathcal{L} of trace class operators in \mathcal{E} defined by the formula $HK = -\hat{H}K + K\hat{H}$ and the equation of motion for the vector $\Psi \in \mathcal{E}$ representing the pure state is $i\frac{d\Psi}{dt} = \hat{H}\Psi$ where \hat{H} is a self-adjoint operator (Hamiltonian). The evolution operator in \mathcal{E} will be denoted by $\hat{U}(t)$; it obeys $i\frac{d\hat{U}}{dt} = \hat{H}\hat{U}$. The evolution operator in \mathcal{L} will be denoted by U(t); it is easy to check that $U(t)K = \hat{U}^{-1}(t)K\hat{U}(t)$.

Notice that in the case at hand pure states have very simple description therefore very often it is convenient to work with pure states and to consider other states as mixtures of pure states. In principle we can work only with pure states for any algebra \mathcal{A} , but in general this is not convenient because the description of pure states is complicated.

For any algebra \mathcal{A} and any state ω we can construct a pre-Hilbert space \mathcal{E} and a representation of \mathcal{A} by operators in this space such that for some cyclic vector $\Phi \in \mathcal{E}$ we have $\omega(A) = \langle \hat{A}\Phi, \Phi \rangle$. (An element $A \in \mathcal{A}$ is represented by operator \hat{A} ; we assume that the map $A \to \hat{A}$ is an algebra homomorphism and is compatible with involution: $\hat{A}^* = (\hat{A})^*$. The vector Φ is cyclic in the following sense: every other vector can be represented in the form $\hat{A}\Phi$ where $A \in \mathcal{A}$.) This construction (GNS-construction) is essentially unique (up to equivalence).

Let us sketch the proof of this theorem. Let us assume that the representation we need is constructed. Let us introduce in \mathcal{A} an inner product by the formula $\langle A,B\rangle=\omega(B^*A)$. It is easy to see that the map $\nu:A\to\mathcal{E}$ sending A to $\hat{A}\Phi$ preserves this inner product. It follows from cyclicity of Φ that this map is surjective; this allows us to identify \mathcal{E} with the quotient of \mathcal{A} with respect to null vectors. (Recall that a null vector is a vector that is orhogonal to all other vectors.) The obvious relation $\nu(BA)=\hat{B}\nu(A)$ allows us to describe our representation in terms of the algebra \mathcal{A} and state ω . Namely we construct \mathcal{E} as \mathcal{A} factorized with respect to null vectors of the inner product $\langle A,B\rangle=\omega(B^*A)$, the operation of the multiplication from the left by A descents to the operator \hat{A} , the unit element of \mathcal{A} corresponds to the vector Φ .

We worked with pre-Hilbert spaces, but we can take a completion of \mathcal{E} to obtain a representation of \mathcal{A} by operators acting in Hilbert space.

We see that every state of \mathcal{A} can be represented by a vector in Hilbert space. However, we cannot consider all states as elements of the same Hilbert space.

If ω is a stationary state (a state invariant with respect to time evolution) then the group U(t) descends to a group $\hat{U}(t)$ of unitary transformations of corresponding space \mathcal{E} . The generator \hat{H} of $\hat{U}(t)$ plays the role of Hamiltonian.

We say that the stationary state ω is a ground state if the spectrum of \hat{H} is non-negative.

This definition agrees with the definition of the ground state in Hilbert space formulation of quantum mechanics. Let us apply the GNS construction to the algebra of bounded operators in Hilbert space \mathcal{E} and to a state represented by a vector $\Phi \in \mathcal{E}$ where Φ is an eigenvector of the Hamiltonian: $\hat{H}\Phi = E\Phi$. Then the space given by GNS construction can be identified with \mathcal{E} and the generator of $\hat{U}(t)$ is equal to $\hat{H} - E$. The condition that Φ is the eigenstate with minimal eigenvalue is equivalent to the positivity of $\hat{H} - E$.

The representation containing the ground state will be called ground state representation. This representation is especially important in quantum field theory: we will consider particles as elementary excitations of ground state.

Let us define the correlation functions in a stationary state ω as functions

$$w_n(t_1,...,t_n) = \omega(A_1(t_1)...A_n(t_n))$$

where $A_1, ..., A_n \in \mathcal{A}$.

The Green functions in the state ω are defined by the formula

$$G_n(t_1,...,t_n) = \omega(T(A_1(t_1)...A_n(t_n))),$$

where T stands for time ordering. It is easy to express them in terms of correlation functions.

The correlation functions in the ground state are called Wightman functions. The properties of particles in quantum field theory can be expressed in terms of these functions and/or corresponding Green functions; the same is true for scattering matrix.

0.3 Classical and quantum

To relate quantum and classical mechanics we consider a family of algebras \mathcal{A}_{\hbar} depending smoothly on the parameter \hbar assuming that for $\hbar=0$ we have a commutative algebra with the product that will be denoted $A\cdot B$. More precisely, we assume that all these algebras are defined on the same vector space, in other words, the addition and multiplication by a number do not depend on \hbar , but the multiplication of elements A,B of the algebra (denoted by $A\cdot_{\hbar}B$) smoothly depends on \hbar . The commutator $[A,B]_{\hbar}=A\cdot_{\hbar}B-B\cdot_{\hbar}A$ vanishes for $\hbar=0$, therefore we can introduce a new operation $\{A,B\}$ (Poisson bracket) using the formula

$$[A, B]_{\hbar} = i\{A, B\}\hbar + O(\hbar^2).$$

It is easy to verify that A_0 (the algebra with commutative multiplication $A \cdot B$ that we have for $\hbar = 0$) with the new operation is Poisson algebra, i.e. the new operation satisfies

the axioms of Lie algebra and

$${A \cdot B, C} = {A, C} \cdot B + A \cdot {B, C}.$$

If there exists an involution $A \to A^*$ compatible with multiplication in all algebras \mathcal{A}_{\hbar} then it is compatible also with Poisson bracket (i.e. the Poisson bracket of two self-adjoint elements is again a self-adjoint element). This statement is one of the reasons why a factor i is included in the definition of the Poisson bracket.

0.4 Quantization. Weyl algebra

We have found that the classical mechanics can be obtained from quantum mechanics in the limit $\hbar \to 0$. Conversely quantum mechanics can be obtained as a deformation of classical mechanics. We can start with Poisson algebra and deform it (this means we would like to construct a family \mathcal{A}_{\hbar} that gives this Poisson algebra in the limit $\hbar \to 0$).

If a Poisson algebra \mathcal{A} is an algebra of polynomial functions on a vector space with coordinates $(u^1, ..., u^n)$ then the Poisson bracket can be written in the form

$$\{A, B\} = \frac{1}{2} \sigma^{kl}(u) \frac{\partial A}{\partial u^k} \frac{\partial B}{\partial u^l}. \tag{6}$$

It specifies a structure of Poisson manifold on the vector space. (Here $\{u^k, u^l\} = \sigma^{kl}(u)$.)

Let us consider the case when the Poisson bracket on polynomial functions on vector space is defined by the formula (6) with constant coefficients σ^{kl} . Moreover, we assume that the matrix σ^{kl} is non-degenerate, then dimension of the vector space is necessarily even. (This is the situation of Section 1.) Then we can define the algebra \mathcal{A}_{\hbar} as a unital associative algebra with generators \hat{u}^k and relations $\hat{u}^k \hat{u}^l - \hat{u}^l \hat{u}^k = i \sigma^{kl}$. This algebra is called Weyl algebra. If the coordinates u^k are considered as real numbers we introduce an involution in Weyl algebra requiring that the generators \hat{u}^k are self-adjoint. If the Poisson bracket is written in the form (??) (we always can write it in this form changing coordinates) then the Weyl algebra is generated by self-adjoint elements $(\hat{p}_1,...,\hat{p}_n,\hat{q}^1,...,\hat{q}^n)$ with relations $\hat{p}_k \hat{p}_l = \hat{p}_l \hat{p}_k, \hat{q}^k \hat{q}^l = \hat{q}^l \hat{q}^k, \hat{p}_k \hat{q}^l - \hat{q}^l \hat{p}_k = \frac{\hbar}{i} \delta_k^l$. These relations are called canonical commutation relations (CCR). Instead of self-adjoint generators $(\hat{p}_1,...,\hat{p}_n,\hat{q}^1,...,\hat{q}^n)$ one can consider generators a_k,a_k^* where $a_k=\frac{1}{\sqrt{2}}(\hat{q}^k+i\hat{p}_k),a_k^*=\frac{1}{\sqrt{2}}(\hat{q}^k-i\hat{p}_k)$. These generators satisfy relations $a_k a_l = a_l a_k, a_k^* a_l^* = a_l^* a_k^*, a_k a_l^* - a_l^* a_k = \hbar \delta_{kl}$. These relations are also called CCR. To say that the family of algebras \mathcal{A}_{\hbar} can be considered as a deformation of the commutative polynomial algebra we should realize their elements as polynomials. This can be done in many different ways. For example, we can notice that using CCR we are able to move all operators \hat{q}^k to the left and all operators \hat{p}_k to the right; "removing hats" in the expression we get we obtain a polynomial called (q-p) symbol of the element of Weyl algebra. This representation of elements Weyl algebra by polynomials does not agree with involution ((q-p)-symbol of self-adjoint element is not necessarily real), however,

it is easy to modify the construction to avoid this drawback. For example, one can write down an element of Weyl algebra in terms of generators a_k , a_k^* and use CCR to move a_k^* to the left and a_k to the right. The expression we get is called normal form of the element of Weyl algebra. Considering a_k , a_k^* in the normal form as complex variables we obtain a polynomial called Wick symbol.

We can go in opposite direction and obtain an element of Weyl algebra from a polynomial. This operation is called quantization. Quantization allows us, for example, to obtain quantum Hamiltonian from classical Hamiltonian. It is important to notice that the quantization depends on the choice of symbol (we have "ordering ambiguity"). However, for some classical Hamiltonians there exists a natural choice of corresponding quantum Hamiltonians. In particular, this is true for Hamiltonians represented as a sum of kinetic energy expressed as a function of momenta and potential energy depending on coordinates (no ordering ambiguity).

0.5 Stationary states

A state that does not depend on time is called stationary state. In what follows we work in the formalism where the states are described by density matrices in Hilbert space \mathcal{E} . The state represented by a density matrix K is stationary if K obeys HK=0 i.e. if K commutes with the Hamiltonian \hat{H} . (Recall that H acts as a commutator with \hat{H} .) An important particular case of stationary state is the Gibbs state $K=Z^{-1}e^{-\beta\hat{H}}$ where $Z=Tre^{-\beta\hat{H}}$. This state corresponds to the equilibrium state with the temperature $T=\beta^{-1}$. It tends to the ground state as $T\to 0$.

Let us assume that the operator \hat{H} has discrete spectrum with orthonormal basis ϕ_n of eigenvectors with eigenvalues E_n . Then it is convenient to work in representation where \hat{H} is represented by a diagonal matrix with entries E_n (it is called \hat{H} - representation). In this representation the eigenvectors of the operator H in the space \mathcal{L} are matrices ψ_{mn} having only one non-zero entry equal to 1 in the position (m,n). Alternatively one can define ψ_{mn} as an operator acting by the formula $\psi_{mn}x = \langle x, \phi_n \rangle \phi_m$ where $x \in \mathcal{E}$. Corresponding eigenvalues are $E_m - E_n$. We see that the vectors ϕ_n and the corresponding density matrices ψ_{nn} are stationary states. It follows that all diagonal density matrices in \hat{H} -representation are stationary states. Moreover, if the spectrum is simple all stationary states are represented by diagonal matrices.

A density matrix K_0 represents a ground state if $Tr\hat{H}K_0 \leq Tr\hat{H}K$ for any density matrix K. If the ground state is unique it is necessarily pure and corresponds to the eigenfunction of \hat{H} with lowest eigenvalue.

0.6 Adiabatic approximation

Let us consider the case of slowly varying Hamiltonian $\hat{H}(t)$. We will assume that the energy levels $E_n(t)$ are distinct and vary continuously with t, corresponding eigenvectors

will be denoted by $\phi_n(t)$. We assume that these eigenvectors constitute an orthonormal system. Then it is easy to prove that in the first approximation the evolution operator $\hat{U}(t)$ transforms eigenvector into eigenvector:

$$\hat{U}(t)\phi_n(0) = e^{-i\alpha_n(t)}\phi_n(t), \frac{d\alpha_n(t)}{dt} = E_n(t)$$
(7)

To verify (7) we check that the RHS satisfies the equation of motion up to terms that are small for slow varying $\hat{H}(t)$ (see section 16 for more detail).

Let us introduce the operators $\psi_{mn}(t)$ by the formula $\psi_{mn}(t)x = \langle x, \phi_n(t)\rangle\phi_m(t)$. (These operators are eigenvectors of the operator H(t) in the space \mathcal{L} .) Applying (7) or analyzing directly the evolution operator U(t) in \mathcal{L} we obtain that U(t) transforms eigenvector into eigenvector:

$$U(t)\psi_{mn}(0) = e^{-i\beta_{mn}(t)}\psi_{mn}(t), \frac{d\beta_{mn}(t)}{dt} = E_m(t) - E_n(t)$$
 (8)

(this equation is true up to terms that can be neglected for slowly varying Hamiltonian). Notice that β_{mm} does not depend on t.

0.7 Decoherence

Let us consider a quantum system (atom, molecule, etc) described by a Hamiltonian \hat{H} with simple discrete spectrum. We assume that the system is "almost closed" in the following sense: the interaction with the environment can be described as adiabatic change of the Hamiltonian \hat{H} . Let us consider the evolution operator U(T) assuming that $\hat{H}(0) = \hat{H}(T)$. If the Hamiltonian is time-independent than for the eigenvector ϕ_n with the eigenvalue E_n we can say that $\hat{U}(T)\phi_n = C_n(T)\phi_n$ where $C_n(T) = e^{-iE_nT}$. If the Hamiltonian is slowly changing we have the same formula with $C_n(T)$ calculated from (7). Hence if we started with pure stationary state we remain in the same state. Similarly, $U(T)\psi_{mn} = C_{mn}(T)\psi_{mn}$ and the phase factor is constant for m=n.

It is natural to assume that the environment is random (the time-dependent Hamiltonian depends on some parameters $\lambda \in \Lambda$ with some probability distribution on Λ , then for $m \neq n$ we have a random phase factor $C_{mn}(\lambda,T)$. If we start with density matrix $K = \sum k_{mn} \psi_{mn}$ (with matrix entries k_{mn} in \hat{H} -representation) then the density matrix $K_{\lambda}(T)$ is equal to $\sum C_{mn}(\lambda,T)k_{mn}\psi_{mn}$, i.e. the matrix entries acquire phase factor $C_{mn}(\lambda,T)$. Now we should take the mixture $\bar{K}(T)$ of states $K_{\lambda}(T)$ (this means that we should take the average of phase factors). It is obvious that non-diagonal entries of $\bar{K}(T)$ are smaller by absolute value than corresponding entries of K. Imposing some mild conditions on the probability distribution on K0 one can prove that the non-diagonal entries of K1 tend to zero as K2. In other words the matrix K3 can be considered as a mixture of pure states, corresponding to the vectors K3 with probabilities K4.

This phenomenon is known as decoherence.

0.8 Observables and probabilities

Until now we did not relate the formalism of quantum mechanics to experiment. We know that (at least in some cases) quantum mechanics can be considered as a deformation of classical mechanics therefore one can conjecture that classical observables correspond to quantum observables. In particular, remembering that the energy, that is represented by Hamiltonian function, is an integral of motion if the system is invariant with respect to time shift should have quantum analog with similar properties. This is mot quite true: quantum system does not have a definite energy and measuring its energy by means of macroscopic device we obtain different values of energy with some probabilities. (A similar thing happens when we are trying to use a thermometer to measure the temperature of a system that is out of equilibrium. Such a system does not have a temperature, but still we can measure it; thermometer readings will be different, but we will obtain some probability distribution of these readings.) The interaction with macroscopic device leads to decoherence (the non-diagonal matrix entries of the density matrix K in \hat{H} - representation die) and we obtain a mixture of pure states with probabilities k_{nn} . If the density matrix K corresponds to a pure state described by a vector ϕ in \mathcal{E} then in general decoherence leads to mixture of pure states corresponding to the vectors ϕ_n with probabilities $p_n = |\langle \phi, \phi_n \rangle|^2$. However, if ϕ coincides with one of eigenfunction ϕ_k all probabilities p_n vanish except $p_k = 1$. Therefore we say that an eigenfunction of H with eigenvalue E has definite value of energy equal to E. For any other normalized vector ϕ we can speak only about a probability to get some value E measuring the energy. This probability is non-zero only for eigenvalues E_n of H; it is equal to $p_n = |\langle \phi, \phi_n \rangle|^2$. For a state represented by density matrix K the probability is given by the formula $p_n = \langle K\phi_n, \phi_n \rangle$.

Other observables are represented by self-adjoint operators; the formulas we have written for energy remain valid for any observable. Again if the physical quantity A is represented by self-adjoint operator \hat{A} in \mathcal{E} the quantity A has definite value a if a state is represented by a eigenvector of \hat{A} with eigenvalue a. Otherwise we can talk only about probabilities. It is convenient to write the density matrix K representing a state in \hat{A} -representation; if the operator \hat{A} has simple discrete spectrum the probabilities are equal to the diagonal entries of K in \hat{A} -representation.

In general case we can specify the probability distribution of the observable A by the formula

$$\overline{f(A)} = TrKf(\hat{A}) \tag{9}$$

where f stands for any piecewise continuous function and $\overline{f(A)} = \int f(a)\rho(a)da$ denotes the mean value of f(A) with respect the probability distribution $\rho(a)da$. (It is called also the expectation value of f(A).) If the operator \hat{A} has simple discrete spectrum (9) is equivalent to the formulas for probabilities we gave in this case.

If $\hat{A}_1,...,\hat{A}_n$ are commuting self-adjoint operators one can define the joint probability distribution of corresponding physical quantities $A_1,...,A_n$ using the formula

$$\overline{f(A_1, ..., A_n)} = TrKf(\hat{A}_1, ..., \hat{A}_n). \tag{10}$$

More generally, if quantum mechanical system is specified by C^* -algebra \mathcal{A} and a state by a positive functional ω then the joint probability distribution of physical quantities $A_1, ..., A_n$ is given by the formula

$$\overline{f(A_1, ..., A_n)} = \omega(f(\hat{A}_1, ..., \hat{A}_n)).$$
 (11)

(Physical quantities A_i correspond to self-adjoint elements \hat{A}_i of \mathcal{A} . The assumption that \mathcal{A} is a C^* -algebra guarantees that the notion of a function of a family of commuting self-adjoint elements makes sense.)

0.9 Integrals of motion

One can work either in Schrödinger picture when states are time-dependent, but observables do not depend on time or in Heisenberg picture where states do not depend on time, but the observables do. These pictures are equivalent:

$$TrK(t)f(\hat{A}) = TrKf(\hat{A}(t))$$

if $\hat{A}(t)$ obeys the Heisenberg equation

$$i\frac{d\hat{A}}{dt} = [\hat{H}, \hat{A}].$$

This implies that the observable \hat{A} commuting with the Hamiltonian \hat{H} is an integral of motion (corresponding probabilities do not depend on time.

Let us suppose that we have a one-parameter family U(t) of symmetries of the system. (A symmetry is an automorphism preserving the equations of motion. In our case we consider it as a unitary operator, commuting with the Hamiltonian.) The operator $i\frac{dU}{dt}$ is an integral of motion - a self-adjoint operator commuting with the Hamiltonian.

The Hamiltonian itself is an integral of motion corresponding to the time translation. We have noticed already that the corresponding observable is energy.

The integrals of motion corresponding to invariance with respect to spatial translations are component of momentum.

The integral of motion corresponding to the invariance with respect to rotation around some axis is a component of angular momentum.

0.10 Weyl and Clifford algebras

In quantum theory in algebraic approach we are starting with a unital associative algebra with involution. We have seen already that a natural candidate for this algebra is Weyl

algebra. Im this section we will study this algebra and its cousin, Clifford algebra. Recall that the Weyl algebra is generated by self-adjoint elements \hat{p}_i , \hat{q}^i with relations

$$\hat{p}_k \hat{p}_l = \hat{p}_l \hat{p}_k, \hat{q}^k \hat{q}^l = \hat{q}^l \hat{q}^k, \hat{p}_k \hat{q}^l - \hat{q}^l \hat{p}_k = \frac{1}{i} \delta_k^l.$$
 (12)

These relations are called canonical commutation relations (CCR). Instead of self-adjoint generators $\hat{p}_i, ..., \hat{q}^i$ one can consider generators a_k, a_k^* where $a_k = \frac{1}{\sqrt{2}}(\hat{q}^k + i\hat{p}_k), a_k^* = \frac{1}{\sqrt{2}}(\hat{q}^k - i\hat{p}_k)$. These generators satisfy relations

$$a_k a_l = a_l a_k, a_k^* a_l^* = a_l^* a_k^*, a_k a_l^* - a_l^* a_k = \delta_{kl}.$$
(13)

Both (12) and (13) are called CCR.

For finite number of degrees of freedom there exists only one irreducible representation of CCR. The relations (12) can be represented in the space $L^2(\mathbb{R}^n)$ by operators of multiplication and differentiation : $\hat{q}^k \psi(q^1,...,q^n) = q^k \psi(q^1,...,q^n), \hat{p}_k \psi(q^1,...,q^n) = \frac{1}{i} \frac{\partial}{\partial q^k} \psi(q^1,...,q^n)$. In non-relativistic quantum mechanics this representation is very convenient. If the classical Hamiltonian has the form T(p) + V(q) where the kinetic energy T(p) is a quadratic function of momenta and the potential energy V(q) has a non-degenerate minimum then in a neighborhood of this minimum the classical system can be approximated by multidimensional harmonic oscillator. Similarly for the quantized Hamiltonian $\hat{H} = T(\hat{p}) + V(\hat{q})$ we can approximate low energy levels as energy levels of quantum oscillator. The Hamiltonian of one-dimensional quantum oscillator can be written in the form

$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{\hat{q}^2}{2} = a^* a + \frac{1}{2}.$$

Noticing that $\hat{H}a^* = a^*(\hat{H}+1)$, $\hat{H}a = a(\hat{H}-1)$ we obtain that the operator a^* transforms an eigenfunction ϕ with eigenvalue E in an eigenfunction with eigenvalue E+1. Similarly, the operator a either sends ϕ to zero (if ϕ is the ground state) or to an eigenfunction with eigenvalue E-1. Using this fact we can check that the ground state θ has energy $\frac{1}{2}$ and the states $\frac{1}{\sqrt{n!}}(a^*)^n\theta$ constitute an orthonormal basis consisting of eigenfunctions of \hat{H} with eigenvalues $n+\frac{1}{2}$.

In appropriate coordinates the Hamiltonian of multidimensional quantum oscillator can be considered as a sum of non-interacting one-dimensional oscillators:

$$\hat{H} = \sum (\omega_k a_k^* a_k + \frac{\omega_k}{2});$$

again applying many times operators a_k^* to the ground state θ we obtain a basis of eigenfunctions.

We see that it is convenient to use the operators a_k^* , a_k in the analysis of excitations of the ground state. In quantum field theory we are interested first of all in excitations of ground state; this is one of many reasons why these operators are so useful.

Let us consider now the Weyl algebra with infinite number of generators. This notion can be made precise in different ways. We can consider simply an algebra with infinite number of generators obeying (13), but it is more convenient to start with some (pre)Hilbert space \mathcal{B} and to consider an algebra with generators a(f), $a^*(f)$ and relations

$$a(\lambda f + \mu g) = \lambda a(f) + \mu a(g), a^*(f) = (a(f))^*,$$

$$a(f)a(g) = a(g)a(f), a^*(f)a^*(g) = a^*(g)a^*(f), a(f)a^*(g) - a^*(g)a(f) = \langle f, g \rangle.$$
(14)

A representation of Weyl algebra (= representation of CCR) is a family of operators in a (pre)Hilbert space obeying (14). (Notice that we use the same notation for elements of Weil algebra and for operators.)

If $\mathcal{B} = l^2$ then $a(f) = \sum f_k a_k$, $a^*(f) = \sum \bar{f}_k a_k^*$ where a_k , a_k^* obey (13). If \mathcal{B} is some space of test functions on \mathbb{R}^n (for example, the Schwartz space) we can say that the formal expression $a(f) = \int f(x) a(x) dx$ specifies a(x) as a generalized operator function on \mathbb{R}^n . We can use these notation and terminology also in other cases when \mathcal{B} is a space of functions on some set.

The theory of Weyl algebra is very similar to the theory of Clifford algebra (an algebra that is defined by canonical anticommutation relations (CAR) where commutators are replaced by anticommutators). The representations of Clifford algebra are called also representations of CAR.

In the simplest form Clifford algebra can be defined as an algebra with generators obeying

$$a_k a_l = -a_l a_k, a_k^* a_l^* = -a_l^* a_k^*, a_k a_l^* + a_l^* a_k = \delta_{kl}.$$
(15)

More generaly, to define the Clifford algebra we start with some (pre)Hilbert space \mathcal{B} and consider an algebra with generators $a(f), a^*(f)$ and relations

$$a(\lambda f + \mu g) = \lambda a(f) + \mu a(g), a^*(f) = (a(f))^*,$$

$$a(f)a(g) = -a(g)a(f), a^*(f)a^*(g) = -a^*(g)a^*(f), a(f)a^*(g) + a^*(g)a(f) = \langle f, g \rangle.$$
(16)

Notice that both Weyl and Clifford algebras can be extended in various ways (for example one can introduce some norm and consider a completion with respect to this norm).

Weyl algebra or Clifford algebra (or tensor product of these algebras) can play the role of the algebra with involution \mathcal{A} in the algebraic description of quantum system. In this description we need also an infinitesimal automorphism H of the algebra. The simplest way to construct it is to take a self-adjoint element h of the algebra and to define a derivation by the formula HA = [h, A]. (This construction works for any algebra; derivations obtained this way are called inner derivations. In C^* -algebra one can prove that an inner derivation is an infinitesimal automorphism considering e^{ith} .) If the algebra is generated by a_k, a_k^* obeying (13) or (15) the element h can be represented in normal form (where a_k are from

the right) by means of finite sum:

$$h = \sum_{mn} \sum_{k_1, \dots, k_m, l_1, \dots, l_n} \Gamma_{k_1, \dots, k_m, l_1, \dots, l_n} a_{k_1}^* \dots a_{k_m}^* a_{l_1} \dots a_{l_n}.$$

$$(17)$$

Here $\Gamma_{k_1,\dots,k_m,l_1,\dots,l_n}=\bar{\Gamma}_{l_n,\dots,l_1,k_m,\dots,k_1}$ (this condition guarantees that h is self-adjoint).

In the case of infinite number of generators one can modify this construction to obtain other infinitesimal automorphisms. Namely, we can consider (17) as a formal expression; if the expressions $[a_k, h]$, $[a_k^*, h]$ can be regarded as elements of \mathcal{A} these formulas specify a derivation of algebra. This happens if for every k there exists only a finite number of summands in (17) where one of indices is equal to k. (Then only a finite number of terms survives in the commutator.) To check that the derivation specifies a one-parameter family of automorphism we should verify that the equations of motion $i\frac{da_k}{dt} = [a_k, h], i\frac{a_k^*}{dt} = [a_k^*, h]$ have a solution. If h is a quadratic hamiltonian the equations of motion are linear and the solution is the same as in classical theory. If h is a sum of quadratic Hamiltonian and a summand multiplied by a parameter g then it is easy to prove can be solved in the framework of perturbation theory with respect to g.

For example, we can take $h = \sum \epsilon_k a_k^* a_k$. Then we obtain an infinitesimal automorphism leading to well defined equations of motion

$$i\frac{da_k}{dt} = -\epsilon_k a_k, i\frac{da_k^*}{dt} = \epsilon_k a_k^*.$$

If $\epsilon_k \geq 0$ the ground state representation is in this case the Fock representation (the representation containing a cyclic vector θ obeying $a_k\theta=0$). To prove this fact we notice that in the space of Fock representation (Fock space) we have an orthogonal basis of eigenvectors $(a_1^*)^{n_1}...(a_k^*)^{n_k}...\theta$ with eigenvalues $\sum \epsilon_k n_k$. Here $n_k=0,1,2,...$ in the case of CCR and $n_k=0,1$ in the case of CAR, only finite number of n_k does not vanish.

If $\epsilon_k < 0$ for some k then in the case of CCR the ground state does not exist. Let us consider the case of CAR. Let us denote by N the set of indices k where $\epsilon_k < 0$. If N is finite one can find ground state Φ in the same Fock space: it it obeys the conditions $a_k \Phi = 0$ for $k \notin N$, and $a_k^* \Phi = 0$ for $k \in N$. If N is infinite we should introduce new system of generators satisfying the same relations (make canonical transformation): $b_k = a_k, b_k^* = a_k^*$ for $k \notin N$, $b_k = a_k^*, b_k^* = a_k$ for $k \in N$. Then the ground state θ' lies in the Fock space constructed by means of b_k, b_k^* and obeys $b_k \theta' = 0$.

The above statements can be easily generalized in various directions. In particular, one can work with algebras defined by relations (14) or (16). Then the Fock representation can be defined as a representation in a (pre)Hilbert space \mathcal{F} that contains a cyclic vector θ obeying $a(f)\theta = 0$. If \mathcal{B} consists of functions on \mathcal{M} we can write formally $a(f) = \int f(k)a(k)dk$ (integration over \mathcal{M}) and consider $a(k), a^*(k)$ as generalized functions on \mathcal{M} .

The equations of motion

$$i\frac{da(k)}{dt} = -\epsilon(k)a(k), i\frac{da^*(k)}{dt} = \epsilon(k)a^*(k)$$
(18)

are coming from the formal Hamiltonian $\int \epsilon(k)a^*(k)a(k)dk$.

Again in the case $\epsilon(k) \geq 0$ the Fock representation is the ground state representation and the vector θ is the ground state. The formal Hamiltonian becomes a self-adjoint operator in Fock space.

More generally any quadratic Hamiltonian leads to linear classical equations of motion that can be considered also as quantum equations of motion. This is true for example for Klein-Gordon equation and for Dirac equation. To construct the ground state representation one should change variables to write the equations in the form (18) where a, a^* obey CCR or CAR.

If a formal Hamiltonian is represented as $H_0 + V$ where H_0 is a quadratic Hamiltonian then in good situations not only H_0 but also the full Hamiltonian is a well defined self-adjoint operator in the ground state representation of H_0 . If we started with a translation-invariant Hamiltonian without ultraviolet divergences then usually we obtain a "good" Hamiltonian after the volume cutoff (infrared cutoff). We can calculate Wightman functions of "good" Hamiltonian (at least in the framework of perturbation theory.) Then taking the limit of Wightman functions as the volume tends to infinity we obtain Wightman functions of the original Hamiltonian (these construction can be considered as a definition of Wightman functions). Finally using Wightman functions and an analog of GNS construction we can construct the ground state representation of the original formal Hamiltonian and of Heisenberg operators in this space. The Heisenberg operators satisfy the equations of motion coming from the formal Hamiltonian. We say that we have obtained an operator realization of formal Hamiltonian (see section 44 for more detail).

0.11 Quantum field theory in algebraic approach

Quantum field theory can be considered as a particular case of quantum mechanics.

To define quantum field theory on d-dimensional space (on (d+1)-dimensional space -time) we assume that the group of space-time translations acts on the algebra of observables. We can say that quantum field theory is quantum mechanics with action of commutative Lie group on the algebra of observables \mathcal{A} . In other words, we assume that operators $\alpha(\mathbf{x},t)$ where $\mathbf{x} \in \mathbb{R}^d$, $t \in \mathbb{R}$ are automorphisms of \mathcal{A} preserving the involution and that $\alpha(\mathbf{x},t)\alpha(\mathbf{x}',t')=\alpha(\mathbf{x}+\mathbf{x}',t+t')$. We will use the notation $A(\mathbf{x},t)$ for $\alpha(\mathbf{x},t)A$ where $A \in \mathcal{A}$.

The action of translation group on \mathcal{A} induces the action of this group on the space of states.

Let us consider now a state ω that is invariant with respect to translation group. We will define (quasi) particles as "elementary excitations" of ω . (If ω is the ground state one

uses the word "particles", if ω is an equilibrium state we are talking about thermal quasiparticles.) To consider collisions of (quasi)particles we should require that ω satisfies the cluster property in some sense. Instead of cluster property one can impose a condition of asymptotic commutativity of the algebra $\mathcal{A}(\omega)$ that consists of operators \hat{A} corresponding to the elements $A \in \mathcal{A}$ in GNS construction. In other words one can require that the commutator $[\hat{A}(\mathbf{x},t),\hat{B}]$ where $A,B\in\mathcal{A}$ is small for $\mathbf{x}\to\infty$.

The weakest form of cluster property is the following condition

$$\omega(A(\mathbf{x},t)B) = \omega(A)\omega(B) + \rho(\mathbf{x},t) \tag{19}$$

where $A, B \in \mathcal{A}$ and ρ in some sense is small for $\mathbf{x} \to \infty$.. For example we can impose the condition that $\int |\rho(\mathbf{x},t)| d\mathbf{x} < c(t)$ where c(t) has at most polynomial growth. Notice that (19) implies asymptotic commutativity in some sense: $\omega([A(\mathbf{x},t),B])$ is small for $\mathbf{x} \to \infty$.

To formulate more general cluster property we introduce the notion of correlation functions in the state ω :

$$w_n(\mathbf{x}_1, t_1, ... \mathbf{x}_n, t_n) = \omega(A_1(\mathbf{x}_1, t_1) \cdots A_n(\mathbf{x}_n, t_n)).$$

where $A_i \in \mathcal{A}$. They generalize Wightman functions of relativistic quantum field theory. We consider corresponding truncated correlation functions $w_n^T(\mathbf{x}_1, t_1, ... \mathbf{x}_n, t_n)$.

We have assumed that the state ω is translation-invariant; it follows that both correlation functions and truncated correlation functions depend on differences $\mathbf{x}_i - \mathbf{x}_j$, $t_i - t_j$. We say that the state ω has cluster property if the truncated correlation functions are small for $\mathbf{x}_i - \mathbf{x}_j \to \infty$. A strong version of cluster property is the assumption that the truncated correlation function tends to zero faster than any power of $||\mathbf{x}_i - \mathbf{x}_j||$. Than its Fourier transform with respect to variables \mathbf{x}_i has the form $\nu_n(\mathbf{p}_2, ..., \mathbf{p}_n, t_1, ..., t_n)\delta(\mathbf{p}_1 + ... + \mathbf{p}_n)$ where the function ν_n is smooth.

Let us show how one can define one-particle excitations of the state ω and the scattering of (quasi)particles.

The action of translation group on \mathcal{A} generates unitary representation of this group on (pre)Hilbert space \mathcal{H} constructed from ω . Generators of this representation \mathbf{P} and -H are identified with momentum operator and Hamiltonian. The vector in the space \mathcal{H} that corresponds to ω will be denoted by Φ . If Φ is a ground state we say that it is the physical vacuum . If ω obeys KMS-condition

$$\omega(A(t)B) = \omega(BA(t+i\beta)) \tag{20}$$

we say that ω is an equilibrium state with the temperature $T = \frac{1}{\beta}$. (It is assumed that A(t) can be analytically continued to the strip $0 \le Imt \le \beta$.)

We say that a state σ is an excitation of ω if it coincides with ω at infinity. More precisely we should require that $\sigma(A(\mathbf{x},t)) \to \omega(A)$ as $\mathbf{x} \to \infty$ for every $A \in \mathcal{A}$. Notice that the state corresponding to any vector $A\Phi$ where $A \in \mathcal{A}$ is an excitation of ω ; this follows from cluster property.

One can define one-particle state (one-particle excitation of the state ω) as a generalized \mathcal{H} -valued function $\Phi(\mathbf{p})$ obeying $\mathbf{P}\Phi(\mathbf{p}) = \mathbf{p}\Phi(\mathbf{p}), H\Phi(\mathbf{p}) = \varepsilon(\mathbf{p})\Phi(\mathbf{p})$. (More precisely, for some class of test functions $f(\mathbf{p})$ we should have a linear map $f \to \Phi(f)$ of this class into \mathcal{H} obeying $\mathbf{P}\Phi(f) = \Phi(\mathbf{p}f), H\Phi(f) = \Phi(\varepsilon(\mathbf{p})f)$ where $\varepsilon(\mathbf{p})$ is a real-valued function. For definiteness we can assume that test functions belong to the Schwartz space $\mathcal{S}(\mathbb{R}^d)$.) We require that there exist an element $B \in \mathcal{A}$ such that $\hat{B}\Phi = \Phi(\phi)$ where ϕ is a non-vanishing function. (The symbol \hat{B} denotes the operator in \mathcal{H} corresponding to the element $B \in \mathcal{A}$.) We assume also that that there exists an element $A \in \mathcal{A}$ and a function $g(\mathbf{x},t) \in \mathcal{S}(\mathbb{R}^{d+1})$ such that $\hat{B} = \int g(\mathbf{x},t)\hat{A}(\mathbf{x},t)d\mathbf{x}dt$ (it follows from this assumption that $\hat{B}(\mathbf{x},t)$ is a smooth function of \mathbf{x},t).

We assume that $\Phi(f)$ is normalized (i.e. $\langle \Phi(f), \Phi(f') \rangle = \langle f, f' \rangle$).

Of course, it is possible that there are several one-particle states; to simplify the notations we assume that there exists only one kind of particles.

Notice that in relativistic theory one-particle states can be identified with irreducible representations of the Poincaré group; our assumption means that we consider a scalar particle.

Let us us fix a function $f(\mathbf{p})$. Define a function $\tilde{f}(\mathbf{x},t)$ as the Fourier transform of the function $f(\mathbf{p})e^{-i\varepsilon(\mathbf{p})t}$ with respect to \mathbf{p} . Let us introduce the notation $B(f,t) = \int \tilde{f}(\mathbf{x},t)B(\mathbf{x},t)d\mathbf{x}$. (We assume that this expression specifies an element of \mathcal{A} such that $\hat{B}(f,t) = \int \tilde{f}(\mathbf{x},t)\hat{B}(\mathbf{x},t)d\mathbf{x}$.) It is easy to check that

$$\hat{B}(f,t)\Phi = \int f(\mathbf{p})\phi(\mathbf{p})\Phi(\mathbf{p})d\mathbf{p}$$
(21)

doest not depend on t.

Let us consider the vectors

$$\Psi(f_1, ..., f_n | t) = B(f_1, t) \cdots B(f_n, t) \Phi$$
(22)

where $f_1, ..., f_n$ satisfy the following condition: if $f_i(\mathbf{p}) \neq 0, f_j(\mathbf{p}') \neq 0, i \neq j$ then $\nabla \varepsilon(\mathbf{p}) \neq \nabla \varepsilon(\mathbf{p}')$. (More precisely we should assume that the distance between $\nabla \varepsilon(\mathbf{p})$ and $\nabla \varepsilon(\mathbf{p}')$ is bounded from below by a positive number). We impose the additional requirement that $\varepsilon(\mathbf{p})$ is a smooth strictly convex function. Then one can derive from cluster property or from asymptotic commutativity of $\mathcal{A}(\omega)$ that these vectors have limits in $\bar{\mathcal{H}}$ as $t \to \pm \infty$; these limits will be denoted by

$$\Psi(f_1,...,f_n|\pm\infty).$$

Let us assume the vectors $\Psi(f_1, ..., f_n | -\infty)$ span a dense subset of \mathcal{H} . (One can hope that this condition is satisfied when ω is the ground state. In other cases one should consider inclusive cross-sections and inclusive scattering matrix; see Chapter 13.) Then we can define in-operators a_{in}^+, a_{in} on \mathcal{H} . In particular, to define $a_{in}^+(f) = \int (f(\mathbf{p})a_{in}^+(\mathbf{p})d\mathbf{p}) d\mathbf{p}$ we can use the formula

$$a_{in}^+(\bar{f}\bar{\phi})\Psi(f_1,...,f_n|-\infty) = \Psi(f,f_1,...,f_n|-\infty),$$

The definition of out-operators is similar. Using these notions we can define the scattering amplitudes by the formula