Session 15

Note Title 11/20/2008

Ohm's law

We have discussed so far about small scale devices and using Hamiltonian and self energy matrices. For large devices we had to consider scattering. The question is how we will get Ohm's law as the device gets bigger and bigger.

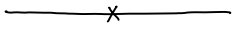
We saw before that: $I \propto \frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2} D \Rightarrow I \propto S$.

$\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2} \propto \frac{1}{L}$, $D \propto V = SL$

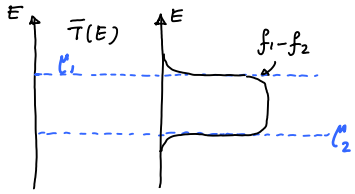
Note that γ is the escape rate at the two contacts. for large channel, electron wavefunction is more spread over the channel. That's why escaping into contacts becomes less easy. Hence $\gamma \propto \frac{1}{L}$.

However, Ohm's law predicts that for a conductor with length L and area S, the conductance changes with $\frac{S}{L}$.

So our $I \propto \frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2} D$ does not predict Ohm's law. In this equation we have assumed the transport to be ballistic, i.e. no scattering inside the device. To address scattering let's compare two conductors: one with 1 scatterer and one with 2:

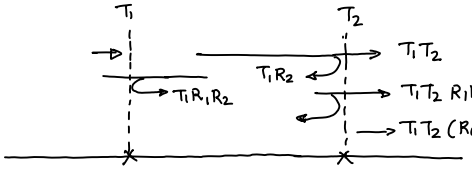


$$I = \frac{2e}{h}\int dE\, \bar{T}(E)(f_1-f_2)$$



Landauer Formula $I \sim \overbrace{\frac{2e}{h}\, T(\mu) \times eV}^{G}$

For transmission through two scatterers we have:



$$\rightarrow T = T_1T_2\left(1 + R_1R_2 + (R_1R_2)^2 + (R_1R_2)^3 + \cdots\right) = \frac{T_1T_2}{1-R_1R_2}$$

$$T_i + R_i = 1 \rightarrow \frac{1}{T} = \frac{1-(1-T_1)(1-T_2)}{T_1T_2} = \frac{1}{T_1} + \frac{1}{T_2} - 1$$

Now we need to see how T changes with length: $T(L) = ?$

From the above relation, we know that if we separate a conductor into two sections of equal length, we must have: $\frac{1}{T(2L)} = \frac{1}{T(L)} + \frac{1}{T(L)} - 1$ This equation satisfies the relation:

$$T(L) = \frac{\lambda}{L+\lambda} \quad \text{as:} \quad \frac{2L+\lambda}{\lambda} = \frac{L+\lambda}{\lambda} + \frac{L+\lambda}{\lambda} - 1$$

λ is the mean free path, MFP, and is defined as: a conductor that has a length of λ, has a transmission of $\frac{1}{2}$.

Does this relation lead to Ohm's law? For a 1D conductor we have:

$$G = \frac{2e^2}{h}T = \frac{2e^2}{h}\frac{\lambda}{L+\lambda} \quad \text{or} \quad R = \frac{h}{2e^2}\left(1+\frac{L}{\lambda}\right)$$

Ohm's law states $G \propto \frac{1}{L}$ for 1D conductor that seems similar to what we have except the term λ in the dinaminator. Based on Ohm's law conductans goes to infinity for $L=0$, but we have a maximum conductance

of $G_{MAX} = \frac{2e^2}{h} \simeq \frac{1}{12.9\,k\Omega}$ this is due to contact resistance as we know. Of course for large L ($L \gg \lambda$), G looks like exactly like Ohm's law.

For a 2D conductor, we have subbands where increasing the number of modes will increase the conductance

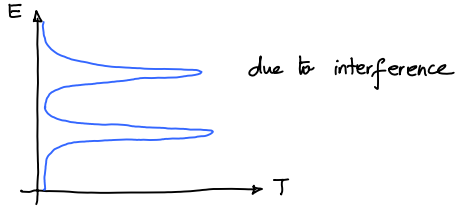
$$R = \frac{h}{2e^2}\frac{1}{M}\left(1+\frac{L}{\lambda}\right) \rightarrow G = \frac{2e^2}{h} M \frac{\lambda}{L+\lambda}$$

$$\frac{S}{L} \Leftarrow \propto S \quad \propto \frac{1}{L} \text{ for large } L$$

M increases with area S, so we get the Ohm's law for 2D.

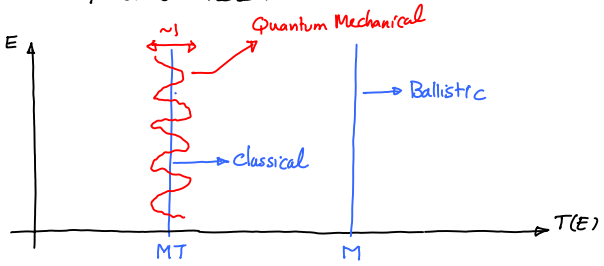
Our picture for conductance has still to be looked into as electrons have also wave characteristics.

Consider for example, a conductor with two scatterers. From particle point of view, transmission must reduce by a factor of 2 when we have two scatterers compared to one. However, this is not completely true. Quantum mechanically the interference between the electron waves changes the picture. For example, if the distance between the two scatterers is quarter of wavelength, two reflections cancel each other, hence we can get more transmission, i.e. constructive interference.



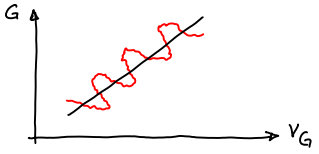
So what do we have if we calculate the transmission quantum mechanically?

For a conductor with 50 modes, for example, if the conductor is ballistic, transmission would be one times number of modes, i.e. 50 here:



Classically for a device with scatterings transmission is constant versus energy. However, quantum mechanically we get fluctuations with height of order 1.

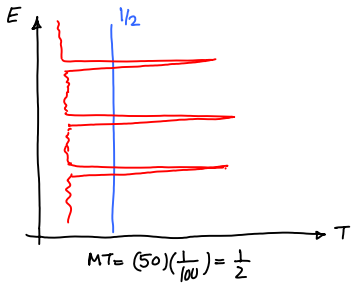
The conduction therefore fluctuates by order of $\frac{2e^2}{h}$. For example for Conductance versus gate voltage for an FET we get:



In fact, quantum mechanical calculation gives a little lower average than the classical because of weak localization.

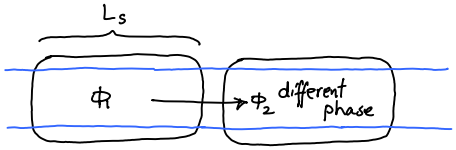
(we won't discuss this further here)

What if transmission per mode is, say, $\frac{1}{100}$ and have 50 modes? For this case MT = 0.5 and fluctuations of order one would give negative transmission, which is impossible. So what does happen? It is believed that quantum mechanical transmission would be zero except that at some energies it has sharp peaks. This is called regime of strong localization.



So we expect, based on this theory, that if we make the channel long enough as T is reduced we should get to the strong localization egime. But this is not what we see in real world. This is because we should also consider phase breaking.

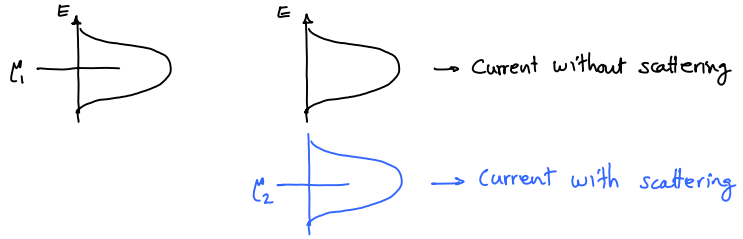
In a wire there are regions of length of order scattering length L_s. Within this length transport is explained quantum mechanically with wave behavior. However these regions are not phase coherent with each other and cannot have destructive interference.



Power Dissipation: where does the heat go?

For a small ballistic device we have a minimum resistance of $\frac{h}{2e^2}$. One may think that this is the channel resistance. However, there is no scattering in the channel. For resistance to occur electron must loose its energy to something.

So what happens to RI^2?

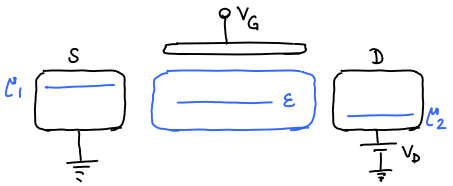


If the energy currents on the left and right contacts are the same, it means no energy was left behind. At present of scattering, the current at right contact flows at a lower energy. For our model that there is no scattering, the energy drop happens at the contact resulted from the contact resistance $\frac{h}{2e^2}$.

Experimental evidance:

In some experiments on carbon nanotubes, the current flow in CNT must result in large enough energy dissipation that must burn the device if the dissipation was in the channel. But this is not observed and the CNT doesn't burn for high current. In fact it is believed that the heat is dissipated in the contacts. How much heat is dissipated in each contact remains to be established.

Self Consistent field and its limitations



$$N = \int dE\, D(E)\, \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \qquad I = \frac{e}{\hbar}\int dE\, D(E) \frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}(f_1 - f_2)$$

$$\downarrow \qquad\qquad \downarrow$$

$$[\rho] = \int \frac{dE}{2\pi}\left(G\Gamma_1 G^+ f_1 + G\Gamma_2 G^+ f_2\right) \qquad I = \frac{e}{\hbar}\int dE\, \text{Trace}\left(\Gamma_1 G \Gamma_2 G^+\right)(f_1 - f_2)$$

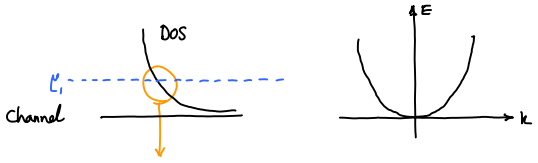
These calculations have to be done self consistently with the Poisson equation:

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

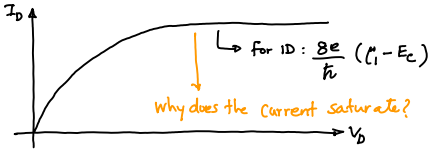
U_L is Laplace potential: the potential in channel if there were no electrons in channel, i.e. insulating channel.

U_0 is the single electron charging energy: the potential change in channel by addition of one electron into the channel.

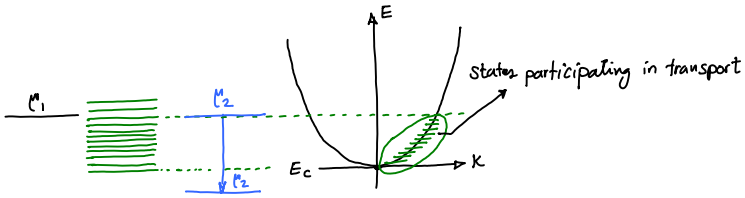
for large conductors U_0 is small and can be ignored, but for small devices it can cause strange things as we will see.

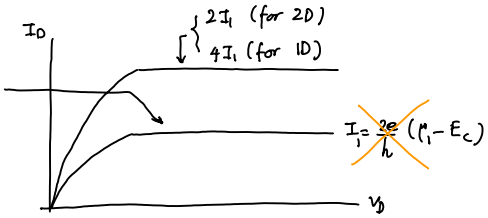


Current flow depends on the number of states available around the chemical potential



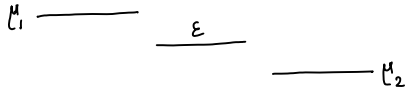
Current Saturation: If the gate is completely coupled to the channel, channel potential is fixed to that of gate and doesn't change with the drain potential. Now by increasing V_{DS} current increases because μ_2 is lowered and DOS increases, but at some point lowering μ_2 does not change DOS between μ_1 and μ_2 and the current saturates:

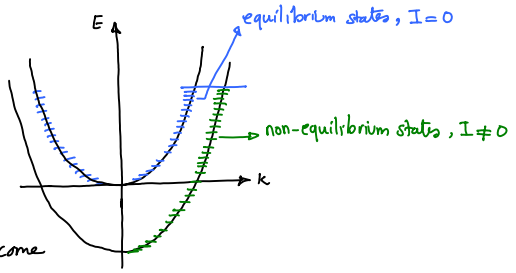




What is the "on" current? One would expect the saturated or "on" current to be $I = \frac{2e}{h}(\mu_1 - E_c)$. However this is not practically correct. The current is quite bigger! This a lot depends on how big the conductor is. The size affects the single electron charging energy U_0: $U_0 = \frac{e^2}{C_E}$ If U_0 is large, N, the number of electrons in channel does not change much from the zero gate value of N_0.

Let's look again at our potential diagram:





If ε is not changing, the number of electrons is reduced to $\frac{1}{2}$ upon turning on voltage as half of the states become empty. Since N wants to remain close to N_0, the E-K diagram shifts down so there is twice as much positive going electrons and the total number is close to N_0. So ε will go down enough to keep N close to N_0. But

as $\mathcal{E}$ goes down, the number of states between μ_1 and μ_2 increases and that increases the current.

$U = U_L + \frac{e^2}{C}\Delta N$

$N_0 = \frac{2}{\pi\hbar}\sqrt{2m(\mu_1 - E_C)}$ in 1D (Note $D(E) \sim \partial N/\partial E \sim 1/\sqrt{E}$)

$N = \frac{1}{\pi\hbar}\sqrt{2m(\mu_1 - E_C + U)}$ ← { x2 gone after turning on the bias

$N = N_0 \Rightarrow 2\sqrt{2m(\mu_1 - E_C)} = \sqrt{2m(\mu_1 - E_C + U)}$

$\rightarrow \mu_1 - E_C + U = 4(\mu_2 - E_C)$

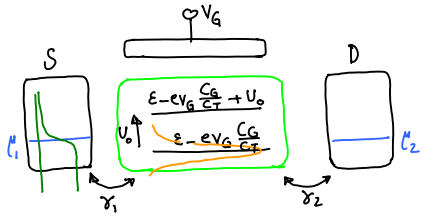
$\rightarrow I_{max} = \frac{2e}{h}(\mu_1 - E_C + U) = 4 \times \frac{2e}{h}(\mu_1 - E_C)$

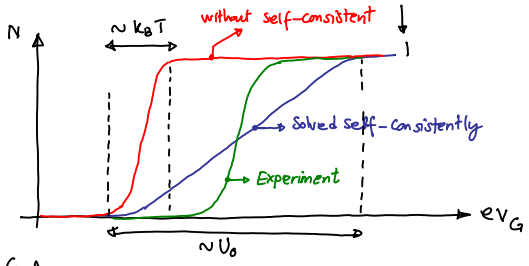
Now we need to also look on how the bias voltage affects the channel potential through self-consistant solution.

Consider U_0 is large :

Assume the broadening is small first:

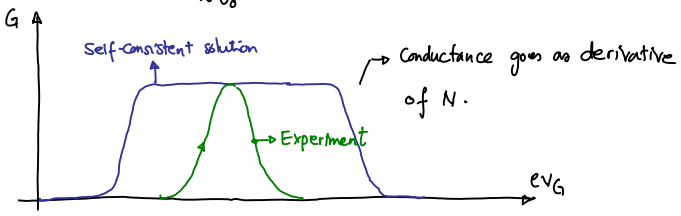
assume one energy level in channel. So $N_{max} = 1$





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

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

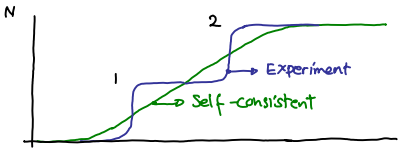


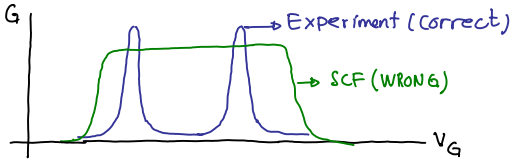
When we solve self-consistently for N, the slope will be slower versus V_G. Why?

Answer: By increasing V_G, the channel starts to gets filled, but that floats up the channel potential by U_0. To increase N, the level has to be lowered below chemical potential that requires larger V_G. That's why the slope becomes slower. We should also compare U_0 with γ and k_BT. If $U_0 \ll k_BT$ or γ, our experiment would look like our self-consistent field calculation. The difference is appeared when the device becomes small so U_0 is larger than k_BT and γ.

$U_0 = \frac{e^2}{C_E}$ becomes large typically for sizes of smaller than 10-20 Å.

Experimentally, we actually have two levels of spin up and down. So this is what we observe for single $\mathcal{E}$ in the channel.



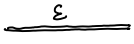


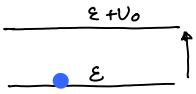
In order to explain this we can take two different approach:

1) The electron picture: more convenient but not exactly correct.

2) Multi electron picture: we take all the electrons as one big system. It's hard to do but is correct.

One electron picture:

Consider two states at energy ε:  two states for spin up and down

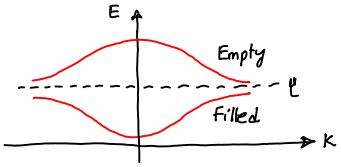
When the first electron fills a state, the level that it occupies doesn't change (an electron doesn't feel its own field), however, the othe state moves up by U_0:  we may include this change by reducing the number of electrons in the second level (or ith level in the general case of having many levels) with Δn_i:

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

→ Since the level floats up, there will be less number of electrons in this state.

This means that different orbitals feel different potentials. As an example, consider a lattice with atomic energy U and nearest neighboor coupling t:

If t is very large ($t \gg U$), the band splits in two and instead of a conductor the material becomes an insulator:



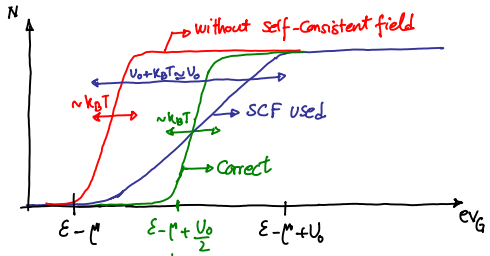
La_2CuO_4 is an example that is insulator based on this effect.

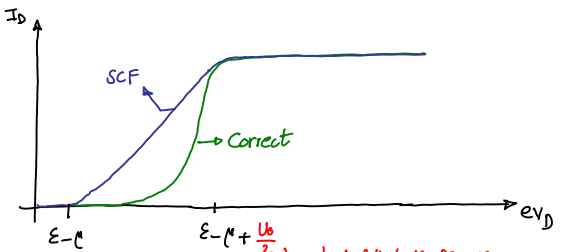
People tried to dope La_2CuO_4 for example with Sr to make it conductor. But instead they got a superconductor with a high critical temperature (T_c) in 1980's that resulted in a nobel prize! But what is happening? Why do we get superconductor than a conductor? People believe transport is in this case neighter in Coulomb blockade nor completely in band conduction regime, but in the border line between the two. They belive that high T_c superconductors are like coupled quantum dots intricately designed to be at this border regime. This is generally not understood at all!

Note: Coulomb blockade is the case where U_0 is comparable to k_BT and γ: $U_0 \gtrsim \gamma, k_BT \rightarrow$ Coulomb blockade

So in the Coulomb blockade regime we will see the following in experiment versus our self-consistent calculation:

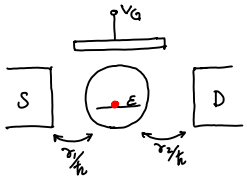
For one level device: ($U_0 \gg k_BT$ and γ)





→ half filled if $\gamma_1 = \gamma_2$

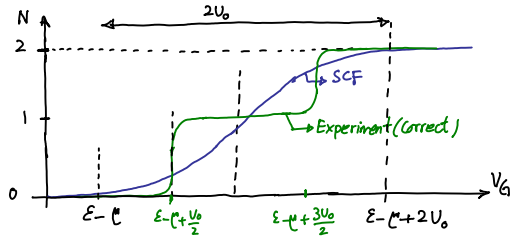
Why transition happens at $\frac{U_0}{2}$ from $\varepsilon - \mu$? The answer is actually easy if we look at the energy that one electron adds to the device:

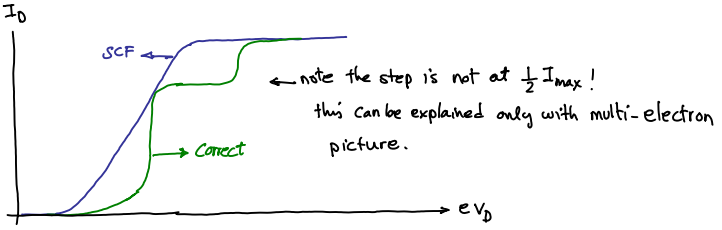


energy stored in a capacitor is: $\frac{q^2}{2C}$ for one electron it is $\frac{e^2}{2C}$

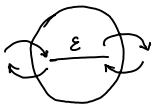
We defined before $U_0 = \frac{e^2}{C}$ → energy added by one electron is $\frac{U_0}{2}$. For the 2nd electron it becomes $\frac{(2e)^2}{2C} = \frac{2e^2}{C} = 2U_0$

For two level device: ($U_0 \gg k_BT$ and γ)

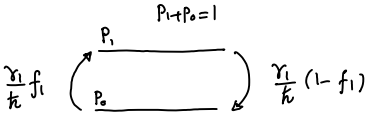




Multi-electron picture



$P_1+P_0=1$



One level muli electron picture:

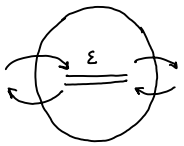
when one electron enters the device, the system goes from state 0 to 1.

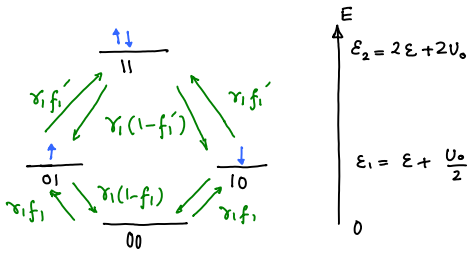
when the electron leaves the system, it goes from state 1 to 0.

At steady state the rates for entering and exiting the system must be equal:

$$\frac{P_1}{P_0} = \frac{(\gamma_1/\hbar)f_1}{(\gamma_1/\hbar)(1-f_1)} = \frac{f_1}{1-f_1} \rightarrow \frac{P_1}{P_1+P_0} = \frac{f_1}{1} \Rightarrow P_1 = f_1 \quad \text{as expected } \checkmark$$

Two level multi particle picture:





$$f_1 = \frac{1}{e^{(\varepsilon_1-\mu)/kT}+1} \Rightarrow \frac{1}{f_1} = e^{(\varepsilon_1-\mu)/kT}+1 \Rightarrow \frac{1-f_1}{f_1} = e^{(\varepsilon_1-\mu)/kT} \Rightarrow \frac{P_{01}}{P_{00}} = \frac{f_1}{1-f_1} = e^{-(\varepsilon_1-\mu)/kT}$$

Note: General principle of equilibrium statistical mechanics is:

The probability of finding a particular state occupied is proportional to the exponential term $e^{-(E_\alpha-\mu N_\alpha)}$:

$$P_\alpha = \frac{1}{Z} e^{-(E_\alpha-\mu N_\alpha)/k_BT}$$

Z is the partition function and is the normalization factor to make the sum of all probabilities equal to one:

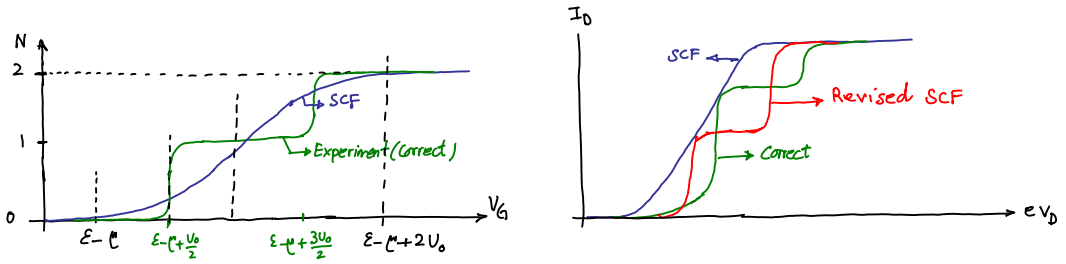
$$Z = \sum_\alpha e^{-(E_\alpha-\mu N_\alpha)/k_BT}$$

---

one may wish to revise the SCF calculation to get the experimental data by assuming that the energy level in the channel is at $\varepsilon+\frac{U_0}{2}$ instead of ε. Then since the electron doesn't see its own potential, in calculating the potential for a give state i, we must remove the state occupation Δn_i from ΔN:

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

But unfortunately this also doesn't give the right plot for $I_D - V_D$. It is shown as "revised SCF" below.



Summary:

For large systems, it is very difficult or impossible to use the multi-electron picture. So we still try to modify the one-electron picture to get a correct result. For this we take out the self interaction (Δn_i) from the SCF. This works for equilibrium but not for non-equilibrium.

Remember that in this course we discussed mostly on transport regime where $U_0 \ll k_B T$ or γ. If U_0 is large or comparable to γ and $k_B T$, Coulomb blockade happens and the right way to solve it is the multi-electron picture. In the intermediate regime of transport many strange thing (such as high T_c superconduction) happens that no one really has a good understanding of how it really works!