Rabi oscillation, Berry phase, and topological insulators

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In this problem, the connection between Rabi oscillation, Berry phase, and topological insulators is discussed.

• Rabi oscillation

The Rabi oscillation is observed in a two-state system, say, a spin-1/2 system, whose dynamics is governed by the Zeeman-coupling Hamiltonian:

$$H = -g\mathbf{S} \cdot \mathbf{B}, \tag{1}$$

where $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$ with $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, where the Pauli matrices are defined as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2}$$

Now, let us imagine that the **B**-field is rotating within the xy-plane:

$$\mathbf{B} = B_0\hat{z} + B_1\left(\cos\omega t\,\hat{x} + \sin\omega t\,\hat{y}\right). \tag{3}$$

Then, the Schrödinger equation can be explicitly written as follows:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \begin{pmatrix} \hbar\Omega/2 & \gamma e^{-i\omega t} \\ \gamma e^{i\omega t} & -\hbar\Omega/2 \end{pmatrix}|\psi\rangle, \tag{4}$$

where $\hbar\Omega/2 = -gB_0$ and $\gamma = -gB_1\hbar/2$.

(a) Show that the general solution of the above Schrödinger equation is given as follows:

$$|\psi(t)\rangle = \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2} \end{pmatrix}\begin{pmatrix} \cos\tilde{\Omega}t - i\cos\theta\sin\tilde{\Omega}t & -i\sin\theta\sin\tilde{\Omega}t \\ -i\sin\theta\sin\tilde{\Omega}t & \cos\tilde{\Omega}t + i\cos\theta\sin\tilde{\Omega}t \end{pmatrix}|\psi(t=0)\rangle, \tag{5}$$

where $\hbar\tilde{\Omega} = \sqrt{\frac{\hbar^2}{4}(\Omega - \omega)^2 + \gamma^2}$ and $\tan\theta = \frac{\gamma}{\hbar(\Omega-\omega)/2}$. Argue that this above solution describes the resonance behavior at $\omega = \Omega$.

(b) Show that, in the adiabatic limit, i.e., $\omega \ll \Omega$, if the state begins initially as an eigenstate of the Hamiltonian at $t = 0$, it remains as the instantaneous eigenstate of the Hamiltonian at a later time t with two phase factors with one being the dynamical phase factor, $\exp\left(-\frac{i}{\hbar}\int_0^t dt' E_\pm(t')\right)$, where $E_\pm(t) = \pm\hbar\Omega_*/2 = \pm\sqrt{\frac{\hbar^2}{4}\Omega^2 + \gamma^2}$, and the other being an geometrical phase factor given by $\exp\left(\pm i\frac{\Omega}{2\Omega_*}\omega t\right)$. Show that, after completing the full rotation at $t = 2\pi/\omega$, the state returns to itself with an additional phase factor given by $\exp\left(\mp\frac{i}{2}S(\theta_0)\right)$, where $\cos\theta_0 = \Omega/\Omega_*$ and $S(\theta_0) = 2\pi(1 - \cos\theta_0)$ is the solid angle enclosed by the closed path of the **B**-field during the full rotation between $t = 0$ and $2\pi/\omega$. This additional phase is called the Berry phase.

• Berry phase

Imagine that a Hamiltonian depends on time through the time-dependent vector, $\mathbf{R}(t)$: $H = H(\mathbf{R}(t))$. Also, let us assume that $\mathbf{R}(t)$ changes very slowly in time compared to an intrinsic time scale in the system, say, the inverse of the energy level spacing between adjacent instantaneous eigenstates.

(a) In this situation, show that, if the state begins as an instantaneous eigenstate of the Hamiltonian, i.e., $H(\mathbf{R}(t = 0))$, it returns to itself with the Berry phase given below after $\mathbf{R}$ completes a closed path C:

$$\Gamma_n = i\oint_C d\mathbf{R} \cdot \langle\psi_{n*}(\mathbf{R})|\nabla_{\mathbf{R}}|\psi_{n*}(\mathbf{R})\rangle, \tag{6}$$

where $|\psi_{n*}(\mathbf{R})\rangle$ is the instantaneous eigenstate of $H(\mathbf{R}(t))$ with the instantaneous eigenvalue $E_{n*}(\mathbf{R})$.

(b) The above equation can be rewritten as follows:

$$\Gamma_n = \oint_C d\mathbf{R} \cdot \mathcal{A}_n(\mathbf{R}), \tag{7}$$

where $\mathcal{A}_n(\mathbf{R}) = i\langle\psi_{n*}(\mathbf{R})|\nabla_{\mathbf{R}}|\psi_{n*}(\mathbf{R})\rangle$ is called the Berry connection. Argue that $\mathcal{A}_n(\mathbf{R})$ can be regarded as the vector potential similar to that appearing in the electromagnetism. By using the Stoke's theorem, the above equation can be again rewritten as follows:

$$\Gamma_n = \int_S d\mathbf{S} \cdot \mathcal{B}_n(\mathbf{R}), \tag{8}$$

where $\mathcal{B}_n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathcal{A}_n(\mathbf{R})$ is called the Berry curvature. Show that

$$\mathcal{B}_n(\mathbf{R}) = -\mathrm{Im} \sum_{m \neq n} \frac{\langle\psi_{n*}(\mathbf{R})| \left[\nabla_{\mathbf{R}} H(\mathbf{R})\right] |\psi_{m*}(\mathbf{R})\rangle \times \langle\psi_{m*}(\mathbf{R})| \left[\nabla_{\mathbf{R}} H(\mathbf{R})\right] |\psi_{n*}(\mathbf{R})\rangle}{[E_{n*}(\mathbf{R}) - E_{m*}(\mathbf{R})]^2}. \tag{9}$$

(c) Show that the Berry phase obtained from the exact solution can be reproduced by using the above equation for $\mathcal{B}_n(\mathbf{R})$. In particular, show that the Berry curvature is generated by the Dirac monopole in the $\mathbf{R}$-space.

• **Topological insulators**

The dynamics of electrons in a two-dimensional topological insulator is described by the Hamiltonian of the following generic form:

$$H_{\uparrow}(\mathbf{k}) = \epsilon_{\mathbf{k}}\mathbb{I} + \mathbf{d}_{\mathbf{k}} \cdot \boldsymbol{\sigma} \tag{10}$$

for spin-up electrons and $H_{\downarrow}(\mathbf{k}) = H_{\uparrow}^*(-\mathbf{k})$ for spin-down electrons. The concrete mathematical forms of $\epsilon_{\mathbf{k}}$ and $\mathbf{d}_{\mathbf{k}}$ depend on specific microscopic models. But, in general, $\mathbf{d}_{\mathbf{k}}$ can be expanded around where the energy gap is minimum, say, $\mathbf{k} = 0$, as follows:

$$\mathbf{d}_{\mathbf{k}} \simeq (Ak_x, Ak_y, M + B(k_x^2 + k_y^2)). \tag{11}$$

Show that the band topology becomes non-trivial if $M/B < 0$ and trivial otherwise.