Quantum Transport: From Atoms to Transistors

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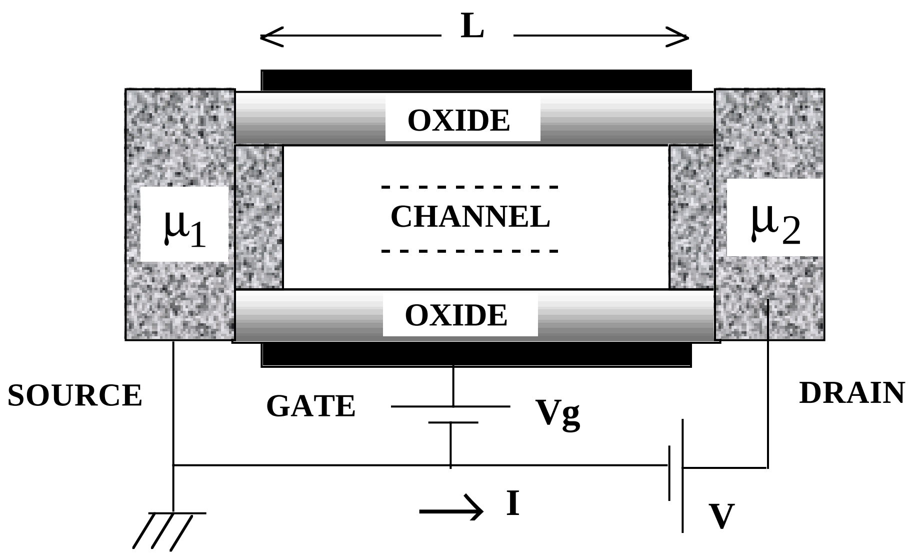
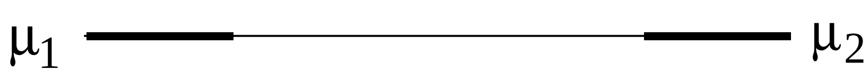
Outline

- Equilibrium
- Current flow as a balancing act
- Broadening
- Charging
- Coulomb blockade
- Capacitance
- Conductance
- Transistors
- Summary: Basic equations

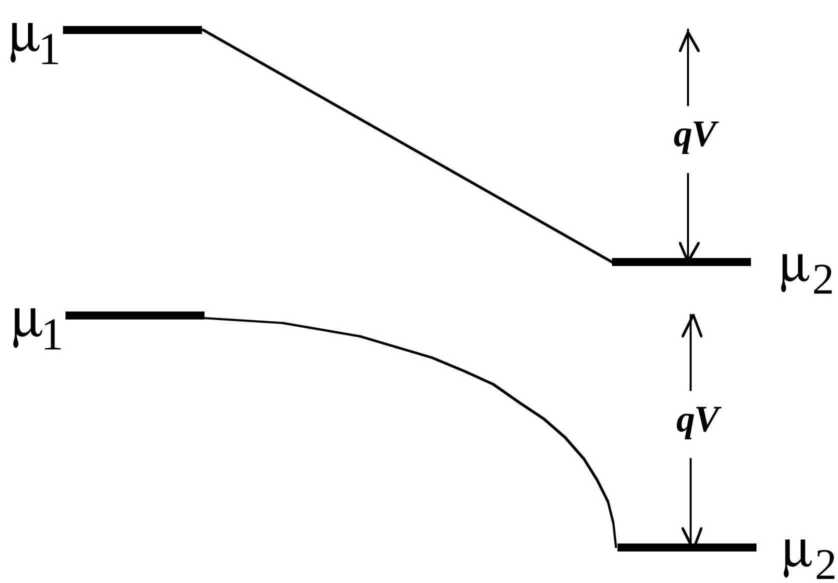
Nanoscale Transistor



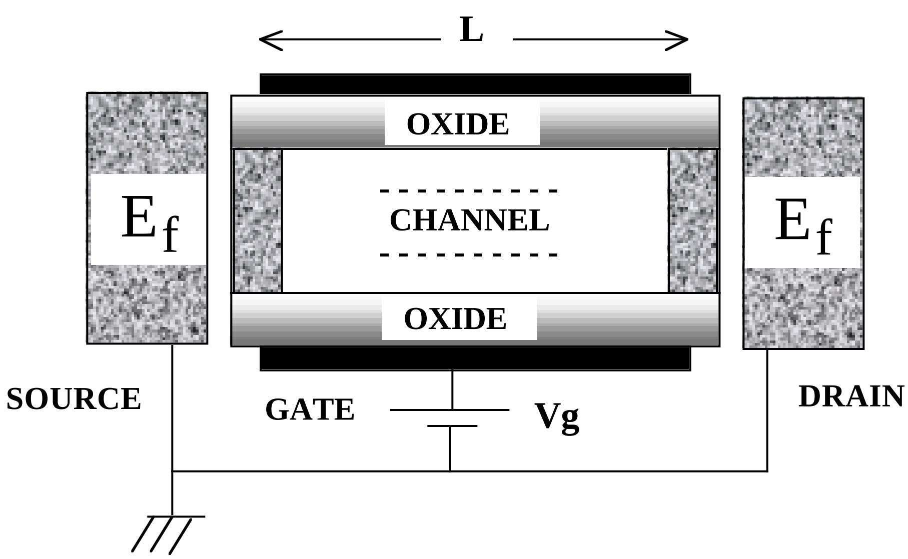
Zero bias, V = 0

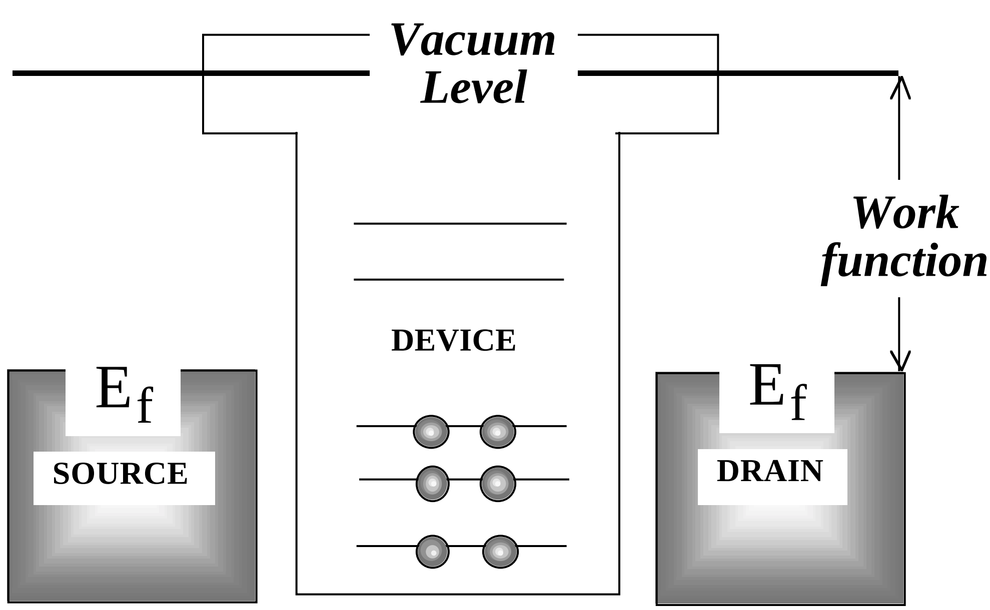


V ≠ 0

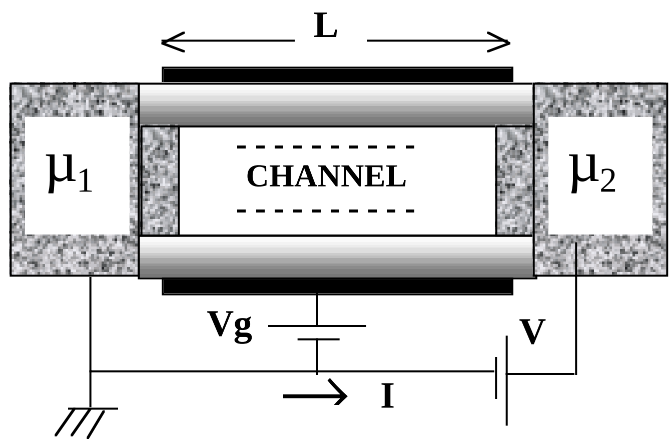


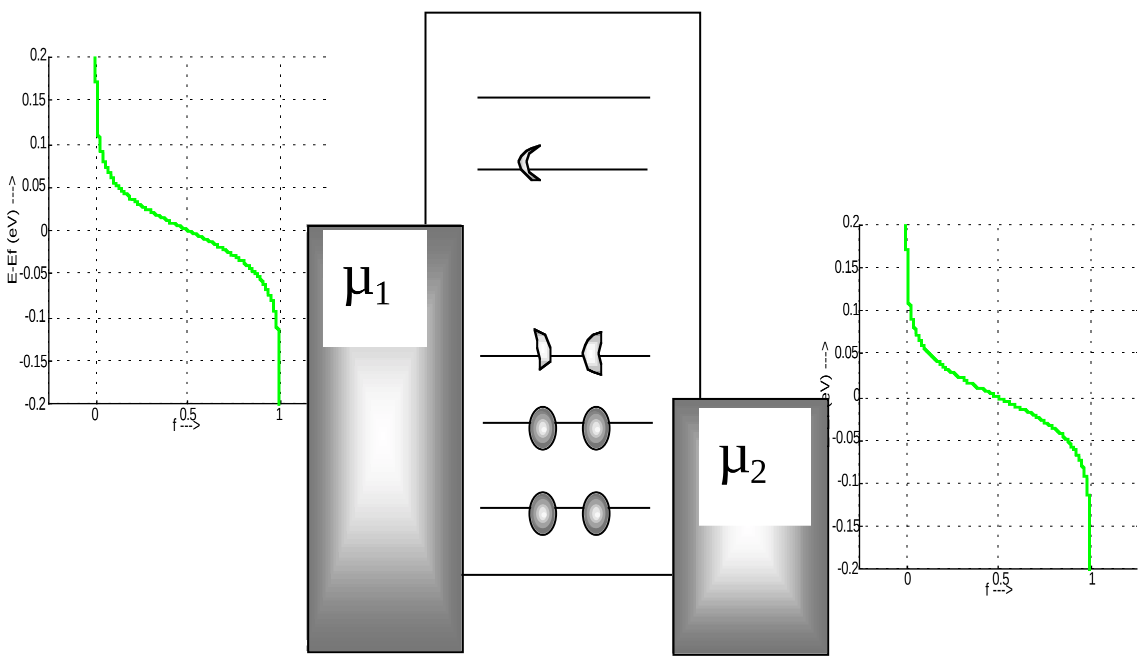
Equilibrium





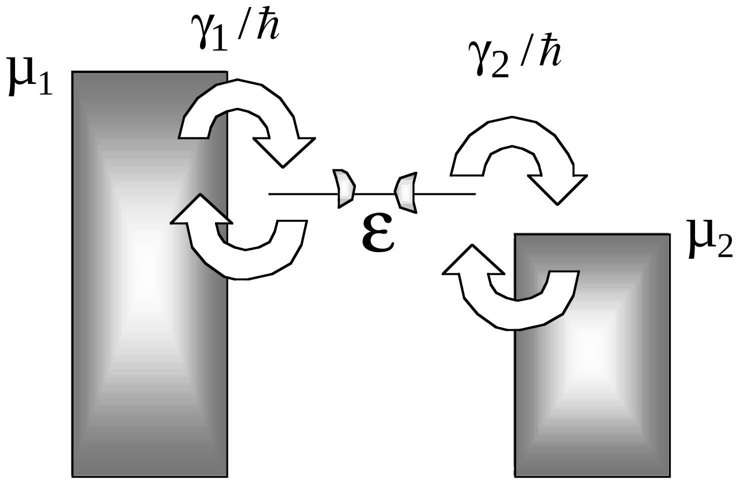
Current flow as a “balancing act”





$$\mu_1 = E_f + (qV/2) \qquad \mu_2 = E_f - (qV/2)$$

One-level Model



$$N_1 = 2\, f_1(\varepsilon) \qquad\qquad N_2 = 2\, f_2(\varepsilon)$$

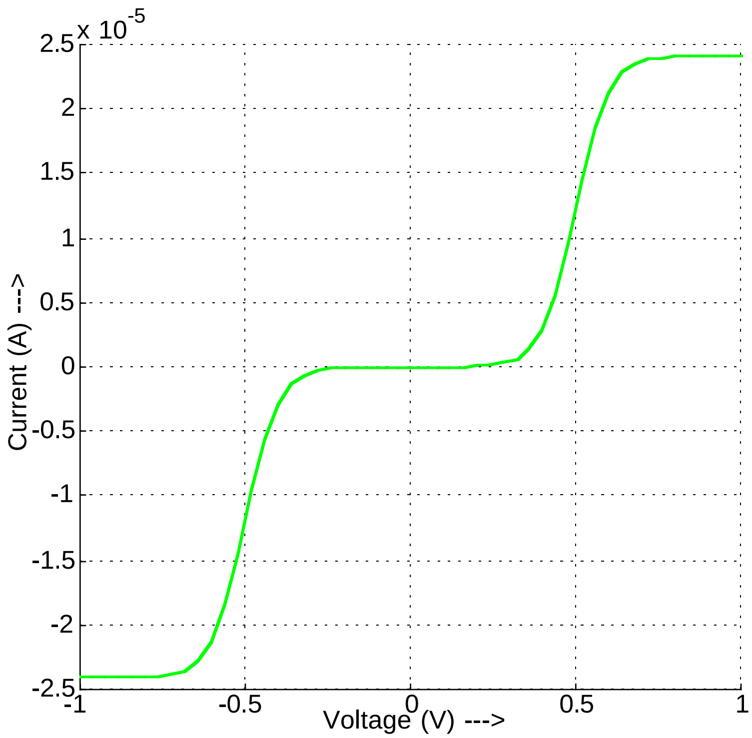
$$I_1 = q\frac{\gamma_1}{\hbar}(N_1 - N) \qquad\qquad I_2 = q\frac{\gamma_2}{\hbar}(N - N_2)$$

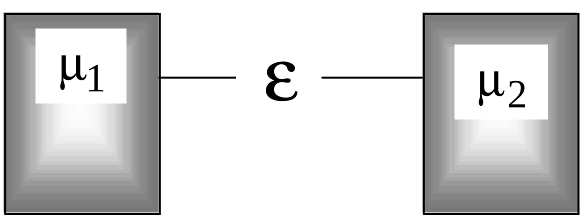
$$N = \frac{\gamma_1 N_1 + \gamma_2 N_2}{\gamma_1 + \gamma_2}$$

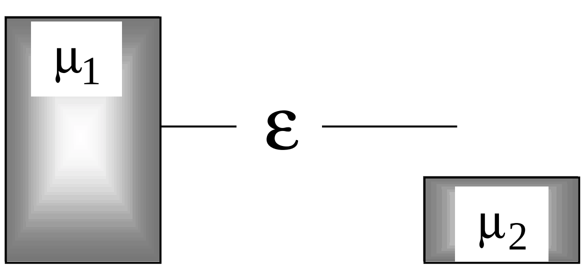
$$I = I_1 = I_2 = \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}(N_1 - N_2)$$

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

One-level Model:
Current (I) vs. Voltage (V)

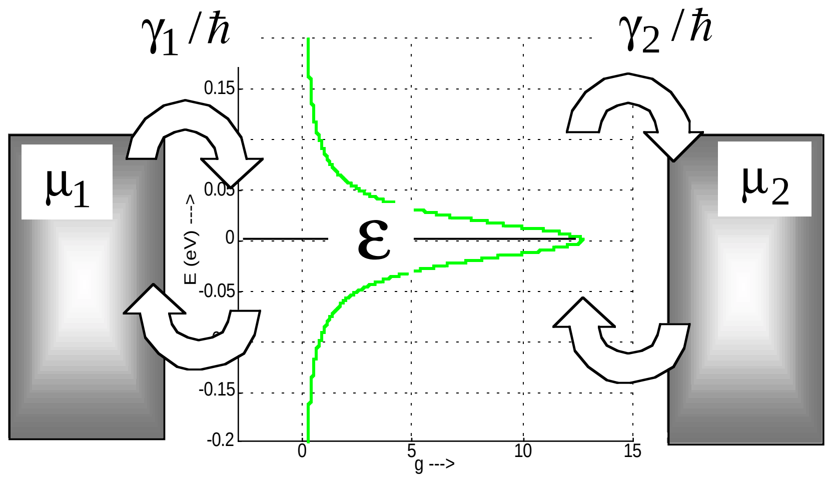






$\mu_1 = E_f + (qV/2)$,
$\mu_2 = E_f - (qV/2)$,
$E_f - \varepsilon = 0.25\ \mathrm{eV}$,
$\gamma_1 = \gamma_2 = 0.1\,\mathrm{eV}$

Broadening



$$\gamma = \gamma_1 + \gamma_2$$

$$D(E) \quad = \quad \frac{\gamma/2\pi}{(E-\varepsilon-\Delta)^2 + (\gamma/2)^2}$$

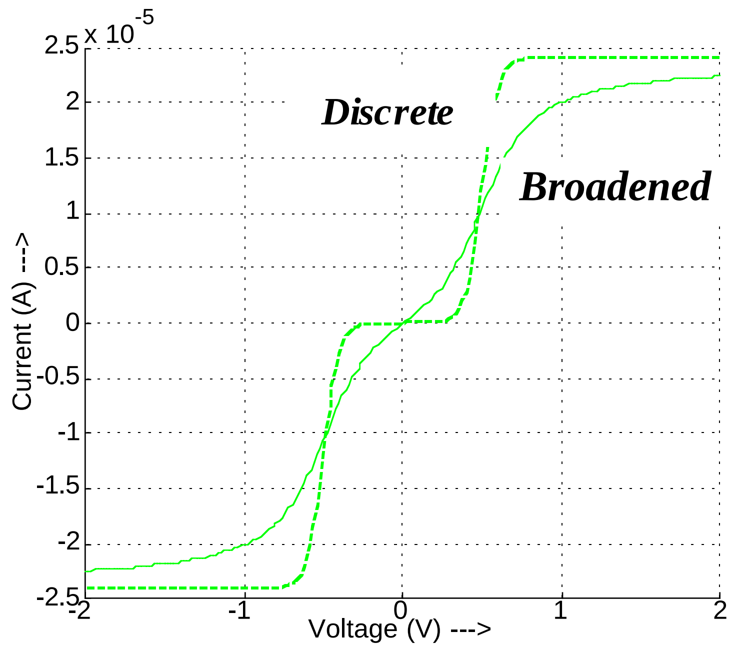
$$I \quad = \quad \frac{2q}{\hbar}\,\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\,[f_1(\varepsilon) - f_2(\varepsilon)]$$

$$I \quad = \quad \frac{2q}{\hbar}\int_{-\infty}^{+\infty} dE\; D(E)\;\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\,[f_1(E) - f_2(E)]$$

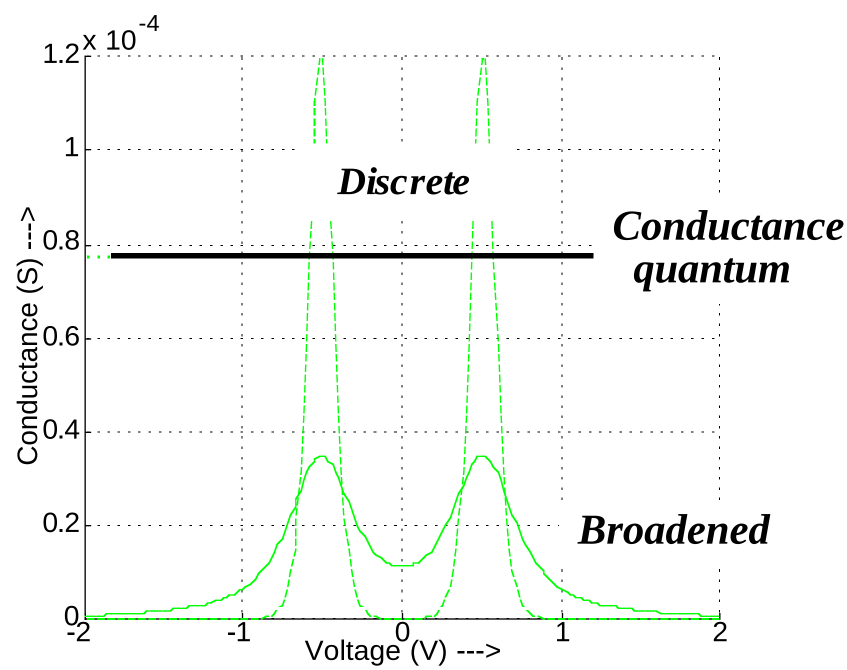
$$N \quad = \quad \frac{\gamma_1 f_1(\varepsilon) + \gamma_2 f_2(\varepsilon)}{\gamma_1+\gamma_2}$$

$$N \quad = \quad \int_{-\infty}^{+\infty}\frac{dE}{2\pi}\;D(E)\;\frac{\gamma_1 f_1(E) + \gamma_2 f_2(E)}{\gamma_1+\gamma_2}$$

One-level Model:
Current (I) vs. Voltage (V)



$E_f - \varepsilon = 0.25\,\text{eV}$,
$\gamma_1 = \gamma_2 = 0.1\,\text{eV}$

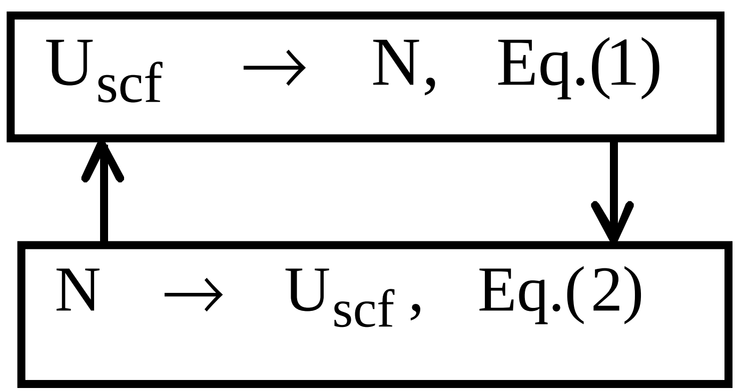


Charging

$$\varepsilon \quad \rightarrow \quad \varepsilon + U_{scf}(N)$$

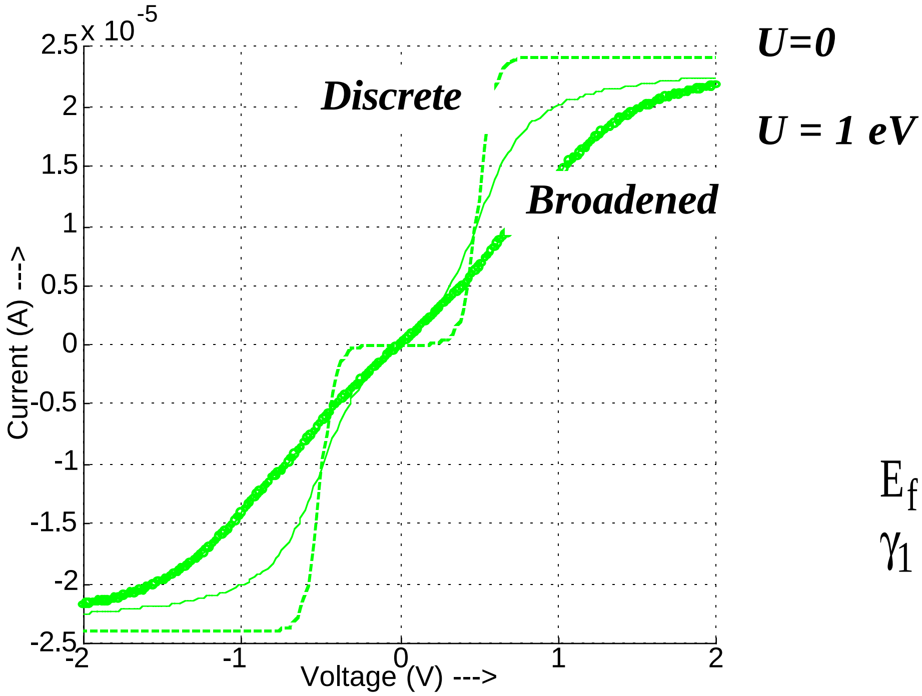
$$D(E) \quad = \quad \frac{\gamma/2\pi}{\left(E - \varepsilon - U_{scf} - \Delta\right)^2 + \left(\gamma/2\right)^2}$$

(1) $$N \quad = \quad \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \; D(E) \; \frac{\gamma_1 f_1(E) + \gamma_2 f_2(E)}{\gamma_1 + \gamma_2}$$

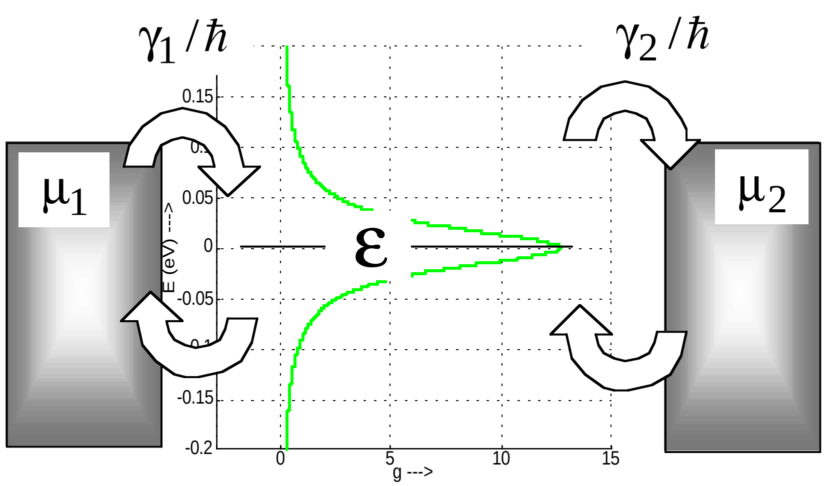


(2) $$U_{scf}(N) \quad = \quad U_a \quad + \quad U\,(N - N_{eq})$$

One-level Model:
Current (I) vs. Voltage (V)

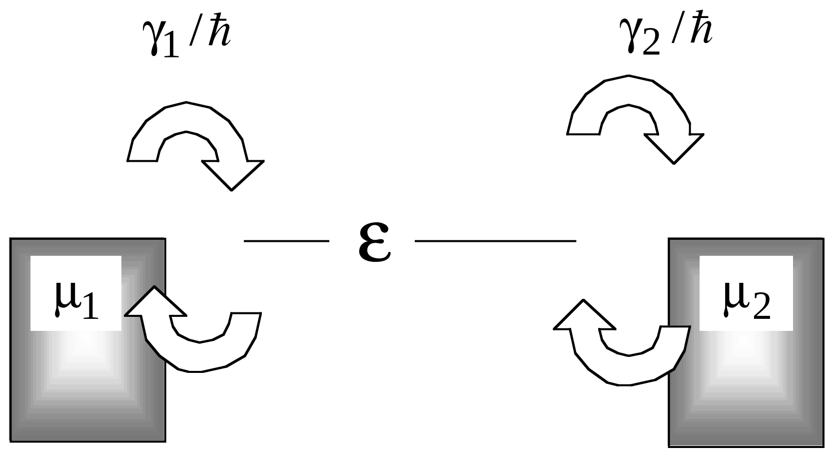


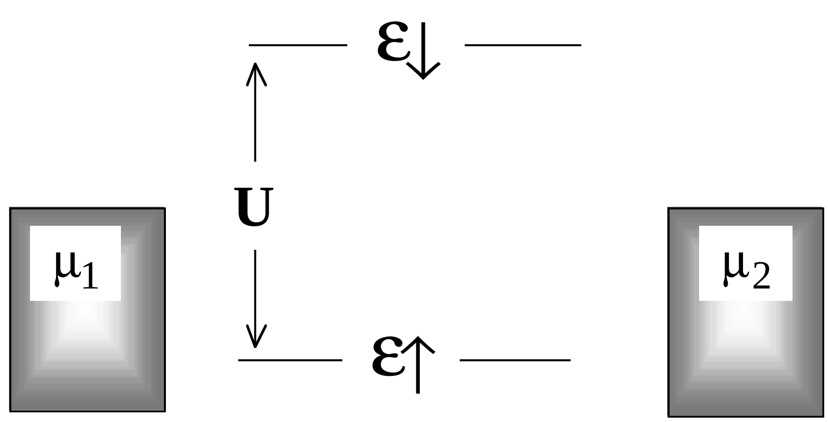
$$E_f - \varepsilon = 0.25\,\text{eV},$$
$$\gamma_1 = \gamma_2 = 0.1\,\text{eV}$$



$$U_{scf}(N) \quad = \quad U_a \quad + \quad U\,(N - N_{eq})$$

Coulomb Blockade

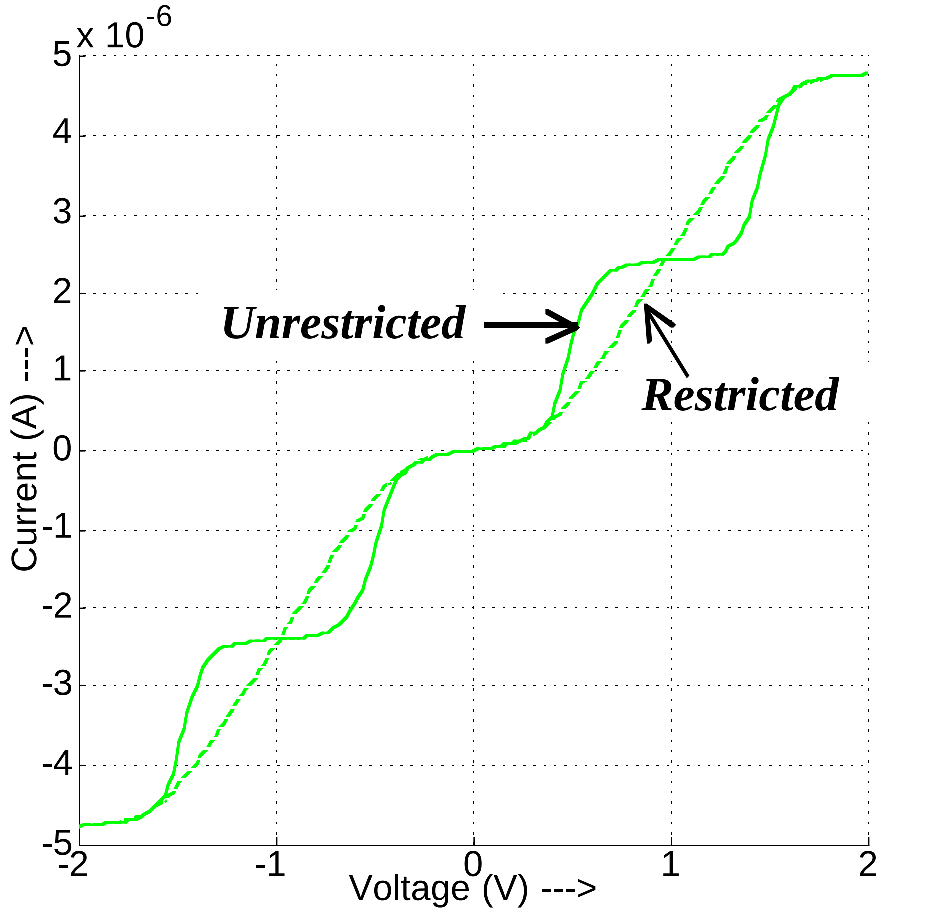




$$\varepsilon_{\uparrow} \;=\; \varepsilon + U\,N_{\downarrow}$$

$$\varepsilon_{\downarrow} \;=\; \varepsilon + U\,N_{\uparrow}$$

One-level model:
Restricted vs. Unrestricted



Unrestricted

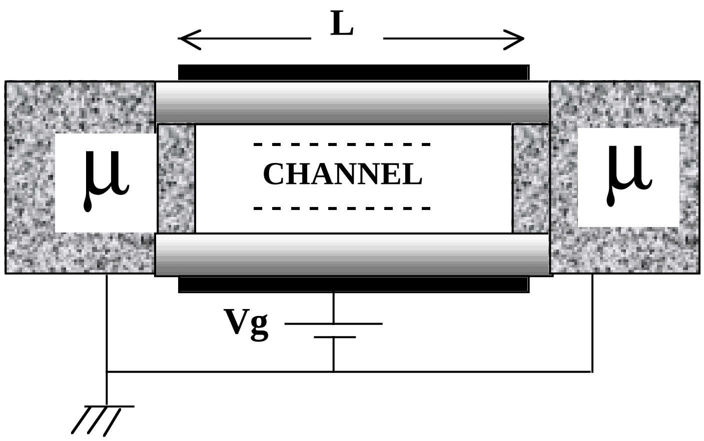
$$\varepsilon_\uparrow \;=\; \varepsilon + U\,N_\downarrow \qquad\qquad \varepsilon_\downarrow \;=\; \varepsilon + U\,N_\uparrow$$

Restricted

$$\varepsilon_{\downarrow,\uparrow} \;=\; \varepsilon + U\left(N_\downarrow + N_\uparrow\right)$$

Current (A) --->

Capacitance

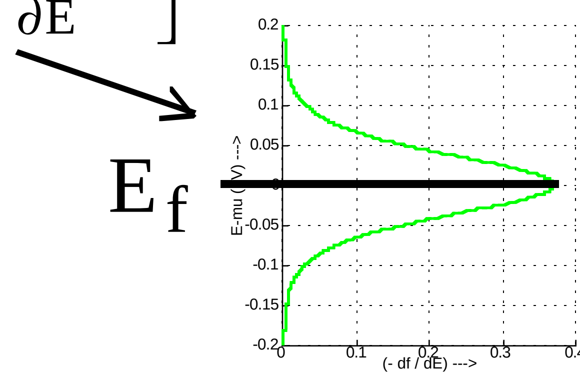


$$C \;\equiv\; q\left[\frac{\partial N}{\partial V_G}\right]_{V=0} \;=\; \frac{1}{\dfrac{1}{C_Q}+\dfrac{1}{C_E}}$$

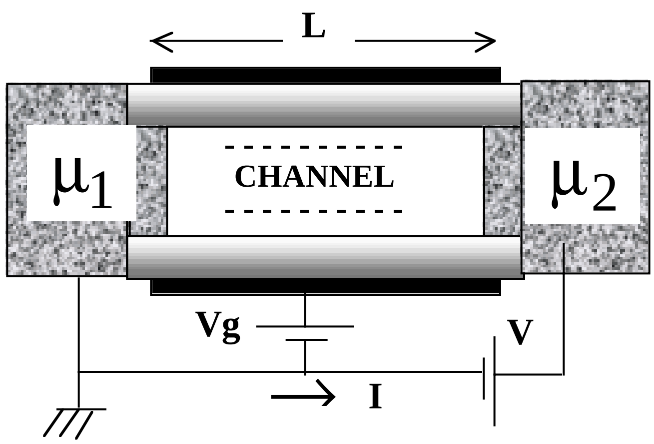
$$N \;=\; \int_{-\infty}^{+\infty} dE\;\; D(E)\, f_0(E-\mu)$$

$$C_Q \;\equiv\; q^2\,\frac{\partial N}{\partial \mu} \;=\; q^2\, D_0$$

$$D_0 \;\equiv\; \int_{-\infty}^{+\infty} dE\; D(E)\left[-\frac{\partial f_0\,(E-\mu)}{\partial E}\right]$$



Conductance

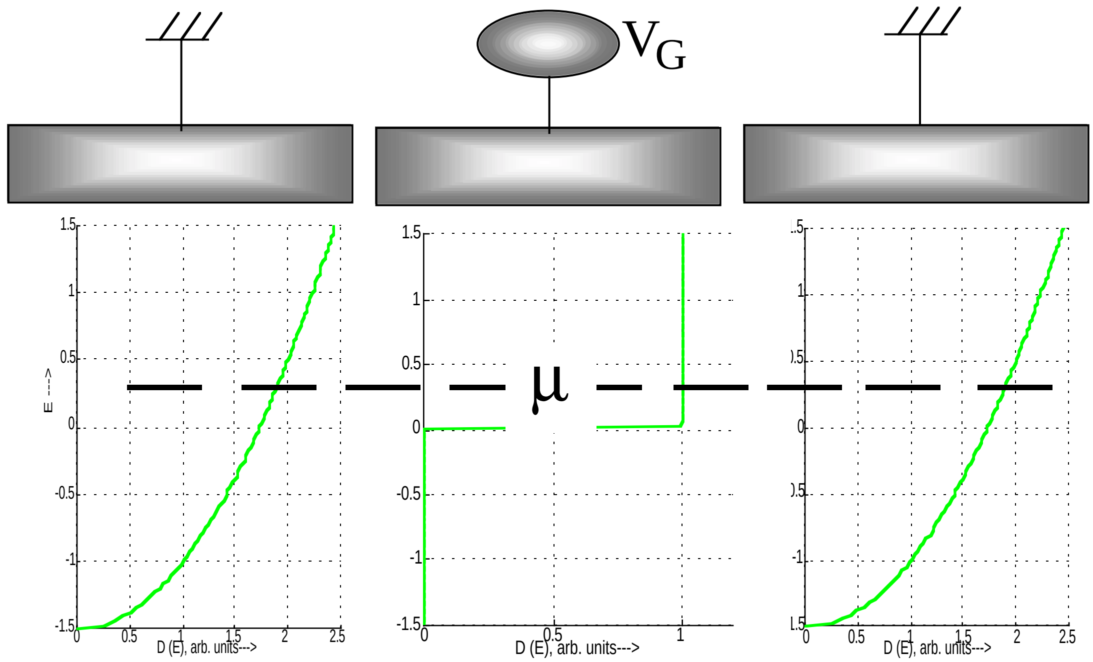


$$I = \frac{2q}{\hbar} \int_{-\infty}^{+\infty} dE \; \overbrace{D(E) \, \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}}^{\overline{T}(E)} \; [f_1(E) - f_2(E)]$$

$$R^{-1} \equiv \left[\frac{\partial I}{\partial V}\right]_{\text{fixed } V_G} = \frac{2q^2}{h} T_0$$

$$T_0 \equiv \int_{-\infty}^{+\infty} dE \; \overline{T}(E) \left[- \frac{\partial f_0 (E - \mu)}{\partial E} \right]$$

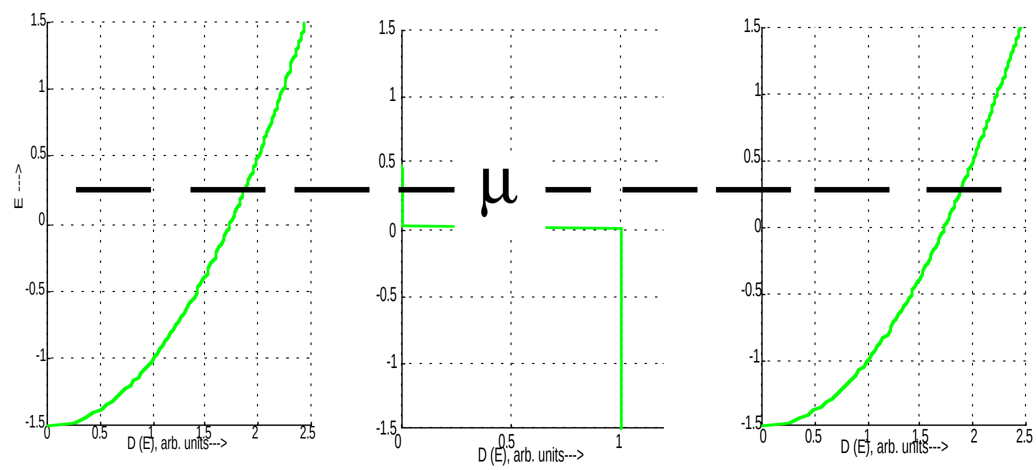
Transistors: n- and p- channel



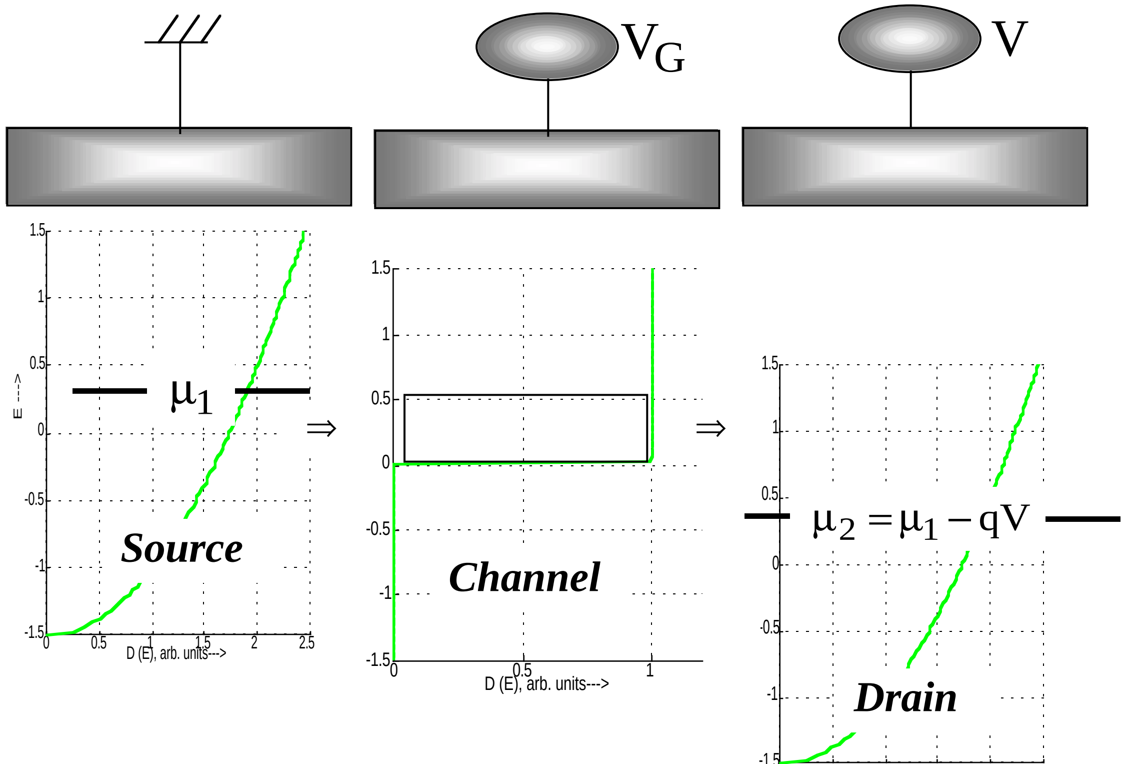
n- channel

Source ***Drain***

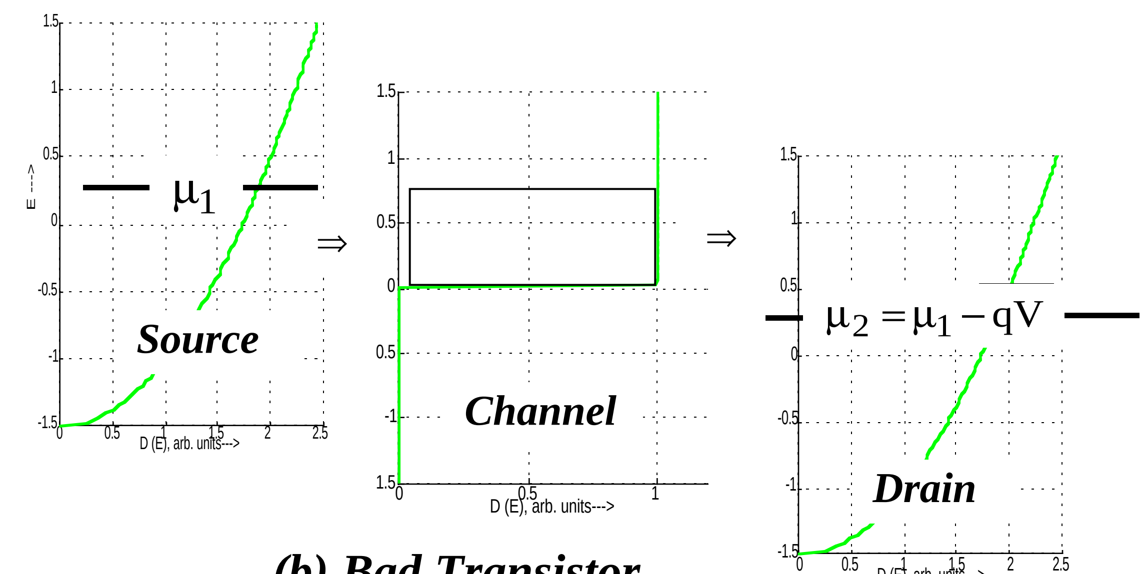
p- channel



“Good” transistors and “bad” transistors

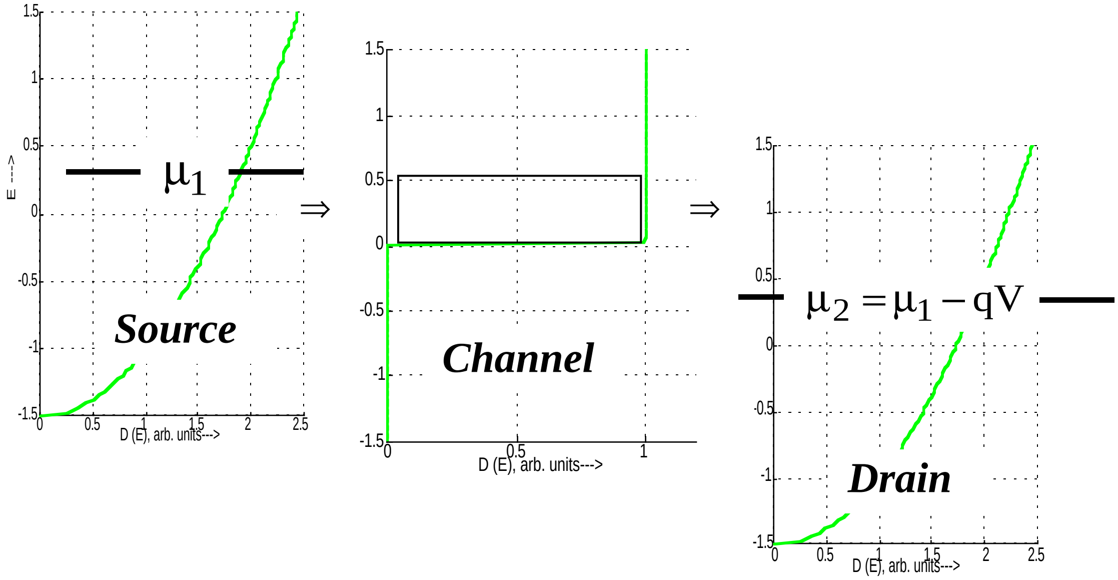


(a) Good Transistor



(b) Bad Transistor

“Good” transistor: On - current



$$I_{ON} = \frac{\langle v \rangle}{L} C\,(V_G - V_T)$$ ***Lundstrom, EDL (1997)***

$$I_{ON} = \frac{2q}{h} \int_{\varepsilon_0}^{\infty} dE\; f_1(E)$$

$$C\,(V_G - V_T) = qN_{eq} = q \int_{\varepsilon_0}^{\infty} dE\; D(E)\, f_1(E)$$

$$\Rightarrow q \int_{\varepsilon_0}^{\infty} dE\; \frac{2L}{\pi \hbar v(E)}\, f_1(E)$$

$$v(E) \Rightarrow \frac{L}{\pi \hbar D(E)}$$

One-level model:

Basic Equations

$$N = \int_{-\infty}^{+\infty} dE \; \left[D_1(E)\, f_1(E) + D_2(E)\, f_2(E) \right]$$

$$I = \frac{2q}{h} \int_{-\infty}^{+\infty} dE \; \overline{T}(E) \; \left[f_1(E) - f_2(E) \right]$$

$$2\pi\, D_1(E) = G\, \gamma_1\, G^*$$

$$2\pi\, D_2(E) = G\, \gamma_2\, G^*$$

$$\overline{T}(E) \equiv \gamma_1\, G\, \gamma_2\, G^*$$

$$G = \frac{1}{E - \varepsilon - U_{scf}(N) - \left(\Delta - i\gamma/2 \right)}$$

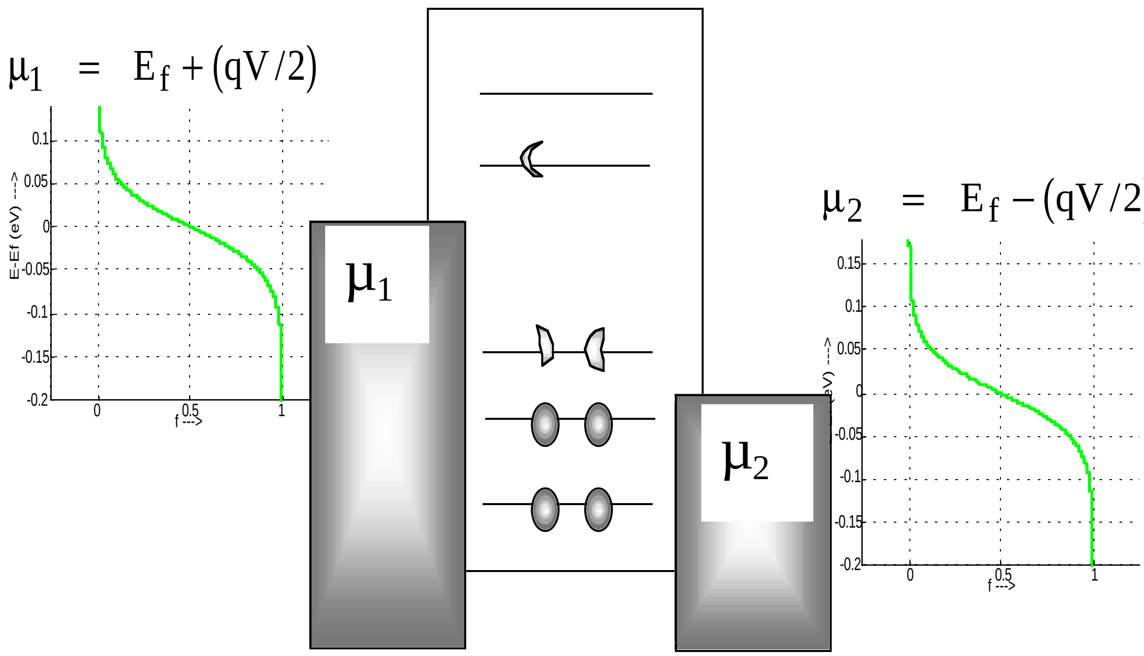
$$\Delta \equiv \Delta_1 + \Delta_2 \quad , \quad \gamma \equiv \gamma_1 + \gamma_2$$

One – level → Multi-level

Numbers → Matrices

$\mu_1 = E_f + (qV/2)$

$\mu_2 = E_f - (qV/2)$



$\varepsilon \rightarrow [H]$

$U_{scf} \rightarrow [U_{scf}]$

$\Delta_1 - i\gamma_1 \rightarrow [\Sigma_1(E)]$

$\Delta_2 - i\gamma_2 \rightarrow [\Sigma_2(E)]$

$N \rightarrow [\rho]$, ***Density matrix***

$2\pi D(E) \rightarrow [A(E)]$ ***Spectral function***

Multi-level Model:
Basic equations

$$[\rho] = \int_{-\infty}^{+\infty} dE \ \{ [A_1(E)] f_1(E) + [A_2(E)] f_2(E) \}$$

$$I = \frac{2q}{h} \int_{-\infty}^{+\infty} dE \ \bar{T}(E) \ [f_1(E) - f_2(E)]$$

$$A_1(E) = G \Gamma_1 G^+$$

$$A_2(E) = G \Gamma_2 G^+$$

$$\bar{T}(E) = \text{Trace}\left[\Gamma_1 G \Gamma_2 G^+\right]$$

$$G = \left[EI - H - U_{scf}([\rho]) - \Sigma_1 - \Sigma_2\right]^{-1}$$

Summary