

Fundamentals of Nanoelectronics

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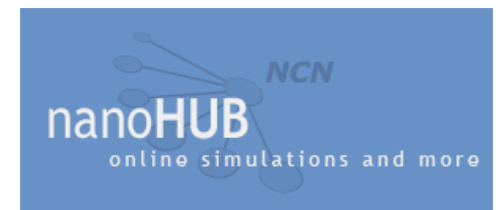
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Lecture 16: Bandstructure 1

Ref. Chapter 5.1



Network for Computational Nanotechnology



Basis Functions

- What we are trying to learn are the energy levels of a given solid. The concept of bandstructure is very useful in understanding the energy levels of periodic solids. Note that the atoms in solids we are interested in are arranged periodically.

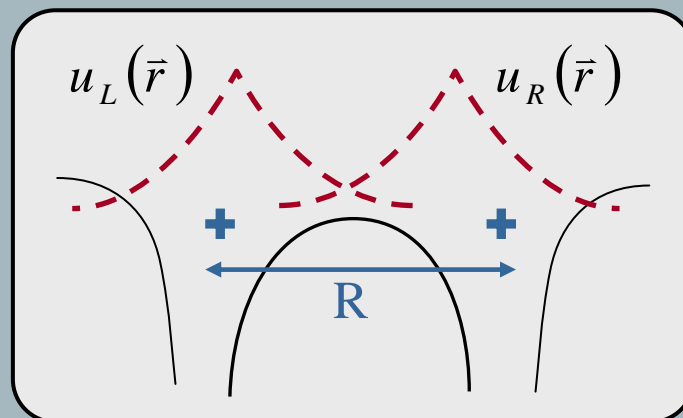
• The starting point is the Schrödinger equation:

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

- The direct way of solving this equation is to set up a lattice of points and turn the equation into a matrix equation. But this direct approach gets intractable because the matrices get huge for problems dealing with more than 1 dimension.
- Instead what is widely used is the method of basis functions: one uses his/her knowledge of the material to write the function Φ in terms of a set of basis functions.

- Example: suppose you are interested in the lowest energy levels of a hydrogen molecule. There, one knows the wavefunctions of 1s levels of each H atom. When the two atoms are brought close to each other the wavefunctions mix up somewhat but the overall wavefunction is composed of the two individual wave functions: $\Phi(\vec{r}) = \sum_m \phi_m u_m(\vec{r})$

- Instead of looking for a function we only need to find the proper coefficients which in the case of H₂ molecule there are only 2 of them.



Basis Functions and the Overall Wavefunction

04:19

- After writing the total wavefunction as some of a set of basis functions one can turn the Schrödinger equation into a matrix equation:

$$E \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix} \mathbf{H} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

- The elements of H can be found by first principles (ab initio) or by the semi empirical method which is easier to deal with. In the case of H₂ molecule we want to find the elements of a 2by2 matrix. From the symmetry of the problem we can name the elements as:

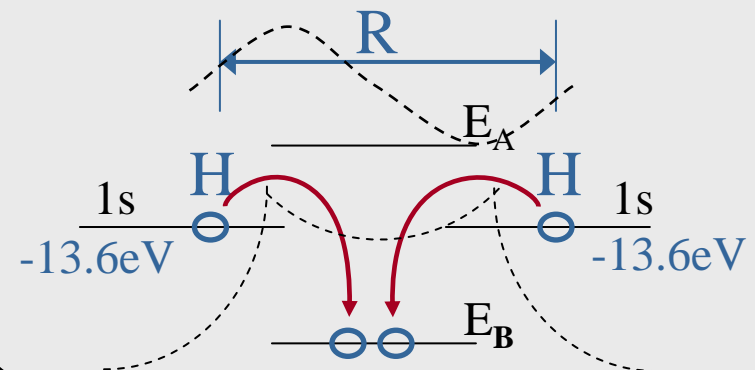
$$\mathbf{H} = \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}$$

The parameters t and ε be found by choosing them in a way that the wavefunction calculated this way would fit the experimental data.

- The advantage of this method is that it is a lot faster.
- The next step is to find the eigenvalues of our 2by2 matrix. Let λ represent the eigenvalues of the matrix. Then $\lambda = \varepsilon \pm t$
- And eigenvectors are:

$$\varepsilon + t \Rightarrow \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \varepsilon - t \Rightarrow \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = (\varepsilon + t) \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = (\varepsilon - t) \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$



A Note on Matrices

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- A note about matrices, their eigenvalues and eigenvectors:
- If a constant number is added to the diagonal elements, then all the eigenvalues are modified by adding that constant value to them and the eigenvectors remain unchanged.

$$[A]\{\phi\} = \lambda\{\phi\}$$

$$[A + c \bullet I]\{\phi\} = [A]\{\phi\} + c\{\phi\} = (\lambda + c)\{\phi\}$$

Periodicity and the Principle of Bandstructure

18:58

- Let's now move on to bandstructure and start with a simple example. Consider a hypothetical solid consisted of an array of hydrogen atoms:

$$\begin{array}{ccccccc}
 -H & -H & -H & -H & -H & -H & -H- \\
 1 & & & & & & N
 \end{array}
 \begin{bmatrix}
 \varepsilon & t & 0 & 0 & 0 & 0 \\
 t & \varepsilon & t & 0 & 0 & \\
 0 & t & \varepsilon & t & & \\
 0 & & \ddots & \ddots & \ddots & \\
 0 & & & \ddots & \ddots & \\
 0 & & & & &
 \end{bmatrix}$$

- Since the solid is periodic, all of the "t"s are actually the same.
- Notice that in general the rest of the matrix elements are not zero but because the coupling between atoms gets weaker the farther they are apart, in some cases people only consider the nearest neighbors.

- One can include more terms to get higher order answers. The important thing to note is that the principles of bandstructure will work regardless. For that to work each row in the matrix should look the same as others (although the elements might be shifted)
- What we'll see in the next couple of lectures is that if H would form a solid like the left figure it would be a metal and conduct very well. But in practice if Hydrogen atoms are put in array together the configuration that minimizes energy will be more like:



- This is what is called a dimerized solid. In this configuration the solid will be a semiconductor.

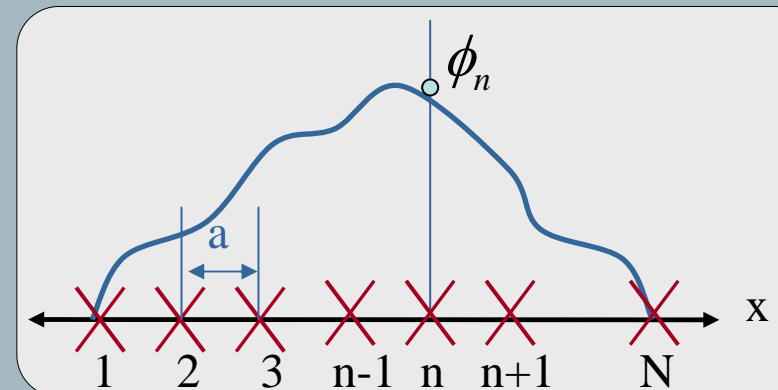
- We want to find the eigenvalues of the Hamiltonian matrix:

$$E \begin{Bmatrix} \phi_1 \\ \vdots \\ \phi_N \end{Bmatrix} = \begin{bmatrix} \varepsilon & t & & \\ t & \varepsilon & t & \\ & t & \varepsilon & \ddots \\ & & \ddots & \ddots \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \vdots \\ \phi_N \end{Bmatrix}$$

- Because the solid is periodic and the matrix looks like above, one can use the principle of bandstructure to find the answers analytically.
- The basic idea is that the matrix equation above can be written as N algebraic equations. For example the nth row gives us the nth equation:

$$E\phi_n = t\phi_{n-1} + \varepsilon\phi_n + t\phi_{n+1} \quad (1)$$

- Now if the solid is periodic, then any row's equation will look like 1 and the following solution will satisfy 1: $\phi_n = e^{inka} \phi_0$



- To check the answer plug it in the equation:

$$E\phi_0 e^{ikna} = t\phi_0 e^{i(n-1)ka} + \varepsilon\phi_0 e^{ikna} + t\phi_0 e^{i(n+1)ka}$$

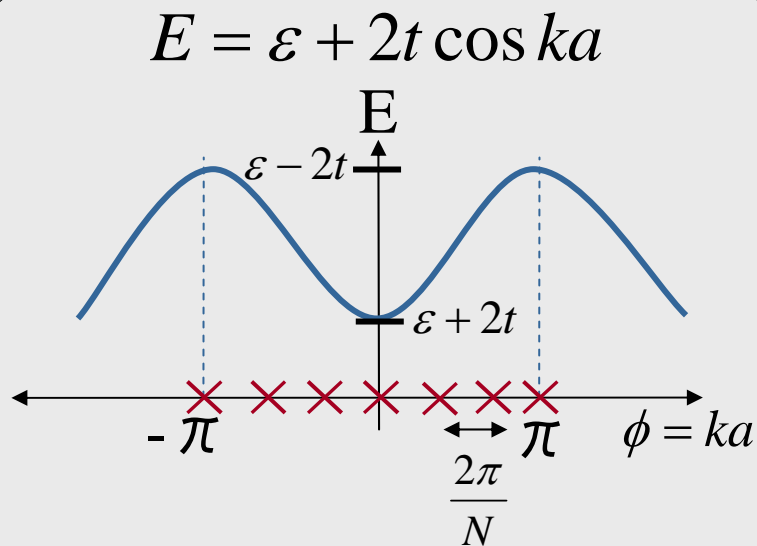
$$E = te^{-ika} + \varepsilon + te^{ika} = \varepsilon + 2t \cos ka$$

- This is called the E-k relationship and our solution satisfies 1 if this relation is satisfied.

Dispersion Relation

43:15

- We can plot the E-k relationship:



- But the above seems to suggest that E-k relationship is a continuous function; hence infinite amount of eigenvalues not N of them. So how do we get N eigenvalues? The point is that there are only specific values of k that are allowed. This is coming from the Periodic Boundary Conditions (PBC):

A horizontal line with arrows at both ends represents a periodic boundary. Points are marked along the line with labels 0, 1, 2, 3, n-1, n, n+1, and N. Below each label is a red 'x' mark. A curved line connects the point at 0 to the point at N, indicating that the system is periodic.

$$e^{inka} = e^{i(n+N)ka} \Rightarrow$$

$$e^{iNka} = 1 = e^{i2\pi(\text{integer})} \Rightarrow$$

$$Nka = 2\pi\nu \quad \nu : \text{integer} \Rightarrow$$

$$k = \frac{2\pi}{Na} \nu \quad (1)$$

- Equation (1) clearly shows that k cannot assume any values and since E is related to k via E-k relation, energy eigenvalues can only assume particular values.