Quantum Transport:

Atom to Transistor

Prof. Supriyo Datta
ECE 659
Purdue University

02.19.2003

Lecture 16: Band Structure, Toy Examples
Ref. Chapter 5.1

Network for Computational Nanotechnology

nanoHUB
online simulations and more

A Chain of Atoms

• In this lecture the topic of band structure shall be introduced i.e. to derive the energy levels of a periodic solid. Note that common semiconductors have periodic crystal structure that allows one to do certain things which will be explored hereon.

• To start take a simple example, in this case a chain of N atoms.

$$\times\quad\times\quad\times\quad\cdots\quad\times\quad\quad\times$$
$$1\quad 2\quad 3\qquad\quad n\text{-}1\quad N$$
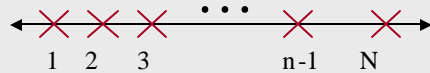
• Let us first assume only one orbital at each atomic site. Using these orbitals centered around each site as our basis set, excluding overlap, we get a diagonal Hamiltonian matrix of size NxN.

$$H=\begin{pmatrix} E_0 & & & \\ & E_0 & & \\ & & E_0 & \\ & & & \ddots \end{pmatrix}$$

If atoms are brought close together, overlap occurs; hence we'll have non-zero off diagonal elements in [H] like what we had for hydrogen molecule:

$$1s \quad \times \quad \times \quad 1s$$

For our 1D solid:

$$H=\begin{pmatrix} E_0 & E_{ss} & & \\ E_{ss} & E_0 & E_{ss} & \\ & E_{ss} & E_0 & \ddots \\ & & \ddots & \ddots & \ddots \end{pmatrix}$$

• So with overlap:

$$H = \begin{bmatrix} E_0 & E_{ss} & & & \\ E_{ss} & E_0 & E_{ss} & & \\ & E_{ss} & E_0 & \ddots & \\ & & \ddots & \ddots & \end{bmatrix}$$

• The periodicity of solid causes the Hamiltonian to have rows that are identical to each other except with a shift. Importantly, this periodicity allows the eigenvalues and eigenvectors of H to be calculated analytically.

• So, the basic equation we are trying to solve is:

$$E \begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \\ \vdots \\ y_N \end{Bmatrix} = \begin{bmatrix} E_0 & E_{ss} & & & \\ E_{ss} & E_0 & E_{ss} & & \\ & E_{ss} & E_0 & \ddots & \\ & & \ddots & \ddots & \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \\ \vdots \\ y_N \end{Bmatrix}$$

where

$$y_n = E_{ss} y_{n-1} + y_n E_0 + E_{ss} y_{n+1}$$

• But one problem still remains, periodicity is not preserved at the first and last rows of H.

- To maintain periodicity we assume periodic boundary conditions; hence:

$$E\begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \\ \vdots \\ y_N \end{Bmatrix} = \begin{bmatrix} E_0 & E_{ss} & & E_{ss} \\ E_{ss} & E_0 & E_{ss} & \\ & E_{ss} & E_0 & \ddots \\ E_{ss} & & \ddots & \ddots \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \\ \vdots \\ y_N \end{Bmatrix}$$

- Each row:

$$E y_n = E_{ss} y_{n-1} + E_0 y_n + E_{ss} y_{n+1}$$

- The above equation can be solved analytically via $y_n = y_0 e^{inf}$ (where f is any real number)
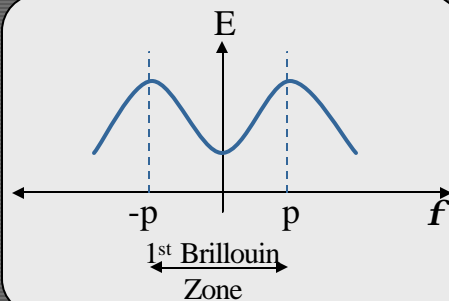
- Substituting in we get,

$$E = E_{ss} \frac{y_{n-1}}{y_n} + E_0 + E_{ss} \frac{y_{n+1}}{y_n}$$

$$= E_{ss} e^{-if} + E_0 + E_{ss} e^{+if}$$

$$= E_0 + 2 E_{ss} \cos(f)$$

- But in this form f gives a continuous infinite number of values for E. What condition should be placed on f such that we have a finite number of eigenvalues like the original finite matrix?

E

$$f$$

-p   p

$$1^{st} \text{ Brillouin}$$
Zone

• To get a finite number of eigenvalues, we have to (1) limit the range of f and (2) discretize the allowed values of f.

• What limits the range of f ?

$$\boldsymbol{y}_n = \boldsymbol{y}_0 e^{in(\boldsymbol{f}+2\boldsymbol{p})} = \boldsymbol{y}_0 e^{in\boldsymbol{f}}$$

$\boldsymbol{f}$ and $(\boldsymbol{f}+2\boldsymbol{p})$ give us the same wave function and we only need: $0 \le \boldsymbol{f} \le 2\boldsymbol{p}$

• But in a finite range we can still have infinite eigen values. Now what? The answer is that eigen values must be discredited because for a periodic solid we have:

$$\boldsymbol{y}_{n+1} = \boldsymbol{y}_0 e^{in(N+1)\boldsymbol{f}} = \boldsymbol{y}_1$$

This tells us: $e^{iN\boldsymbol{f}} = 1$

Which means: $N\boldsymbol{f} = 2\boldsymbol{p}\boldsymbol{n} \Rightarrow \boldsymbol{f} = v\dfrac{2\boldsymbol{p}}{N}$
($\boldsymbol{n}$ is an integer)

• What we have now is a discrete set of eigen values in a finite range which results in a finite number just as the size of [H] matrix which was finite.
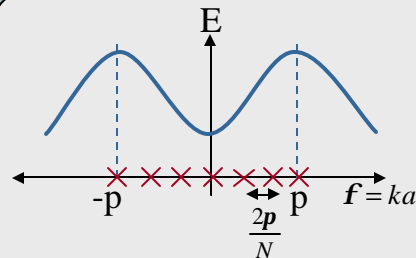
• Summarizing, we have:

$$\boldsymbol{f} = v\frac{2\boldsymbol{p}}{N}$$

which looks like....

Usually $\boldsymbol{f}$ is written as $\boldsymbol{f}$=ka where 'a' is the spacing between lattice points

• How does the value of E_{ss} affect E? For Ess > 0 E has upward curvature in the region of $-\boldsymbol{p} \leq ka \leq \boldsymbol{p}$ and downward curvature for Ess < 0.
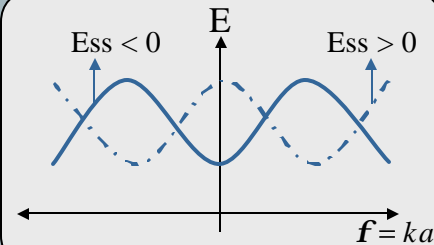
Positive / Negative overlap

- For which cases is $E_{ss}>0$ and $E_{ss}<0$? In general the sign of E_{ss} depends on the sign of the potential and on the symmetry of the overlapping wave functions.

- Example 1:

Consider two 1s Hydrogen wave functions:

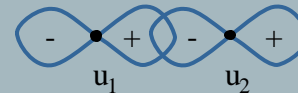With the interaction potential U<0 (since U depends mostly on the nuclear forces).

- Example 1 contd:
So we have,

$$\int d\bar{r}\, u_1^* U u_2 < 0 \qquad \text{and } E_{ss}<0$$

since $u_1 \cap u_2 > 0$ and $U < 0$

Likewise, take 2 px hydrogen wave functions
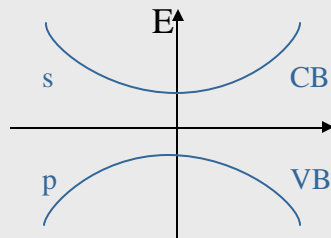

Thus,

$$\int d\bar{r}\, u_1^* U u_2 > 0 \qquad \text{and } E_{ss}>0$$

Since again U<0 and $u_1 \cap u_2 < 0$

• One last point, roughly in semiconductors one could say that the valance band is composed of 'p' orbitals and the conduction band of 's' orbitals. Hence the well known curvature.

Semiconductor Conductance(CB) and Valance (VB) Bands

E

s   CB

p   VB

• What if we had two atoms at each lattice site? i.e.

$$1 \quad 1' \qquad 2 \quad 2' \qquad 3 \quad 3' \qquad N \quad N'$$

• In this case the Schrödinger equation becomes:

$$E\left\{\begin{array}{c} y_1 \\ y_1' \\ \vdots \\ y_N \\ y_N' \end{array}\right\} = \left[\begin{array}{ccccc} E_o & E_{ss} & & & E_{ss'} \\ E_{ss} & E_o & E_{ss'} & & \\ & E_{ss'} & E_o & \ddots & \\ & & & \ddots & \ddots \\ E_{ss'} & & & & \end{array}\right]\left\{\begin{array}{c} y_1 \\ y_1' \\ \vdots \\ y_N \\ y_N' \end{array}\right\}$$

• The primary difference is $E_{ss} \neq E_{ss}'$ which results in only even/odd rows to be the same.

• How do we handle the two atom unit cell Hamiltonian?

The previous relation

$$\boldsymbol{y}_n = E_{ss}\boldsymbol{y}_{n-1} + \boldsymbol{y}_n E_0 + E_{ss}\boldsymbol{y}_{n+1}$$

does not easily apply.

Ans: Collect elements $\boldsymbol{y}_n$ and $\boldsymbol{y}'_n$ into the form $\boldsymbol{f}_n$.

• Reorganizing the Schrödinger equation we get:

$$E\begin{Bmatrix} \boldsymbol{f}_1 \\ \boldsymbol{f}_2 \\ \vdots \\ \boldsymbol{f}_N \end{Bmatrix} = \begin{bmatrix} H_{11} & H_{12} & & \\ H_{21} & H_{22} & H_{23} & \\ & H_{32} & H_{33} & \ddots \\ & & \ddots & \ddots \end{bmatrix} \begin{Bmatrix} \boldsymbol{f}_1 \\ \boldsymbol{f}_2 \\ \vdots \\ \boldsymbol{f}_N \end{Bmatrix}$$

• Where,

$$H_{nn} = \begin{bmatrix} E_0 & E_{ss} \\ E_{ss} & E_0 \end{bmatrix}$$

$$H_{n,n+1} = \begin{bmatrix} 0 & 0 \\ E'_{ss} & 0 \end{bmatrix}$$

$$H_{n,n-1} = \begin{bmatrix} 0 & E'_{ss} \\ 0 & 0 \end{bmatrix}$$

and,

$$\{\boldsymbol{f}_n\} = \begin{Bmatrix} \boldsymbol{y}_n \\ \boldsymbol{y}'_n \end{Bmatrix}$$

• To solve this set of equations now apply the equality

$$E\{\boldsymbol{f}_n\} = H_{n,n-1}\{\boldsymbol{f}_{n-1}\} + H_{nn}\{\boldsymbol{f}_n\} + H_{n,n+1}\{\boldsymbol{f}_{n+1}\}$$

and the ansatz

$$\{\boldsymbol{f}_n\} = \{\boldsymbol{f}_0\}e^{ikna}$$

where a is:
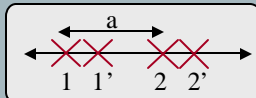
Combined these equations give:

$$E\{\boldsymbol{f}_0\}e^{inka} = [H_{n,n-1}]\{\boldsymbol{f}_0\}e^{i(n-1)ka}$$
$$+ [H_{n,n}]\{\boldsymbol{f}_0\}e^{inka}$$
$$+ [H_{n,n+1}]\{\boldsymbol{f}_0\}e^{i(n+1)ka}$$
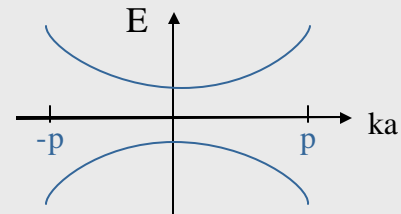
• Or in a simplified form:

$$E\{\boldsymbol{f}_0\} = \lfloor h(\vec{k}) \rfloor\{\boldsymbol{f}_0\}$$

where

$$h(\vec{k}) = H_{n,n} + H_{n,n-1}e^{-ika} + H_{n,n+1}e^{+ika}$$

and the eigenvalues, for each $\vec{k}$ now come in pairs.

Paired Eigenvalues of Two Atom Unit Cell

• Why are there two eigenvalues for each value of k?

Ans: The number of eigenvalues per $\bar{k}$ has a one to one ratio with the number of basis functions per unit cell. In this case we have two basis functions(two atoms with one orbitals each) per unit cell.

• Next Lecture:

- Look at two dimensional structures.
- Particularly graphite, which has the structure