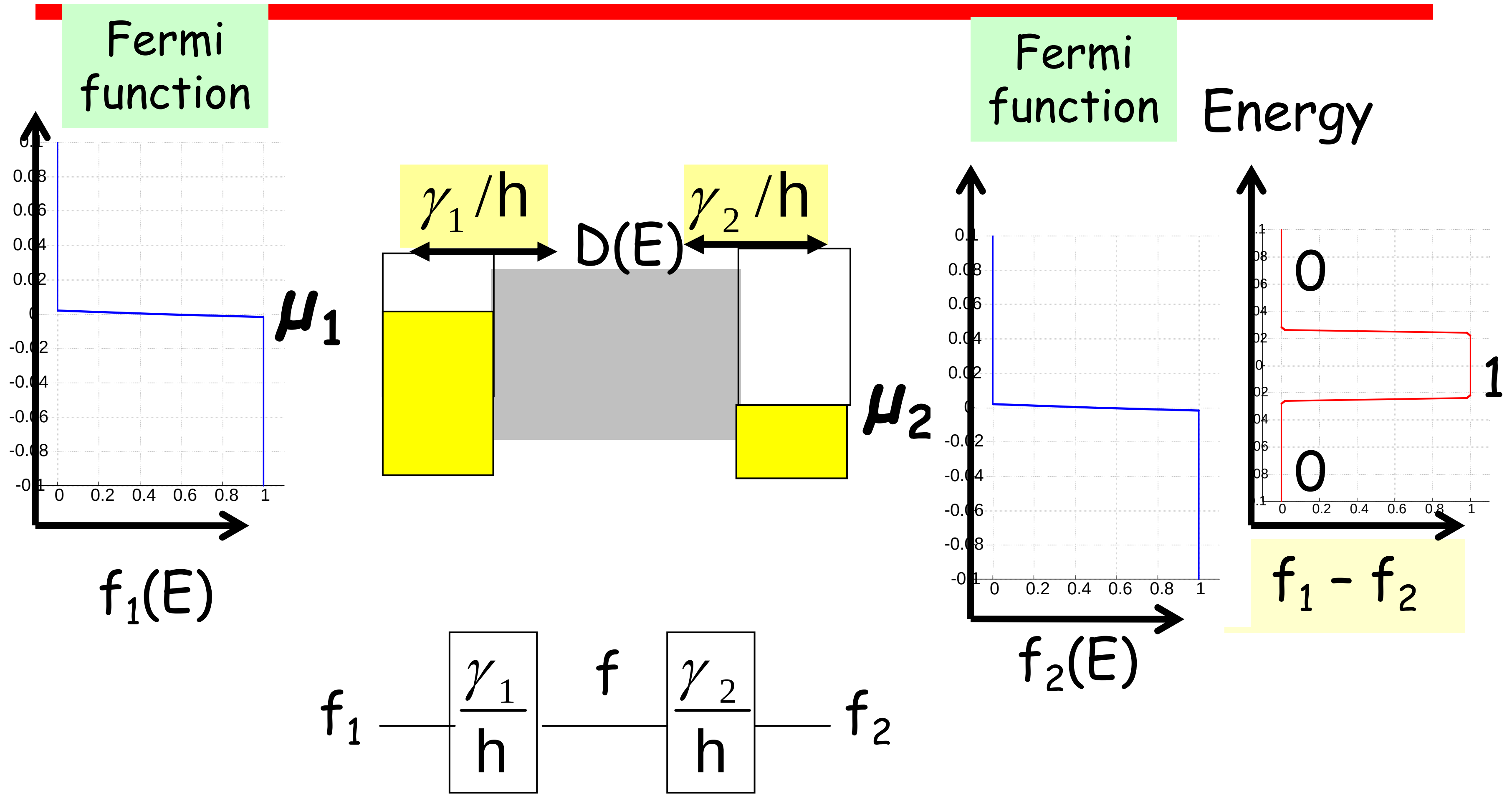
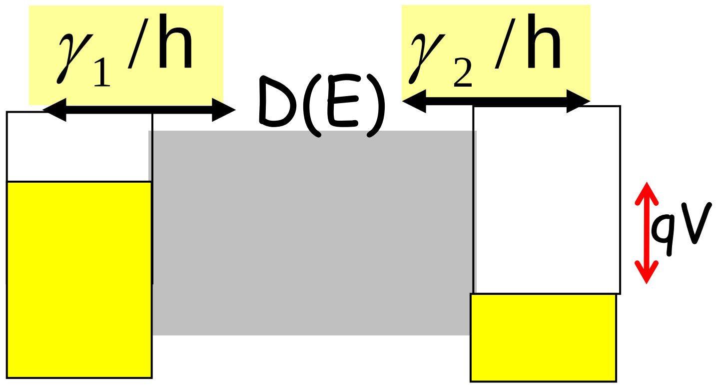
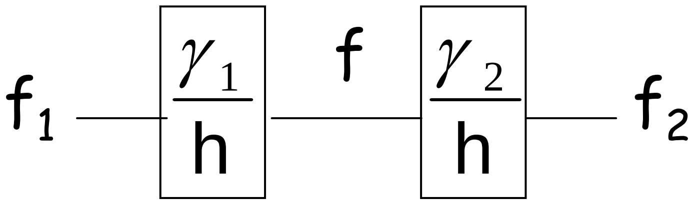
** Quantitative model



Quantitative model





$$f(E) = \left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

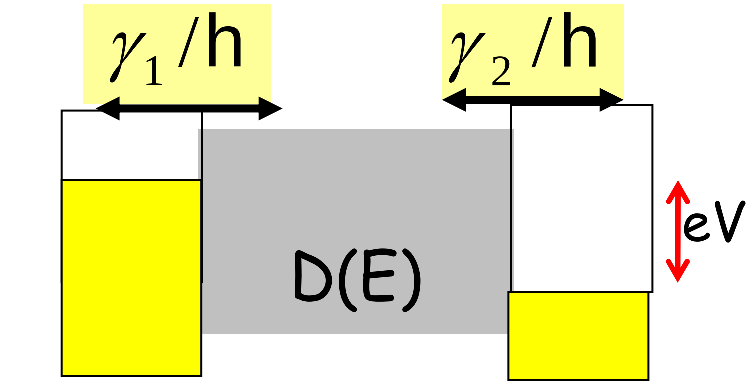
$$I(E) \sim \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}\left[f_1 - f_2\right]$$

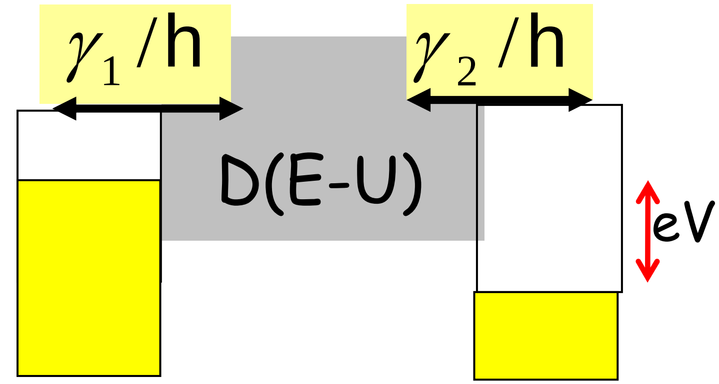
$$f(E) \equiv \frac{n(E)}{D(E)} = \left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

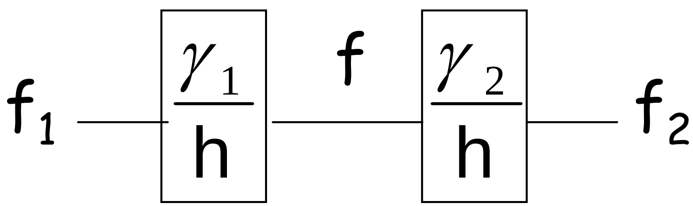
$$I(E) = \frac{q}{h} D(E) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}\left[f_1 - f_2\right]$$

$$\rightarrow \frac{q\gamma}{2h} D \left[f_1 - f_2\right]$$

Quantitative model: Introducing U



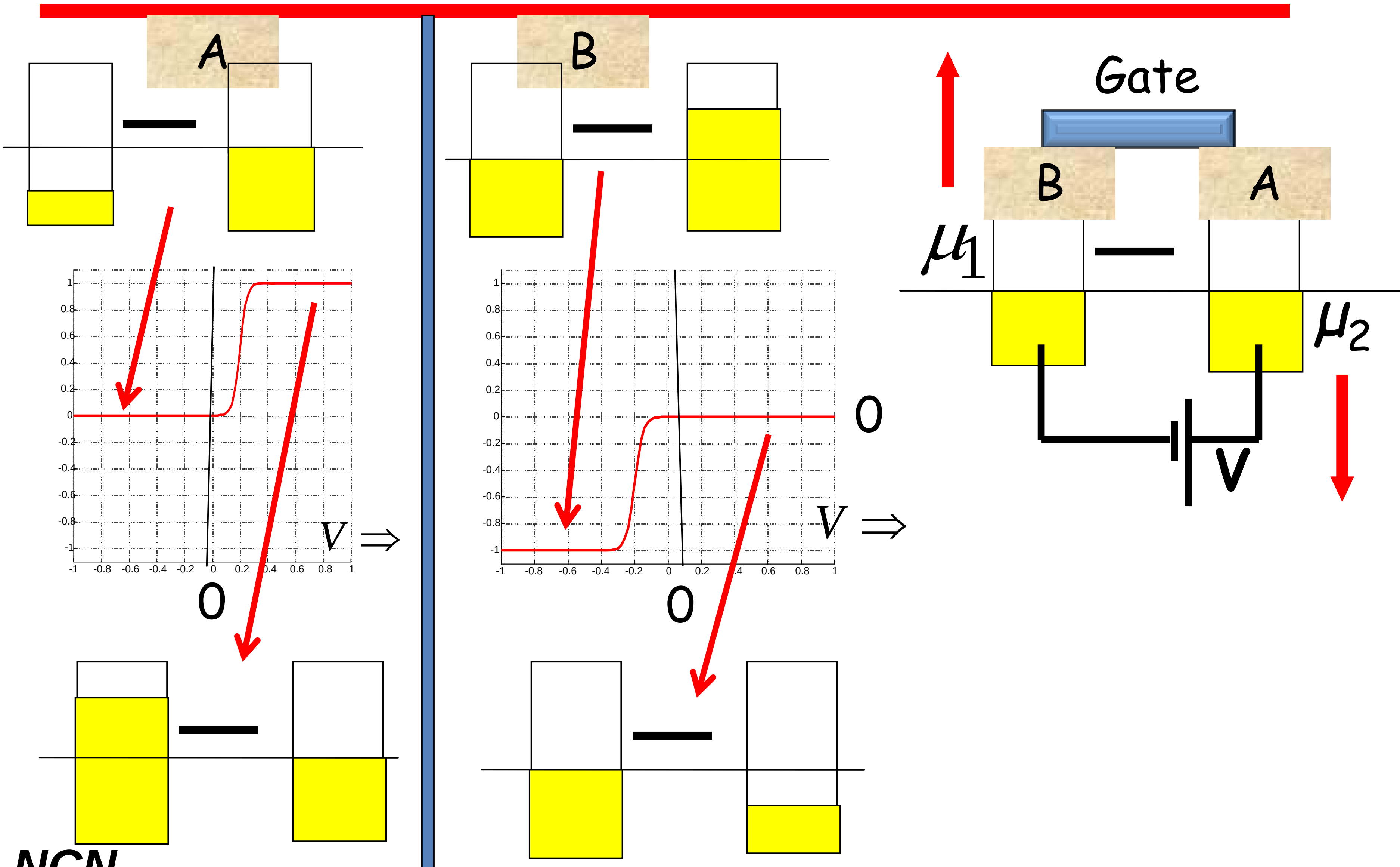




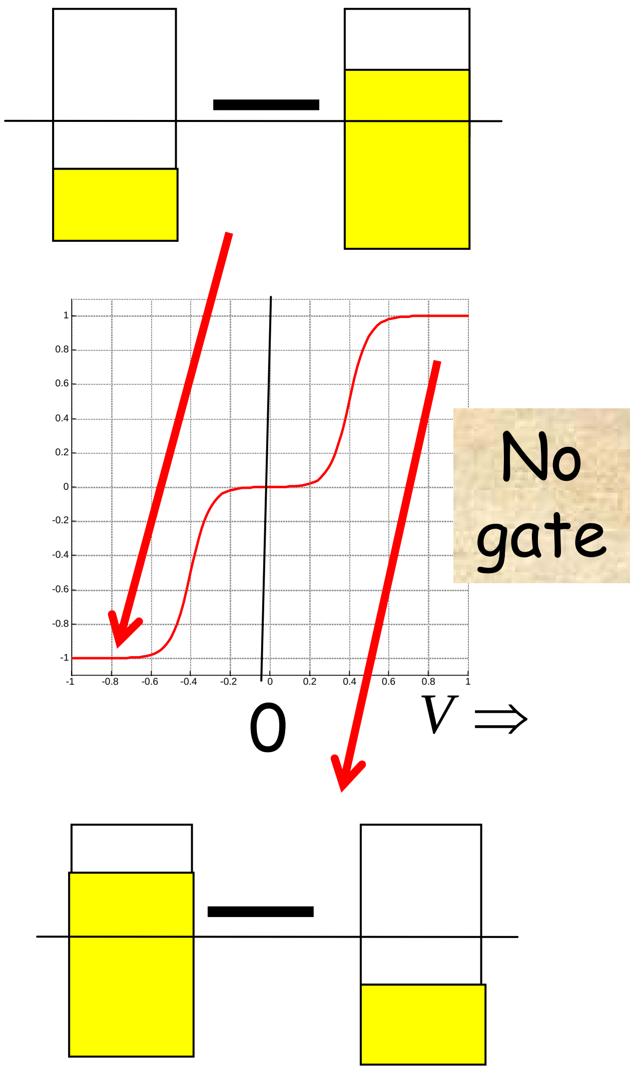
$$n(E) = \quad D(E)\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right] \quad \rightarrow \quad D(E-U)\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

$$I(E) = \quad \frac{q}{h}\, D(E)\, \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}\left[f_1 - f_2\right] \quad \rightarrow \quad \frac{q}{h}\, D(E-U)\, \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}\left[f_1 - f_2\right]$$

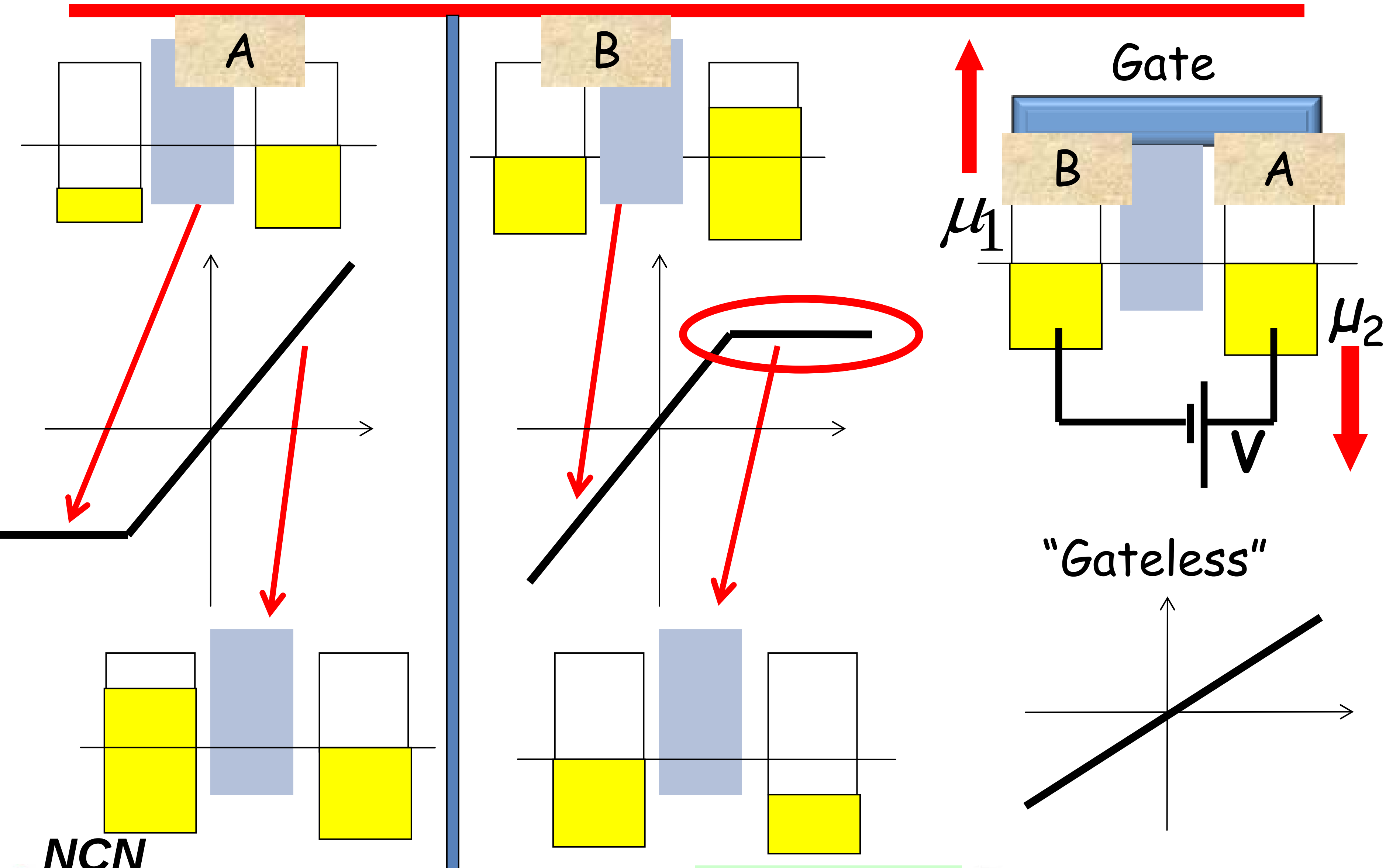
Current through ONE level



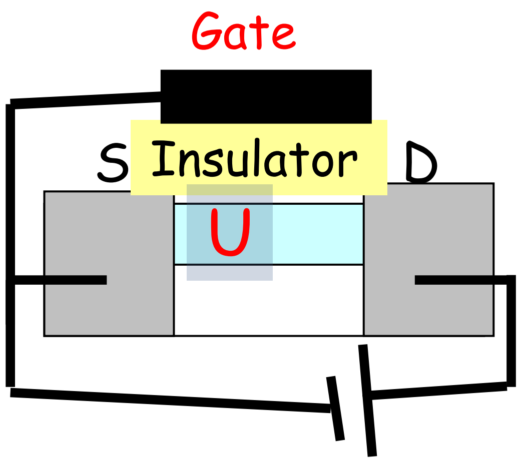
"Gateless" conduction through ONE level

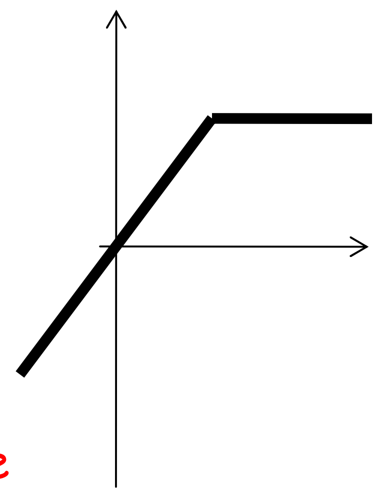


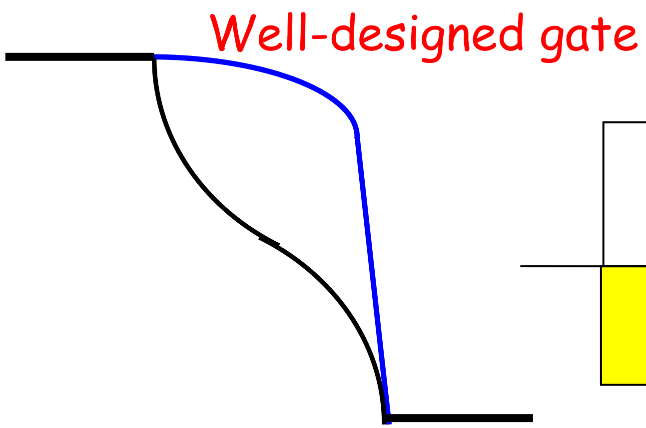
Current through a 2-D conductor

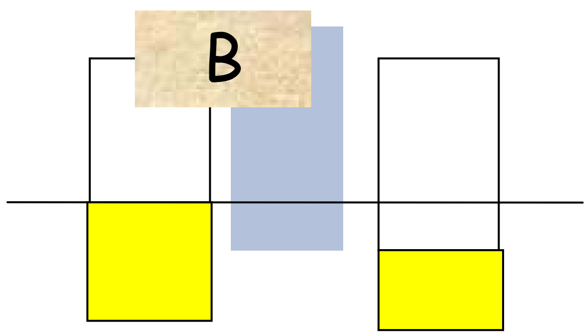


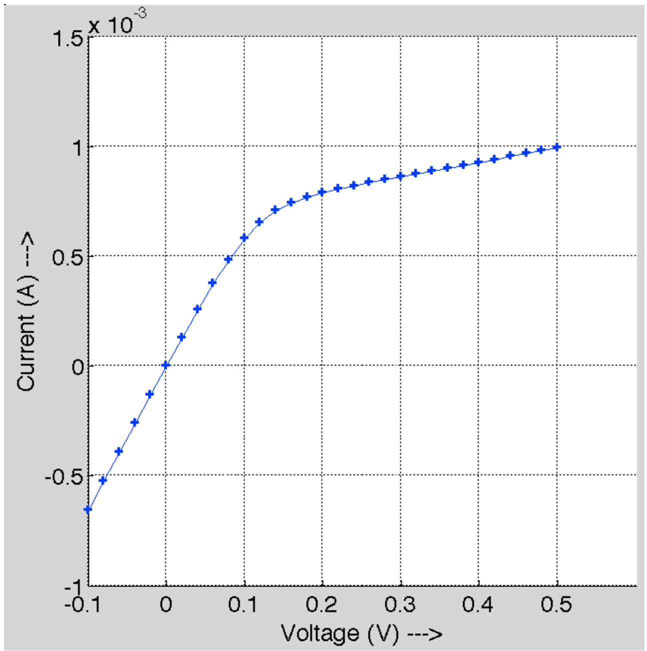
Electrostatics of nanotransistors









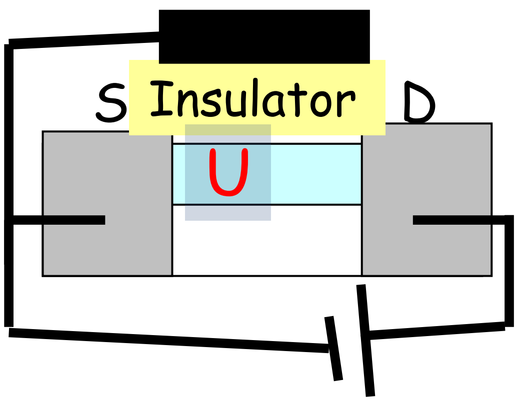


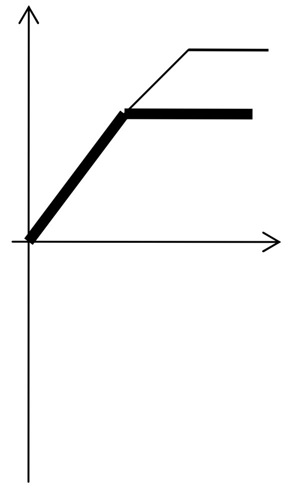
$$n(E) = D(E-U)\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

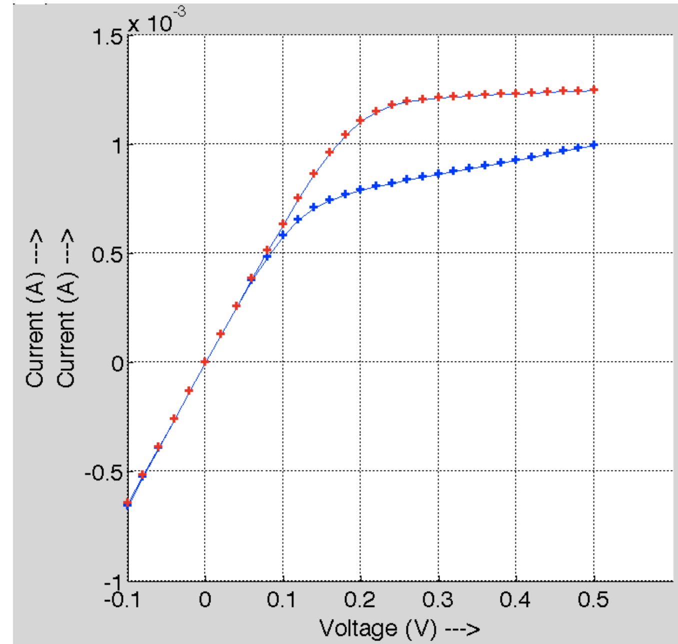
$$I = \frac{q}{\hbar} D(E-U)\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\left[f_1 - f_2\right]$$

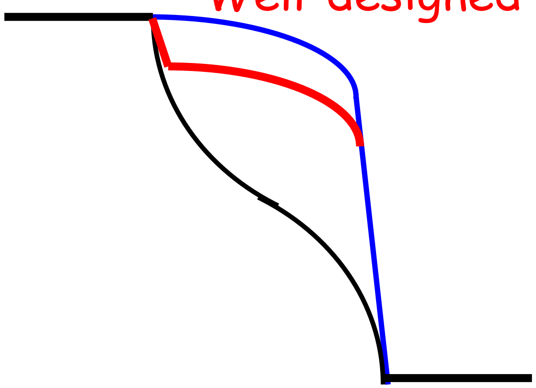
$$\nabla^2 U = 0 \quad \rightarrow \quad U = U_L$$

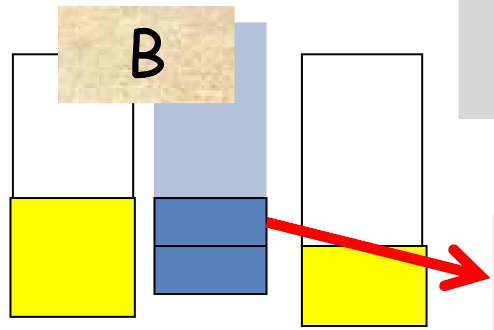
Electrostatics of nanotransistors











Semi-depleted of electrons

$$\nabla^2 U \sim n \quad \rightarrow \quad U = \quad U_L + U_0 (n - n_0)$$

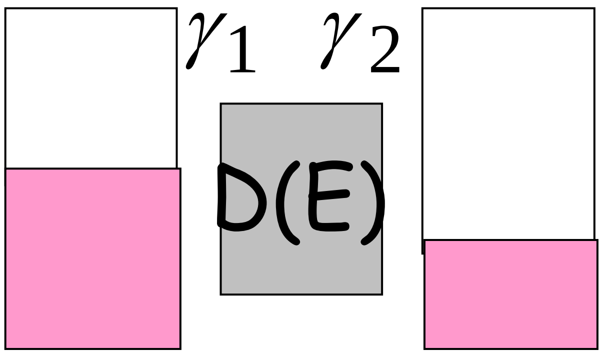
NCN

http://www.nanohub.org/courses/cqt

Supriyo Datta

PURDUE UNIVERSITY

Self-consistent field (scf) method

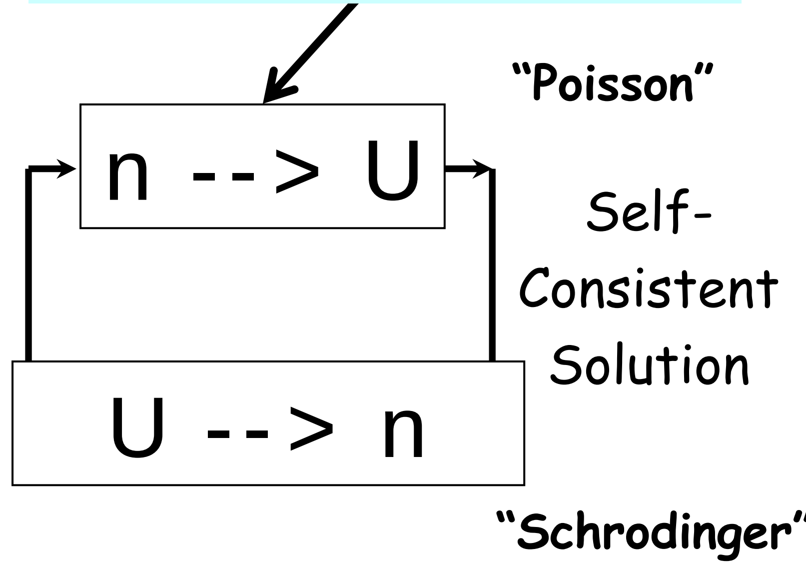


$$U = U_L + U_0(n - n_0)$$

$$n = D(E-U)\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

$$I = \frac{q}{\hbar} D(E-U)\frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}[f_1 - f_2]$$

Simplified treatment of a very complicated problem



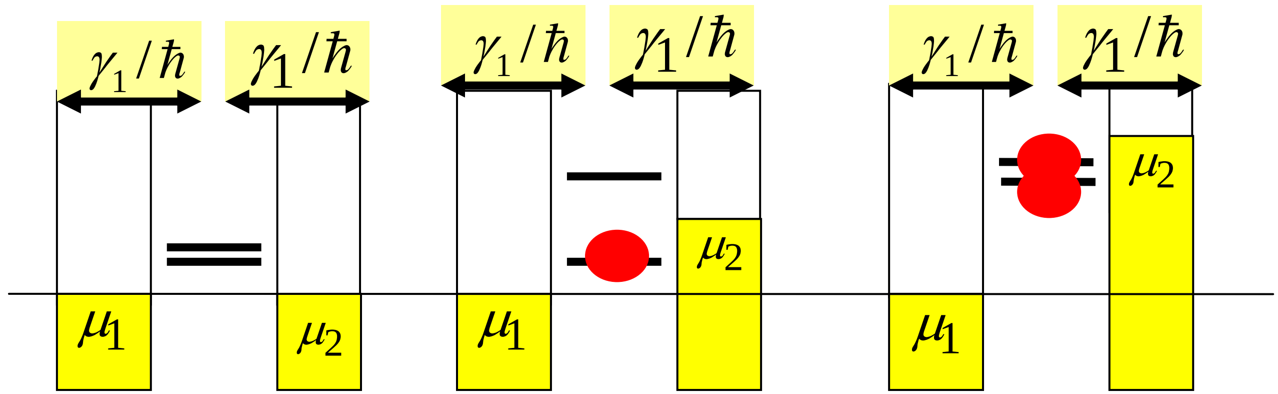
U --> I

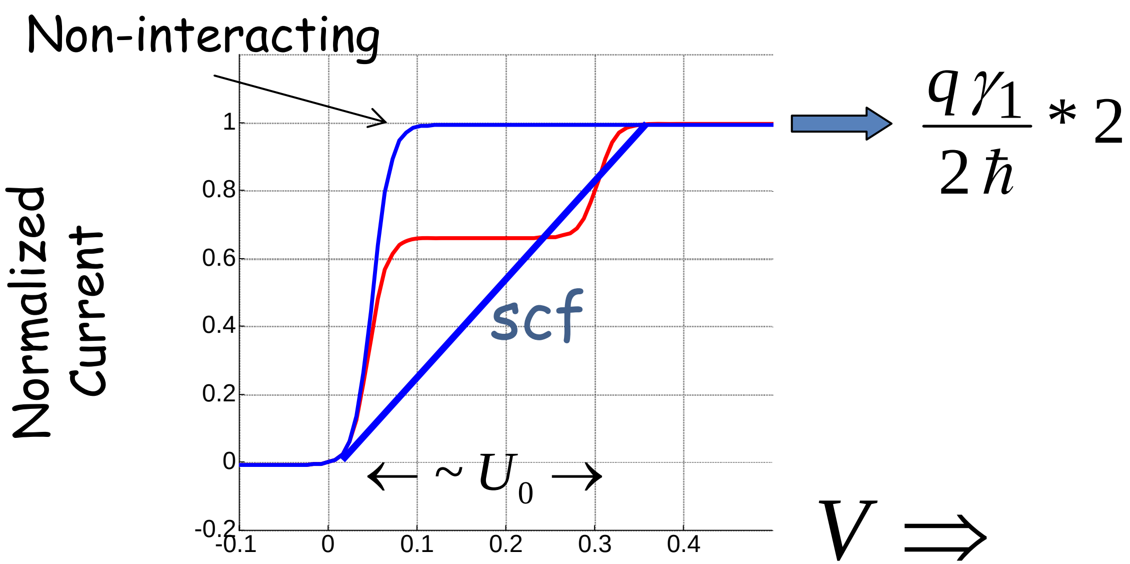
Nanowires / Nanotubes / Molecules

** Single-electron charging

U_0 : *Increase in potential due to SINGLE electron* $>> \gamma, kT$

"Self-interaction Correction"





NCN

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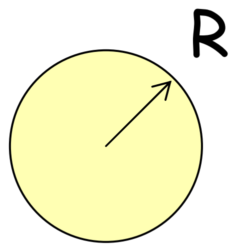
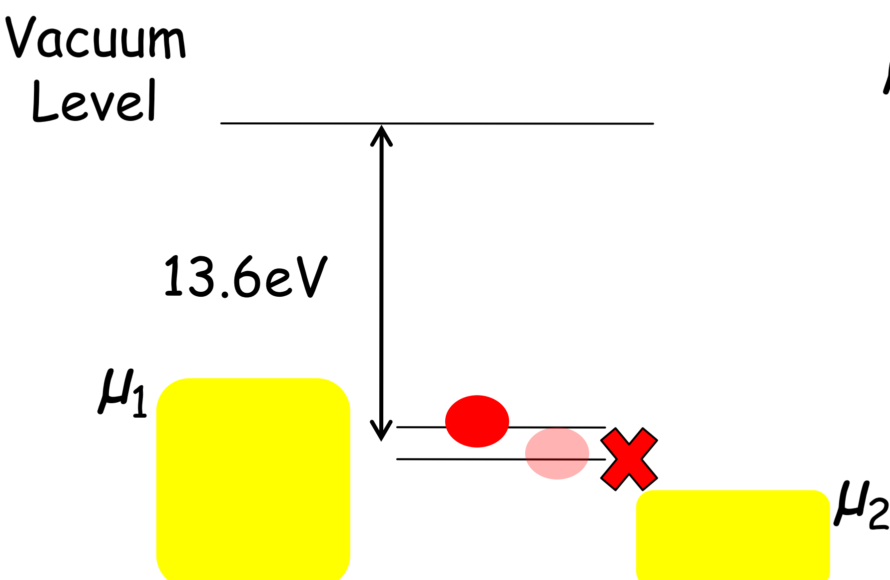
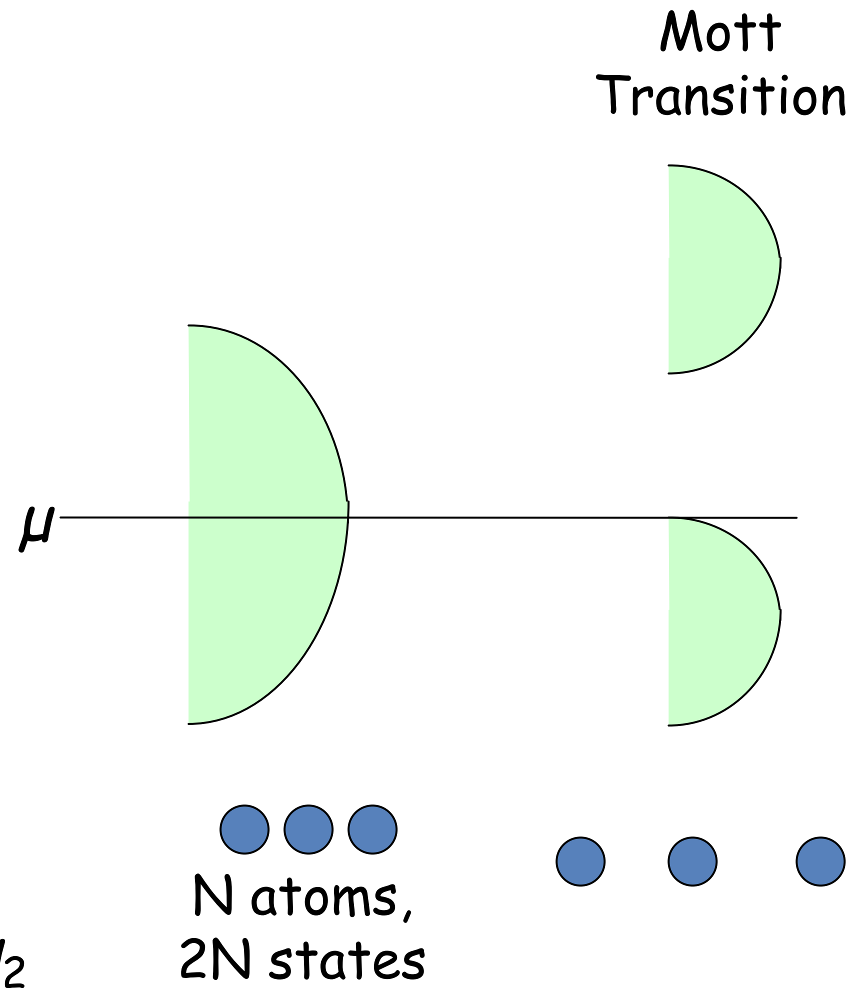
Single-electron charging energy

$$U_0 \sim \frac{q^2}{4\pi\varepsilon_0 R}$$

$$\rightarrow \quad 1.6\, eV \quad for\ R = 1\, nm$$



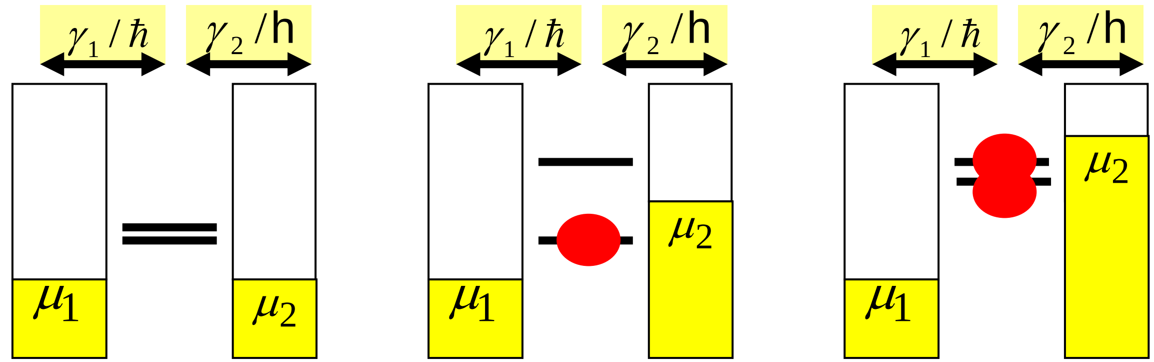




2 levels: SCF versus Exact

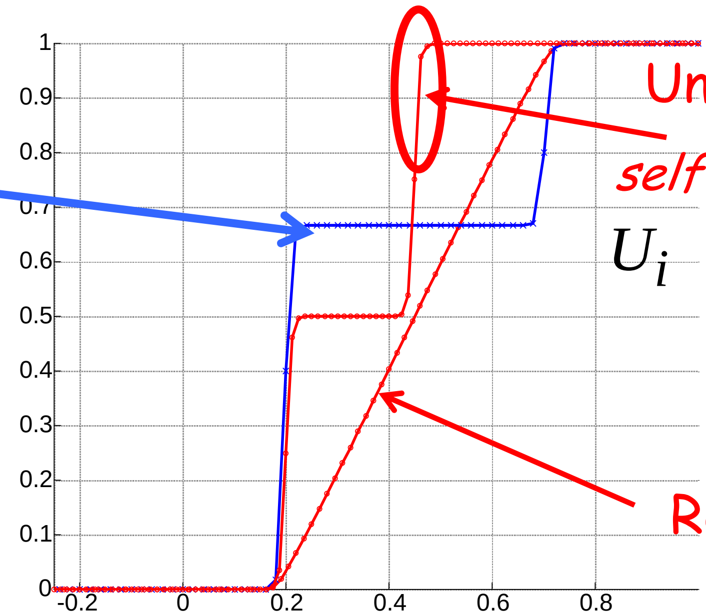
SCF works fine as long as

U_0 : Single electron charging energy $\leq \gamma, kT$



Exact
Needs picture in “Fock” space:

Lectures 5



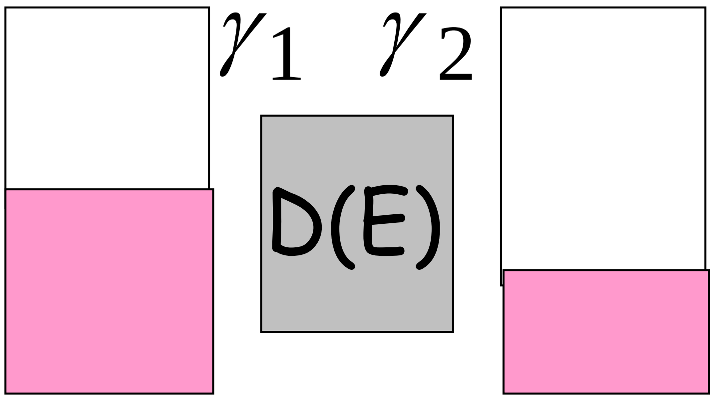
Unrestricted SCF for *self-interaction correction*

$$U_i = U_0 (N - N_i)$$

Restricted SCF

$$U_i = U_0 N$$

Summary: Self-consistent field method

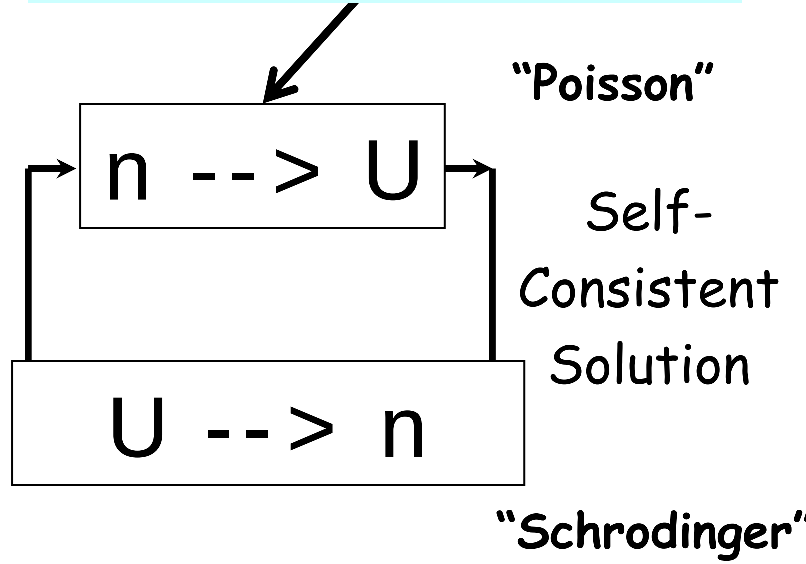


$$U = U_L + U_0 (n - n_0)$$

$$n = \quad D(E-U) \left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \right]$$

$$I \quad = \quad \frac{q}{\hbar} D(E-U) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} [f_1 - f_2]$$

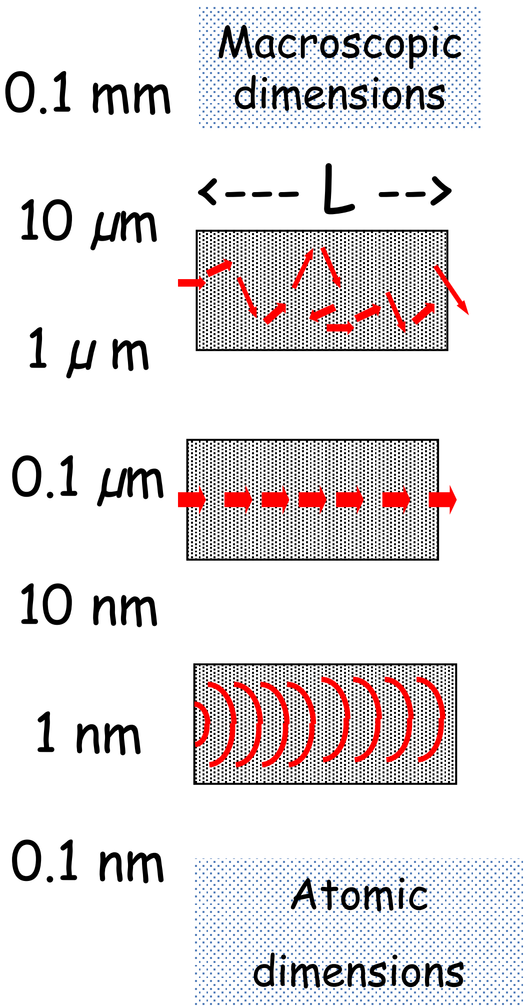
Simplified treatment of a very complicated problem



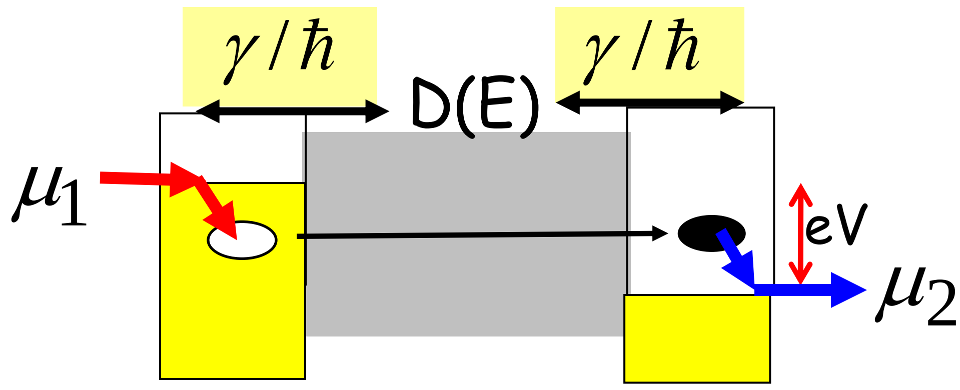
U --> I

Nanowires / Nanotubes / Molecules

** Where is the heat (I^2R) ?



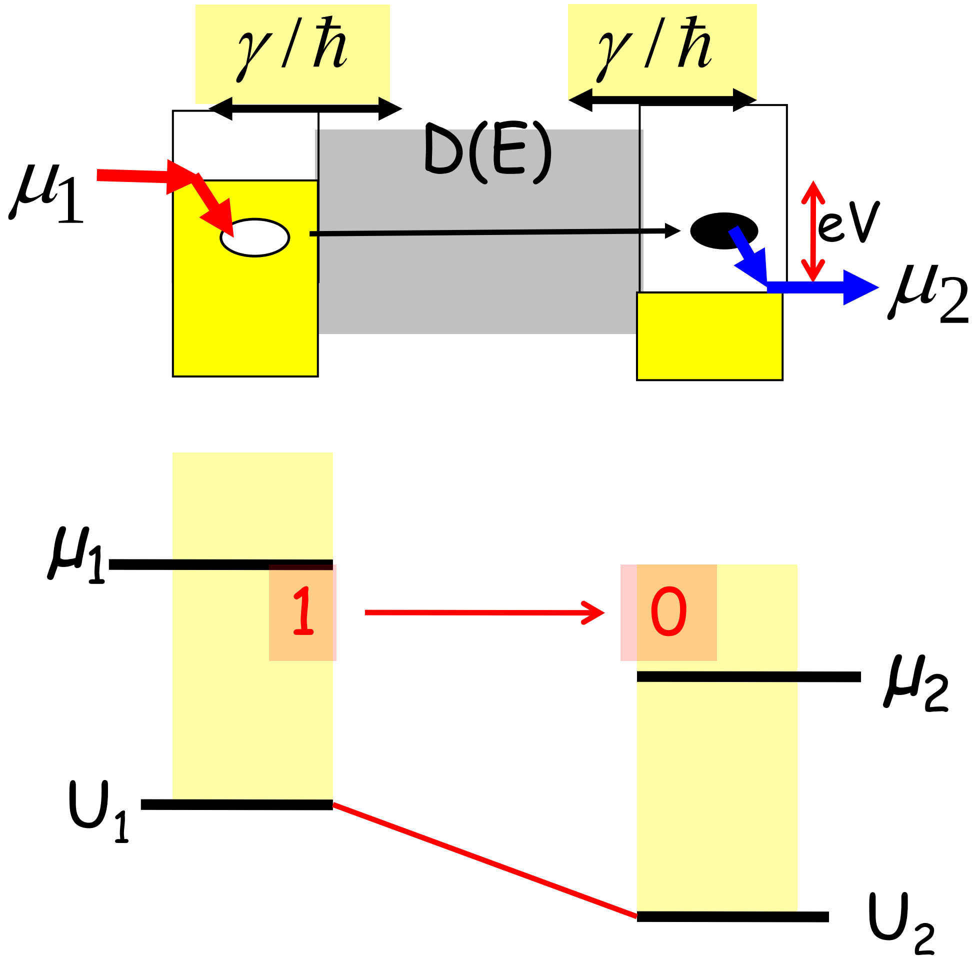
$$V/I = \frac{25.8\ K\Omega}{2}\ \frac{1}{M}$$



$$P = V\,I$$

$$= eV * \frac{N}{t}$$

Where is the voltage ?

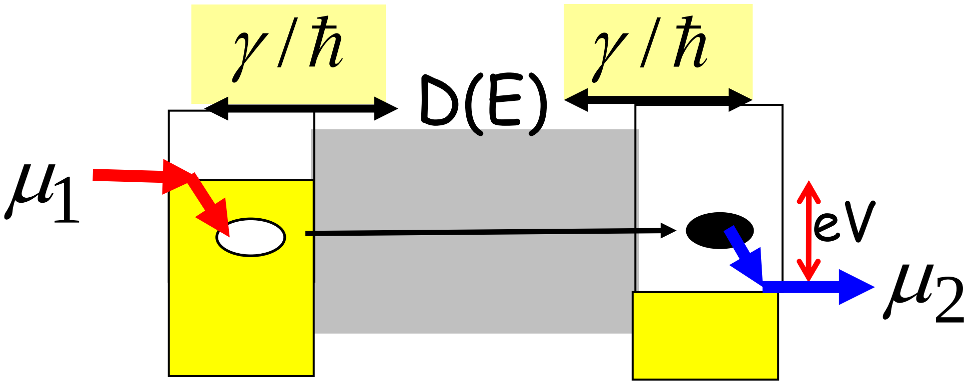


"Voltage"

U or μ ?

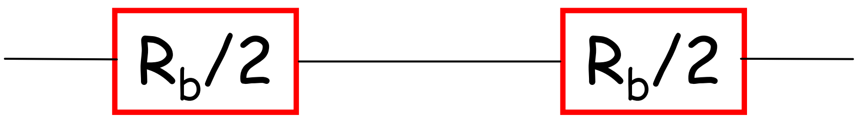
Answer: f

Where is the voltage ?



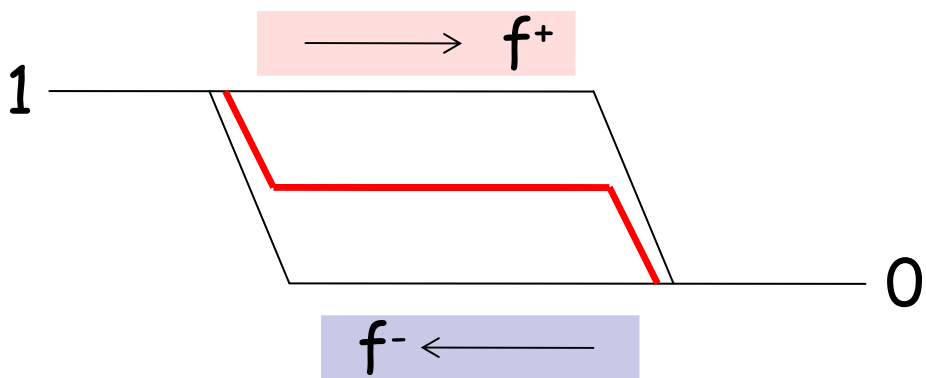
$$R_b \equiv V / I_b$$

$$I_b = (2q^2 V / h) \; M$$

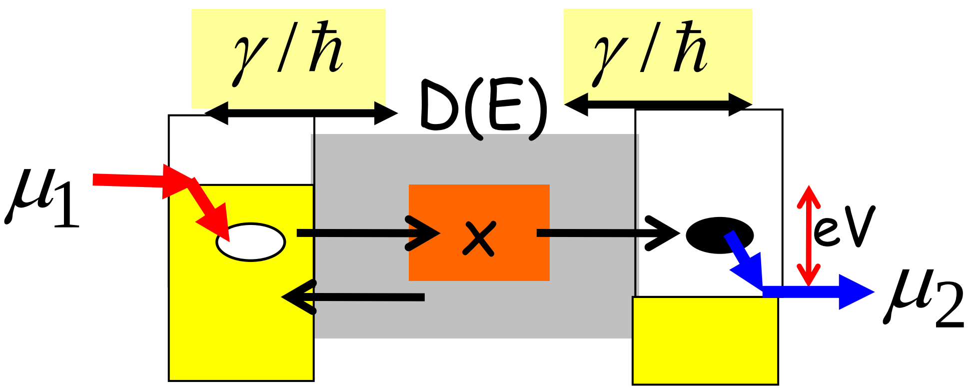


$$I^+ = I_b \; f^+$$

$$I^- = I_b \; f^-$$



Voltage across a scatterer



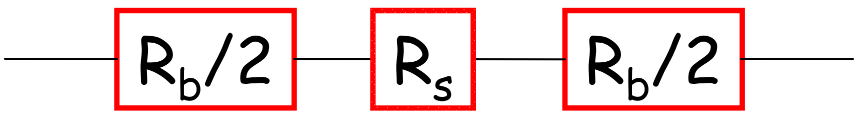
$$R_b \equiv V/I_b$$

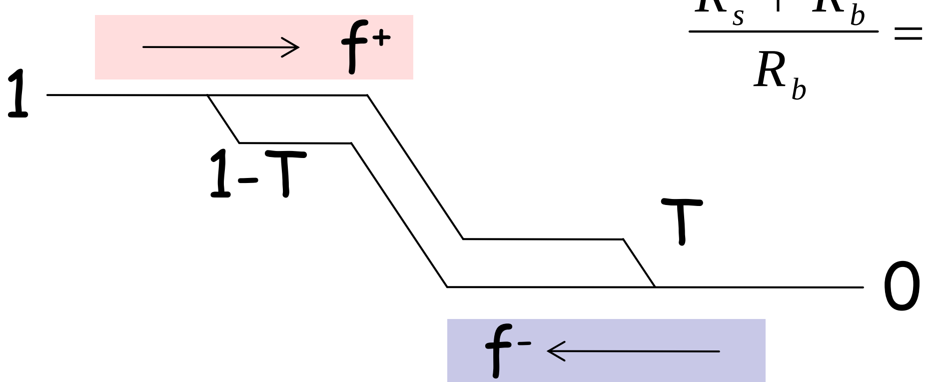
$$I_b = (2q^2V/h)\ M$$

$$I^+/I_b \equiv f^+$$

$$I^-/I_b \equiv f^-$$

$$I/I_b \equiv f^+ - f^-$$





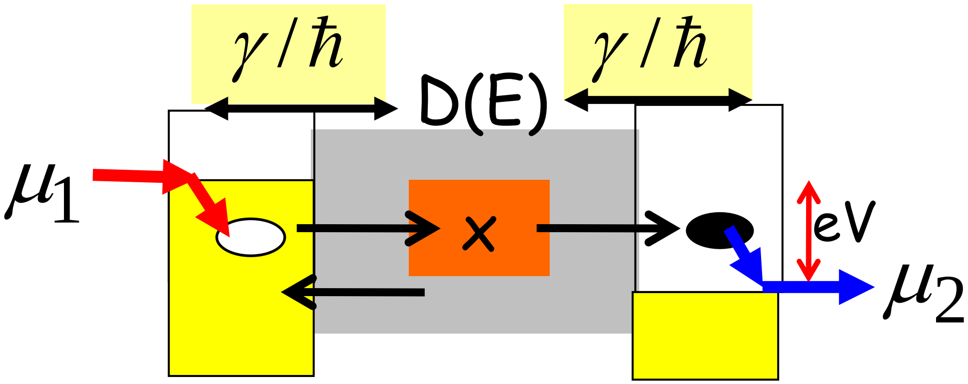
$$\frac{R_s + R_b}{R_b} = \frac{1}{T}$$

$$R_s + R_b = \frac{R_b}{T}$$

Landauer formula

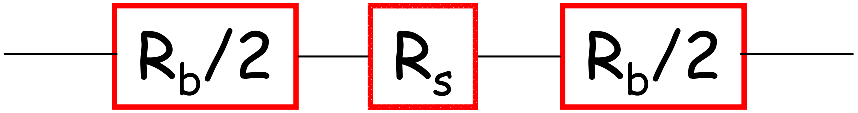
$$R_s = R_b \frac{1-T}{T}$$

Where is the resistance?



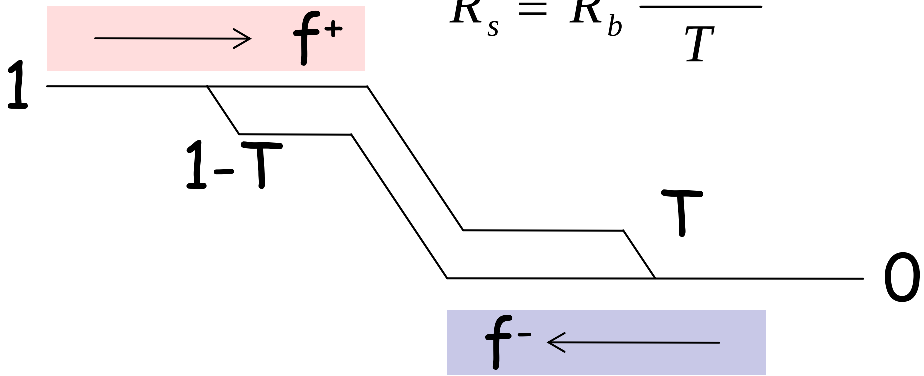
$$R_b \equiv V/I_b$$

$$I_b = (2q^2V/h)\ M$$

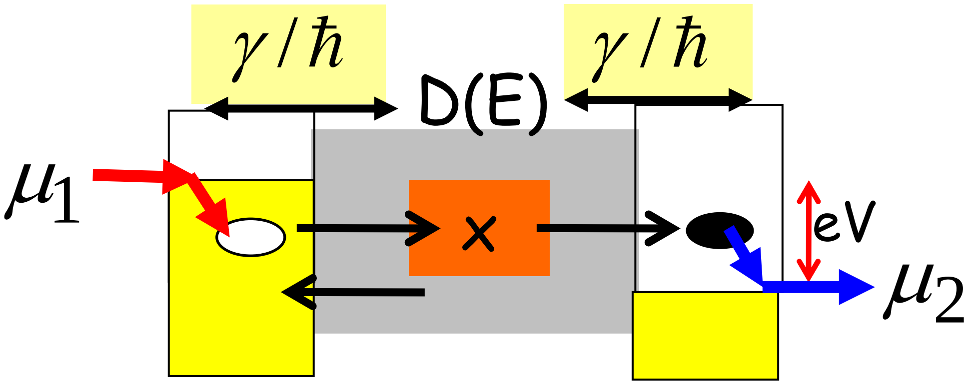


$$R_s = R_b \frac{1-T}{T}$$

"I^2R" lost in the contacts, but "voltage" drops at scatterer too.

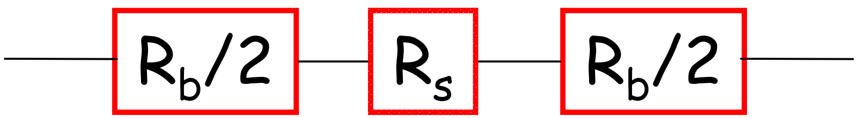


Electrostatic Potential

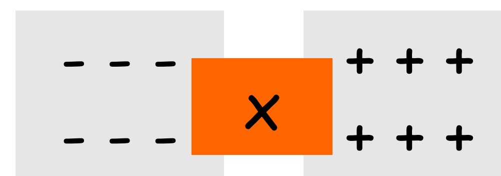


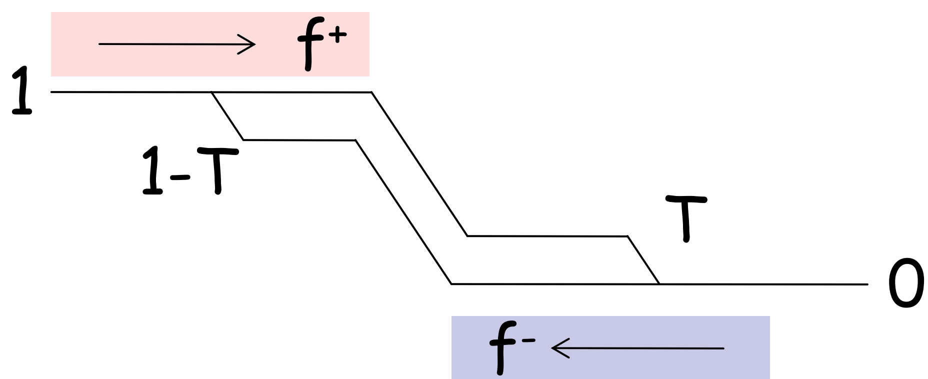
$$I / I_b \equiv f^+ - f^-$$

$$n \sim f^+ + f^-$$

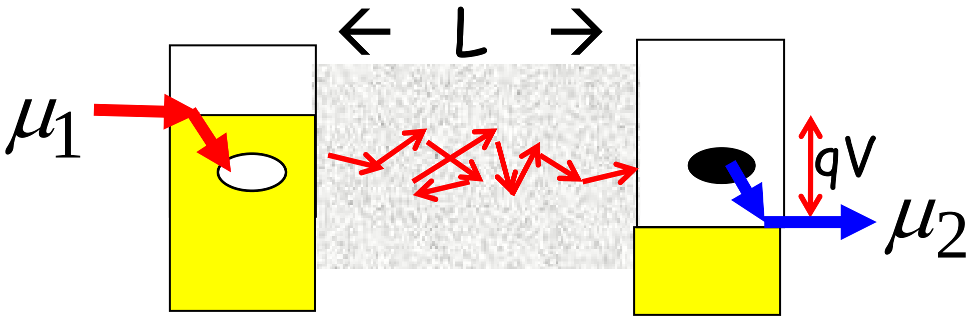


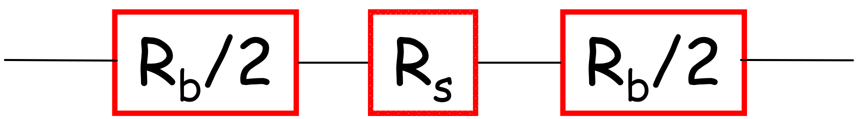
Resistivity dipole

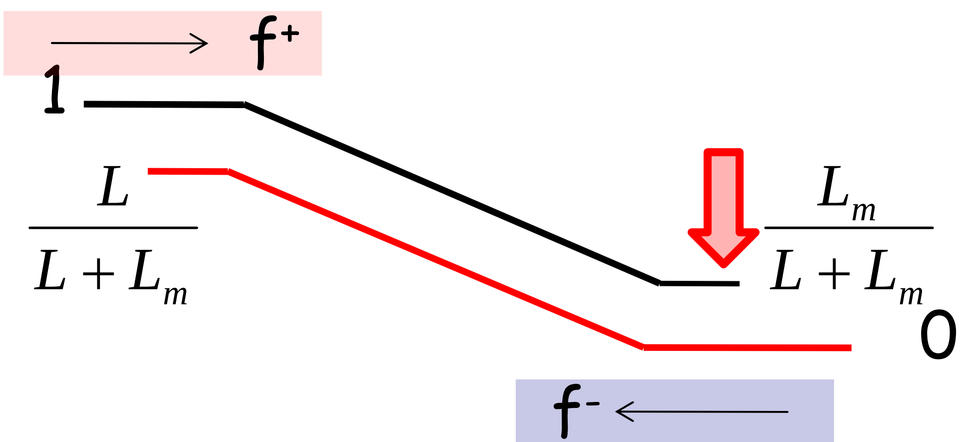




Continuous scattering







$$R_b \equiv V/I_b$$

$$I_b = (2q^2V/h)\ M$$

$$I/I_b \equiv f^+ - f^-$$

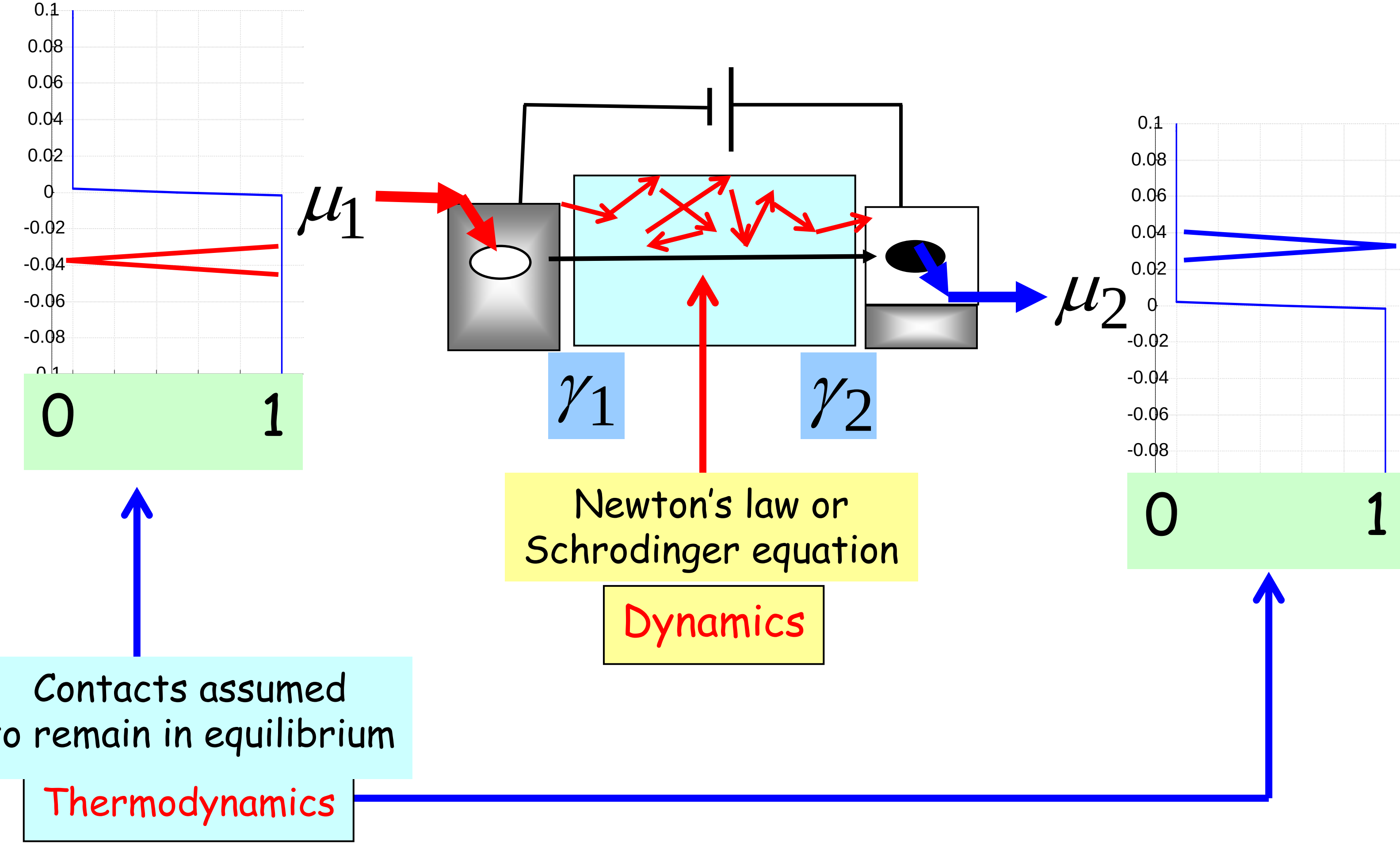
$$df^+ = -\frac{dx}{L_m}(f^+ - f^-)$$

$$\frac{R_s + R_b}{R_b} = \frac{1}{L_m/(L+L_m)}$$

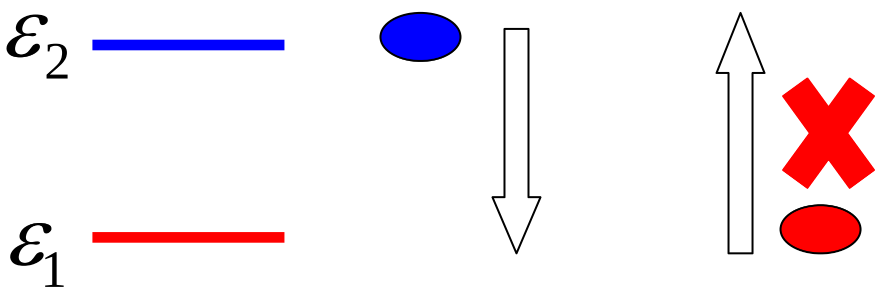
$$R_s = \frac{L}{L_m} R_b$$

Ohm's law

** "Landauer model"



Pure dynamics is not enough



Down > Up

Isolated

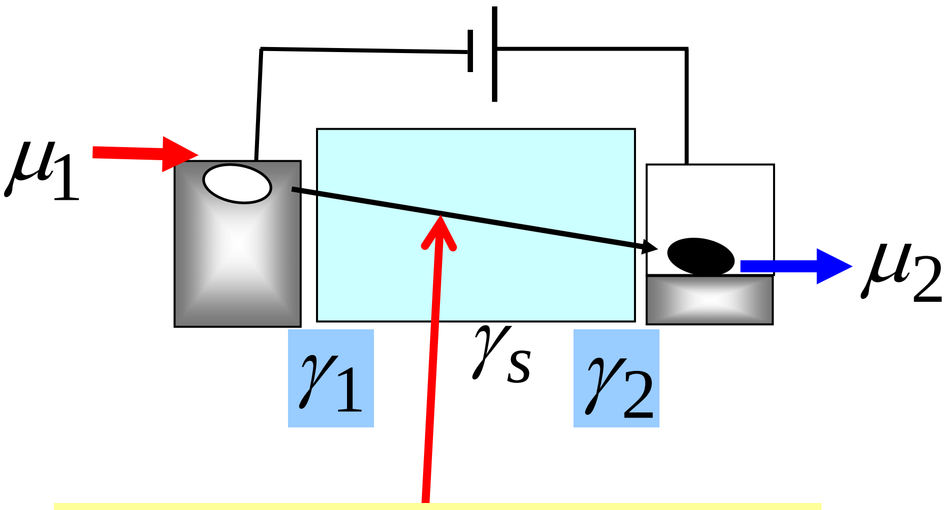
$$i\hbar\frac{\partial}{\partial t}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}=\begin{bmatrix}\varepsilon_1 & 0\\ 0 & \varepsilon_2\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

Interaction

$$i\hbar\frac{\partial}{\partial t}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}=\begin{bmatrix}\varepsilon_1 & a\\ a^* & \varepsilon_2\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

"Unidirectionality"
does NOT follow from
Schrodinger equation

Combining dynamic and "entropic forces"

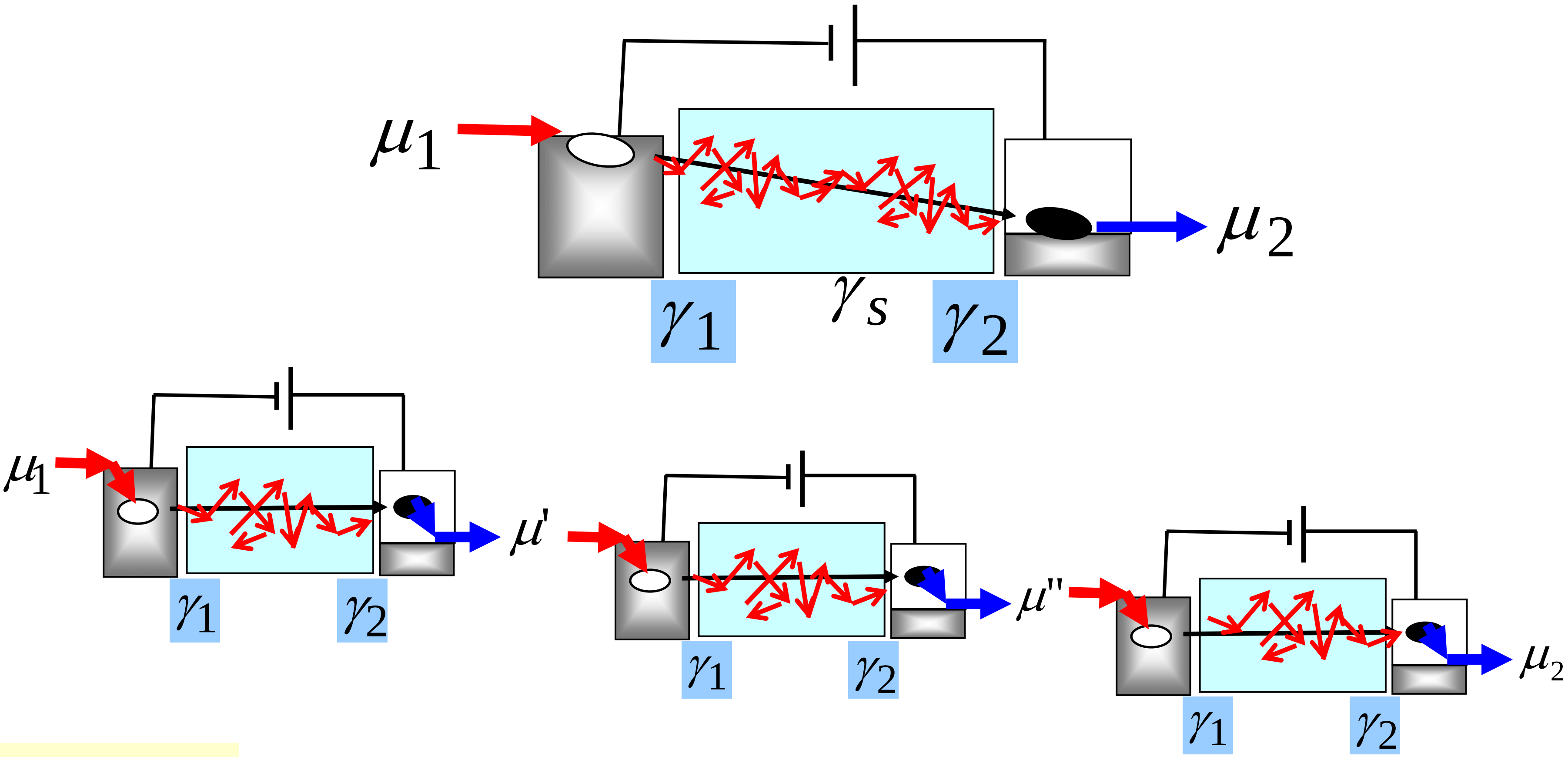


Newton's law + "Entropic forces"
= Boltzmann Equation

Schrodinger equation
+ "Entropic forces" = NEGF

Schwinger, Keldysh,
Kadanoff, Baym (1960's)

Long devices → "Landauer devices" in series

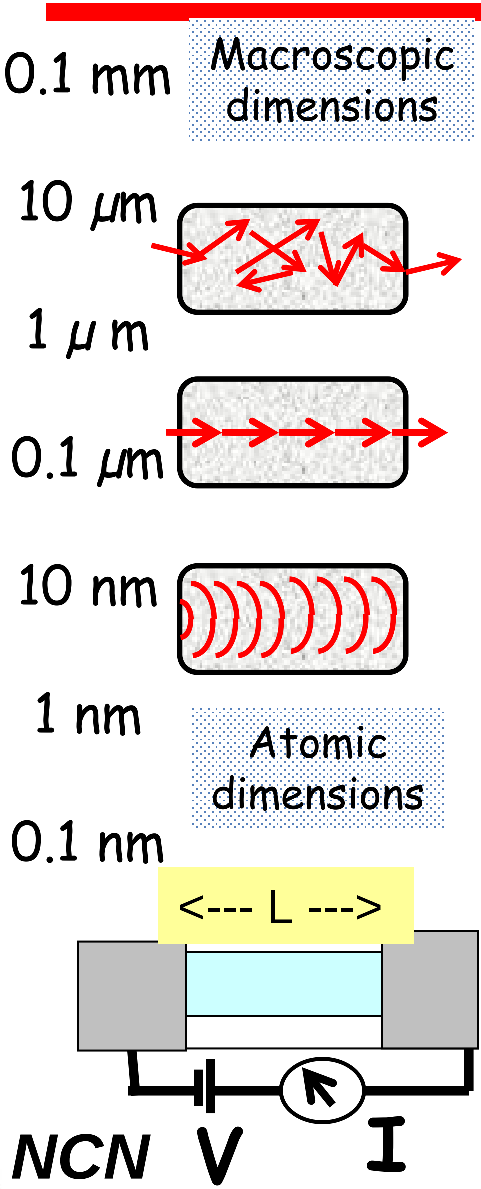


What drives the current?

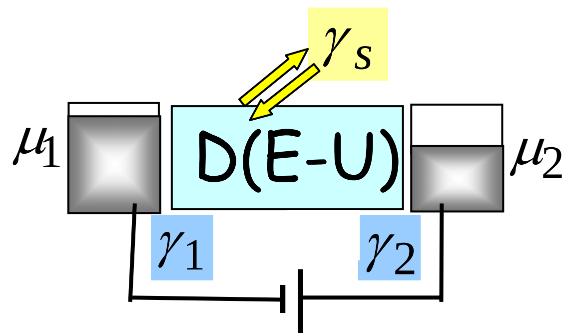
$$\frac{\Delta f}{\Delta \mu} \rightarrow \frac{\partial f}{\partial \mu} \rightarrow \left(-\frac{\partial f}{\partial E}\right)$$

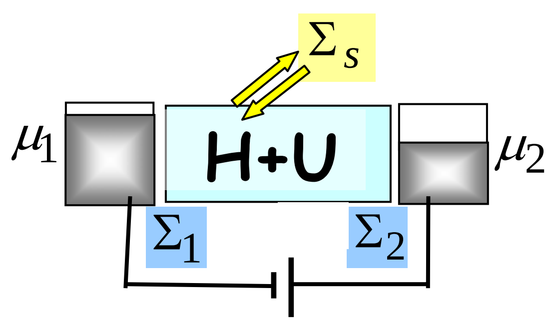
$$Or, \quad \frac{\Delta f}{\Delta T} \rightarrow \frac{\partial f}{\partial T} \rightarrow \left(-\frac{\partial f}{\partial E}\right)$$

Nanoelectronics and the meaning of Resistance :



Lectures 1a,b:
Simple model





Lectures 2a,b:
Microscopic model

<u>Materials</u>

Semiconductors
Graphene / CNT
Molecules
...

1 μm = .001 mm
1 nm = .001 μm

End of Lectures 1a,b