Fundamentals of Nanoelectronics

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Lecture 19: Bandstructure
Ref. Chapter 5.1 & 5.2

Network for Computational Nanotechnology

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• The bandstructure principle helps us to understand the energy levels of large solids and serves as a background to understand the energy levels of nanostructures. For electrical conduction we need to understand the energy levels and we need to know where the Fermi level lies because the energy levels around the Fermi level determine the I-V characteristics.

• We always start from Schrödinger equation:

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

• As long as there is spherical symmetry for the potential we can reduce this equation to three 1D equations. Solving each equation numerically then involves turning the equation to a matrix equation. To so we first set up a lattice of points.

• By doing this we have discretized the quantities we are dealing with. For example the wavefunction will have a value at each lattice point.
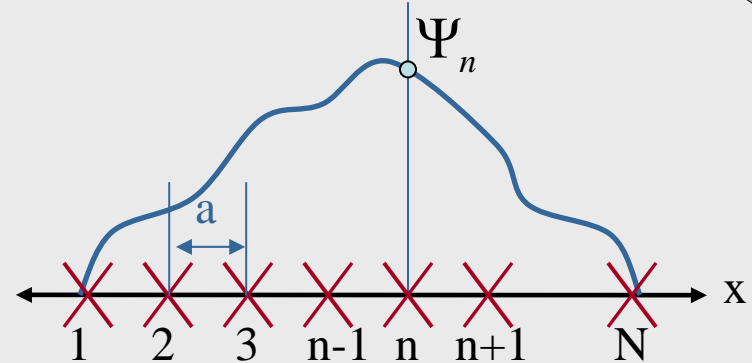

• Notice that without the spherical symmetry the problem is not separable; hence we have to deal with the 3D equation which easily gets out of hand.

• To solve the problem we turn into another method, namely the idea of basis functions.

$$\Psi(\vec{r}) = \sum_m \psi_m u_m(\vec{r})$$

• A good example for use of basis functions is to use it for the Hydrogen molecule. The separate Hydrogen atoms are have these 1s orbital. We can use these as our basis functions keeping in mind that the wavefunction of the Hydrogen molecule will be some linear combination of these two.

2s,2p

$u_1(\vec{r})$

1s

$U_1(\vec{r})$

$+$ H

2s,2p

$u_2(\vec{r})$

1s

$U_2(\vec{r})$

$+$ H
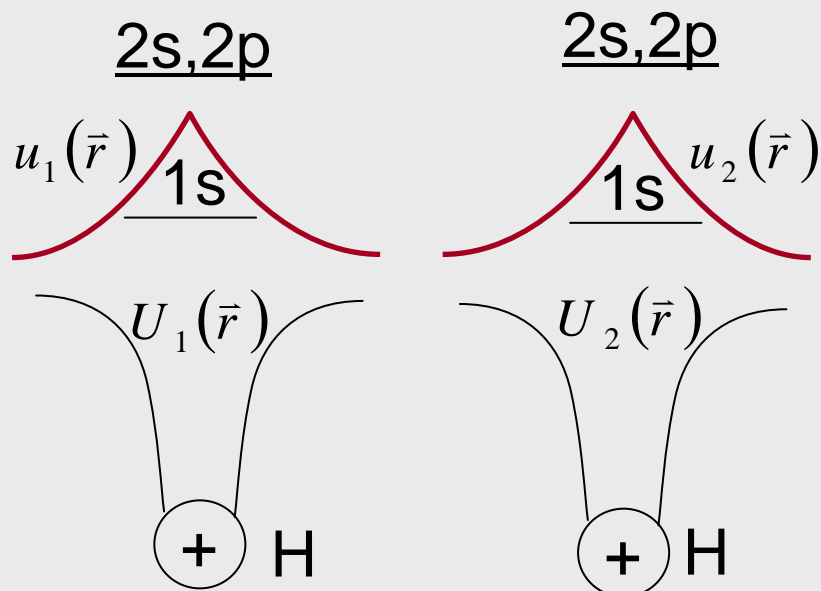
• Again Schrödinger equation becomes a matrix equation:

$$E\left\{\ \right\} = \left[\ bN^*bN\ \right]\left\{\ \right\}$$

• With this background we get into the concept of bandstructure. Consider a 2D solid:

y

$\vec{a}_2$

t

$\mathcal{E}$ ✖ $\vec{a}_1$

n

x

m
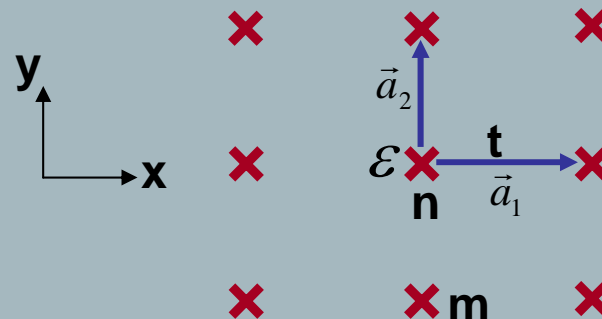
• The number of basis functions is b*N where b is the number of atoms and N is the number of orbitals per atom.
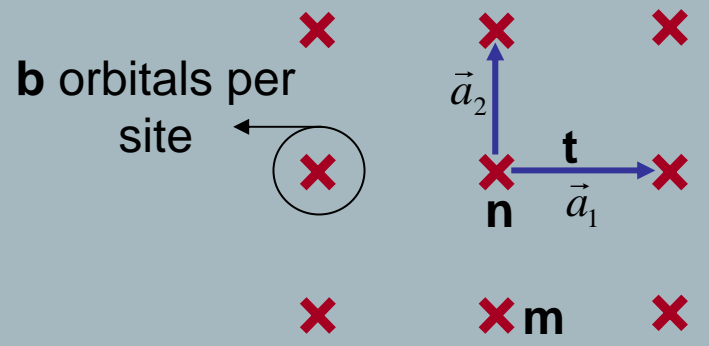
- The principle of bandstructure helps us to find the eigenvalues of a periodic matrix in a simple way. This is important for us because solids that we are interested in have periodic structures so the Hamiltonian matrix looks periodic. For example:

$$E \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} \boxed{b*b} & & \\ & \boxed{b*b} & \\ & & \\ & & \text{N*N} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

This matrix equation is a set of algebraic equations each of which can be written as:

$$E \underbrace{\{\phi_n\}}_{b \times 1} = \sum_m \underbrace{[H_{nm}]}_{b \times b} \underbrace{\{\phi_m\}}_{b \times 1}$$

b orbitals per site

- We can now think of the matrix as an N by N matrix where each element is b by b. In doing so what we've gained is the periodicity of the matrix. Once the matrix is periodic we can use the principle of bandstructure and find the energy levels in a relatively easy manner. To see this start with the wavefunction: we can write the solution to the Schrödinger equation as:

$$\{\phi_m\} = \{\phi_0\} e^{i\vec{k} \bullet \vec{d}_m}$$

$$E\{\phi_n\} = \sum_m [H_{nm}]\{\phi_m\} \quad (1)$$
$$\underbrace{\phantom{E\{\phi_n\}}}_{b\times 1} \quad \underbrace{\phantom{[H_{nm}]}}_{b\times b} \underbrace{\phantom{\{\phi_m\}}}_{b\times 1}$$

$$\{\phi_m\} = \{\phi_0\}e^{i\vec{k}\bullet\vec{d}_m} \quad (2)$$

- Substituting 2 in 1, we have:

- Where:

$$E\{\phi_0\} = [h(\vec{k})]\{\phi_0\}$$
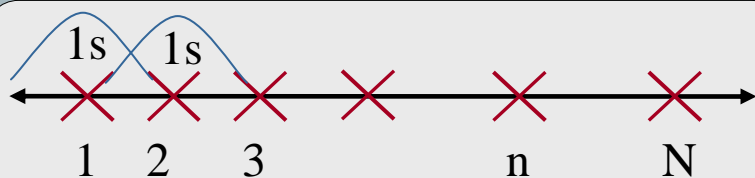
$$[h(\vec{k})] = \sum_m [H_{nm}]e^{i\vec{k}\bullet(\vec{d}_m - \vec{d}_n)}$$

- What has happened is that finding the eigenvalues of h(k) has now become more tractable . Since for a particular k, h(k) is b*b we can easily find its eigenvalues. k runs from 1 to N based on the number of lattice points. So for each k we get b*b eigenvalues. Altogether we have Nb*Nb eigenvalues which is exactly what we were after.
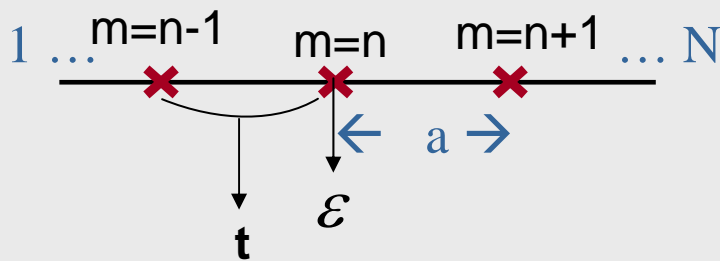
• Let's apply what we've learned to a special case. Consider a 1D lattice with 1 orbital per unit cell.

$1s$ $1s$

1   2   3   n   N

• The general expression for h(k) is:

$$\left[h\!\left(\vec{k}\right)\right]=\sum_{m}\left[H_{nm}\right]e^{i\vec{k}\bullet\left(\vec{d}_m-\vec{d}_n\right)}$$

• Fix a point "n" and write the summation:

1 … m=n-1   m=n   m=n+1   … N

$\leftarrow$ a $\rightarrow$

t ε

• h(k) becomes:

$$\left[h(k)\right]=\varepsilon+te^{-ika}+te^{ika}=\varepsilon+2t\cos ka$$

• We can now draw the dispersion relation:

E

k_a
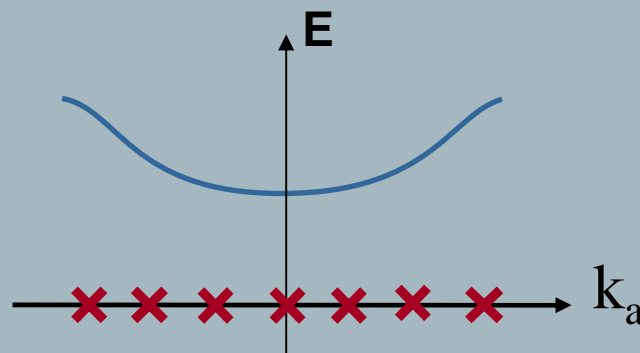
• Let's apply this to another example, namely the dimerized solid.
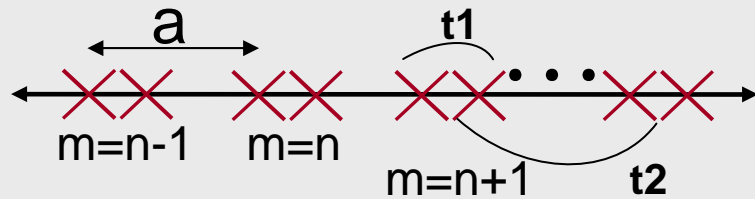
• Again the general h(k) can be written as:

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

• h(k) for the dimerized solid can be written as:

$$[h(k)] = \overbrace{\begin{bmatrix} \varepsilon & t_1 \\ t_1 & \varepsilon \end{bmatrix}}^{m=n} + \begin{matrix} n,1 \\ n,2 \end{matrix} \overbrace{\begin{bmatrix} \overset{m,1}{0} & \overset{m,2}{t_1} \\ 0 & 0 \end{bmatrix}}^{m=n-1} e^{-ika} + \overbrace{\begin{bmatrix} 0 & 0 \\ t_2 & 0 \end{bmatrix}}^{m=n+1} e^{ika}$$

$$[h(k)] = \begin{bmatrix} \varepsilon & \Delta(k) \\ \Delta^*(k) & \varepsilon \end{bmatrix} \qquad \left(\Delta \equiv t_1 + t_2 e^{-ika}\right)$$
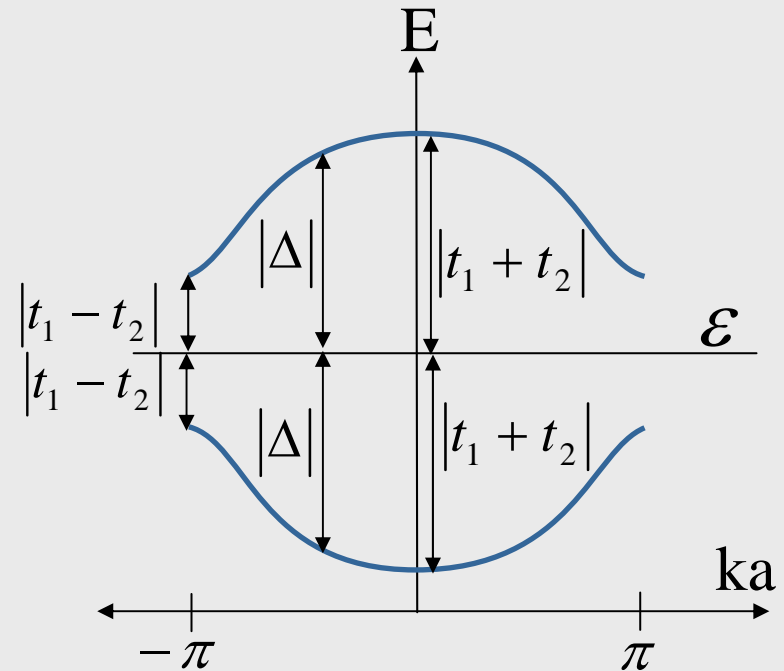
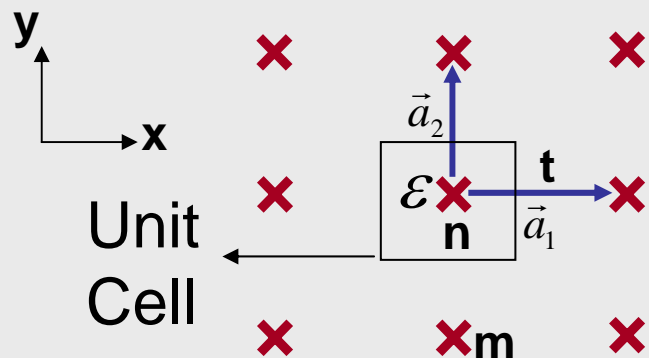- Next we want to find the eigenvalues.

$$[h(k)] = \begin{bmatrix} \varepsilon & t_1 + t_2 e^{-ika} \\ t_1 + t_2 e^{+ika} & \varepsilon \end{bmatrix}$$
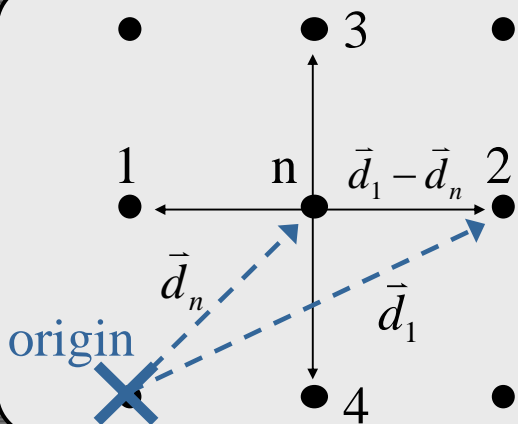
- Eigenvalues are:

$$E = \varepsilon \pm |\Delta| \qquad \Delta \equiv t_1 + t_2 e^{-ika}$$

Example: 2D Square Solid

Unit Cell

• Take $\vec{k} = k_x \hat{x} + k_y \hat{y}$ and set the origin as shown…

Want to evaluate: $h(\vec{k}) = \sum_m H_{nm} e^{i\vec{k} \bullet (\vec{d}_m - \vec{d}_n)}$

Evaluating H$_{nn}$ results in ε (self-energy) and evaluating H$_{nm}$ results in a value that we call t. So we have 5 terms in our summation:

$$h(\vec{k}) = \varepsilon + \sum_{m=1}^{4} t e^{i\vec{k}(\vec{d}_m - \vec{d}_n)}$$

$$= \varepsilon + t e^{i\vec{k} \cdot (-\hat{x}a)} + t e^{i\vec{k} \cdot (\hat{x}a)}$$

$$+ t e^{i\vec{k} \cdot (\hat{y}a)} + t e^{i\vec{k} \cdot (-\hat{y}a)}$$

• Thus, after adding all of them we get:

$$h(\vec{k}) = \varepsilon + 2t(\cos k_x a + \cos k_y b)$$