Theory of Berry phase

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1 General theory

Let us consider a Hamiltonian $\hat{H}(r)$. Assume that the multi–component parameter r slowly depends on time. Then it is possible to search the solution of Schrodinger equation in the form

$$\Psi(t) = \exp\left\{-i\int_0^t \epsilon_m(r(t))\,dt + i\gamma(t)\right\} u_m(r(t)) \tag{1}$$

Here u_m is the wavefunction of the m–th level state, and ϵ_m is its energy.

After substituting to the Schrodinger equation $i\partial_t\Psi = \hat{H}(r(t))\Psi$ we get the following equation:

$$-\frac{\partial\gamma}{\partial t}u_m + i\frac{\partial u_m}{\partial r_i}\dot{r}_i = 0 \tag{2}$$

Multiplying it by $\langle u_m|$ we obtain

$$\frac{\partial\gamma}{\partial t} = i\langle u_m\frac{\partial}{\partial r_i}u_m\rangle\dot{r_i} \tag{3}$$

The solution is

$$\gamma = \int \mathcal{A}_i\,dr_i \tag{4}$$

where

$$\mathcal{A}_i = i\langle u_m\frac{\partial}{\partial r_i}u_m\rangle \tag{5}$$

is so called Berry connection. It is a real quantity, because

$$0 = \partial_i\langle u_m|u_m\rangle = \langle u_m|\partial_i u_m\rangle + \langle\partial_i u_m|u_m\rangle, \tag{6}$$

so

$$\langle u_m|\partial_i u_m\rangle = -\langle u_m|\partial_i u_m\rangle* \tag{7}$$

Let us introduce gauge transformations $u'_m = u_m e^{i\chi_0(r)}$. Under such transformations, Berry connection changes:

$$\mathcal{A'}_i = i\langle\Psi'_0\frac{\partial}{\partial r_i}\Psi'_0\rangle = i\langle\Psi_0\frac{\partial}{\partial r_i}\Psi_0\rangle - \frac{\partial\chi_0}{\partial r_i} = \mathcal{A}_i - \frac{\partial\chi_0}{\partial r_i} \tag{8}$$

However, all physical quantities are defined not by Berry connection but by Berry curvature:

$$\Omega_{ij} \equiv \frac{\partial \mathcal{A}_j}{\partial r_i} - \frac{\partial \mathcal{A}_i}{\partial r_j} \tag{9}$$

Obviously, it is gauge invariant:

$$\Omega'_{ij} = \Omega_{ij} - (\partial_i \partial_j - \partial_j \partial_i)\chi_0 = \Omega_{ij} \tag{10}$$

It is possible to derive an expression for Ω_{ij} which is explicitely gauge invariant. First of all, from (5) and (9) follows

$$\Omega_{ij} = i(\langle \partial_i u_m | \partial_j u_m \rangle - \langle \partial_j u_m | \partial_i u_m \rangle \tag{11}$$

Inserting the unity:

$$\Omega_{ij} = i \sum_n (\langle \partial_i u_m | u_n \rangle \langle u_n | \partial_j u_m \rangle - \langle \partial_j u_m | u_n \rangle \langle u_n | \partial_i u_m \rangle \tag{12}$$

Let us drive a nice expression for the matrix elements in the equation above. For that, let us differentiate the stationary Schrodinger equation:

$$\partial_i \hat{H} u_m + \hat{H} \partial_i u_m = \partial_i E_m u_m + E_m \partial_i u_m \tag{13}$$

Multplying by $\langle u_n|$,$n \neq m$, we get

$$\langle u_n | \partial_i u_m \rangle = -\frac{\langle u_n | \partial_i \hat{H} u_m \rangle}{E_n - E_m} \tag{14}$$

The contibution of $\langle u_m \partial_i u_m \rangle$ to (12) is zero, therefore,

$$\Omega_{ij} = i \sum_n \frac{\langle u_m | \partial_i \hat{H} | u_n \rangle \langle u_n | \partial_j \hat{H} | u_m \rangle - \langle u_m | \partial_j \hat{H} | u_n \rangle \langle u_n | \partial_i \hat{H} | u_m \rangle}{(E_n - E_m)^2} \tag{15}$$

In the particular case of three–dimensional parameter space, it is possible to define a curvature vector:

$$\Omega_i \equiv \frac{1}{2} \epsilon_{ijk} \Omega_{jk} = \epsilon_{ijk} \partial_j \mathcal{A}_k = \tag{16}$$

$$\vec{\Omega} = i \sum_n \frac{\langle u_m | \vec{\nabla} \hat{H} | u_n \rangle \times \langle u_n | \vec{\nabla} \hat{H} | u_m \rangle}{(E_n - E_m)^2} \tag{17}$$

2 The case of spin in magnetic field

In this section, we will compute the Berry phase for the Hamiltonian

$$\hat{H} = \mu \vec{B} \cdot \vec{\sigma} = \mu B \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \tag{18}$$

It is quite obvious that the eigenvalues are $\pm\mu B$, and the eigenvectors —

$$\begin{aligned} u_\uparrow &= \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix} \\ u_\downarrow &= \begin{pmatrix} -\sin\frac{\theta}{2} e^{-i\phi} \\ \cos\frac{\theta}{2} \end{pmatrix} \end{aligned} \tag{19}$$

(as in the first problem from this assignment) The Berry connection for the **upper state** can be easily calculated from the definition:

$$\begin{aligned} A_r &= 0 \\ A_\theta &= 0 \\ A_\phi &= -\sin^2\frac{\theta}{2} \end{aligned} \tag{20}$$

The curvature —

$$\Omega_{\theta\phi} = -\frac{\sin\theta}{2} \tag{21}$$

That implies that the phase after a 2π rotation will be

$$\gamma_{\text{upper}} = -2\pi \sin^2\frac{\theta}{2} \tag{22}$$

It is gauge invariant as an integral of $\mathcal{A}$ over closed path.

For **lower state**,

$$\begin{aligned} A_r &= 0 \\ A_\theta &= 0 \\ A_\phi &= \sin^2\frac{\theta}{2} \end{aligned} \tag{23}$$

Therefore,

$$\gamma_{\text{lower}} = 2\pi \sin^2\frac{\theta}{2} \tag{24}$$

It is also interesting to compute the vector $\vec{\Omega}$. To make a transformation to cartesian coordinates, let us write Ω as a form:

$$\Omega = \mp\frac{1}{2}\sin\theta d\theta \wedge d\phi = \pm\frac{1}{2} d\cos\theta \wedge d\phi \tag{25}$$

Here minus is for upper and plus for lower state. After making transrormation to Cartesian coordinates, we obtain

$$\Omega = \mp\frac{1}{2r^3}\epsilon_{ijk} x_i dx_j \wedge dx_k \tag{26}$$

Therefore,

$$\vec{\Omega} = \mp\frac{\vec{r}}{2r^3} \tag{27}$$