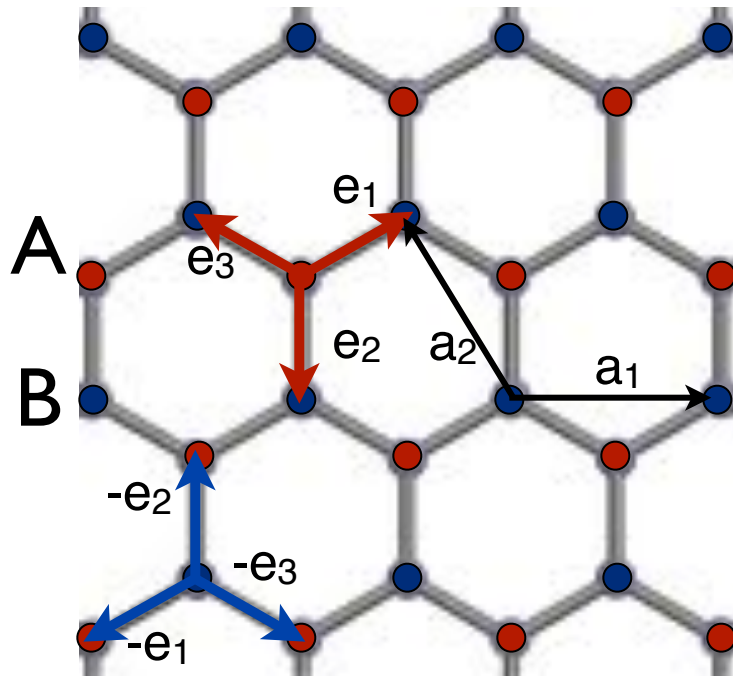


# Graphene



- electronic properties?
- Carbon has  $Z=6$ ,  $(\text{He}) 2s^2 2p^2 = (\text{He}) sp^2\pi$
- $1 \pi = p^z$  electron per C atom not tied up in covalent  $sp^2$  bonds
- Can treat this via tight-binding model

# Graphene

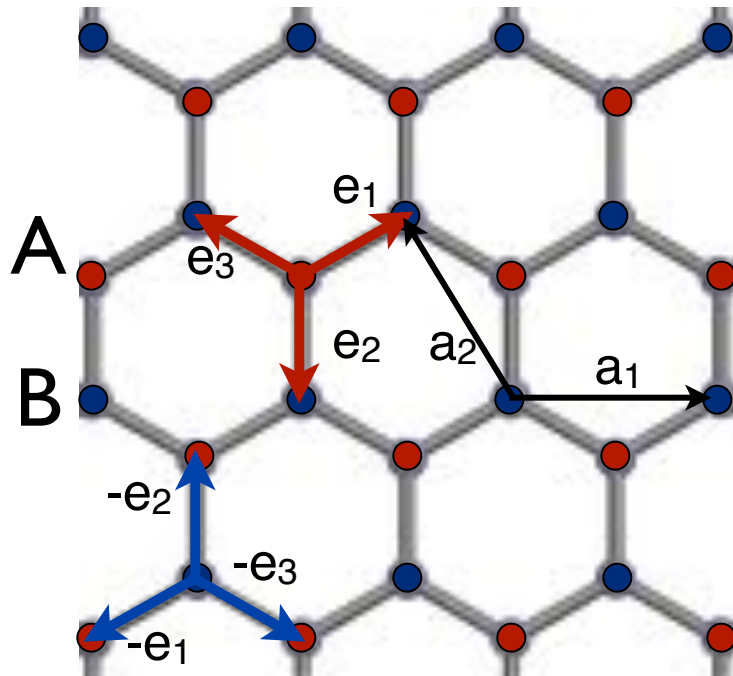


*Bipartite: A sites hop to B sites, and vice versa*

$$\hat{H}\psi_R = \epsilon_0\psi_R - \gamma \sum_{i=1}^3 \psi_{R+e_i} = \epsilon\psi_R \quad R \in A$$

$$\hat{H}\psi_R = \epsilon_0\psi_R - \gamma \sum_{i=1}^3 \psi_{R-e_i} = \epsilon\psi_R \quad R \in B$$

# Graphene



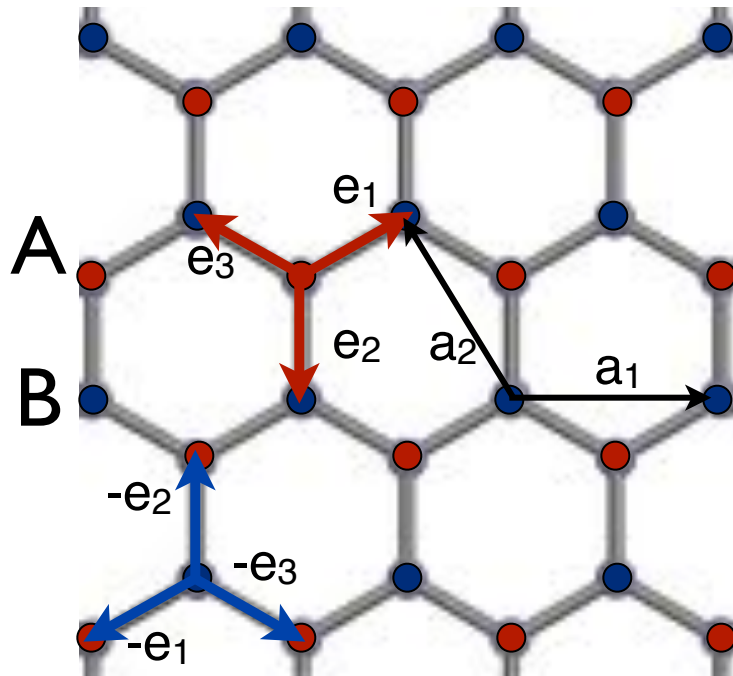
*Bloch form:*

$$\psi_R = \begin{cases} \psi_A e^{ik \cdot R} & R \in A \\ \psi_B e^{ik \cdot R} & R \in B \end{cases}$$

$$\hat{H}\psi_R = \epsilon_0\psi_R - \gamma \sum_{i=1}^3 \psi_{R+e_i} = \epsilon\psi_R \quad R \in A$$

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# Graphene



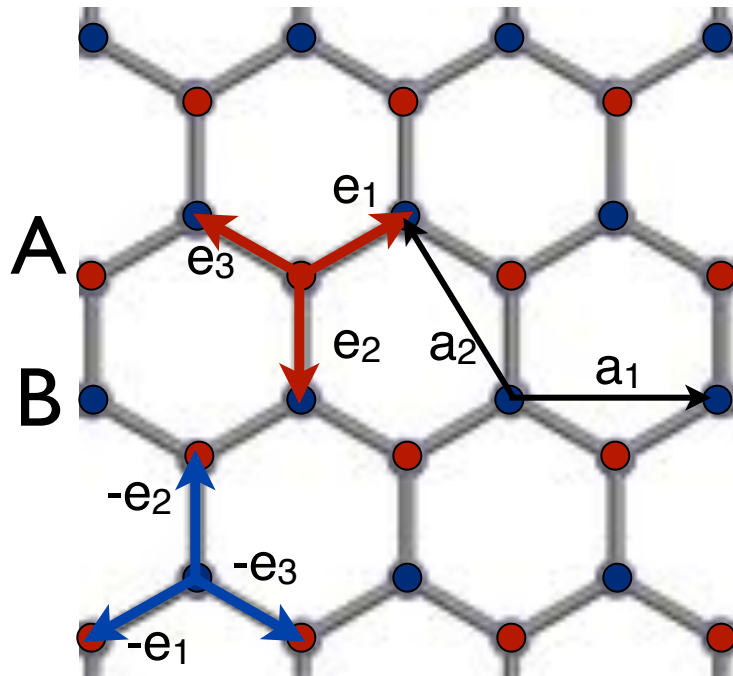
*Bloch form:*

$$\psi_R = \begin{cases} \psi_A e^{ik \cdot R} & R \in A \\ \psi_B e^{ik \cdot R} & R \in B \end{cases}$$

$$\begin{pmatrix} \epsilon_0 & f(k) \\ f^*(k) & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \epsilon \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

$$f(k) = -\gamma \sum_{i=1}^3 e^{ik \cdot e_i}$$

# Graphene



*Bloch form:*

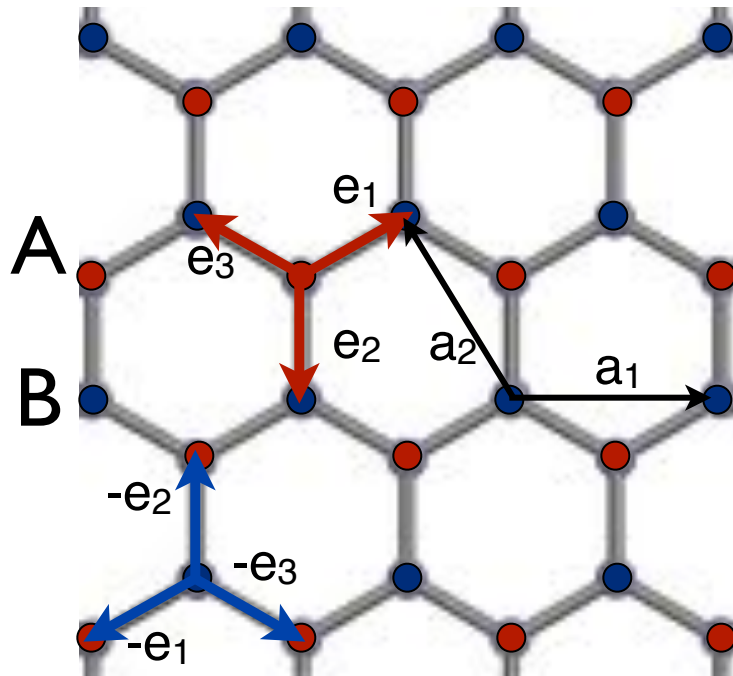
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energy bands

$$\epsilon_{\pm}(k) = \epsilon_0 \pm |f(k)|$$

$$f(k) = -\gamma \sum_{i=1}^3 e^{ik \cdot e_i}$$

# Graphene



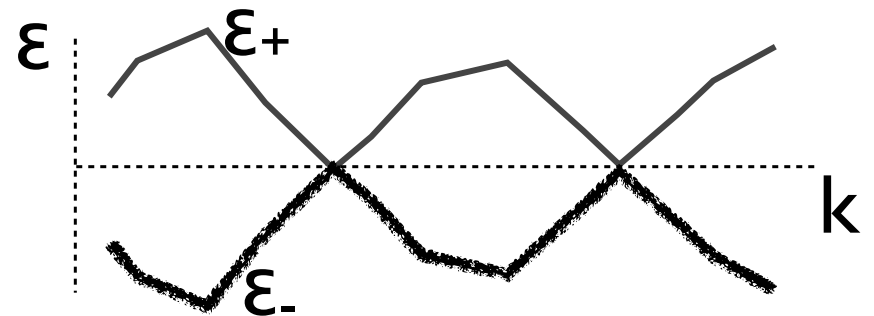
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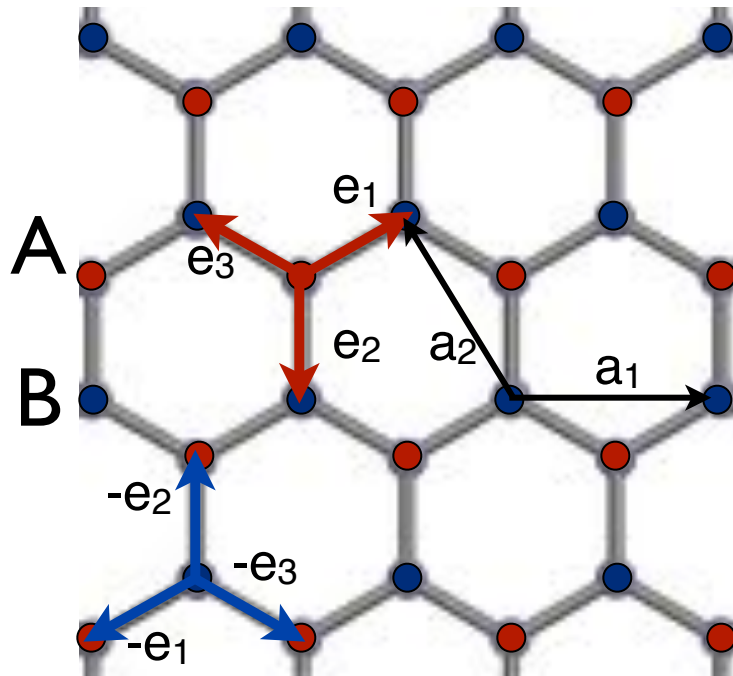
$$\epsilon_{\pm}(k) = \epsilon_0 \pm |f(k)|$$

$$f(k) = -\gamma \sum_{i=1}^3 e^{ik \cdot e_i}$$



conduction and valence  
band touch if and only if  $f=0$

# Graphene



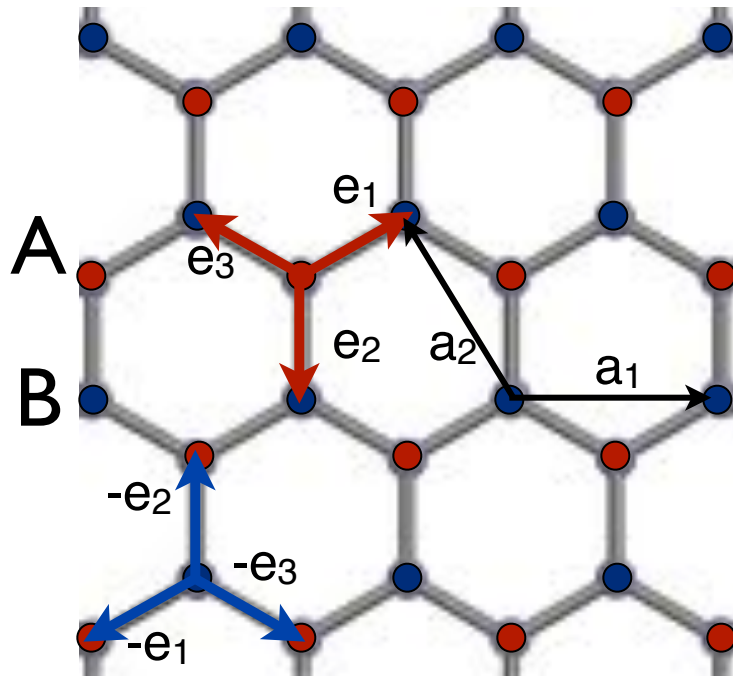
$$e_1 = a_0 \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right)$$

$$e_2 = a_0 (0, -1)$$

$$e_3 = a_0 \left( -\frac{\sqrt{3}}{2}, \frac{1}{2} \right) = -e_1 - e_2$$

$$\begin{aligned} f(k) &= -\gamma \left[ e^{-ik_y a_0} + 2 \cos \left( \frac{\sqrt{3} k_x a_0}{2} \right) e^{ik_y a_0 / 2} \right] \\ &= -\gamma e^{\frac{i}{2} k_y a_0} \left[ e^{-\frac{3}{2} i k_y a_0} + 2 \cos \left( \frac{\sqrt{3} k_x a_0}{2} \right) \right] \end{aligned}$$

# Graphene



$$e_1 = a_0 \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right)$$

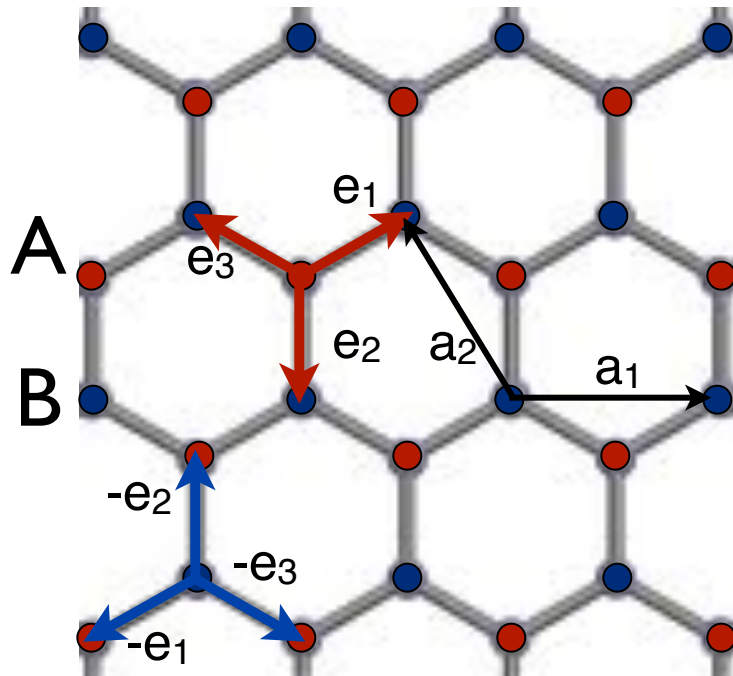
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$$\sin \left( \frac{3}{2} k_y a_0 \right) = 0 \quad \longrightarrow \quad k_y = 0, \pm \frac{4\pi}{3a_0}, \dots$$

$$\cos \left( \frac{3}{2} k_y a_0 \right) + 2 \cos \left( \frac{\sqrt{3}}{2} k_x a_0 \right) = 0$$

# Graphene



$$e_1 = a_0 \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right)$$

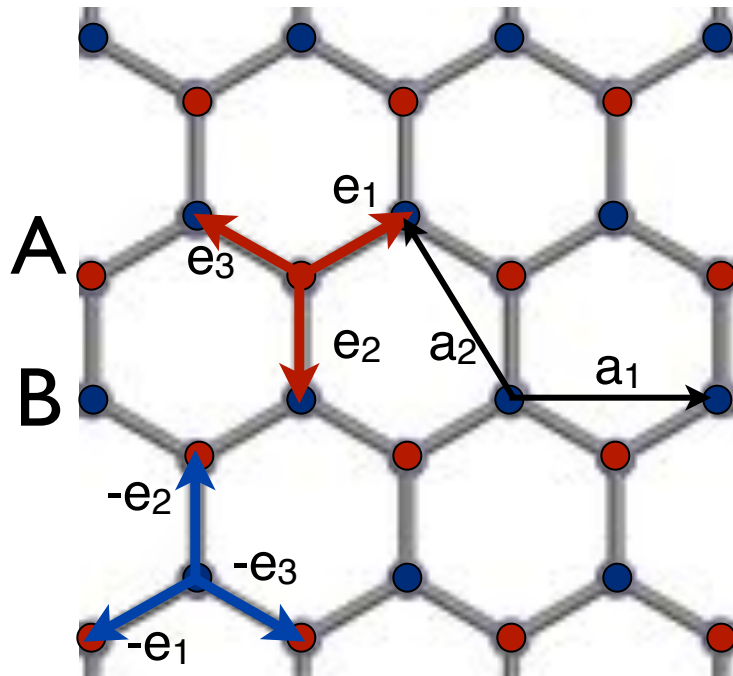
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$$\sin \left( \frac{3}{2} k_y a_0 \right) = 0 \quad \longrightarrow \quad k_y = 0, \pm \frac{2\pi}{3a_0}, \dots$$

$$\pm 1 + 2 \cos \left( \frac{\sqrt{3}}{2} k_x a_0 \right) = 0 \quad k_x = \pm \frac{4\pi}{3\sqrt{3}a_0}, \pm \frac{2\pi}{3\sqrt{3}a_0}, \dots$$

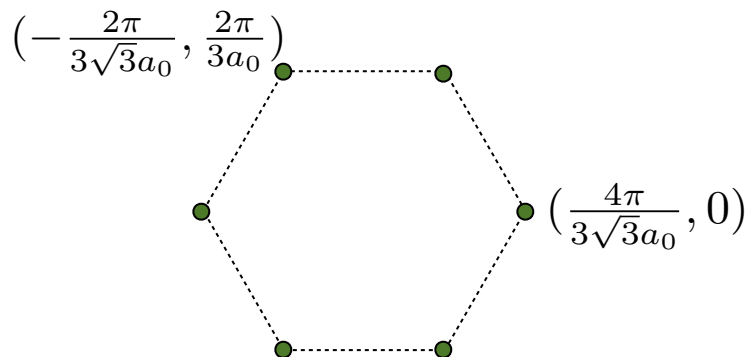
# Graphene



$$e_1 = a_0 \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right)$$

$$e_2 = a_0 (0, -1)$$

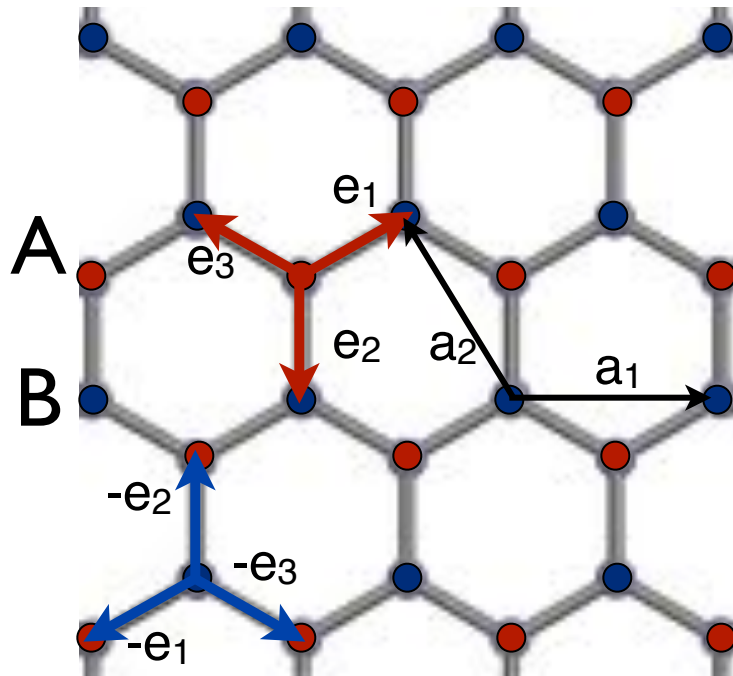
$$e_3 = a_0 \left( -\frac{\sqrt{3}}{2}, \frac{1}{2} \right) = -e_1 - e_2$$



$$k_y = 0, \pm \frac{2\pi}{3a_0}, \dots$$

$$k_x = \pm \frac{4\pi}{3\sqrt{3}a_0}, \pm \frac{2\pi}{3\sqrt{3}a_0}, \dots$$

# Graphene



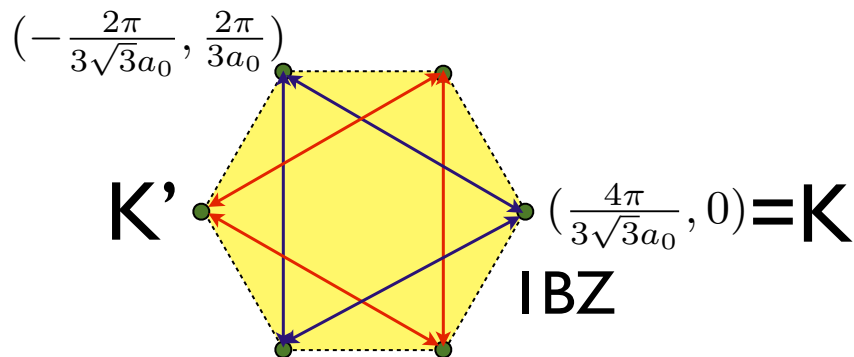
$$e_1 = a_0 \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right)$$

$$e_2 = a_0 (0, -1)$$

$$e_3 = a_0 \left( -\frac{\sqrt{3}}{2}, \frac{1}{2} \right) = -e_1 - e_2$$

$$a_1 = e_1 - e_3 = \sqrt{3}a_0 (1, 0)$$

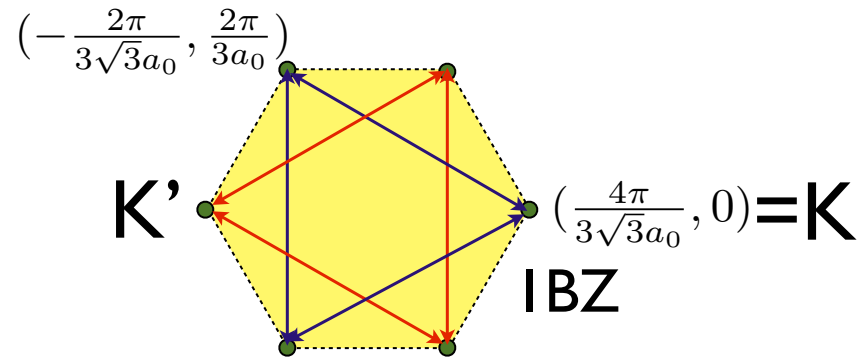
$$a_2 = e_3 - e_2 = \sqrt{3}a_0 \left( -\frac{1}{2}, \frac{\sqrt{3}}{2} \right)$$



$$b_1 = \left( \frac{2\pi}{\sqrt{3}a_0}, \frac{2\pi}{3a_0} \right)$$

$$b_2 = \left( 0, \frac{4\pi}{3a_0} \right)$$

# Graphene

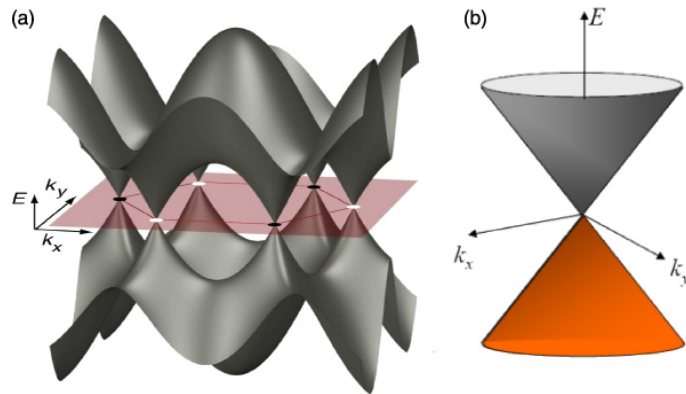


- Result: zero gap semiconductor with *Fermi points*
- Low energy excitations?

$$f(K + q) \approx \frac{3}{2}\gamma a_0(q_x + iq_y) \quad f(K' + q) \approx -\frac{3}{2}\gamma a_0(q_x - iq_y)$$

$$\epsilon_{\pm}(K(K') + q) \approx \pm v|q| \quad v = \frac{3}{2}\gamma a_0$$

# Graphene



“Dirac” cones

- Result: zero gap semiconductor with *Fermi points*
- Low energy excitations?

$$f(K + q) \approx \frac{3}{2} \gamma a_0 (q_x + i q_y) \quad f(K' + q) \approx -\frac{3}{2} \gamma a_0 (q_x - i q_y)$$

$$\epsilon_{\pm}(K(K') + q) \approx \pm v |q| \quad v = \frac{3}{2} \gamma a_0$$

# Dirac equation

$$\begin{pmatrix} \epsilon_0 & f(k) \\ f^*(k) & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \epsilon \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

**Expand near K point:**  $f(K + q) \approx \frac{3}{2}\gamma a_0(q_x + iq_y)$

$$[\epsilon_0 + v(q_x \underline{\sigma}^x - q_y \underline{\sigma}^y)] \psi = \epsilon \psi$$

$$[\epsilon_0 + v(q_x \gamma^x + q_y \gamma^y)] \psi = \epsilon \psi \quad \text{2d Dirac equation}$$

$$\gamma^x = \sigma^x \quad \gamma^y = \sigma^y$$

for K point

$$\gamma^x = -\sigma^x \quad \gamma^y = \sigma^y$$

for K' point

Many interesting properties follow from the Dirac form