

ECE 495N

**Fundamentals of
Nanoelectronics**

Fall 2008

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**Lecture: 7
Title: Quantum Capacitance/
Schrödinger's Equation
Date: September 10, 2008**

**Video Lectures posted at:
<https://www.nanohub.org/resources/5346/>**

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Quantum Capacitance / Schrödinger Equation Lecture 7

Sept. 10, 2008

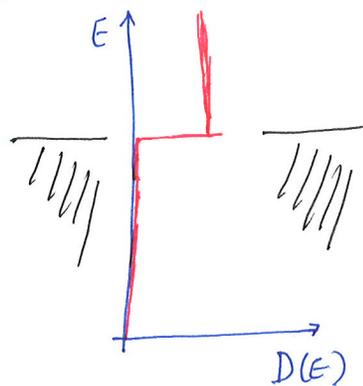
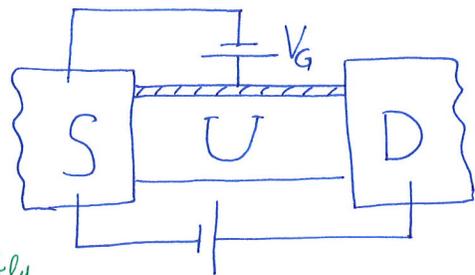
$$I = \frac{q}{h} \int dE \cdot D(E-U) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2)$$

$$N = \int dE \cdot D(E-U) \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

we have to solve them self-consistently

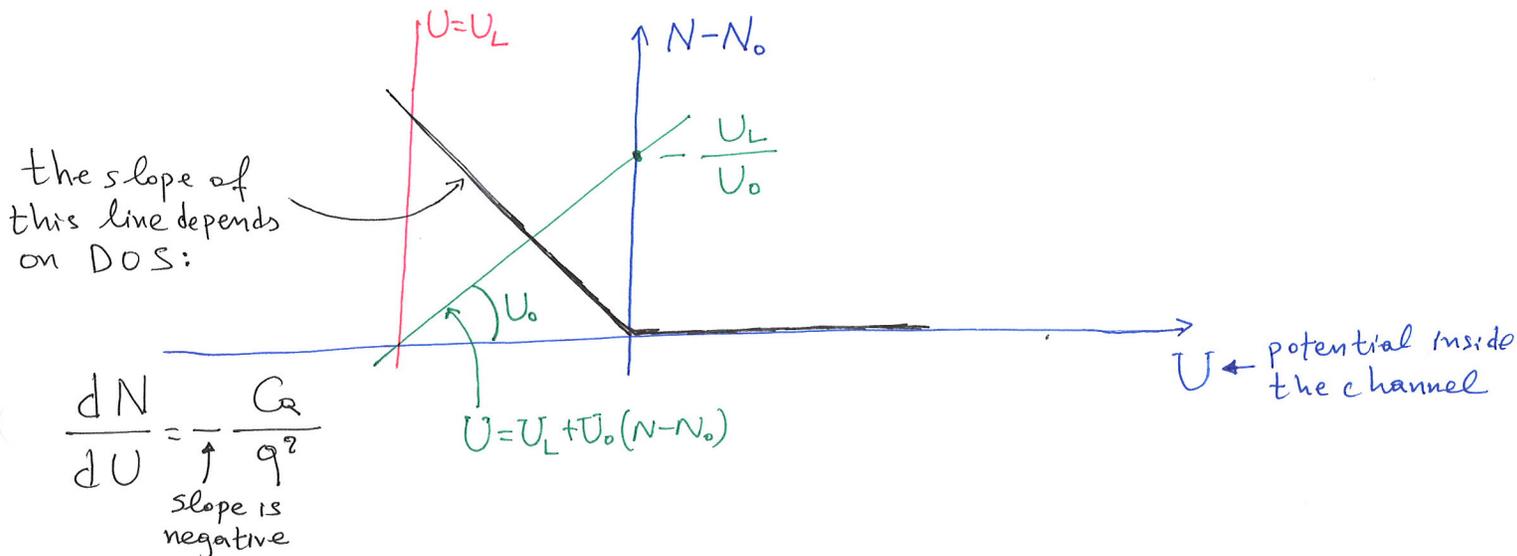
$$U = U_L + U_0 (N - N_0)$$

($\nabla^2 U_L = 0$ plus [boundary conditions] $V_g = 1, V_s = 0, V_D = \dots$)



N depends on U . U is the potential energy inside the channel. The question is if we apply $V_g = 1$ how much the potential energy inside the channel will change? The first term of that is U_L , which ideally means that the energy will change be 1eV

Positive Voltage (V_g) \Rightarrow lower U



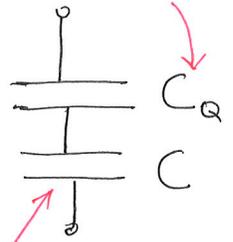
$$\frac{dU}{dU_L} = 1 + U_0 \frac{dN}{dU_L} = 1 + U_0 \frac{dN}{dU} \cdot \frac{dU}{dU_L}$$

$$\Rightarrow \frac{dU}{dU_L} = \frac{1}{1 - U_0 \frac{dN}{dU}} = \frac{1}{1 + U_0 \frac{C_a}{q^2}} = \frac{1}{1 + \frac{q^2}{C}}$$

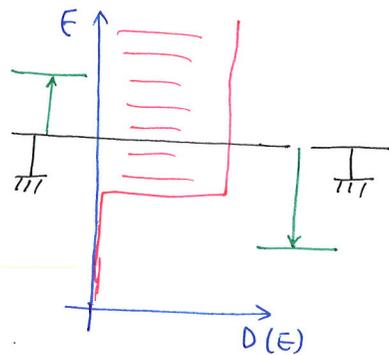
Hence, $\frac{dU}{dU_L} = \frac{1}{1 + \frac{C_a}{C}} = \frac{C}{C + C_a}$

Finally $\frac{dN}{dU_L} = \frac{dN}{dU} \cdot \frac{dU}{dU_L} \sim C_a \frac{C}{C + C_a}$

It is related to the density of states



It comes from electron-electron interaction.



add the same constant to all	equivalent $\left\{ \begin{array}{l} +0.5 \\ 0 \end{array} \right.$	0	-0.5	not equivalent $\left\{ \begin{array}{l} -1 \\ -1 \end{array} \right.$
	0	-0.5	-1	
	0	0	-1	

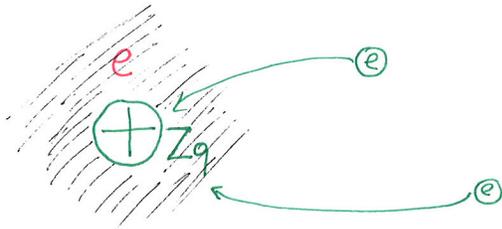
Schrödinger Equation

Electrons inside the atoms have ~~discrete~~ discrete energy levels:

$$\frac{E_0}{n^2}$$

$$h\nu = E_0 \left(\frac{1}{n^2} - \frac{1}{m^2} \right)$$

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + U(r)\Psi$$



$$\frac{\sum q^2}{4\pi\epsilon r}$$

How to solve this equation?

- Analytically (only for hydrogen atom, by Schrödinger)
- Numerically (for all the other atoms.)

* One dimensional version of this equation (1-D Schrödinger) is:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

Solution: $\Psi = A e^{-iEt/\hbar} e^{ikx}$

$$i\hbar \cdot \frac{-iE}{\hbar} \cdot \cancel{\Psi} = -\frac{\hbar^2}{2m} (ik)^2 \cdot \cancel{\Psi} \Rightarrow E = \frac{\hbar^2 k^2}{2m}$$

this is called dispersion relationship

* 2-D Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial y^2}$$

as long as we have constant coefficient we can write the solution as ~~product~~ ^{product} of exponentials: (the 'k' is different)

$$\Psi = e^{-iEt/\hbar} e^{ik_x x} \cdot e^{ik_y y}$$

Setting the solution back:

$$E \Psi = \frac{\hbar^2 k_x^2}{2m} \Psi + \frac{\hbar^2 k_y^2}{2m} \Psi$$

$$\Rightarrow E = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m}$$

* If the coefficients depend on time and/or space then we cannot apply this approach

* If the coefficients depend only on space and not on time then: the Schrödinger Equation's ^{solution} can be written as:

$$\Psi(r, t) = \Phi(r) e^{-iEt/\hbar}$$

Setting the solution back to S.E.:

$$e^{-iEt/\hbar} \left[E \Phi(r) = -\frac{\hbar^2}{2m} \nabla^2 \Phi + U(r) \Phi(r) \right]$$

$$\Rightarrow E \Phi(r) = -\frac{\hbar^2}{2m} \nabla^2 \Phi + U(r) \Phi(r)$$

← Time independent Schrödinger Equation

This is the equation that Schrödinger solved for H atom using $U(r) = -\frac{Zq^2}{4\pi\epsilon_0 r}$. This equation gives non-zero (trivial) solutions

only if energy E is taking ~~some~~ certain values, which are called eigenvalues and are solution of this equation given by $E = \frac{-E_0}{n^2} \rightarrow 13.6 \text{ eV}$