Quantum Transport:
Atom to Transistor

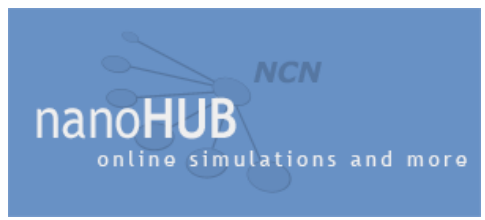
Prof. Supriyo Datta
ECE 659
Purdue University

03.24.2004

Lecture 24: Electron Density

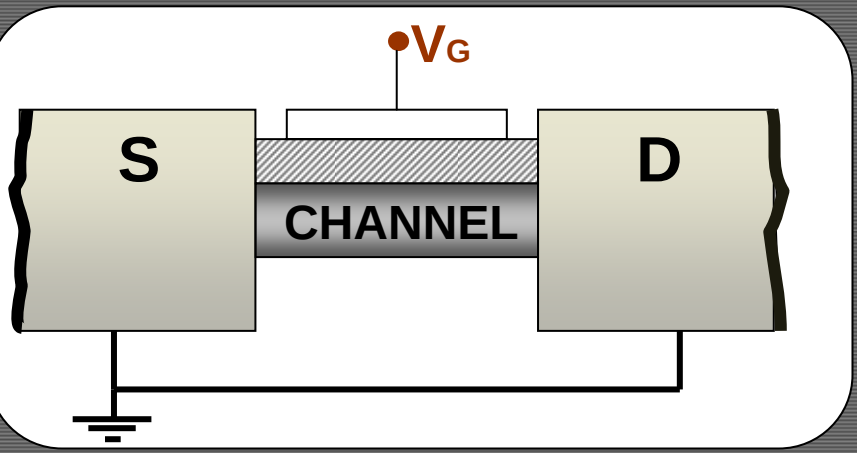
Ref. Chapter 7.2

Network for Computational Nanotechnology



Self Consistent Solution

00:00



• The objective is to calculate the electron density as a function of gate voltage.

• Quantum Mechanical way at equilibrium: $\rho = f_0(H - \mu I)$

• Effective mass Hamiltonian for this device:

$$\begin{bmatrix} E_c + 2t & -t & & \\ -t & E_c + 2t & -t & \\ & -t & \ddots & \\ & & & \end{bmatrix}_{n*n}$$

• To get the complete picture, this has to be solved self consistently with Poisson equation because the surrounding imposes a potential and that has to be included.

$$H = H_0 + U$$

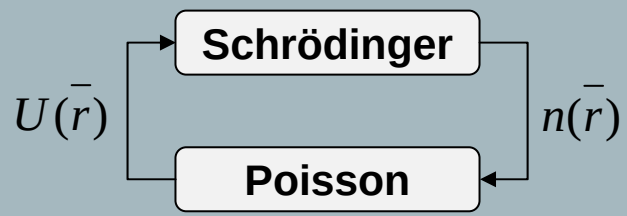
$$\nabla^2 \cdot V = -\frac{\rho}{\varepsilon}$$ Electromagnetic Texts

U = - qV

$$-\nabla^2 \cdot U = q^2 \frac{n}{\varepsilon}$$ Our Form

• Allowing variation of dielectric constant, $-\vec{\nabla} \cdot (\varepsilon \vec{\nabla} U) = q^2 n$

• Self Consistent Solution

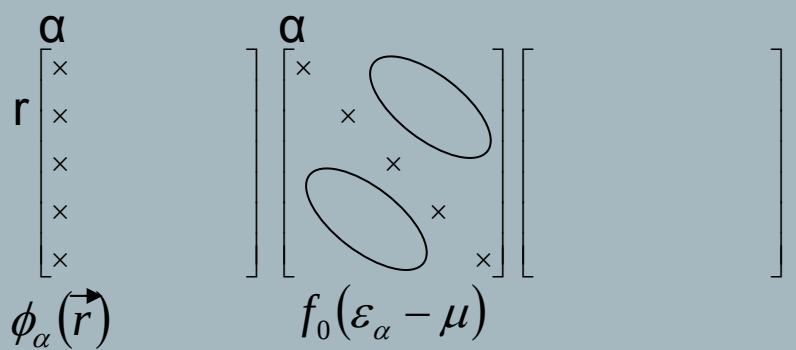


Electron Density Homogeneous Solid

09:30

• Given a particular H, we want to find the electron density matrix whose diagonal elements are electron densities at different points.

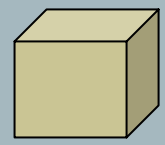
$$\rho = f_0(H - \mu I) \Rightarrow$$



$$\Rightarrow \rho(r,r') = \sum_\alpha \phi_\alpha(r)\phi_\alpha^*(r') f_0(\varepsilon_\alpha - \mu)$$

$$n(r) = \sum_\alpha |\phi_\alpha(\vec{r})|^2 f_0(\varepsilon_\alpha - \mu)$$

• <u>Electron density in a homogeneous material</u>



Homogeneous Silicon

$$\left(E_c - \frac{\hbar^2}{2m_c}\nabla^2\right)\psi_\alpha = \varepsilon_\alpha \psi_\alpha$$

• Note that for differential equations with constant coefficients, solutions can be written as plane waves.

• Solution

$$\psi_k(\vec{r}) = \frac{e^{ikx}\, e^{iky}\, e^{ikz}}{\sqrt{L_x L_y L_z}}$$

$$n(r) = \sum_{k_x k_y k_z} \frac{1}{L_x L_y L_z} f_0(\varepsilon_k - \mu)$$

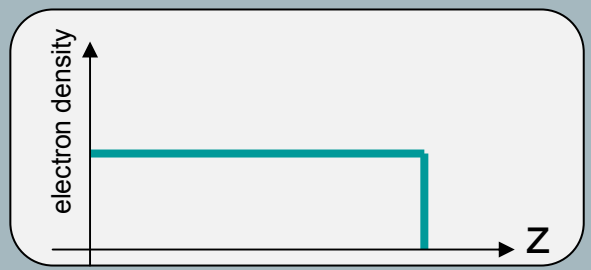
• What this tells us is that for a homogeneous solid the electron density is position invariant.

Boundary Conditions Inhomogeneous Device

18:00

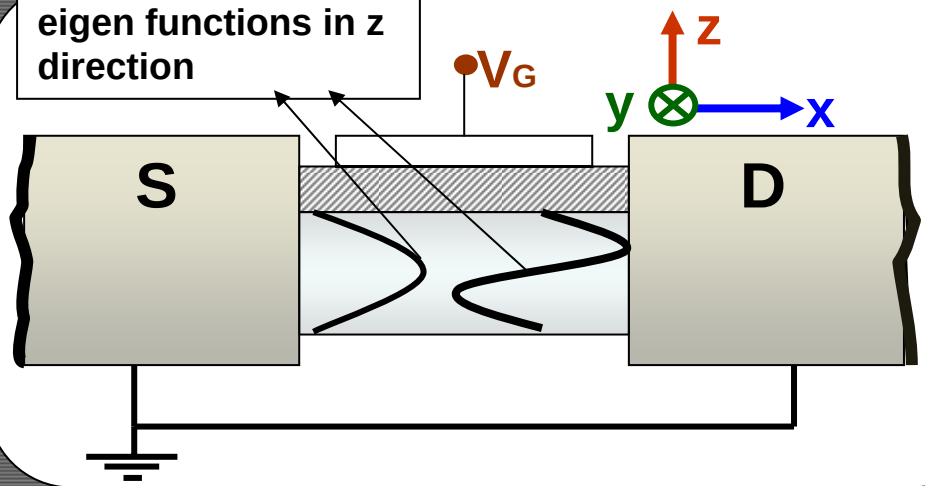
• Periodic versus box boundary conditions:

• n(r) for box boundary conditions:



• n(r) for periodic boundary conditions:

First and second eigen functions in z direction



• We'll assume x and y dimensions to be infinite and use periodic boundary conditions for them. How ever we want to treat z more carefully.

• Eigen Functions:

$$\psi_k(r) = \frac{e^{ikx}e^{iky}}{\sqrt{L_x L_y}}\phi_m(z)$$

Inhomogeneous Eigen Functions

- We want to find eigen functions in z direction, $\left[E_c - \frac{\hbar^2}{2m_c}\frac{d^2}{dz^2} + U(z)\right]\phi_\alpha(z) = E\phi_\alpha(z)$
- The plane waves in x and y direction satisfy the following:

$$\left(-\frac{\hbar^2}{2m_c}\frac{d^2}{dx^2}\right)e^{ik_x x} = \frac{\hbar^2 k_x^2}{2m_c}e^{ik_x x}$$

- Replace x with y to get the expression for y.
- Remember we are assuming that the potential is separable in x, y and z and therefore Schrödinger equation can be broken into three coordinates.
- For homogenous material we had:

$$n(r) = \sum_\alpha \frac{1}{L_x L_y L_z} f_0(\varepsilon_\alpha - \mu)$$

- For our device,

$$n(r) = \sum_{k_x k_y m} \frac{1}{L_x L_y} |\phi_m(z)|^2 f_0\left(\varepsilon_m + \varepsilon_{\vec{k}_t} - \mu\right)$$

In this case summing the Fermi functions over the two dimensions of x and y can be done analytically.

- **Schrödinger**

$$\left[E_c - \frac{\hbar^2}{2m_c}\frac{d^2}{dz^2} + U(z)\right]\phi_m(z) = \varepsilon_m\phi_m(z)$$

$$n(z) = \sum_m |\phi_m(z)|^2 f_{2D}(\varepsilon_m - \mu)$$

- **Poisson**

$$-\frac{d}{dz}\cdot\left(\varepsilon\frac{d}{dz}U\right) = q^2 n$$

Potential Change due to Changes in V_G

- Schrödinger

$$\psi_0 = 0$$

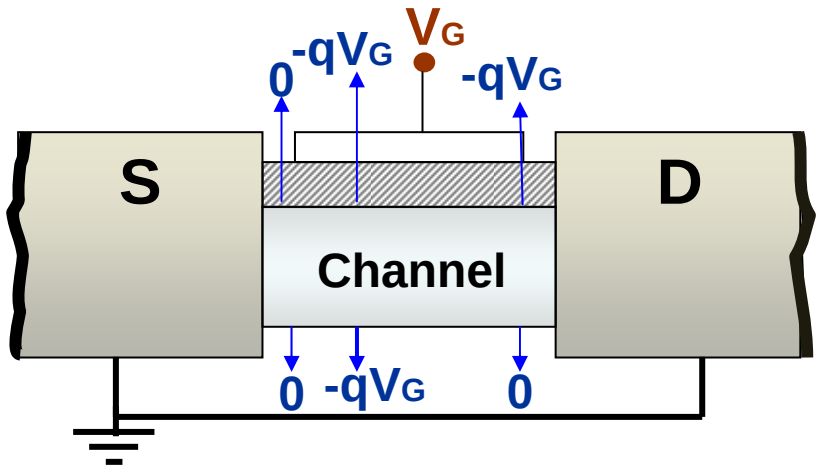
$$E\{\psi\} = \begin{pmatrix} E_c+2t & -t \\ -t & E_c+2t \end{pmatrix}\{\psi\}$$

- Poisson

$$\otimes \begin{pmatrix} & U_0 & \\ & & \\ & & \end{pmatrix}\{U\} = \{n\} + \begin{Bmatrix} \times \\ \\ \times \end{Bmatrix}$$

- What we are after is to monitor the electron density as the gate voltage changes. But how can we see the effect of these changes in our equations?
- Answer: **The additional term (boundary term of the Poisson equation),** which depends on V_G .

Different possible boundary conditions



- Next day we will discuss the physics behind this. i.e. when you change the gate voltage what determines the rate at which electron density changes. We will also discuss the quantum capacitance which is a very important physical concept.

Electron Density Inhomogeneous Device

41:50

- Now we want to talk about the function: f_{2D}

$$n(r) = \sum_{k_x k_y m} \frac{1}{L_x L_y} \left|\phi_m(z)\right|^2 f_0\left(\varepsilon_m + \varepsilon_{\vec{k}t} - \mu\right)$$

- We want to evaluate this summation:

$$\frac{1}{L_x L_y} \sum_{k_t} \frac{1}{1 + \exp\left(\frac{\varepsilon_m - \mu + \varepsilon_{k_t}}{k_B T}\right)}$$

Where $\left(\varepsilon_{k_t} = \frac{\hbar^2}{2m_c}\left(k_t^2\right)\right)$

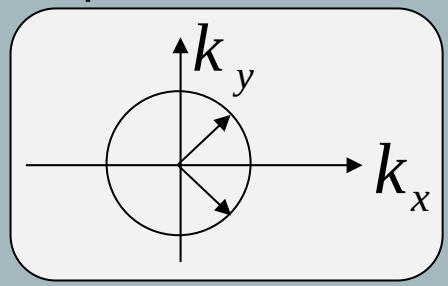
- For big devices, we convert to integral,

$$\int \frac{dk_x k_y}{4\pi^2} \frac{1}{1 + Ae^X}$$

- Where

$$A \equiv \exp\left(\frac{\varepsilon_m - \mu}{k_B T}\right) \qquad X \equiv \frac{\hbar^2 k_t^2}{2m_c k_b T}$$

- Since the integrand does not depend on the angle of $\vec{k}$, but only its magnitude, we can do the integral in spherical coordinates.



- Then,

$$\int \frac{\overbrace{2\pi k_t dk_t}^{dX}}{4\pi^2} \frac{1}{1 + Ae^X}$$

Electron Density as a Function of V_G

48:07

$$A \equiv \exp\left(\frac{\varepsilon_m - \mu}{k_B T}\right) \quad X \equiv \frac{\hbar^2 k_t^2}{2 m_c k_B T}$$

- **Details of integration:**

$$\int_0^\infty \frac{2\pi k_t \, dk_t}{4\pi^2} \frac{1}{1 + Ae^X}$$

$$= \frac{m_c k_B T}{2\pi\hbar^2} \int_0^\infty \frac{dX}{1 + Ae^X}$$

$$= \frac{m_c k_B T}{2\pi\hbar^2} \left\{ \ln\left[A + e^{-X}\right] \right\}_\infty^0$$

$$= \frac{m_c k_B T}{2\pi\hbar^2} \ln\left[1 + e^{-E/k_B T}\right]$$

$$f_{2D}(E) = \frac{m_c k_B T}{2\pi\hbar^2} \left\{ \ln\left[1 + e^{-E/k_B T}\right] \right\}$$

$$E = \varepsilon_m - k_B T$$

- Similar integral comes up in the case of a homogenous material and we have to sum over a three dimensional k vector.

$$n(r) = \sum_{k_x k_y k_z} \frac{1}{L_x L_y L_z} f_0(\varepsilon_k - \mu)$$

How ever in this case the integral doesn't come out to be as simple and it cannot be done analytically. It can be tabulated and found numerically.

- For the integrand in three dimensions, instead of kdk, you'll have k^2 dk and after the change of variable, we end up with $dx\sqrt{x}$ which can't be solved analytically. This is tabulated and is called "f half" integral.
- In one dimensional case we end up with $dx\sqrt{x}$ which is called "f minus half" integral. *It is worth remembering the important result of how to do the summation over the Fermi function analytically.*