Quantum Transport:

Atom to Transistor

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Lecture 40: Self-Consistent Field Method and Its Limitations

Ref. Chapter 1.5 & 11.4

Network for Computational Nanotechnology

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online simulations and more

Retouch on Concepts

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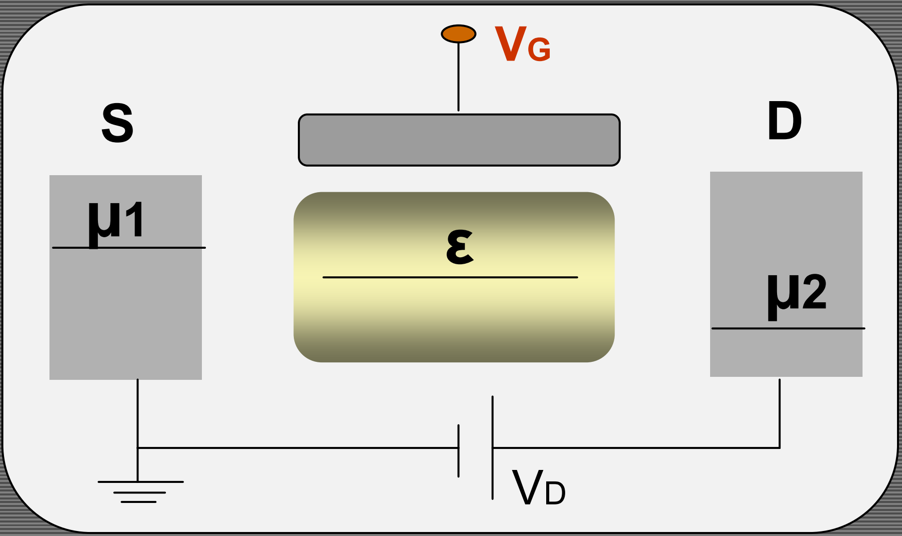


- Number of electrons for the one level device with a drain to source voltage:

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

- Later in the course we discussed this more in general where the Hamiltonian matrix replaces the single level to describe the channel.

- For N we obtained this matrix equation for the number of electrons:

$$[\rho] = \int \frac{dE}{2\pi} \left[\left(G\Gamma_1 G^+ \right) f_1 + \left(G\Gamma_2 G^+ \right) f_2 \right]$$

- Similarly for current we have:

One level

$$I = \frac{q}{\hbar} \int dE D_\varepsilon(E) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2)$$

General

$$I = \frac{q}{\hbar} \int dE Trace \left(\Gamma_1 G \Gamma_2 G^+ \right) (f_1 - f_2)$$

- It is very important to note that these calculations have to be solved self consistently with the Poisson equation.

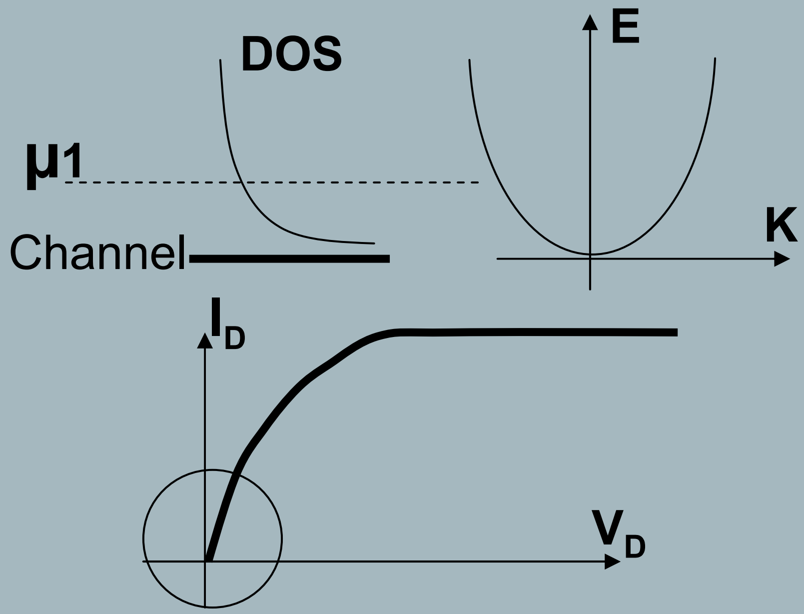
Example on the Importance of Self-Consistent Field

- In order to derive the answer self consistently we include this equation:

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

- Laplace potential is the potential in the channel if the channel was insulator.
- U_0 is called the Single Electron Charging Energy. It tells us how much the potential will be changed if the number of electrons is changed by one.
- Later we'll discuss the case for which, U_0 becomes large and strange things that happen as the result of this. For large conductors this quantity is small and doesn't influence the picture as in small devices.
- For now consider an example to appreciate the importance of self consistent solution:

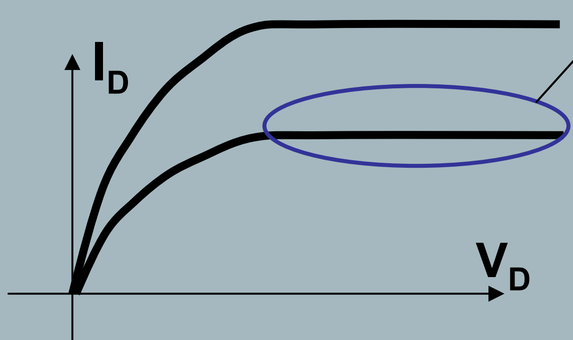
On-current of a Transistor



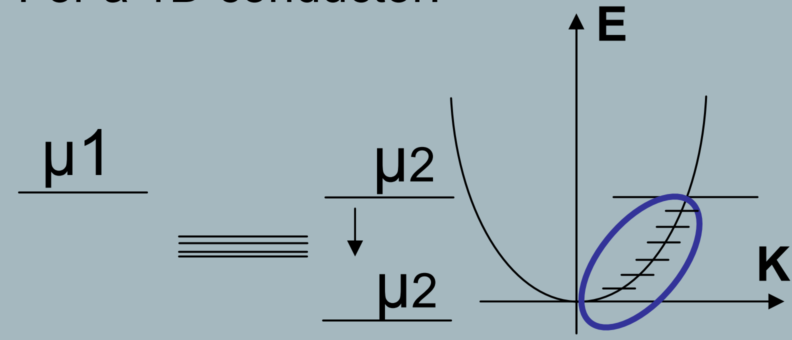
- Here, current flow depends on the availability of the states around the chemical potential. Higher DOS will result in higher current and low DOS will result in a small current. But why does the current saturate?

Example Cont'd

- Why does the current saturate?
- Answer: If the channel is well coupled to the gate, gate's potential will keep channel's potential constant as the drain voltage is changed. Current increases primarily because DOS is increases, but since channel 's potential is fixed, after some point lowering μ2 will not change DOS between μ1 and μ2, hence the current will saturate.
- What is the "On" current?



- For a 1D conductor:



You would expect the current to be:

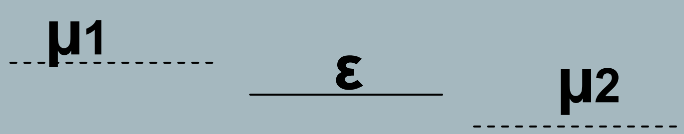
$$I = \frac{2q}{h}\mu_1$$

- How ever this is not correct; in fact current could **be quite bigger**. Note that a lot depends on how big the single electron charging energy is. U_0 is the amount by which the potential changes inside the channel due to addition of one electron.

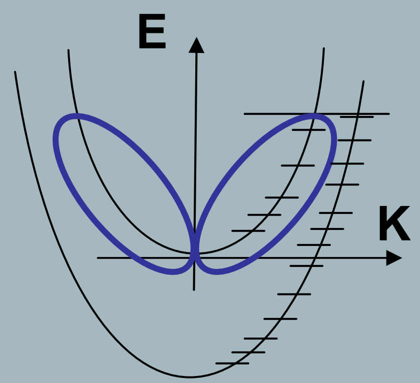
$$U_0 = \frac{q^2}{C_E}$$

Why can current be bigger?

• If U_0 is large, then N does not deviate much form N_0 and it tends to stay close to N_0. Now let's go back to our potential profile:



• If epsilon sticks where it is right now, then the number of electrons will be reduced by a factor of ½. The reason being that at equilibrium there are two equal amount of electrons that are positive and negative going. After applying the bias, half of the states will become empty. And since N wants to remain close to N_0, the E-K diagram shifts down such that there are twice as much positive going electrons and the total number is close to N_0.



• So epsilon will slide down enough to keep the number of electrons the same. And since it is sliding down, the number of states between μ1 and μ2 increases and this will result in the increase of current.

• To understand current-voltage characteristics, one needs to know how the potential divides in the channel and what it will be after self-consistent solution.

Large U_0

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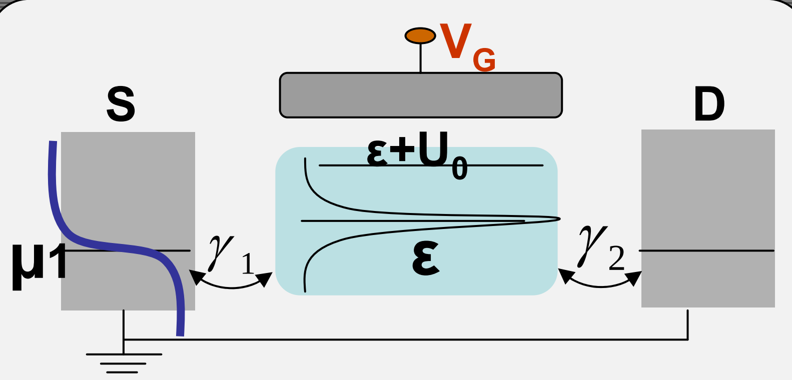
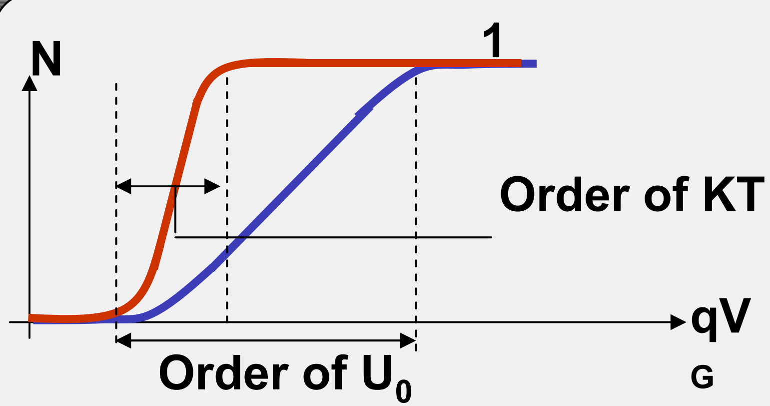
- Large U_0 for a one level channel with small broadening.





- Finding N as a function of gate voltage self consistently will result in a slower increase in N as V_G increases. Why?
- Answer: As the channel gets filled, the potential will float up and to increase N, the level ($\varepsilon+U_0$) will have to be lowered below chemical potential and this requires more gate voltage.

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

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

- We are comparing U_0 with γ and kT. New issues are involved when U_0 is much bigger than Gamma and kT. So what are these issues and what happens if U_0 is much bigger than Gamma and kT?

Expectation vs. Experiment

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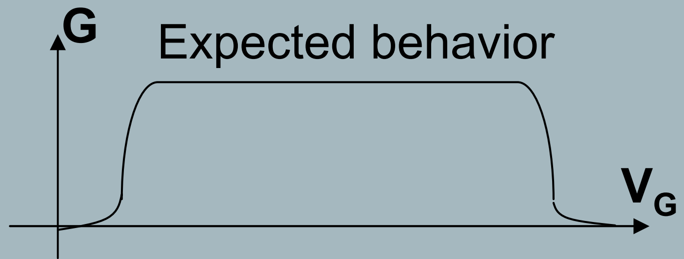
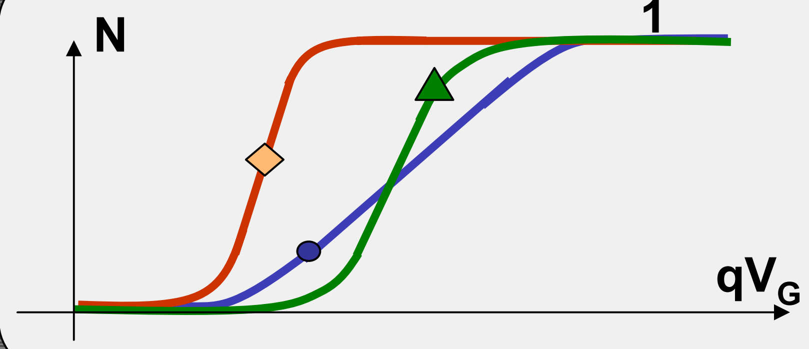
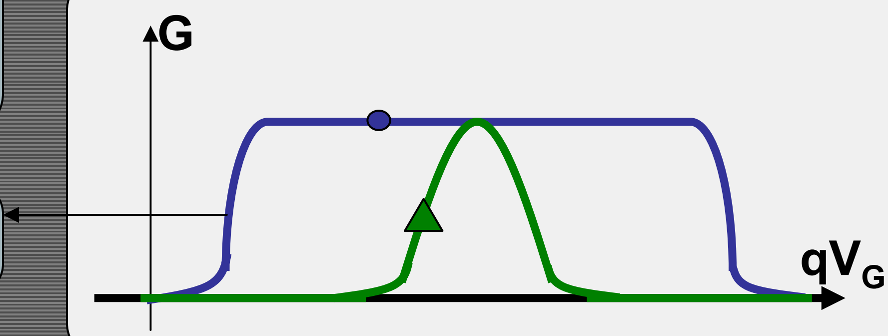
- So how should the conductance look like as a function of gate voltage?



- How ever this is not observed in experiment at all. The experiment's result is indicated on the graph.



- **Conductance goes as derivative of N.**

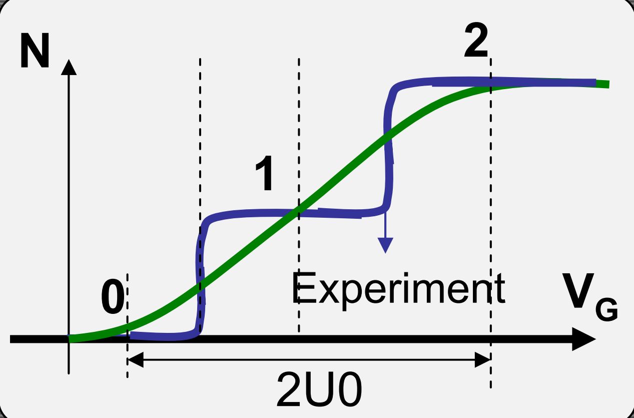


- This experiment has not been done exactly. What has been done involves two levels of up and down spin.
- See next page for the results.

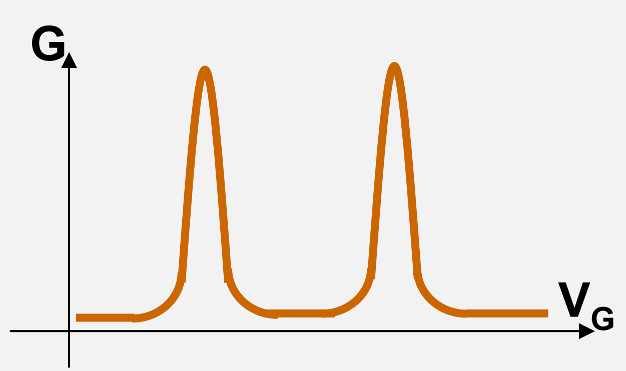
◇ Self consistent solution is not used.
● Solved self consistently.
▲ Experiment

Experimental Observations and Understanding Them

Experimental Observations



Coulomb Blockade Peaks



- Normally we don't worry about these differences between theory and experiment because thus far we've assumed that Gamma and kT are bigger or comparable to U0. This is usually the case either because of the temperature or because of good coupling to the contacts.
- This really becomes important as the size of channel gets smaller and smaller because for smaller channel, total capacitance is lower and that results in higher U0. ($U_0 = q^2/C_E$) Sizes of about 10 to 20 Å are the ones that need care and attention in terms of U0.
- There are two ways to explain all these:
- 1) One electron picture. It is more convenient but it's not exactly correct.
- 2) Multi electron picture. You think of electrons as one big system. This gives the correct answer; but it's hard to do.

One Electron Picture

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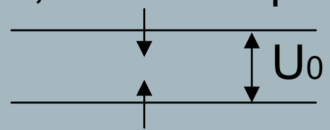
- We know that no electron feels any potential due to itself. So when you put an electron inside the channel, the level that it occupies does not change but the other one, up-spin or down-spin based on what was filled first, will float up by an amount U_0.



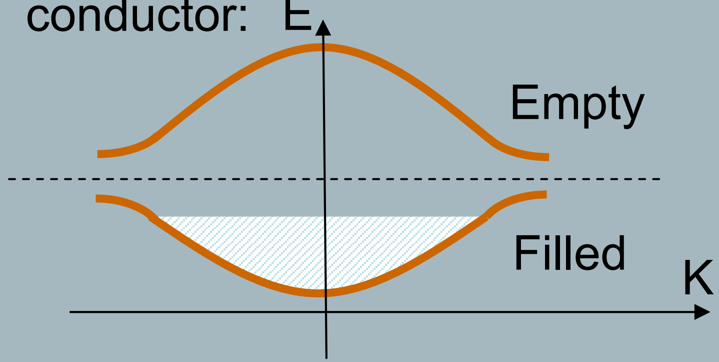
- So to include this fact, we subtract Δn**i**, change in the number of electrons in level (i) from ΔN in the potential equation.

$$U_i = U_L + U_0(N - N_0 - \Delta n_i)$$

- This means that different orbitals feel different potentials.
- But this is not something you can trust very much. Coulomb Blockade regime of transport must be considered which will be discussed next day.

- Similar situation is observable in solids. For example consider the **Kronig-Penny Model:**

- If t is much bigger than U_0, then the band will split in two and become an insulator instead of a conductor:



- La_2CuO_4 is an example where this behavior has been observed.

Intermediate Regime

• Intermediate regime is the border line between coulomb blockade and band conduction and it is generally not understood at all. Most people believe that high T_C superconductors are a set of coupled Quantum Dots which are intricately designed to be at this border line.

• In this course we've used the self consistent field method where U0 is smaller than γ and kT.

• Coulomb Blockade must be considered in cases for which U0 is comparable to γ or kT. This topic will be discussed in the next class.