Fundamentals of Nanoelectronics

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ECE 453
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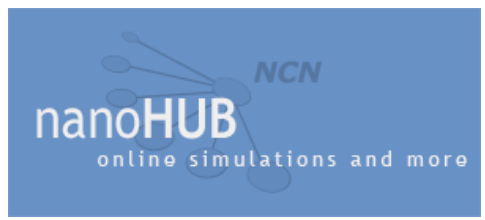
Lecture 29: Effective Mass Equation

Ref. Chapter 7.1

Network for Computational Nanotechnology



Overview

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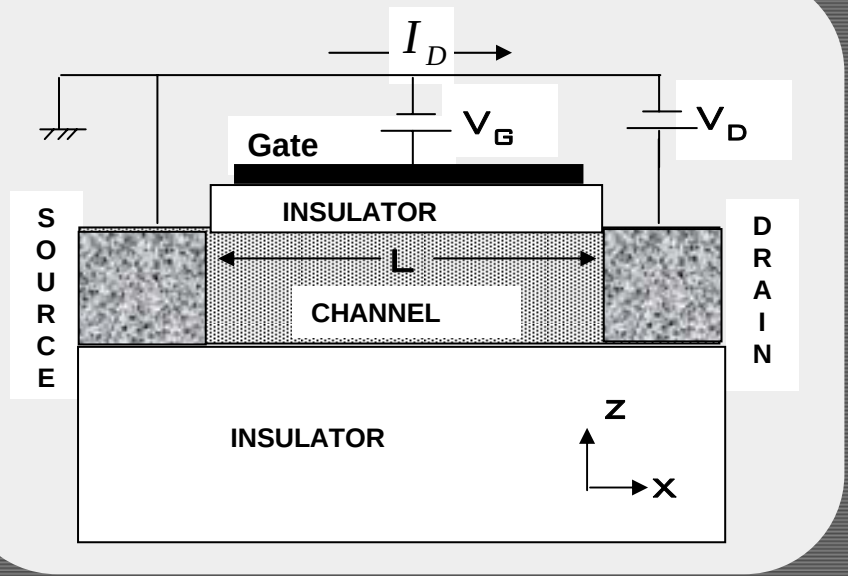
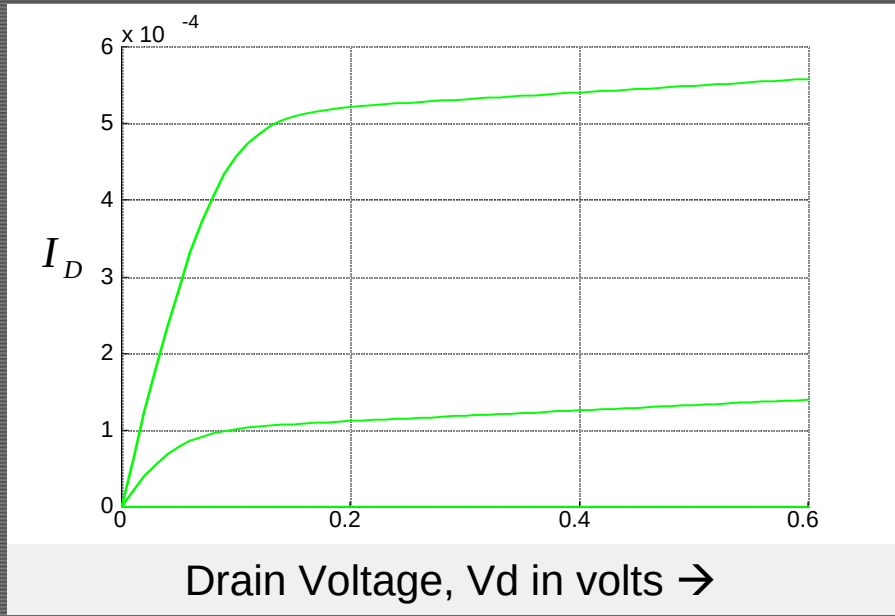
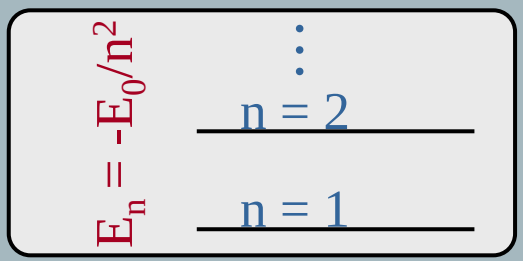




• To understand how well a transistor conductance, we need to have a knowledge about the energy levels of the channel and their relative positioning with respect to the Fermi level.

Atoms

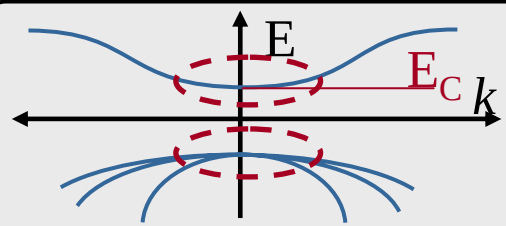


Nano Structures

Bottom Up

Top Down

Solids



Parabolic Approximation Effective Mass Equation

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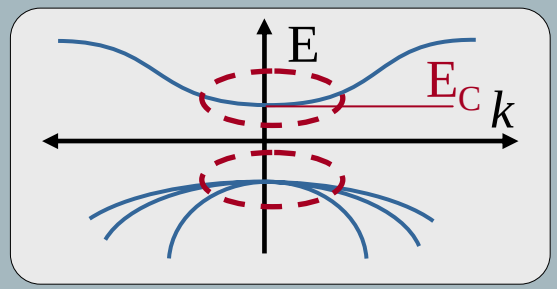


• Considering the energy range close to the bottom of conduction band we can approximate the band as a parabola:

$$E = E_c + \frac{\hbar^2 k^2}{2m_c}$$

• Notice that the starting point for Schrödinger equation is:

0: Vacuum

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

• Where

$$\psi = \psi_0 e^{i\vec{k}\cdot\vec{r}} = \psi_0 e^{ik_x x} e^{ik_y y} e^{ik_z z}$$

• Given that:

$$E = U_0 + \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{\hbar^2 k^2}{2m} + U_0$$

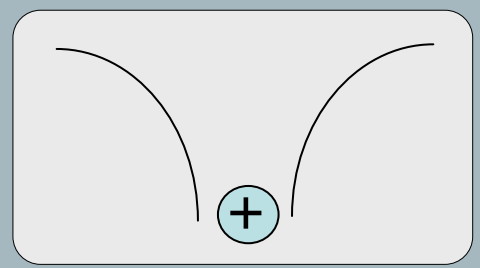
• For an electron in the conduction band in the indicated energy range we can start from a Schrödinger equation of the from:

$$\left[E_c - \frac{\hbar^2}{2m_c}\nabla^2 \right]\psi = E\psi$$

• Whereas the real problem would be a lot harder: $\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) \right]\psi = E\psi$

• Potential due to an impurity:

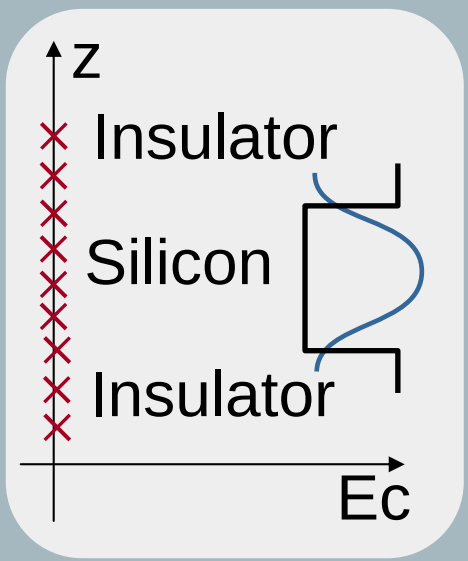
$$E_{1s} \propto -\frac{m}{\varepsilon_0^2}$$



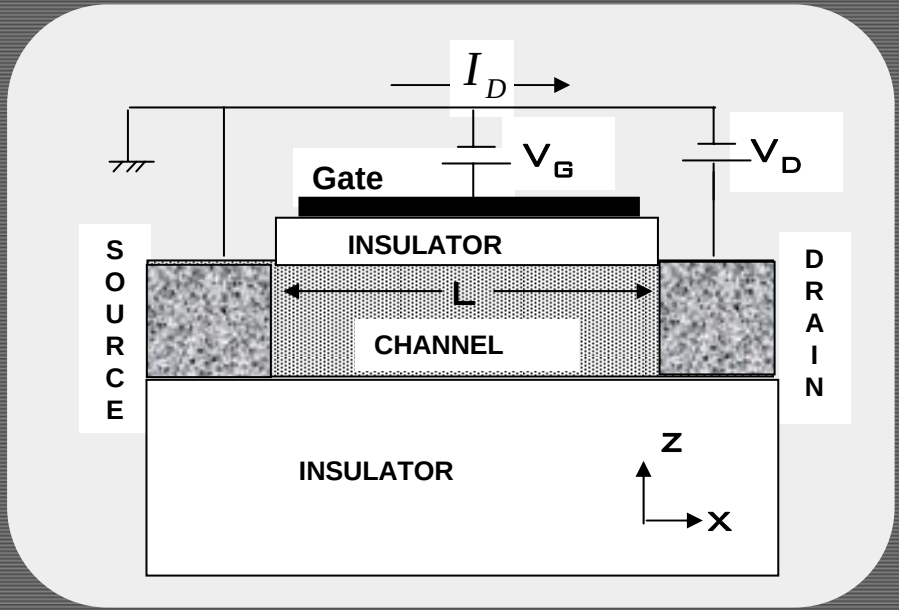
Effective Mass Equation

• To describe the energy levels, we can use the effective mass equation with a position dependent Ec.

$$\left[E_c(z) - \frac{\hbar^2}{2m_c} \nabla^2 \right] \psi = E\psi$$

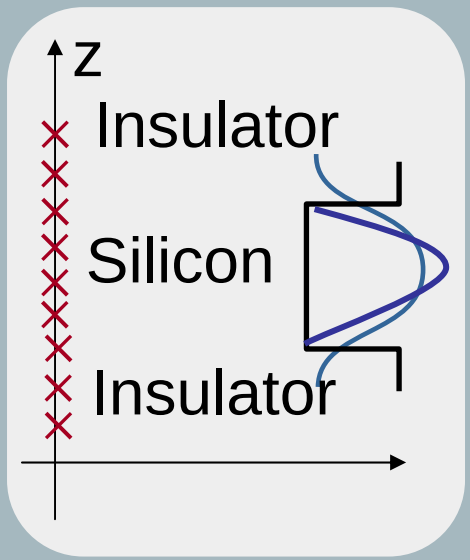


• Next step is to solve this equation…



Solution of Effective Mass Equation

- In 1D:



$$\left[E_C(z) - \frac{\hbar^2}{2m_C}\frac{d^2}{dz^2}\right]\Psi = E\Psi \qquad t_0 \equiv \frac{\hbar^2}{2m_c a^2}$$

$$\begin{bmatrix} 2t_0 + E_c(z_1) & -t_0 & \cdots & \cdots & \cdots & -t_0 \\ -t_0 & 2t_0 + E_c(z_2) & \cdots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & & & \vdots \\ \vdots & \vdots & & \ddots & & \vdots \\ \vdots & \vdots & & & \ddots & -t_0 \\ -t_0 & \cdots & \cdots & \cdots & -t_0 & 2t_0 + E_c(z_N) \end{bmatrix} \{\Psi\} = E\{\Psi\}$$

- To account for x and y direction rewrite Schrödinger equation including x and y:

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

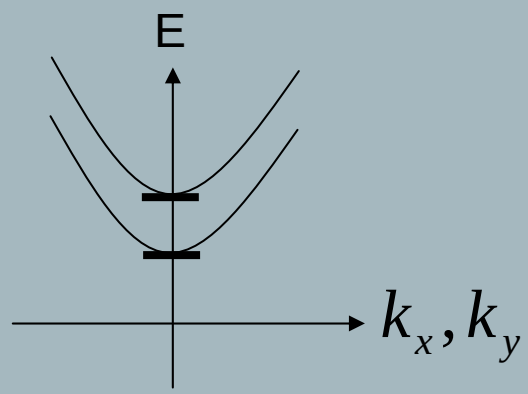
- As long as Ec doesn't vary in x and y:

$$\Phi = \Psi(z)e^{ik_x x}e^{ik_y y} \Rightarrow$$

$$\left[E_C(z) - \frac{\hbar^2}{2m_C}\frac{d^2}{dz^2} + \frac{\hbar^2\left(k_x^2 + k_y^2\right)}{2m_C}\right]\Psi = E\Psi$$

Energy Levels

- We can write energy levels as:

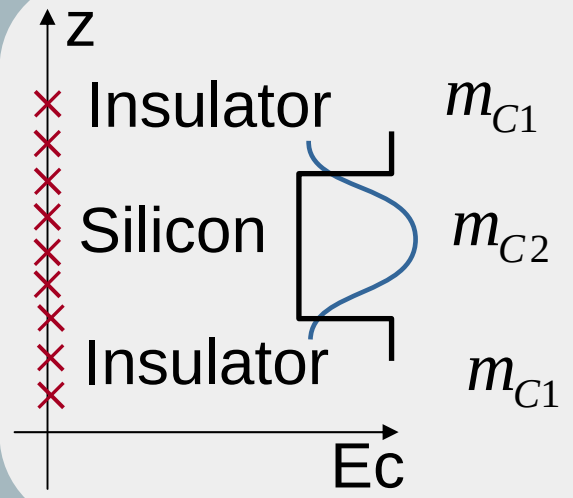


$$E = 1D\,\text{Solution} + \frac{\hbar^2\left(k_x^2 + k_y^2\right)}{2m_C}$$

Variation of Effective Mass

• If the effective mass changes as a function of position, Then:

$$H=\begin{bmatrix} 2t_1+E_c(z_1) & -t_2 & \cdots & \cdots & \cdots & \\ -t_1 & t_1+t_2+E_c(z_2) & -t_2 & \cdots & \cdots & \vdots \\ \vdots & -t_2 & & & & \vdots \\ \vdots & \vdots & & \ddots & & \vdots \\ \vdots & \vdots & & & \ddots & -t_1 \\ & \cdots & \cdots & \cdots & -t_1 & 2t_0+E_c(z_N) \end{bmatrix}$$



• Where t1 and t2 is defined based on he proper effective mass:

$$t_1 \equiv \frac{\hbar^2}{2m_{c1}a^2} \qquad t_1 \equiv \frac{\hbar^2}{2m_{c2}a^2}$$

• The correct form of the differential equation that will lead to the correct answer written above is:

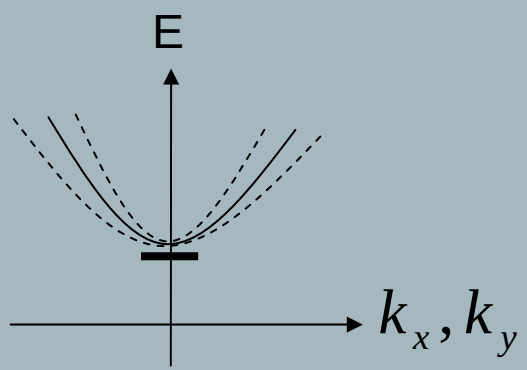
$$\left[E_C(z)-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_C(z)}\frac{d}{dz}\right)\right]\Psi=E\Psi$$

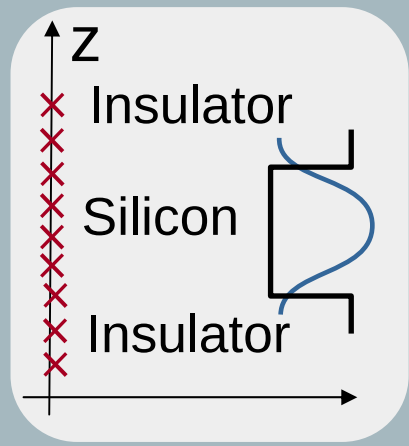
Variation of Effective Mass

• Consider the old equation:

$$E\Psi = \left[E_C(z) - \frac{\hbar^2}{2m_C}\frac{d^2}{dz^2} - \frac{\hbar^2\left(k_x^2 + k_y^2\right)}{2m_C} \right]\Psi$$

• Effective mass appears in 2 places. If it is position dependent, the both terms involving it will be position dependent. So the Schrödinger equation has to be solved once for each value of k. We will not have the simple parabolic form any more.





• There will be 2 curves surrounding the old parabola based on the mass of Si and SiO2. The real curve is something between the two. What determines how close the real curve is to each one is the confinement of the wave function. If it is completely confined in the Si region, then the curve will have effective mass of Si. As wavefunction leaks out more and more the contribution of the oxide curve increases.