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NOTES

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DEPARTMENT OF PHYSICS

Quantum Theory of Matter

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Happy New Term :D

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- Geometric and dynamical phases under adiabatic evolution.

1.1 Adiabatic Evolution

1.1.1 Berry Connection

Consider the Hamiltonian $\hat{H}$ with parameter $\boldsymbol{R}$. The system has a discrete set of energy eigenstates, labelled by ν, then

$$\hat{H}(\boldsymbol{R})\,|\nu,\boldsymbol{R}\rangle = E_\nu(\boldsymbol{R})\,|\nu,\boldsymbol{R}\rangle \tag{1}$$

Consider slow variation in $\boldsymbol{R}(t)$ in time t, system prepared in state ν stays in state ν in the adiabatic regime, *i.e.*, $|\nu,\boldsymbol{R}+\delta\boldsymbol{R}\rangle \simeq |\nu,\boldsymbol{R}\rangle$. The eigenstates $|\nu,\boldsymbol{R}(t)\rangle$ are defined as **instantaneous eigenstates** at time t.

Consider time evolution in the adiabatic regime

$$i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle = \hat{H}(\boldsymbol{R}(t))\,|\psi(t)\rangle \tag{2}$$

We prepare the system in eigenstate

$$|\psi(t=0)\rangle = |\nu,\boldsymbol{R}(t=0)\rangle \tag{3}$$

For a constant $\boldsymbol{R}$, we have $|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar}E_\nu(\boldsymbol{R})t\right]|\nu,\boldsymbol{R}\rangle$. So we guess

$$|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar}\int_0^t E_\nu(\boldsymbol{R}(t'))\mathrm{d}t'\right]|\nu,\boldsymbol{R}(t=0)\rangle \tag{4}$$

Suppose

$$|\psi(t)\rangle = \mathrm{e}^{i\gamma(t)}\,|\nu,\boldsymbol{R}(t)\rangle \tag{5}$$

Consider the Eq.(2),

$$\text{RHS} = \hat{H}(\boldsymbol{R}(t))\,|\psi(t)\rangle = \mathrm{e}^{i\gamma}E_\nu(\boldsymbol{R}(t))\,|\nu,\boldsymbol{R}(t)\rangle \tag{6}$$

$$\begin{aligned}\text{LHS} = i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle &= \mathrm{e}^{i\gamma}\left(-\hbar\dot{\gamma} + i\hbar\frac{\partial}{\partial t}\right)|\nu,\boldsymbol{R}(t)\rangle \\ &= \mathrm{e}^{i\gamma}\left(-\hbar\dot{\gamma} + i\hbar\dot{\boldsymbol{R}}\cdot\boldsymbol{\nabla}_{\boldsymbol{R}}\right)|\nu,\boldsymbol{R}(t)\rangle\end{aligned} \tag{7}$$

Then we have

$$\mathrm{e}^{i\gamma}E_\nu(\boldsymbol{R}(t))\,|\nu,\boldsymbol{R}(t)\rangle = \mathrm{e}^{i\gamma}\left(-\hbar\dot{\gamma} + i\hbar\dot{\boldsymbol{R}}\cdot\boldsymbol{\nabla}_{\boldsymbol{R}}\right)|\nu,\boldsymbol{R}(t)\rangle \tag{8}$$

Take overlap with $\langle\nu,\boldsymbol{R}|$, we have

$$E_\nu(\boldsymbol{R}) = -\hbar\dot{\gamma} + i\hbar\dot{\boldsymbol{R}}\cdot\langle\nu,\boldsymbol{R}|\,\boldsymbol{\nabla}_{\boldsymbol{R}}\,|\nu,\boldsymbol{R}\rangle \tag{9}$$

Rearranging this equation

$$\hbar\dot{\gamma} = -E_\nu(\boldsymbol{R}) + i\hbar\dot{\boldsymbol{R}} \cdot \langle \nu, \boldsymbol{R}| \boldsymbol{\nabla_R} |\nu, \boldsymbol{R}\rangle \tag{10}$$

so

$$\begin{aligned}\gamma(t) =& -\frac{1}{\hbar}\int_0^t E(\boldsymbol{R}(t'))\mathrm{d}t' + i\int_0^t \langle \nu, \boldsymbol{R}| \boldsymbol{\nabla_R} |\nu, \boldsymbol{R}\rangle \cdot \frac{\mathrm{d}\boldsymbol{R}}{\mathrm{d}t'}\mathrm{d}t' \\ =& -\frac{1}{\hbar}\int_0^t E(\boldsymbol{R}(t'))\mathrm{d}t' + i\int_C \langle \nu, \boldsymbol{R}| \boldsymbol{\nabla_R} |\nu, \boldsymbol{R}\rangle \cdot \mathrm{d}\boldsymbol{R} \\ =&\gamma_{\text{dyn}} + \gamma_{\text{geom}}\end{aligned} \tag{11}$$

Here, we get two phases. The first term is *dynamic phase*

$$\gamma_{\text{dyn}} = -\frac{1}{\hbar}\int_0^t E(\boldsymbol{R}(t'))\mathrm{d}t' \tag{12}$$

and the second term is *geometric phase*.

$$\gamma_{\text{geom}} = i\int_C \langle \nu, \boldsymbol{R}| \nabla_{\boldsymbol{R}} |\nu, \boldsymbol{R}\rangle \cdot \mathrm{d}\boldsymbol{R} = \int_C \boldsymbol{A}(\boldsymbol{R}) \cdot \mathrm{d}\boldsymbol{R} \tag{13}$$

Here $\boldsymbol{A}(\boldsymbol{R})$ is called Berry connection

$$\boldsymbol{A}_\nu(\boldsymbol{R}) = i\,\langle \nu, \boldsymbol{R}| \nabla_{\boldsymbol{R}} |\nu, \boldsymbol{R}\rangle \tag{14}$$

1.1.2 Example: Spin-half Electron in Zeeman Field

In magnetic field, $\boldsymbol{d} = (d_x, d_y, 0) = d(\cos\phi, \sin\phi, 0)$. The Zeeman Hamiltonian can be expressed as

$$\hat{H} = \boldsymbol{d}(t) \cdot \hat{\sigma} = d_x\hat{\sigma}_x + d_y\hat{\sigma}_y = \sum_{s,s'=\uparrow,\downarrow} h_{ss'}\,|s\rangle\,\langle s'| \tag{15}$$

where

$$h = \begin{pmatrix} 0 & d_x - id_y \\ d_x + id_y & 0 \end{pmatrix} = d\begin{pmatrix} 0 & \mathrm{e}^{-i\phi} \\ \mathrm{e}^{i\phi} & 0 \end{pmatrix} \tag{16}$$

We choose $\phi(t) = 2\pi t/T$, and d is a constant when the system evolves from $t = 0$ to $t = T$. The instantaneous eigenstates at given ϕ

$$|+, \phi\rangle = \frac{1}{\sqrt{2}}(+\mathrm{e}^{-i\phi}\,|\uparrow\rangle + |\downarrow\rangle) \tag{17}$$

$$|-, \phi\rangle = \frac{1}{\sqrt{2}}(-\mathrm{e}^{-i\phi}\,|\uparrow\rangle + |\downarrow\rangle) \tag{18}$$

Prepare the system in the excited state $|+\rangle$, the instantaneous eigenstate is

$$|+, \phi\rangle = \frac{1}{\sqrt{2}}(\mathrm{e}^{-i\phi}\,|\uparrow\rangle + |\downarrow\rangle) \tag{19}$$

with eigenvalue $E_+ = d$. After one full 2π-rotation of d, The phases are

$$\gamma_{\text{dyn}} = -\frac{1}{\hbar}\int_0^T E_+\mathrm{d}t = -\frac{d}{\hbar}T \tag{20}$$

$$\gamma_{\text{geom}} = i\int_0^{2\pi} \langle +, \phi|\, \partial_\phi\, |+, \phi\rangle\, \mathrm{d}\phi = i\int_0^{2\pi} \langle\uparrow|\, \frac{\mathrm{e}^{i\phi}}{\sqrt{2}}(-i)\frac{\mathrm{e}^{-i\phi}}{\sqrt{2}}\,|\uparrow\rangle\, \mathrm{d}\phi = \pi \tag{21}$$

1.2 Berry Curvature

1.2.1 Gauge Choice

The instantaneous eigenstates chosen to be single-valued and differentiable. If we change instantaneous eigenstates by a single-valued, differentiable phase factor

$$|\nu, \boldsymbol{R}\rangle \to \mathrm{e}^{i\chi(\boldsymbol{R})}\,|\nu, \boldsymbol{R}\rangle \tag{22}$$

$$\boldsymbol{A}_\nu(\boldsymbol{R}) \to \boldsymbol{A}_\nu(\boldsymbol{R}) - \boldsymbol{\nabla}_{\boldsymbol{R}}\chi(\boldsymbol{R}) \tag{23}$$

For a closed path C over parameter space, the geometry phase

$$\gamma_{\text{geom}} = \oint_C \boldsymbol{A}_\nu(\boldsymbol{R}) \cdot \mathrm{d}\boldsymbol{R} \to \oint_C \boldsymbol{A}_\nu(\boldsymbol{R}) \cdot \mathrm{d}\boldsymbol{R} - \underbrace{[\chi(\boldsymbol{R}(T)) - \chi(\boldsymbol{R}(0))]}_{\Delta\chi=2\pi n} \tag{24}$$

Hence, geometric phase γ_{geom} changes, but $\mathrm{e}^{i\gamma_{\text{geom}}}$ is invariant.