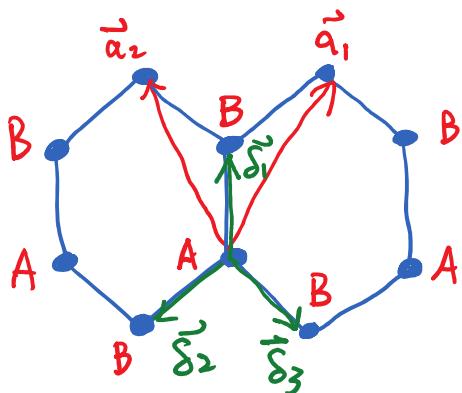


§3. Band electrons

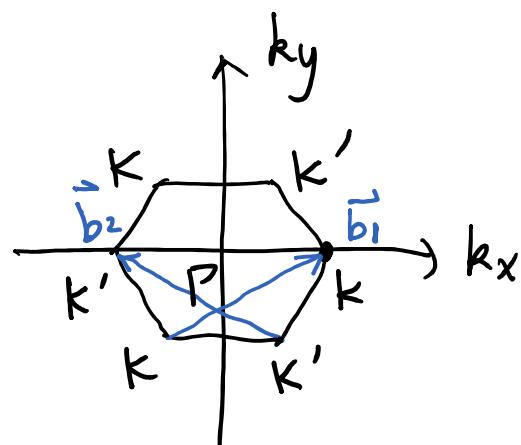
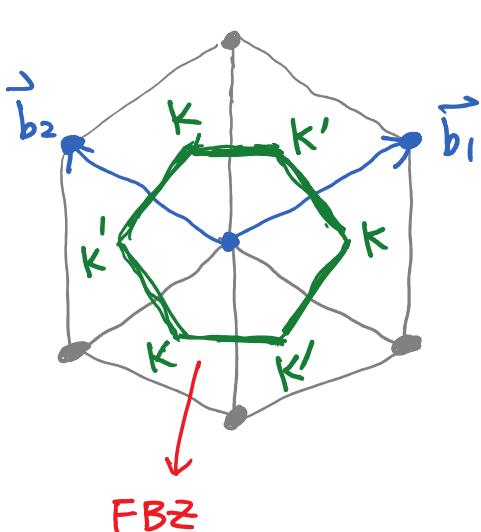
* Energy bands in graphene



$$\left\{ \begin{array}{l} \vec{\delta}_1 = \vec{a} = \frac{\sqrt{3}}{3} a \hat{y} \\ \vec{\delta}_2 = -\frac{1}{2} a \hat{x} - \frac{\sqrt{3}}{2} a \hat{y} \\ \vec{\delta}_3 = \frac{1}{2} a \hat{x} - \frac{\sqrt{3}}{6} a \hat{y} \end{array} \right.$$

Reciprocal lattice: $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$ ($i, j = 1, 2$)

$$\left\{ \begin{array}{l} \vec{a}_1 = a \left(\frac{1}{2}, \frac{\sqrt{3}}{2} \right) \\ \vec{a}_2 = a \left(-\frac{1}{2}, \frac{\sqrt{3}}{2} \right) \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \vec{b}_1 = \frac{2\pi}{a} \left(1, \frac{\sqrt{3}}{3} \right) \\ \vec{b}_2 = \frac{2\pi}{a} \left(-1, \frac{\sqrt{3}}{3} \right) \end{array} \right.$$



$$K: \frac{2\pi}{a} \left(\frac{2}{3}, 0 \right)$$

$$K': \frac{2\pi}{a} \left(-\frac{2}{3}, 0 \right)$$

Diagonalize the Hamiltonian :

$$H_{\pi} = t \sum_{\vec{r} \in R_n} \sum_{\vec{\delta}=\vec{\delta}_1, \vec{\delta}_2, \vec{\delta}_3} (C_{\vec{r},A}^+ C_{\vec{r}+\vec{\delta},B} + C_{\vec{r}+\vec{\delta},B}^+ C_{\vec{r},A}) \\ + \varepsilon \sum_{\vec{r} \in R_n} (C_{\vec{r},A}^+ C_{\vec{r},A} + C_{\vec{r}+\vec{\delta},B}^+ C_{\vec{r}+\vec{\delta},B})$$

$$\left\{ \begin{array}{l} C_{\vec{r},A} = \frac{1}{N} \sum_{\vec{k}} C_{\vec{k},A} e^{i \vec{k} \cdot \vec{r}} \\ C_{\vec{r}+\vec{\delta},B} = \frac{1}{N} \sum_{\vec{k}} C_{\vec{k},B} e^{i \vec{k} \cdot (\vec{r}+\vec{\delta})} \end{array} \right. \quad \vec{R} \in FBZ$$

$$+ \sum_{\vec{r}} \sum_{\vec{\delta}=\vec{\delta}_1, \vec{\delta}_2, \vec{\delta}_3} C_{\vec{r},A}^+ C_{\vec{r}+\vec{\delta},B} \\ = t \sum_{\vec{r}} \sum_{\vec{\delta}} \underbrace{\frac{1}{N} \sum_{\vec{k}, \vec{k}'} C_{\vec{k},A}^+ C_{\vec{k}',B} e^{-i \vec{k} \cdot \vec{r} + i \vec{k}' \cdot (\vec{r}+\vec{\delta})}}_{= \sum_{\vec{k}'} e^{i (\vec{k}' - \vec{k}) \cdot \vec{r}} = \delta_{\vec{k}, \vec{k}'}} \\ = t \sum_{\vec{k}} \sum_{\vec{s}} C_{\vec{k},A}^+ C_{\vec{k},B} e^{i \vec{k} \cdot \vec{s}}$$

$$\varepsilon \sum_{\vec{r}} C_{\vec{r},A}^+ C_{\vec{r},A} = \varepsilon \sum_{\vec{k}} C_{\vec{k},A}^+ C_{\vec{k},A}$$

$$\varepsilon \sum_{\vec{r}} C_{\vec{r}+\vec{\delta},B}^+ C_{\vec{r},B} = \varepsilon \sum_{\vec{k}} C_{\vec{k},B}^+ C_{\vec{k},B}$$

$$\begin{aligned}
 H_{\pi} &= + \sum_{\vec{k}} C_{\vec{R}A}^+ C_{\vec{R}B} \left(\sum_{\vec{\delta}} e^{i\vec{k} \cdot \vec{\delta}} \right) + C_{\vec{R}B}^+ C_{\vec{E}A} \left(\sum_{\vec{\delta}} e^{-i\vec{k} \cdot \vec{\delta}} \right) \\
 &\quad + \varepsilon \sum_{\vec{k}} (C_{\vec{R}A}^+ C_{\vec{E}A} + C_{\vec{R}B}^+ C_{\vec{E}B}) \\
 &= \sum_{\vec{k}} (C_{\vec{R}A}^+, C_{\vec{R}B}^+) \begin{pmatrix} \varepsilon & \Delta_{\vec{k}} \\ \Delta_{\vec{k}}^* & \varepsilon \end{pmatrix} \begin{pmatrix} C_{\vec{R}A} \\ C_{\vec{R}B} \end{pmatrix} \\
 \Delta_{\vec{k}} &= + \sum_{\vec{\delta}=\vec{\delta}_1, \vec{\delta}_2, \vec{\delta}_3} e^{i\vec{k} \cdot \vec{\delta}} \quad \downarrow \\
 &= t \left(e^{i\frac{\sqrt{3}}{3}ak_y} + e^{-\frac{i}{2}ak_x - \frac{i}{6}\sqrt{3}aky} + e^{\frac{i}{2}ak_x - \frac{i}{6}\sqrt{3}aky} \right) \\
 &= + e^{i\frac{\sqrt{3}}{3}aky} \left[1 + 2 \cos\left(\frac{a}{2}k_x\right) e^{-i\frac{\sqrt{3}}{2}aky} \right]
 \end{aligned}$$

$$\begin{cases} \vec{\delta}_1 = \frac{\sqrt{3}}{3}a\hat{y} \\ \vec{\delta}_2 = -\frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{6}a\hat{y} \\ \vec{\delta}_3 = \frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{6}a\hat{y} \end{cases}$$

Eigenvalue of the single-particle Hamiltonian:

$$\det \begin{pmatrix} \varepsilon - E & \Delta_{\vec{k}} \\ \Delta_{\vec{k}}^* & \varepsilon - E \end{pmatrix} = 0$$

$$\Rightarrow E_{\vec{k}}^{\pm} = \varepsilon \pm |\Delta_{\vec{k}}|$$

$$U_{\vec{K}} \begin{pmatrix} \varepsilon & \Delta_{\vec{K}}^+ \\ \Delta_{\vec{K}}^* & \varepsilon \end{pmatrix} U_{\vec{K}}^+ = \begin{pmatrix} E_{\vec{K}}^+ & 0 \\ 0 & E_{\vec{K}}^- \end{pmatrix}$$

\downarrow
2x2 unitary matrix

$$\Rightarrow H_{\pi} = \sum_{\vec{K}} (C_{\vec{K}A}^+, C_{\vec{K}B}^+) \begin{pmatrix} \varepsilon & \Delta_{\vec{K}}^+ \\ \Delta_{\vec{K}}^* & \varepsilon \end{pmatrix} \begin{pmatrix} C_{\vec{K}A} \\ C_{\vec{K}B} \end{pmatrix}$$

$$= \sum_{\vec{K}} (C_{\vec{K}A}^+, C_{\vec{K}B}^+) U_{\vec{K}}^+ U_{\vec{K}} \begin{pmatrix} \varepsilon & \Delta_{\vec{K}}^+ \\ \Delta_{\vec{K}}^* & \varepsilon \end{pmatrix} U_{\vec{K}}^+ U_{\vec{K}} \begin{pmatrix} C_{\vec{K}A} \\ C_{\vec{K}B} \end{pmatrix}$$

$\underbrace{(d_{\vec{K},1}^+, d_{\vec{K},2}^+)}_{||}$ $\underbrace{\left(\begin{matrix} E_{\vec{K}}^+ & 0 \\ 0 & E_{\vec{K}}^- \end{matrix} \right)}_{||}$ $\underbrace{\left(\begin{matrix} d_{\vec{K},1} \\ d_{\vec{K},2} \end{matrix} \right)}_{||} = U_{\vec{K}} \begin{pmatrix} C_{\vec{K}A} \\ C_{\vec{K}B} \end{pmatrix}$

$$\left\{ \begin{array}{l} \{d_{\vec{K},\mu}^+, d_{\vec{K}',\mu'}^+\} = \{d_{\vec{K},\mu}, d_{\vec{K}',\mu'}\} = 0 \\ \{d_{\vec{K},\mu}^+, d_{\vec{K}',\mu'}^+\} = \delta_{\vec{K},\vec{K}'} \delta_{\mu\mu'} \quad (\mu=1,2) \end{array} \right.$$

$$\Rightarrow H_{\pi} = \sum_{\vec{K}} (d_{\vec{K},1}^+, d_{\vec{K},2}^+) \begin{pmatrix} E_{\vec{K}}^+ & 0 \\ 0 & E_{\vec{K}}^- \end{pmatrix} \begin{pmatrix} d_{\vec{K},1} \\ d_{\vec{K},2} \end{pmatrix}$$

$$= \sum_{\vec{K}} (E_{\vec{K}}^+ d_{\vec{K},1}^+ d_{\vec{K},1} + E_{\vec{K}}^- d_{\vec{K},2}^+ d_{\vec{K},2})$$

\downarrow \swarrow
single-particle energies (energy bands)!

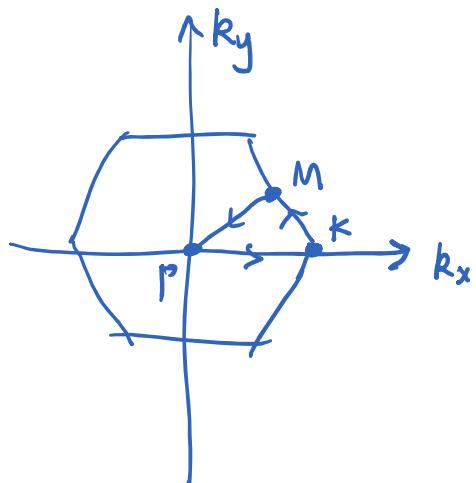
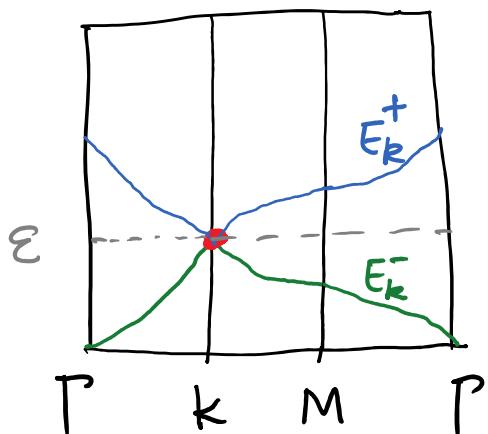
$$E_{\vec{k}}^{\pm} = \varepsilon \pm |\Delta_{\vec{k}}|$$

\downarrow
 $2p_z$ orbital energy

$$|\Delta_{\vec{k}}| = |t| \cdot \left| 1 + 2 \cos\left(\frac{\alpha}{2}k_x\right) e^{-\frac{i\sqrt{3}\alpha}{2}ky} \right|$$

k, k' point: $|\Delta_{\vec{k}}| = 0$

$$\begin{aligned} k: & \frac{2\pi}{a} \left(\frac{2}{3}, 0 \right) \\ k': & \frac{2\pi}{a} \left(-\frac{2}{3}, 0 \right) \end{aligned}$$



Near k and k' (Dirac points)

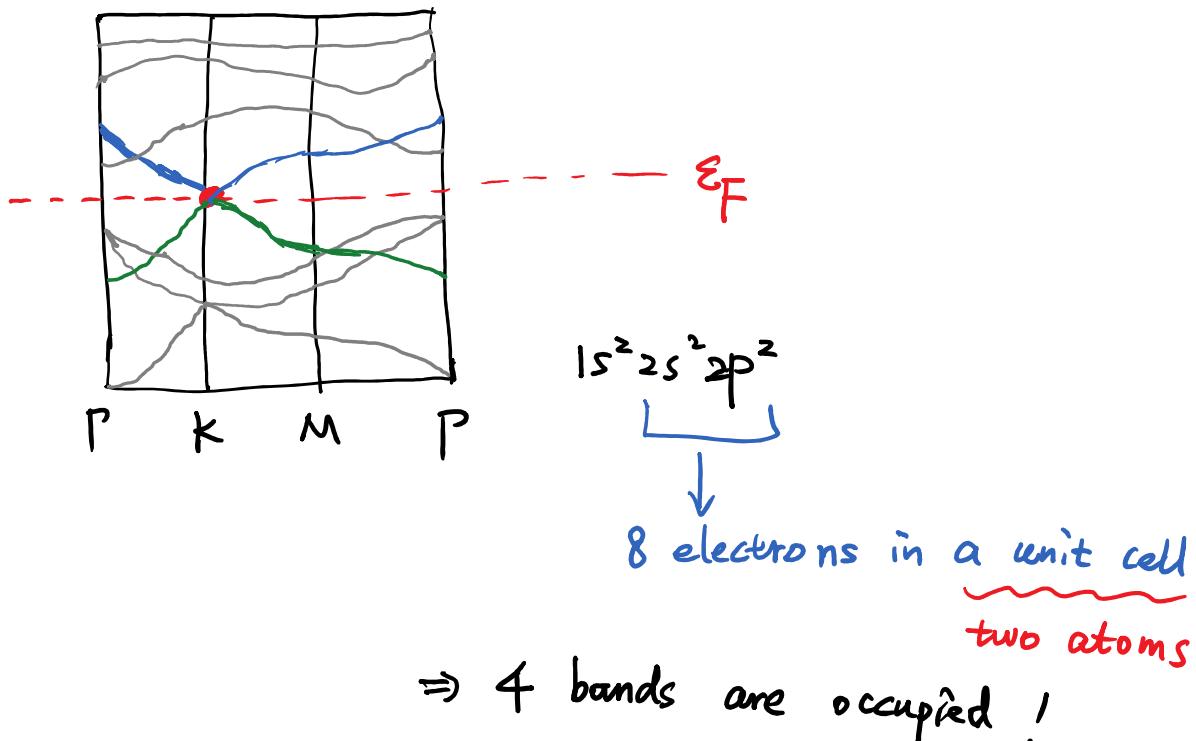
$$E_{\vec{k}}^{\pm} \simeq \pm v_F \hbar \Delta k, \quad \Delta k = \sqrt{\Delta k_x^2 + \Delta k_y^2}$$

Band electrons behave like relativistic Dirac fermions (linear dispersion).

Fermi velocity $v_F \simeq 8 \times 10^5 \text{ m/s} \ll c = 3 \times 10^8 \text{ m/s}$

\downarrow
velocity of light

Band structure with both σ and π electrons:



\Rightarrow Fermi energy is precisely at the Dirac point!

Graphene is a semimetal.

\hookrightarrow DOS small near ϵ_F

At low temperature, two Dirac cones near K and K' are most relevant.

Experimental realization:

Geim & Novoselov, Nobel Prize (2010)