

# Fundamentals of Nanoelectronics

ECE495 - Session 19, Oct 9, 2009

## Bandstructure I

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### Review

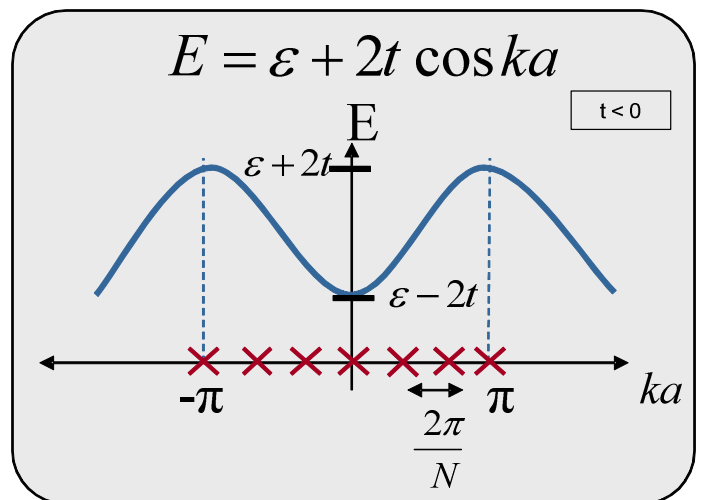
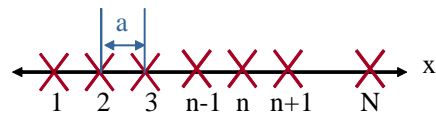
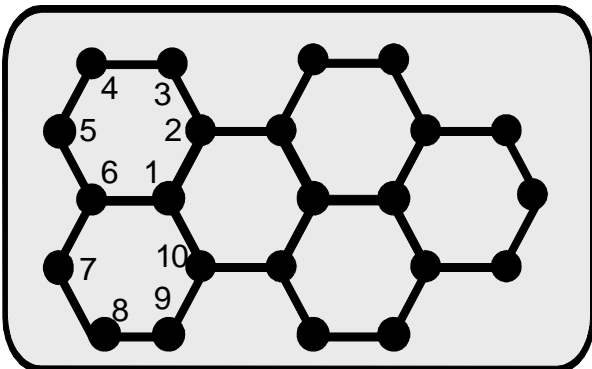
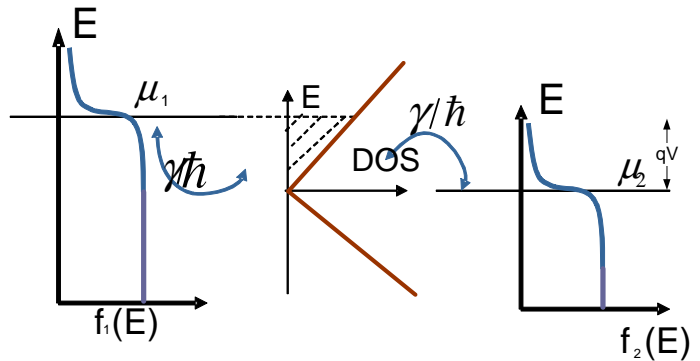
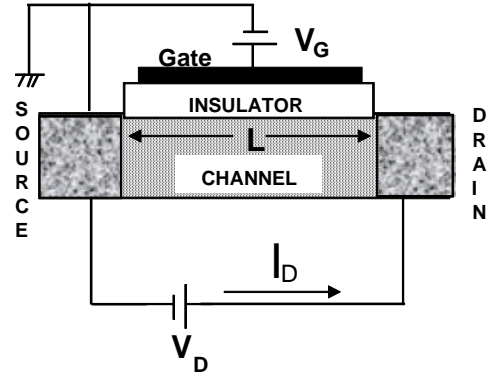
$$E\Psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + U_N(\vec{r}) + U_e(\vec{r}) \right) \Psi$$

$$E \begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_N \end{Bmatrix} = \begin{bmatrix} \epsilon & & \\ & \epsilon & \\ & & \ddots \\ & & & \epsilon \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_N \end{Bmatrix} \Rightarrow E(k) \Rightarrow D(E)$$

$$M(E)$$

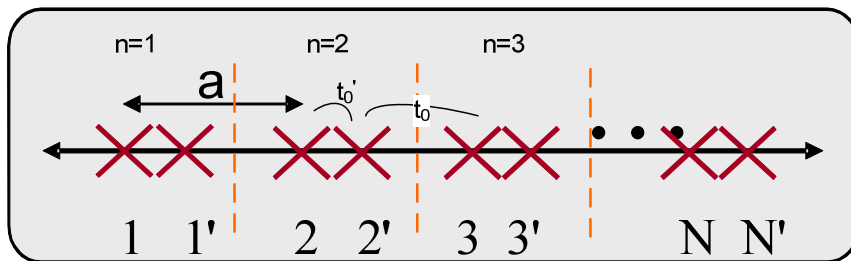
How starting from Schrodinger equation we can get D(E)?

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



## Generalization of Bandstructure Method

What we'll learn today is a generalization of bandstructure method to a solid where the **unit cell** consists of two atoms.



It is periodic

Next we want to find the dispersion relation for this solid:

$$E \begin{Bmatrix} \psi_1 \\ \psi'_1 \\ \vdots \\ \psi_N \\ \psi'_N \end{Bmatrix} = \begin{bmatrix} \epsilon & t'_0 \\ t'_0 & \epsilon \\ 0 & t_0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ t_0 & 0 \\ \epsilon & t'_0 \\ t'_0 & \epsilon \\ 0 & t_0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ t_0 & 0 \\ \epsilon & t'_0 \\ t'_0 & \epsilon \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi'_1 \\ \vdots \\ \psi_N \\ \psi'_N \end{Bmatrix}$$

Matrix is **Hermitian** and tri-diagonal.

A **Hermitian matrix** (or **self-adjoint matrix**) is a square matrix with complex entries which is equal to its own conjugate transpose – that is, the element in the  $i^{\text{th}}$  row and  $j^{\text{th}}$  column is equal to the complex conjugate of the element in the  $j^{\text{th}}$  row and  $i^{\text{th}}$  column. If matrix elements are real then matrix would be symmetric also.

We see that now every other row in the matrix is the same not every row. To use the principle of bandstructure every row must look the same. To get this configuration we can do this:

$$\Rightarrow E \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{Bmatrix} = \begin{bmatrix} \alpha & \beta & & \\ \beta^+ & \alpha & \beta & \\ & \beta^+ & \alpha & \ddots \\ & & \ddots & \ddots \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{Bmatrix}$$

What has happened is that by combining two elements of the wavevector into a new one, we get:

$$\phi_1 = \begin{Bmatrix} \psi_1 \\ \psi'_1 \end{Bmatrix}, \alpha \equiv \begin{bmatrix} \epsilon & t'_0 \\ t'_0 & \epsilon \end{bmatrix} \text{ and } \beta \equiv \begin{bmatrix} 0 & 0 \\ t_0 & 0 \end{bmatrix}$$

We can now use the principle of bandstructure to write the solution to the set of equations:

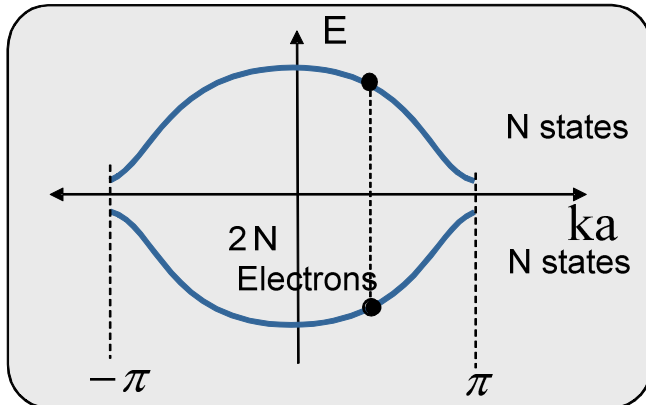
$$E\{\phi_n\} = [\beta^+]\{\phi_{n-1}\} + [\alpha]\{\phi_n\} + [\beta]\{\phi_{n+1}\} \quad (1)$$

$$\{\varphi_n\} = \{\varphi_0\} e^{inka} \quad (\text{II})$$

$$\Rightarrow E\{\varphi_0\} e^{inka} = [\beta^+ \{\varphi_0\} e^{i(n-1)ka} + [\alpha] \{\varphi_0\} e^{inka} + [\beta] \{\varphi_0\} e^{i(n+1)ka}]$$

$$\Rightarrow E\{\varphi_0\} = [\beta^+ \{\varphi_0\} e^{-ika} + [\alpha] \{\varphi_0\} + [\beta] \{\varphi_0\} e^{ika}] \quad \text{a is distance between two unit cells.}$$

$E\{\varphi_0\} = [\beta^+ e^{-ika} + \alpha + \beta e^{ika}] \{\varphi_0\}$  we **can't** drop  $\{\varphi_0\}$  from both sides due to it is a column vector but we can calculate eigenvalues for  $E$ .



How many branches we have shows how many basis function we have. For silicon it is 20.

$$E\{\varphi_0\} = [\beta^+ e^{-ika} + \alpha + \beta e^{ika}] \{\varphi_0\}$$

$$E\{\varphi_0\} = \begin{bmatrix} 0 & t_0 e^{-ika} \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} \varepsilon & t'_0 \\ t'_0 & \varepsilon \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ t_0 e^{-ika} & 0 \end{bmatrix} \{\varphi_0\}$$

$$[h(k)] = \begin{bmatrix} \varepsilon & t'_0 + t_0 e^{-ika} \\ t'_0 + t_0 e^{+ika} & \varepsilon \end{bmatrix} \quad \text{This matrix is Hermitian.}$$

Eigenvalues are:

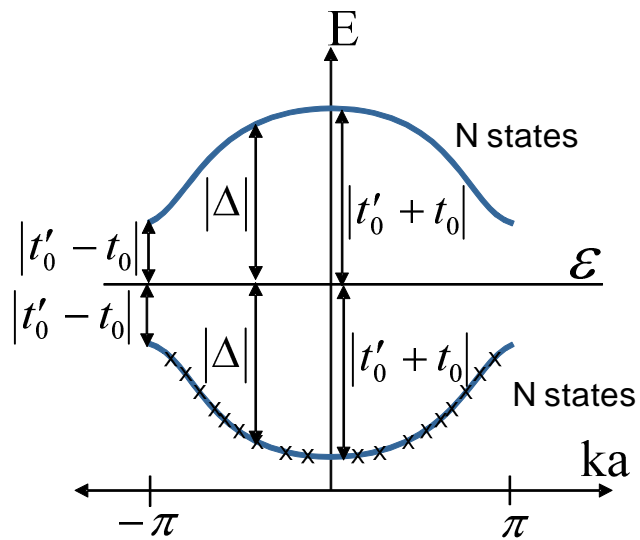
$$E = \varepsilon \pm |\Delta| \quad \Delta \equiv t'_0 + t_0 e^{-ika}$$

$$\Rightarrow E(k) = \varepsilon \pm \sqrt{t_0'^2 + t_0^2 + \frac{2t_0't_0 \cos ka}{2t_0't_0 \cos ka}}$$

$$\begin{pmatrix} \varepsilon & c \\ c^* & \varepsilon \end{pmatrix} \rightarrow \text{eigenvalues } \varepsilon \pm |c|$$

$$\Rightarrow \det \begin{pmatrix} \varepsilon - \lambda & c \\ c^* & \varepsilon - \lambda \end{pmatrix} = 0 \Rightarrow (\varepsilon - \lambda)^2 - cc^* = 0$$

$$\Rightarrow (\varepsilon - \lambda)^2 = cc^* \Rightarrow \lambda = \varepsilon \pm |c|$$



$N$  is number of unit cells.

There are  $2N$  states available. There are total of  $2N$  electrons. Each state can take two electrons (up spin and down spin). At temperature, the lower band is filled and the upper band is empty. Fermi level ( $\mu$ ) lies between the two bands ( $\epsilon = \mu$ ). Since there are no states around the Fermi level then solid will conduct well.