Fundamentals of Nanoelectronics

ECE495 - Session 22, Oct 16, 2009

Density of States I

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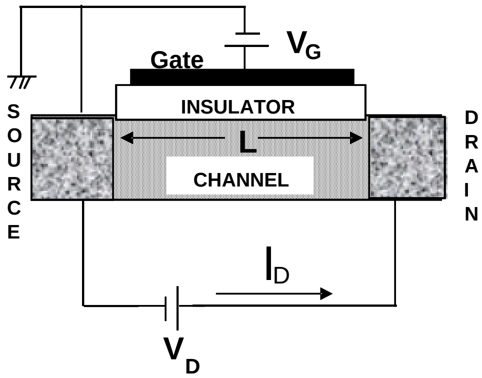
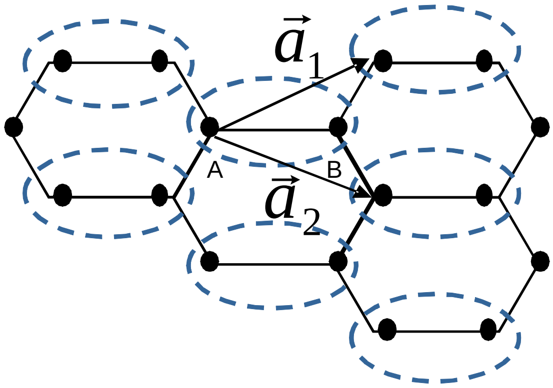
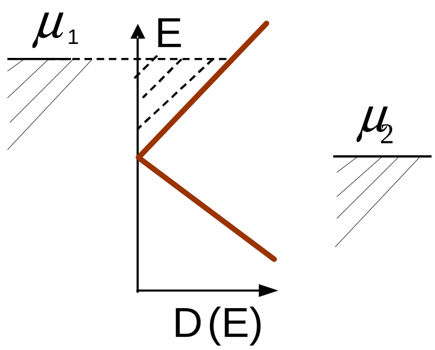


Review

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



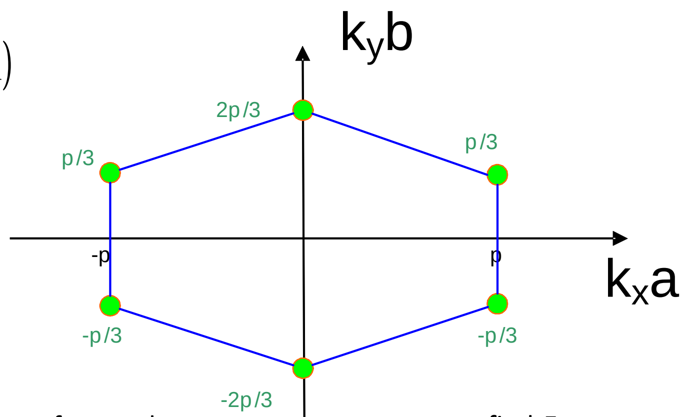


$\vec{a}_1 = \hat{x}a + \hat{y}b$ *and* $\vec{a}_2 = \hat{x}a - \hat{y}b$

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

$h_0(k_x, k_y) \approx -iat_0(k_x - i\beta_y)$ where $\beta_y = k_y - \frac{2\pi}{3b}$

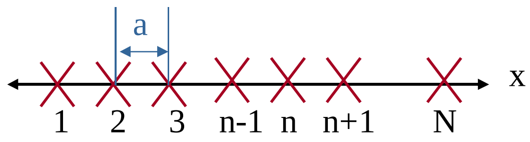
$$h(\vec{k}) = \sum_m [H_{nm}] e^{i\vec{k}(\vec{d}_m - \vec{d}_n)}$$

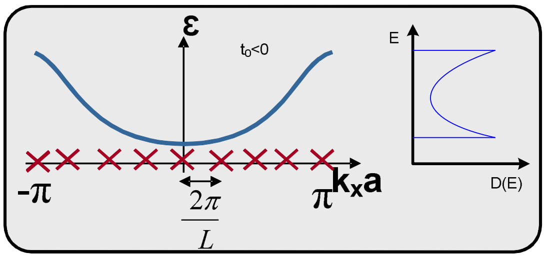


Then for $E = \varepsilon \pm \left|h_0(\vec{k})\right|$ where $\left|h_0(\vec{k})\right| = 0$ is important for us then we want to find E-k diagram around ε.

One Dimensional Density of State

$$\varepsilon = \varepsilon_0 + 2t_0 \cos ka$$





In low slop of energies we have lots of states.

$$D(E) = \frac{L}{\left({}^{d\varepsilon}/_{dk}\right)_{\varepsilon=E}}$$

$$\varepsilon = \varepsilon_0 + 2t_0 \cos ka \quad (I) \Rightarrow \frac{d\varepsilon}{dk} = -2at_0 \sin ka \qquad (II)$$

$$(I) \Rightarrow \cos ka = \frac{\varepsilon - \varepsilon_0}{2t_0} \Rightarrow \sin ka = \sqrt{1 - \left(\frac{\varepsilon - \varepsilon_0}{2t_0}\right)^2} \quad (III)$$

$$(II)\&(III) \Rightarrow \frac{d\varepsilon}{dk} = -2at_0 \sqrt{1 - \left(\frac{\varepsilon - \varepsilon_0}{2t_0}\right)^2}$$

$D(E) = \sum_k \underbrace{\delta(E - \varepsilon(k))}_{/eV} \Rightarrow \int \underbrace{dk}_{/m} \underbrace{\delta(E - \varepsilon(k))}_{/eV}$ then the integral dimensionally is not match so we change it to $\frac{\Delta k}{{}^{2\pi}/_L} \delta(E - \varepsilon(k))$ then:

$$D(E) = \int_{-\infty}^{\infty} \frac{dk}{{}^{2\pi}/_L} \delta(E - \varepsilon(k)) = \int_0^{\infty} 2 \frac{d\varepsilon}{{}^{2\pi}/_L} \delta(E - \varepsilon(k)) \frac{dk}{d\varepsilon}$$

If we assume $\frac{d\varepsilon}{dk} = \hbar v$ then

$$D(E) = \frac{L}{\pi} \left[\frac{dk}{d\varepsilon}\right]_{\varepsilon=E} = \frac{L}{\pi \hbar v}$$

$$\boxed{\int_{-\infty}^{\infty} f(x)\, \delta(x - x_0) dx = f(x_0)}$$

If we assume spin we should multiply D(E) by 2.