### Física de Semiconductores

Lección 12

### Position operator

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

$$r\Psi(r) = \int d\mathbf{k}\Psi(\mathbf{k})re^{i\mathbf{k}\cdot\mathbf{r}}$$

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

• where we have integrated by parts. Then the position operator in momentum  $\partial$ 

representation is 
$$\hat{m{r}}=irac{\partial}{\partial m{k}}$$

## Bloch wave expansion

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

$$egin{aligned} \Psiig(oldsymbol{r}ig) &= \sum_n \int doldsymbol{k} \Psi_nig(oldsymbol{k}ig) \psi_{noldsymbol{k}}ig(oldsymbol{r}ig) \ &= \sum_{n,m} \int doldsymbol{k} \delta_{nm} \Psi_nig(oldsymbol{k}ig) \psi_{moldsymbol{k}}ig(oldsymbol{r}ig) \end{aligned}$$

An operator is then

$$\hat{O}\Psiig(m{r}ig) = \sum \int dm{k} \hat{O}_{nm}ig(m{k}ig)\Psi_{n}ig(m{k}ig)\psi_{mm{k}}ig(m{r}ig)$$

we would like to find this for the position operator

### Position operator in Bloch wave basis (I)

This means

$$\begin{split} \boldsymbol{r}\Psi\left(\boldsymbol{r}\right) &= \sum_{n} \int d\boldsymbol{k} \Psi_{n}\left(\boldsymbol{k}\right) u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) \boldsymbol{r} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \\ &= \sum_{n} \int d\boldsymbol{k} \Psi_{n}\left(\boldsymbol{k}\right) u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) \left(-i\frac{\partial}{\partial \boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\right) \\ &= \sum_{n} \int d\boldsymbol{k} \left(i\frac{\partial}{\partial \boldsymbol{k}} \Psi_{n}\left(\boldsymbol{k}\right) u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \\ &= \sum_{n} \int d\boldsymbol{k} \left(iu_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) \frac{\partial \Psi_{n}\left(\boldsymbol{k}\right)}{\partial \boldsymbol{k}} + i\Psi_{n}\left(\boldsymbol{k}\right) \frac{\partial u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \end{split}$$

## Position operator in Bloch wave basis (II)

$$\begin{split} &= \sum_{n} \int d\boldsymbol{k} \left[ iu_{nk} \left( \boldsymbol{r} \right) \frac{\partial \Psi_{n} \left( \boldsymbol{k} \right)}{\partial \boldsymbol{k}} + i\Psi_{n} \left( \boldsymbol{k} \right) \frac{\partial u_{nk} \left( \boldsymbol{r} \right)}{\partial \boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \right. \\ &= \sum_{n} \int d\boldsymbol{k} \left[ i\psi_{nk} \left( \boldsymbol{r} \right) \frac{\partial \Psi_{n} \left( \boldsymbol{k} \right)}{\partial \boldsymbol{k}} + i\Psi_{n} \left( \boldsymbol{k} \right) \int d\boldsymbol{r}' \delta \left( \boldsymbol{r} - \boldsymbol{r}' \right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \frac{\partial u_{nk} \left( \boldsymbol{r}' \right)}{\partial \boldsymbol{k}} \right) \\ &= \sum_{n} \int d\boldsymbol{k} \left[ i\psi_{nk} \left( \boldsymbol{r} \right) \frac{\partial \Psi_{n} \left( \boldsymbol{k} \right)}{\partial \boldsymbol{k}} + i\Psi_{n} \left( \boldsymbol{k} \right) \int d\boldsymbol{r}' \sum_{m} u_{mk}^{*} \left( \boldsymbol{r}' \right) u_{mk} \left( \boldsymbol{r} \right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \frac{\partial u_{nk} \left( \boldsymbol{r}' \right)}{\partial \boldsymbol{k}} \right. \\ &= \sum_{n} \int d\boldsymbol{k} \left[ i\psi_{nk} \left( \boldsymbol{r} \right) \frac{\partial \Psi_{n} \left( \boldsymbol{k} \right)}{\partial \boldsymbol{k}} + i\Psi_{n} \left( \boldsymbol{k} \right) \sum_{m} \psi_{mk} \left( \boldsymbol{r} \right) \int d\boldsymbol{r}' u_{mk}^{*} \left( \boldsymbol{r}' \right) \frac{\partial u_{nk} \left( \boldsymbol{r}' \right)}{\partial \boldsymbol{k}} \right. \\ &= \sum_{n} \int d\boldsymbol{k} \left[ i\psi_{nk} \left( \boldsymbol{r} \right) \frac{\partial \Psi_{n} \left( \boldsymbol{k} \right)}{\partial \boldsymbol{k}} + i\Psi_{n} \left( \boldsymbol{k} \right) \sum_{m} \mathcal{A}_{mn} \left( \boldsymbol{k} \right) \psi_{mk} \left( \boldsymbol{r} \right) \right] \end{split}$$

## Berry connection

We have defined the Berry connection as

$$\mathcal{A}_{mn}\left(oldsymbol{k}
ight) = i \int doldsymbol{r} \, u_{moldsymbol{k}}^*\left(oldsymbol{r}
ight) rac{\partial}{\partial oldsymbol{k}} \, u_{noldsymbol{k}}\left(oldsymbol{r}
ight)$$

We will examine the meaning of this expression later

# Final expression for position opp

$$m{r}\Psiig(m{r}ig) = \sum_{n,m}\int dm{k}igg[irac{\partial}{\partialm{k}}\delta_{nm} + \mathcal{A}_{mn}ig(m{k}ig)ar{\Psi}_{n}ig(m{k}ig)\psi_{mm{k}}ig(m{r}ig)$$

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 
$$\hat{m{r}}_{nm} = \left(irac{\partial}{\partial m{k}}\delta_{nm} + \mathcal{A}_{mn}\left(m{k}
ight)
ight)$$

In many cases  $\Psi_m(\mathbf{k}) = 0$  for  $m \neq n$ . Then we only need

$$\hat{m{r}}_{nn} \equiv \hat{m{r}}_{n} = \left(irac{\partial}{\partialm{k}} + \mathcal{A}_{nn}\left(m{k}
ight)
ight) \equiv \left(irac{\partial}{\partialm{k}} + \mathcal{A}_{n}\left(m{k}
ight)
ight)$$

## Explanation for the extra term I

The Bloch wave function is a solution of

$$-\left[rac{\hbar^2
abla^2}{2m} + V(m{r})
ight]\psi_{nm{k}}(m{r}) = E_{nm{k}}\psi_{nm{k}}(m{r})$$

Let's consider

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

Accordingly, observables cannot depend on phase

## Explanation for the extra term II

Suppose that I change the phase of the Bloch function

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

• with  $\psi_{nm{k}}'(m{r}) = e^{i\phi(m{k})}\psi_{nm{k}}(m{r})$  . Then

$$\Psi_{n}'\left(oldsymbol{k}
ight) = e^{-i\phi\left(oldsymbol{k}
ight)}\Psi_{n}\left(oldsymbol{k}
ight)$$

## **Explanation II**

Then suppose I ignore the A term

$$\int d\mathbf{r} \Psi^{*}(\mathbf{r}) \hat{\mathbf{r}} \Psi(\mathbf{r}) = \int d\mathbf{r} \int d\mathbf{k} \Psi_{n}^{\prime *}(\mathbf{k}) \psi_{nk}^{\prime *}(\mathbf{r}) i \frac{\partial \Psi_{n}^{\prime}(\mathbf{k})}{\partial \mathbf{k}} \psi_{nk}^{\prime}(\mathbf{r}) 
= \int d\mathbf{r} \int d\mathbf{k} \Psi_{n}^{\prime *}(\mathbf{k}) \psi_{nk}^{*}(\mathbf{r}) i \frac{\partial \Psi_{n}^{\prime}(\mathbf{k})}{\partial \mathbf{k}} \psi_{nk}(\mathbf{r}) 
= \int d\mathbf{r} \int d\mathbf{k} \Psi_{n}^{\prime *}(\mathbf{k}) \psi_{nk}^{*}(\mathbf{r}) i \left[ \frac{\partial \Psi_{n}(\mathbf{k})}{\partial \mathbf{k}} e^{-i\phi(\mathbf{k})} - i\Psi_{n}(\mathbf{k}) e^{-i\phi(\mathbf{k})} \frac{\partial \phi(\mathbf{k})}{\partial \mathbf{k}} \right] \psi_{nk}(\mathbf{r}) 
= \int d\mathbf{r} \int d\mathbf{k} \Psi_{n}^{\prime *}(\mathbf{k}) e^{-i\phi(\mathbf{k})} \psi_{nk}^{*}(\mathbf{r}) i \frac{\partial \Psi_{n}(\mathbf{k})}{\partial \mathbf{k}} \psi_{nk}(\mathbf{r}) 
+ \int d\mathbf{r} \int d\mathbf{k} \Psi_{n}^{\prime *}(\mathbf{k}) e^{-i\phi(\mathbf{k})} \psi_{nk}^{*}(\mathbf{r}) \left[ \Psi_{n}(\mathbf{k}) \frac{\partial \phi(\mathbf{k})}{\partial \mathbf{k}} \right] \psi_{nk}(\mathbf{r})$$

## **Explanation III**

$$= \int d\boldsymbol{r} \int d\boldsymbol{k} \Psi_{n}^{\prime*}(\boldsymbol{k}) e^{-i\phi(\boldsymbol{k})} \psi_{n\boldsymbol{k}}^{*}(\boldsymbol{r}) i \frac{\partial \Psi_{n}(\boldsymbol{k})}{\partial \boldsymbol{k}} \psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

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

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

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

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

## **Explanation IV**

But let's see how the Berry connection transforms

$$\mathcal{A}'_{n}(\mathbf{k}) = i \int d\mathbf{r} u_{n\mathbf{k}}^{\prime*}(\mathbf{r}) \frac{\partial}{\partial \mathbf{k}} u_{n\mathbf{k}}^{\prime}(\mathbf{r}) 
= i \int d\mathbf{r} e^{-i\phi(\mathbf{k})} u_{n\mathbf{k}}^{*}(\mathbf{r}) \frac{\partial}{\partial \mathbf{k}} e^{i\phi(\mathbf{k})} u_{n\mathbf{k}}(\mathbf{r}) = 
= i \left[ \int d\mathbf{r} u_{n\mathbf{k}}^{*}(\mathbf{r}) \left[ \frac{\partial u_{n\mathbf{k}}(\mathbf{r})}{\partial \mathbf{k}} + u_{n\mathbf{k}}(\mathbf{r}) i \frac{\partial \phi(\mathbf{k})}{\partial \mathbf{k}} \right] \right] 
= i \int d\mathbf{r} u_{n\mathbf{k}}^{*}(\mathbf{r}) \frac{\partial u_{n\mathbf{k}}(\mathbf{r})}{\partial \mathbf{k}} - \frac{\partial \phi(\mathbf{k})}{\partial \mathbf{k}} = \mathcal{A}_{n}(\mathbf{k}) - \frac{\partial \phi(\mathbf{k})}{\partial \mathbf{k}}$$

## **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:

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

Then

$$m{A} 
ightarrow m{A}' = m{A} + m{\nabla}\phiig(m{r}ig)$$
 $m{arphi} 
ightarrow m{arphi}' = m{arphi} - rac{1}{c} rac{\partial \phiig(m{r}ig)}{\partial t}$ 
 $m{\psi} 
ightarrow \psi' = \psi e^{irac{ec}{\hbar}\phiig(m{r}ig)}$ 

## The velocity and force operators

The quantities we are interested in are

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

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

Hamiltonian of a charge:

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

## Semiclassical equations

$$\frac{d\mathbf{k}}{dt} = -e\mathbf{E} - \frac{e}{c}(\mathbf{v} \times \mathbf{H})$$

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

### Berry curvature

We define the Berry curvature as

$$\Omega_{n}ig(m{k}ig)\equivrac{\partial}{\partialm{k}} imes\mathcal{A}_{n}ig(m{k}ig)$$
 so

$$\begin{split} &\hbar\frac{d\boldsymbol{k}}{dt} = -e\boldsymbol{E} - \frac{e}{c} \left(\boldsymbol{v} \times \boldsymbol{H}\right) \\ &\frac{d\hat{\boldsymbol{r}}_{n}}{dt} = \frac{1}{\hbar} \frac{\partial E_{n} \left(\boldsymbol{k}\right)}{\partial \boldsymbol{k}} - \frac{d\boldsymbol{k}}{dt} \times \Omega_{n} \left(\boldsymbol{k}\right) \end{split}$$

#### Electric field

In the presence of an electric field only

$$oldsymbol{v}_{n}ig(oldsymbol{k}ig) = rac{doldsymbol{r}_{n}}{dt} = rac{1}{\hbar}rac{\partial E_{n}ig(oldsymbol{k}ig)}{\partialoldsymbol{k}} + rac{eoldsymbol{E}}{\hbar} imes\Omega_{n}ig(oldsymbol{k}ig)$$

#### Current

The electric current is

$$egin{aligned} oldsymbol{j}_n &= \left(-e
ight) \int rac{doldsymbol{k}}{\left(2\pi
ight)^d} oldsymbol{v}_nig(oldsymbol{k}ig) f_nig(oldsymbol{k}ig) \ &= \left(-e
ight) \int rac{doldsymbol{k}}{\left(2\pi
ight)^d} rac{1}{\hbar} rac{\partial E_nig(oldsymbol{k}ig)}{\partial oldsymbol{k}} f_nig(oldsymbol{k}ig) \ &+ ig(-eig) \int rac{doldsymbol{k}}{\left(2\pi
ight)^d} f_nig(oldsymbol{k}ig) rac{eoldsymbol{E}}{\hbar} imes \Omega_nig(oldsymbol{k}ig) \end{aligned}$$

#### Filled band

For a filled band

$$oldsymbol{j}_n = \left(-e\right) \int rac{doldsymbol{k}}{\left(2\pi\right)^d} oldsymbol{v}_n\left(oldsymbol{k}
ight)$$

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

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

• But

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

#### Filled band

Therefore

$$egin{align} oldsymbol{j}_{n}^{ ext{filled}} &= \left(-e
ight) \int rac{doldsymbol{k}}{\left(2\pi
ight)^{d}} rac{eoldsymbol{E}}{\hbar} imes \Omega_{n}\left(oldsymbol{k}
ight) \ &= -rac{e^{2}}{\hbar} oldsymbol{E} imes rac{1}{\left(2\pi
ight)^{d}} \int doldsymbol{k} \Omega_{n}\left(oldsymbol{k}
ight) \ &= -rac{e^{2}}{\hbar} oldsymbol{E} imes rac{1}{\left(2\pi
ight)^{d}} \int doldsymbol{k} \Omega_{n}\left(oldsymbol{k}
ight) \end{aligned}$$

When is this integral zero?

## Defining phase differences

Suppose I have two complex numbers

$$z_{_{1}}=\left|z_{_{1}}
ight|e^{i\phi_{_{1}}}; \quad z_{_{2}}=\left|z_{_{2}}
ight|e^{i\phi_{_{2}}}$$

Then

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

#### Parametric Hamiltonian

The periodic part of the wave function satisfies

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

$$H(\mathbf{k}) u_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_{n\mathbf{k}} u_{n\mathbf{k}}(\mathbf{r})$$

Then we can define

$$e^{-i\Delta\phi_{12}^n} = rac{\int dr u_{noldsymbol{k}_1}^*ig(oldsymbol{r}ig) u_{noldsymbol{k}_2}ig(oldsymbol{r}ig) u_{noldsymbol{k}_2}ig(oldsymbol{r}ig)}{\left|ig\langle noldsymbol{k}_1ig| noldsymbol{k}_2ig
angle} = rac{ig\langle noldsymbol{k}_1ig| noldsymbol{k}_2ig
angle}{\left|ig\langle noldsymbol{k}_1ig| noldsymbol{k}_2ig
angle}$$

Taking logs

$$-i\Delta\phi_{12}^{n}=\ln\left\langle noldsymbol{k}_{1}\left|noldsymbol{k}_{2}
ight
angle -\ln\left|\left\langle noldsymbol{k}_{1}\left|noldsymbol{k}_{2}
ight
angle 
ight|$$

#### Phase definition

• But since 
$$\left| \frac{\left\langle n \mathbf{k}_1 \middle| n \mathbf{k}_2 \right\rangle}{\left| \left\langle n \mathbf{k}_1 \middle| n \mathbf{k}_2 \right\rangle \right|} = 1$$

•  $\Delta\phi^n_{12}$  is real. Then

$$egin{aligned} \Delta\phi_{12}^n &= -\operatorname{Im}\!\left[\ln\left\langle noldsymbol{k}_{\!\scriptscriptstyle 1}\!\left|noldsymbol{k}_{\!\scriptscriptstyle 2}
ight
angle
ight] + \operatorname{Im}\!\left[\ln\left|\left\langle noldsymbol{k}_{\!\scriptscriptstyle 1}\!\left|noldsymbol{k}_{\!\scriptscriptstyle 2}
ight
angle
ight] \\ \Delta\phi_{12}^n &= -\operatorname{Im}\!\left[\ln\left\langle noldsymbol{k}_{\!\scriptscriptstyle 1}\!\left|noldsymbol{k}_{\!\scriptscriptstyle 2}
ight
angle
ight] \end{aligned}$$

 This phase difference can be changed arbitrarily.

### Closed path: Berry phase

For a closed path, we define

$$\begin{split} \gamma &= \Delta \phi_{12} + \Delta \phi_{23} + \Delta \phi_{34} + \Delta \phi_{41} \\ \gamma &= -\operatorname{Im} \left( \ln \left( \left\langle n \boldsymbol{k}_1 \middle| n \boldsymbol{k}_2 \right\rangle \right) \right) - \operatorname{Im} \left( \ln \left( \left\langle n \boldsymbol{k}_2 \middle| n \boldsymbol{k}_3 \right\rangle \right) \right) \\ &- \operatorname{Im} \left( \ln \left( \left\langle n \boldsymbol{k}_3 \middle| n \boldsymbol{k}_4 \right\rangle \right) \right) - \operatorname{Im} \left( \ln \left( \left\langle n \boldsymbol{k}_4 \middle| n \boldsymbol{k}_1 \right\rangle \right) \right) \\ &= -\operatorname{Im} \left[ \left\langle n \boldsymbol{k}_1 \middle| n \boldsymbol{k}_2 \right\rangle \left\langle n \boldsymbol{k}_2 \middle| n \boldsymbol{k}_3 \right\rangle \left\langle n \boldsymbol{k}_3 \middle| n \boldsymbol{k}_4 \right\rangle \left\langle n \boldsymbol{k}_4 \middle| n \boldsymbol{k}_1 \right\rangle \right] \end{split}$$

This is independent of choice of phase.

## Infinitesimal displacement in k

• Consider two states very close in k 
$$e^{-id\phi} \simeq 1 - id\phi = \frac{\left\langle n m{k} \middle| n m{k} + d m{k} \right\rangle}{\left| \left\langle n m{k} \middle| n m{k} + d m{k} \right\rangle \right|}$$

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

Therefore

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

# Berry phase as an integral

Therefore

$$\gamma = \oint d\phi = \oint \mathcal{A}_{n}ig(oldsymbol{k}ig)doldsymbol{k}$$

#### Alternative derivation

Suppose that at time 0 I am in a state

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

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

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

But there could be an additional phase, so

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

#### Time evolution I

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

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

$$\theta(t) = \int_{0}^{t} \varepsilon(\mathbf{k}(t')) dt' - ih \int_{0}^{t} dt' \langle n\mathbf{k}(t') | \frac{\partial}{\partial t'} | n\mathbf{k}(t') \rangle$$

$$\theta(t) = \int_{0}^{t} \varepsilon(\mathbf{k}(t')) dt' - i\hbar \int_{0}^{t} dt' \langle n\mathbf{k}(t') | \frac{\partial}{\partial \mathbf{k}} | n\mathbf{k}(t') \rangle \frac{\partial \mathbf{k}}{\partial t'}$$

$$= \int_{0}^{t} \varepsilon \left( \boldsymbol{k}(t') \right) dt' - i h \int_{C} \left\langle n \boldsymbol{k} \right| \frac{\partial}{\partial \boldsymbol{k}} \left| n \boldsymbol{k} \right\rangle d\boldsymbol{k}$$

$$=\int_{0}^{t} \varepsilon(\mathbf{k}(t'))dt' - ih\int_{C} \mathcal{A}_{n}(\mathbf{k})d\mathbf{k}$$

## Berry connection

• Notice that 
$$e^{-id\phi} \simeq 1 - id\phi = rac{\left\langle nm{k} \middle| nm{k} + dm{k} \right
angle}{\left| \left\langle nm{k} \middle| nm{k} + dm{k} \right
angle}$$

$$= \frac{\partial}{\partial \mathbf{k}} \langle n\mathbf{k} | n\mathbf{k} \rangle = 0 = \frac{\partial \langle n\mathbf{k} |}{\partial \mathbf{k}} |n\mathbf{k} \rangle + \langle n\mathbf{k} | \frac{\partial |n\mathbf{k} \rangle}{\partial \mathbf{k}} \rangle$$

But the two terms in the rhs are complex

conjugate, so 
$$\left\langle n\mathbf{k} \middle| \frac{\partial \middle| n\mathbf{k} \middle\rangle}{\partial \mathbf{k}} \right\rangle \equiv \left\langle n\mathbf{k} \middle| \frac{\partial}{\partial \mathbf{k}} \middle| n\mathbf{k} \middle\rangle$$

• is purely imaginary.

## Berry phase I

• Then, since

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

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

• If k is 3D:

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

Next we use

$$(\vec{A} \times \vec{B})_i = \varepsilon_{ijk} A_j B_k$$

## Berry phase II

Then

$$\gamma = -\mathrm{Im}\int\limits_{\Sigma}dS_{i}arepsilon_{ijk}\cdotrac{\partial}{\partial k_{j}}ig\langle nm{k}igg|rac{\partial}{\partial k_{k}}igg|nm{k}igg
angle$$

• But

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

• But since  $\varepsilon_{ijk} = -\varepsilon_{ikj}$   $\frac{\partial}{\partial k_i} \langle n \boldsymbol{k} | \frac{\partial}{\partial k_k} | n \boldsymbol{k} \rangle = \frac{\partial \langle n \boldsymbol{k} |}{\partial k_i} \frac{\partial |n \boldsymbol{k} \rangle}{\partial k_k}$ 

## Berry phase III

• So 
$$\gamma = -\operatorname{Im} \int_{\Sigma} dS_{i} \varepsilon_{ijk} \cdot \frac{\partial \left\langle n\mathbf{k} \right|}{\partial k_{j}} \frac{\partial \left| n\mathbf{k} \right\rangle}{\partial k_{k}}$$

$$= -\operatorname{Im} \sum_{n'} \int_{\Sigma} dS_{i} \varepsilon_{ijk} \cdot \frac{\partial \left\langle n\mathbf{k} \right|}{\partial k_{j}} \left| n'\mathbf{k} \right\rangle \left\langle n'\mathbf{k} \right| \frac{\partial \left| n\mathbf{k} \right\rangle}{\partial k_{k}}$$
• But 
$$E_{n} \left\langle n'\mathbf{k} \middle| \nabla n\mathbf{k} \right\rangle = \left\langle n'\mathbf{k} \middle| \nabla \left( H \middle| n\mathbf{k} \right) \right\rangle$$

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

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

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

## Berry phase IV

This means

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

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

$$\begin{split} \gamma &= -\operatorname{Im} \sum_{n'} \int_{\Sigma} dS_{i} \varepsilon_{ijk} \cdot \frac{\left\langle n\boldsymbol{k} \middle| \left(\nabla_{j} H\right) \middle| n'\boldsymbol{k} \right\rangle}{\left(E_{n} - E_{n'}\right)} \frac{\left\langle n'\boldsymbol{k} \middle| \left(\nabla_{k} H\right) \middle| n\boldsymbol{k} \right\rangle}{\left(E_{n} - E_{n'}\right)} \\ &= -\operatorname{Im} \sum_{n'} \int_{\Sigma} dS_{i} \varepsilon_{ijk} \cdot \frac{\left\langle n\boldsymbol{k} \middle| \left(\nabla_{j} H\right) \middle| n'\boldsymbol{k} \right\rangle \left\langle n'\boldsymbol{k} \middle| \left(\nabla_{k} H\right) \middle| n\boldsymbol{k} \right\rangle}{\left(E_{n} - E_{n'}\right)^{2}} \end{split}$$

Also

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

## Berry phase VI

Therefore

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