

Fundamentals of Nanoelectronics

ECE495 - Session 17, Oct 4, 2009

Basis Function I

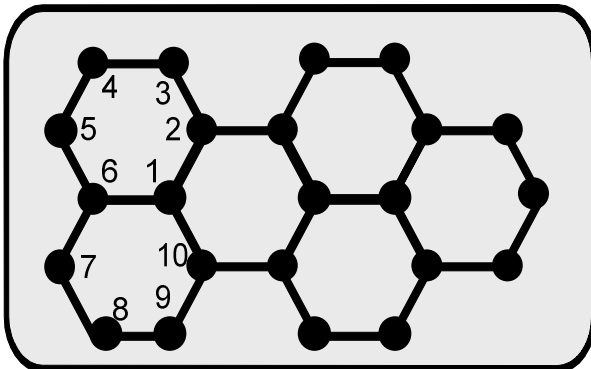
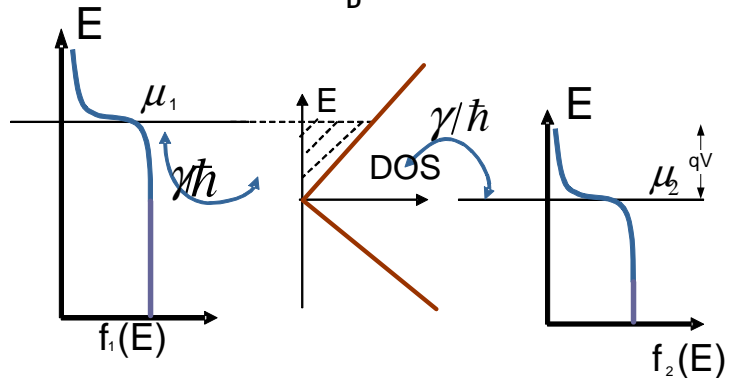
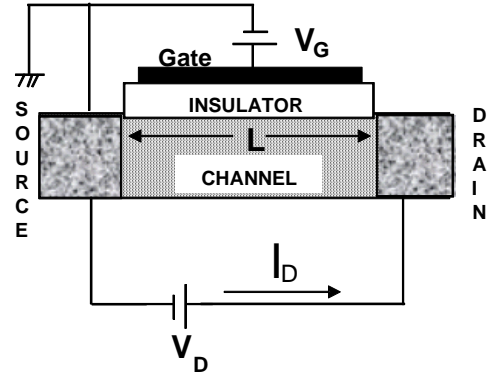
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Review

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

Density of state for Graphene is depicted. Graphite is multilayer of Graphene.

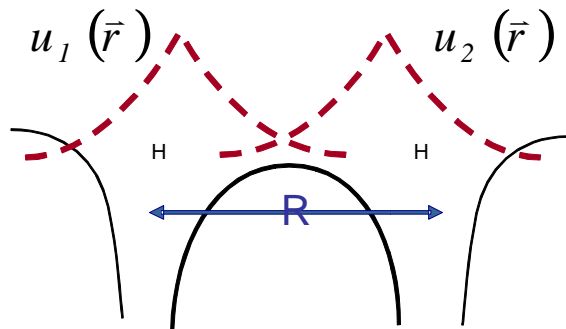


$$E \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix} = \begin{bmatrix} & & & \\ & H & & \\ & & & \\ & & & N \times N \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix}$$

The direct way of solving Schrodinger 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 or for small distance between points ($a = 0.1\text{\AA}$).

Then, what is widely used is the method of basis functions: one uses his/her knowledge of the material to write the function Ψ in terms of a set of basis functions.

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



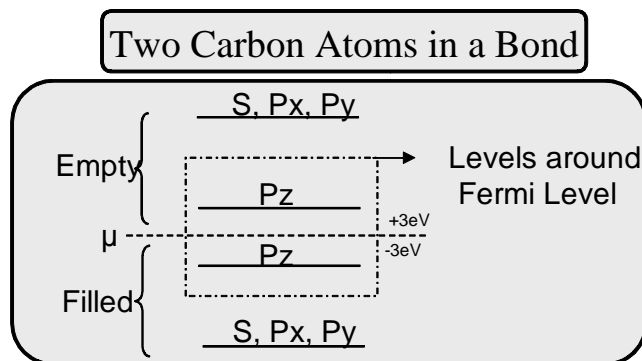
$$\Psi(\vec{r}) = \psi_1 u_1(\vec{r}) + \psi_2 u_2(\vec{r})$$

$$\begin{bmatrix} H \\ N \times N \end{bmatrix}$$

N is number of atoms

Based on periodicity we can do eigenvalue calculation analytically.

Principle of Bandstructure



How many basis functions do we need per atom? The basis functions are the atomic orbitals. There are 4 orbitals for the valence electrons of a carbon atom.

C6: $\begin{array}{l} \underline{\quad 4 \quad} \text{2p} \\ \underline{\quad 2 \quad} \text{2s} \\ \underline{\quad 2 \quad} \text{1s} \end{array}$

As it turns out we can talk only one of these four orbitals for our basis set. This makes the problem easier and tractable analytically. The reason that we can ignore the other 3 is that the "Pz" orbital does not mix with the other ones (the structure is planar). So the problem can be separated into two parts: the one for Pz orbital; and the one for S, Px, Py. Practically, it turns out that only the Pz orbitals play a major role in determining the electronic and optical properties.

For Silicon (^{14}Si) 3s 3p levels are important.

$$E\{\Psi\} = [H]\{\Psi\}$$

There are two approaches to write [H]:

1. First principle methods (Ab initio)
 - a. $H_{mn} = \int dV u_m^*(r)(H_{op}u_n(r))$
2. Semi-empirical methods
 - a. H_{mn} is determined based on experimental achievements.

Nearest neighbour

Consider a hypothetical solid consisted of an array of hydrogen atoms:

$$\begin{array}{cccccccc}
 & \varepsilon & & \varepsilon & & & & \\
 - & H & - & H & - & H & - & H & - & H & - & H & - & \\
 & & & t_0 & & t_0 & & & & & & & & \\
 \left[\begin{array}{cccccccc}
 \varepsilon & t_0 & 0 & 0 & 0 & 0 \\
 t_0 & \varepsilon & t_0 & 0 & 0 & \\
 0 & t_0 & \varepsilon & t_0 & & \\
 0 & & \ddots & \ddots & \ddots & \\
 0 & & & \ddots & \ddots & \\
 0 & & & & \ddots & \ddots & \\
 0 & & & & & & &
 \end{array} \right]
 \end{array}$$

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.