

Berry phase

If the Hamiltonian H is independent on time, then when the system starts from a non-degenerated eigenstate $\psi_n(\vec{r})$

$$H\psi_n(\vec{r}) = E_n\psi_n(\vec{r})$$

In time it remains in the same state, picking up a phase factor

$$\psi_n(\vec{r}, t) = \psi_n(\vec{r})e^{-i\frac{E_n t}{\hbar}}$$

If we change the parameters of the Hamiltonian very gradually in time, the system remains in the same eigenstate assuming that it remains nondegenerated (the energy gap between this state and any other states remains finite)

That is the *adabatic principle*.

We consider a physical system with a general time-varying Hamiltonian $H(\mathbf{R})$ that depends on time through several parameters (such as magnetic field, electric field, flux, and strain) labeled by a vector $\mathbf{R}=(R_1, R_2, , \dots)$ where $R_i = R_i(t)$. We are interested in the adiabatic evolution of the system-the evolution of the system as the parameters $\mathbf{R}(t)$ are varried very slowly (compared to other energy scales-gaps-in the problem) along a path C in the parameter space. For our purposes, C can now be any path, closed or open. We introduce an instantaneous orthonormal basis of the instantaneous eigenstates $|n(\mathbf{R})\rangle$ of $H(\mathbf{R})$ at each point \mathbf{R} obtained by diagonalizing $H(\mathbf{R})$ at each value \mathbf{R} :

$$H(\mathbf{R})|n(\mathbf{R})\rangle = E_n(\mathbf{R})|n(\mathbf{R})\rangle$$

It determines the basic function $|n(\mathbf{R})\rangle$ up to a phase.

We want to analyze the phase of the wave function of a system prepared in an initial pure state $|n(\mathbf{R}(t))\rangle$ as we slowly move $\mathbf{R}(t)$ along the path C .

Per the adiabatic theorem, a system starting in an eigenstate $|n(\mathbf{R}(0))\rangle$ will evolve with $H(\mathbf{R})$ and hence stay as an instantaneous eigenstate of the Hamiltonian $H(\mathbf{R}(t))$ throughout the process.

Let the phase $\theta(t)$ of the state $|\psi(t)\rangle = e^{-i\theta(t)}|n(\mathbf{R}(t))\rangle$

The time evolution of the system is given by

$$H(\mathbf{R}(t))|\psi(t)\rangle = i\hbar \frac{d}{dt} |\psi(t)\rangle$$

$$E_n(\mathbf{R}(t))|n(\mathbf{R}(t))\rangle = \hbar \left(\frac{d}{dt} \theta(t) \right) |n(\mathbf{R}(t))\rangle + i\hbar \frac{d}{dt} |n(\mathbf{R}(t))\rangle$$

Taking the scalar product with $\langle n(\mathbf{R}(t)) |$ and assuming the state is normalized

$$E_n(\mathbf{R}(t)) - i\hbar \langle n(\mathbf{R}(t)) | \frac{d}{dt} |n(\mathbf{R}(t))\rangle = \hbar \left(\frac{d}{dt} \theta(t) \right)$$

The solution for the phase $\theta(t)$ is

$$\theta(t) = \frac{1}{\hbar} \int_0^t E_n(\mathbf{R}(t')) dt' - i \int_0^t \langle n(\mathbf{R}(t')) | \frac{d}{dt'} |n(\mathbf{R}(t'))\rangle dt'$$

The first part of the phase is the conventional dynamical phase. The negative of the second part is called the Berry phase. If we write

$$|\psi(t)\rangle = \exp\left(\frac{1}{\hbar} \int_0^t E_n(\mathbf{R}(t')) dt'\right) \exp(i\gamma_n) |n(\mathbf{R}(t))\rangle$$

Then the Berry phase is γ_n

$$\gamma_n = i \int_0^t \langle n(\mathbf{R}(t')) | \frac{d}{dt'} |n(\mathbf{R}(t'))\rangle dt'$$

Time can be removed explicitly from the equation- the only thing needed being the dependence of the eigenstates on the parameters R_i , which are implicitly time dependent.

$$\gamma_n = i \int_0^{t_f} \langle n(\mathbf{R}(t')) | \frac{d}{dt'} |n(\mathbf{R}(t'))\rangle \frac{d\mathbf{R}}{dt'} dt' = i \int_C \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} |n(\mathbf{R})\rangle d\mathbf{R}$$

The Berry phase γ_n is real, because $\langle n(\mathbf{R}) | \nabla_{\mathbf{R}} |n(\mathbf{R})\rangle$ is itself imaginary.

We can define a vector function called Berry connection, or Berry vector potential:

$$\mathbf{A}_n(\mathbf{R}) = i \langle n(\mathbf{R}) | \frac{\partial}{\partial \mathbf{R}} |n(\mathbf{R})\rangle, \quad \gamma_n = \int_C \mathbf{A}_n(\mathbf{R}) d\mathbf{R}$$

The Berry connection $\mathbf{A}_n(\mathbf{R})$ is obviously gauge dependent. Under gauge transformation $|n(\mathbf{R})\rangle \rightarrow e^{i\zeta(\mathbf{R})} |n(\mathbf{R})\rangle$, the Berry connection transforms in the usual way:

$$\mathbf{A}_n(\mathbf{R}) \rightarrow \mathbf{A}_n(\mathbf{R}) - \frac{\partial}{\partial \mathbf{R}} \zeta(\mathbf{R})$$

The γ_n can not be cancelled by a smart choice of the gauge factor $\zeta(\mathbf{R})$ from the following reason:

We can consider closed path C in parameter space for which, after a long time T we return to the original parameters: $\mathbf{R}(T) = \mathbf{R}(0)$. For such paths, the fact that the eigenstates basis to be single-valued means that when we return to the original parameter configuration, the basis state must be the same $|n(\mathbf{R}(T))\rangle = |n(\mathbf{R}(0))\rangle$. Gauge transformations must maintain this property, so

$$e^{i\zeta(\mathbf{R}(0))} |n(\mathbf{R}(0))\rangle = e^{i\zeta(\mathbf{R}(T))} |n(\mathbf{R}(T))\rangle = e^{i\zeta(\mathbf{R}(T))} |n(\mathbf{R}(0))\rangle \text{ and hence } \zeta(\mathbf{R}(T)) - \zeta(\mathbf{R}(0)) = 2\pi m, \text{ with } m \text{ an integer.}$$

Let the parameter space three-dimensional. For a closed path, the Berry phase is a gauge-invariant quantity independent of the specific form of how \mathbf{R} varies in time. Because C is a closed path, application of Stokes theorem gives

$$\begin{aligned}\gamma_n &= \int d\mathbf{S} (\nabla \times \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} | n(\mathbf{R}) \rangle) = \int dS_i \epsilon_{ijk} \nabla_j \langle n(\mathbf{R}) | \nabla_k | n(\mathbf{R}) \rangle \\ &= \int d\mathbf{S} (\langle \nabla n(\mathbf{R}) | \times | \nabla n(\mathbf{R}) \rangle)\end{aligned}$$

where $\langle \nabla n(\mathbf{R}) | \times | \nabla n(\mathbf{R}) \rangle$ is the Berry curvature (to be precise, $F_{jk} = \langle \nabla_j n(\mathbf{R}) | \nabla_k n(\mathbf{R}) \rangle - (j \leftrightarrow k)$ is the Berry curvature). We can think of F_{jk} as a magnetic field in parameter space (the curl of the Berry connection)