Quantum Transport:
Atom to Transistor

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Lecture 2: What Makes Electrons Flow?

Ref. Chapter 1.2

Network for Computational Nanotechnology

NCN nanoHUB online simulations and more

Retouch on Concepts

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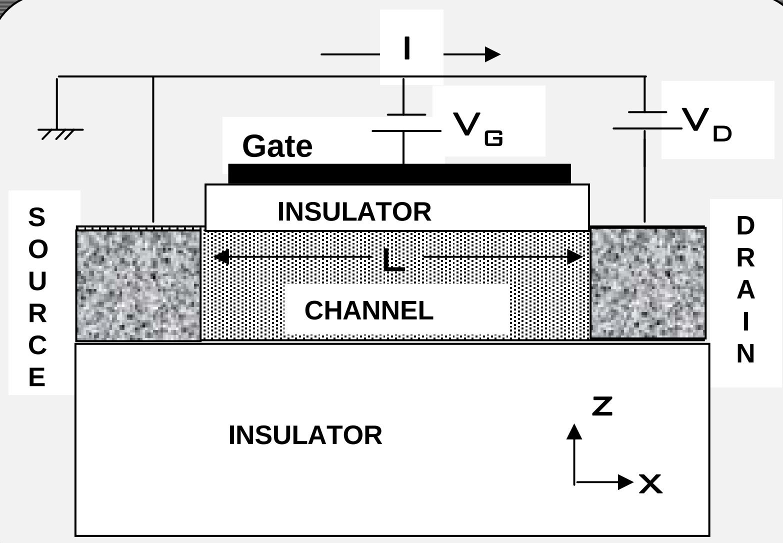
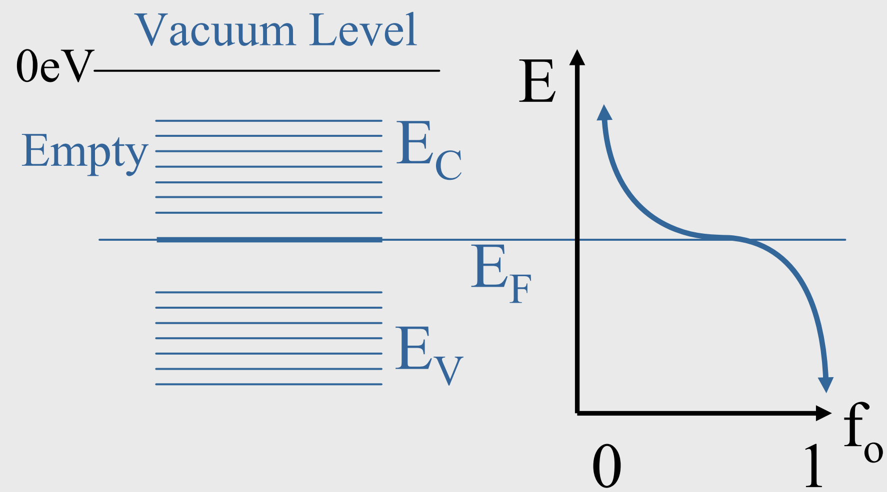
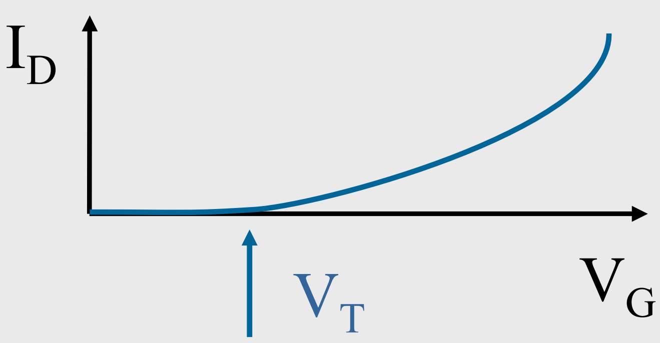
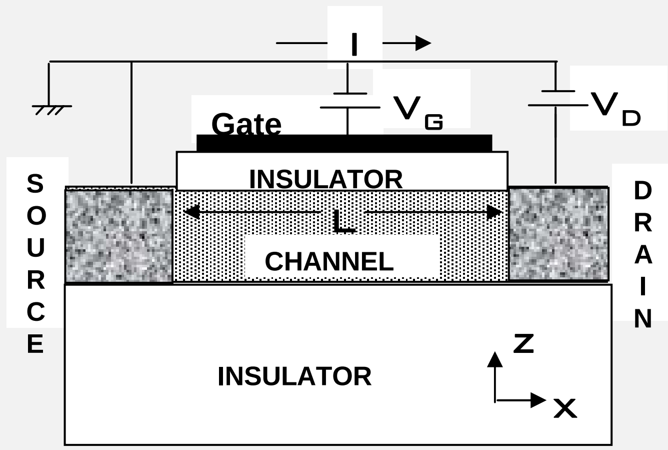


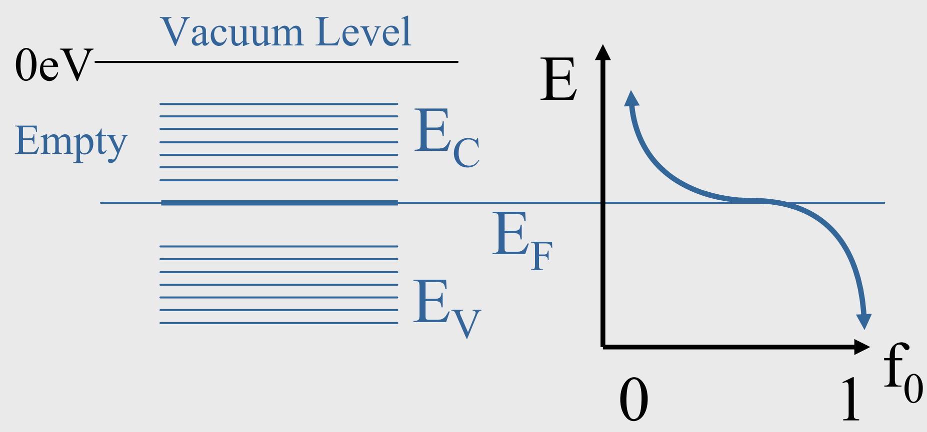




- Key Concepts: V_D and V_G Bias, Empty and full energy levels, Threshold voltage V_T, and Fermi energy
- Basic Fermi function centered at E=0: $f_0(E) = 1/(e^{E/k_BT} + 1)$. To get it centered at Ef, one could shift it in energy: $f_0(E-E_F)$

Retouch on Concepts





- Pauli Exclusion Principle allows two electrons per energy level (one spin up and one spin down)

- Positive gate voltage lowers these levels and negative gate voltage raises them

- At equilibrium, there is no bias voltage between the source and drain, the Fermi energy is fixed at the same level in source, channel and drain
- **Very Important**: The amount of current flow does not depend on number of electrons. It is the amount of states around the Fermi energy that determines how much current flows.

Band Diagram for a Simple Molecule

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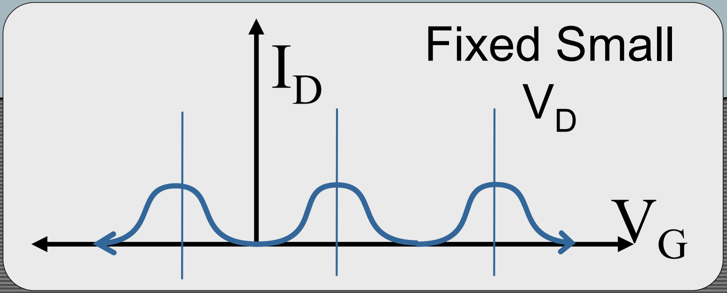
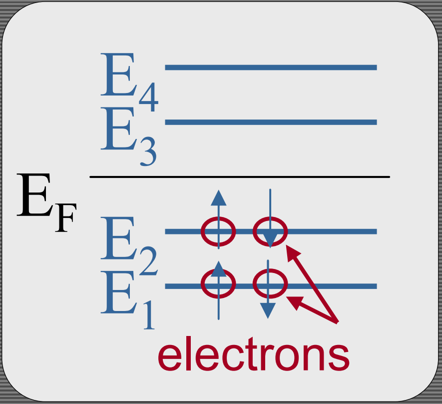
• Consider a simple system with wide spacing of electron energy levels (a small molecule)

• 4 electrons in the system considering spin up and down fill the first 2 energy levels.

• The Fermi energy is a level for which at T=0K the levels below it are full and the levels above it are empty. For our system at 0 K, the Fermi level will be half way between levels 2 and 3.

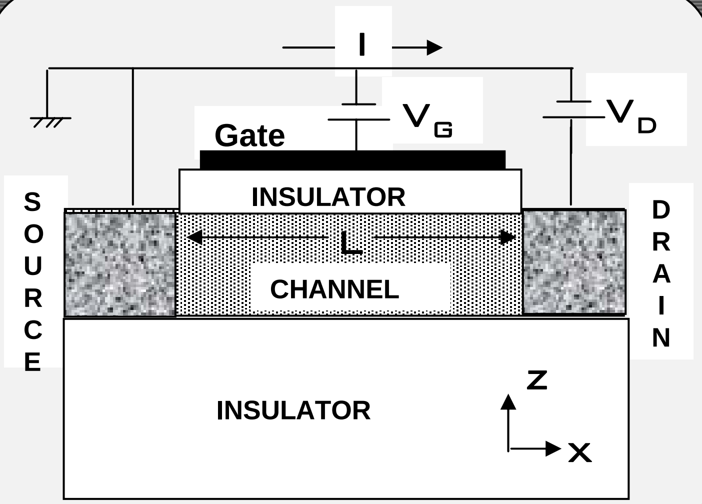


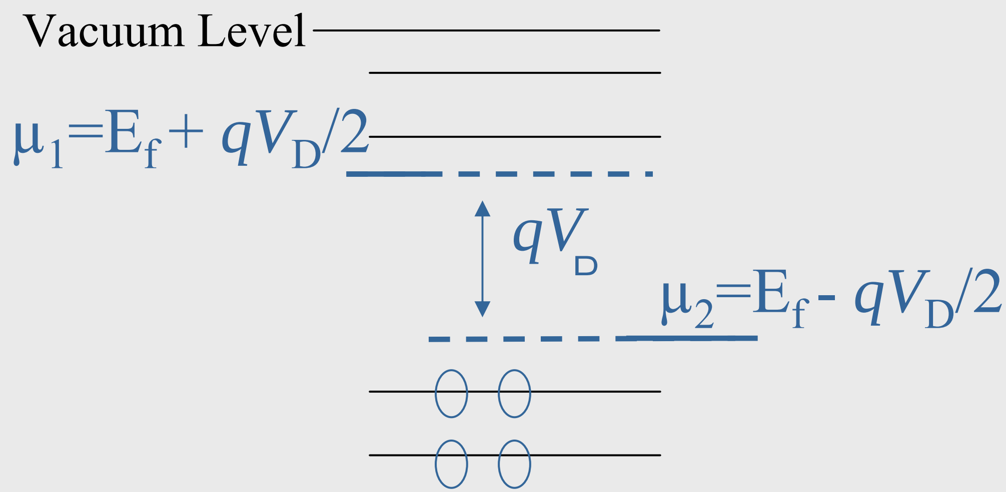
• The smaller the system, the more the spacing between the energy levels.



• The picks observed in the current are due to the overlap of energy levels and the Fermi level: As the gate voltage is applied these energy levels move up or down based on the sign of the voltage; hence they cross over the Fermi level and the result will be higher current because of higher availability of states at the Fermi energy.

Away from Equilibrium





- When V_D is applied between the source and drain, system is driven out of equilibrium; the Fermi energies in the source and drain will not be at the same level any more.
- Total energy difference between the two Fermi levels (chemical potentials) μ_1 and μ_2 is qV_D.
- i.e. $1V \times q = 1eV = 1.6 \times 10^{-19}$J

- The reason why the shift in Fermi levels is symmetric will be discussed later. For now consider the fact that division of voltage is very important for large bias but not so important for small bias which is in fact the case here.

Current Flow due to Difference in Agenda

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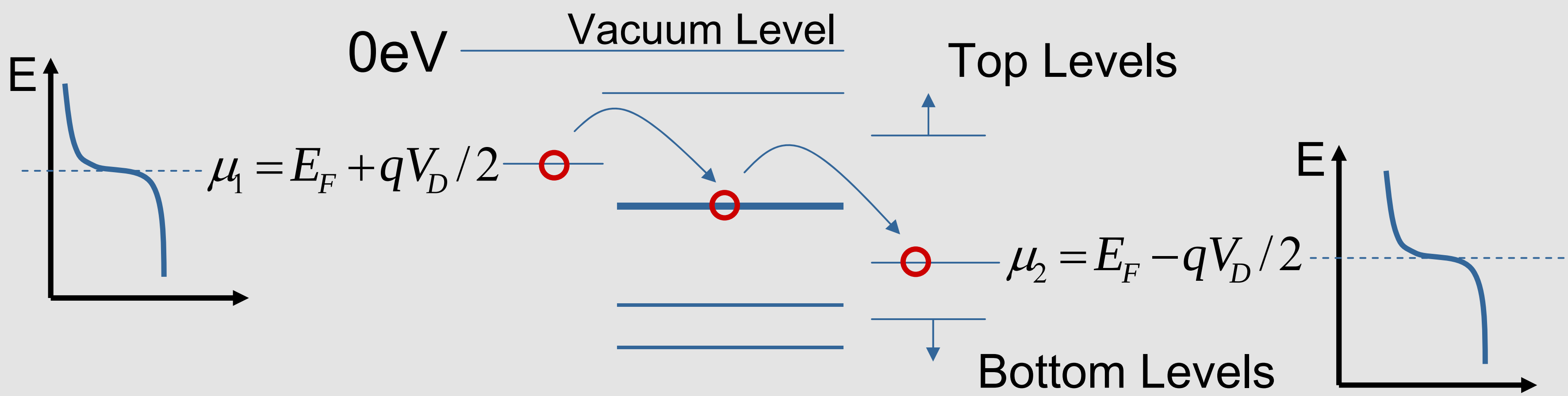


- If you do not have any levels between μ1 and μ2 then current will not flow
- If you have a level between μ1 and μ2 current will flow because left side (at μ_1) keeps filling up the level and right side (at μ_2) keeps emptying it.

- Why **don't** bottom and top levels contribute to current? Since we have two different Fermi levels, we have two different Fermi functions. Consider their value for high energies and for low energies; you'll find that they have the same value of 0 (For high E) and 1 (For low E) - In other words, **both contacts have the same agenda** for these levels; hence no current flow due to these levels.

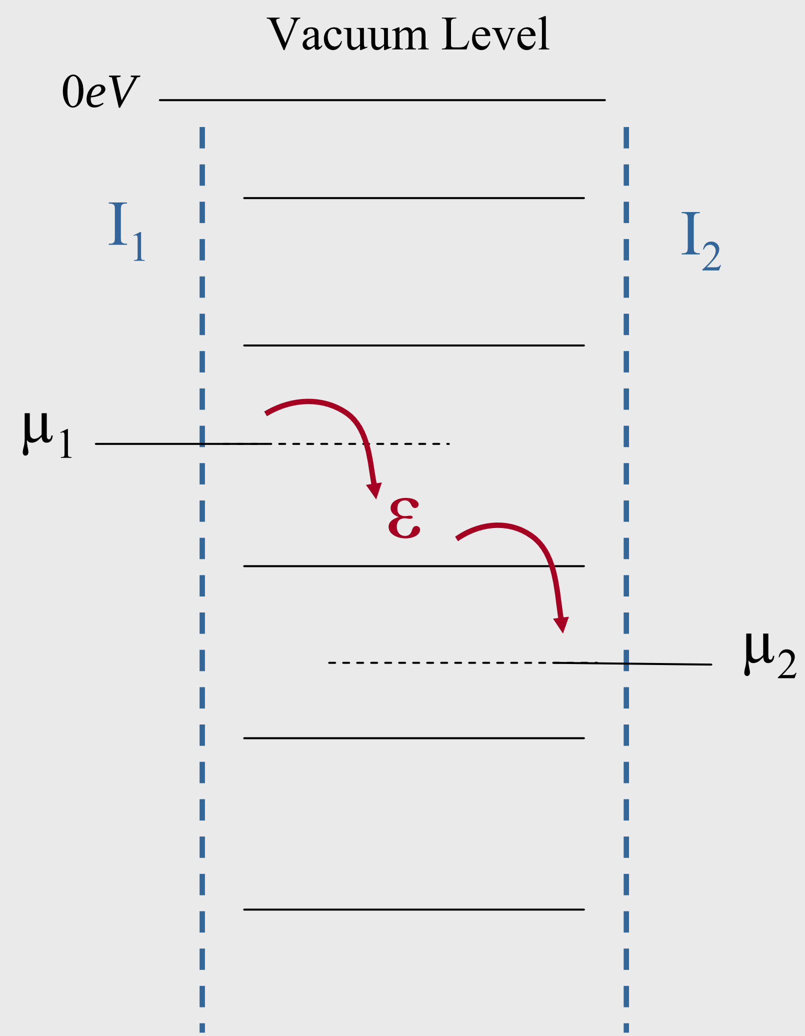
Average Number of Electrons

- What is the average number of electrons in the level ε ?

- N_1: the average number of electrons that the *left* contact would like to see
  - $N_1 = 2f_1(\varepsilon) = 2f_0(\varepsilon - \mu_1)$

- N_2: the average number of electrons that the *right* contact would like to see
  - $N_2 = 2f_2(\varepsilon) = 2f_0(\varepsilon - \mu_2)$

- Note: factor of two is due to the fact that we can put two electrons of up and down spin in the same level.



Current Flow Left and Right

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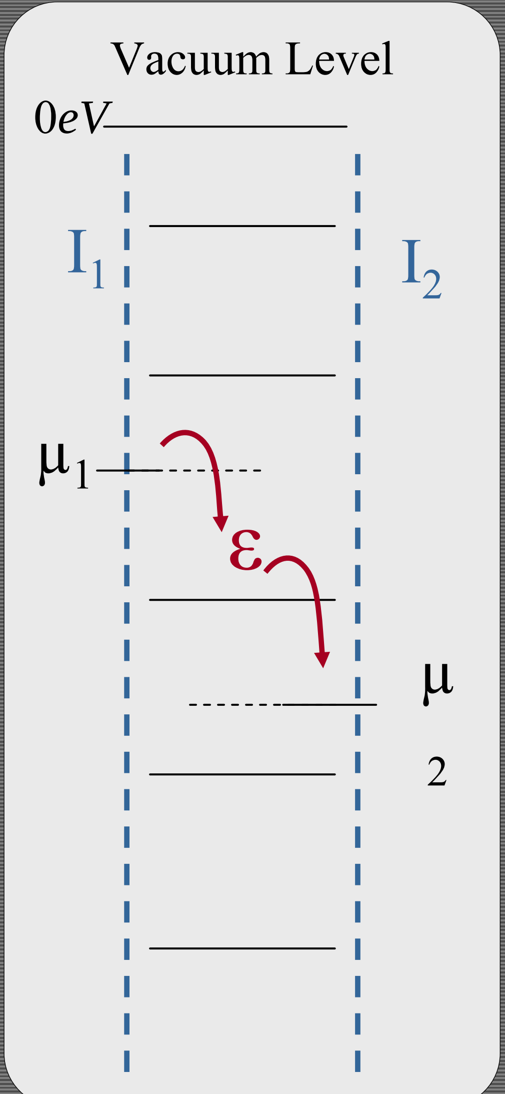
- N is the actual number of electrons at steady state in the channel
- Current from left side: $I_1 = q\dfrac{\gamma_1}{\hbar}(N_1 - N)$

  Where $\gamma_1/\hbar$ is the rate at which electrons cross from μ_1 to ε.
- Current to right side: $I_2 = q\dfrac{\gamma_2}{\hbar}(N - N_2)$

  Where $\gamma_2/\hbar$ is the rate at which electrons cross from ε to μ_2 .
- $\hbar = h/2\pi = 1.06\times10^{-34}\ J\cdot\sec$
- So $\gamma_1 + \gamma_2$ are in units of Joules
- Take $\gamma_1 = 1meV$, we have:

$$\gamma_1/\hbar = \frac{1.6\times10^{-19}\times10^{-3}\ J}{1.06\times10^{-34}\ J\cdot\sec} \cong 10^{12}/\sec$$

Therefore, it takes ~1 pico second for electrons to escape into the channel



Steady State Current

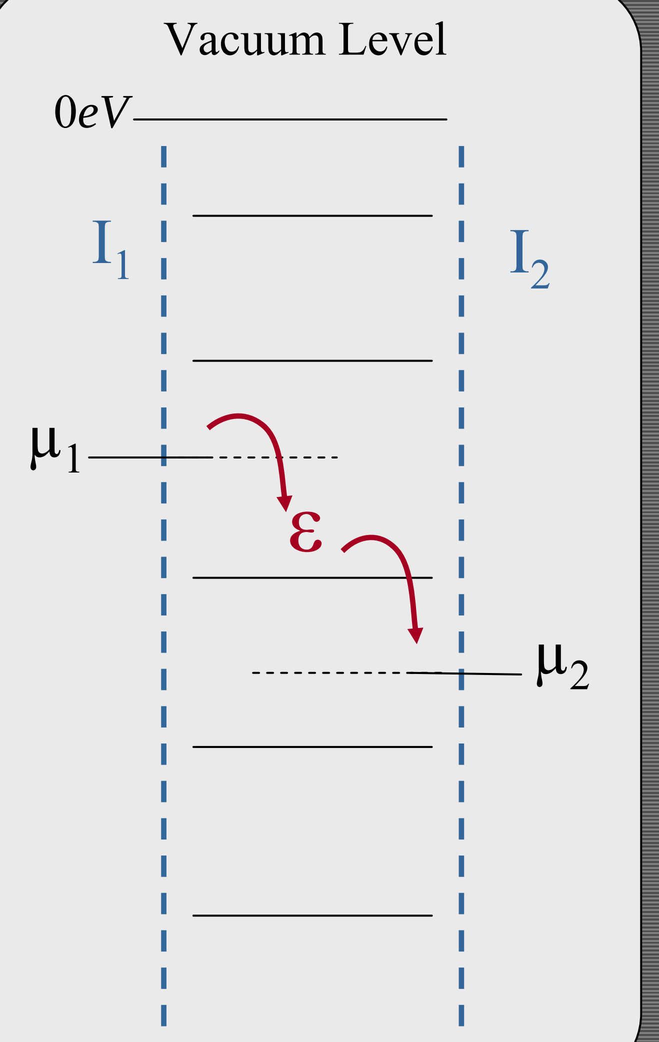
- Equating I_1 and I_2 for a steady state solution we get

$$N = \frac{\gamma_1 N_1 + \gamma_2 N_2}{\gamma_1 + \gamma_2}$$

- $$\therefore I = I_1 = I_2 = \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}(N_1 - N_2)$$

$$= \frac{2q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}[f_1(\varepsilon) - f_2(\varepsilon)]$$

- Remember, in order for current to flow, f_1 must differ from f_2
- N-Type conduction: Go through a level that is *empty at equilibrium*
- P-Type conduction: Go through a level that is *full at equilibrium*



Current at Small Voltages

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- Use Taylor expansion to get an expression for current at small voltages:

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

$f_2(\varepsilon) = f_0(\varepsilon - \mu_2)$ therefore:

$f_1 - f_2 = (df_0 / dE)(\mu_2 - \mu_1)$

$= -(df_0 / dE)\, qV_D$

Therefore for small voltages:

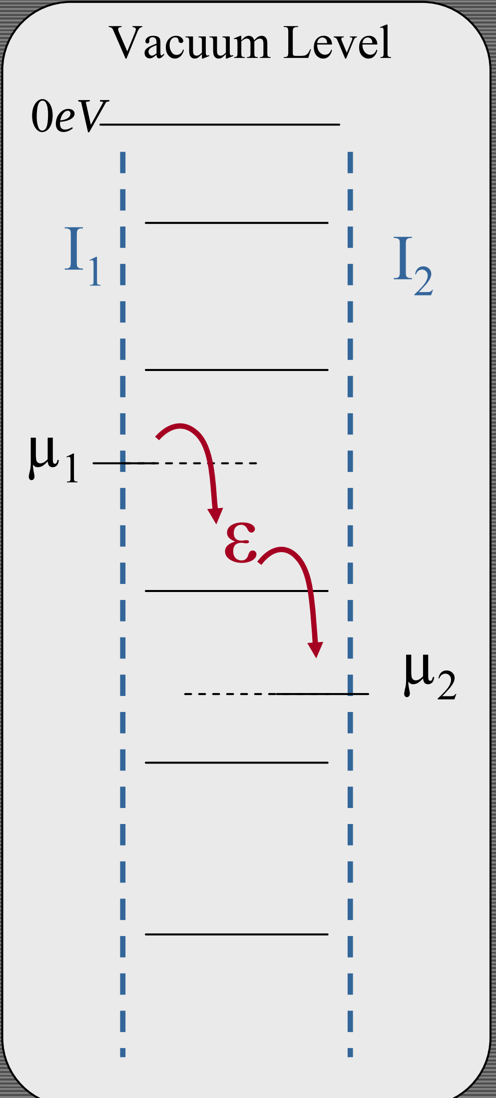
$$I = \frac{2q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}[f_1(\varepsilon) - f_2(\varepsilon)] = V\,\frac{2q^2}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\left[-\frac{df_0}{dE}\right]_{E=\varepsilon-E_f}$$

Use $E = \varepsilon - E_f$ since $\mu_1 = E_f + qV_D/2$ and $\mu_2 = E_f - qV_D/2$

- Note: $2q^2/\hbar$, dimensions of conductance

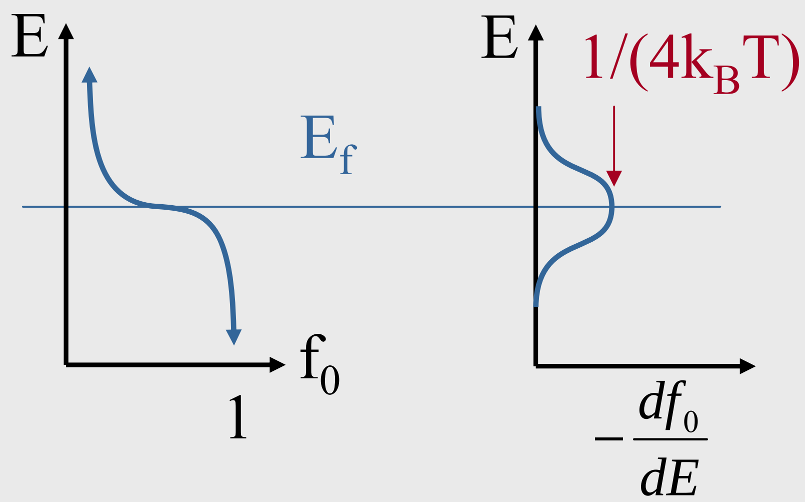
$\dfrac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}$, dimensions of energy

$\left[\dfrac{df_0}{dE}\right]_{E=\varepsilon-E_f}$, dimensions of inverse energy



No Upper Limit?

What does $-\frac{df_0}{dE}$ look like?



Peak $\cong 1/(4kBT)$; Width $\cong$ kBT Area = 1.
As t→0, it can be approximated as a delta function.

- From the equation

$$I = V\frac{2q^2}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\left[-\frac{df_0}{dE}\right]_{E=\varepsilon-E_f}$$

it would appear that there is no upper limit on the conductance

$$\frac{2q^2}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\left[-\frac{df_0}{dE}\right]_{E=\varepsilon-E_f}$$

- However, this is not true. An upper limit does occur due to **energy broadening.** The maximum value of conductance for one level device is:

$$\frac{2q^2}{h}\cong 77.4\,\mu S \cong 1/12.9\,k\Omega$$

…to be discussed in more detail next