Fundamentals of Nanoelectronics

ECE495 - Session 20, Oct 12, 2009

Bandstructure II

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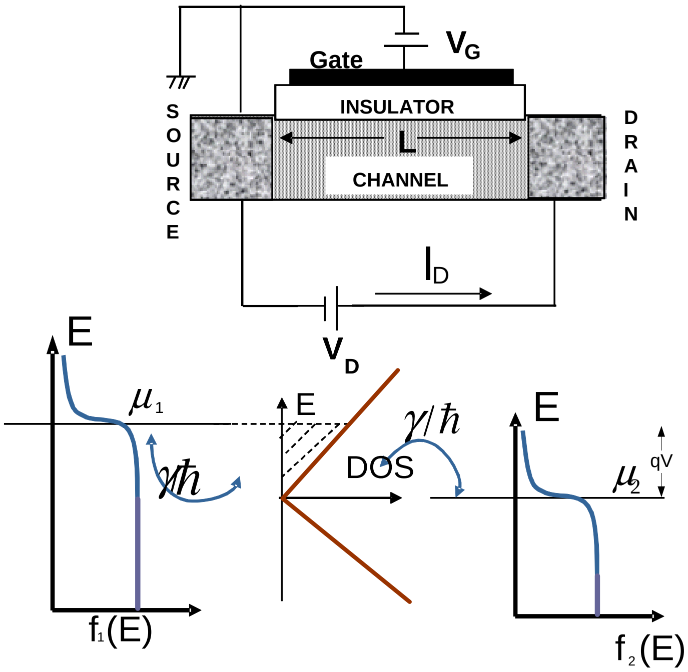
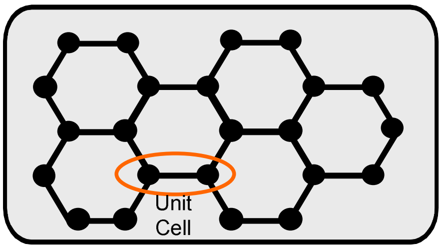
<u>Review</u>



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

$$E\{\psi\} = [H]\{\psi\} \Rightarrow E(k) \Rightarrow$$

How starting from Schrodinger equation we can get D(E)?



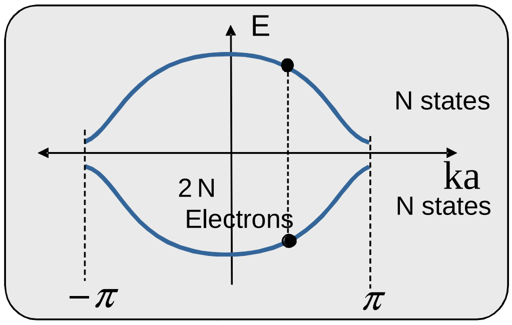
$$\Psi(\vec{r}) = \sum_m \psi_m u_m(\vec{r}) \qquad u_m = b \times N_A$$

Unit cell: two atoms here contribute two basis functions. Then

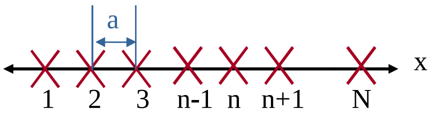
$$\Psi(\vec{r}) = \psi_1 u_1(\vec{r}) + \psi_2 u_2(\vec{r})$$

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

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

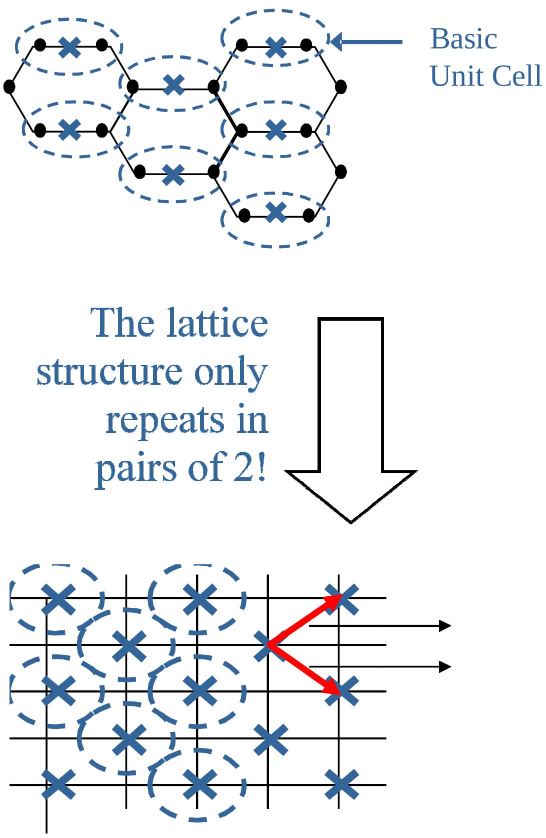


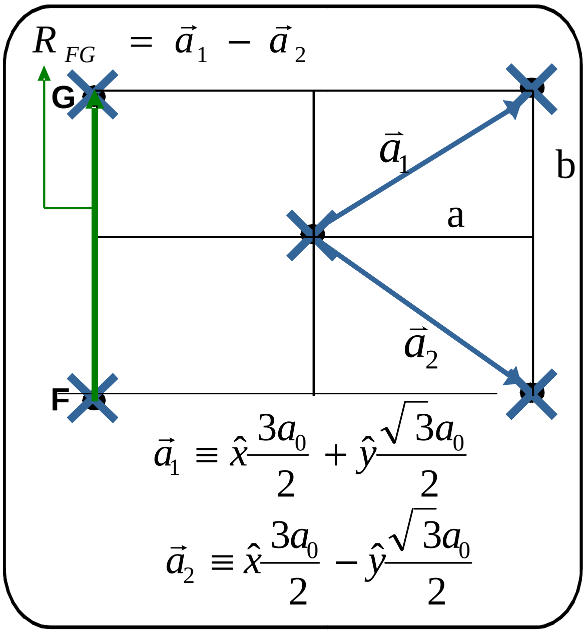
$$h(\vec{k}) = \sum_m [H_{nm}] e^{i\vec{k}(\vec{r}_m-\vec{r}_n)} \;\Rightarrow\; E\{\psi_0\} = [h(\vec{k})]\{\psi_0\}$$



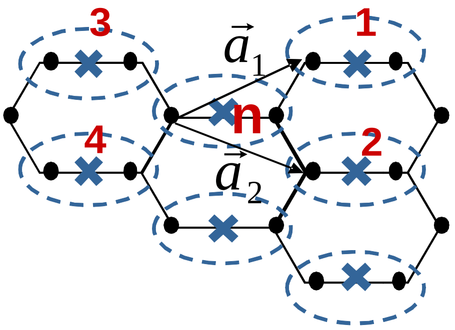
$$h(\vec{k}) = \underbrace{\varepsilon}_{m=n} + \underbrace{t_0 e^{ika}}_{m=n+1} + \underbrace{t_0 e^{-ika}}_{m=n-1} = \varepsilon + 2t_0\cos(ka)$$

Graphene h(k)





To evaluate h(k), we choose any unit cell n and then perform the summation over its nearest neighbors including n itself:



m=n	n,1	n,2
n,1	ε	t
n,2	t	ε

Phase factor is 1

m=1	m,1	m,2
n,1	0	0
n,2	t	0

To write the phase factor notice that $\boldsymbol{r_m}$-$\boldsymbol{r_n}$ for m=2 is actually $\boldsymbol{a_1}$. Continuing like this, we can write all of the 4 terms that run through neighbors 1 to 4:

$$[h(\vec{k})] = \begin{bmatrix} \varepsilon & t_0 \\ t_0 & \varepsilon \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ t_0 & 0 \end{bmatrix} e^{i\vec{k}\bullet\vec{a}_1} + \begin{bmatrix} 0 & t_0 \\ 0 & 0 \end{bmatrix} e^{i\vec{k}\bullet(-\vec{a}_2)} + \begin{bmatrix} 0 & t_0 \\ 0 & 0 \end{bmatrix} e^{i\vec{k}\bullet(-\vec{a}_1)} + \begin{bmatrix} 0 & 0 \\ t_0 & 0 \end{bmatrix} e^{i\vec{k}\bullet\vec{a}_2}$$

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

Then eigenvalue will be

$$\mathrm{E} = \varepsilon \pm \left|h_0\right|$$

E- k Relationship