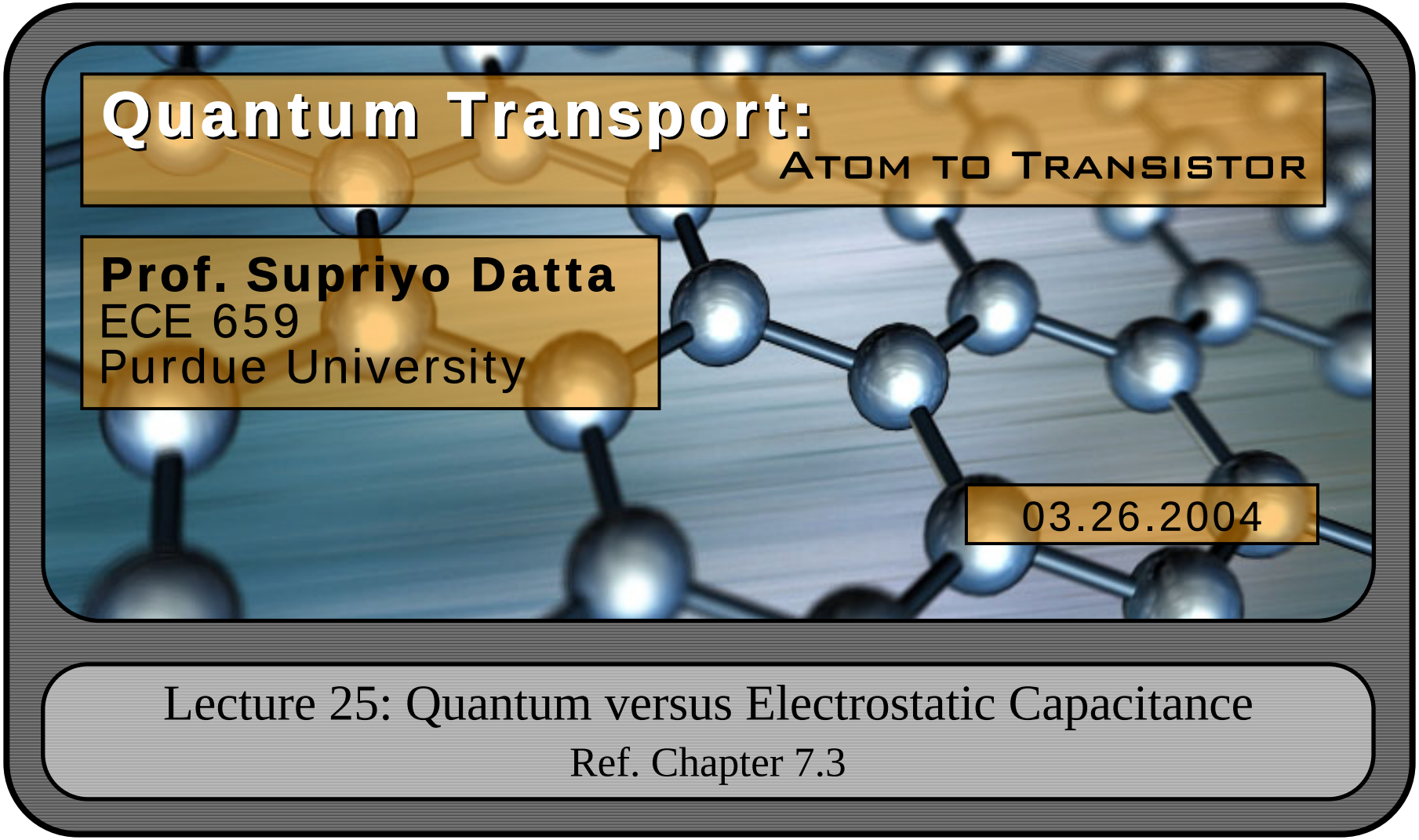


Quantum Transport:
Atom to Transistor

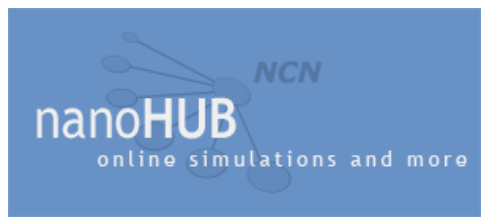
Prof. Supriyo Datta
ECE 659
Purdue University

03.26.2004

Lecture 25: Quantum versus Electrostatic Capacitance

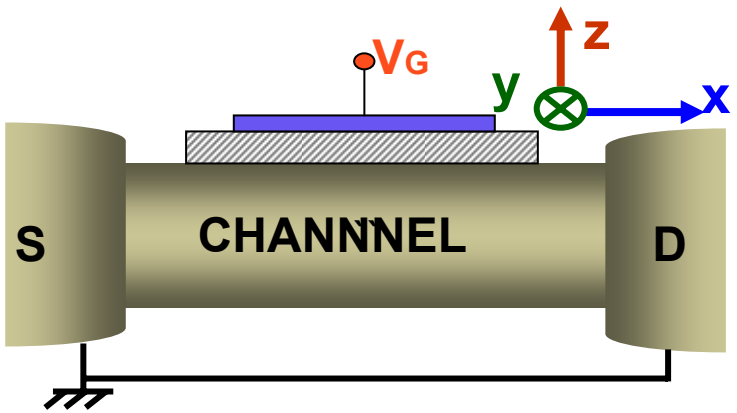
Ref. Chapter 7.3

Network for Computational Nanotechnology



Schrödinger / Poisson

00:00



• System at equilibrium: source and drain shorted together.
• Last day we discussed how electron density changes as a response to a certain gate potential. Today we'll discuss the physics behind this.
• The usual procedure is to use the Schrödinger / Poisson solver.

• Assuming the x and y directions to be infinite; hence getting the periodic boundary conditions and solving the 1D problem we derived at:

• **Schrödinger**

$$n(z) = \sum_m \underbrace{|\phi_m(z)|^2}_{[/m]} \underbrace{f_{2D}(\varepsilon_m - \mu)}_{[/m]^2}$$

• Solving the Schrödinger equation for x and y results in plane wave solutions. The main effect of the x, y part appears in the f2D function in the above equation.

• From previous day we have:

$$f_{2D} = \frac{1}{A} \sum_{\vec{k}} f_0\left(\varepsilon_{\vec{k}} - \mu\right)$$

• **Poisson**

$$-\frac{d}{dz}\left(\varepsilon_r \frac{dU}{dZ}\right) = \frac{q^2 n(z)}{\varepsilon_0}$$

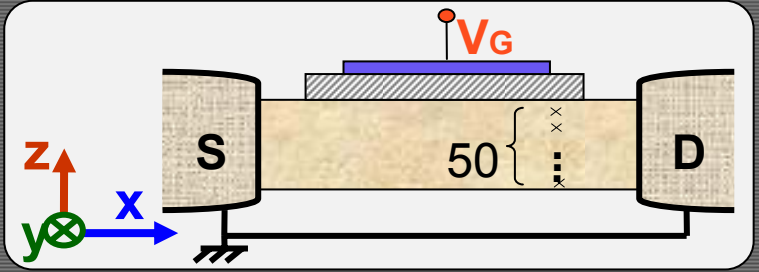
Self Consistent Solution

09:10

• Hamiltonian in the Schrödinger equation

$\underbrace{H_0}$ + $\underbrace{U(z)}$

Describes the channel and the insulator — From Poisson



• **Self Consistent Solution**

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

$$-\frac{d}{dz}\left(\varepsilon_r \frac{dU}{dZ}\right) = \frac{q^2 n(z)}{\varepsilon_0}$$

• To solve this problem numerically we set up a lattice. For instance you can have 50 lattice points across the device in the z direction which would give you a 50*50 Hamiltonian matrix.

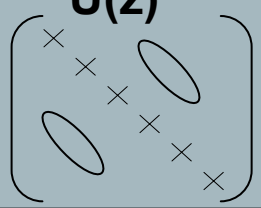
• Same goes for U(z); namely we will have a 50*50 diagonal matrix whose diagonal elements give us the potential at different lattice points.

• Notice that U(z) is purely diagonal while the Hamiltonian is not because it does include the interaction of lattice points with their nearest neighbors. These interactions are represented by off-diagonal terms.

H0

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

U(z)

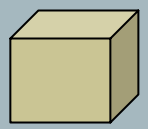


Poisson / Boltzmann

14:40

• For the purpose of comparison it is useful to do a semi-classical calculation because standard device solvers (Poisson / Boltzman solvers) use this method.

Poisson/ Boltzman Solver



Uniform Silicon in 3D

For n we have: $n = f_{3D}(E_c - \mu)$

• E_c is the bottom of conduction band and in the presence of a **constant** potential, it will float up.

---------- $E_c + U$

———— E_c

Then: $n = f_{3D}(E_c + U - \mu)$

• The semi-classical approximation goes like this: if the potential is varying with position (in our case in the z direction) then n also is changing with position. Therefore, $n(z) = f_{3D}(E_c + U(z) - \mu)$

One might miss the quantum effects but for thick devices this method gives a good approximation.

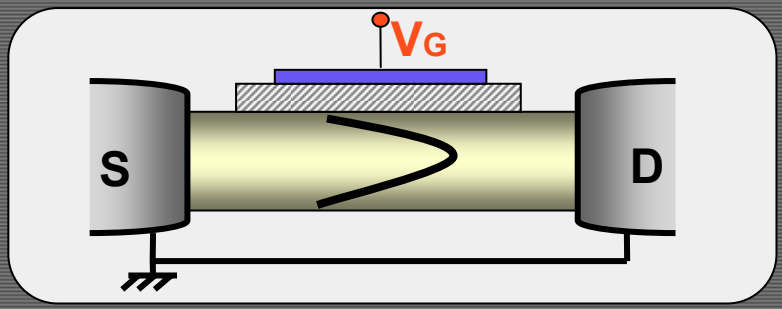
• For very small devices, the difference between the quantum mechanical solution and the semi-classical approach becomes more distinct. One can compare the two methods by investigating the resulting electron density form each solution.

• On the next page we will look at this crucial difference.

Quantum vs. Semi-Classical

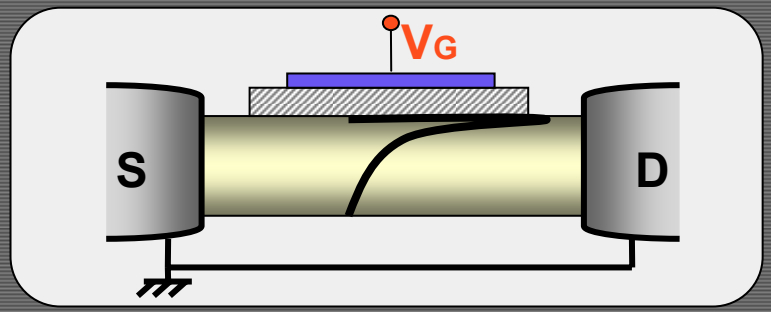
18:05

Quantum Mechanical Approach



- Wave function goes to 0 at the boundaries; therefore electron density will be 0 at the boundaries.
- For **big** devices the quantum solution will have the various Fourier components which add up together and give rise to an electron density looking like the semi-classical solution. Remember that the device has to be sufficiently wide.

Semi-Classical Approach



- There is no concept of wave function here. Electron density has a pick at the boundary. Intuitively, one can think of this as the electron pill-up at the boundary due to a positive gate voltage. This is the concept of Delta Function approximation discussed in Semiconductor Device texts.

Electron Density as Function of Gate Voltage

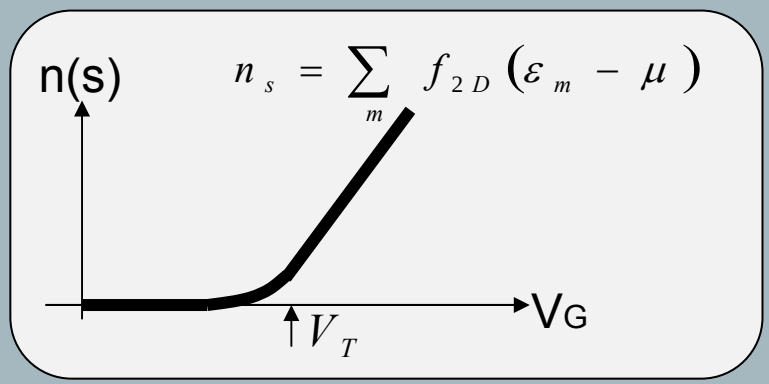
21:35

• Having n(z), the next step is to calculate n(s) which is the electron density per unit area.

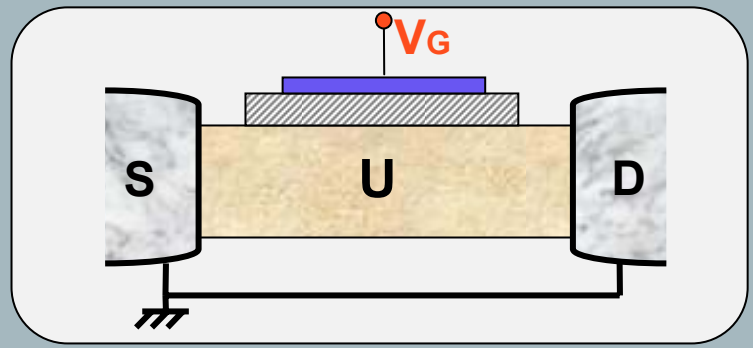
$$n(s) = \int n(z)dz$$

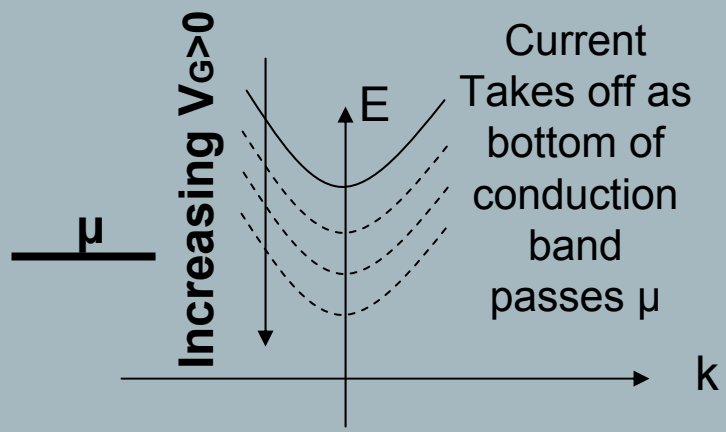
$$n(z) = \sum_m |\phi_m(z)|^2 f_{2D}(\varepsilon_m - \mu)$$

• The motivation for doing this comes from the fact that if you think of the device as a capacitor, the n(s) will give you charge density per unit area and you'll have a capacitance per unit area..



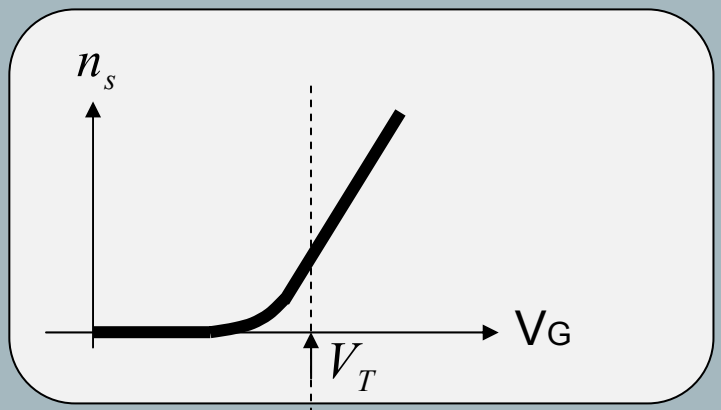
VG Changes the average potential inside the channel

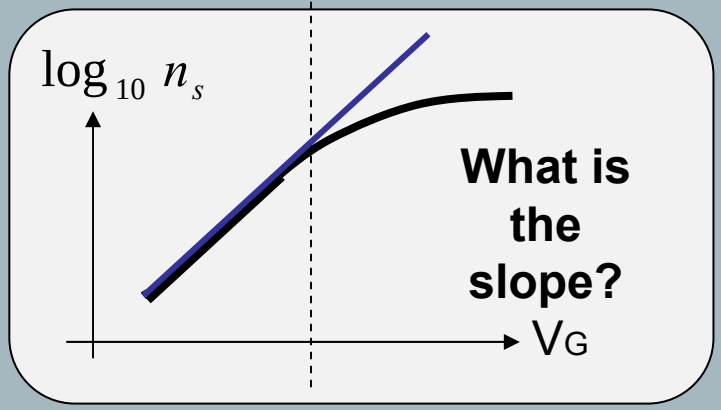




Electron Density vs. Gate Voltage (slope)

27:50

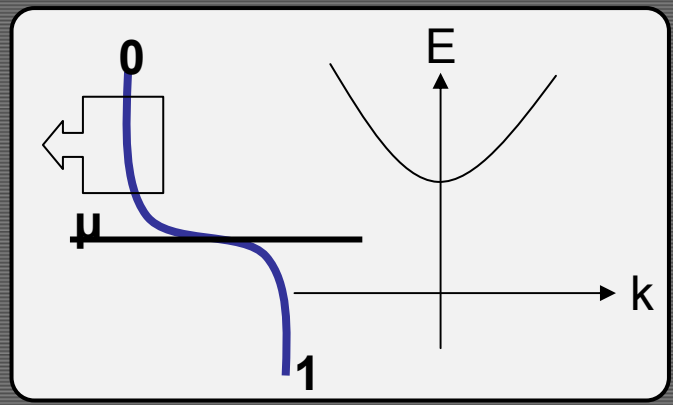




• The slope goes as exp(-E/kT). (as you know the Fermi function becomes this exponential via Boltzmann approximation.)

• Boltzmann Approximation

$$f \approx e^{-E/kT}$$



• As the potential U is changed inside the channel, the probability of electron filling the bottom of conduction band changes as

$$e^{-(E_c+U)/k_BT}$$

$$n_s \propto e^{\frac{-E_c+U}{k_BT}}$$

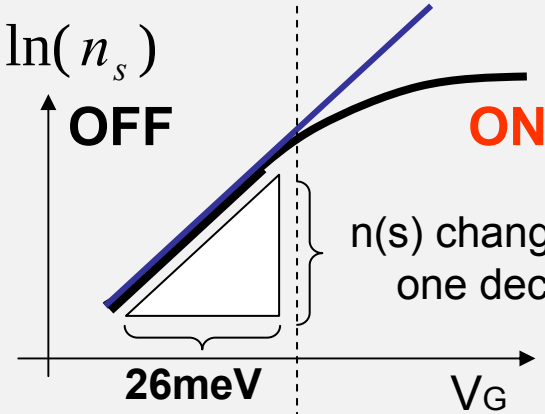
C: Constant

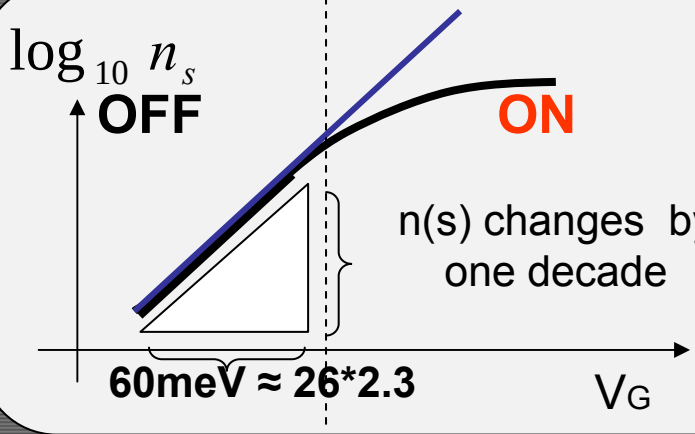
U=-qVG

$$\ln n_s = C - \frac{E_c - qV_G}{k_BT}$$

$$\ln n_s = C + \frac{qV_G}{k_BT_{room}} = \frac{qV_G}{26\ meV}$$

n_s vs. V_G Slope (Cont'd)





$$\ln(n_s) = \ln(10) \times \log_{10}(n_s) = 2.3 \log_{10}(n_s)$$

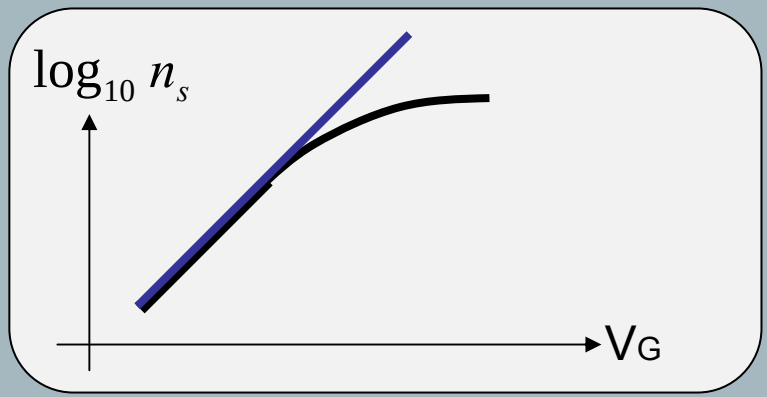
$$\ln n_s \propto \frac{qV_G}{k_B T_{room}} = \frac{V_G}{26\ meV}$$

$$\log_{10} n_s \propto \frac{V_G}{2.3 \times 26\ meV}$$

- On the log(ns) vs. VG plot, in the off region, the electron density changes at the rate of one decade per 60meV.
- **Important Issue**: Is there any way of getting a rate higher than one decade per 60meV for small devices? This is of significance because as devices are getting smaller, smaller operating power is desired, hence a smaller voltage range is available. At the current rate, it takes 300meV to turn the device off by 5 orders of magnitude. What we want is to turn it off by less voltage. But as long as we operate on the basis of electrostatic principles, we're stuck with 60meV per decade.

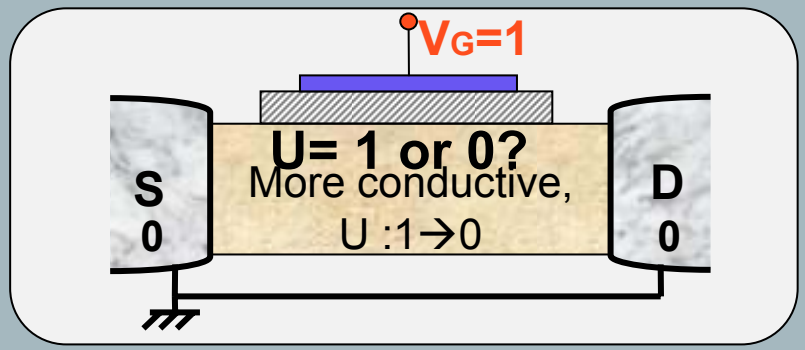
Insulator to Conductor

• Next question: why doesn't electron density obey the same rule as it increases? i.e. why does it roll off?



• Part of it is because the Fermi function doesn't increase as fast as exponential for the whole region. But there is a more important point:

• We've assumed that $U = -qV_G$, however as the channel gets more conductive, this will not be the case.



• As the channel becomes more conductive it becomes more like a metal, hence shorted to the contacts. Therefore potential gradually decreases to 0.

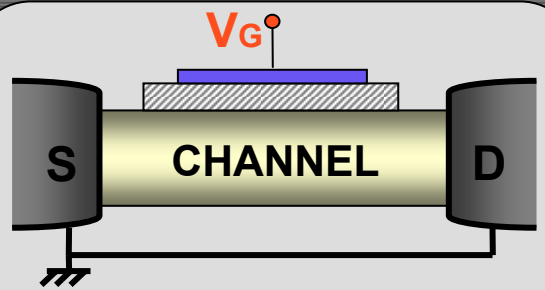
• Now the question is at what point does it start to behave like a metal and what determines it. We'll see the results first and then try to understand them. See next page.

Insulator to Conductor (cont'd)

39:22

LOW DOS

• Low DOS results in low quantum capacitance. For a small capacitance, since caps behave as inverse resistors (conductors), conductance is low (open) and the entire voltage appears across C_Q.



$$C_Q = q^2 D$$

HIGH DOS

• For high DOS, the capacitor is large, hence more metallic; acts as a short, node C becomes 0. And there will be low voltage drop across C_Q.

INSULATOR **METAL**

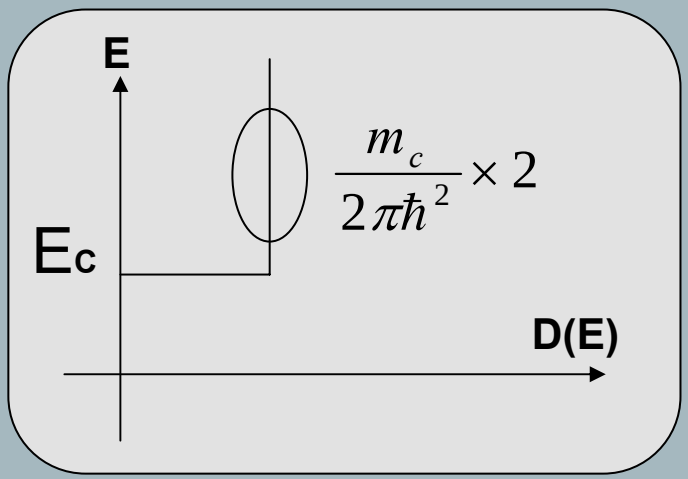
• This is now becoming an important issue in the small devices. In the past Cins was small relative to C_Q; hence effect of C_Q wasn't significant. Consider the equation for Cins: $Cins = \varepsilon_{ins}/t_{ins}$. Over the years, t_{ins} has become smaller. Through making t_{ins} smaller (Hence increasing Cins) people were able to control the channel. How ever at some point Cins will become big relative to C_Q. C_Q will then have more influence and the channel can't really be controlled by Cins. It is the Quantum Capacitance that controls now.

Quantum Capacitance

• **DIMENSIONS**

$$C_Q = \underbrace{q}^{2}\,\underbrace{D}$$
$$\left[Coul.^2\right]\left[\frac{1}{eV \cdot m^2}\right]$$

• DOS in a 2D system is constant.



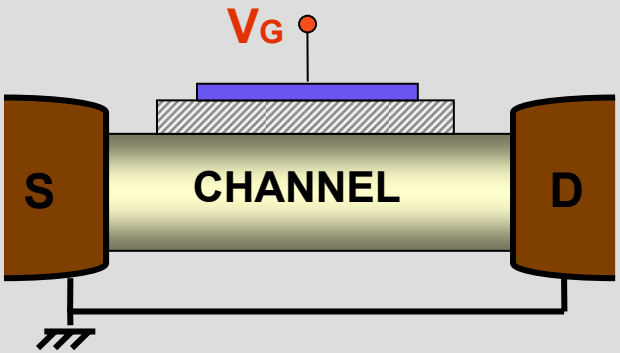
• For the corresponding Quantum Capacitance we have:

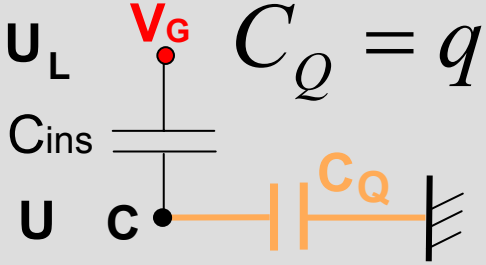
$$C_Q = q^2 \frac{m_c}{\pi\hbar^2} = \frac{\varepsilon}{d}$$

Once the thickness gets comparable to 10 Å, one has to worry about the Quantum Capacitance. (Quantum Capacitance is like a parallel plate capacitor whose plates are separated by the quantity d)

• But how do we get the expression for the Quantum Capacitance?
• This is done on the next page.

Quantum Capacitance (cont'd)





$$C_Q = q^2 D$$

- For the potential, we had:

$$U = U_L + \frac{q^2}{C_E}\Delta N \quad \textbf{(1)}$$

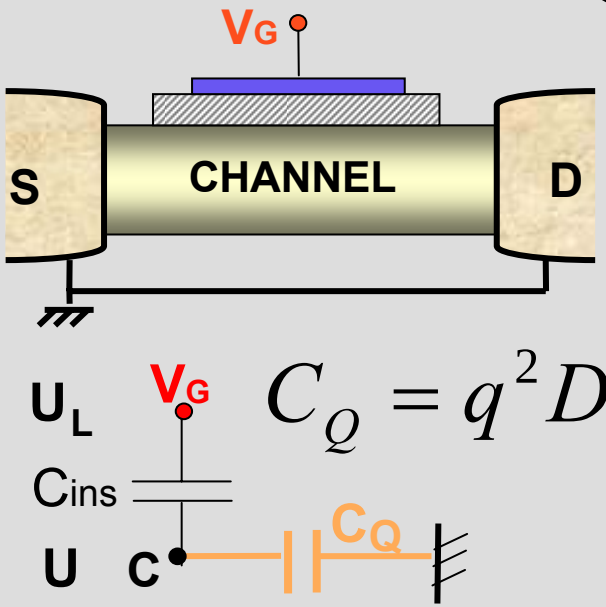
- The amount of change in ΔN depends on U. This dependence is non-linear but any nonlinear curve can be approximated by a line over a small region. Therefore we have:

$$\Delta N = -D\Delta U \quad \textbf{(2)}$$

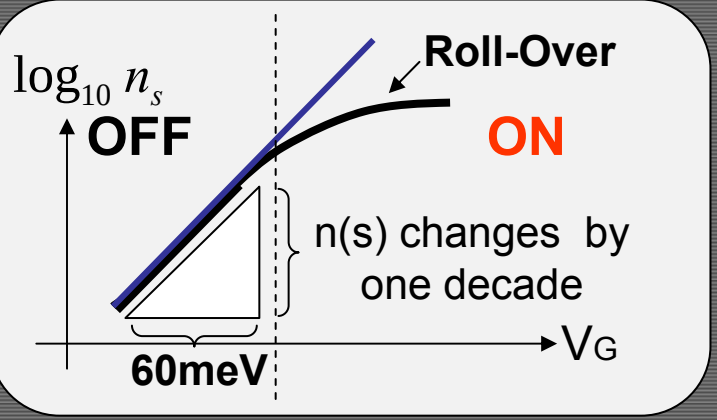
$$1\&2 \Rightarrow U = U_L - \frac{C_Q}{C_E}U$$

- This is what we would get if we'd solve for the potential at node C.

n_s vs. Gate Voltage; Quantum Capacitance



$$C_Q = q^2 D$$



Roll-Over in the ON region

- One reason is the Fermi function that doesn't change as fast as an exponential.
- The more important reason is that once the channel gets conductive, it is very hard to change the potential in the channel. The amount of change is decided by the ratio of insulator versus quantum capacitance.

Quantum Capacitance

- The Quantum capacitance is a very important concept especially for small devices where it is a small value; hence the voltage drop over it is big and influential; whereas in big devices Quantum Capacitance is very big which results in a short and one doesn't have to worry about it as much.