Fundamentals of Nanoelectronics

ECE495 - Session 18, Oct 7, 2009

Basis Function II

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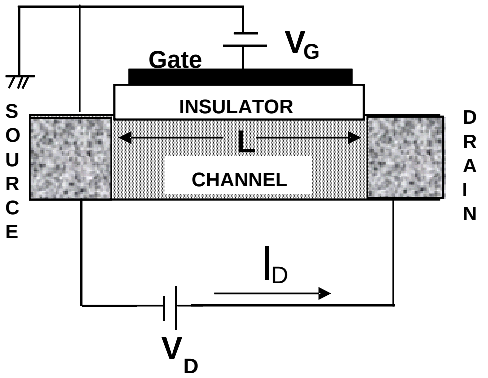
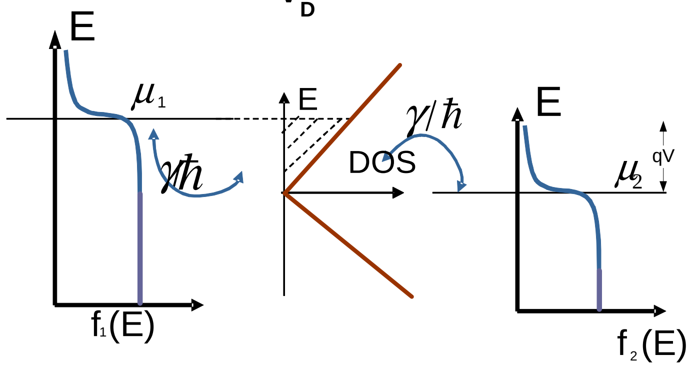
Review

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

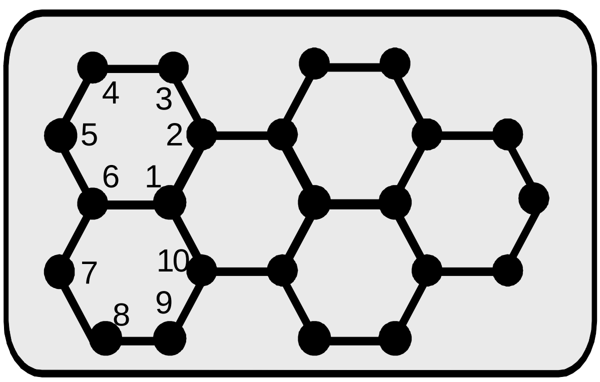


$$E\begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_N \end{Bmatrix} = \begin{bmatrix} \varepsilon & & & \\ & \varepsilon & & \\ & & \varepsilon & \ddots \\ & & \ddots & \ddots \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_N \end{Bmatrix}$$



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

$$\Psi(\vec{r}) = \sum_m \psi_m u_m(\vec{r})$$ ***u_m is a known function***



A note about matrices, their eigenvalues and eigenvectors:

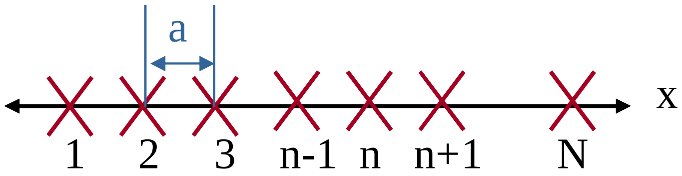
If a constant number is added to the diagonal elements, then all the eigenvalues are modified by adding that constant value to them and the eigenvectors remain unchanged.

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

One dimensional example

Consider a hypothetical solid consisted of an array of atoms:

$$\begin{bmatrix} \varepsilon & t_0 & 0 & 0 & 0 & 0 \\ t_0 & \varepsilon & t_0 & 0 & 0 & \\ 0 & t_0 & \varepsilon & t_0 & & \\ 0 & & \ddots & \ddots & \ddots & \\ 0 & & & \ddots & \ddots & \\ 0 & & & & & \end{bmatrix}$$



Since the solid is periodic, all of the “t_0”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***.

We want to find the eigenvalues of the Hamiltonian matrix:

$$E\begin{Bmatrix} \psi_1 \\ \\ \\ \psi_N \end{Bmatrix} = \begin{bmatrix} \varepsilon & t_0 & & \\ t_0 & \varepsilon & t_0 & \\ & t_0 & \varepsilon & \ddots \\ & & \ddots & \ddots \end{bmatrix}\begin{Bmatrix} \psi_1 \\ \\ \\ \psi_N \end{Bmatrix}$$

Because the solid is periodic and the matrix looks like above , one can use the principle of bandstructure to find the answers analytically.

$$E\psi_2 = t_0\psi_1 + \varepsilon\psi_2 + t_0\psi_3$$

$$E\psi_3 = t_0\psi_2 + \varepsilon\psi_3 + t_0\psi_4$$

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:

$$E\psi_n = t_0\psi_{n-1} + \varepsilon\psi_n + t_0\psi_{n+1} \quad (I)$$

Now if the solid is periodic, then any row's equation will look like ***(I)*** and the following solution will satisfy ***(I)***:

$$\psi_n = e^{inka}\psi_0$$

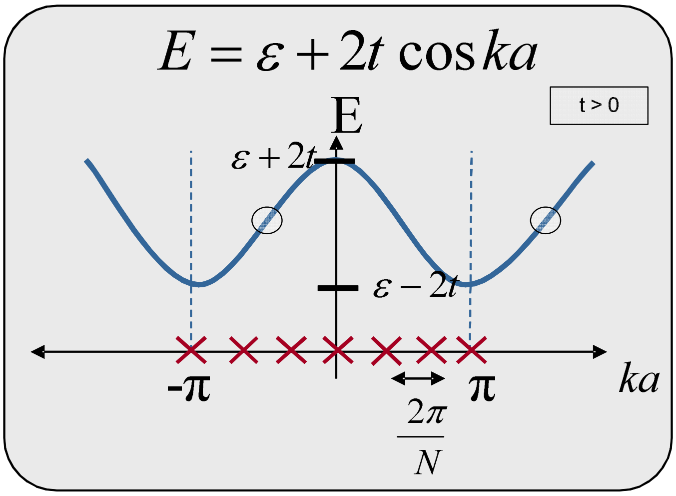
To check the answer plug it in the equation:

$$E\psi_0 e^{ikna} = t\psi_0 e^{i(n-1)ka} + \varepsilon\psi_0 e^{ikna} + t\psi_0 e^{i(n+1)ka} \Rightarrow E = te^{-ika} + \varepsilon + te^{ika} = \varepsilon + 2t\cos ka$$

$$\Rightarrow E = \varepsilon + 2t\cos ka$$

This is called the E-k relationship and our solution satisfies ***(I)*** if this relation is satisfied.

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):

$$\psi_n = \psi_{n+N} \Rightarrow e^{inka} = e^{i(n+N)ka} \Rightarrow e^{iNka} = 1 = e^{i2\pi(\text{integer})} \Rightarrow Nka = 2\pi\nu \quad \nu: \text{integer} \Rightarrow$$

$$k = \frac{2\pi}{Na}\nu$$

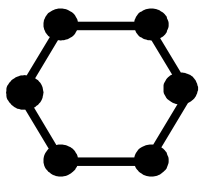
This equation clearly shows that ***k*** cannot assume any values and since ***E*** is related to ***k*** via E-k relation, energy eigenvalues can only assume particular values.

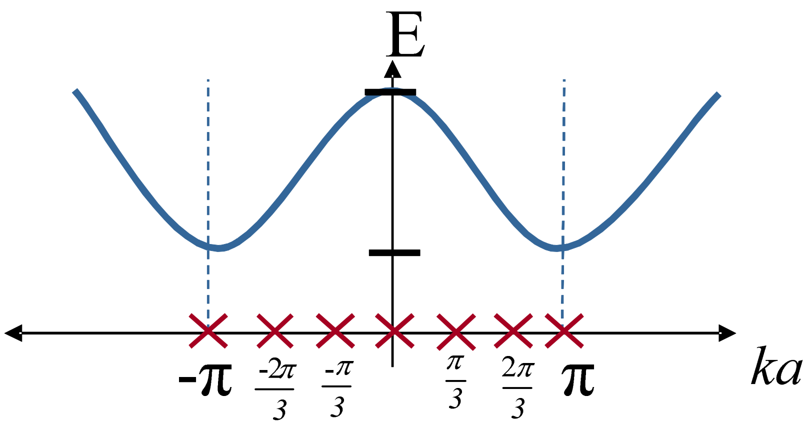
For eigenvalues we should only look over between –π and π. Two circled points in E-k diagram have same wavefunction; not only same energy.

$\psi_0 e^{inka}$ and the other $\psi_0 e^{i(k+\frac{2\pi}{a})na} = \psi_0 e^{ikna} e^{i2\pi n} = \psi_0 e^{ikna}$

Benzene Molecule

For Benzene molecule (carbon),





$E = \varepsilon + 2t_0$	(1)
$E = \varepsilon + t_0$	(2)
$E = \varepsilon - t_0$	(2)
$E = \varepsilon - 2t_0$	(1)
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	(6)

$$E\{\psi\} = \begin{bmatrix} \varepsilon & t & 0 & 0 & 0 & t \\ t & \varepsilon & t & 0 & 0 & 0 \\ 0 & t & \varepsilon & t & 0 & 0 \\ 0 & 0 & t & \varepsilon & t & 0 \\ 0 & 0 & 0 & t & \varepsilon & t \\ t & 0 & 0 & 0 & t & \varepsilon \end{bmatrix} \{\psi\}$$

To write eigenfunctions for ka = π/3 then

$$\begin{Bmatrix} e^{i\pi/3} \\ e^{2i\pi/3} \\ e^{i\pi} \\ e^{4i\pi/3} \\ e^{5i\pi/3} \\ e^{2i\pi} \end{Bmatrix}$$