

Lecture 2 : Berry Phase and Chern number

Berry Phase review

Assuming a physical system is depended on some parameters $\mathbf{R} = (R_1, R_2, \dots, R_N)$, we have the *snapshot* Hamiltonian $H(\mathbf{R})$, its eigen-values and eigen-states:

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

where $|n(\mathbf{R})\rangle$ can have an arbitrary phase prefactor.

The parameters $\mathbf{R}(\mathbf{t})$ are slowly changed with time t , then the adiabatic evolution of time-dependent Schrodinger equation:

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

Take the Ansatz: $|\psi(t)\rangle = e^{i\gamma_n(t)} e^{-i \int_0^t E_n(\mathbf{R}(\mathbf{t}')) dt'} |n(\mathbf{R}(\mathbf{t}))\rangle$, we have

$$- \left(\frac{d}{dt} \gamma_n \right) |n\rangle + i \left| \frac{d}{dt} n \right\rangle = 0$$

That gives the Berry phase expression:

$$\gamma_n(\mathcal{C}) = \int_{\mathcal{C}} i \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle d\mathbf{R}$$

Define *Berry connection*:

$$\mathbf{A}^{(n)}(\mathbf{R}) = i \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle = -Im \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle$$

Gauge transformation:

$$|n(\mathbf{R})\rangle \rightarrow e^{i\alpha(\mathbf{R})} |n(\mathbf{R})\rangle$$

$$\mathbf{A}^{(n)}(\mathbf{R}) \rightarrow \mathbf{A}^{(n)}(\mathbf{R}) - \nabla_{\mathbf{R}} \alpha(\mathbf{R})$$

$\gamma = \oint \mathbf{A}(\mathbf{R}) d\mathbf{R}$ is gauge invariant.

Gauge and Parallel transportation: recalling the arbitrary phase

$$|n(\mathbf{R})\rangle \rightarrow e^{i\alpha(\mathbf{R})} |n(\mathbf{R})\rangle$$

why shouldn't we choose one which makes

$$\frac{d}{dt}|n\rangle \equiv 0$$

from

$$-\left(\frac{d}{dt}\gamma_n\right)|n\rangle + i\left|\frac{d}{dt}n\right\rangle = 0$$

then we have

$$\gamma_n = 0$$

There is no Berry Phase in this frame, which is called *inertial frame*, the condition $\frac{d}{dt}|n\rangle \equiv 0$ is called *parallel transportation*. All the information resorted to $|n(\mathbf{R})\rangle$, similar to a transformation from *active frame* to *passive frame*.

Berry curvature

Define the *Berry curvature*:

$$\mathbf{B}(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathbf{A}^{(n)}(\mathbf{R})$$

Using Stokes theorem, we have for the Berry Phase:

$$\gamma_n(\mathcal{C}) = \int_{\mathcal{S}} \mathbf{B}^{(n)}(\mathbf{R}) d\mathcal{S}$$

where \mathcal{S} is any surface whose boundary is the loop \mathcal{C} .

Two useful formula:

- $B_j = \epsilon_{jkl} \partial_k A_l = -Im \epsilon_{jkl} \partial_k \langle n | \partial_l n \rangle = -Im \epsilon_{jkl} \langle \partial_k n | \partial_l n \rangle$, that is $\mathbf{B}^{(n)} = -Im \sum_{n' \neq n} \langle \nabla n | n' \rangle \times \langle n' | \nabla n \rangle$.

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- $\mathbf{B}^{(n)} = -Im \sum_{n' \neq n} \langle \nabla n | n' \rangle \times \langle n' | \nabla n \rangle$ to calculate $\langle n' | \nabla n \rangle$, start from:

$$\begin{aligned} H(\mathbf{R})|n\rangle &= E_n|n\rangle \\ \Rightarrow (\nabla H)|n\rangle + H|\nabla n\rangle &= (\nabla E_n)|n\rangle + E_n|\nabla n\rangle \\ \Rightarrow \langle n' | \nabla H | n \rangle + \langle n' | H | \nabla n \rangle &= E_n \langle n' | \nabla n \rangle \\ \Rightarrow \langle n' | \nabla n \rangle &= \frac{\langle n' | \nabla H | n \rangle}{E_n - E_{n'}} \end{aligned}$$

then we get:

$$\mathbf{B}^{(n)} = -Im \sum_{n' \neq n} \langle \nabla n | n' \rangle \times \langle n' | \nabla n \rangle = -Im \sum_{n' \neq n} \frac{\langle n | \nabla H | n' \rangle \times \langle n' | \nabla H | n \rangle}{(E_n - E_{n'})^2}$$

which is gauge invariant!

Berry curvature from perturbation theory

We can use time-independent perturbation theory to derive the changes of instant snapshot basis:

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

we have

$$|n(\mathbf{R} + \Delta\mathbf{R})\rangle = |n(\mathbf{R})\rangle + \sum_{m \neq n} \frac{\langle m | H(\mathbf{R} + \Delta\mathbf{R}) - H(\mathbf{R}) | n \rangle}{E_n - E_m} |m(\mathbf{R})\rangle$$

We see that $\langle n | \Delta n(\mathbf{R}) \rangle = 0$ which means we have used *parallel transport* gauge, more general, we should add a arbitrary phase factor in the above equation for $|n(\mathbf{R} + \Delta\mathbf{R})\rangle$.

$$\nabla_{\mathbf{R}} |n\rangle = \sum_{m \neq n} \frac{\langle m | \nabla_{\mathbf{R}} H | n \rangle}{E_n - E_m} |m\rangle$$

From $\mathbf{B}^{(n)} = -Im \sum_{n' \neq n} \langle \nabla n | n' \rangle \times \langle n' | \nabla n \rangle$ we also get:

$$\mathbf{B}^{(n)} = -Im \sum_{n' \neq n} \frac{\langle n | \nabla H | n' \rangle \times \langle n' | \nabla H | n \rangle}{(E_n - E_{n'})^2}$$

Also notice:

$$\begin{aligned} \sum_n \mathbf{B}^{(n)} &= -Im \sum_n \sum_{n' \neq n} \frac{\langle n | \nabla H | n' \rangle \times \langle n' | \nabla H | n \rangle}{(E_n - E_{n'})^2} \\ &= -Im \sum_n \sum_{n' < n} \frac{\langle n | \nabla H | n' \rangle \times \langle n' | \nabla H | n \rangle + \langle n' | \nabla H | n \rangle \times \langle n | \nabla H | n' \rangle}{(E_n - E_{n'})^2} \\ &= 0 \end{aligned}$$

Which gives:

$$\sum_n \gamma_n(\mathcal{C}) = \int_{\mathcal{S}} \sum_n \mathbf{B}^{(n)}(\mathbf{R}) d\mathcal{S} = 0$$

Benchmark: Spin-1/2

Gauge!Gauge!Gauge!

2-level Hamiltonian $H(\mathbf{R}) = h_0(\mathbf{R})\sigma_0 + \mathbf{h}(\mathbf{R}) \cdot \boldsymbol{\sigma}$, we can set $h_0 = 0$, because it does not affect the eigenstates, eigen-energy are $\pm|\mathbf{h}|$, introduce the unit vector: $\hat{\mathbf{h}} = \mathbf{h}/|\mathbf{h}|$, the endpoints of $\hat{\mathbf{h}}$ map out the surface of a unit sphere, called the *Bloch sphere* shows below:

