Física de Semiconductores

Lección 13

Dirac magnetic monopole

- Let us suppose that there exists a magnetic monopole at the center of our coordinate system. Then the magnetic field produced by such monopole is

$$\boldsymbol{B} = q_m \frac{\boldsymbol{r}}{r^3} = \frac{\left(x, y, z\right)}{\left(x^2 + y^2 + z^2\right)}$$

- The vector potential must be such that

$$\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$$

Possible vector potential I

- Let's try $$\boldsymbol{A} = q_m \frac{\left(y, -x, 0\right)}{r\left(r - z\right)}$$

$$\boldsymbol{\nabla} \times \boldsymbol{A} = \begin{vmatrix} \hat{\mathbf{i}} & \hat{\mathbf{j}} & \hat{\mathbf{k}} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ \dfrac{y}{r\left(r - z\right)} & \dfrac{-x}{r\left(r - z\right)} & 0 \end{vmatrix}$$

Possible vector potential II

- Calculating the curl

$$\boldsymbol{B} = \left(-\frac{\partial}{\partial z}\left[\frac{-x}{r\left(r-z\right)}\right], \frac{\partial}{\partial z}\left[\frac{y}{r\left(r-z\right)}\right], \frac{\partial}{\partial x}\left[\frac{-x}{r\left(r-z\right)}\right] - \frac{\partial}{\partial y}\left[\frac{y}{r\left(r-z\right)}\right]\right)$$

- The first term, for example, is

$$\frac{\partial}{\partial z}\left[\frac{x}{r\left(r-z\right)}\right] = x\frac{\partial}{\partial z}\left[\frac{1}{r\left(r-z\right)}\right] = x\left\{\frac{1}{r}\frac{\partial}{\partial z}\left[\frac{1}{r-z}\right] + \frac{1}{r-z}\frac{\partial}{\partial z}\left[\frac{1}{r}\right]\right\}$$

$$= x\left\{\frac{1}{r}\left[-\frac{1}{\left(r-z\right)^2}\left(\frac{z}{r}-1\right)\right] + \frac{1}{r-z}\left(-\frac{1}{r^2}\right)\frac{z}{r}\right\}$$

Possible vector potential III

$$= -\frac{x}{r^3}\left\{\frac{r}{\left(r-z\right)^2}\left(z-r\right)+\frac{z}{r-z}\right\}$$

$$= -\frac{x}{r^3}\left\{\frac{r}{\left(r-z\right)^2}\left(z-r\right)+\frac{z\left(r-z\right)}{\left(r-z\right)^2}\right\}$$

$$= -\frac{x}{r^3}\left\{\frac{\left(z-r\right)}{\left(r-z\right)^2}\left(r-z\right)\right\} = \frac{x}{r^3}$$

Singularity

- However, the vector potential

$$\boldsymbol{A} = q_m \frac{\left(y, -x, 0\right)}{r\left(r - z\right)}$$

- is singular for *z* = *r*. We can use

$$\boldsymbol{A} = q_m \frac{\left(-y, x, 0\right)}{r\left(r + z\right)}$$

- but this is singular for *z* = -*r*. There is always a singular point no matter what the choice of vector potential is.

Using two vector potentials I

- We can then use different vector potentials for the northern and southern hemispheres:

$$\boldsymbol{A}_N = q_m \frac{\left(-y, x, 0\right)}{r\left(r+z\right)} \qquad \boldsymbol{A}_S = q_m \frac{\left(y, -x, 0\right)}{r\left(r-z\right)}$$

- Now

$$\boldsymbol{A}_N - \boldsymbol{A}_S = q_m \frac{\left(-y, x, 0\right)\left(r-z\right)}{r\left(r+z\right)\left(r-z\right)} - q_m \frac{\left(y, -x, 0\right)\left(r+z\right)}{r\left(r-z\right)\left(r+z\right)}$$

$$= \frac{q_m}{r\left(r+z\right)\left(r-z\right)}\left[-y\left(r-z\right) - y\left(r+z\right), x\left(r-z\right) + x\left(r+z\right), 0\right]$$

Using two vector potentials II

- Or

$$\boldsymbol{A}_N - \boldsymbol{A}_S = \frac{q_m}{r\left(r+z\right)\left(r-z\right)}\left[-2yr, 2xr\right]$$

$$= \frac{2q_m}{\left(r+z\right)\left(r-z\right)}\left[-y, x, 0\right]$$

$$= \frac{2q_m}{r^2 - z^2}\left[-y, x, 0\right] = \frac{2q_m}{x^2 + y^2}\left[-y, x, 0\right]$$

- But

$$\boldsymbol{\nabla} \tan^{-1}\left(\frac{y}{x}\right) = \frac{1}{1+\left(y/x\right)^2}\left(\frac{y}{-x^2}\right) + \frac{1}{1+\left(y/x\right)^2}\left(\frac{1}{x}\right) = \frac{1}{x^2+y^2}\left[-y, x, (\right.$$

$$\boldsymbol{A}_N = \boldsymbol{A}_S + 2q_m \boldsymbol{\nabla}\left[\tan^{-1}\left(\frac{y}{x}\right)\right] = \boldsymbol{A}_S + \boldsymbol{\nabla}\left(2q_m \phi\right)$$

Using two vector potentials III

- Because the two vector potentials differ by a gradient, they describe the same physics. Now if I make the switch

$$\boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \boldsymbol{\nabla}\Lambda \quad \varphi \to \varphi' = \varphi - \frac{1}{c}\frac{\partial \Lambda}{\partial t}$$

$$\Psi \to \Psi' = \Psi e^{-i\frac{e}{c\hbar}\Lambda} = \Psi e^{-i\frac{e}{c\hbar}2q_m\phi}$$

- But the wave function must be the same if I change ϕ by 2π, so

$$\frac{2q_m e}{c\hbar} = m$$

The flux or B (I)

- The flux through the surface of a domain *D* is

$$\iint_D \boldsymbol{B} \cdot d\boldsymbol{S} = \iint_D \left(\boldsymbol{\nabla} \times \boldsymbol{A}\right) \cdot d\boldsymbol{S}$$

- Applying Stokes theorem

$$\iint_D \left(\boldsymbol{\nabla} \times \boldsymbol{A}\right) \cdot d\boldsymbol{S} = \int_{\partial D} \boldsymbol{A} \cdot d\boldsymbol{l}$$

- A closed domain can be seen as the combination of two parts D_1 and D_2, so

$$4\pi q_m = \oiint \left(\boldsymbol{\nabla} \times \boldsymbol{A}\right) \cdot d\boldsymbol{S} = \int_{\partial D_1} \boldsymbol{A}_1 \cdot d\boldsymbol{l} + \int_{\partial D_2} \boldsymbol{A}_2 \cdot d\boldsymbol{l}$$

The flux or B (II)

- But $\partial D_1 = -\partial D_2$
- Then $4\pi q_m = \oiint (\boldsymbol{\nabla} \times \boldsymbol{A}) \cdot d\boldsymbol{S} = \int_{\partial D_1} (\boldsymbol{A}_1 - \boldsymbol{A}_2) \cdot d\boldsymbol{l}$
- If A is non singular and we can use the same expression over the entire domain, then

$$\oiint (\boldsymbol{\nabla} \times \boldsymbol{A}) \cdot d\boldsymbol{S} = \int_{\partial D_1} (\boldsymbol{A} - \boldsymbol{A}) \cdot d\boldsymbol{l} = 0$$

- So if there is a magnetic monopole the vector potential must be singular somewhere.

Chern number

- If q_m is not zero

$$4\pi q_m = \oiint \left(\boldsymbol{\nabla} \times \boldsymbol{A}\right) \cdot d\boldsymbol{S} = \int_{\partial D_1} \left(\boldsymbol{A}_1 - \boldsymbol{A}_2\right) \cdot d\boldsymbol{l}$$

$$= \int_{\partial D_1} \boldsymbol{\nabla}\left(2q_m \phi\right) \cdot d\boldsymbol{l} = 2q_m \int_{\partial D_1} \boldsymbol{\nabla}\left(\phi\right) \cdot d\boldsymbol{l} = 2q_m \left(2\pi\right)$$

- The integral

$$C = \frac{1}{2\pi q_m} \oiint \left(\boldsymbol{\nabla} \times \boldsymbol{A}\right) \cdot d\boldsymbol{S}$$

- is called the Chern number

Berry phase I

- We have

$$\mathcal{A}_n(\boldsymbol{k}) = i\int d\boldsymbol{r}\, u^*_{n\boldsymbol{k}}(\boldsymbol{r}) \frac{\partial}{\partial \boldsymbol{k}} u_{n\boldsymbol{k}}(\boldsymbol{r}) = i\left\langle n\boldsymbol{k}\right| \frac{\partial}{\partial \boldsymbol{k}} \left| n\boldsymbol{k}\right\rangle$$

$$\gamma = \oint \mathcal{A}_n(\boldsymbol{k})\cdot d\boldsymbol{k} = \int_\Sigma \left(\frac{\partial}{\partial \boldsymbol{k}} \times \mathcal{A}_n(\boldsymbol{k})\right)\cdot d\boldsymbol{S}$$

$$= \int_\Sigma \Omega_n(\boldsymbol{k})\cdot d\boldsymbol{S}$$

- Therefore

$$\boldsymbol{\Omega}_n(\boldsymbol{k}) = i\frac{\partial}{\partial \boldsymbol{k}} \times \left\langle n\boldsymbol{k}\right| \frac{\partial}{\partial \boldsymbol{k}} \left| n\boldsymbol{k}\right\rangle$$

Berry phase II

Using $\left(\vec{A} \times \vec{B}\right)_{\alpha} = \sum_{\beta\gamma} \varepsilon_{\alpha\beta\gamma} A_{\beta} B_{\gamma}$

$$\left(\Omega_{n}\right)_{\alpha} = \sum_{\beta\gamma} \varepsilon_{\alpha\beta\gamma} \frac{\partial}{\partial k_{\beta}} \left\langle n\boldsymbol{k} \right| \frac{\partial}{\partial k_{\gamma}} \left| n\boldsymbol{k} \right\rangle =$$

$$= \sum_{\beta\gamma} \varepsilon_{\alpha\beta\gamma} \left\{ \frac{\partial \left\langle n\boldsymbol{k} \right|}{\partial k_{\beta}} \frac{\partial \left| n\boldsymbol{k} \right\rangle}{\partial k_{\gamma}} + \left\langle n\boldsymbol{k} \right| \frac{\partial}{\partial k_{\beta}} \frac{\partial}{\partial k_{\gamma}} \left| n\boldsymbol{k} \right\rangle \right\}$$

$$= \sum_{\beta\gamma} \varepsilon_{\alpha\beta\gamma} \frac{\partial \left\langle n\boldsymbol{k} \right|}{\partial k_{\beta}} \frac{\partial \left| n\boldsymbol{k} \right\rangle}{\partial k_{\gamma}}$$

Because

$$\varepsilon_{\alpha\beta\gamma} = -\varepsilon_{\alpha\beta\gamma}$$

Berry phase III

- Inserting the identity

$$\left(\Omega_n\right)_\alpha = \sum_{n'} \sum_{\beta\gamma} \varepsilon_{\alpha\beta\gamma} \frac{\partial \left\langle n\boldsymbol{k}\right|}{\partial k_\beta} \left| n'\boldsymbol{k} \right\rangle \left\langle n'\boldsymbol{k} \right| \frac{\partial \left| n\boldsymbol{k}\right\rangle}{\partial k_\gamma}$$

- But

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

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

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

Berry phase IV

- This means

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

- Similarly (taking the complex conjugate)

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

Berry phase V

- Inserting back

$$\left(\Omega_n\right)_\alpha = \sum_{n'}\sum_{\beta\gamma}\varepsilon_{\alpha\beta\gamma}\frac{\left\langle n\boldsymbol{k}\right|\frac{\partial H}{\partial k_\beta}\left|n'\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)}\frac{\left\langle n'\boldsymbol{k}\right|\frac{\partial H}{\partial k_\gamma}\left|n\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)}$$

- Or

$$\boldsymbol{\Omega}_n = \sum_{n'}\frac{\left\langle n\boldsymbol{k}\right|\frac{\partial H}{\partial \boldsymbol{k}}\left|n'\boldsymbol{k}\right\rangle \times \left\langle n'\boldsymbol{k}\right|\frac{\partial H}{\partial \boldsymbol{k}}\left|n\boldsymbol{k}\right\rangle}{\left(E_n - E_{n'}\right)^2}$$

Degeneracies

- If there is a dgeneracy, the Berry curvature diverges, as the magnetic field of a monopole diverges at the monopole location.

Tight binding models

- The Bloch function for an electron within the tight binding model is

$$\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=\sum_{aj}C_{n,aj}\left(\boldsymbol{k}\right)\phi_{aj,\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

$$=\frac{1}{\sqrt{N}}\sum_{aj}C_{n,aj}\left(\boldsymbol{k}\right)\sum_{\boldsymbol{R}}e^{i\boldsymbol{k}\cdot\left(\boldsymbol{R}+\boldsymbol{d}_j\right)}\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)$$

- Therefore, the periodic part of the wave function is $u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$

$$u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)=\frac{1}{\sqrt{N}}\sum_{aj}C_{n,aj}\left(\boldsymbol{k}\right)\sum_{\boldsymbol{R}}e^{i\boldsymbol{k}\cdot\left(\boldsymbol{R}+\boldsymbol{d}_j-\boldsymbol{r}\right)}\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)$$

Derivatives of u

- For the Berry connnection we need the derivative

$$\frac{\partial u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}} = \frac{1}{\sqrt{N}}\sum_{aj}\frac{dC_{n,aj}\left(\boldsymbol{k}\right)}{d\boldsymbol{k}}\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\left(\boldsymbol{R}+\boldsymbol{d}_j-\boldsymbol{r}\right)}\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)$$

$$+\frac{i}{\sqrt{N}}\sum_{aj}C_{n,aj}\left(\boldsymbol{k}\right)\sum_{\boldsymbol{R}}\left(\boldsymbol{R}+\boldsymbol{d}_j-\boldsymbol{r}\right)e^{i\boldsymbol{k}\cdot\left(\boldsymbol{R}+\boldsymbol{d}_j-\boldsymbol{r}\right)}\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)$$

Berry connection I

- Therefore

$$u^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)\frac{du_{n\boldsymbol{k}}}{d\boldsymbol{k}} =$$

$$= \frac{1}{N}\sum_{\substack{a'j'\\aj}} C^*_{n,a'j'}\left(\boldsymbol{k}\right)\frac{dC_{n,aj}\left(\boldsymbol{k}\right)}{d\boldsymbol{k}}\sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}\left(\boldsymbol{R}-\boldsymbol{R}'\right)}e^{-i\boldsymbol{k}\cdot\left(\boldsymbol{d}_j-\boldsymbol{d}_{j'}\right)}\phi^*_{a'}\left(\boldsymbol{r}-\boldsymbol{R}'-\boldsymbol{d}_{j'}\right)\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)$$

$$+\frac{i}{N}\sum_{\substack{a'j'\\aj}} C^*_{n,a'j'}\left(\boldsymbol{k}\right)C_{n,aj}\left(\boldsymbol{k}\right)\sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}\left(\boldsymbol{R}-\boldsymbol{R}'\right)}e^{-i\boldsymbol{k}\cdot\left(\boldsymbol{d}_j-\boldsymbol{d}_{j'}\right)}\left(\boldsymbol{R}+\boldsymbol{d}_j\right)\phi^*_{a'}\left(\boldsymbol{r}-\boldsymbol{R}'-\boldsymbol{d}_{j'}\right)\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)$$

$$-\frac{i}{N}\sum_{\substack{a'j'\\aj}} C^*_{n,a'j'}\left(\boldsymbol{k}\right)C_{n,aj}\left(\boldsymbol{k}\right)\sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}\left(\boldsymbol{R}-\boldsymbol{R}'\right)}e^{-i\boldsymbol{k}\cdot\left(\boldsymbol{d}_j-\boldsymbol{d}_{j'}\right)}\phi^*_{a'}\left(\boldsymbol{r}-\boldsymbol{R}'-\boldsymbol{d}_{j'}\right)\boldsymbol{r}\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)$$

Berry connection II

- Integrating

$$\int d\boldsymbol{r} u^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)\frac{du_{n\boldsymbol{k}}}{d\boldsymbol{k}} =$$

$$= \frac{1}{N}\sum_{\substack{a'j'\\aj}} C^*_{n,a'j'}\left(\boldsymbol{k}\right)\frac{dC_{n,aj}\left(\boldsymbol{k}\right)}{d\boldsymbol{k}}\sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}\left(\boldsymbol{R}-\boldsymbol{R}'\right)}e^{-i\boldsymbol{k}\cdot\left(\boldsymbol{d}_j-\boldsymbol{d}_{j'}\right)}\int d\boldsymbol{r}\phi^*_{a'}\left(\boldsymbol{r}-\boldsymbol{R}'-\boldsymbol{d}_{j'}\right)\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)$$

$$+ \frac{i}{N}\sum_{\substack{a'j'\\aj}} C^*_{n,a'j'}\left(\boldsymbol{k}\right)C_{n,aj}\left(\boldsymbol{k}\right)\sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}\left(\boldsymbol{R}-\boldsymbol{R}'\right)}e^{-i\boldsymbol{k}\cdot\left(\boldsymbol{d}_j-\boldsymbol{d}_{j'}\right)}\left(\boldsymbol{R}+\boldsymbol{d}_j\right)\int d\boldsymbol{r}\phi^*_{a'}\left(\boldsymbol{r}-\boldsymbol{R}'-\boldsymbol{d}_{j'}\right)\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}\right.$$

$$- \frac{i}{N}\sum_{\substack{a'j'\\aj}} C^*_{n,a'j'}\left(\boldsymbol{k}\right)C_{n,aj}\left(\boldsymbol{k}\right)\sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}\left(\boldsymbol{R}-\boldsymbol{R}'\right)}e^{-i\boldsymbol{k}\cdot\left(\boldsymbol{d}_j-\boldsymbol{d}_{j'}\right)}\int d\boldsymbol{r}\phi^*_{a'}\left(\boldsymbol{r}-\boldsymbol{R}'-\boldsymbol{d}_{j'}\right)\boldsymbol{r}\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)$$

Berry connection III

- Using the orthogonality of the orbitals

$$\int d\boldsymbol{r} u^*_{n\boldsymbol{k}}(\boldsymbol{r}) \frac{du_{n\boldsymbol{k}}}{d\boldsymbol{k}} =$$

$$= \frac{1}{N} \sum_{\substack{a'j' \\ aj}} C^*_{n,a'j'}(\boldsymbol{k}) \frac{dC_{n,aj}(\boldsymbol{k})}{d\boldsymbol{k}} \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}(\boldsymbol{R}-\boldsymbol{R}')} e^{-i\boldsymbol{k}\cdot(\boldsymbol{d}_j - \boldsymbol{d}_{j'})} \delta_{aa'} \delta_{\boldsymbol{R}',\boldsymbol{R}} \delta_{jj'}$$

$$+ \frac{i}{N} \sum_{\substack{a'j' \\ aj}} C^*_{n,a'j'}(\boldsymbol{k}) C_{n,aj}(\boldsymbol{k}) \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}(\boldsymbol{R}-\boldsymbol{R}')} e^{-i\boldsymbol{k}\cdot(\boldsymbol{d}_j - \boldsymbol{d}_{j'})} (\boldsymbol{R} + \boldsymbol{d}_j) \delta_{aa'} \delta_{\boldsymbol{R}',\boldsymbol{R}} \delta_{jj'}$$

$$- \frac{i}{N} \sum_{\substack{a'j' \\ aj}} C^*_{n,a'j'}(\boldsymbol{k}) C_{n,aj}(\boldsymbol{k}) \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}(\boldsymbol{R}-\boldsymbol{R}')} e^{-i\boldsymbol{k}\cdot(\boldsymbol{d}_j - \boldsymbol{d}_{j'})} \int d\boldsymbol{r} \phi^*_{a'}(\boldsymbol{r} - \boldsymbol{R}' - \boldsymbol{d}_{j'}) \boldsymbol{r} \phi_a(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{d}_j)$$

Simplifying

- Using the orthogonality of the orbitals

$$\int d\boldsymbol{r} u^*_{n\boldsymbol{k}}(\boldsymbol{r}) \frac{du_{n\boldsymbol{k}}}{d\boldsymbol{k}} =$$

$$= \sum_{aj} C^*_{n,aj}(\boldsymbol{k}) \frac{dC_{n,aj}(\boldsymbol{k})}{d\boldsymbol{k}}$$

$$+ \frac{i}{N} \sum_{aj} C^*_{n,aj}(\boldsymbol{k}) C_{n,aj}(\boldsymbol{k}) \sum_{\boldsymbol{R}} (\boldsymbol{R} + \boldsymbol{d}_j)$$

$$- \frac{i}{N} \sum_{\substack{a'j' \\ aj}} C^*_{n,a'j'}(\boldsymbol{k}) C_{n,aj}(\boldsymbol{k}) \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\boldsymbol{k}(\boldsymbol{R}-\boldsymbol{R}')} e^{-i\boldsymbol{k}\cdot(\boldsymbol{d}_j - \boldsymbol{d}_{j'})} \int d\boldsymbol{r} \phi^*_{a'}(\boldsymbol{r} - \boldsymbol{R}' - \boldsymbol{d}_{j'}) \boldsymbol{r} \phi_a(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{d}_j)$$

Dipole matrix element

- If we now make we the approximation

$$\int d\boldsymbol{r}\phi_a^*\left(\boldsymbol{r}-\boldsymbol{R}'-\boldsymbol{d}_{j'}\right)\boldsymbol{r}\phi_a\left(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{d}_j\right)\simeq\left(\boldsymbol{R}-\boldsymbol{d}_j\right)\delta_{\boldsymbol{R}\boldsymbol{R}'}\delta_{jj'}\delta_{aa'}$$

- as discussed in Tight-Binding Formalism in the Context of the PythTB Package (Yusufaly et al) and justified in detail by Schulz PRB 73, 245327: $\int d\boldsymbol{r}u_{n\boldsymbol{k}}^*\left(\boldsymbol{r}\right)\frac{du_{n\boldsymbol{k}}}{d\boldsymbol{k}}=$

$$=\sum_{aj}C_{n,aj}^*\left(\boldsymbol{k}\right)\frac{dC_{n,aj}\left(\boldsymbol{k}\right)}{d\boldsymbol{k}}+\frac{i}{N}\sum_{aj}C_{n,aj}^*\left(\boldsymbol{k}\right)C_{n,aj}\left(\boldsymbol{k}\right)\sum_{\boldsymbol{R}}\left(\boldsymbol{R}+\boldsymbol{d}_j\right)$$

$$-\frac{i}{N}\sum_{\substack{a'j'\\aj}}C_{n,a'j'}^*\left(\boldsymbol{k}\right)C_{n,aj}\left(\boldsymbol{k}\right)\sum_{\boldsymbol{R}}\left(\boldsymbol{R}+\boldsymbol{d}_j\right)=\sum_{aj}C_{n,aj}^*\left(\boldsymbol{k}\right)\frac{dC_{n,aj}\left(\boldsymbol{k}\right)}{d\boldsymbol{k}}$$

Simplest tight binding model

- Let us consider the hamiltonian

$$H = \begin{pmatrix} k_z & k_x - ik_y \\ k_x - ik_y & -k_z \end{pmatrix} = \boldsymbol{k} \cdot \boldsymbol{\sigma}$$

- The eigenvalues are $\pm k \equiv \sqrt{k_x^2 + k_y^2 + k_z^2}$
- With eigenvectors

$$u_+ = \begin{pmatrix} \sqrt{\dfrac{k+k_z}{2k}} e^{-i\delta/2} \\ \sqrt{\dfrac{k-k_z}{2k}} e^{i\delta/2} \end{pmatrix} = \begin{pmatrix} \cos\dfrac{\theta}{2} e^{-i\phi/2} \\ \sin\dfrac{\theta}{2} e^{i\phi/2} \end{pmatrix}; \quad u_- = \begin{pmatrix} \sqrt{\dfrac{k-k_z}{2k}} e^{-i\delta/2} \\ -\sqrt{\dfrac{k+k_z}{2k}} e^{i\delta/2} \end{pmatrix} = \begin{pmatrix} \sin\dfrac{\theta}{2} e^{-i\phi/2} \\ -\cos\dfrac{\theta}{2} e^{i\phi/2} \end{pmatrix}$$

$$\delta = \tan^{-1}\left(k_y / k_x\right)$$

Berry curvature calculation I

- We need $$\frac{\partial H}{\partial \boldsymbol{k}} = \frac{\partial}{\partial \boldsymbol{k}}\left(\boldsymbol{k}\cdot\boldsymbol{\sigma}\right) = \boldsymbol{\sigma}$$
- So for example

$$\left\langle u_+^\dagger \left| \frac{\partial H}{\partial k_x} \right| u_- \right\rangle =$$

$$= \left(\sqrt{\frac{k+k_z}{2k}} e^{i\delta/2}, \sqrt{\frac{k-k_z}{2k}} e^{-i\delta/2} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{\frac{k-k_z}{2k}} e^{-i\delta/2} \\ -\sqrt{\frac{k+k_z}{2k}} e^{i\delta/2} \end{pmatrix}$$

$$= \left(\sqrt{\frac{k+k_z}{2k}} e^{i\delta/2}, \sqrt{\frac{k-k_z}{2k}} e^{-i\delta/2} \right) \begin{pmatrix} -\sqrt{\frac{k+k_z}{2k}} e^{i\delta/2} \\ \sqrt{\frac{k-k_z}{2k}} e^{-i\delta/2} \end{pmatrix}$$

$$= -\left(\frac{k+k_z}{2k} \right) e^{i\delta} + \left(\frac{k-k_z}{2k} \right) e^{-i\delta}$$

Berry curvature calculation II

- We also get

$$\left\langle u_+^\dagger \right| \frac{\partial H}{\partial k_y} \left| u_- \right\rangle = \left(\frac{k + k_z}{2k} \right) i e^{i\delta} + \left(\frac{k - k_z}{2k} \right) e^{-i\delta}$$

$$\left\langle u_+^\dagger \right| \frac{\partial H}{\partial k_z} \left| u_- \right\rangle = \frac{\sqrt{k^2 - k_z^2}}{k}$$

$$\left\langle u_-^\dagger \right| \frac{\partial H}{\partial k_x} \left| u_+ \right\rangle = \left(\frac{k - k_z}{2k} \right) e^{i\delta} - \left(\frac{k + k_z}{2k} \right) e^{-i\delta}$$

$$\left\langle u_-^\dagger \right| \frac{\partial H}{\partial k_y} \left| u_+ \right\rangle = -\left(\frac{k - k_z}{2k} \right) i e^{i\delta} - \left(\frac{k + k_z}{2k} \right) i e^{-i\delta}$$

$$\left\langle u_-^\dagger \right| \frac{\partial H}{\partial k_z} \left| u_+ \right\rangle = \frac{\sqrt{k^2 - k_z^2}}{k}$$

Berry curvature calculation III

- Then

$$\boldsymbol{\Omega} = \frac{1}{4k^2}\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ -\left(\frac{k+k_z}{2k}\right)e^{i\delta} + \left(\frac{k-k_z}{2k}\right)e^{-i\delta} & \left(\frac{k-k_z}{2k}\right)e^{i\delta} - \left(\frac{k+k_z}{2k}\right)e^{-i\delta} & \frac{\sqrt{k^2-k_z^2}}{k} \\ \left(\frac{k-k_z}{2k}\right)e^{i\delta} - \left(\frac{k+k_z}{2k}\right)e^{-i\delta} & -\left(\frac{k-k_z}{2k}\right)ie^{i\delta} - \left(\frac{k+k_z}{2k}\right)ie^{-i\delta} & \frac{\sqrt{k^2-k_z^2}}{k} \end{vmatrix}$$

$$= \frac{\boldsymbol{k}}{2k^3}$$

Berry connection I

- We can also write

$$u_+ = \begin{pmatrix} \cos\dfrac{\theta}{2} e^{-i\phi/2} \\ \sin\dfrac{\theta}{2} e^{i\phi/2} \end{pmatrix}; \quad u_- = \begin{pmatrix} \sin\dfrac{\theta}{2} e^{-i\phi/2} \\ -\cos\dfrac{\theta}{2} e^{i\phi/2} \end{pmatrix}$$

- The gradient in spherical coordinates is

$$\boldsymbol{\nabla} f = \frac{\partial f}{\partial r}\hat{\boldsymbol{r}} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\boldsymbol{\theta}} + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \varphi}\hat{\boldsymbol{\varphi}}$$

Berry connection II

- Then

$$\mathcal{A}_{+} = i\left\langle u_{+}\left|\frac{\partial}{\partial \boldsymbol{k}}\right|u_{+}\right\rangle = i\hat{\boldsymbol{r}}\left(\cos\frac{\theta}{2}e^{i\phi/2}, \sin\frac{\theta}{2}e^{-i\phi/2}\right)\frac{\partial}{\partial k}\left(\begin{array}{c}\cos\frac{\theta}{2}e^{-i\phi/2}\\ \sin\frac{\theta}{2}e^{+i\phi/2}\end{array}\right)$$

$$+i\frac{\hat{\boldsymbol{\theta}}}{k}\left(\cos\frac{\theta}{2}e^{i\phi/2}, \sin\frac{\theta}{2}e^{-i\phi/2}\right)\frac{\partial}{\partial \theta}\left(\begin{array}{c}\cos\frac{\theta}{2}e^{-i\phi/2}\\ \sin\frac{\theta}{2}e^{+i\phi/2}\end{array}\right)$$

$$+i\frac{\hat{\boldsymbol{\varphi}}}{k\sin\theta}\left(\cos\frac{\theta}{2}e^{i\phi/2}, \sin\frac{\theta}{2}e^{-i\phi/2}\right)\frac{\partial}{\partial \varphi}\left(\begin{array}{c}\cos\frac{\theta}{2}e^{-i\phi/2}\\ \sin\frac{\theta}{2}e^{+i\phi/2}\end{array}\right)$$

Berry connection III

- Then

$$\mathcal{A}_{+} = i\left\langle u_{+}\middle|\frac{\partial}{\partial \boldsymbol{k}}\middle|u_{+}\right\rangle = 0$$

$$+i\frac{\hat{\boldsymbol{\theta}}}{k}\left(\cos\frac{\theta}{2}e^{i\phi/2}, \sin\frac{\theta}{2}e^{-i\phi/2}\right)\begin{pmatrix} -\frac{1}{2}\sin\frac{\theta}{2}e^{-i\phi/2} \\ \frac{1}{2}\cos\frac{\theta}{2}e^{+i\phi/2} \end{pmatrix}$$

$$+i\frac{\hat{\boldsymbol{\varphi}}}{k\sin\theta}\left(\cos\frac{\theta}{2}e^{i\phi/2}, \sin\frac{\theta}{2}e^{-i\phi/2}\right)\left(-\frac{i}{2}\right)\begin{pmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ -\sin\frac{\theta}{2}e^{+i\phi/2} \end{pmatrix}$$

Berry connection IV

- Then $\mathcal{A}_{+} = \frac{1}{2}\frac{\hat{\boldsymbol{\varphi}}}{k\sin\theta}\left(2\cos^2\frac{\theta}{2} - 1\right) = \frac{\hat{\boldsymbol{\varphi}}}{k\sin\theta}\left(\cos^2\frac{\theta}{2} - \frac{1}{2}\right)$

$$\nabla\times\mathcal{A}_{+} = \frac{1}{r\sin\theta}\left(\frac{\partial}{\partial\theta}\left(A_{\varphi}\sin\theta\right) - \frac{\partial A_{\theta}}{\partial\varphi}\right)\hat{\boldsymbol{r}}$$

$$+\frac{1}{k}\left(\frac{1}{\sin\theta}\frac{\partial A_{k}}{\partial\varphi} - \frac{\partial}{\partial r}\left(kA_{\varphi}\right)\right)\hat{\boldsymbol{\theta}} + \frac{1}{k}\left(\frac{\partial}{\partial r}\left(kA_{\theta}\right) - \frac{\partial A_{k}}{\partial\theta}\right)\hat{\boldsymbol{\varphi}}$$

$$= \frac{1}{k\sin\theta}\left(\frac{\partial}{\partial\theta}\left(A_{\varphi}\sin\theta\right)\right)\hat{\boldsymbol{k}}$$

$$\frac{1}{k^2\sin\theta}\left(\frac{\partial}{\partial\theta}\left(\cos^2\frac{\theta}{2} - \frac{1}{2}\right)\right)\hat{\boldsymbol{k}} = -\frac{1}{k^2\sin\theta}\cos\frac{\theta}{2}\sin\frac{\theta}{2}\hat{\boldsymbol{k}}$$

$$= -\frac{1}{2k^2\sin\theta}2\cos\frac{\theta}{2}\sin\frac{\theta}{2}\hat{\boldsymbol{k}} = -\frac{\hat{\boldsymbol{k}}}{2k^2}$$