ADIABATIC PHASES IN QUANTUM MECHANICS

Hauptseminar: Geometric phases
Prof. Dr. Michael Keyl
Ana Škerjanc, 05. June 2014

Conditions in adiabatic process are changing gradually and therefore the infinitely slow evolution of the system allows the system to adapt its configuration during the process.

The adiabatic theorem describes the long time behavior of solutions of Schrödinger equation \( i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \), where \( \Psi(t) \) represents the state of the system at time \( t \).

We consider a time-dependent self-adjoint Hamiltonian \( H = H(t) \) and assume that the spectrum of \( H \) is discrete and non-degenerate:

\[
H(t)|n(t)\rangle = E_n(t)|n(t)\rangle
\]

where eigenvectors orthogonal to each other i.e.

\[
\langle n(t)|m(t)\rangle = \delta_{nm} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases}
\]

The time-dependent phase-transformation may be performed since eigenvectors not uniquely defined i.e.

\[
|n(t)\rangle \rightarrow e^{i\lambda_n(t)}|n(t)\rangle
\]

The adiabatic theorem now states, that if the Hamiltonian changes in time slowly enough, then a system initially in the eigenstate \( |n(0)\rangle \) will remain (up to a phase) in an instantaneous eigenstate \( |n(t)\rangle \) of \( H(t) \) i.e.

\[
\Psi(t) = e^{i\alpha_n(t)}|n(t)\rangle
\]

The state of the system at time \( t \) may be expanded in the orthonormal base \( |n(t)\rangle \):

\[
\Psi(t) = \sum_m c_m(t)e^{\phi_m} = \sum_m c_m(t)\exp\left(-\frac{i}{\hbar} \int_a^t E_m(\tau)d\tau\right)|m(t)\rangle
\]

By Substitution of (3) into SE: \( \hbar \frac{\partial \Psi}{\partial t} = H\Psi \) we obtain the following equation:

\[
i\hbar \sum_m (c'_m|m(t)\rangle + c_m|\dot{n}(t)\rangle) + \frac{i}{\hbar} c_m|m(t)\rangle(-E_m)e^{\phi_m} = \sum_m (c_m e^{\phi_m}|m(t)\rangle H)
\]

The third term of left hand side cancels out with the right hand side leaving

\[
\sum_m (c'_m|m(t)\rangle)e^{\phi_m} = - \sum_m (c_m|\dot{n}(t)\rangle)e^{\phi_m}
\]

now taking the inner product with an arbitrary eigenfunction \( |k(t)\rangle \), the on the left \( \langle m|k \rangle \) gives \( \delta_{nm} \) which is 1 only for \( m = n \) otherwise vanishes. The part that remains is:

\[
c'_m = -\sum_m c_m\langle m(t)|\frac{d}{dt}|k(t)\rangle e^{i(\phi_k - \phi_m)}
\]

Differentiating (1) with respect to time, we get:
\[
\hat{H}|k\rangle + H|\dot{k}\rangle = \hat{E}_k|k\rangle + E_k|\dot{k}\rangle
\]

Multiplying by \( |m\rangle \) gives us the following equation:

\[
\langle m|\dot{k}\rangle = \frac{1}{E_k - E_m}\langle m|\hat{H}|k\rangle \text{ for } m \neq k
\]

The evolution generated by \( H(t) \) is considered **adiabatic** if

\[
|\langle m|\dot{H}|k\rangle| \ll \frac{|E_k - E_m|}{\Delta T_{km}}
\]

where \( \Delta T_{km} \) is a characteristic time of transition between states \( k \) and \( m \).

In the adiabatic limit \( \Delta T_{km} \to \infty \) the changes of \( H \) are infinitely slow \( |\langle m|\dot{H}|k\rangle| \to 0 \) and hence \( \langle m|\dot{k}\rangle \to 0 \).

Therefore, in the adiabatic limit, (4) simplifies to

\[
c_m = -c_m\langle m|\dot{m}\rangle
\]

With the initial condition \( c_m(0) = \delta_{nm} \) it follows that \( c_m = 0 \) for \( m \neq k \) and together with (3) the adiabatic theorem is shown:

\[
\Psi(t) = c_n(t)\exp(-\frac{i}{\hbar}\int_0^t E_n(\tau)d\tau)|n(t)\rangle
\]

\( \Rightarrow \) During the adiabatic evolution \( \Psi(t) \) remains in the \( n \)-th eigenstate of \( H(t) \).

We are now interested in the coefficients \( c_n(t) \). It is clear from differential equation (6) that \( c_n(t) \) is a pure phase factor \( c_n(t) = e^{i\phi_n(t)} \), where the phase \( \phi_n(t) \) satisfies \( \dot{\phi}_n = i\langle n|\dot{n}\rangle \).

\( \phi_n(t) \) represents geometric phase, so called **Berry’s phase** - it is a phase difference acquired over the course of a cycle, when the system is subjected to cyclic adiabatic processes, which results from the geometrical properties of the parameter space of the Hamiltonian.

Pure quantum states are represented by vectors in a complex Hilbert space \( \tilde{H} \). Two vectors \( \Psi \) and \( \varphi \) describe the same physical state if \( \Psi = \lambda \varphi \) and two normalized state vectors \( \Psi \) and \( \varphi \) are physically equivalent \( \Psi \sim \varphi \) if \( \Psi = e^{i\alpha} \varphi \). We call \( \alpha \) a relative phase between states \( \Psi \) and \( \varphi \). \( \alpha \) can be measured.

We may equivalently represent pure quantum states as one-dimensional projectors in \( H \): \( \Psi \to P_\Psi := \langle \Psi | \Psi \rangle \).

Now we consider a curve \( C \) on a manifold of external parameters \( M \): \( t \to x_t \in M \) and the adiabatic evolution along \( C \) described by Hamiltonian, whose parameter \( x_t \) is time dependent, i.e. \( H(t) = H(x_t) \). We also suppose that for any \( x \in M \) the Hamiltonian \( H(x) \) fulfills (1) and (2) and that the eigenvectors \( |n(x)\rangle \) are single valued as Functions of \( x \in M \) we assume the locally existence of the map

\[
M \ni x \to |n(x)\rangle \in \tilde{H} \text{ (system’s Hilbert space)}.
\]

Let \( E_n(x) \) be nondegenerable and \( P_n(x) \) the corresponding one-dimensional projector onto the \( n \)-th eigenspace \( \tilde{H}_n(x) \).

\[
\tilde{H}_n(x) := \text{Range } P_n(x) = \{ \alpha |n(x)\rangle | \alpha \in \mathbb{C} \}.
\]
One may arbitrary change the phase of $|n(x)\rangle$, since they are not uniquely defined by (1) and (2): $|n(x)\rangle \rightarrow |n'(x)\rangle = e^{i\alpha_n(x)|n(x)\rangle}$ where $\alpha_n : M \rightarrow \mathbb{R}$. Phase transformation does not change $P_n(x)$.

If $\Psi(0) = |n(x_0)\rangle$ then due to adiabatic theorem $\Psi(t)$ stays in $n$-th eigenspace of $H(x_t)$ during the adiabatic evolution, i.e. $\Psi(t) \in \tilde{H}_n(x_t)$.

Therefore, if the evolution is cyclic, then $\Psi(0)$ and $\Psi(T)$, for some $T$ where $x_0 = x_1$, both belong to $\tilde{H}_n(x_t) = \tilde{H}_n(x_0)$ and so may differ only by a phase factor: $\psi(T) = e^{i\gamma}\psi(0)$.

The possible guess would be a dynamical phase

$$\gamma = -\frac{1}{\hbar} \int_0^T E_n(t) dt$$

but as shown by Berry (1984) there is still an additional component with a purely geometric origin missing.

To find it, let us take (7) with coefficients $c_n(t) = e^{i\phi_n}$:

$$\Psi(t) = \exp\left(-\frac{i}{\hbar} \int_0^t E_m(\tau)d\tau \right) e^{i\phi_n(t)} |n(x_t)\rangle$$

and

$$\dot{\phi}_n = i \langle n|\dot{n} \rangle$$

Last formula defines the following one-form on $M$:

$$A^{(n)} := i \langle n|dn \rangle$$

in local coordinates $(x_1, ..., x_n)$:

$$A^{(n)} = A^{(n)}_k dx^k$$

with $A^{(n)}_k := i \langle n|\partial_k n \rangle$

Now we can solve (9) by integrating $\phi_n(t)$:

$$\phi_n(t) = i \int_0^t \langle n(\tau)|\dot{n}(\tau) \rangle d\tau = \int_C A^n$$

and find out that (8) is supplemented by $\gamma_n(c) := \phi_n(T) = \oint_C A^{(n)}$

$$\Rightarrow \gamma = -\frac{1}{\hbar} \int_0^T E_n(t) dt + \gamma_n(C).$$

The phase factor depends upon the geometry of the manifold $M$ and the circuit $C$ itself.

With Stokes theorem we may write Berry’s phase $\gamma_n(C)$ as

$$\gamma_n(C) = \int_\Sigma F^n$$

where $\Sigma$ = arbitrary two-dim submanifold in M, such that $\partial \Sigma = C$ and

$$F^n = dA^n = -I m\langle dn| \wedge |dn \rangle$$

or in local coordinates

$$F^n = \frac{1}{2} F^n_{ij} dx^i \wedge dx^j$$

with

$$F^n_{ij} = -I m(\langle \partial_i n|\partial_j n \rangle - \langle \partial_j n|\partial_i n \rangle)$$
Performing a phase transformation \( |n'(x)\rangle = e^{i\alpha_n(x)} |n(x)\rangle \) the quantity \( A^n \) transforms accordingly

\[
A^n \rightarrow A'(n) = A^n - d\alpha_n
\]

using component notation

\[
A'^n_k = A^n_k - \partial_k \alpha_n
\]

Since \( d^2\alpha_n = 0 \) the two-form \( F^n \) gauge invariant and due to (11) Berry’s phase \( \gamma_n(C) \) as well. \( F^n \) represents the magnetic field for the potential \( A^n \) and so follows with (11) that

Berry’s phase \( \gamma_n(C) = \) flux of \( F^n \) through \( \Sigma \)

We can express magnetic field with energy eigenvalues \( E_k \). Inserting \( 1 = \sum_m |m\rangle \langle m| \) into (12) and (5) one gets

\[
F^n = -\text{Im} \sum_{m \neq n} \frac{|\langle n|dH|m\rangle \wedge \langle m|dH|n\rangle|}{(E_n - E_m)^2}
\]

(13)

Proposition: The two form \( F^n \) satisfies the following property

\[
\sum_n F^n = 0 \quad (14)
\]

**Example:** Adiabatic evolution of a spin-half particle in a magnetic field

The Hamiltonian is given by

\[
H(B) = \frac{1}{2} \mu \sigma \cdot B,
\]

\( \sigma \) represents a three-vector of Pauli matrices and magnetic field \( B \in \mathbb{R} \) plays the role of external parameter and can be rewritten in spherical coordinates as

\[
B = B(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta).
\]

If \( B = B e_3 \) then we get \( \pm \frac{1}{2} \mu B \) as eigenvalues and \( |+(e_3)\rangle = |0\rangle \), \( |-(e_3)\rangle = |1\rangle \) corresponding eigenvectors.

If \( B \) is parametrized by spherical angles \((\theta, \varphi)\), then it may be obtained from \( e_3 \) by the \( SO(3) \) rotation. With corresponding unitary operator acting in \( \mathbb{C}^2 \) we get eigenvectors now written in spherical angles as following:

\[
|+(\theta, \varphi)\rangle = |\cos \frac{\theta}{2}, e^{i\varphi} \sin \frac{\theta}{2}\rangle, \quad |-(\theta, \varphi)\rangle = |\frac{\sin \theta}{2} \rangle e^{i\varphi} \cos \frac{\theta}{2} \rangle
\]

(15)

But the parametrization of eigenvectors is not global (consider \( \theta = 0 \) at north and south pole). Hence we have two well defined maps:

\[
|\pm\rangle : S^2 - \{(0, 0, \pm B)\} \rightarrow S^3 \subset \mathbb{C}^2
\]
Now inserting (15) into (10) one obtains

\[ A^{(\pm)} = \mp \frac{1}{2} (1 \mp \cos \theta) d\varphi \]

and so the corresponding berry curvature is given by

\[ F^{(\pm)} = \mp \frac{1}{2} \sin \theta \, d\theta \wedge d\varphi \]

and therewith the formula for the Berry phase for a spin-half particle follows:

\[ \gamma^{\pm}(C) = \int_{\Sigma} F^{(\pm)} = \mp \pi (1 - \cos \theta) \]

Observing the angle \( \theta = \frac{\pi}{2} \) we have \( \gamma^{\pm}(C) = \mp \pi \Rightarrow e^{i\gamma^{\pm}(C)} = -1 \Rightarrow \) wave function changes sign after coming back to the initial point of the parameter manifold. The same result follows directly from (12).

Notes:

Literature:

- Dariusz Chruściński, Andrzej Jamiołkowski, Geometric Phases in Classical and Quantum Mechanics, Birkhäuser, 2004
- Torsten Fließbach, Quantenmechanik, Spektrum Akademischer Verlag, 3 Auflage 2000