Física de Semiconductores

Lección 12

Position operator

- Let's write $\Psi\left(\boldsymbol{r}\right)=\int d\boldsymbol{k}\Psi\left(\boldsymbol{k}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$
- Then

$$\boldsymbol{r}\Psi\left(\boldsymbol{r}\right)=\int d\boldsymbol{k}\Psi\left(\boldsymbol{k}\right)\boldsymbol{r}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$=\int d\boldsymbol{k}\Psi\left(\boldsymbol{k}\right)\left(-i\frac{\partial}{\partial\boldsymbol{k}}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}=\int d\boldsymbol{k}\left(i\frac{\partial\Psi\left(\boldsymbol{k}\right)}{\partial\boldsymbol{k}}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

- where we have integrated by parts. Then the position operator in momentum representation is $\hat{\boldsymbol{r}}=i\frac{\partial}{\partial\boldsymbol{k}}$

Bloch wave expansion

- Let's suppose that we expand in terms of Bloch waves instead of plane waves:

$$\Psi\left(\boldsymbol{r}\right) = \sum_{n} \int d\boldsymbol{k} \Psi_{n}\left(\boldsymbol{k}\right) \psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

$$= \sum_{n,m} \int d\boldsymbol{k} \delta_{nm} \Psi_{n}\left(\boldsymbol{k}\right) \psi_{m\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- An operator is then

$$\hat{O}\Psi\left(\boldsymbol{r}\right) = \sum_{n,m} \int d\boldsymbol{k} \hat{O}_{nm}\left(\boldsymbol{k}\right) \Psi_{n}\left(\boldsymbol{k}\right) \psi_{m\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- we would like to find this for the position operator

Position operator in Bloch wave basis (I)

- This means

$$\boldsymbol{r}\Psi\left(\boldsymbol{r}\right)=\sum_n\int d\boldsymbol{k}\Psi_n\left(\boldsymbol{k}\right)u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)\boldsymbol{r}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$=\sum_n\int d\boldsymbol{k}\Psi_n\left(\boldsymbol{k}\right)u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)\left(-i\frac{\partial}{\partial\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\right)$$

$$=\sum_n\int d\boldsymbol{k}\left(i\frac{\partial}{\partial\boldsymbol{k}}\Psi_n\left(\boldsymbol{k}\right)u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$=\sum_n\int d\boldsymbol{k}\left(iu_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)\frac{\partial\Psi_n\left(\boldsymbol{k}\right)}{\partial\boldsymbol{k}}+i\Psi_n\left(\boldsymbol{k}\right)\frac{\partial u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial\boldsymbol{k}}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

Position operator in Bloch wave basis (II)

$$= \sum_n \int d\boldsymbol{k} \left(i u_{n\boldsymbol{k}}(\boldsymbol{r}) \frac{\partial \Psi_n(\boldsymbol{k})}{\partial \boldsymbol{k}} + i\Psi_n(\boldsymbol{k}) \frac{\partial u_{n\boldsymbol{k}}(\boldsymbol{r})}{\partial \boldsymbol{k}} \right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$= \sum_n \int d\boldsymbol{k} \left(i\psi_{n\boldsymbol{k}}(\boldsymbol{r}) \frac{\partial \Psi_n(\boldsymbol{k})}{\partial \boldsymbol{k}} + i\Psi_n(\boldsymbol{k}) \int d\boldsymbol{r}' \delta(\boldsymbol{r} - \boldsymbol{r}') e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \frac{\partial u_{n\boldsymbol{k}}(\boldsymbol{r}')}{\partial \boldsymbol{k}} \right)$$

$$= \sum_n \int d\boldsymbol{k} \left(i\psi_{n\boldsymbol{k}}(\boldsymbol{r}) \frac{\partial \Psi_n(\boldsymbol{k})}{\partial \boldsymbol{k}} + i\Psi_n(\boldsymbol{k}) \int d\boldsymbol{r}' \sum_m u^*_{m\boldsymbol{k}}(\boldsymbol{r}') u_{m\boldsymbol{k}}(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \frac{\partial u_{n\boldsymbol{k}}(\boldsymbol{r}')}{\partial \boldsymbol{k}} \right.$$

$$= \sum_n \int d\boldsymbol{k} \left(i\psi_{n\boldsymbol{k}}(\boldsymbol{r}) \frac{\partial \Psi_n(\boldsymbol{k})}{\partial \boldsymbol{k}} + i\Psi_n(\boldsymbol{k}) \sum_m \psi_{m\boldsymbol{k}}(\boldsymbol{r}) \int d\boldsymbol{r}' u^*_{m\boldsymbol{k}}(\boldsymbol{r}') \frac{\partial u_{n\boldsymbol{k}}(\boldsymbol{r}')}{\partial \boldsymbol{k}} \right)$$

$$= \sum_n \int d\boldsymbol{k} \left(i\psi_{n\boldsymbol{k}}(\boldsymbol{r}) \frac{\partial \Psi_n(\boldsymbol{k})}{\partial \boldsymbol{k}} + \Psi_n(\boldsymbol{k}) \sum_m \mathcal{A}_{mn}(\boldsymbol{k}) \psi_{m\boldsymbol{k}}(\boldsymbol{r}) \right)$$

Berry connection

- We have defined the Berry connection as

$$\mathcal{A}_{mn}\left(\boldsymbol{k}\right) = i\int dr\, u^{*}_{m\boldsymbol{k}}\left(\boldsymbol{r}\right)\frac{\partial}{\partial \boldsymbol{k}}u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- We will examine the meaning of this expression later

Final expression for position opp

$$\boldsymbol{r}\Psi\left(\boldsymbol{r}\right)=\sum_{n,m}\int d\boldsymbol{k}\left(i\frac{\partial}{\partial\boldsymbol{k}}\delta_{nm}+\mathcal{A}_{mn}\left(\boldsymbol{k}\right)\right)\Psi_{n}\left(\boldsymbol{k}\right)\psi_{m\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

Comparing with

$$\hat{O}\Psi\left(\boldsymbol{r}\right)=\sum_{n,m}\int d\boldsymbol{k}\hat{O}_{nm}\left(\boldsymbol{k}\right)\Psi_{n}\left(\boldsymbol{k}\right)\psi_{m\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

We conclude $$\hat{\boldsymbol{r}}_{nm}=\left(i\frac{\partial}{\partial\boldsymbol{k}}\delta_{nm}+\mathcal{A}_{mn}\left(\boldsymbol{k}\right)\right)$$

In many cases $\Psi_{m}\left(\boldsymbol{k}\right)=0 \quad \text{for } m\neq n$. Then we only need

$$\hat{\boldsymbol{r}}_{nn}\equiv\hat{\boldsymbol{r}}_{n}=\left(i\frac{\partial}{\partial\boldsymbol{k}}+\mathcal{A}_{nn}\left(\boldsymbol{k}\right)\right)\equiv\left(i\frac{\partial}{\partial\boldsymbol{k}}+\mathcal{A}_{n}\left(\boldsymbol{k}\right)\right)$$

Explanation for the extra term I

- The Bloch wave function is a solution of

$$-\left[\frac{\hbar^2\nabla^2}{2m}+V\left(\boldsymbol{r}\right)\right]\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=E_{n\boldsymbol{k}}\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- Let's consider

$$\psi'_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=e^{i\phi\left(\boldsymbol{k}\right)}\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- Then

$$-\left[\frac{\hbar^2\nabla^2}{2m}+V\left(\boldsymbol{r}\right)\right]\psi'_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=E_{n\boldsymbol{k}}\psi'_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- Accordingly, observables cannot depend on phase

Explanation for the extra term II

- Suppose that I change the phase of the Bloch function

$$\Psi\left(\boldsymbol{r}\right)=\sum_{n}\int d\boldsymbol{k}\Psi_{n}\left(\boldsymbol{k}\right)\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=\sum_{n}\int d\boldsymbol{k}\Psi'_{n}\left(\boldsymbol{k}\right)\psi'_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- with $\psi'_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=e^{i\phi\left(\boldsymbol{k}\right)}\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$. Then

$$\Psi'_{n}\left(\boldsymbol{k}\right)=e^{-i\phi\left(\boldsymbol{k}\right)}\Psi_{n}\left(\boldsymbol{k}\right)$$

Explanation II

- Then suppose I ignore the A term

$$\int d\boldsymbol{r}\Psi^*(\boldsymbol{r})\hat{\boldsymbol{r}}\Psi(\boldsymbol{r}) = \int d\boldsymbol{r}\int d\boldsymbol{k}\Psi'^*_n(\boldsymbol{k})\psi'^*_{n\boldsymbol{k}}(\boldsymbol{r})\, i\frac{\partial\Psi'_n(\boldsymbol{k})}{\partial\boldsymbol{k}}\psi'_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$= \int d\boldsymbol{r}\int d\boldsymbol{k}\Psi'^*_n(\boldsymbol{k})\psi^*_{n\boldsymbol{k}}(\boldsymbol{r})\, i\frac{\partial\Psi'_n(\boldsymbol{k})}{\partial\boldsymbol{k}}\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$= \int d\boldsymbol{r}\int d\boldsymbol{k}\Psi'^*_n(\boldsymbol{k})\psi^*_{n\boldsymbol{k}}(\boldsymbol{r})\, i\left[\frac{\partial\Psi_n(\boldsymbol{k})}{\partial\boldsymbol{k}}e^{-i\phi(\boldsymbol{k})} - i\Psi_n(\boldsymbol{k})e^{-i\phi(\boldsymbol{k})}\frac{\partial\phi(\boldsymbol{k})}{\partial\boldsymbol{k}}\right]\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$= \int d\boldsymbol{r}\int d\boldsymbol{k}\Psi'^*_n(\boldsymbol{k})e^{-i\phi(\boldsymbol{k})}\psi^*_{n\boldsymbol{k}}(\boldsymbol{r})\, i\frac{\partial\Psi_n(\boldsymbol{k})}{\partial\boldsymbol{k}}\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$+\int d\boldsymbol{r}\int d\boldsymbol{k}\Psi'^*_n(\boldsymbol{k})e^{-i\phi(\boldsymbol{k})}\psi^*_{n\boldsymbol{k}}(\boldsymbol{r})\left[\Psi_n(\boldsymbol{k})\frac{\partial\phi(\boldsymbol{k})}{\partial\boldsymbol{k}}\right]\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

Explanation III

$$= \int d\boldsymbol{r} \int d\boldsymbol{k} \Psi'^{*}_{n}\left(\boldsymbol{k}\right) e^{-i\phi\left(\boldsymbol{k}\right)} \psi^{*}_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) i \frac{\partial \Psi_{n}\left(\boldsymbol{k}\right)}{\partial \boldsymbol{k}} \psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

$$+ \int d\boldsymbol{r} \int d\boldsymbol{k} \Psi'^{*}_{n}\left(\boldsymbol{k}\right) e^{-i\phi\left(\boldsymbol{k}\right)} \psi^{*}_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) \left[\Psi_{n}\left(\boldsymbol{k}\right) \frac{\partial \phi\left(\boldsymbol{k}\right)}{\partial \boldsymbol{k}} \right] \psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

$$= \int d\boldsymbol{r} \int d\boldsymbol{k} \Psi^{*}_{n}\left(\boldsymbol{k}\right) \psi^{*}_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) i \frac{\partial \Psi_{n}\left(\boldsymbol{k}\right)}{\partial \boldsymbol{k}} \psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

$$+ \int d\boldsymbol{r} \int d\boldsymbol{k} \Psi^{*}_{n}\left(\boldsymbol{k}\right) \psi^{*}_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) \left[\Psi_{n}\left(\boldsymbol{k}\right) \frac{\partial \phi\left(\boldsymbol{k}\right)}{\partial \boldsymbol{k}} \right] \psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

This is a problem because all properties should be independent of phase. But

Explanation IV

But let's see how the Berry connection transforms

$$\mathcal{A}'_n(\boldsymbol{k}) = i\int dr u'^*_{n\boldsymbol{k}}(\boldsymbol{r})\frac{\partial}{\partial \boldsymbol{k}}u'_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$= i\int dr e^{-i\phi(\boldsymbol{k})}u^*_{n\boldsymbol{k}}(\boldsymbol{r})\frac{\partial}{\partial \boldsymbol{k}}e^{i\phi(\boldsymbol{k})}u_{n\boldsymbol{k}}(\boldsymbol{r}) =$$

$$= i\left[\int d\boldsymbol{r}u^*_{n\boldsymbol{k}}(\boldsymbol{r})\left[\frac{\partial u_{n\boldsymbol{k}}(\boldsymbol{r})}{\partial \boldsymbol{k}} + u_{n\boldsymbol{k}}(\boldsymbol{r})i\frac{\partial \phi(\boldsymbol{k})}{\partial \boldsymbol{k}}\right]\right]$$

$$= i\int d\boldsymbol{r}u^*_{n\boldsymbol{k}}(\boldsymbol{r})\frac{\partial u_{n\boldsymbol{k}}(\boldsymbol{r})}{\partial \boldsymbol{k}} - \frac{\partial \phi(\boldsymbol{k})}{\partial \boldsymbol{k}} = \mathcal{A}_n(\boldsymbol{k}) - \frac{\partial \phi(\boldsymbol{k})}{\partial \boldsymbol{k}}$$

Explanation V

But

$$-\int d\boldsymbol{r}\int d\boldsymbol{k}\Psi_{n}^{*}\left(\boldsymbol{k}\right)\psi_{n\boldsymbol{k}}^{*}\left(\boldsymbol{r}\right)\frac{\partial\phi\left(\boldsymbol{k}\right)}{\partial\boldsymbol{k}}\Psi_{n}\left(\boldsymbol{k}\right)\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

so that the Berry connection exactly compensates for the phase, and the result for the average position becomes independent of phase, as it should.

Analogía con el potencial vector

- Hamiltonian of a charge:

$$H = \frac{1}{2m}\left[\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\left(\boldsymbol{r}\right)\right]^2 - e\varphi\left(\boldsymbol{r}\right)$$

- Then

$$\boldsymbol{A} \rightarrow \boldsymbol{A}' = \boldsymbol{A} + \boldsymbol{\nabla}\phi\left(\boldsymbol{r}\right)$$

$$\varphi \rightarrow \varphi' = \varphi - \frac{1}{c}\frac{\partial\phi\left(\boldsymbol{r}\right)}{\partial t}$$

$$\psi \rightarrow \psi' = \psi e^{i\frac{ec}{\hbar}\phi\left(\boldsymbol{r}\right)}$$

The velocity and force operators

- The quantities we are interested in are

$$\frac{d\hat{\boldsymbol{r}}_n}{dt} = \frac{i}{\hbar}\left[H, \hat{\boldsymbol{r}}_n\right] = \frac{i}{\hbar}\left[H, i\frac{\partial}{\partial \boldsymbol{k}} + \mathcal{A}_n\left(\boldsymbol{k}\right)\right]$$

$$\hbar\frac{d\boldsymbol{k}}{dt} = \frac{d\boldsymbol{\pi}}{dt} = \frac{i}{\hbar}\left[H, \boldsymbol{\pi}\right] + \frac{\partial \boldsymbol{\pi}}{\partial t} = \frac{i}{\hbar}\left[H, \boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right] + \frac{e}{c}\frac{\partial \boldsymbol{A}}{\partial t}$$

- Hamiltonian of a charge:

$$H = \frac{1}{2m}\boldsymbol{\pi}^2 - e\varphi\left(\boldsymbol{r}\right) = \frac{1}{2m}\left[\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\left(\boldsymbol{r}\right)\right]^2 - e\varphi\left(\boldsymbol{r}\right)$$

Semiclassical equations

$$\hbar \frac{d\boldsymbol{k}}{dt} = -e\boldsymbol{E} - \frac{e}{c}\left(\boldsymbol{v} \times \boldsymbol{H}\right)$$

$$\frac{d\hat{\boldsymbol{r}}_n}{dt} = \frac{1}{\hbar}\frac{\partial E_n\left(\boldsymbol{k}\right)}{\partial \boldsymbol{k}} - \frac{d\boldsymbol{k}}{dt} \times \left[\frac{\partial}{\partial \boldsymbol{k}} \times \mathcal{A}_n\left(\boldsymbol{k}\right)\right]$$

Berry curvature

- We define the Berry curvature as

$$\Omega_n(\boldsymbol{k}) \equiv \frac{\partial}{\partial \boldsymbol{k}} \times \mathcal{A}_n(\boldsymbol{k})$$

- so

$$\hbar \frac{d\boldsymbol{k}}{dt} = -e\boldsymbol{E} - \frac{e}{c}\left(\boldsymbol{v} \times \boldsymbol{H}\right)$$

$$\frac{d\hat{\boldsymbol{r}}_n}{dt} = \frac{1}{\hbar}\frac{\partial E_n(\boldsymbol{k})}{\partial \boldsymbol{k}} - \frac{d\boldsymbol{k}}{dt} \times \Omega_n(\boldsymbol{k})$$

Electric field

- In the presence of an electric field only

$$\boldsymbol{v}_n\left(\boldsymbol{k}\right)=\frac{d\boldsymbol{r}_n}{dt}=\frac{1}{\hbar}\frac{\partial E_n\left(\boldsymbol{k}\right)}{\partial\boldsymbol{k}}+\frac{e\boldsymbol{E}}{\hbar}\times\Omega_n\left(\boldsymbol{k}\right)$$

Current

- The electric current is

$$\boldsymbol{j}_n = \left(-e\right)\int \frac{d\boldsymbol{k}}{\left(2\pi\right)^d}\boldsymbol{v}_n\left(\boldsymbol{k}\right)f_n\left(\boldsymbol{k}\right)$$

$$= \left(-e\right)\int \frac{d\boldsymbol{k}}{\left(2\pi\right)^d}\frac{1}{\hbar}\frac{\partial E_n\left(\boldsymbol{k}\right)}{\partial \boldsymbol{k}}f_n\left(\boldsymbol{k}\right)$$

$$+\left(-e\right)\int \frac{d\boldsymbol{k}}{\left(2\pi\right)^d}f_n\left(\boldsymbol{k}\right)\frac{e\boldsymbol{E}}{\hbar}\times\Omega_n\left(\boldsymbol{k}\right)$$

Filled band

- For a filled band

$$\boldsymbol{j}_n = (-e)\int \frac{d\boldsymbol{k}}{(2\pi)^d}\boldsymbol{v}_n(\boldsymbol{k})$$

$$= (-e)\int \frac{d\boldsymbol{k}}{(2\pi)^d}\frac{1}{\hbar}\frac{\partial E_n(\boldsymbol{k})}{\partial \boldsymbol{k}}$$

$$+(-e)\int \frac{d\boldsymbol{k}}{(2\pi)^d}\frac{e\boldsymbol{E}}{\hbar}\times\Omega_n(\boldsymbol{k})$$

- But

$$\int d\boldsymbol{k}\frac{\partial E_n(\boldsymbol{k})}{\partial \boldsymbol{k}} = 0$$

Filled band

- Therefore

$$\boldsymbol{j}_n^{\text{filled}} = \left(-e\right)\int \frac{d\boldsymbol{k}}{\left(2\pi\right)^d}\frac{e\boldsymbol{E}}{\hbar}\times\Omega_n\left(\boldsymbol{k}\right)$$

$$= -\frac{e^2}{\hbar}\boldsymbol{E}\times\frac{1}{\left(2\pi\right)^d}\int d\boldsymbol{k}\,\Omega_n\left(\boldsymbol{k}\right)$$

- When is this integral zero?

Defining phase differences

- Suppose I have two complex numbers

$$z_1 = |z_1| e^{i\phi_1}; \quad z_2 = |z_2| e^{i\phi_2}$$

- Then

$$\frac{z_1^* z_2}{|z_1||z_2|} = e^{i(\phi_2 - \phi_1)} \equiv e^{i\Delta\phi_{12}}$$

Parametric Hamiltonian

- The periodic part of the wave function satisfies

$$\left[-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}+\frac{\hbar}{m}\boldsymbol{k}\cdot\boldsymbol{p}+V\left(\boldsymbol{r}\right)\right]u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=\varepsilon_{n\boldsymbol{k}}u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

$$H\left(\boldsymbol{k}\right)u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=\varepsilon_{n\boldsymbol{k}}u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- Then we can define

$$e^{-i\Delta\phi_{12}^{n}}=\frac{\int dr u_{n\boldsymbol{k}_1}^{*}\left(\boldsymbol{r}\right)u_{n\boldsymbol{k}_2}\left(\boldsymbol{r}\right)}{\left|\int dr u_{n\boldsymbol{k}_1}^{*}\left(\boldsymbol{r}\right)u_{n\boldsymbol{k}_2}\left(\boldsymbol{r}\right)\right|}=\frac{\left\langle n\boldsymbol{k}_1\middle|n\boldsymbol{k}_2\right\rangle}{\left|\left\langle n\boldsymbol{k}_1\middle|n\boldsymbol{k}_2\right\rangle\right|}$$

- Taking logs

$$-i\Delta\phi_{12}^{n}=\ln\left\langle n\boldsymbol{k}_1\middle|n\boldsymbol{k}_2\right\rangle-\ln\left|\left\langle n\boldsymbol{k}_1\middle|n\boldsymbol{k}_2\right\rangle\right|$$

Phase definition

- But since $$\left|\frac{\langle n\boldsymbol{k}_1 | n\boldsymbol{k}_2\rangle}{\left|\langle n\boldsymbol{k}_1 | n\boldsymbol{k}_2\rangle\right|}\right| = 1$$
- $\Delta\phi_{12}^n$ is real. Then

$$\Delta\phi_{12}^n = -\mathrm{Im}\left[\ln\langle n\boldsymbol{k}_1 | n\boldsymbol{k}_2\rangle\right] + \mathrm{Im}\left[\ln\left|\langle n\boldsymbol{k}_1 | n\boldsymbol{k}_2\rangle\right|\right]$$
$$\Delta\phi_{12}^n = -\mathrm{Im}\left[\ln\langle n\boldsymbol{k}_1 | n\boldsymbol{k}_2\rangle\right]$$

- This phase difference can be changed arbitrarily.

Closed path: Berry phase

- For a closed path, we define

$$\gamma = \Delta\phi_{12} + \Delta\phi_{23} + \Delta\phi_{34} + \Delta\phi_{41}$$

$$\begin{aligned}\gamma = &-\mathrm{Im}\left(\ln\left(\left\langle n\boldsymbol{k}_1 \middle| n\boldsymbol{k}_2\right\rangle\right)\right) - \mathrm{Im}\left(\ln\left(\left\langle n\boldsymbol{k}_2 \middle| n\boldsymbol{k}_3\right\rangle\right)\right)\\ &-\mathrm{Im}\left(\ln\left(\left\langle n\boldsymbol{k}_3 \middle| n\boldsymbol{k}_4\right\rangle\right)\right) - \mathrm{Im}\left(\ln\left(\left\langle n\boldsymbol{k}_4 \middle| n\boldsymbol{k}_1\right\rangle\right)\right)\\ = &-\mathrm{Im}\left[\left\langle n\boldsymbol{k}_1 \middle| n\boldsymbol{k}_2\right\rangle\left\langle n\boldsymbol{k}_2 \middle| n\boldsymbol{k}_3\right\rangle\left\langle n\boldsymbol{k}_3 \middle| n\boldsymbol{k}_4\right\rangle\left\langle n\boldsymbol{k}_4 \middle| n\boldsymbol{k}_1\right\rangle\right]\end{aligned}$$

- This is independent of choice of phase.

Infinitesimal displacement in k

- Consider two states very close in k

$$e^{-id\phi} \simeq 1 - id\phi = \frac{\left\langle n\boldsymbol{k} \middle| n\boldsymbol{k} + d\boldsymbol{k} \right\rangle}{\left| \left\langle n\boldsymbol{k} \middle| n\boldsymbol{k} + d\boldsymbol{k} \right\rangle \right|}$$

$$= \frac{\left\langle n\boldsymbol{k} \middle| n\boldsymbol{k} \right\rangle + \left\langle n\boldsymbol{k} \middle| \frac{\partial}{\partial \boldsymbol{k}} \middle| n\boldsymbol{k} \right\rangle d\boldsymbol{k}}{\left| \left\langle n\boldsymbol{k} \middle| n\boldsymbol{k} \right\rangle \right|} = 1 + \left\langle n\boldsymbol{k} \middle| \frac{\partial}{\partial \boldsymbol{k}} \middle| n\boldsymbol{k} \right\rangle d\boldsymbol{k}$$

- Therefore

$$d\phi = i \left\langle n\boldsymbol{k} \middle| \frac{\partial}{\partial \boldsymbol{k}} \middle| n\boldsymbol{k} \right\rangle d\boldsymbol{k} = \mathcal{A}_n\left(\boldsymbol{k}\right) d\boldsymbol{k}$$

Berry phase as an integral

- Therefore

$$\gamma = \oint d\phi = \oint \mathcal{A}_n \left(\boldsymbol{k} \right) d\boldsymbol{k}$$

Alternative derivation

- Suppose that at time 0 I am in a state

$$\left|n\boldsymbol{k}\left(0\right)\right\rangle$$

- If I change k very slowly, then the adiabatic theorem says that at time *t* I will be in

$$\left|n\boldsymbol{k}\left(t\right)\right\rangle$$

- But there could be an additional phase, so

$$\left|\psi\left(t\right)\right\rangle = e^{-i\theta\left(t\right)}\left|n\boldsymbol{k}\left(t\right)\right\rangle$$

Time evolution I

- But $$H\left(\boldsymbol{k}\left(t\right)\right)\left|\psi\left(t\right)\right\rangle = ih\frac{\partial}{\partial t}\left|\psi\left(t\right)\right\rangle$$

$$H\left(\boldsymbol{k}\left(t\right)\right)\left|\psi\left(t\right)\right\rangle = i\hbar\left[-i\frac{d\theta}{dt}e^{i\theta\left(t\right)}\left|n\boldsymbol{k}\left(t\right)\right\rangle + e^{i\theta\left(t\right)}\frac{\partial}{\partial t}\left|n\boldsymbol{k}\left(t\right)\right\rangle\right]$$

$$\left(\boldsymbol{k}\left(t\right)\right)e^{i\theta\left(t\right)}\left|n\boldsymbol{k}\left(t\right)\right\rangle = i\hbar\left[-i\frac{d\theta}{dt}e^{i\theta\left(t\right)}\left|n\boldsymbol{k}\left(t\right)\right\rangle + e^{i\theta\left(t\right)}\frac{\partial}{\partial t}\left|n\boldsymbol{k}\left(\right.\right.\right.$$

$$\left(\boldsymbol{k}\left(t\right)\right)\left|n\boldsymbol{k}\left(t\right)\right\rangle = i\hbar\left[-i\frac{d\theta}{dt}\left|n\boldsymbol{k}\left(t\right)\right\rangle + \frac{\partial}{\partial t}\left|n\boldsymbol{k}\left(t\right)\right\rangle\right]$$

$$\left(\boldsymbol{k}\left(t\right)\right) = \hbar\frac{d\theta}{dt} + ih\left\langle n\boldsymbol{k}\left(t\right)\right|\frac{\partial}{\partial t}\left|n\boldsymbol{k}\left(t\right)\right\rangle$$

Time evolution II

$$\varepsilon\left(\boldsymbol{k}\left(t\right)\right) = \hbar\frac{d\theta}{dt} + ih\left\langle n\boldsymbol{k}\left(t\right)\right|\frac{\partial}{\partial t}\left|n\boldsymbol{k}\left(t\right)\right\rangle$$

$$\theta\left(t\right) = \int_0^t \varepsilon\left(\boldsymbol{k}\left(t'\right)\right)dt' - ih\int_0^t dt'\left\langle n\boldsymbol{k}\left(t'\right)\right|\frac{\partial}{\partial t'}\left|n\boldsymbol{k}\left(t'\right)\right\rangle$$

$$\theta\left(t\right) = \int_0^t \varepsilon\left(\boldsymbol{k}\left(t'\right)\right)dt' - ih\int_0^t dt'\left\langle n\boldsymbol{k}\left(t'\right)\right|\frac{\partial}{\partial \boldsymbol{k}}\left|n\boldsymbol{k}\left(t'\right)\right\rangle\frac{\partial \boldsymbol{k}}{\partial t'}$$

$$= \int_0^t \varepsilon\left(\boldsymbol{k}\left(t'\right)\right)dt' - ih\int_C \left\langle n\boldsymbol{k}\right|\frac{\partial}{\partial \boldsymbol{k}}\left|n\boldsymbol{k}\right\rangle d\boldsymbol{k}$$

$$= \int_0^t \varepsilon\left(\boldsymbol{k}\left(t'\right)\right)dt' - ih\int_C \mathcal{A}_n\left(\boldsymbol{k}\right)d\boldsymbol{k}$$

Berry connection

- Notice that

$$e^{-id\phi} \simeq 1 - id\phi = \frac{\langle n\boldsymbol{k} | n\boldsymbol{k} + d\boldsymbol{k} \rangle}{\left| \langle n\boldsymbol{k} | n\boldsymbol{k} + d\boldsymbol{k} \rangle \right|}$$

$$= \frac{\partial}{\partial \boldsymbol{k}} \langle n\boldsymbol{k} | n\boldsymbol{k} \rangle = 0 = \frac{\partial \langle n\boldsymbol{k} |}{\partial \boldsymbol{k}} | n\boldsymbol{k} \rangle + \left\langle n\boldsymbol{k} \left| \frac{\partial | n\boldsymbol{k} \rangle}{\partial \boldsymbol{k}} \right. \right\rangle$$

- But the two terms in the rhs are complex conjugate, so

$$\left\langle n\boldsymbol{k} \left| \frac{\partial | n\boldsymbol{k} \rangle}{\partial \boldsymbol{k}} \right. \right\rangle \equiv \left\langle n\boldsymbol{k} \left| \frac{\partial}{\partial \boldsymbol{k}} \right| n\boldsymbol{k} \right\rangle$$

- is purely imaginary.

Berry phase I

- Then, since

$$d\phi = i\left\langle n\boldsymbol{k}\right|\frac{\partial}{\partial \boldsymbol{k}}\left|n\boldsymbol{k}\right\rangle d\boldsymbol{k} = \mathcal{A}_n\left(\boldsymbol{k}\right)d\boldsymbol{k}$$

$$\gamma = -\mathrm{Im}\oint\left\langle n\boldsymbol{k}\right|\frac{\partial}{\partial \boldsymbol{k}}\left|n\boldsymbol{k}\right\rangle \cdot d\boldsymbol{k}$$

- If k is 3D:

$$\gamma = -\mathrm{Im}\int_{\Sigma} d\boldsymbol{S}\cdot\frac{\partial}{\partial \boldsymbol{k}}\times\left\langle n\boldsymbol{k}\right|\frac{\partial}{\partial \boldsymbol{k}}\left|n\boldsymbol{k}\right\rangle$$

- Next we use

$$\left(\vec{A}\times\vec{B}\right)_i = \varepsilon_{ijk}A_jB_k$$

Berry phase II

- Then

$$\gamma = -\mathrm{Im}\int_{\Sigma} dS_i \varepsilon_{ijk} \cdot \frac{\partial}{\partial k_j}\left\langle n\boldsymbol{k}\right|\frac{\partial}{\partial k_k}\left|n\boldsymbol{k}\right\rangle$$

- But

$$\frac{\partial}{\partial k_j}\left\langle n\boldsymbol{k}\right|\frac{\partial}{\partial k_k}\left|n\boldsymbol{k}\right\rangle = \frac{\partial\left\langle n\boldsymbol{k}\right|}{\partial k_j}\frac{\partial\left|n\boldsymbol{k}\right\rangle}{\partial k_k} + \left\langle n\boldsymbol{k}\right|\frac{\partial}{\partial k_j}\frac{\partial}{\partial k_k}\left|n\boldsymbol{k}\right\rangle$$

- But since $\varepsilon_{ijk} = -\varepsilon_{ikj}$

$$\frac{\partial}{\partial k_j}\left\langle n\boldsymbol{k}\right|\frac{\partial}{\partial k_k}\left|n\boldsymbol{k}\right\rangle = \frac{\partial\left\langle n\boldsymbol{k}\right|}{\partial k_j}\frac{\partial\left|n\boldsymbol{k}\right\rangle}{\partial k_k}$$

Berry phase III

- So

$$\gamma = -\mathrm{Im}\int_{\Sigma} dS_i \varepsilon_{ijk} \cdot \frac{\partial\left\langle n\boldsymbol{k}\right|}{\partial k_j}\frac{\partial\left|n\boldsymbol{k}\right\rangle}{\partial k_k}$$

$$= -\mathrm{Im}\sum_{n'}\int_{\Sigma} dS_i \varepsilon_{ijk} \cdot \frac{\partial\left\langle n\boldsymbol{k}\right|}{\partial k_j}\left|n'\boldsymbol{k}\right\rangle\left\langle n'\boldsymbol{k}\right|\frac{\partial\left|n\boldsymbol{k}\right\rangle}{\partial k_k}$$

- But

$$E_n\left\langle n'\boldsymbol{k}\middle|\nabla n\boldsymbol{k}\right\rangle = \left\langle n'\boldsymbol{k}\middle|\nabla\left(H\middle|n\boldsymbol{k}\right\rangle\right)$$

$$= \left\langle n'\boldsymbol{k}\middle|\left(\nabla H\right)\middle|n\boldsymbol{k}\right\rangle + E_n\left\langle n'\boldsymbol{k}\middle|H\nabla\middle|n\boldsymbol{k}\right\rangle$$

$$= \left\langle n'\boldsymbol{k}\middle|\left(\nabla H\right)\middle|n\boldsymbol{k}\right\rangle + E_n\left\langle n'\boldsymbol{k}\middle|H\nabla\middle|n\boldsymbol{k}\right\rangle$$

$$= \left\langle n'\boldsymbol{k}\middle|\left(\nabla H\right)\middle|n\boldsymbol{k}\right\rangle + E_{n'}\left\langle n'\boldsymbol{k}\middle|\nabla\middle|n\boldsymbol{k}\right\rangle$$

Berry phase IV

- This means

$$\left\langle n'\boldsymbol{k}\middle|\nabla\, n\boldsymbol{k}\right\rangle = \frac{\left\langle n'\boldsymbol{k}\middle|\left(\nabla H\right)\middle|n\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)}$$

- Also

$$\left\langle \nabla n'\boldsymbol{k}\middle|n\boldsymbol{k}\right\rangle = \frac{\left\langle n\boldsymbol{k}\middle|\left(\nabla H\right)\middle|n'\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)}$$

Berry phase V

- Inserting back

$$\gamma = -\mathrm{Im}\sum_{n'}\int_{\Sigma} dS_i \varepsilon_{ijk} \cdot \frac{\left\langle n\boldsymbol{k}\middle|\left(\nabla_j H\right)\middle|n'\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)} \frac{\left\langle n'\boldsymbol{k}\middle|\left(\nabla_k H\right)\middle|n\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)}$$

$$= -\mathrm{Im}\sum_{n'}\int_{\Sigma} dS_i \varepsilon_{ijk} \cdot \frac{\left\langle n\boldsymbol{k}\middle|\left(\nabla_j H\right)\middle|n'\boldsymbol{k}\right\rangle\left\langle n'\boldsymbol{k}\middle|\left(\nabla_k H\right)\middle|n\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)^2}$$

- Also

$$\gamma = -\mathrm{Im}\sum_{n'}\int_{\Sigma} d\boldsymbol{S} \cdot \frac{\left\langle n\boldsymbol{k}\middle|\left(\boldsymbol{\nabla} H\right)\middle|n'\boldsymbol{k}\right\rangle \times \left\langle n'\boldsymbol{k}\middle|\left(\boldsymbol{\nabla} H\right)\middle|n\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)^2}$$

Berry phase VI

- Therefore

$$\Omega_n\left(\boldsymbol{k}\right) = \frac{\left\langle n\boldsymbol{k}\middle|\left(\boldsymbol{\nabla} H\right)\middle|n'\boldsymbol{k}\right\rangle \times \left\langle n'\boldsymbol{k}\middle|\left(\boldsymbol{\nabla} H\right)\middle|n\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)^2}$$