# Quantum Transport:
## Atom to Transistor

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# Lecture 4: Charging / Coulomb Blockade

Ref. Chapter 1.4 & 1.5

*Network for Computational Nanotechnology*

NCN nanoHUB online simulations and more

# Retouch on Concepts

00:00

## Current flow through only one level

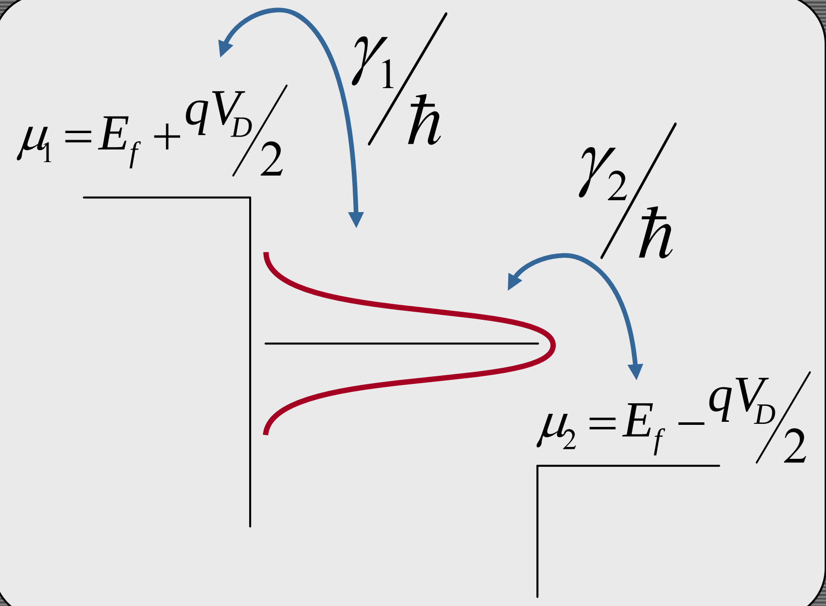
- Important Issue: Current flows when Fermi functions differ.

$$f_1(E) = f_0(E - \mu_1)$$

$$f_2(E) = f_0(E - \mu_2)$$

$$f_0(E) = 1 \Big/ \left(e^{E/k_B T} + 1\right)$$

$$F_T(E) = -\frac{df_0}{dE} = \frac{1}{4k_B T} \bullet \frac{1}{\cosh^2(E/2k_B T)}$$




- One level equations:

$$I = \frac{2q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \int dE \cdot D_\varepsilon(E)(f_1 - f_2)$$

$$N = 2 \int dE \cdot D_\varepsilon(E) \left[ \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \right]$$

# Retouch on Concepts

04:07

- One level equations:

$$I = \frac{2q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\int dE \cdot D_\varepsilon(E)(f_1 - f_2)$$

$$N = 2\int dE \cdot D_\varepsilon(E)\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1+\gamma_2}\right]$$

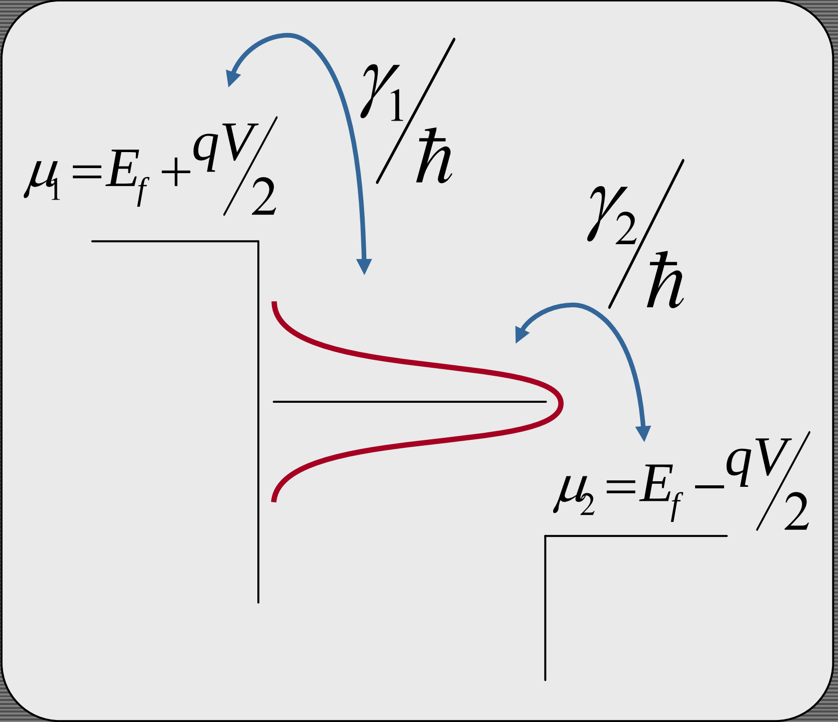
- For one level:

$$D_\varepsilon(E) = \frac{\gamma/2\pi}{(E-\varepsilon)^2 + (\gamma/2)^2}, \gamma = \gamma_1 + \gamma_2$$

- Note: If $\mu_1$ and $\mu_2$ are equal, then the number of electrons, N, is given by

$$N = 2\int dE \cdot D_\varepsilon(E) f_1 = 2\int dE \cdot D_\varepsilon(E) f_2$$

## Current flow through only one level



# Electrostatics of the Channel

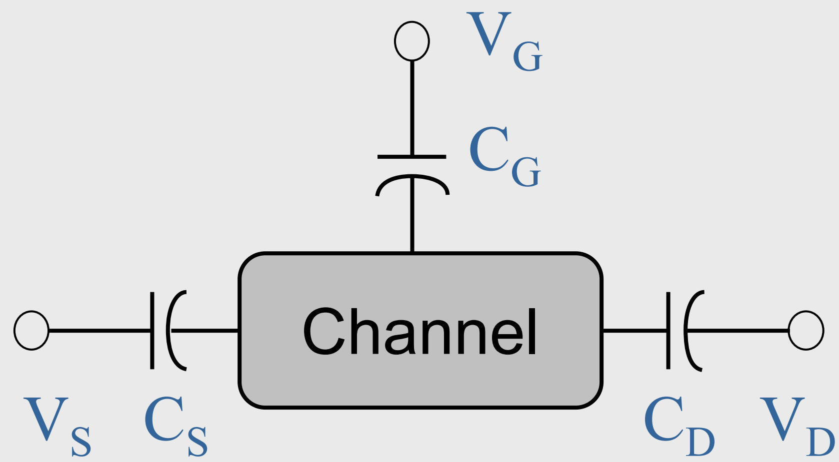


- Remember: Gate voltage moves levels up and down but by how much? And what will the potential be?
- By an approximation you can visualize capacitances $C_s$, $C_G$, and $C_D$ between the three terminals

- Might think of potential as a weighted average:

$$V = \frac{C_S V_S + C_G V_G + C_D V_D}{C_S + C_G + C_D}$$

## Channel with Capacitances



# External Voltages: Effect on Energy Levels



• Set $V_S$=0; the grounded reference potential, therefore the effect on channel energy levels by $C_S$, $C_G$, and $C_D$ is given by

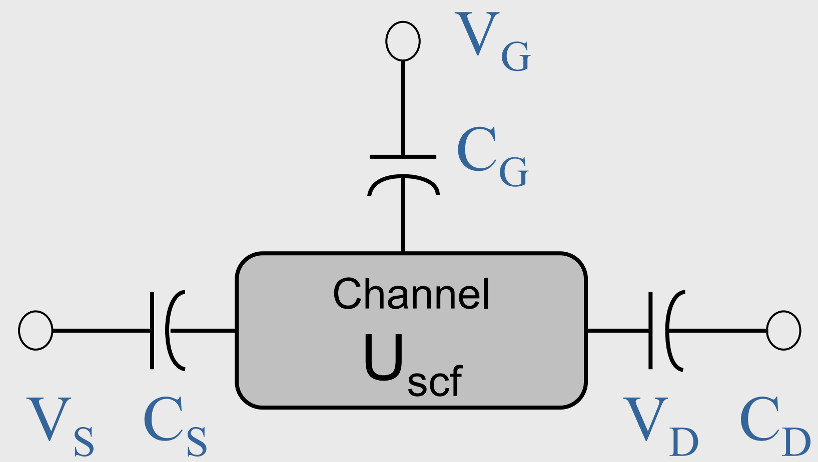
$U_{ext} = (C_G/C_T)(-qV_G) + (C_D/C_T)(-qV_D)$,

where $C_T = C_S + C_G + C_D$

and $V_S = 0$ such that it is excluded.

• The above would be correct if the number of electrons in the channel was not changing (i.e. an insulator such that $U_{scf} = U_{ext}$)

## Capacitances and energy levels



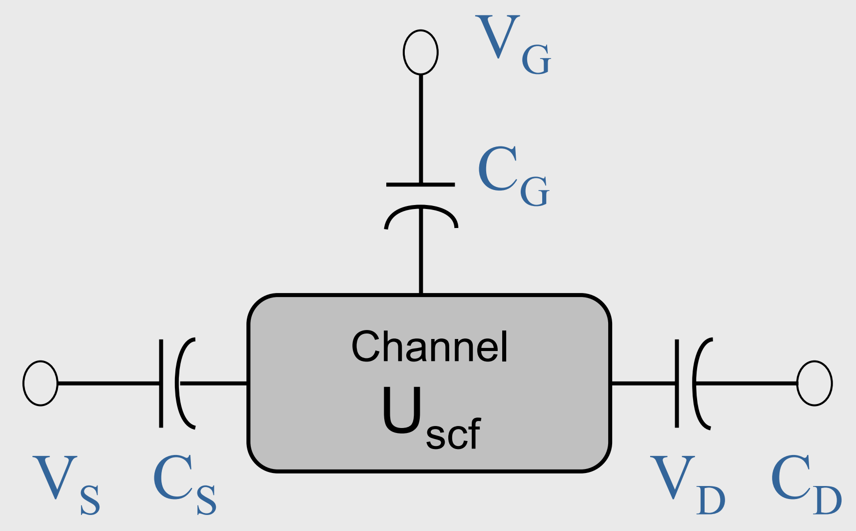
# Effect on Energy Levels due to change in number of electrons



• Increase in electrons raises levels; decrease lowers levels.

• Electron-electron electrostatics causes: $U_{scf} = U_{ext} + (q^2/C_T)\,(N\text{-}N_0)$ where $N_0$ is the number of electrons under equilibrium and $U_{ext} = (C_G/C_T)(-qV_G) + (C_D/C_T)(-qV_D)$

## Capacitances and energy levels



# Self Consistent Field

20:08

- Why use the term "self consistent field" (scf)? Because equation A must be solved self consistently with equation B.

(A)

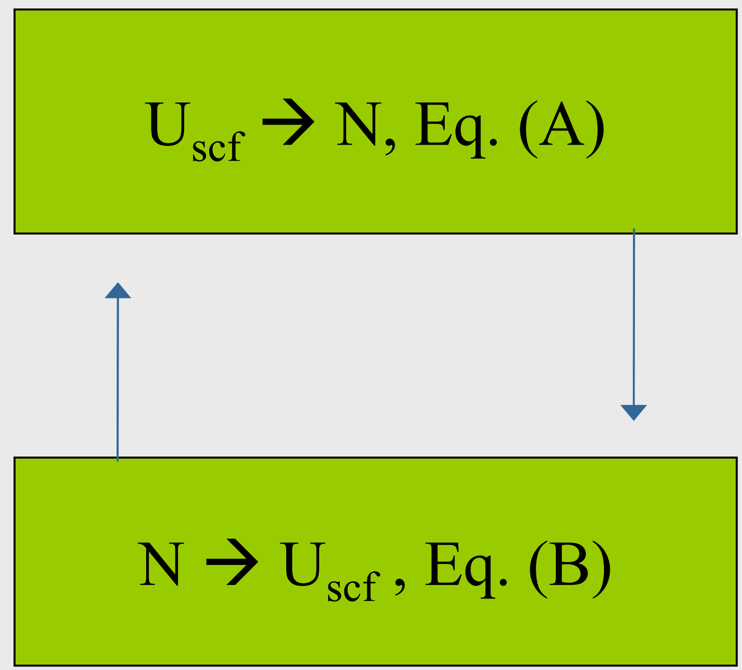
$$N = 2\int dE \cdot D_{\varepsilon}\left(E - U_{scf}\right)\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

(B)

$$U_{scf} = U_{ext} + \frac{q^2}{C_T}\left(N - N_0\right)$$

Note:
(B) is a simplified version of Poisson's equation

## Self Consistent Iteration



# Effect on Conductance vs. Gate Voltage

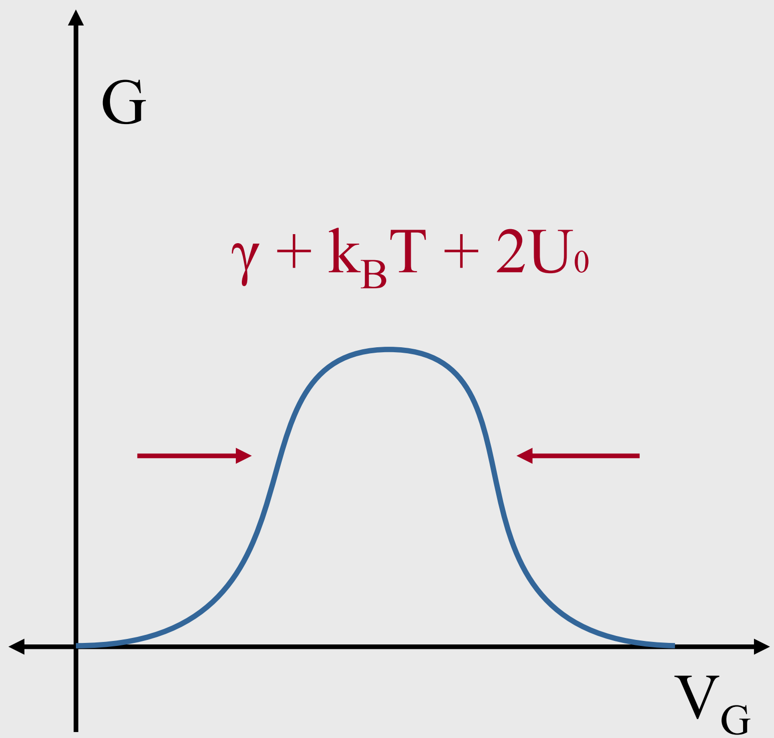


- What effect would this have on conductance vs. gate voltage?

i.e. Assume that the gate is very closely coupled to the device. So, $C_G/C_T \approx 1$ and $C_D/C_T \approx 0$ in $U_{ext}$.

- Then conductance vs. gate voltage peak is determined by:
  - Broadening, $\gamma$
  - Temperature, $k_BT$
  - $U_0 = q^2/C_T$ in $U_{scf} = U_{ext} + q^2/C_T(N-N_0)$ from electrons placed in levels

Conductance vs. Gate Voltage (very small $V_G$)



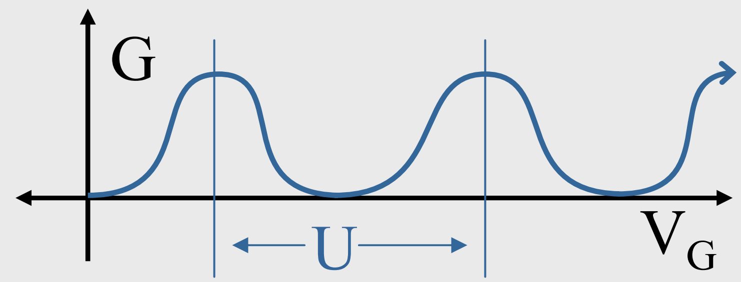
# Coulomb Blockade



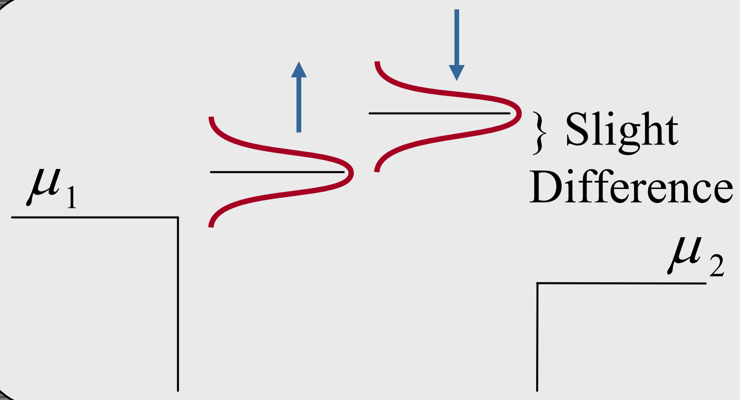
- Rather than a single peak, sometimes experimentally we see two peaks of width $\gamma + k_B T$ (Coulomb Blockade)
- Occurs when $U >> k_B T + \gamma$
- Reason: there are two levels: spin up and spin down. When one level is filled and the other is not, this will result in floating up of the level which is NOT initially filled but feels the potential due to the filled level. Note that the filled level doesn't feel a potential due to itself.

- For illustration, in this figure, assume spin up (↑) and spin down (↓) start out with slightly different energies

## Coulomb Blockade G vs. $V_G$




## Coulomb Blockade: Spreading of Spin Levels



# Coulomb Blockade Cont.

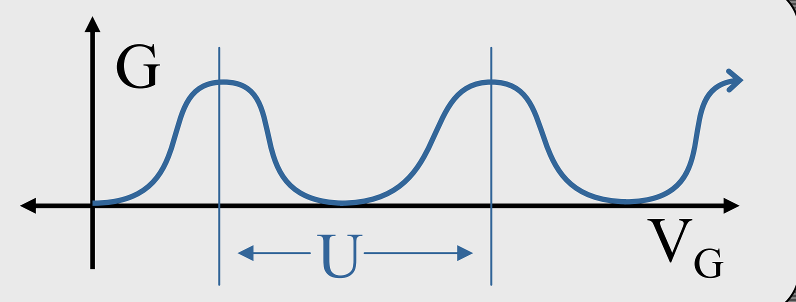


- As current flows say the spin up gets filled first and pushes up the energy level of spin down as the bottom figure illustrates. So what's happening is the splitting of up and down spin levels and this is what's called coulomb blockade.
- Note: for small devices $U = q^2/C_T$ can become very large as $C_T$ becomes very small, hence affecting the condition $U >> k_B T + \gamma$ under which Coulomb Blockade occurs

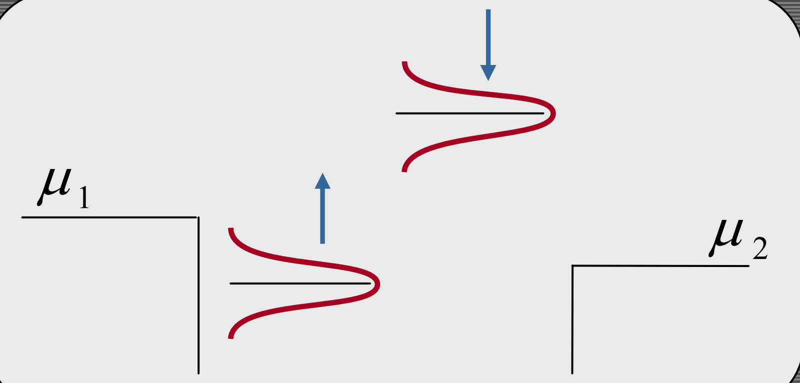
- An example:

$$\frac{q^2}{C_T} = \frac{1.6\times10^{-19}C^2}{10^{-18}F} = 0.16eV$$

Coulomb Blockade G vs. $V_G$




Coulomb Blockade: Spreading of Spin Levels



# Conclusions



- Primary Equations are:

(A)
$$N = 2\int dE \cdot D_{\varepsilon}\left(E - U_{\text{scf}}\right)\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

(B)
$$U_{\text{scf}} = U_{\text{ext}} + \frac{q^2}{C_T}\left(N - N_0\right)$$

And
$$I = \frac{2q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}\int dE \cdot D_{\varepsilon}(E - U_{\text{scf}})\left(f_1 - f_2\right)qV$$

- (A) and (B) must be solved self consistently.
- One further point: the effect of $U_{ext} = C_G/C_T(-qV_G) + C_D/C_T(-qV_D)$ can be quite dramatic. There are many important factors in electrostatics which can create very different I-V curves.

# Questions & Answers