TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Solid State Theory (SS2020)

Lecture 13: Graphene

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June 4th, 2020

§ 3.6 Energy bands in graphene

- Last lecture: tight-binding model for graphene

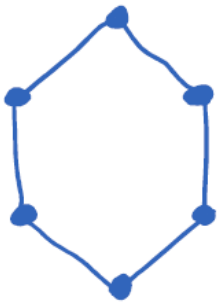
σ-electron part : $2s, 2p_x, 2p_y$

$$H_\sigma = \sum_{\langle j,\ell\rangle} \sum_{n,n'=1,2,3} t_{(j,n);(\ell,n')}\, C^+_{j,n} C_{\ell,n'} + \sum_{j,n=1,2,3} \varepsilon_n C^+_{j,n} C_{j,n}$$

π-electron part :

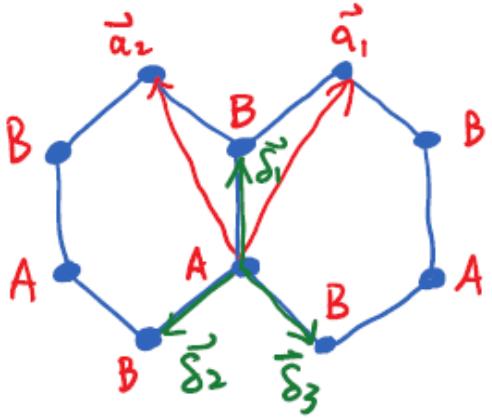
$$H_\pi = \sum_{\langle j\ell\rangle} t_{j\ell}\, C_j^+ C_\ell + \sum_j \varepsilon\, C_j^+ C_j$$

$2p_z$ ($n=4$ suppressed)



§ 3.6 Energy bands in graphene

- Reciprocal lattice and FBZ:



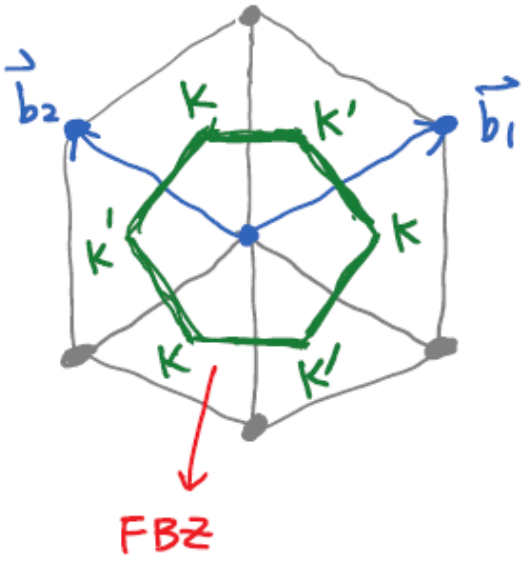
$$\begin{cases} \vec{\delta}_1 = \vec{d} = \frac{\sqrt{3}}{3} a\,\hat{y} \\ \vec{\delta}_2 = -\frac{1}{2} a\,\hat{x} - \frac{\sqrt{3}}{6} a\,\hat{y} \\ \vec{\delta}_3 = \frac{1}{2} a\,\hat{x} - \frac{\sqrt{3}}{6} a\,\hat{y} \end{cases}$$

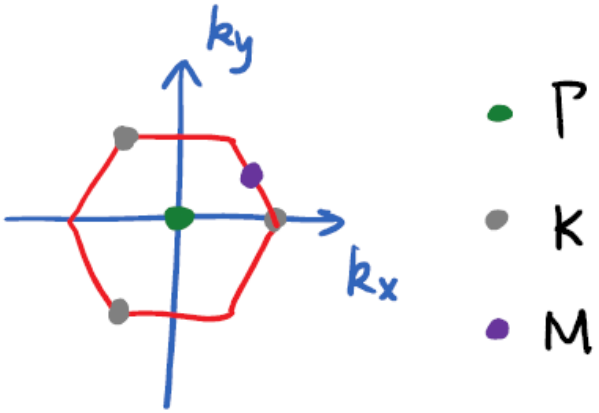
Reciprocal lattice: $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \quad (i, j = 1, 2)$

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

§ 3.6 Energy bands in graphene

- Reciprocal lattice and FBZ:





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

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

§ 3.6 Energy bands in graphene

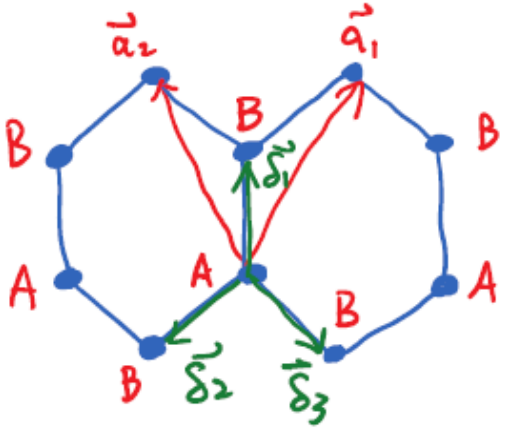
- Tight-binding Hamiltonian for π-electrons:

$$H_\pi = t \sum_{\vec{r}\in\vec{R}_n} \sum_{\vec{\delta}=\vec{\delta}_1,\vec{\delta}_2,\vec{\delta}_3} \left(C^{+}_{\vec{r},A} C_{\vec{r}+\vec{\delta},B} + C^{+}_{\vec{r}+\vec{\delta},B} C_{\vec{r},A} \right)$$

$$+ \varepsilon \sum_{\vec{r}\in\vec{R}_n} \left(C^{+}_{\vec{r},A} C_{\vec{r},A} + C^{+}_{\vec{r}+\vec{\delta}_1,B} C_{\vec{r}+\vec{\delta}_1,B} \right)$$

  - Fourier transform:

$$\begin{cases} C_{\vec{r},A} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} C_{\vec{k},A}\, e^{i\vec{k}\cdot\vec{r}} \\ C_{\vec{r}+\vec{\delta},B} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} C_{\vec{k},B}\, e^{i\vec{k}\cdot(\vec{r}+\vec{\delta})} \end{cases}$$



§ 3.6 Energy bands in graphene

$$t\sum_{\vec{r}}\sum_{\vec{\delta}=\vec{\delta}_1,\vec{\delta}_2,\vec{\delta}_3} C^{+}_{\vec{r},A}\, C_{\vec{r}+\vec{\delta},B}$$

$$= t\sum_{\vec{r}}\sum_{\vec{\delta}}\frac{1}{N}\sum_{\vec{k},\vec{k}'} C^{+}_{\vec{k},A}\, C_{\vec{k}',B}\; e^{-i\vec{k}\cdot\vec{r}+i\vec{k}'\cdot(\vec{r}+\vec{\delta})}$$

$$= t\sum_{\vec{k}}\sum_{\vec{\delta}} C^{+}_{\vec{k},A}\, C_{\vec{k},B}\; e^{i\vec{k}\cdot\vec{\delta}}$$

$$\frac{1}{N}\sum_{\vec{r}} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} = \delta_{\vec{k},\vec{k}'}$$

§ 3.6 Energy bands in graphene

$$t\sum_{\vec{r}}\sum_{\vec{\delta}=\vec{\delta}_1,\vec{\delta}_2,\vec{\delta}_3} C^{+}_{\vec{r},A}\, C_{\vec{r}+\vec{\delta},B}$$

$$= t\sum_{\vec{r}}\sum_{\vec{\delta}}\frac{1}{N}\sum_{\vec{k},\vec{k}'} C^{+}_{\vec{k},A}\, C_{\vec{k}',B}\; e^{-i\vec{k}\cdot\vec{r}+i\vec{k}'\cdot(\vec{r}+\vec{\delta})}$$

$$= t\sum_{\vec{k}}\sum_{\vec{\delta}} C^{+}_{\vec{k},A}\, C_{\vec{k},B}\; e^{i\vec{k}\cdot\vec{\delta}}$$

$$\frac{1}{N}\sum_{\vec{r}} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} = \delta_{\vec{k},\vec{k}'}$$

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

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

§ 3.6 Energy bands in graphene

$$H_\pi = t\sum_{\vec{k}} C^+_{\vec{k}A} C_{\vec{k}B}\left(\sum_{\delta} e^{i\vec{k}\cdot\vec{\delta}}\right) + C^+_{\vec{k}B} C_{\vec{k}A}\left(\sum_{\delta} e^{-i\vec{k}\cdot\vec{\delta}}\right)$$

$$+ \varepsilon \sum_{\vec{k}}\left(C^+_{\vec{k}A} C_{\vec{k}A} + C^+_{\vec{k}B} C_{\vec{k}B}\right)$$

$$= \sum_{\vec{k}} \left(C^+_{\vec{k}A}\ ,\ C^+_{\vec{k}B}\right)\begin{pmatrix} \varepsilon & \Delta_{\vec{k}} \\ \Delta^*_{\vec{k}} & \varepsilon \end{pmatrix}\begin{pmatrix} C_{\vec{k}A} \\ C_{\vec{k}B} \end{pmatrix}$$

§ 3.6 Energy bands in graphene

$$H_\pi = t\sum_{\vec{k}} c^+_{\vec{k}A} c_{\vec{k}B}\left(\sum_{\delta} e^{i\vec{k}\cdot\vec{\delta}}\right) + c^+_{\vec{k}B} c_{\vec{k}A}\left(\sum_{\delta} e^{-i\vec{k}\cdot\vec{\delta}}\right)$$

$$+ \varepsilon \sum_{\vec{k}} \left(c^+_{\vec{k}A} c_{\vec{k}A} + c^+_{\vec{k}B} c_{\vec{k}B}\right)$$

$$= \sum_{\vec{k}} \left(c^+_{\vec{k}A},\ c^+_{\vec{k}B}\right) \begin{pmatrix} \varepsilon & \Delta_{\vec{k}} \\ \Delta^*_{\vec{k}} & \varepsilon \end{pmatrix} \begin{pmatrix} c_{\vec{k}A} \\ c_{\vec{k}B} \end{pmatrix}$$

$$\Delta_{\vec{k}} = t\sum_{\vec{\delta}=\vec{\delta}_1,\vec{\delta}_2,\vec{\delta}_3} e^{i\vec{k}\cdot\vec{\delta}}$$

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

$$= t\left(e^{i\frac{\sqrt{3}}{3}ak_y} + e^{-\frac{i}{2}ak_x - \frac{i}{6}\sqrt{3}ak_y} + e^{\frac{i}{2}ak_x - \frac{i}{6}\sqrt{3}ak_y}\right)$$

$$= t\,e^{i\frac{\sqrt{3}}{3}ak_y}\left[1 + 2\cos\left(\frac{a}{2}k_x\right)e^{-i\frac{\sqrt{3}}{2}ak_y}\right]$$

§ 3.6 Energy bands in graphene

$$H_\pi = t\sum_{\vec{k}} c^+_{\vec{k}A} c_{\vec{k}B}\left(\sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}}\right) + c^+_{\vec{k}B} c_{\vec{k}A}\left(\sum_{\vec{\delta}} e^{-i\vec{k}\cdot\vec{\delta}}\right)$$

$$+ \varepsilon \sum_{\vec{k}}\left(c^+_{\vec{k}A} c_{\vec{k}A} + c^+_{\vec{k}B} c_{\vec{k}B}\right)$$

$$= \sum_{\vec{k}} \left(c^+_{\vec{k}A},\ c^+_{\vec{k}B}\right) \begin{pmatrix} \varepsilon & \Delta_{\vec{k}} \\ \Delta^*_{\vec{k}} & \varepsilon \end{pmatrix} \begin{pmatrix} c_{\vec{k}A} \\ c_{\vec{k}B} \end{pmatrix}$$

Eigenvalue of the single-particle Hamiltonian:

$$\det \begin{pmatrix} \varepsilon - E & \Delta_{\vec{k}} \\ \Delta^*_{\vec{k}} & \varepsilon - E \end{pmatrix} = 0 \quad \Rightarrow \quad E^{\pm}_{\vec{k}} = \varepsilon \pm |\Delta_{\vec{k}}|$$

§ 3.6 Energy bands in graphene

$$\Rightarrow H_T = \sum_{\vec{k}} \left(C^+_{\vec{k}A},\ C^+_{\vec{k}B} \right) \begin{pmatrix} \varepsilon & \Delta_{\vec{k}} \\ \Delta^*_{\vec{k}} & \varepsilon \end{pmatrix} \begin{pmatrix} C_{\vec{k}A} \\ C_{\vec{k}B} \end{pmatrix}$$

$$= \sum_{\vec{k}} \left(C^+_{\vec{k}A},\ C^+_{\vec{k}B} \right) U^+_{\vec{k}}\, U_{\vec{k}} \begin{pmatrix} \varepsilon & \Delta_{\vec{k}} \\ \Delta^*_{\vec{k}} & \varepsilon \end{pmatrix} U^+_{\vec{k}}\, U_{\vec{k}} \begin{pmatrix} C_{\vec{k}A} \\ C_{\vec{k}B} \end{pmatrix}$$

$$\| \qquad\qquad \| \qquad\qquad \|$$

$$\left(d^+_{\vec{k},1},\ d^+_{\vec{k},2} \right) \qquad \begin{pmatrix} E^+_{\vec{k}} & 0 \\ 0 & E^-_{\vec{k}} \end{pmatrix} \qquad \begin{pmatrix} d_{\vec{k},1} \\ d_{\vec{k},2} \end{pmatrix} = U_{\vec{k}} \begin{pmatrix} C_{\vec{k}A} \\ C_{\vec{k}B} \end{pmatrix}$$

$$\begin{cases} \left\{ d^+_{\vec{k},\mu},\ d^+_{\vec{k}',\mu'} \right\} = \left\{ d_{\vec{k},\mu},\ d_{\vec{k}',\mu'} \right\} = 0 \\ \left\{ d_{\vec{k},\mu},\ d^+_{\vec{k}',\mu'} \right\} = \delta_{\vec{k},\vec{k}'}\, \delta_{\mu\mu'} \end{cases} \qquad (\mu = 1, 2)$$

§ 3.6 Energy bands in graphene

$$\Rightarrow \quad H_{\pi} = \sum_{\vec{k}} \left(d^{+}_{\vec{k},1} \;,\; d^{+}_{\vec{k},2} \right) \begin{pmatrix} E^{+}_{\vec{k}} & 0 \\ 0 & E^{-}_{\vec{k}} \end{pmatrix} \begin{pmatrix} d_{\vec{k},1} \\ d_{\vec{k},2} \end{pmatrix}$$

$$= \sum_{\vec{k}} \left(E^{+}_{\vec{k}}\, d^{+}_{\vec{k},1}\, d_{\vec{k},1} + E^{-}_{\vec{k}}\, d^{+}_{\vec{k},2}\, d_{\vec{k},2} \right)$$

single-particle energies (energy bands)!

§ 3.6 Energy bands in graphene

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

↓

$2p_z$ orbital energy

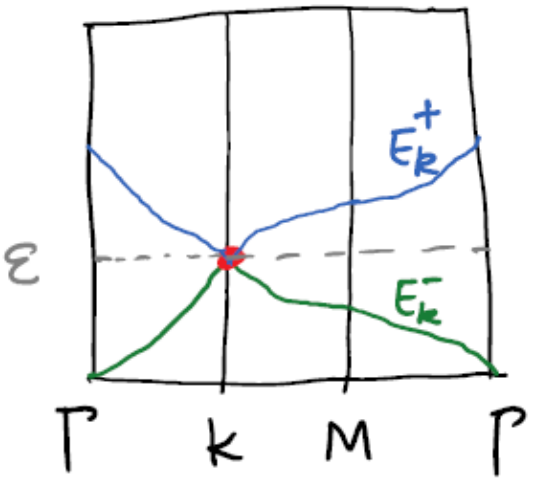
$$|\Delta_{\vec{k}}| = |t| \cdot \left| 1 + 2\cos\left(\frac{a}{2}k_x\right) e^{-i\frac{\sqrt{3}}{2}ak_y} \right|$$

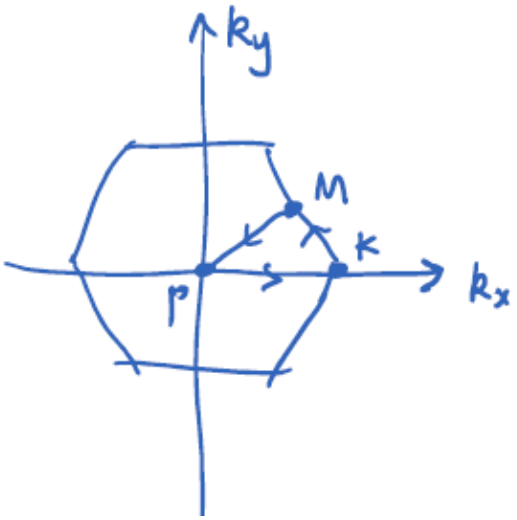
K, K' point: $|\Delta_{\vec{k}}| = 0$

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

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

§ 3.6 Energy bands in graphene



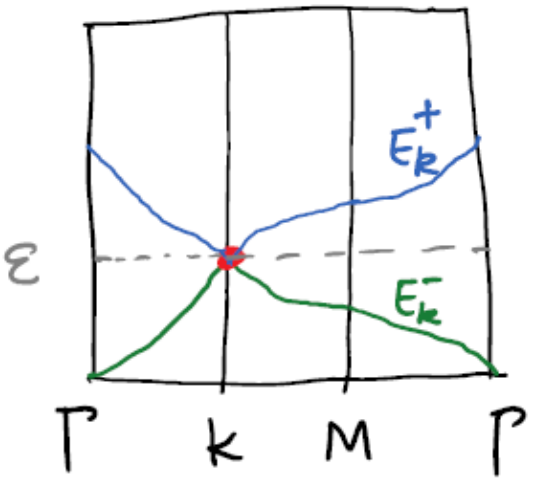


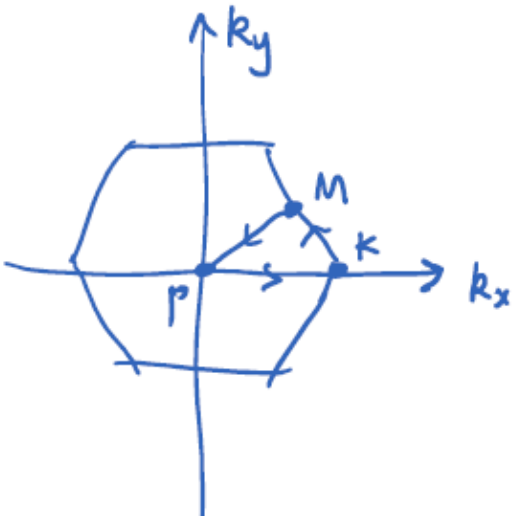
Near K and K′ (Dirac points)

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

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

§ 3.6 Energy bands in graphene





Near K and K′ (Dirac points)

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

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

↓

velocity of light

§ 3.6 Energy bands in graphene

- Band structure with both σ and π electrons:

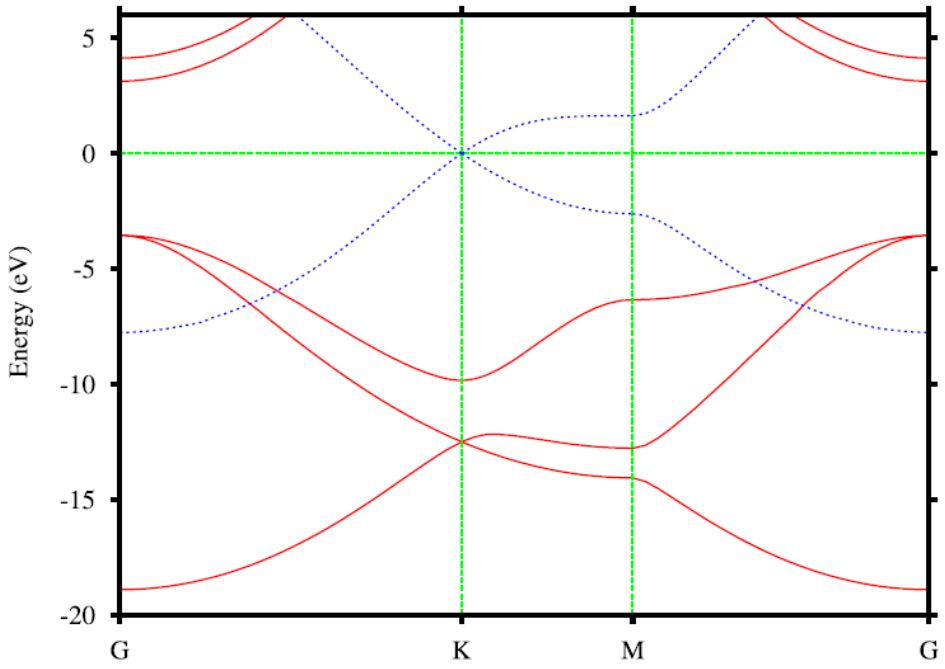


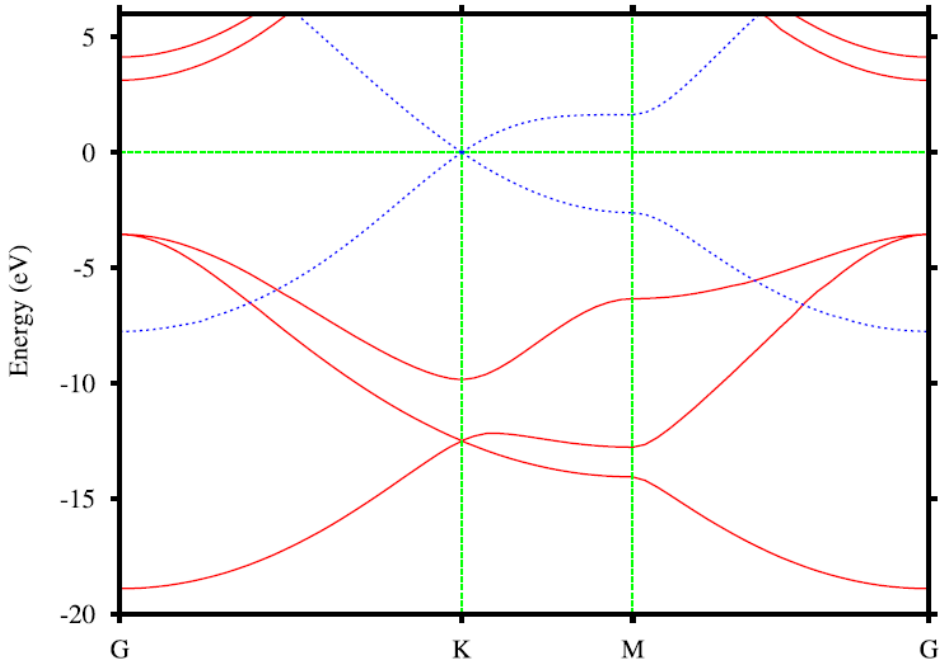
FIG. 1. (Color online) Band structure of a single graphene layer. Solid red lines are σ bands and dotted blue lines are π bands.

two π-bands
six σ-bands

Figure from Phys. Rev. B 77, 035427 (2008)

§ 3.6 Energy bands in graphene

- Band structure with both σ and π electrons:



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➢ Where is the Fermi energy?

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§ 3.6 Energy bands in graphene

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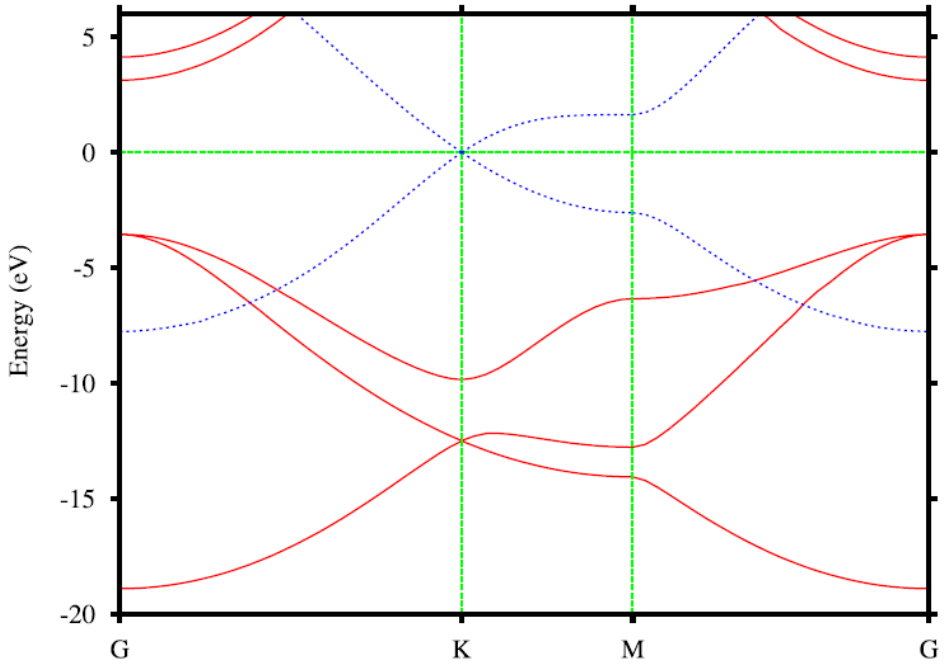

FIG. 1. (Color online) Band structure of a single graphene layer. Solid red lines are σ bands and dotted blue lines are π bands.

Figure from [Phys. Rev. B 77, 035427 (2008)]

- Where is the Fermi energy?

$1s^2 2s^2 2p^2$

8 electrons in a unit cell

two atoms

4 bands are occupied !

§ 3.6 Energy bands in graphene

⇒ Fermi energy is precisely at the Dirac point!

Graphene is a semimetal.

↳ DOS small near ε_F

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

Experimental realization: see Nobel Prize webpage

Geim & Novoselov, Nobel Prize (2010)