

Let us consider the case of slowly varying (adiabatic) 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:

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

To verify this fact we check that the RHS satisfies the equation of motion if we neglect $\dot{\phi}_n(t)$.

More accurate consideration

Consider a smooth family of Hamiltonians $\hat{H}(g)$ with eigenvectors $\phi_n(g)$ and eigenvalues $E_n(g)$ smoothly depending on g . The family

$$\hat{H}(t) = \hat{H}(g(t))$$

is an adiabatic family if $\dot{g}(t)$ can be neglected.

(For example, we can fix a function $g(t)$ and consider a family of functions $g_a(t) = g(at)$ with $a \rightarrow 0$.) Then

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

because $\dot{\phi}_n(g(t))$ can be neglected.

$U(t)$ -evolution operator of density matrix K .

$$\frac{dK}{dt} = H(t)K(t) = \frac{1}{i\hbar}[\hat{H}(t), K]$$

Introduce 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 adiabatic approximation $U(t)$ transforms eigenvector into eigenvector:

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

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

It follows that $K(t) = U(t)K$ where

$K = \sum k_{mn}\psi_{mn}$ is given by the formula

$K(t) = \sum k_{mn}(t)\psi_{mn}(t)$ where

$k_{mn}(t) = e^{-i\beta_{mn}(t)}k_{mn},$

$\beta_{mn}(t) = \int_0^t (E_m(\tau) - E_n(\tau))d\tau$

If $\hat{H}(T) = \hat{H}(0)$ we can assume that

$\phi_n(T) = \phi_n(0)$. Then we see that diagonal entries of K do not change, but non-diagonal entries are multiplied by a phase factor.

If $\hat{H}(t)$ is an unknown adiabatic deformation of Hamiltonian \hat{H} the non-diagonal entries of $K(T)$ are unpredictable.

If we consider linear combination (superposition) $\alpha_0\phi_0 + \alpha_1\phi_1$ of eigenvectors of $\hat{H} = \hat{H}(0)$ then evolving it with respect to the Hamiltonian \hat{H} we get phase factors : $\alpha_k(t) = e^{-iE_k t}\alpha_k$. If we evolve this linear combination with respect to unknown adiabatic deformation $\hat{H}(t)$ the absolute value $|\alpha_k(t)|$ remains constant ,but the phase factors are unpredictable.

Decoherence.

We model interaction with environment by random adiabatic perturbation of Hamiltonian \hat{H} . We assume that random time-dependent Hamiltonian depends on some parameters $\lambda \in \Lambda$ with some probability distribution on Λ . If we start with density matrix (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 Λ one can prove that the non-diagonal entries of $\bar{K}(T)$ tend to zero when the adiabatic parameter α tends to zero. In other words the matrix $\bar{K}(T)$ tends to a diagonal matrix \bar{K} having the same diagonal entries as K . The matrix \bar{K} can be considered as a mixture of pure states, corresponding to the vectors ϕ_n with probabilities k_{nn} .

Let us include the Hamiltonian \hat{H} in a family of Hamiltonians $\hat{H}(g)$, where $g \in \Lambda$. We assume that $\hat{H}(0) = \hat{H}$. Let us consider a time dependent Hamiltonian $\hat{H}(g(t))$ where $g(0) = 0, g(1) = 0$. We can construct an adiabatic Hamiltonian by the formula

$$\hat{H}_\alpha(t) = \hat{H}(g(\alpha t)) \text{ where } \alpha \rightarrow 0.$$

It is clear that $\hat{H}_\alpha(0) = \hat{H}_\alpha(T) = \hat{H}$ where $T = \alpha^{-1}$.

Denote by $E_n(g)$ the eigenvalues of $\hat{H}(g)$. Then the eigenvalues of $\hat{H}_\alpha(t)$ are equal to $E_n(g(\alpha t))$. The evolution of matrix entries of the density matrix with respect to the Hamiltonian $\hat{H}_\alpha(t)$ is governed by phase factors $e^{-i\beta_{mn}(t)}$ where for

$$t = T$$

$$\begin{aligned}\beta_{mn} &= \int_0^T d\tau (E_m(g(\alpha\tau)) - E_n(g(\alpha\tau))) = \\ &\frac{1}{\alpha} \int_0^1 d\tau (E_m(g(\tau)) - E_m(g(\tau)))\end{aligned}$$

Introducing probability distribution on the set Λ we obtain random adiabatic Hamiltonian.

The average phase factor vanishes for $m \neq n$.

Geometric approach to quantum theory

We start with a bounded closed convex set

$\mathcal{C}_0 \subset \mathcal{L}$ (set of states) and a subgroup \mathcal{V} of the automorphism group of \mathcal{C}_0

Here \mathcal{L} is a Banach space and automorphisms of \mathcal{C}_0 are invertible linear operators in \mathcal{L} mapping \mathcal{C}_0 onto itself.

The evolution operator $\sigma(t) \in \mathcal{V}$ transforms the state in the moment 0 into the state in the moment t

Equation of motion

$$\frac{d\sigma}{dt} = H(t)\sigma(t)$$

This formula can be considered as a definition of $H(t)$ ("Hamiltonian"), but usually we want to find the evolution operator knowing the "Hamiltonian". If H does not depend on time then $\sigma(t) = \exp(Ht)$.

Observable - a pair (A, a) where $A \in \text{Lie}(\mathcal{V})$ and a is an A -invariant linear functional on \mathcal{L}
 $A \in \text{Lie}(\mathcal{V})$ if A generates a one-parameter subgroup of \mathcal{V} denoted by $\sigma_A(t) = \exp(At)$

In textbook QM \mathcal{C}_0 consists of density matrices, \mathcal{V} is unitary group.

Observables are pairs (A, a) where A is self-adjoint operator, $a(K) = \text{tr}(AK)$.

In algebraic approach \mathcal{C}_0 consists of positive linear functionals ω on unital associative algebra with involution denoted by \mathcal{A} (positive means that $\omega(A^*A) \geq 0$).

Observable is a pair (A, a) where A is a self-adjoint elements of \mathcal{A} and $a(\omega) = \omega(A)$.

Decoherence in geometric approach

Let us fix a time independent "Hamiltonian" H .

Evolution operator $\sigma(t) = e^{tH}$

We assume that H is diagonalizable (there exists a basis of \mathcal{L} consisting of eigenvectors of H). Let us denote by (ψ_j) such a basis:

$$H\psi_j = \epsilon_j \psi_j$$

The eigenvalues ϵ_j are purely imaginary.

Let us assume that $H(g)$ is a family of "Hamiltonians" such that $H(0) = H$ and there exists a basis $(\psi_j(g))$ depending smoothly on g in such a way that $\psi_j(0) = \psi_j$ and

$$H\psi_j(g) = \epsilon_j(g)\psi_j(g)$$

We say ψ_j is a robust zero mode of H if $\epsilon_j(g) \equiv 0$.

Let us model the interaction with environment by random "Hamiltonian" $H(g(t))$. Then neglecting $\dot{g}(t)$ (in the adiabatic approximation) we obtain

$$\sigma(t)\psi_j = e^{\rho_j(t)}\psi_j(g(t)),$$

where $\frac{d\rho_j}{dt} = \epsilon_j(g(t))$.

If ψ_j is a robust zero mode of H then

$\sigma(t)\psi_j = \psi_j(g(t))$. If $g(T) = g(0)$ we have

$\sigma(T)\psi_j = \psi_j$.

All other modes acquire phase factors. If we have an unknown adiabatic perturbation it is impossible to predict these phase factors.

Imposing some conditions on the random Hamiltonian $H(t)$ we can prove that in average the random phase factors $e^{\rho_j(t)}$ vanish unless ϕ_j is a robust zero mode of H .

In textbook quantum mechanics robust zero modes of H are diagonal entries of density matrix in \hat{H} -representation.

Decoherence

Let us denote by P' a linear operator leaving intact robust zero modes of H and sending to zero all other eigenvectors of H . If $x \in \mathcal{C}_0$ one can prove that $P'x \in \mathcal{C}_0$. One can represent $P'x$ as a mixture of extreme points u_i of $P'(\mathcal{C}_0)$ (of pure robust zero modes): $P'x = \sum p_i u_i$. The coefficients p_i should be interpreted as probabilities.

If all zero modes of H are robust $P' = P$ where

$$P = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sigma(t) dt$$

Take observable (A, a) where $A \in \mathcal{V}$, a is a functional obeying $a(Ax) = 0$.

x is a robust zero mode of A if $Ax = 0$ and for every A' that is close to A there exists x' that is close to x and obeys $A'x' = 0$.

Assume that all zero modes of A are robust.

Consider the set \mathcal{C}_A of all states that are zero modes of A :

$$\mathcal{C}_A = (\text{Ker } A) \cap \mathcal{C} = \text{Im}(P_A) \text{ where}$$

$$P_A = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt e^{At}.$$

Represent $P_A(x)$ as a mixture of pure zero modes of A (of extreme points of \mathcal{C}_A):

$$P_A(x) = \sum p_i u_i.$$

In non-degenerate case p_i is the probability of $a(u_i)$ in the state x .

L-functionals

Weyl algebra with generators \hat{u}^i obeying

$$\hat{u}^k \hat{u}^l - \hat{u}^l \hat{u}^k = i\hbar \sigma^{k,l}$$

K -density matrix in representation of Weyl algebra

$$L_K(\alpha) = \text{tr} e^{i\alpha_k \hat{u}^k} K = \text{tr} V_\alpha K$$

$V_\alpha = e^{i\alpha_k \hat{u}^k} = e^{i\alpha u}$ where α_k are real is a unitary operator

$$V_\alpha V_\beta = e^{-i\frac{\hbar}{2}\alpha\sigma\beta} V_{\alpha+\beta} \text{ where } \alpha\sigma\beta = \alpha_k \sigma^{k,l} \beta_k.$$

\mathcal{L} -space of all linear functionals on Weyl algebra

$L_K \in \mathcal{L}$ specifies a positive functional (state). It is normalized: $L_K(0) = 1$.

Every element A of an algebra with involution specifies two operators on linear functionals: one (denoted by the same symbol) transforms the functional $\omega(x)$ into the functional

$(A\omega)(x) = \omega(Ax)$, another (denoted by \tilde{A}) transforms it into the functional
 $(\tilde{A}\omega)(x) = \omega(xA^*)$.

Denote by \mathcal{C} the cone of positive (not necessary normalized) linear functionals.

The operator $\tilde{A}A$ transforms \mathcal{C} into \mathcal{C} .

If $A = e^{tH}$ then $\tilde{A} = e^{t\tilde{H}}$. Hence the evolution operator defined as solution of equation

$d\sigma/dt = (H + \tilde{H})\sigma$

also acts in \mathcal{C} .

It is easy to calculate that

$$(V_\beta L)(\alpha) = e^{-i\frac{\hbar}{2}\alpha\sigma\beta} L(\alpha + \beta),$$

$$(\tilde{V}_\beta L)(\alpha) = e^{i-\frac{\hbar}{2}\alpha\sigma\beta} L(\alpha - \beta).$$

An element of Weyl algebra $\hat{H} = \int d\beta h(\beta) V_\beta$ is self-adjoint if $h(-\beta) = h(\beta)^*$. Taking $H = -\frac{i}{\hbar} \hat{H}$ we obtain the equation of motion

$$i\hbar \frac{d\sigma}{dt} = (\hat{H} - \tilde{\hat{H}})\sigma , \text{ hence}$$

$$\begin{aligned}
& i\hbar \frac{dL}{dt} = \\
& \int d\beta h(\beta) e^{-i\frac{\hbar}{2}\alpha\sigma\beta} L(\alpha+\beta) - \int d\beta h(-\beta) e^{-i\frac{\hbar}{2}\alpha\sigma\beta} L(\alpha-\beta) \\
& = \int d\beta h(\beta) (e^{-i\frac{\hbar}{2}\alpha\sigma\beta} - e^{i\frac{\hbar}{2}\alpha\sigma\beta}) L(\alpha + \beta)
\end{aligned}$$

Finally,

$$\frac{dL}{dt} = \int d\beta h(\beta) \frac{2 \sin(\frac{\hbar}{2}\alpha\sigma\beta)}{\hbar} L(\alpha + \beta)$$

L-functionals. Another definition.

Take representation of Weyl algebra (of CCR) in Hilbert space \mathcal{H} . (We understand CCR as relations $[a_k, a_l^+] = \delta_{kl}$, $[a_k, a_l] = [a_k^+, a_l^+] = 0$, where k, l run over a discrete set M .)

To a density matrix K (or more generally to any trace class operator in \mathcal{H}) we can assign a functional $L_K(\alpha^*, \alpha)$ defined by the formula

$$L_K(\alpha^*, \alpha) = \text{tr} e^{-\alpha a^+} e^{\alpha^* a} K = e^{\frac{1}{2}\alpha^* \alpha} \text{tr} e^{-\alpha a^+ + \alpha^* a} K$$

Here αa^+ stands for $\sum \alpha_k a_k^+$ and $\alpha^* a$ for $\sum \alpha_k^* a_k$, where k

One can say that L_K is a generating functional of correlation functions.

One can consider also a more general case when CCR are written in the form

$$[a(k), a^+(k')] = \hbar\delta(k, k'), [a(k), a(k')] = [a^+(k), a^+(k')] = 0$$

k, k' run over a measure space M . We are using the exponential form of CCR; in this form a representation of CCR is specified as a collection of unitary operators $e^{-\alpha a^+ + \alpha^* a}$ obeying appropriate commutation relations. Here $\alpha(k)$ is a complex function on the measure space M , the expressions of the form $\alpha^* a, \alpha a^+$ can be written as integrals $\int \alpha^*(k) a(k) dk, \int \alpha(k) a^+(k) dk$ over M . We assume that α is square-integrable, then the expression for L_K is well defined.

An action of Weyl algebra \mathcal{A} on \mathcal{L} (on the space of L -functionals) can be specified by operators

$$b^+(k) = \hbar c_1^+(k) - c_2(k), b(k) = c_1(k)$$

obeying CCR. Here $c_i^+(k)$ are multiplication operators by α_k^* , α_k and $c_i(k)$ are derivatives with respect to α_k^* , α_k . This definition is prompted by relations

$$L_{a(k)K} = b(k)L_K, L_{a^+(k)K} = b^+(k)L_K,$$

Another representation of \mathcal{A} on \mathcal{L} . is specified by the operators

$$\tilde{b}^+(k) = -\hbar c_2^+(k) + c_1(k), \tilde{b}(k) = -c_2(k),$$

obeying CCR and satisfying

$$L_{K a^+(k)} = \tilde{b}(k)L_K, L_{K a(k)} = \tilde{b}^+(k)L_K,$$

Let us consider a Hamiltonian \hat{H} in a space of representation of CCR. We will write \hat{H} in the form

$$\hat{H} = \sum_{m,n} \sum_{k_i, l_j} H_{m,n}(k_1, \dots, k_m | l_1, \dots, l_n) a_{k_1}^+ \dots a_{k_m}^+ a_{l_1} \dots a_{l_n} \quad (1)$$

There are two operators in \mathcal{L} corresponding to \hat{H} :

$$\hat{H} = \sum_{m,n} \sum_{k_i, l_j} H_{m,n}(k_1, \dots, k_m | l_1, \dots, l_n) b_{k_1}^+ \dots b_{k_m}^+ b_{l_1} \dots b_{l_n} \quad (2)$$

(we denote it by the same symbol) and

$$\tilde{H} = \sum_{m,n} \sum_{k_i, l_j} H_{m,n}(k_1, \dots, k_m | l_1, \dots, l_n) \tilde{b}_{k_1}^+ \dots \tilde{b}_{k_m}^+ \tilde{b}_{l_1} \dots \tilde{b}_{l_n} \quad (3)$$

The equation of motion for the L -functional $L(\alpha^*, \alpha)$ has the form

$$i\hbar \frac{dL}{dt} = HL = \hat{H}L - \tilde{H}L$$

(We introduced the notation $H = \hat{H} - \tilde{H}$.)
It corresponds to the equation for density matrices.

The equations of motion for L -functionals make sense even in the situation when the equations of motion in the Fock space are ill-defined (but there are no ultraviolet divergences). This is related to the fact that vectors and density matrices from all representations of CCR are described by L -functionals. This means that applying the formalism of L -functionals we can avoid the problems related to the existence of inequivalent representations of CCR.

In perturbation theory for translation-invariant Hamiltonians these problems appear as divergences related to infinite volume. Therefore in the standard formalism it is necessary to consider at first a Hamiltonian in finite volume V (to make volume cutoff or, in another terminology, infrared cutoff) and to take the limit $V \rightarrow \infty$ in physical quantities.

In the formalism of L -functionals we can work directly in infinite volume. We can define adiabatic S -matrix and adiabatic generalized Green functions repeating the standard definitions. If the adiabatic parameter a tends to zero then the adiabatic S -matrix multiplied by some factors tends to inclusive scattering matrix. The adiabatic Green functions in the formalism of L -functionals tend to GGreen functions. This gives a very simple derivation of the diagram techniques for the calculation of GGreen functions.