Fundamentals of Nanoelectronics

ECE495 - Session 21, Oct 14, 2009

Graphene Bandstructure

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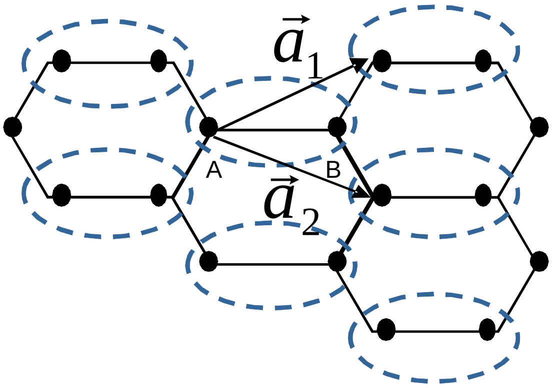
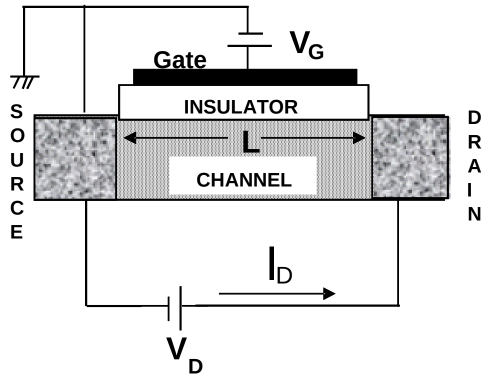
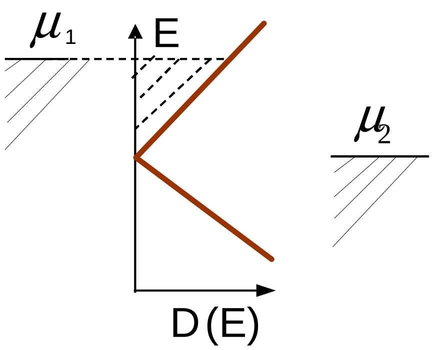
Review

$$E\Psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_N(\vec{r}) + U_e(\vec{r})\right)\Psi$$







$\vec{a}_1 = \hat{x}a + \hat{y}b$ and $\vec{a}_2 = \hat{x}a - \hat{y}b$

$$E\{\psi_n\} = \sum_m [H_{nm}]\{\psi_n\} \quad where\ \{\psi_n\} = \{\psi_0\}e^{i\vec{k}\vec{d}_n}\ and\ H_{nm}\ is\ 2\times 2\ and\ we\ have\ 2N\ \{\psi_n\}$$

$$\Rightarrow E e^{i\vec{k}\vec{r}_n}\{\psi_0\} = \sum_m [H_{nm}]e^{i\vec{k}\vec{r}_m}\{\psi_0\} \Rightarrow E\{\psi_0\} = \underbrace{\sum_m [H_{nm}]e^{i\vec{k}(\vec{r}_m - \vec{r}_n)}}_{h(\vec{k})}\{\psi_0\}$$

$$h(\vec{k}) = \sum_m [H_{nm}]e^{i\vec{k}(\vec{d}_m - \vec{d}_n)} \Rightarrow E\{\psi_0\} = [h(\vec{k})]\{\psi_0\}$$

Based on periodic structure we can write eignevalues analytically.

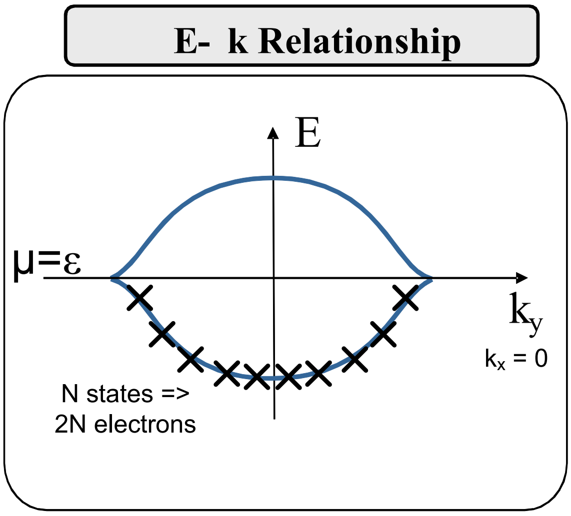
Graphene h(k)

$$[h(\vec{k})] = \begin{bmatrix} \varepsilon & h_0^* \\ h_0 & \varepsilon \end{bmatrix} \text{ where } h_0(\vec{k}) \equiv t_0\left(e^{i\vec{k}\bullet\vec{a}_1} + e^{i\vec{k}\bullet\vec{a}_2} + 1\right)$$

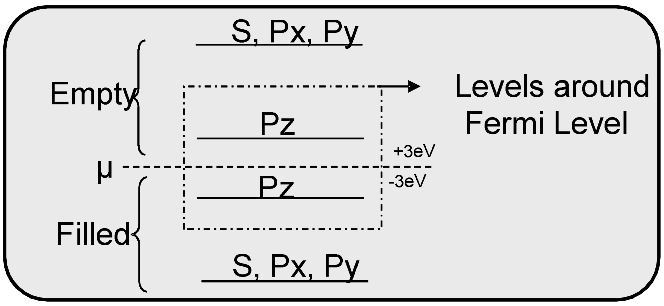
Then eigenvalue will be

$$\mathrm{E} = \varepsilon \pm \left| h_0(\vec{k}) \right|$$

There are several approaches to plot this E-k diagram.



μ=ε is the line separate occupied states from empty states.



For C: $1s^2$

$2s^2\ 2p_x^{\ 2}\ 2p_y^{\ 2}\ \ 2p_z^{\ 2}$

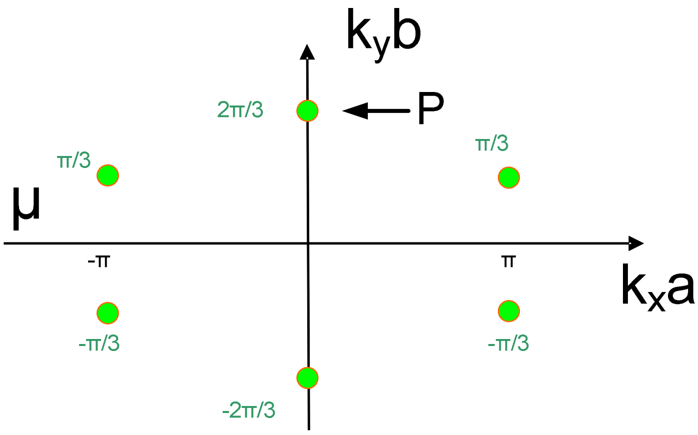
States around μ is important due to we may apply a small voltage.

Then for $\mathrm{E} = \varepsilon \pm \left| h_0(\vec{k}) \right|$ where $\left| h_0(\vec{k}) \right| = 0$ is important for us then we want to find E-k diagram around ε.

$$h_0(\vec{k}) \equiv t_0\left(e^{i\vec{k}\bullet\vec{a}_1} + e^{i\vec{k}\bullet\vec{a}_2} + 1\right) = t_0\left(1 + e^{ik_x a}e^{ik_y b} + e^{ik_x a}e^{-ik_y b}\right) = t_0(1 + 2e^{ik_x a}\cos(k_y B)) = 0$$

K_x and k_y =??

We assume k_x a=0 and k_yb= ±2 π /3 then:



$$h_0(k_x,k_y) = t_0\left(1+2e^{ik_xa}\cos(k_yb)\right) \approx 0 + \left[\frac{\partial h}{\partial k_x}\right]_P k_x + \left[\frac{\partial h}{\partial k_y}\right]_P k_y \qquad (I)$$

$$\left[\frac{\partial h}{\partial k_x}\right]_P k_x = (2t_0\cos(k_yb).\,iae^{ik_xa})_P = -iat_0 \qquad (II)$$

$$\left[\frac{\partial h}{\partial k_y}\right]_P k_y = (2t_0e^{ik_xa}.\,b\sin(k_yb))_P = -\sqrt{3}bt_0 \qquad (III)$$

$$b = \frac{\sqrt{3}}{2}a_0$$

$$a = \frac{3}{2}a_0$$

Then $h_0(k_x,k_y) \approx -iat_0k_x - \sqrt{3}bt_0k_y = -iat_0(k_x - ik_y)$

Then $E = \varepsilon \pm at_0\sqrt{{k_x}^2 + {k_y}^2}$