Física de Semiconductores

Lección 14

Time reversal symmetry I

- Time dependent Schrödinger equation

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

- Reverse time

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

- Take complex conjugate:

$$\left[\frac{-\hbar^2\boldsymbol{\nabla}^2}{2m}+V\left(\boldsymbol{r}\right)\right]\psi^*_{n\boldsymbol{k}}\left(\boldsymbol{r},-t\right)=i\hbar\frac{\partial\psi^*_{n\boldsymbol{k}}\left(\boldsymbol{r},-t\right)}{\partial t}$$

Time reversal symmetry II

- Choose $\psi^*_{n\boldsymbol{k}}\left(\boldsymbol{r},-t\right)=\psi^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)e^{-iE_n\left(\boldsymbol{k}\right)/\hbar}$
- Then

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

- This means that

$$\psi^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right),\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- have the same energy eigenvalue. Are they different Bloch functions?

Time reversal symmetry III

- For any Bloch function

$$\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}+\boldsymbol{R}\right)=e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- Then

$$\psi^{*}_{n\boldsymbol{k}}\left(\boldsymbol{r}+\boldsymbol{R}\right)=e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}\psi^{*}_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- This means that

$$\psi^{*}_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- is a Bloch function with wavevector –***k*** and energy $E_n(\boldsymbol{k})$

$$\psi_{n,-\boldsymbol{k}}\left(\boldsymbol{r}\right)=\psi^{*}_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)\Rightarrow E_{n}\left(-\boldsymbol{k}\right)=E_{n}\left(\boldsymbol{k}\right)$$

Spatial inversion symmetry I

- If system has inversion symmetry $V(\boldsymbol{r}) = V(-\boldsymbol{r})$

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

- Invert ***r***:

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

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

Time-reversed Berry connection

- Let $\mathcal{T}$ be time-reversal operator. Then

$$\mathcal{T}\mathcal{A}_n(\boldsymbol{k}) = i\int dr\left[\mathcal{T}u^*_{n\boldsymbol{k}}(\boldsymbol{r})\right]\frac{\partial}{\partial\boldsymbol{k}}\left[\mathcal{T}u_{n\boldsymbol{k}}(\boldsymbol{r})\right]$$

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

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

- But if system has time-reversal symmetry

$$\mathcal{T}\mathcal{A}_n(\boldsymbol{k}) = \mathcal{A}_n(\boldsymbol{k}) + \nabla\chi(\boldsymbol{k})$$

- so

$$\mathcal{A}_n(-\boldsymbol{k}) = \mathcal{A}_n(\boldsymbol{k}) + \nabla\chi(\boldsymbol{k})$$

Time-reversed Berry curvature

$$\Omega\left(\boldsymbol{k}\right) = i\int d\boldsymbol{r}\,\frac{\partial u^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}} \times \frac{\partial u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}}$$

$$\mathcal{T}\Omega\left(\boldsymbol{k}\right) = i\int d\boldsymbol{r}\,\frac{\partial \mathcal{T}u^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}} \times \frac{\partial \mathcal{T}u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}}$$

$$= i\int d\boldsymbol{r}\,\frac{\partial u_{n-\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}} \times \frac{\partial u^*_{n-\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}} = -i\int d\boldsymbol{r}\,\frac{\partial u^*_{n-\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}} \times \frac{\partial u_{n-\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial \boldsymbol{k}}$$

$$= -i\int d\boldsymbol{r}\,\frac{\partial u^*_{n-\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial\left(-\boldsymbol{k}\right)} \times \frac{\partial u_{n-\boldsymbol{k}}\left(\boldsymbol{r}\right)}{\partial\left(-\boldsymbol{k}\right)} = -\Omega\left(-\boldsymbol{k}\right)$$

- So if there is time reversal symmetry:

$$\Omega\left(\boldsymbol{k}\right) = -\Omega\left(-\boldsymbol{k}\right)$$

Point group symmetry

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

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

- Therefore $\psi_{n\boldsymbol{k}}\left(S\boldsymbol{r}\right)$ is an eigenfunction with eigenvalue $E_n\left(\boldsymbol{k}\right)$ Now

$$\psi_{n\boldsymbol{k}}\left(S\left(\boldsymbol{r}+\boldsymbol{R}\right)\right)=\psi_{n\boldsymbol{k}}\left(S\boldsymbol{r}+S\boldsymbol{R}\right)$$

- But since $\psi_{n\boldsymbol{k}}\left(S\boldsymbol{r}\right)$ is a Bloch function and S***R*** is a lattice vector,

Point symmetry (II)

$$\psi_{n\boldsymbol{k}}\left(S\boldsymbol{r}+S\boldsymbol{R}\right)=e^{i\boldsymbol{k}\cdot S\boldsymbol{R}}\psi_{n\boldsymbol{k}}\left(S\boldsymbol{r}\right)=$$

$$=e^{iS^{-1}S\boldsymbol{k}\cdot S\boldsymbol{R}}\psi_{n\boldsymbol{k}}\left(S\boldsymbol{r}\right)=e^{iS^{-1}\boldsymbol{k}\cdot\boldsymbol{R}}\psi_{n\boldsymbol{k}}\left(S\boldsymbol{r}\right)$$

- So that $\psi_{n\boldsymbol{k}}\left(S\boldsymbol{r}\right)$ is a Bloch function with energy $E_n\left(\boldsymbol{k}\right)$ and wave vector $S^{-1}\boldsymbol{k}$

$$\psi_{n\boldsymbol{k}}\left(S\boldsymbol{r}\right)=\psi_{nS^{-1}\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- So

$$E_n\left(\boldsymbol{k}\right)=E_n\left(S^{-1}\boldsymbol{k}\right)$$

Inversion Berry connection

- If the point symmetry is the inversion $\mathcal{J}$

$$\mathcal{J}u_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) = u_{n-\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- One can then show that

$$\mathcal{J}\mathcal{A}\left(\boldsymbol{k}\right) = \mathcal{A}\left(-\boldsymbol{k}\right)$$

$$\mathcal{J}\boldsymbol{\Omega}\left(\boldsymbol{k}\right) = \boldsymbol{\Omega}\left(-\boldsymbol{k}\right)$$

- If the system is invariant under inversion

$$\mathcal{J}\mathcal{A}\left(\boldsymbol{k}\right) = \mathcal{A}\left(\boldsymbol{k}\right) + \nabla\chi\left(\boldsymbol{k}\right) = \mathcal{A}\left(-\boldsymbol{k}\right)$$

$$\mathcal{J}\boldsymbol{\Omega}\left(\boldsymbol{k}\right) = \boldsymbol{\Omega}\left(\boldsymbol{k}\right) = \boldsymbol{\Omega}\left(-\boldsymbol{k}\right)$$

Chern number I

- 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 then an integer.

Chern number II

- By analogy we define the Chern number as

$$C = \frac{1}{2\pi} \oiint \boldsymbol{\Omega}\left(\boldsymbol{k}\right) \cdot d\boldsymbol{S}$$

- If we identify the "surface" with the BZ, and consider that the integral of an odd function of k over the BZ is zero, then we conclude that the Chern number is zero if there is time inversion symmetry.

Chern number III

- If there is both time reversal and inversion symmetry

$$\Omega\left(\boldsymbol{k}\right) = -\Omega\left(-\boldsymbol{k}\right)$$ TR

$$\Omega\left(\boldsymbol{k}\right) = \Omega\left(-\boldsymbol{k}\right)$$ Inversion

$$\Omega\left(\boldsymbol{k}\right) = 0$$

Effect on magnetic field

- If we move an electron in a closed loop in the presence of a magnetic field, the electron picks up a phase

$$\phi = \frac{e}{c\hbar} \oint \boldsymbol{A} \cdot d\boldsymbol{l} = \frac{e}{c\hbar} \iint \boldsymbol{B} \cdot d\boldsymbol{S}$$

- Under time reversal the phase changes sign, so

$$\mathcal{T} \iint \boldsymbol{B} \cdot d\boldsymbol{S} = -\iint \boldsymbol{B} \cdot d\boldsymbol{S}$$
$$\Rightarrow \mathcal{T}\boldsymbol{B} = -\boldsymbol{B}$$

Phase with time reversal symmetry

- If a system has time-reversal symmetry, we tentatively say

$$e^{i\phi} = e^{-i\phi} \Rightarrow \phi = -\phi \Rightarrow \phi = 0 \Rightarrow B = 0$$

- But true condition is

$$\phi = -\phi + 2m\pi$$

- So that to preserve time-reversal symmetry we only need $\phi = m\pi$, so we can have

$$B = \frac{c\hbar}{e} \sum_i m_i \pi \delta\left(r - r_i\right)$$

Application to Berry curvature

- Under time reversal symmetry

$$\Omega\left(\boldsymbol{k}\right)=\sum_{i} m_{i}\pi\delta\left(k-k_{i}\right)$$

Dirac point

- Consider a hamiltonian

$$H = v_F \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} = v_F k \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}$$

- Eigenvalues: $\pm v_F k$
- Eigenvectors: $u_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix}; \quad u_- = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-i\phi} \\ 1 \end{pmatrix}$

Berry connection at Dirac point

- The Berry connection in polar coordinates has components k and ϕ:

$$\mathcal{A}_k^+ = i\left\langle u_+ \left| \frac{\partial}{\partial k} \right| u_+ \right\rangle = 0$$

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

$$= \frac{i}{2k}\left(e^{i\phi}, 1\right)\frac{\partial}{\partial \phi}\begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix} = \frac{i}{2k}\left(e^{i\phi}, 1\right)\begin{pmatrix} -ie^{-i\phi} \\ 0 \end{pmatrix} = \frac{1}{2k}$$

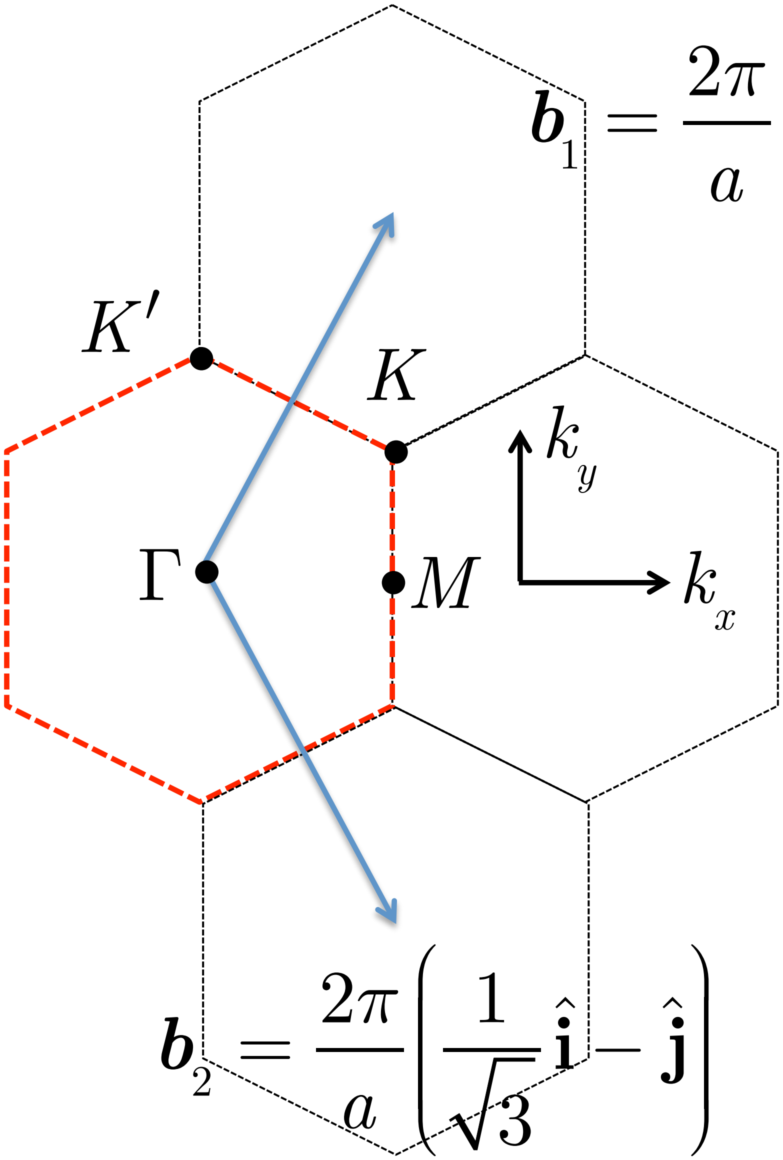
Berry flux

$$\iint \boldsymbol{\Omega}\left(\boldsymbol{k}\right) \cdot d\boldsymbol{S} = \oint \mathcal{A} \cdot d\boldsymbol{l}$$

- Taking a circle around k=0

$$\oint \mathcal{A} \cdot d\boldsymbol{l} = \int_{0}^{2\pi} \frac{1}{2k} k d\phi = \pi$$

Brillouin zone del grafeno



$$\boldsymbol{b}_1 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)$$

$$\boldsymbol{b}_2 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{\mathbf{i}} - \hat{\mathbf{j}}\right)$$

$$\Gamma = 0$$

$$M = \frac{1}{2}\left(\boldsymbol{b}_1 + \boldsymbol{b}_2\right) = \frac{2\pi}{a\sqrt{3}}\mathbf{i}$$

$$K = \frac{2}{3}\boldsymbol{b}_1 + \frac{1}{3}\boldsymbol{b}_2 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\mathbf{i} + \frac{1}{3}\mathbf{j}\right)$$

$$K' = \frac{1}{3}\boldsymbol{b}_1 - \frac{1}{3}\boldsymbol{b}_2 = \frac{2\pi}{a}\left(\frac{2}{3}\mathbf{j}\right)$$

Graphene

- The hamiltonian matrix for graphene is

$$H = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix}$$

$$H_{AA} = H_{BB} = \begin{pmatrix} \varepsilon_s & 0 & 0 & 0 \\ 0 & \varepsilon_{p\sigma} & 0 & 0 \\ 0 & 0 & \varepsilon_{p\sigma} & 0 \\ 0 & 0 & 0 & \varepsilon_{p\pi} \end{pmatrix}$$

$$H_{AB} = H_{BA}^{*}$$

$$\left(\begin{array}{cccc} V_{ss\sigma}\left(g_1 + g_2 + g_3\right) & V_{sp\sigma}\left[g_1 - \frac{1}{2}\left(g_2 + g_3\right)\right] & \frac{\sqrt{3}}{2} V_{sp\sigma}\left(g_2 - g_3\right) & 0 \\ -V_{sp\sigma}\left[g_1 - \frac{1}{2}\left(g_2 + g_3\right)\right] & g_1 V_{pp\sigma} + \left(g_2 + g_3\right)\left[\frac{3}{4} V_{pp\pi} + \frac{1}{4} V_{pp\sigma}\right] & \frac{\sqrt{3}}{4}\left(V_{pp\sigma} - V_{pp\pi}\right)\left(g_3 - g_2\right) & 0 \\ -\frac{\sqrt{3}}{2} V_{sp\sigma}\left(g_2 - g_3\right) & \frac{\sqrt{3}}{4}\left(V_{pp\sigma} - V_{pp\pi}\right)\left(g_3 - g_2\right) & g_1 V_{pp\pi} + \left(g_2 + g_3\right)\left[\frac{1}{4} V_{pp\pi} + \frac{3}{4} V_{pp\sigma}\right] & 0 \\ 0 & 0 & 0 & \left(g_1 + g_2 + g_3\right) V_{p} \end{array}$$

The pπ submatrix

$$H = \begin{pmatrix} \varepsilon_{p\pi} & \left(g_1 + g_2 + g_3\right) V_{pp\pi} \\ \left(g_1 + g_2 + g_3\right)^* V_{pp\pi} & \varepsilon_{p\pi} \end{pmatrix}$$

$$g_1 \equiv e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}}$$

$$g_2 \equiv e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}}$$

$$g_3 \equiv e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}}$$

$$\boldsymbol{n}_{AB}^{(1)} = -\boldsymbol{n}_{BA}^{(1)} = \left(a/\sqrt{3}\right)\hat{\mathbf{i}}$$

$$\boldsymbol{n}_{AB}^{(2)} = -\boldsymbol{n}_{BA}^{(2)} = \left(a/\sqrt{3}\right)\left[-\left(1/2\right)\hat{\mathbf{i}} + \left(\sqrt{3}/2\right)\hat{\mathbf{j}}\right]$$

$$\boldsymbol{n}_{AB}^{(3)} = -\boldsymbol{n}_{BA}^{(3)} = \left(a/\sqrt{3}\right)\left[-\left(1/2\right)\hat{\mathbf{i}} = \left(\sqrt{3}/2\right)\hat{\mathbf{j}}\right]$$

Pauli matrix formulation

$$H=\begin{pmatrix} \varepsilon_{p\pi} & \left(g_1+g_2+g_3\right)V_{pp\pi} \\ \left(g_1+g_2+g_3\right)^* V_{pp\pi} & \varepsilon_{p\pi} \end{pmatrix}$$

$$=\begin{pmatrix} H_{11}\left(\boldsymbol{k}\right) & H_{12}\left(\boldsymbol{k}\right) \\ H_{21}\left(\boldsymbol{k}\right) & H_{22}\left(\boldsymbol{k}\right) \end{pmatrix}$$

We can write this as

$$g_1+g_2+g_3=$$

$$=H_0\left(\boldsymbol{k}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}+H_x\left(\boldsymbol{k}\right)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}+H_y\left(\boldsymbol{k}\right)\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}+H_z\left(\boldsymbol{k}\right)\begin{pmatrix} 1 & 0 \\ 0 & - \end{pmatrix}$$

The pπ submatrix II

Then

$$H_{11}(\boldsymbol{k}) = H_0(\boldsymbol{k}) + H_z(\boldsymbol{k}); \quad H_{22}(\boldsymbol{k}) = H_0(\boldsymbol{k}) - H_z(\boldsymbol{k})$$

$$H_{12}(\boldsymbol{k}) = H_x(\boldsymbol{k}) - iH_y(\boldsymbol{k}); \quad H_{21}(\boldsymbol{k}) = H_x(\boldsymbol{k}) + iH_y(\boldsymbol{k})$$

$$H_0(\boldsymbol{k}) = \frac{H_{11}(\boldsymbol{k}) + H_{22}(\boldsymbol{k})}{2} = \frac{\varepsilon_{pA} + \varepsilon_{pB}}{2} = \varepsilon_p$$

$$H_z(\boldsymbol{k}) = \frac{H_{11}(\boldsymbol{k}) - H_{22}(\boldsymbol{k})}{2} = \frac{\varepsilon_{pA} - \varepsilon_{pB}}{2} = \Delta_p$$

$$H_x(\boldsymbol{k}) = \frac{H_{12}(\boldsymbol{k}) + H_{21}(\boldsymbol{k})}{2}$$

$$= \mathrm{Re}\left[H_{12}(\boldsymbol{k})\right] = V_{pp\pi}\left[\cos\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}\right) + \cos\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}\right) + \cos\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}\right)\right]$$

$$H_y(\boldsymbol{k}) = i\,\frac{H_{12}(\boldsymbol{k}) - H_{21}(\boldsymbol{k})}{2} = -\mathrm{Im}\left[H_{12}(\boldsymbol{k})\right]$$

$$= -V_{pp\pi}\left[\sin\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}\right) + \sin\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}\right) + \sin\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}\right)\right]$$

The pπ submatrix III

Expanding

$$H_x(\boldsymbol{k}) = V_{pp\pi}\left[\cos\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}\right) + \cos\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}\right) + \cos\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}\right)\right] =$$

$$= V_{pp\pi}\left[\cos\left(k_x a/\sqrt{3}\right) + \cos\left(-\tfrac{1}{2}k_x a/\sqrt{3} + \tfrac{1}{2}k_y a\right) + \cos\left(-\tfrac{1}{2}k_x a/\sqrt{3} - \tfrac{1}{2}k_y a\right)\right]$$

$$= V_{pp\pi}\left[\cos\left(k_x a/\sqrt{3}\right) + 2\cos\left(\tfrac{1}{2}k_x a/\sqrt{3}\right)\cos\left[\tfrac{1}{2}k_y a\right]\right]$$

$$H_y(\boldsymbol{k}) = -V_{pp\pi}\left[\sin\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}\right) + \sin\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}\right) + \sin\left(\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}\right)\right]$$

$$= -V_{pp\pi}\left[\sin\left(k_x a/\sqrt{3}\right) + \sin\left(-\tfrac{1}{2}k_x a/\sqrt{3} + \tfrac{1}{2}k_y a\right) + \sin\left(-\tfrac{1}{2}k_x a/\sqrt{3} - \tfrac{1}{2}k_y a\right)\right]$$

$$H_y(\boldsymbol{k}) = -V_{pp\pi}\left[\sin\left(k_x a/\sqrt{3}\right) - 2\sin\left(\tfrac{1}{2}k_x a/\sqrt{3}\right)\cos\left[\tfrac{1}{2}k_y a\right]\right]$$

Near K (I)

- We propose $K = k_x = \dfrac{2\pi}{a\sqrt{3}} + \delta k_x ; k_y = \dfrac{2\pi}{3a} + \delta k_y$

$$H_x(\boldsymbol{k}) = V_{pp\pi}\left[\cos\left(k_x a/\sqrt{3}\right) + 2\cos\left(\tfrac{1}{2}k_x a/\sqrt{3}\right)\cos\left[\tfrac{1}{2}k_y a\right]\right]$$

$$= V_{pp\pi}\left[\cos\left(\left\{\frac{2\pi}{a\sqrt{3}} + \delta k_x\right\}a/\sqrt{3}\right) + 2\cos\left(\tfrac{1}{2}\left\{\frac{2\pi}{a\sqrt{3}} + \delta k_x\right\}a/\sqrt{3}\right)\cos\left[\tfrac{1}{2}\left\{\frac{2\pi}{3a} + \delta k_y\right\}a\right]\right]$$

$$= V_{pp\pi}\left[\cos\left(\frac{2\pi}{3} + \delta k_x a/\sqrt{3}\right) + 2\cos\left(\frac{\pi}{3} + \tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\cos\left(\frac{\pi}{3} + \frac{\delta k_y a}{2}\right)\right]$$

$$= V_{pp\pi}\left[\cos\left(\frac{2\pi}{3}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \sin\left(\frac{2\pi}{3}\right)\sin\left(\delta k_x a/\sqrt{3}\right) + \right.$$

$$\left. + 2\left\{\cos\left(\frac{\pi}{3}\right)\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \sin\left(\frac{\pi}{3}\right)\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\cos\left(\frac{\pi}{3} + \frac{\delta k_y a}{2}\right)\right]$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\delta k_x a/\sqrt{3}\right) + \right.$$

$$\left. 2\left\{\frac{1}{2}\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\left\{\cos\left(\frac{\pi}{3}\right)\cos\left(\frac{\delta k_y a}{2}\right) - \sin\left(\frac{\pi}{3}\right)\sin\left(\frac{\delta k_y a}{2}\right)\right\}\right]$$

Near K (II)

- We propose $K = k_x = \frac{2\pi}{a\sqrt{3}} + \delta k_x ; k_y = \frac{2\pi}{3a} + \delta k_y$

$$= V_{pp\pi}\left[\cos\left(\frac{2\pi}{3}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \sin\left(\frac{2\pi}{3}\right)\sin\left(\delta k_x a/\sqrt{3}\right) + 2\left\{\cos\left(\frac{\pi}{3}\right)\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \sin\left(\frac{\pi}{3}\right)\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\cos\left(\frac{\pi}{3} + \frac{\delta k_y a}{2}\right)\right]$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\delta k_x a/\sqrt{3}\right) + 2\left\{\frac{1}{2}\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\left\{\cos\left(\frac{\pi}{3}\right)\cos\left(\frac{\delta k_y a}{2}\right) - \sin\left(\frac{\pi}{3}\right)\sin\left(\frac{\delta k_y a}{2}\right)\right\}\right]$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\delta k_x a/\sqrt{3}\right) + 2\left\{\frac{1}{2}\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\left\{\frac{1}{2}\cos\left(\frac{\delta k_y a}{2}\right) - \frac{\sqrt{3}}{2}\sin\left(\frac{\delta k_y a}{2}\right)\right\}\right]$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right) - \frac{\sqrt{3}}{2}\left(\delta k_x a/\sqrt{3}\right) + \left\{1 - \sqrt{3}\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\left\{\frac{1}{2} - \frac{\sqrt{3}}{4}\delta k_y a\right\}\right]$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right) - \frac{\delta k_x a}{2} + \left\{\frac{1}{2} - \frac{\sqrt{3}}{4}\delta k_y a - \frac{1}{2}\left(\tfrac{1}{2}\delta k_x a\right)\right\}\right]$$

$$= V_{pp\pi}\left[-\frac{\delta k_x a}{2} + \left\{-\frac{\sqrt{3}}{4}\delta k_y a - \frac{\delta k_x a}{4}\right\}\right] = V_{pp\pi}\left[-\frac{3\delta k_x a}{4} - \frac{\sqrt{3}}{4}\delta k_y a\right] = -\frac{V_{pp\pi}a}{4}\left[3\delta k_x + \sqrt{3}\delta k_y\right] = -\frac{3V_{pp\pi}a}{4}\left[\delta k_x + \frac{\delta k_y}{\sqrt{3}}\right]$$

Axis rotation K point

- We have

$$H_x\left(\boldsymbol{k}\right) = -\frac{3V_{pp\pi}a}{4}\left[\delta k_x + \frac{\delta k_y}{\sqrt{3}}\right]$$

$$H_y\left(\boldsymbol{k}\right) = -\frac{3V_{pp\pi}a}{4}\left[-\frac{\delta k_x}{\sqrt{3}} + \delta k_y\right]$$

- Define

$$\begin{pmatrix} q_x \\ q_y \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix} \begin{pmatrix} \delta k_x \\ \delta k_y \end{pmatrix}$$

$$H_x\left(\boldsymbol{k}\right) = -\frac{3V_{pp\pi}a}{4}\left[\delta k_x + \frac{\delta k_y}{\sqrt{3}}\right] = -\frac{3V_{pp\pi}a}{4}\left(\frac{2q_x}{\sqrt{3}}\right) = -\frac{\sqrt{3}V_{pp\pi}a}{2}q_x$$

$$H_y\left(\boldsymbol{k}\right) = -\frac{3V_{pp\pi}a}{4}\left[-\frac{\delta k_x}{\sqrt{3}} + \delta k_y\right] = -\frac{3V_{pp\pi}a}{4}\left(\frac{2q_y}{\sqrt{3}}\right) = -\frac{\sqrt{3}V_{pp\pi}a}{2}q_y$$

K' (I)

- We propose $K = k_x = \frac{2\pi}{a\sqrt{3}} + \delta k_x ; k_y = -\frac{2\pi}{3a} + \delta k_y$

$$H_x\left(\boldsymbol{k}\right) = V_{pp\pi}\left[\cos\left(k_x a/\sqrt{3}\right) + 2\cos\left(\tfrac{1}{2}k_x a/\sqrt{3}\right)\cos\left[\tfrac{1}{2}k_y a\right]\right]$$

$$= V_{pp\pi}\left[\cos\left(\left\{\frac{2\pi}{a\sqrt{3}} + \delta k_x\right\}a/\sqrt{3}\right) + 2\cos\left(\tfrac{1}{2}\left\{\frac{2\pi}{a\sqrt{3}} + \delta k_x\right\}a/\sqrt{3}\right)\cos\left[\tfrac{1}{2}\left\{-\frac{2\pi}{3a} + \delta k_y\right\}a\right]\right]$$

$$= V_{pp\pi}\left[\cos\left(\frac{2\pi}{3} + \delta k_x a/\sqrt{3}\right) + 2\cos\left(\frac{\pi}{3} + \tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\cos\left(-\frac{\pi}{3} + \frac{\delta k_y a}{2}\right)\right]$$

$$= V_{pp\pi}\left[\cos\left(\frac{2\pi}{3}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \sin\left(\frac{2\pi}{3}\right)\sin\left(\delta k_x a/\sqrt{3}\right) + 2\left\{\cos\left(\frac{\pi}{3}\right)\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \sin\left(\frac{\pi}{3}\right)\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\} \mathrm{co}$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\delta k_x a/\sqrt{3}\right) + 2\left\{\frac{1}{2}\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\right]\left\{\cos\left(\frac{\pi}{3}\right)\cos\left(\frac{\delta k_y a}{2}\right)\right.$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\delta k_x a/\sqrt{3}\right) + 2\left\{\frac{1}{2}\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\right]\left\{\frac{1}{2}\cos\left(\frac{\delta k_y a}{2}\right) + \frac{\sqrt{3}}{2}\right.$$

K’ (II)

- We propose $K = k_x = \frac{2\pi}{a\sqrt{3}} + \delta k_x ; k_y = -\frac{2\pi}{3a} + \delta k_y$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\delta k_x a/\sqrt{3}\right)\right.$$

$$\left. +2\left\{\frac{1}{2}\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\left\{\cos\left(\frac{\pi}{3}\right)\cos\left(\frac{\delta k_y a}{2}\right) + \sin\left(\frac{\pi}{3}\right)\sin\left(\frac{\delta k_y a}{2}\right)\right\}\right]$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right)\cos\left(\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\delta k_x a/\sqrt{3}\right)\right.$$

$$\left. +2\left\{\frac{1}{2}\cos\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right) - \frac{\sqrt{3}}{2}\sin\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\left\{\frac{1}{2}\cos\left(\frac{\delta k_y a}{2}\right) + \frac{\sqrt{3}}{2}\sin\left(\frac{\delta k_y a}{2}\right)\right\}\right]$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right) - \frac{\sqrt{3}}{2}\left(\delta k_x a/\sqrt{3}\right) + \left\{1 - \sqrt{3}\left(\tfrac{1}{2}\delta k_x a/\sqrt{3}\right)\right\}\left\{\frac{1}{2} + \frac{\sqrt{3}}{4}\delta k_y a\right\}\right]$$

$$= V_{pp\pi}\left[\left(-\frac{1}{2}\right) - \frac{\delta k_x a}{2} + \left\{\frac{1}{2} + \frac{\sqrt{3}}{4}\delta k_y a - \frac{1}{2}\left(\tfrac{1}{2}\delta k_x a\right)\right\}\right]$$

$$= V_{pp\pi}\left[-\frac{\delta k_x a}{2} + \left\{+\frac{\sqrt{3}}{4}\delta k_y a - \frac{\delta k_x a}{4}\right\}\right] = V_{pp\pi}\left[-\frac{3\delta k_x a}{4} + \frac{\sqrt{3}}{4}\delta k_y a\right] = -\frac{V_{pp\pi} a}{4}\left[3\delta k_x - \sqrt{3}\delta k_y\right] = -\frac{3V_{pp\pi} a}{4}\left[\delta k_x - \frac{\delta k_y}{\sqrt{3}}\right.$$

Point K' (I)

- We propose $K = k_x = \frac{2\pi}{a\sqrt{3}} + \delta k_x ; k_y = -\frac{2\pi}{3a} + \delta k_y$

$$H_y(\boldsymbol{k}) = -V_{pp\pi}\left[\sin\left(k_x a/\sqrt{3}\right) - 2\sin\left(\tfrac{1}{2}k_x a/\sqrt{3}\right)\cos\left[\tfrac{1}{2}k_y a\right]\right]$$

$$= -V_{pp\pi}\left[\sin\left(\left\{\frac{2\pi}{a\sqrt{3}} + \delta k_x\right\}a/\sqrt{3}\right) - 2\sin\left(\tfrac{1}{2}\left\{\frac{2\pi}{a\sqrt{3}} + \delta k_x\right\}a/\sqrt{3}\right)\cos\left[\tfrac{1}{2}\left\{-\frac{2\pi}{3a} + \delta k_y\right\}a\right]\right]$$

$$= -V_{pp\pi}\left[\sin\left(\frac{2\pi}{3} + \frac{\delta k_x a}{\sqrt{3}}\right) - 2\sin\left(\frac{\pi}{3} + \frac{\delta k_x a}{2\sqrt{3}}\right)\cos\left(-\frac{\pi}{3} + \frac{\delta k_y a}{2}\right)\right]$$

$$= -V_{pp\pi}\left[\sin\left(\frac{2\pi}{3}\right)\cos\left(\frac{\delta k_x a}{\sqrt{3}}\right) + \cos\left(\frac{2\pi}{3}\right)\sin\left(\frac{\delta k_x a}{\sqrt{3}}\right)\right.$$

$$\left. -2\left[\sin\left(\frac{\pi}{3}\right)\cos\left(\frac{\delta k_x a}{2\sqrt{3}}\right) + \cos\left(\frac{\pi}{3}\right)\sin\left(\frac{\delta k_x a}{2\sqrt{3}}\right)\right]\left[\cos\left(-\frac{\pi}{3}\right)\cos\left(\frac{\delta k_y a}{2}\right) - \sin\left(-\frac{\pi}{3}\right)\sin\left(\frac{\delta k_y a}{2}\right)\right]\right]$$

$$= -V_{pp\pi}\left[\frac{\sqrt{3}}{2}\cos\left(\frac{\delta k_x a}{\sqrt{3}}\right) + \left(-\frac{1}{2}\right)\sin\left(\frac{\delta k_x a}{\sqrt{3}}\right) - 2\left[\frac{\sqrt{3}}{2}\cos\left(\frac{\delta k_x a}{2\sqrt{3}}\right) + \left(\frac{1}{2}\right)\sin\left(\frac{\delta k_x a}{2\sqrt{3}}\right)\right]\left[\left(\frac{1}{2}\right)\cos\left(\frac{\delta k_y a}{2}\right) + \left(\frac{\sqrt{3}}{2}\right)\sin\left(\frac{\delta k_y a}{2}\right)\right]\right]$$

Alternative K' (II)

- We propose $K = k_x = \frac{2\pi}{a\sqrt{3}} + \delta k_x ; k_y = -\frac{2\pi}{3a} + \delta k_y$

$$= -V_{pp\pi}\left[\sin\left(\frac{2\pi}{3}\right)\cos\left(\frac{\delta k_x a}{\sqrt{3}}\right) + \cos\left(\frac{2\pi}{3}\right)\sin\left(\frac{\delta k_x a}{\sqrt{3}}\right) - 2\left[\sin\left(\frac{\pi}{3}\right)\cos\left(\frac{\delta k_x a}{2\sqrt{3}}\right) + \cos\left(\frac{\pi}{3}\right)\sin\left(\frac{\delta k_x a}{2\sqrt{3}}\right)\right]\left[\cos\left(-\frac{\pi}{3}\right)\cos\left(\frac{\delta k_y a}{2}\right) - \sin\left(-\frac{\pi}{3}\right)\sin\left(\frac{\delta k_y a}{2}\right)\right]\right]$$

$$= -V_{pp\pi}\left[\frac{\sqrt{3}}{2}\cos\left(\frac{\delta k_x a}{\sqrt{3}}\right) + \left(-\frac{1}{2}\right)\sin\left(\frac{\delta k_x a}{\sqrt{3}}\right) - 2\left[\frac{\sqrt{3}}{2}\cos\left(\frac{\delta k_x a}{2\sqrt{3}}\right) + \left(\frac{1}{2}\right)\sin\left(\frac{\delta k_x a}{2\sqrt{3}}\right)\right]\left[\left(\frac{1}{2}\right)\cos\left(\frac{\delta k_y a}{2}\right) + \left(\frac{\sqrt{3}}{2}\right)\sin\left(\frac{\delta k_y a}{2}\right)\right]\right]$$

$$= -V_{pp\pi}\left[\frac{\sqrt{3}}{2} + \left(-\frac{1}{2}\right)\left(\frac{\delta k_x a}{\sqrt{3}}\right) - \left[\sqrt{3} + \left(\frac{\delta k_x a}{2\sqrt{3}}\right)\right]\left[\left(\frac{1}{2}\right) + \left(\frac{\sqrt{3}}{2}\right)\left(\frac{\delta k_y a}{2}\right)\right]\right]$$

$$= -V_{pp\pi}\left[\frac{\sqrt{3}}{2} + \left(-\frac{1}{2}\right)\left(\frac{\delta k_x a}{\sqrt{3}}\right) - \left\{\left(\frac{\sqrt{3}}{2}\right) + \left(\frac{3}{2}\right)\left(\frac{\delta k_y a}{2}\right)\right\} + \left(\frac{\delta k_x a}{4\sqrt{3}}\right)\right] = -V_{pp\pi}\left[\frac{\sqrt{3}}{2} - \left(\frac{\delta k_x a}{2\sqrt{3}}\right) - \left(\frac{\sqrt{3}}{2}\right) - \left(\frac{3}{2}\right)\left(\frac{\delta k_y a}{2}\right) - \left(\frac{\delta k_x a}{4\sqrt{3}}\right)\right]$$

$$= -V_{pp\pi}\left[-\left(\frac{3\delta k_x a}{4\sqrt{3}}\right) - \left(\frac{3}{2}\right)\left(\frac{\delta k_y a}{2}\right)\right] = -\frac{3V_{pp\pi}a}{4}\left[-\frac{\delta k_x}{\sqrt{3}} - \delta k_y\right]$$

Axis rotation K' point

- We have

$$H_x(\boldsymbol{k}) = -\frac{3V_{pp\pi}a}{4}\left[\delta k_x - \frac{\delta k_y}{\sqrt{3}}\right]$$

$$H_y(\boldsymbol{k}) = -\frac{3V_{pp\pi}a}{4}\left[-\frac{\delta k_x}{\sqrt{3}} - \delta k_y\right]$$

- Define

$$\begin{pmatrix} q'_x \\ q'_y \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix}\begin{pmatrix} \delta k_x \\ \delta k_y \end{pmatrix}$$

$$H_x(\boldsymbol{k}) = -\frac{3V_{pp\pi}a}{4}\left[\delta k_x - \frac{\delta k_y}{\sqrt{3}}\right] = -\frac{3V_{pp\pi}a}{4}\left(\frac{2q'_x}{\sqrt{3}}\right) = -\frac{\sqrt{3}V_{pp\pi}a}{2}q'_x$$

$$H_y(\boldsymbol{k}) = -\frac{3V_{pp\pi}a}{4}\left[-\frac{\delta k_x}{\sqrt{3}} - \delta k_y\right] = -\frac{3V_{pp\pi}a}{4}\left(-\frac{2q'_y}{\sqrt{3}}\right) = -\frac{\sqrt{3}V_{pp\pi}a}{2}\left(-q'_y\right)$$

Near Dirac point hamiltonian

- For the K point:

$$H_K(\boldsymbol{q}) = \begin{pmatrix} \varepsilon_{pA} & 0 \\ 0 & \varepsilon_{pB} \end{pmatrix} - \frac{\sqrt{3}V_{pp\pi}a}{2} q_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \frac{\sqrt{3}V_{pp\pi}a}{2} q_x \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

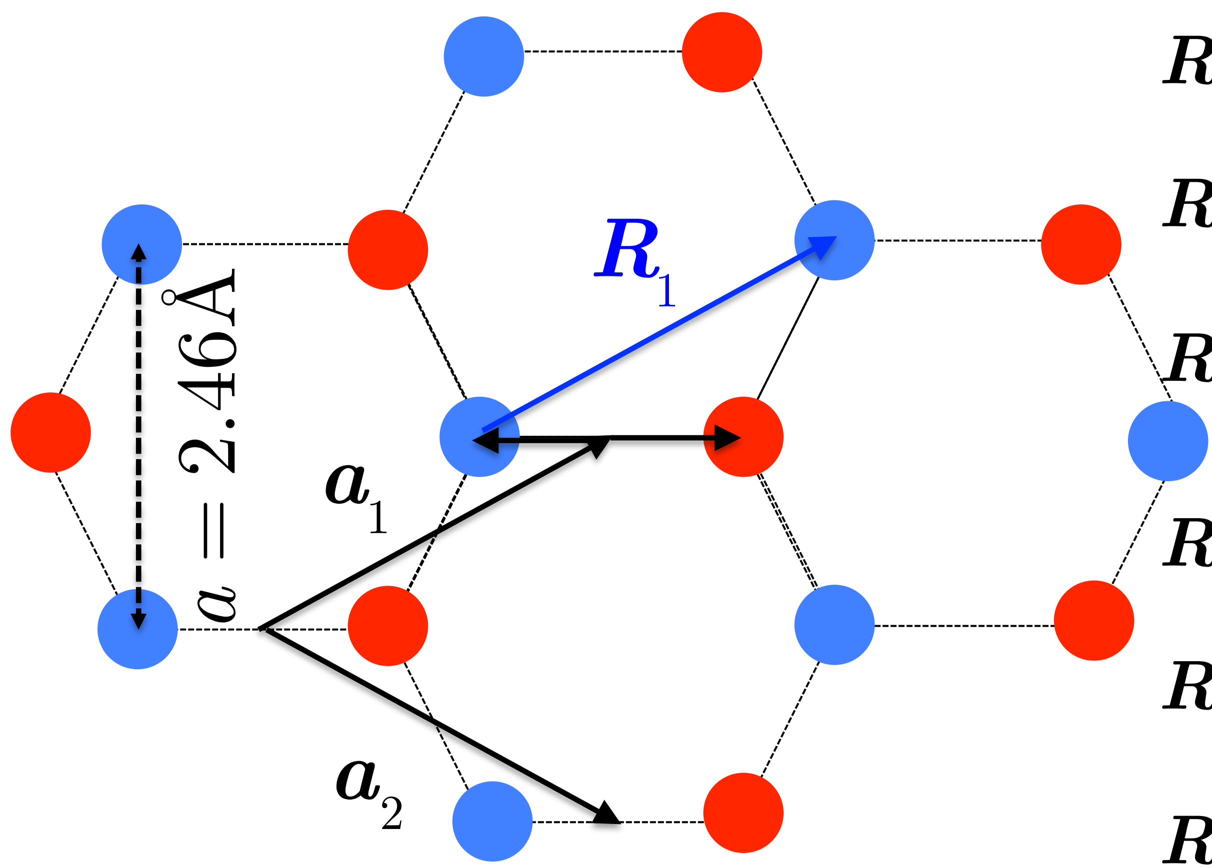
$$= \varepsilon_p I - \frac{\sqrt{3}V_{pp\pi}a}{2}\left(\sigma_x q_x + \sigma_y q_y\right) + \sigma_z \Delta_p$$

- For the K' point:

$$H_{K'}(\boldsymbol{q}) = \begin{pmatrix} \varepsilon_{pA} & 0 \\ 0 & \varepsilon_{pB} \end{pmatrix} - \frac{\sqrt{3}V_{pp\pi}a}{2} q_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{\sqrt{3}V_{pp\pi}a}{2} q_x \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$= \varepsilon_p I - \frac{\sqrt{3}V_{pp\pi}a}{2}\left(\sigma_x q_x - \sigma_y q_y\right) + \sigma_z \Delta_p$$

Graphene second neighbors



$$\boldsymbol{R}_1 = \frac{a}{2}\left(\sqrt{3}\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)$$

$$\boldsymbol{R}_2 = a\hat{\mathbf{j}}$$

$$\boldsymbol{R}_3 = \frac{a}{2}\left(-\sqrt{3}\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)$$

$$\boldsymbol{R}_4 = \frac{a}{2}\left(-\sqrt{3}\hat{\mathbf{i}} - \hat{\mathbf{j}}\right) = -\boldsymbol{R}_1$$

$$\boldsymbol{R}_5 = -a\hat{\mathbf{j}} = -\boldsymbol{R}_2$$

$$\boldsymbol{R}_6 = \frac{a}{2}\left(\sqrt{3}\hat{\mathbf{i}} - \hat{\mathbf{j}}\right) = -\boldsymbol{R}_3$$

Second neighbor H

- Second neighbors belong to the same sublattice, so this will only add diagonal elements:

$$H_{jj} = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R})} \int d\boldsymbol{r}\, \phi^{*}_{j,\boldsymbol{0}}(\boldsymbol{r}) H \phi_{j,\boldsymbol{R}}(\boldsymbol{r})$$

$$= \sum_{k} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_k} \int d\boldsymbol{r}\, \phi^{*}_{j,\boldsymbol{0}}(\boldsymbol{r}) H \phi_{j,\boldsymbol{nn}_k}(\boldsymbol{r})$$

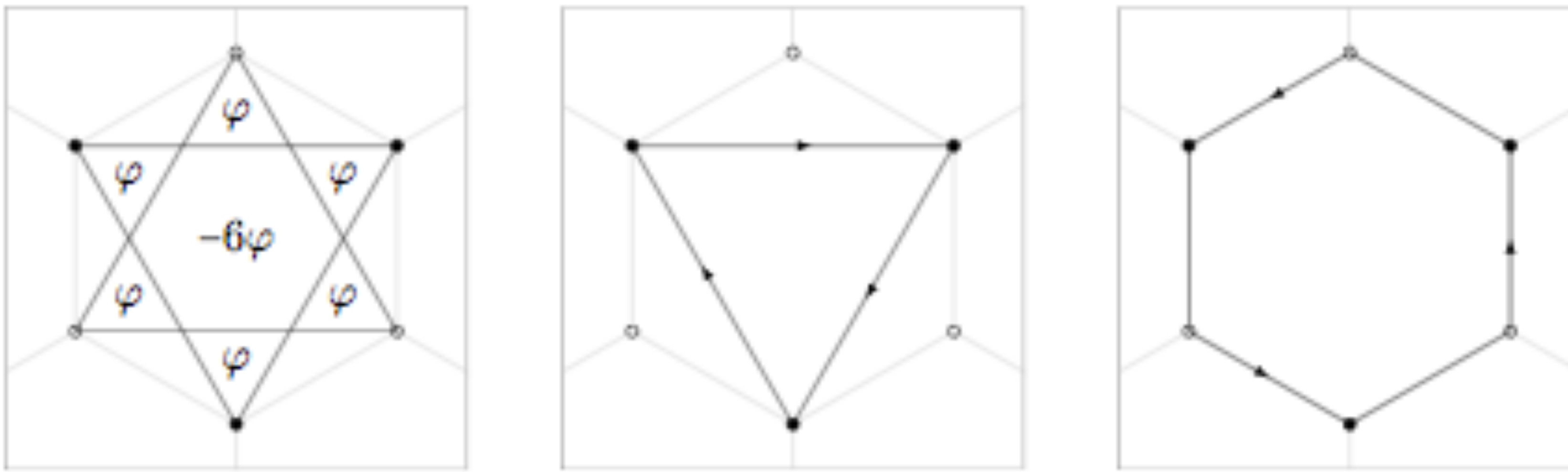
Matrix element

- Let us now assume:

$$\int d\boldsymbol{r}\,\phi^{*}_{A,\boldsymbol{0}}\left(\boldsymbol{r}\right)H\phi_{A,\boldsymbol{R}_k}\left(\boldsymbol{r}\right)=\begin{cases} V_2 e^{i\alpha} & \text{for } i=1,3,4 \\ V_2 e^{-i\alpha} & \text{for } i=2,4,6 \end{cases}$$

$$\int d\boldsymbol{r}\,\phi^{*}_{B,\boldsymbol{0}}\left(\boldsymbol{r}\right)H\phi_{B,\boldsymbol{R}_k}\left(\boldsymbol{r}\right)=\begin{cases} V_2 e^{-i\alpha} & \text{for } i=1,3,4 \\ V_2 e^{+i\alpha} & \text{for } i=2,4,6 \end{cases}$$

How do we get this?



arXiv:1310.0255v2

H(k)

- Then

$$H_{AA} = V_2\left[e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_1+\alpha)} + e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_3+\alpha)} + e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_5+\alpha)}\right]$$
$$+V_2\left[e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_2-\alpha)} + e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_4-\alpha)} + e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_6-\alpha)}\right]$$
$$= 2V_2\left[\cos(\boldsymbol{k}\cdot\boldsymbol{R}_1+\alpha) + \cos(\boldsymbol{k}\cdot\boldsymbol{R}_3+\alpha) + \cos(\boldsymbol{k}\cdot\boldsymbol{R}_5+\alpha)\right]$$

$$H_{BB} = V_2\left[e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_1-\alpha)} + e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_3-\alpha)} + e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_5-\alpha)}\right]$$
$$+V_2\left[e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_2+\alpha)} + e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_4+\alpha)} + e^{i(\boldsymbol{k}\cdot\boldsymbol{R}_6+\alpha)}\right]$$
$$= 2V_2\left[\cos(\boldsymbol{k}\cdot\boldsymbol{R}_1-\alpha) + \cos(\boldsymbol{k}\cdot\boldsymbol{R}_3-\alpha) + \cos(\boldsymbol{k}\cdot\boldsymbol{R}_5-\alpha)\right]$$

New elements

- This second neighbor interaction contributes an additional

$$
\begin{aligned}
H_0(\boldsymbol{k}) &= \frac{H_{AA}(\boldsymbol{k}) + H_{BB}(\boldsymbol{k})}{2} = \\
&= V_2\left[\cos(\boldsymbol{k}\cdot\boldsymbol{R}_1+\alpha)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_3+\alpha)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_5+\alpha)\right]+ \\
&\quad V_2\left[\cos(\boldsymbol{k}\cdot\boldsymbol{R}_1-\alpha)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_3-\alpha)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_5-\alpha)\right] \\
&= 2V_2\cos\alpha\left[\cos(\boldsymbol{k}\cdot\boldsymbol{R}_1)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_3)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_5)\right]
\end{aligned}
$$

$$
\begin{aligned}
H_z(\boldsymbol{k}) &= \frac{H_{AA}(\boldsymbol{k}) - H_{BB}(\boldsymbol{k})}{2} = \\
&= V_2\left[\cos(\boldsymbol{k}\cdot\boldsymbol{R}_1+\alpha)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_3+\alpha)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_5+\alpha)\right] \\
&\quad -V_2\left[\cos(\boldsymbol{k}\cdot\boldsymbol{R}_1-\alpha)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_3-\alpha)+\cos(\boldsymbol{k}\cdot\boldsymbol{R}_5-\alpha)\right] \\
&= 2V_2\sin\alpha\left[\sin(\boldsymbol{k}\cdot\boldsymbol{R}_1)+\sin(\boldsymbol{k}\cdot\boldsymbol{R}_3)+\sin(\boldsymbol{k}\cdot\boldsymbol{R}_5)\right]
\end{aligned}
$$

At K (I)

- We have $K = k_x = \dfrac{2\pi}{a\sqrt{3}}; k_y = \dfrac{2\pi}{3a}$

$$\boldsymbol{R}_1 = \frac{a}{2}\left(\sqrt{3}\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)$$

$$\boldsymbol{R}_3 = \frac{a}{2}\left(-\sqrt{3}\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)$$

$$\boldsymbol{R}_5 = -a\hat{\mathbf{j}} = -\boldsymbol{R}_2$$

$$H_0\left(\boldsymbol{k}\right) = 2V_2 \cos\alpha\left[\cos\left(\boldsymbol{k}\cdot\boldsymbol{R}_1\right) + \cos\left(\boldsymbol{k}\cdot\boldsymbol{R}_3\right) + \cos\left(\boldsymbol{k}\cdot\boldsymbol{R}_5\right)\right]$$

$$= 2V_2\cos\alpha\left[\cos\left[\left(\frac{2\pi}{a\sqrt{3}}\right)\left(\frac{\sqrt{3}a}{2}\right) + \left(\frac{2\pi}{3a}\right)\frac{a}{2}\right] + \cos\left[\left(\frac{2\pi}{a\sqrt{3}}\right)\left(\frac{-\sqrt{3}a}{2}\right) + \left(\frac{2\pi}{3a}\right)\frac{a}{2}\right] + \cos\left[+\left(\frac{2\pi}{3a}\right)\left(-a\right)\right]\right]$$

$$= 2V_2\cos\alpha\left[\cos\left[\pi + \frac{\pi}{3}\right] + \cos\left[-\pi + \frac{\pi}{3}\right] + \cos\left[-\frac{2\pi}{3}\right]\right]$$

$$= 2V_2\cos\alpha\left[\cos\left[\frac{4\pi}{3}\right] + \cos\left[-\frac{2\pi}{3}\right] + \cos\left[-\frac{2\pi}{3}\right]\right]$$

$$= 2V_2\cos\alpha\left[\cos\left[\frac{4\pi}{3}\right] + \cos\left[-\frac{2\pi}{3}\right] + \cos\left[-\frac{2\pi}{3}\right]\right]$$

$$-3V_2\cos\alpha$$

At K (II)

- We have $$K = k_x = \frac{2\pi}{a\sqrt{3}}; k_y = \frac{2\pi}{3a}$$

$$H_z\left(\boldsymbol{k}\right) = 2V_2 \sin\alpha\left[\sin\left(\boldsymbol{k}\cdot\boldsymbol{R}_1\right) + \sin\left(\boldsymbol{k}\cdot\boldsymbol{R}_3\right) + \sin\left(\boldsymbol{k}\cdot\boldsymbol{R}_5\right)\right]$$

$$= 2V_2 \sin\alpha\left[\sin\left[\left(\frac{2\pi}{a\sqrt{3}}\right)\left(\frac{\sqrt{3}a}{2}\right) + \left(\frac{2\pi}{3a}\right)\frac{a}{2}\right] + \sin\left[\left(\frac{2\pi}{a\sqrt{3}}\right)\left(\frac{-\sqrt{3}a}{2}\right) + \left(\frac{2\pi}{3a}\right)\frac{a}{2}\right] + \sin\left[+\left(\frac{2\pi}{3a}\right)\left(-a\right)\right.\right.$$

$$= 2V_2 \sin\alpha\left[\sin\left[\pi + \frac{\pi}{3}\right] + \sin\left[-\pi + \frac{\pi}{3}\right] + \sin\left[-\frac{2\pi}{3}\right]\right]$$

$$= 2V_2 \cos\alpha\left[\sin\left[\frac{4\pi}{3}\right] + \sin\left[-\frac{2\pi}{3}\right] + \sin\left[-\frac{2\pi}{3}\right]\right]$$

$$= -3\sqrt{3}V_2 \sin\alpha$$

At K' (II)

- We have $K' = k_x = \frac{2\pi}{a\sqrt{3}}; k_y = -\frac{2\pi}{3a}$

$$H_z\left(\boldsymbol{k}\right) = 2V_2 \sin\alpha\left[\sin\left(\boldsymbol{k}\cdot\boldsymbol{R}_1\right) + \sin\left(\boldsymbol{k}\cdot\boldsymbol{R}_3\right) + \sin\left(\boldsymbol{k}\cdot\boldsymbol{R}_5\right)\right]$$

$$= 2V_2 \sin\alpha\left[\sin\left[\left(\frac{2\pi}{a\sqrt{3}}\right)\left(\frac{\sqrt{3}a}{2}\right) - \left(\frac{2\pi}{3a}\right)\frac{a}{2}\right] + \sin\left[\left(\frac{2\pi}{a\sqrt{3}}\right)\left(\frac{-\sqrt{3}a}{2}\right) - \left(\frac{2\pi}{3a}\right)\frac{a}{2}\right] + \sin\left[+\left(-\frac{2\pi}{3a}\right)(-a\right.\right.$$

$$= 2V_2 \sin\alpha\left[\sin\left[\pi - \frac{\pi}{3}\right] + \sin\left[-\pi - \frac{\pi}{3}\right] + \sin\left[\frac{2\pi}{3}\right]\right]$$

$$= 2V_2 \cos\alpha\left[\sin\left[\frac{2\pi}{3}\right] + \sin\left[-\frac{4\pi}{3}\right] + \sin\left[\frac{2\pi}{3}\right]\right]$$

$$= 3\sqrt{3}V_2 \sin\alpha$$

Hamiltonian matrix

- The whole hamiltonian is

$$H = \begin{pmatrix} H_0 + H_z & H_x - iH_y \\ H_x + iH_y & H_0 - H_z \end{pmatrix}$$

$$H_z = \Delta_p - 3\sqrt{3}V_2 \sin\alpha \quad (K)$$

$$H_z = \Delta_p + 3\sqrt{3}V_2 \sin\alpha \quad (K')$$

- with

$$\varepsilon_\pm = H_0 \pm \sqrt{H_x^2 + H_y^2 + H_z^2} = H_0 \pm H$$

- and

$$u_- = \begin{pmatrix} -\sin\frac{\theta}{2} \\ e^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix}$$

$$H_x = H\sin\theta\cos\varphi$$

$$H_x = H\sin\theta\sin\varphi$$

$$H_z = H\cos\theta$$