Quantum Transport:
Atom to Transistor

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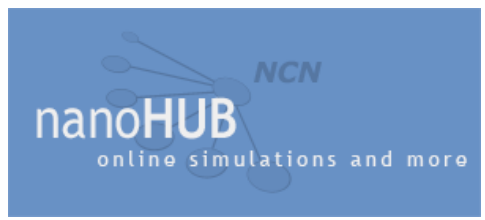
Lecture 23: Capacitance: Model Hamiltonian

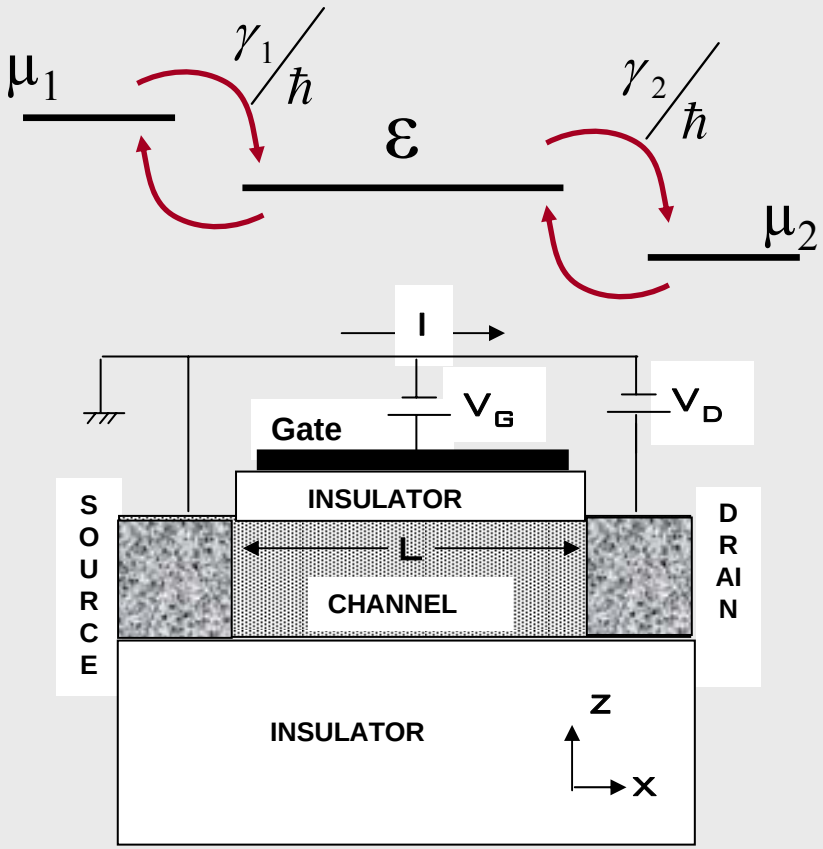
Ref. Chapter 7.1

Network for Computational Nanotechnology



Introduction

00:00



• At the beginning of this course we started with a basic FET example ←

• In this simple model we discussed the basic factors of current flow. Two different levels for μ_1 and μ_2 in the source and drain respectively results in the difference of agenda in the contacts: one keeps pumping in electrons while the other takes them out which leads to a net flow of electrons, through a level ε.

• To make all this quantitative, we need to understand 1) where the levels in the channel are coming from and how to model them; 2) how the coupling to the contacts works.

Device Hamiltonian

03:00

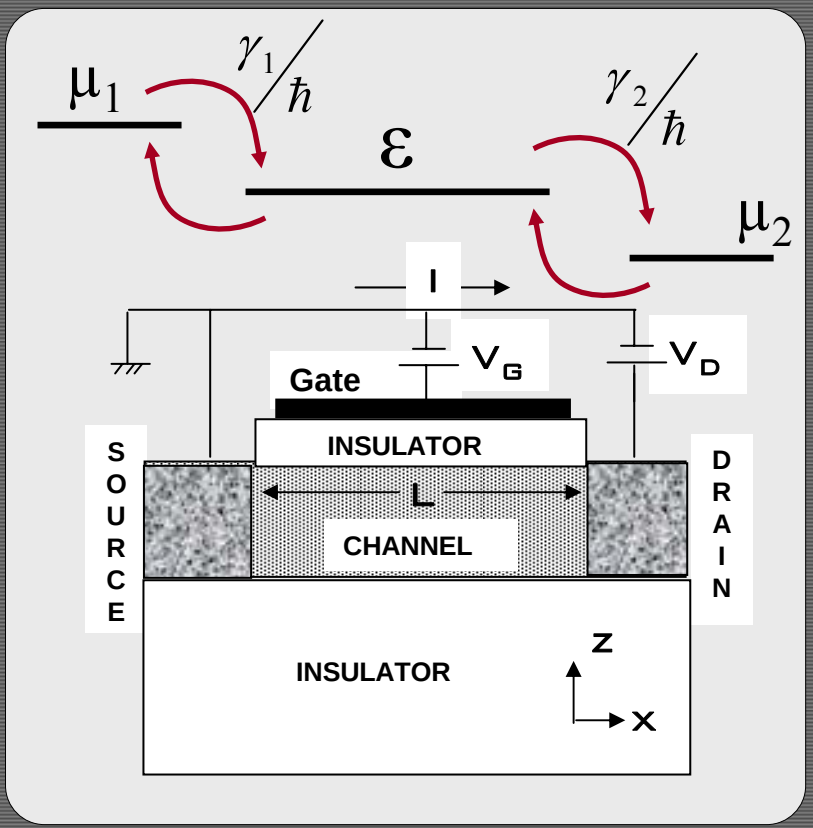
- This week we are going to derive the Hamiltonian [H] for the FET example. This matrix [H] replaces the single number ε in the toy example.

- From [H] we will show how to calculate electron density in the channel at equilibrium, that is

$$\rho = f_0(H - \mu I)$$

- Later on we will incorporate factors such as broadening and self-consistent charging as we move towards a non-equilibrium model.

FET Model



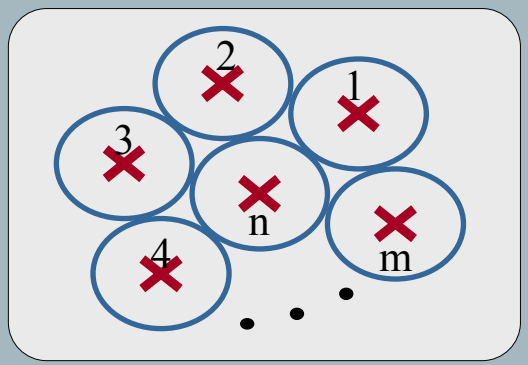
Today we start by showing how to write H for the active region of a device.

Atomistic Hamiltonian

07:01

• How can we calculate [H] for the active region of a device?

• One method, reviewed in previous lectures, is the atomistic model that can be derived from first principles. Recall, a bulk solid may be viewed as a periodic arrangement of unit cells. For common semiconductors there are two atoms in each unit cell. The N^{th} unit cell is surrounded by m unit cells:



• For the purely atomistic model our Hamiltonian will be bN X bN in size, where b is the number of basis functions per unit cell and N is the number of unit cells.

$$[H] = \begin{matrix} \\ bxN \downarrow \end{matrix} \overset{bxN \rightarrow}{\begin{bmatrix} \ddots & & \\ H_{no}\ldots & H_{nn}\ldots & H_{nm}\ldots \\ & & \ddots \end{bmatrix}}$$

• Silicon gives 2 atoms per unit cell and under the sp^3s^* model 5 basis functions per atom, for a total of 10 basis functions per unit cell. Therefore, applied to silicon the atomistic model gives a Hamiltonian of size 10Nx10N and individual H_{nm} matrices of size 10x10

Periodic Solids

• For materials having periodic structure, such as silicon, using the ansatz

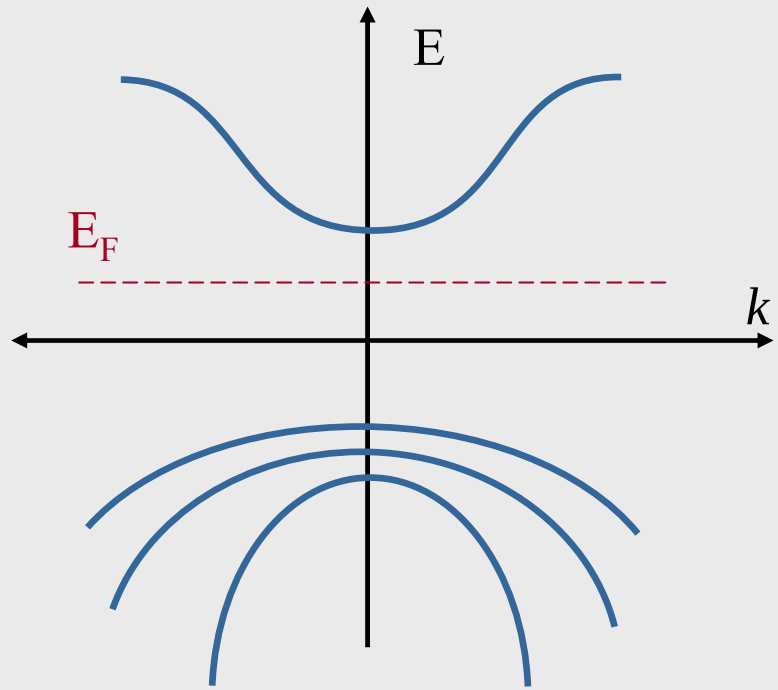
$$\{\varphi_m\} = \{\varphi_0\} e^{i\vec{k}\cdot\vec{d}_m}$$

The large atomistic Hamiltonian may be solved relatively easily

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

Resulting in the familiar $E(\vec{k})$ band diagram.

Band Structure

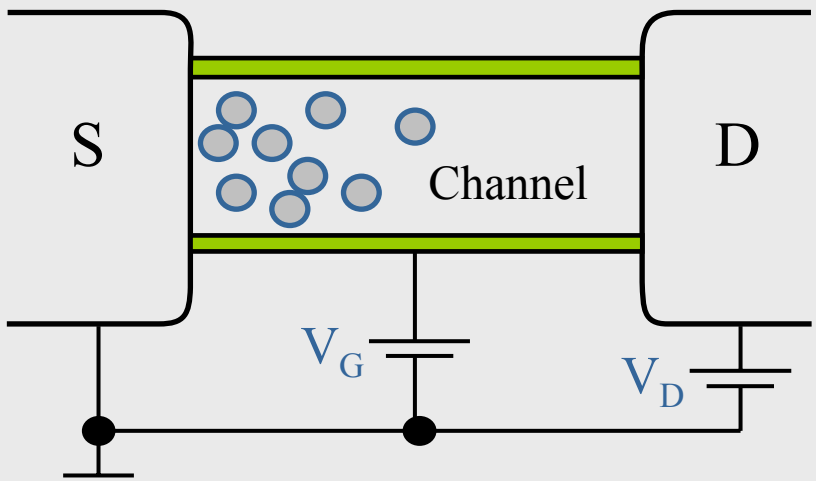


Devices

12:30

- In devices it is often not practical to use the atomistic model.
- For example, the FET shown earlier has an atomistic Hamiltonian of size 10XN, where N is the number of unit cells. Since N is huge, [H] is too large.

Unit Cells in the FET Channel

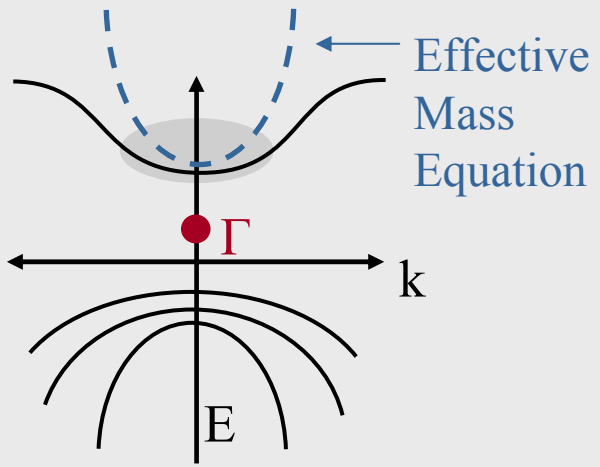


Effective Mass Equation

15:33

• A widely used alternative to atomistic Hamiltonian is the effective mass equation.
• The idea for the effective mass equation goes like this: say you have an n-type semiconductor that has the band structure like the picture. The important part for conduction and electronic properties is the shaded area so we don't worry about getting the Hamiltonian right every where but only near the bottom of conduction band.

Lowest Conduction Band Effective Mass Equation



• For now we are only interested in the lowest conduction band, and therefore concentrate on its effective mass equation, which for silicon is

$$h(\vec{k}) = E_C + \frac{\hbar^2}{2m_C}\left(k_x^2 + k_y^2 + k_z^2\right)$$

Note: isotropic nature

• This works well for bulk solids; however for inhomogeneous structures like our device, we try to use this relation to and modify in a way so as to describe the device.

Convert E(k) to a Differential Equation

• How do we handle variations of dimension and external potentials (i.e. voltage) that might be placed on a periodic bandstructure? *Ans: Convert the effective mass equation to a differential equation*

• Recall the free space Schrödinger equation

$$\frac{-\hbar^2}{2m}\nabla^2\Psi = E\Psi$$

has the solution $\Psi = \phi e^{i\vec{k}\cdot\vec{r}}$

such that $\frac{\hbar^2 k^2}{2m}\Psi = E\Psi$

• How did we get the dispersion relation E(k) from the Schrödinger equation? Basically, the following replacements were made:

$$\partial/\partial x \rightarrow ik_x \qquad \partial/\partial y \rightarrow ik_y \qquad \partial/\partial z \rightarrow ik_z$$

• We may reverse the above process to go from E(k) relation

$$h(\vec{k}) = E_C + \frac{\hbar^2}{2m_C}\left(k_x^2 + k_y^2 + k_z^2\right)$$

to a differential equation:

$$E\Psi = \left[E_C - \frac{\hbar^2}{2m_C}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\right]\Psi$$

More on the Differential Effective Mass Equation

• Conceptually, the differential effective mass equation

$$E\Psi = \left[E_C - \frac{\hbar^2}{2m_C}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \right] \Psi$$

is usually taken to be the equation which an electron obeys (for a given band) in a solid. To get the effective mass equation for different materials we simply vary E_C and m_C.

• Notice that any external potential U_{ext}, resulting, for instance, from a voltage applied across the solid, is easily incorporated into this equation and one does not have to worry about the atomic potentials which DO appear in the Schrödinger equation. (The usage of effective mass is a way to incorporate the solid's potential and structural effects on electron density)

• But what have we lost in adopting this method? Primarily that our results will only be accurate in the energy range for which the original analytical approximation fits the conduction (or valence) band of interest and now where else.

• Finally, this method is not always applied so simply. For instance, an isotropic parabolic approximation is often not sufficient for valence bands

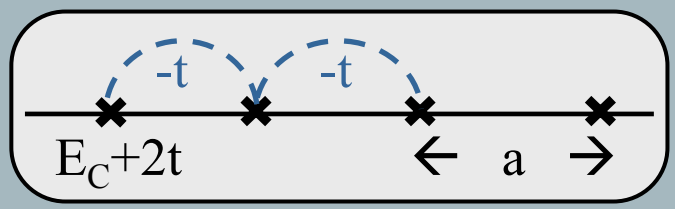
Finite Differences Applied to the Effective Mass Equation

27:30

• Method of finite differences may be applied to the effective mass equation

$$E\Psi = \left(E_C - \frac{\hbar^2}{2m_C}\nabla^2 \right)\Psi$$

• Taking a one dimensional lattice of the form



we get an effective mass equation Hamiltonian of the form…

$$[H] = \begin{bmatrix} E_C + 2t & -t & \cdots & -t \\ -t & E_C + 2t & -t & \\ \vdots & -t & E_C + 2t & \ddots \\ -t & & \ddots & \ddots \end{bmatrix}$$

and any external potential is simply incorporated as

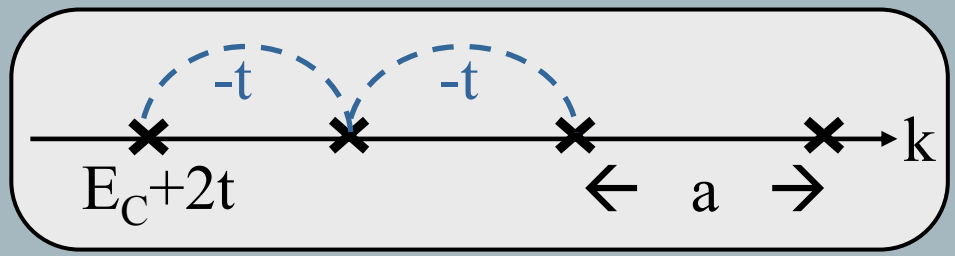
$$[H] = \begin{bmatrix} E_C+2t+U_{ext}(x_1) & -t & \cdots & -t \\ -t & E_C+2t+U_{ext}(x_2) & -t & \\ \vdots & & \ddots & \ddots \\ -t & & & \end{bmatrix}$$

Where $t = \hbar^2 / 2m_C a^2$

Visualizing Effective Mass Equation

• Essentially the effective mass equation is a way to model the behavior of conduction band electrons

• One way to look at the method of finite differences applied to the effective mass equation in 1-D…

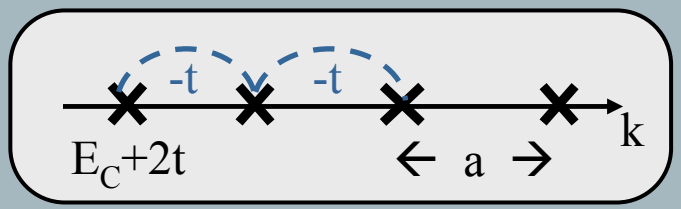


As with atoms, -t may be viewed as the site-to-site nearest neighbor coupling and E_C+2t as the site self-coupling

• There are two main advantages which this method has over the atomistic approach. First, the Hamiltonian matrix tends to be much smaller. Second, the lattice spacing need not be atomistic, though it can be, and only depends upon the energy range over which accuracy is desired.

Dispersion Relation

• What is the dispersion relation for a lattice with the 1-D spacing?



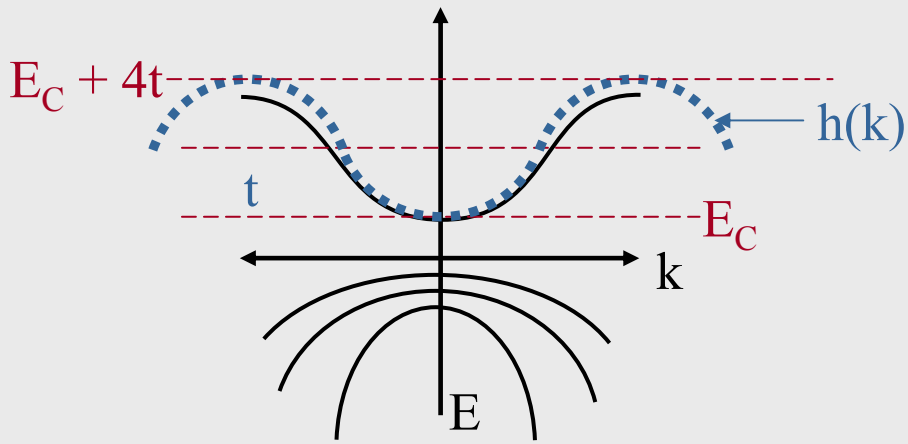
• From the Hamiltonian matrix developed earlier we know that the eigenvalues are given by

$$h(k) = E_C + 2t - te^{ika} - te^{-ika}$$

$$= E_C + 2t(1 - \cos ka)$$

Observing the above equation it is apparent that the accuracy which with the "cosine" wave fits the original bandstructure depends heavily on the spacing of "a"

Conduction Band Dispersion Fit



• Generally, a dispersion fit tends only to be accurate for a range "t" above E_C. Notice that $t = \hbar^2 / 2 m_C a^2$

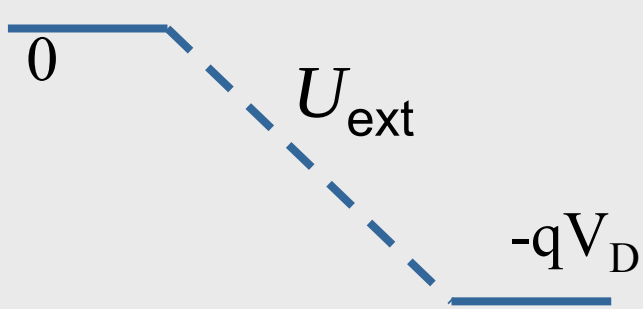
• This means that for a given energy range we can use a larger 'a' if the effective mass m_C is small.

Overall Message

- The bandstructure E(k) applies to uniform solids.
- Often devices are not uniform, in the simplest case due to an applied voltage, and so the bandstructure cannot be used directly.
- How do we get around this problem?
- For the conduction band we create the “effective mass equation” which gives the correct E(k) relation in the energy range of interest for a periodic solid.

- The effective mass equation is converted into a differential equation or a difference equation, using the method of finite differences. External potentials such as an applied voltage or impurity atom may then be easily added to the Hamiltonian

Applied External Bias



Valence Band

• One last comment:
The effective mass equation is easily applied to the conduction band, what about the valence band? It turns out that, because the levels are so closely spaced, modeling in the valence band is in fact much more difficult. When looking at the E-k relationship it turns out to not be parabolic but rather something like

$$E(\vec{k}) = \cdots + \sqrt{k_y^2 k_z^2 + k_x^2 k_z^2 + \ldots}$$

which is not easily converted into a differential equation. This is largely because multiple bands are all mixed up together (light hole, heavy hole, split off).

• Instead of a simple parabola the eigen-energies are usually approximated by a 4x4 or 6x6 matrix of the form

$$\left[h(\vec{k})\right] = \begin{bmatrix} P+Q & 0 & -S & \cdots \\ 0 & P+Q & R^+ & \\ \vdots & & & \ddots \end{bmatrix}$$

where P,Q,R,S are functions of $\vec{k}$ such that the matrix may be solved by the method of finite differences replacing

$$k_x \rightarrow -i\partial/\partial x \quad k_y \rightarrow -i\partial/\partial y \quad k_z \rightarrow -i\partial/\partial z$$

We use a 4x4 matrix for the 4-band model and a 6x6 for the 6-band model. We'll get more into this later when talking about optical properties. For now focus on the conduction band.