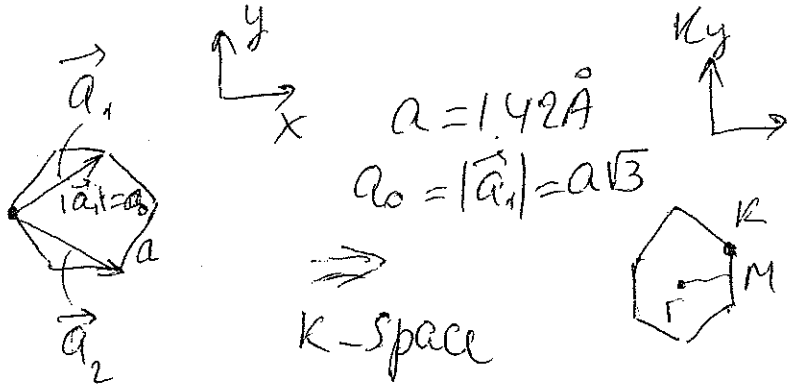
PH673 Nano

Lecture #8

Organic (carbon-based) materials. Graphene

Start from graphene $\Rightarrow$ 2 nonequivalent atoms per unit cell



$a = 1.42\text{Å}$

$a_0 = |\vec{a}_1| = a\sqrt{3}$

$\Rightarrow$ K-space

a – C–C bond length

a_0 – lattice parameter

Solve $H\psi = E\psi \Rightarrow \psi = C_A u_A + C_B u_B$

E ↑ energy of electrons in the π orbitals

$$u_{A(B)} = \frac{1}{\sqrt{N}} \sum_{A(B)} e^{i\vec{K}\cdot\vec{r}_{A(B)}} \chi(\vec{r} - \vec{r}_{A(B)})$$

↑ Block functions

u_A^* / $\int$: all space

$$\int u_A^* H (C_A u_A + C_B u_B) d\tau = E \int u_A^* (C_A u_A + C_B u_B) d\tau$$

$$\int u_A^* u_A d\tau = \int u_B^* u_B d\tau = 1 \; ; \; \int u_{A\,B}^* u_{B\,A} d\tau = 0$$

↑ neglect p_z-wave function overlap between A & B

$$H_{ij} = \int u_i^* H u_j \, d\tau$$

↑ A or B → j

$$C_A H_{AA} + C_B H_{AB} = E C_A$$

$\times \psi_B^*$, $\int$:

$$C_A H_{BA} + C_B H_{BB} = E C_B \Rightarrow$$

$$\begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix} \begin{pmatrix} C_A \\ C_B \end{pmatrix} = E \begin{pmatrix} C_A \\ C_B \end{pmatrix} \Rightarrow$$

has solution if $\det \begin{vmatrix} H_{AA} - E & H_{AB} \\ H_{BA} & H_{BB} - E \end{vmatrix} = 0$

Symmetry: $H_{AA} = H_{BB}$ (A's B are not distinguishable)

Also, $H_{AB} = H_{BA}^*$ $\Rightarrow$ $\underline{E = H_{AA} \mp |H_{AB}|}$

$$H_{AA} = \frac{1}{N} \sum_{A, A^*} e^{i\vec{k}\cdot(\vec{r}_A - \vec{r}_{A^*})} \int \chi^*(\vec{r} - \vec{r}_A) H \chi(\vec{r} - \vec{r}_{A^*}) d\tau$$

tight-binding approximation: take into account interactions with nearest neighbors only: 3 of them which belong to B lattice (for an A atom) $\Rightarrow$

$$H_{AA} \approx \int \chi^*(\vec{r} - \vec{r}_A) H \chi(\vec{r} - \vec{r}_A) d\tau = \underline{E_0}$$

just a shift in energy $\rightarrow$ typically set to 0

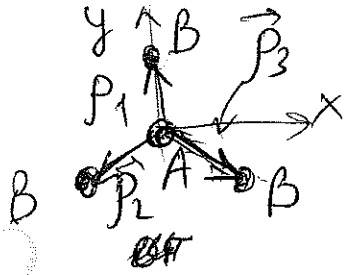
$$H_{AB} = \frac{1}{N} \sum_A \sum_B e^{i\vec{K}(\vec{r}_A - \vec{r}_B)} \int X^*(\vec{r}-\vec{r}_A) H X(\vec{r}-\vec{r}_B)\, d\tau =$$

$$= \frac{1}{N} \sum_A \sum_i e^{i\vec{K}\cdot\vec{\rho}_i} \int X^*(\vec{r}) H X(\vec{r}-\vec{\rho}_i)\, d\tau =$$

$\vec{\rho}_i$: to 3 nearest neighbors

$\int X^* H X\, d\tau$: tight-binding, or transfer, integral $\rightarrow t$

$$= (e^{i\vec{K}\cdot\vec{\rho}_1} + e^{i\vec{K}\cdot\vec{\rho}_2} + e^{i\vec{K}\cdot\vec{\rho}_3})\, t =$$



$$\vec{\rho}_1 = (0, a)$$

$$\vec{\rho}_2 = \left(-\frac{a\sqrt{3}}{2}, -\frac{a}{2}\right)$$

$$\vec{\rho}_3 = \left(a\frac{\sqrt{3}}{2}, -\frac{a}{2}\right)$$

$$= t\left(e^{iK_y a} + e^{-i\left(K_x\frac{a\sqrt{3}}{2} + K_y\frac{a}{2}\right)} + e^{i\left(K_x\frac{a\sqrt{3}}{2} - K_y\frac{a}{2}\right)}\right) =$$

$$= \left(e^{iK_y a} + e^{-i\frac{K_y a}{2}} \cdot 2\cos\frac{K_x a\sqrt{3}}{2}\right) t$$

$$E = \pm |H_{AB}| = \pm t \sqrt{1 + 4\cos^2\frac{K_x a\sqrt{3}}{2} + 4\cos\frac{K_x a\sqrt{3}}{2} \cdot \cos\frac{K_y \cdot 3a}{2}}$$

When is $E = 0$? $\Rightarrow$ solve $\Rightarrow$

find (K_x, K_y) $\Rightarrow$ K-points $\Rightarrow$

$$(k_x, k_y) = \left(\pm\frac{4\pi}{3\sqrt{3}a}, 0\right); \left(\pm\frac{2\pi}{3\sqrt{3}a}, \pm\frac{2\pi}{3a}\right) \quad (4)$$

(1)

K-points $\Rightarrow$ 6 pairs (2 non-equivalent)

$$\left.\frac{dE}{dk}\right|_{K\text{-points}} = \hbar v_F$$

$K: \frac{2\pi}{3a}\left(\frac{1}{\sqrt{3}}, 1\right)$ $K': \frac{2\pi}{3a}\left(-\frac{1}{\sqrt{3}}, 1\right)$

↑ Fermi velocity

$v_F \sim 10^6 \frac{m}{s}$ in graphene

$$E = \hbar v_F \underbrace{\sqrt{k_x^2 + k_y^2}}_{k}$$

↑ compare to energy of massless relativistic particle! $\Rightarrow E = \sqrt{(mc^2)^2 + p^2c^2} = pc = \hbar k c$

($mc^2 = 0$)

$$N_{2D}(E) = \frac{1}{A} \cdot 2 \cdot \frac{2\pi k\, dk/dE}{\left(\frac{2\pi}{A}\right)^2} \sim k\frac{dk}{dE} = \frac{E}{(\hbar v_F)^2} \sim E$$

$\frac{E}{\hbar v_F}$ $\frac{dE}{dk} = \hbar v_F$

Graphene in B-field

$$H\Psi = v_F \begin{pmatrix} -\vec{\sigma}^* \cdot \vec{p} & 0 \\ 0 & \vec{\sigma}\cdot\vec{p} \end{pmatrix} \Psi \qquad (1)$$

4-comp. spinor

$$\vec{\sigma} = (\sigma_x, \sigma_y) \quad \text{Pauli}$$

$$\begin{pmatrix} \psi_A^{K'} \\ \psi_B^{K'} \\ \psi_A^{K} \\ \psi_B^{K'} \end{pmatrix}$$

$$H = v_F \begin{pmatrix} 0 & -(p_{ox} + i p_{oy}) & 0 & 0 \\ -(p_{ox} - i p_{oy}) & 0 & 0 & 0 \\ 0 & 0 & 0 & p_{ox} - i p_{oy} \\ 0 & 0 & p_{ox} + i p_{oy} & 0 \end{pmatrix}$$

Landau gauge

$$\vec{A} = (-B_y, 0)$$

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

$$\vec{A} = \tfrac{1}{2} \vec{B} \times \vec{r}$$

$$[H, p_x] \neq 0$$

$$p_{oi} = p_i - \frac{e}{c} A_i$$

$$E \psi_A^K = v_F (\hat{p}_{ox} - i \hat{p}_{oy}) \psi_B^K$$

$$E \psi_B^K = v_F (p_{ox} + i p_{oy}) \psi_A^K$$

$$E^2 \psi_A^K = v_F^2 (p_{ox} - i p_{oy})(p_{ox} + i p_{oy}) \psi_A^K$$

$$E^2 \psi_B^K = v_F^2 (p_{ox} + i p_{oy})(p_{ox} - i p_{oy}) \psi_B^K$$

$e = -e_0$

$$\frac{E^2}{v_F^2} \psi_B^K = \left(p_x + \frac{e}{c} B y\right) + i p_y \Big) \left(\left(p_x + \frac{e}{c} B y\right) - i p_y \right) \psi_B^K$$

$$= \left(\left(p_x + \frac{eB}{c} y\right)^2 + \frac{\hbar e B}{c} + p_y^2 \right) \psi_B^K$$

$$\frac{1}{2m} \left(\frac{E^2}{v_F^2} + \frac{\hbar e_0 B}{c} \right) \psi_B^K = \left(\frac{K}{2} (y - y_0)^2 + \frac{p_y^2}{2m} \right) \psi_B^K$$

$k = \frac{e_0 B}{c\sqrt{m}}$; $y_0 = \frac{P_x c}{e_0 B}$ (2)

$\tilde{E}\Psi = H\Psi$

$\uparrow$

$\hbar\omega_c \left(n + \frac{1}{2}\right) = \frac{1}{2m}\left(\frac{E^2}{v_F^2} + \frac{\hbar e_0 B}{c}\right)$

($n = 0, 1, 2, \ldots$; $\frac{\hbar e_0 B}{c} = \frac{\hbar\omega_c}{2}$)

$\omega_c = \sqrt{\frac{k}{m}} = \frac{e_0 B}{mc}$

$\Downarrow$

$\frac{E^2}{v_F^2} = \frac{\hbar e_0 B}{c}(2n + 1 - 1)$

$\Downarrow$

$E = \pm \sqrt{\frac{2\hbar e_0 B}{c}}\, v_F \sqrt{n}$

For $\Psi_A^K \rightarrow \sqrt{n+1}$ ← E=0 level lacks

$n \neq 0 \rightarrow$ both A & B sublattices

$n = 0 \rightarrow$ B for K & A for K'

Bilayer : $E = \pm \hbar\omega_c \sqrt{n(n-1)} \sim n$

but with E=0 level