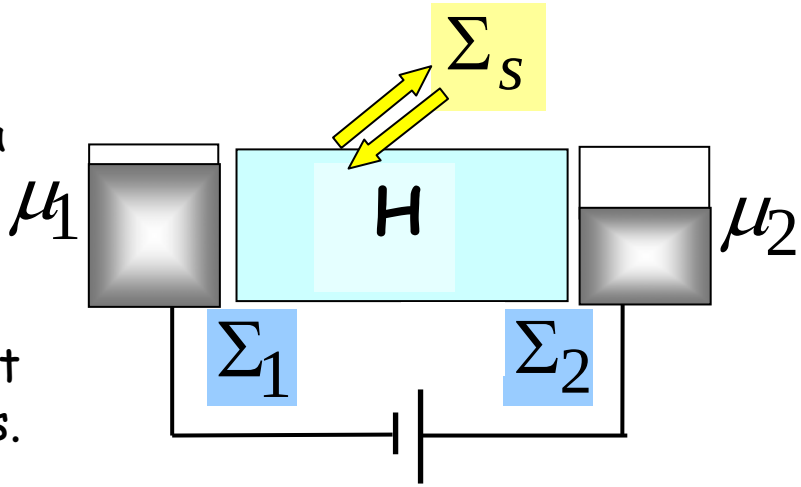
CQT, Lecture#4:

Coulomb blockade and Fock space

U: Self-consistent Field (SCF)

Objective:
To illustrate the limitations of the model described in Lectures 2,3 and introduce a completely different approach based on the concept of Fock space.



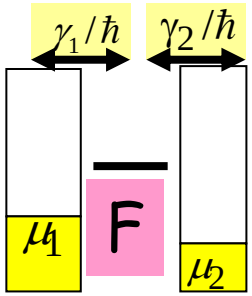
I believe this will be a key concept in the next stage of development of transport physics.

Approach based on
(1)Beenakker, Phys.Rev.B44,1646 (1991), (2) Averin & Likharev, J.LowTemp.Phys. 62, 345 (1986)

"QTAT"
Datta, Quantum Transport: Atom to Transistor, Cambridge (2005)

Reference: QTAT, Chapter 3.4.

Current through a very small conductor

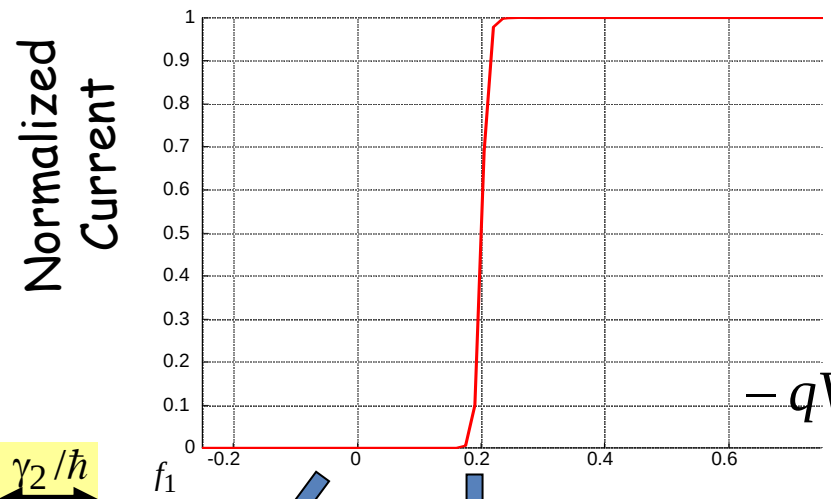


$$F = \left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

$$I = \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}[f_1 - f_2]$$

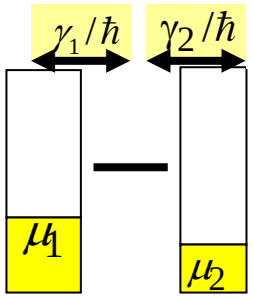
$$\max I = \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}$$

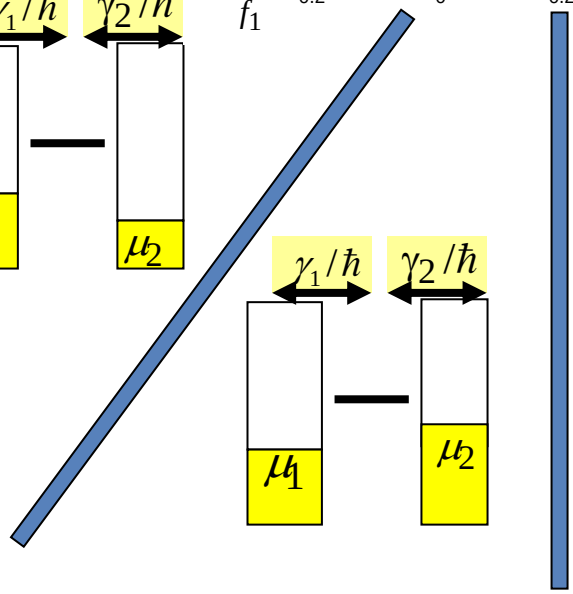
$$\Rightarrow \frac{q\gamma_1}{2\hbar} \quad if\ \gamma_2 = \gamma_1$$

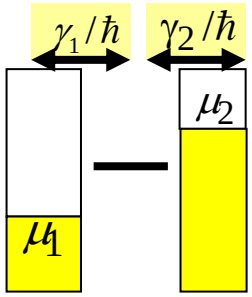


$$\Rightarrow \frac{q\gamma_1}{2\hbar}$$

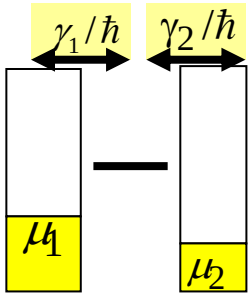
$$-qV_D \Rightarrow$$







Conductance of a very small conductor



$$Conductance = \frac{\partial I}{\partial V_D}$$

$$\sim \frac{q\gamma_1/2\hbar}{2\gamma_1 + 4k_BT}$$

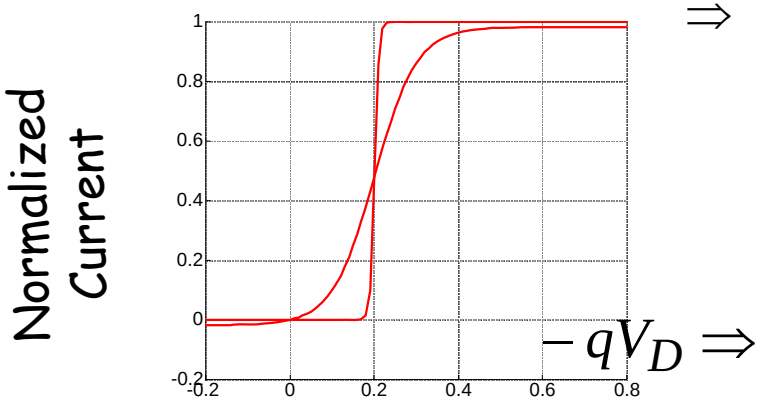
$$\sim q^2/4\hbar \quad if \quad \gamma_1 >> k_BT$$

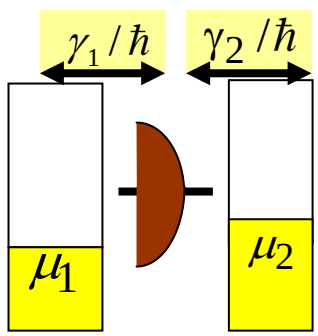
$$Conductance\ quantum$$

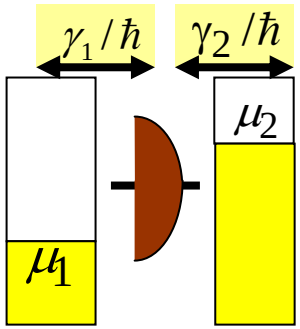
$$\sim q^2/2\pi\hbar$$

$$Assume\ \gamma_2 = \gamma_1$$

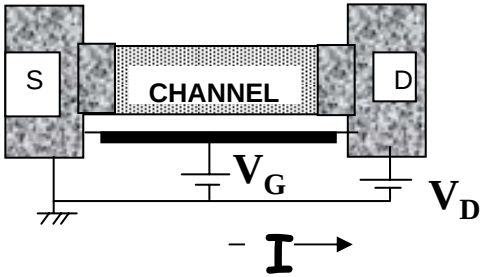
$$2\gamma_1 + 4k_BT \Rightarrow \frac{q\gamma_1}{2\hbar}$$



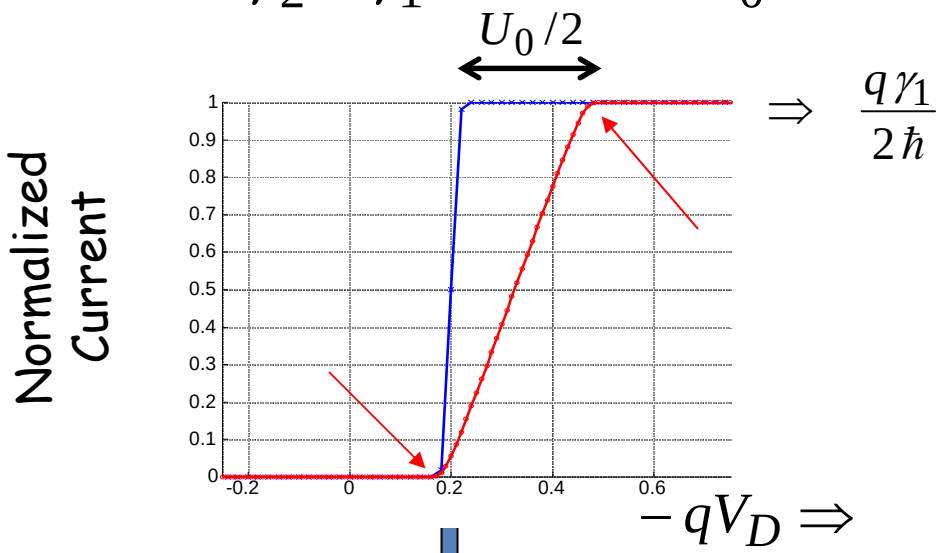




Effect of "U" on conductance



$$\text{Assume } \gamma_2 = \gamma_1 \qquad U_0 = 0.5\ eV$$

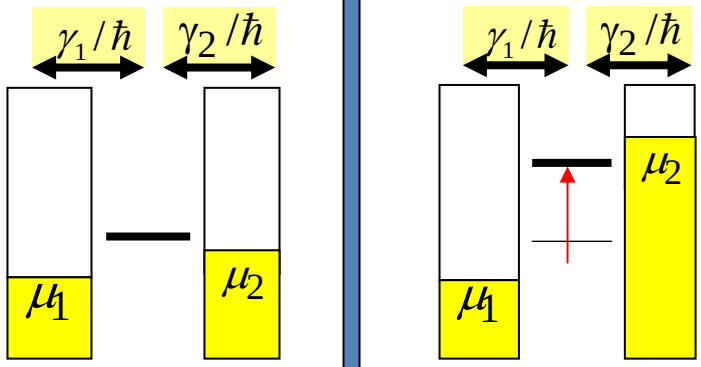


$$\Rightarrow \frac{q\gamma_1}{2\hbar}$$

U_0 : *Increase in potential due to SINGLE electron*

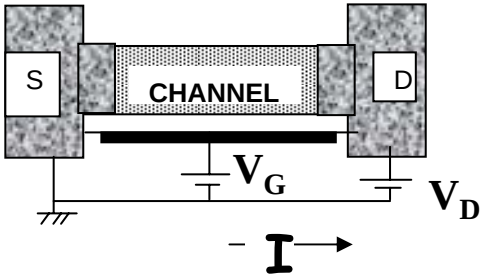
Assume

$$U_0 >> k_B T, \gamma_1, \gamma_2$$



Level floats up by $U_0 \dfrac{\gamma_2}{\gamma_1 + \gamma_2}$

SCF with self-interaction correction



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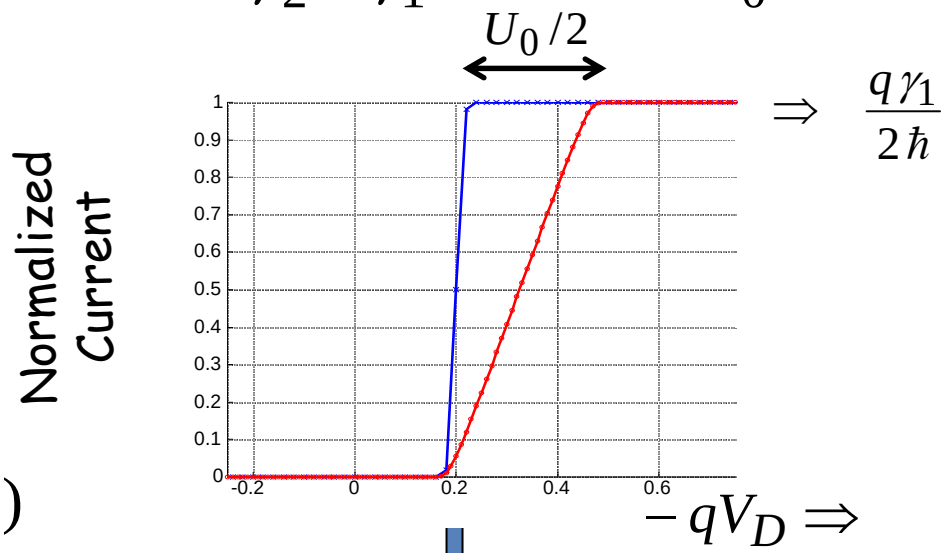
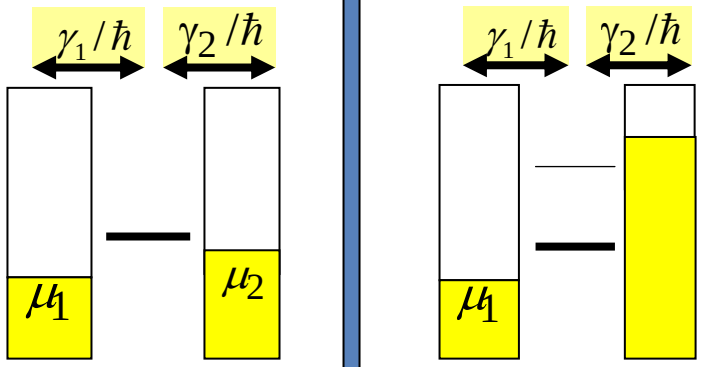


$$\Rightarrow \frac{q\gamma_1}{2\hbar}$$

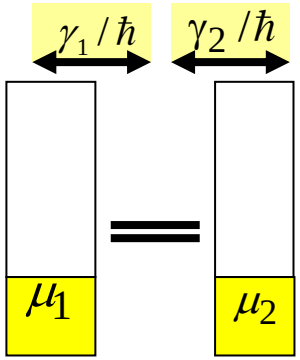
$$U_i = U_0 (N - N_i)$$

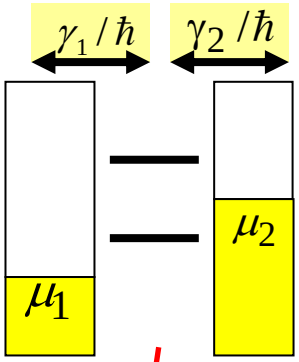
Self-interaction Correction

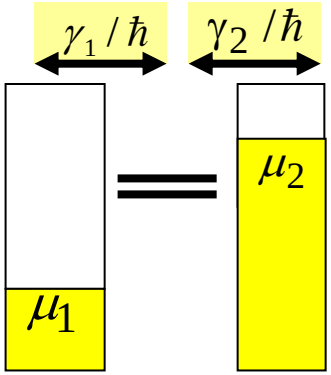


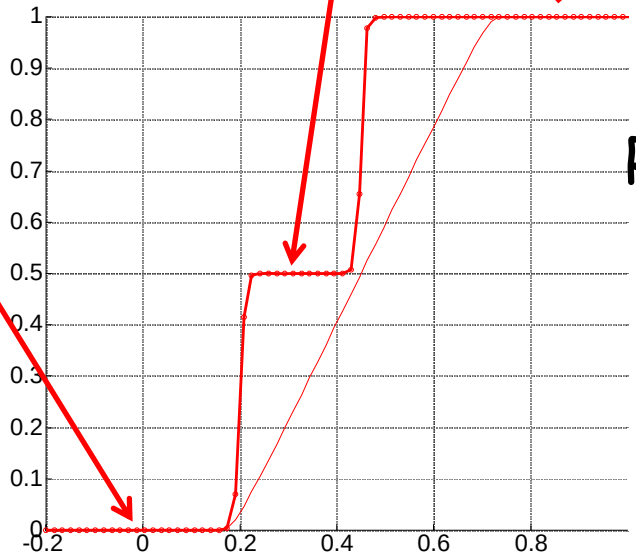
Level does NOT float up

2 levels: Unrestricted SCF









Unrestricted SCF

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

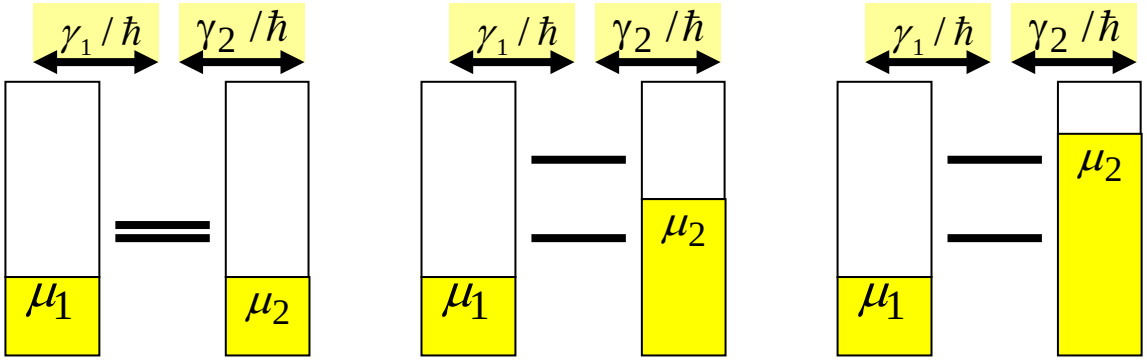
Self-interaction Correction

Restricted SCF

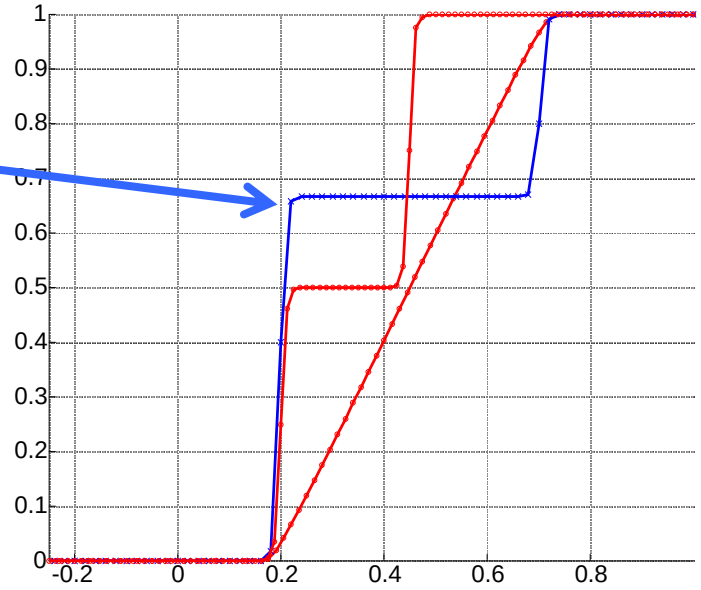
$$U_i = U_0 N$$

2 levels: SCF versus exact

One-electron energy levels

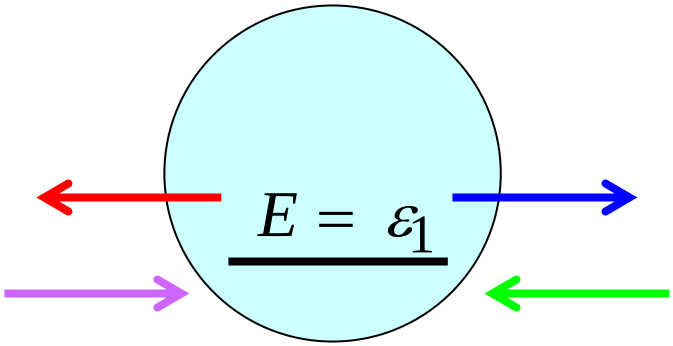


Exact
Needs picture
in "Fock" space



1-level: the view from "Fock space"

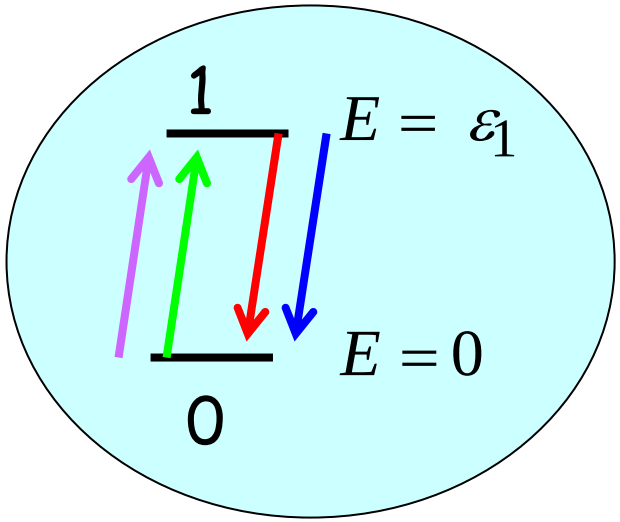
One-electron picture



Most of our thinking

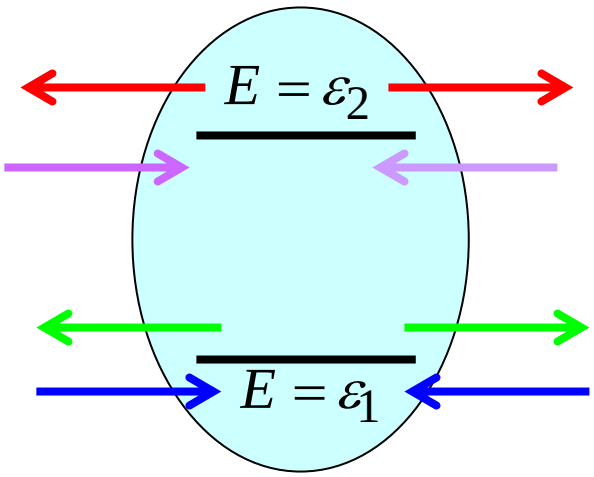
is based on this picture

"Fock space"

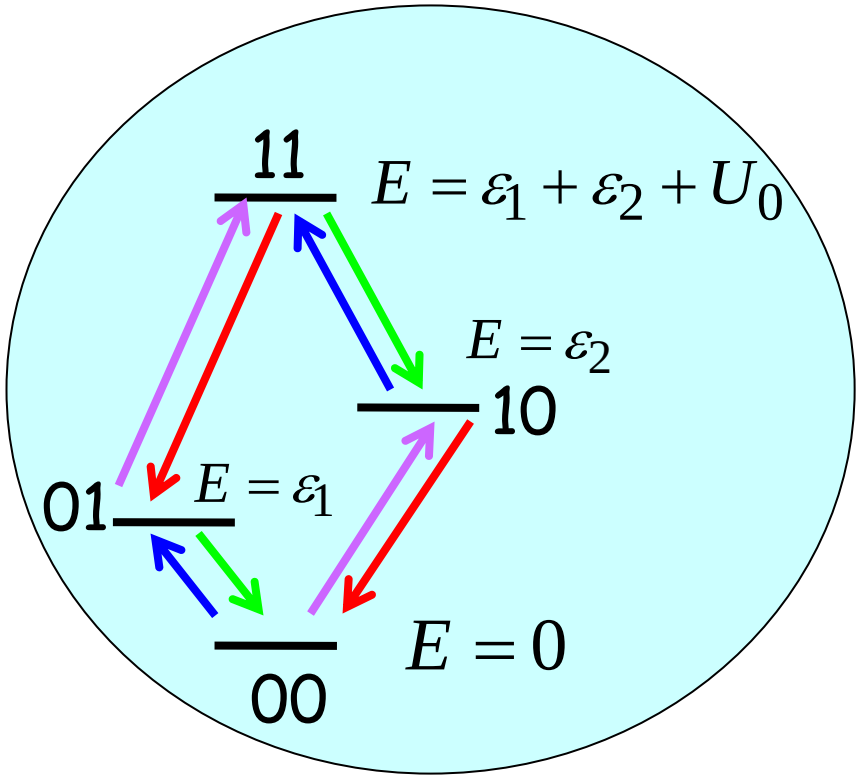


2 levels: the view from "Fock space"

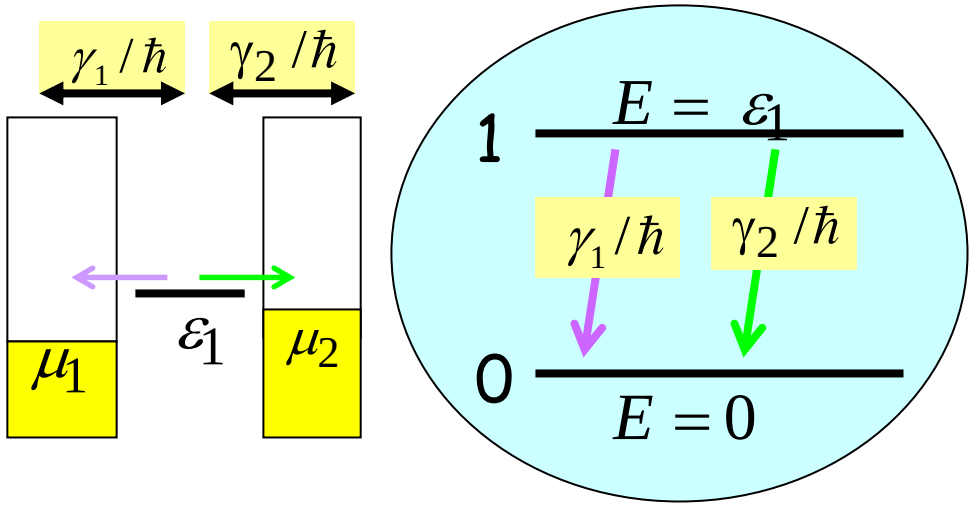
2 one-electron levels



2^2 many-electron levels



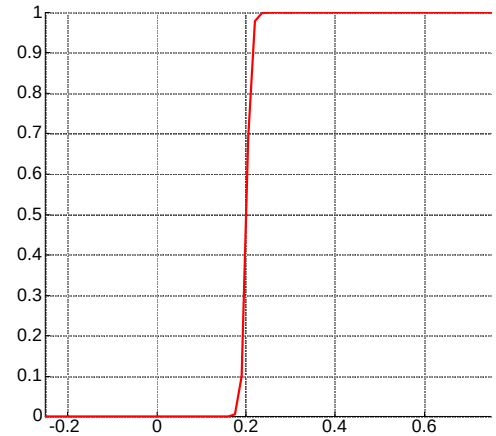
1-level: Current flow in "Fock space"

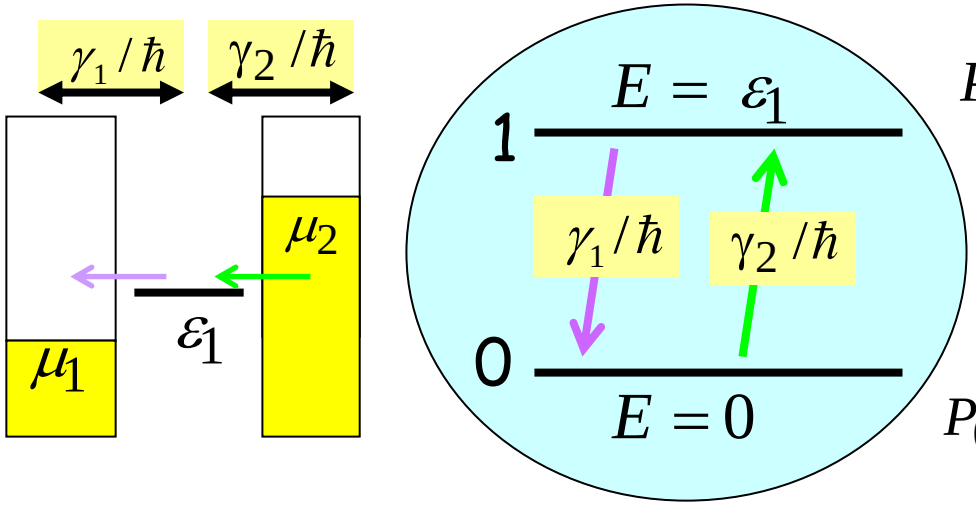


$P_1 = 0$

$P_0 = 1$

$$I = \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}$$



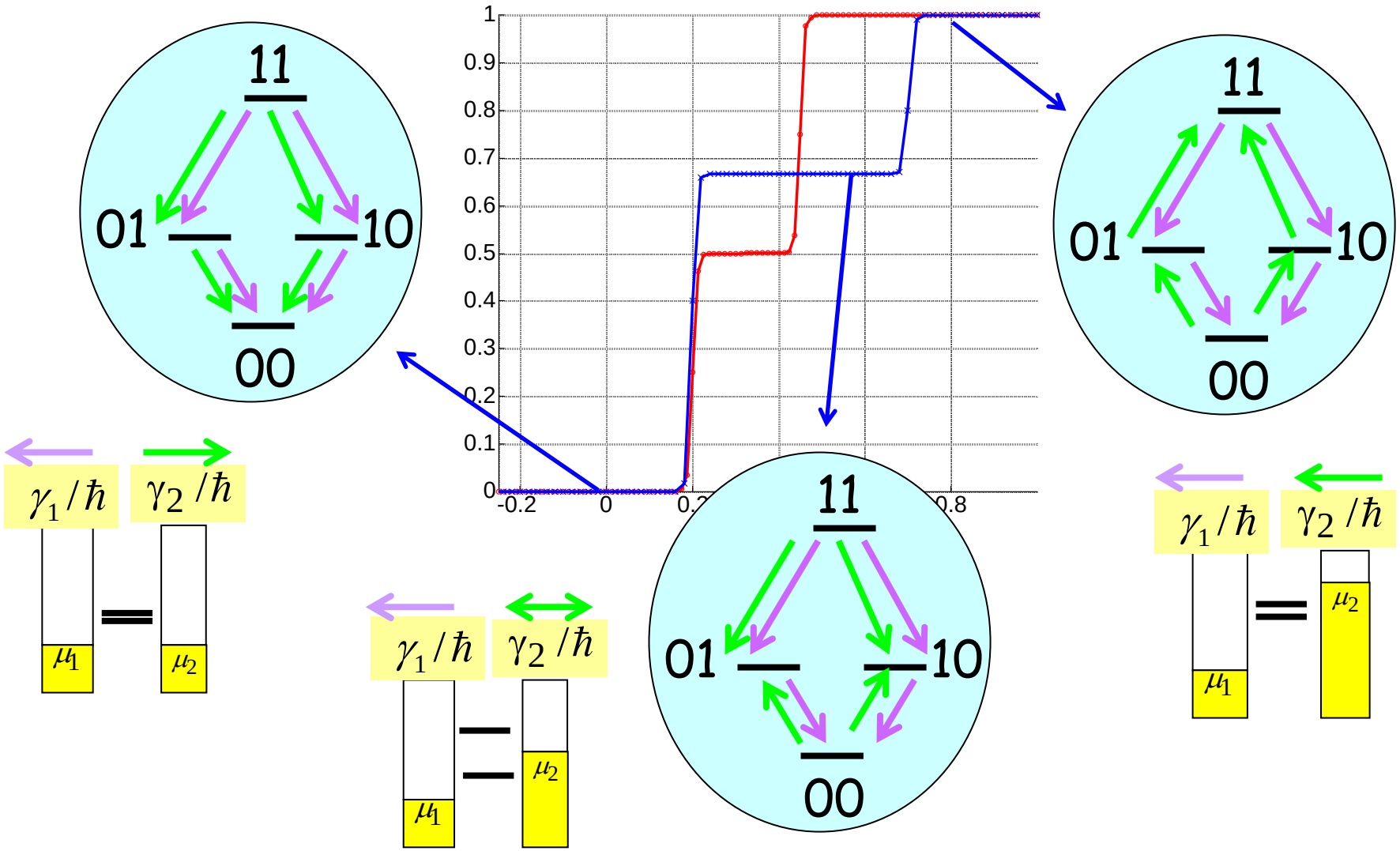


$P_1 = \gamma_2/(\gamma_1+\gamma_2)$

$$I = (q/\hbar)\,\gamma_1 P_1 = (q/\hbar)\,\gamma_2 P_0$$

$P_0 = \gamma_1/(\gamma_1+\gamma_2)$

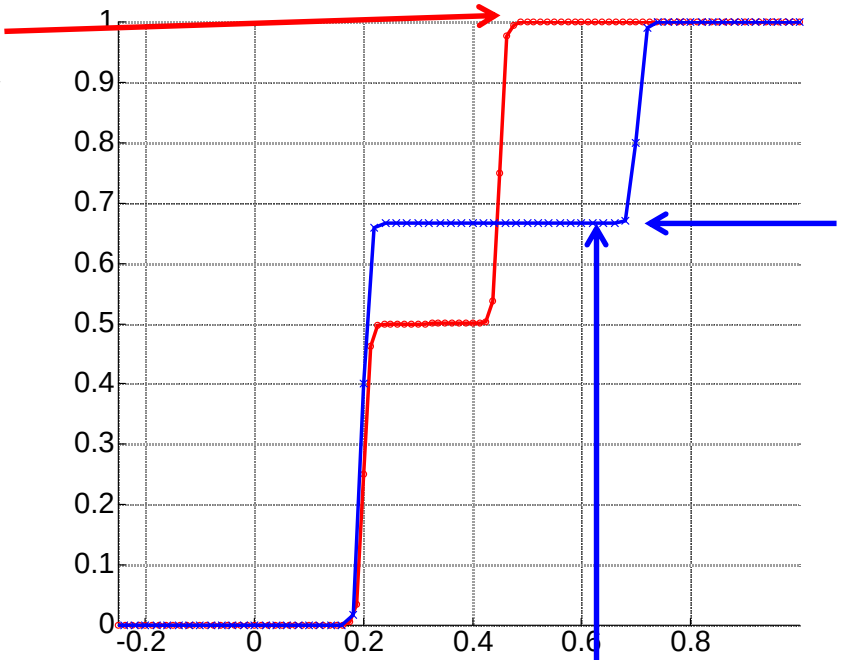
2 levels: Current flow in "Fock space"



2 levels: Current flow in "Fock space"

$$I = \frac{q}{\hbar}\frac{2\gamma_1\gamma_2}{\gamma_1+\gamma_2}$$

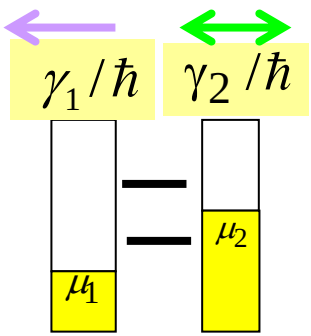
$$\rightarrow \quad (q\gamma_1/\hbar)$$

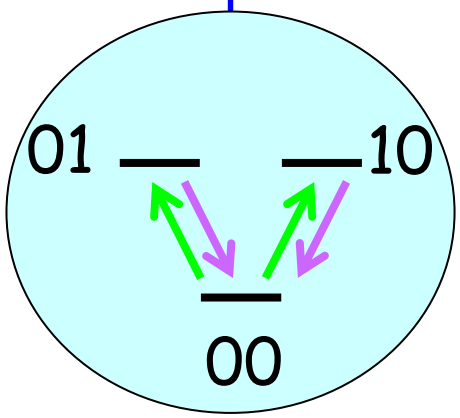


$$I = \frac{q}{\hbar}\frac{2\gamma_1\gamma_2}{\gamma_1+2\gamma_2}$$

$$\rightarrow \quad (2/3)\,(q\gamma_1/\hbar)$$

$$I = (q/\hbar)\,\gamma_1\,P_1$$
$$= (q/\hbar)\,2\gamma_2\,P_0$$

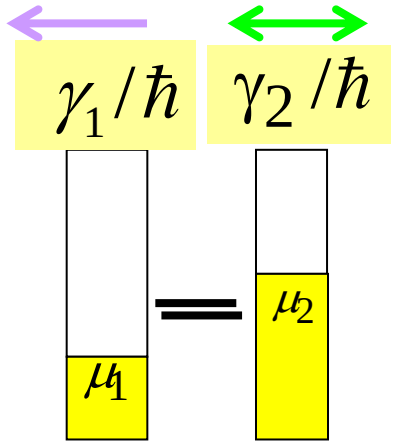




$$P_1 = 2\gamma_2/(\gamma_1+2\gamma_2)$$

$$P_0 = \gamma_1/(\gamma_1+2\gamma_2)$$

Coulomb blockade and strong correlation



$f\uparrow$ and $f\downarrow$

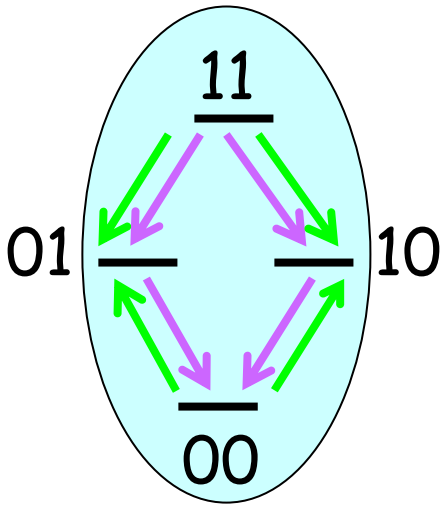
$$P_{00} = (1 - f\uparrow) * (1 - f\downarrow)$$

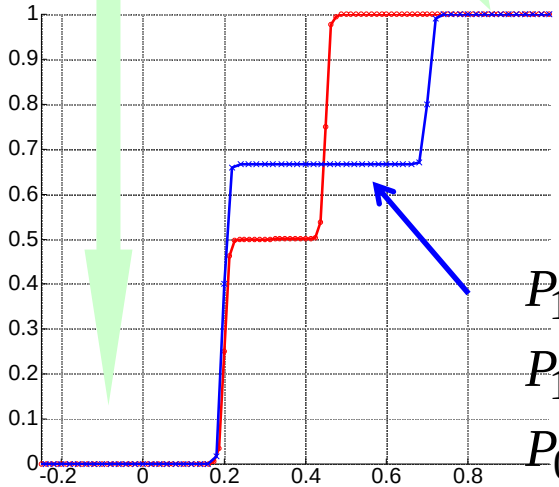
$$P_{10} = f\uparrow * (1 - f\downarrow)$$

$$P_{01} = (1 - f\uparrow) * f\downarrow$$

$$P_{11} = f\uparrow * f\downarrow$$

"UNCORRELATED"





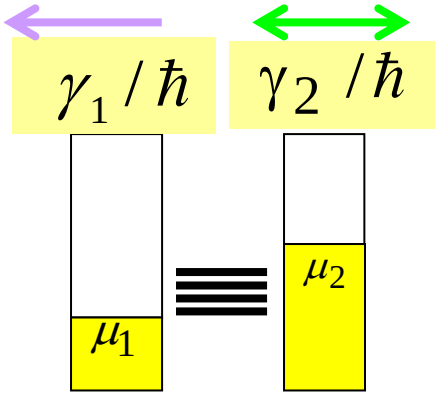
STRONGLY CORRELATED

$$P_{11} = 0$$

$$P_{10} = P_{01} = \gamma_2 / (\gamma_1 + 2\gamma_2)$$

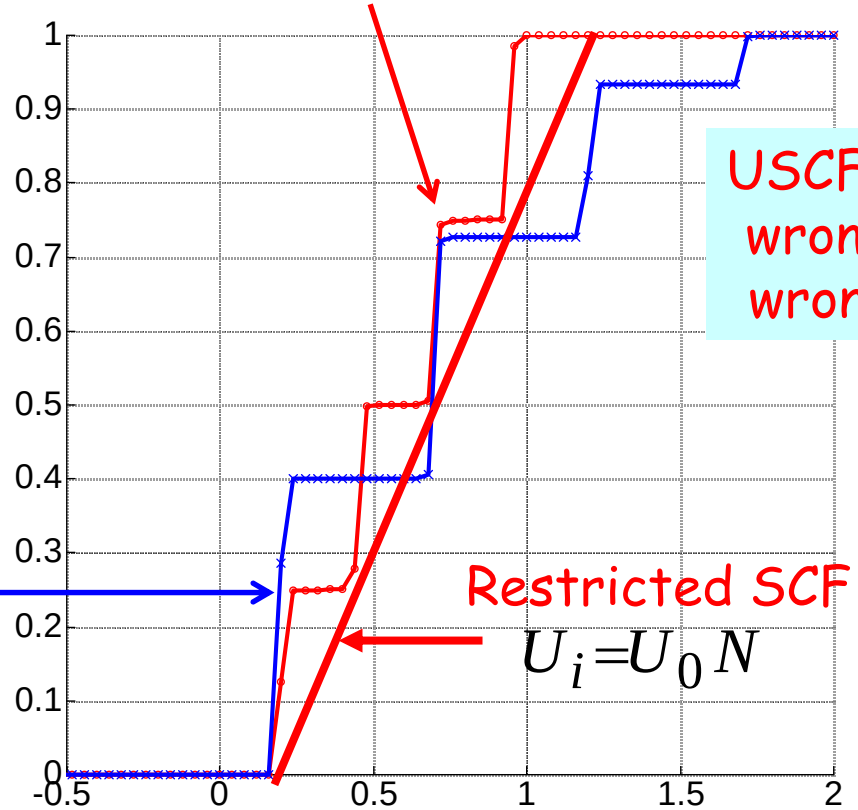
$$P_{00} = \gamma_1 / (\gamma_1 + 2\gamma_2)$$

4 levels: USCF versus exact



Unrestricted SCF

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



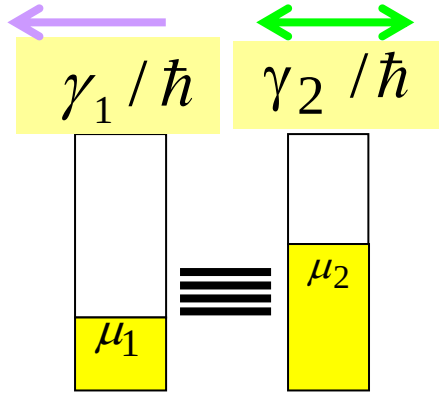
USCF plateaus have
wrong width: $U_0/2$
wrong height: 1/N

Exact
Fock space
approach

Restricted SCF

$$U_i = U_0 N$$

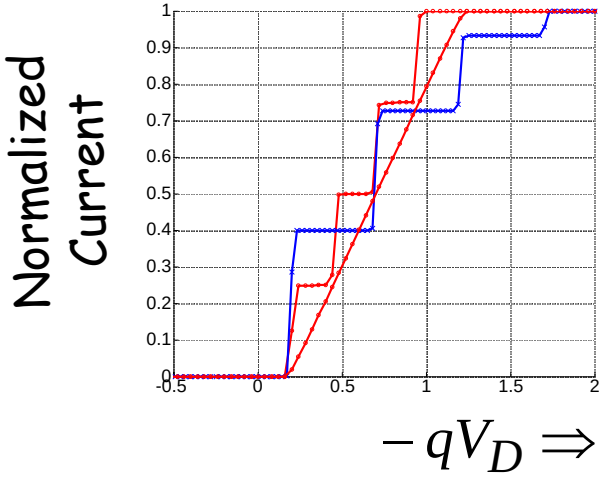
Equilibrium is different …

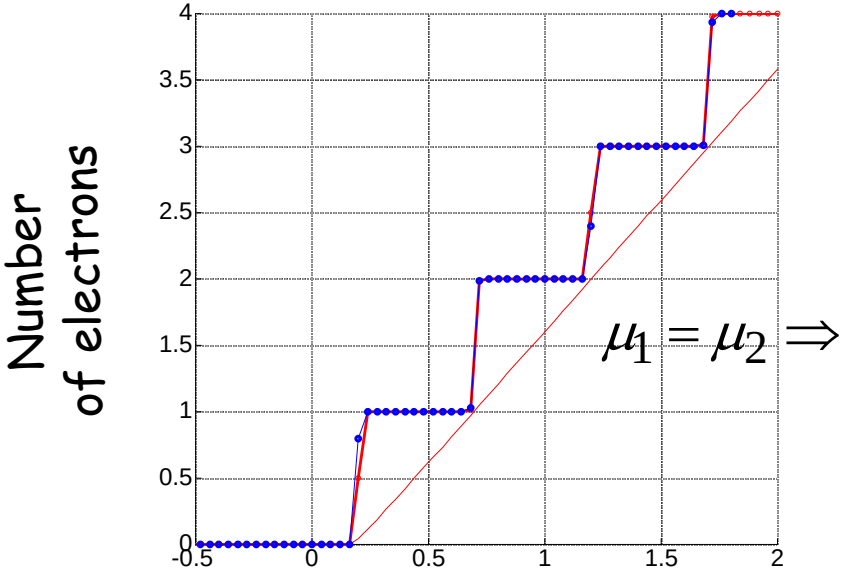


Exact

SCF: Restricted and unrestricted

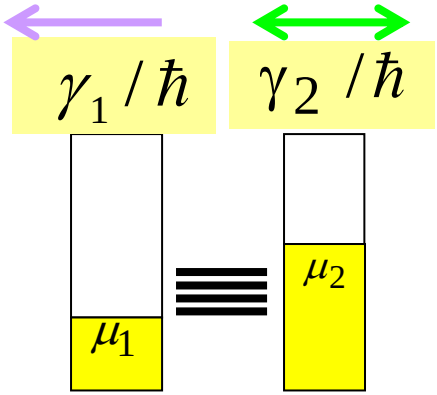
Non-equilibrium





Equilibrium

Being "close" to equilibrium helps too

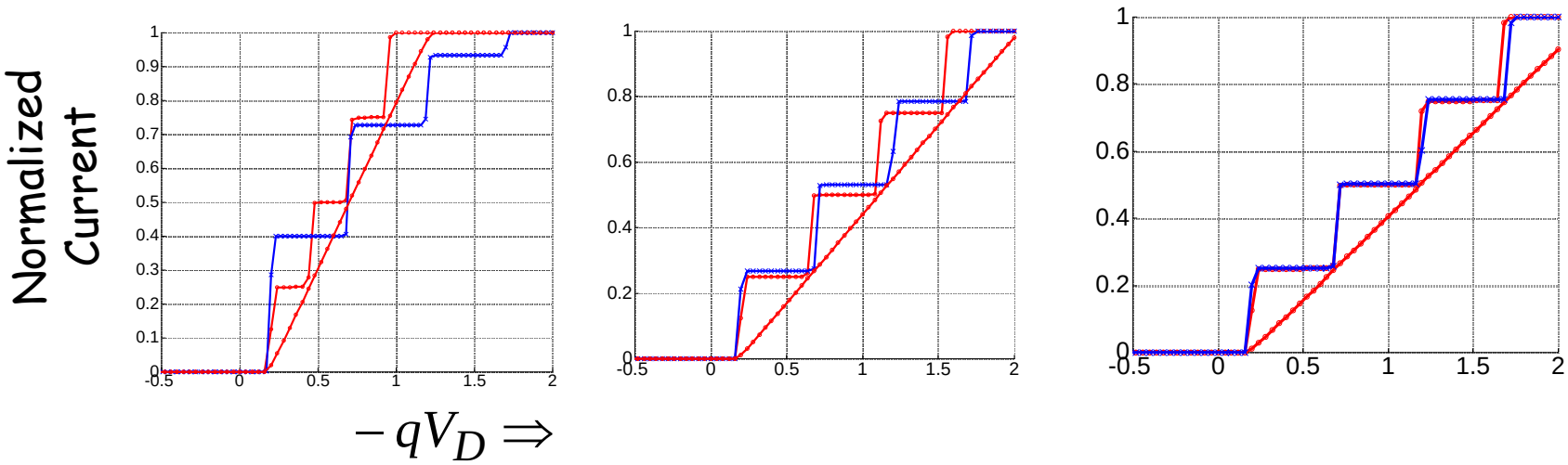


Exact

SCF: Restricted and unrestricted

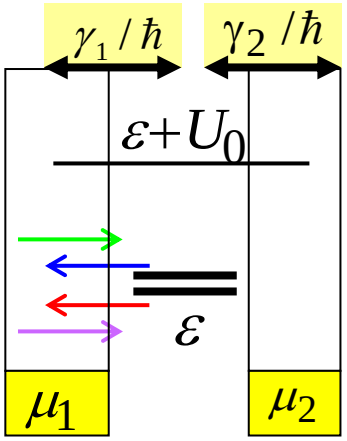
---> Closer ---> to equilibrium --->

$\gamma_2 = \gamma_1$ $\qquad$ $\gamma_2 = 10\,\gamma_1$ $\qquad$ $\gamma_2 = 100\,\gamma_1$

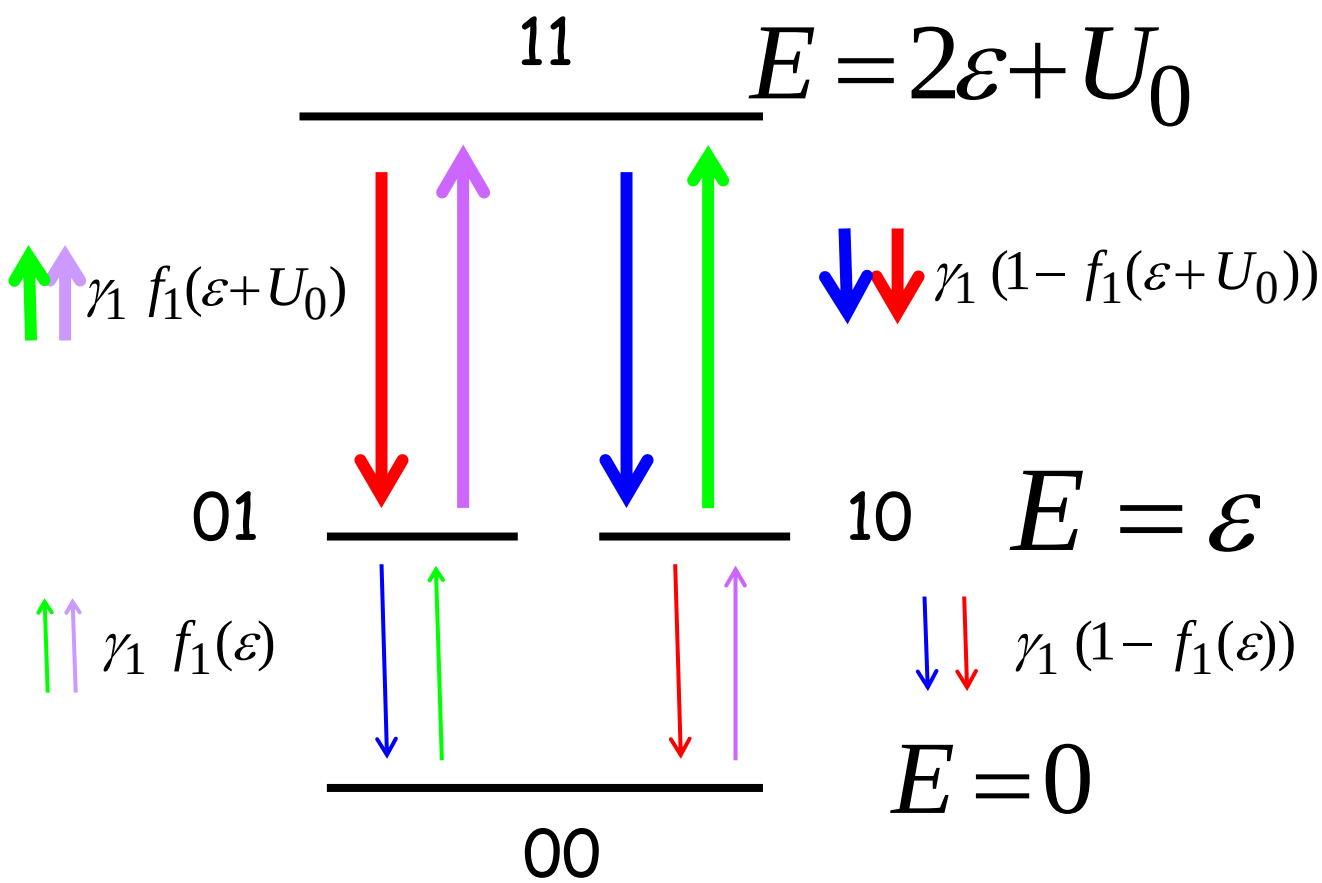


General "Fock space" approach

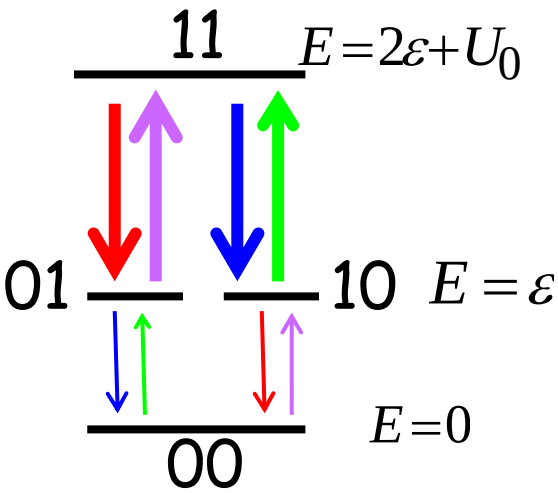
2 one-electron levels

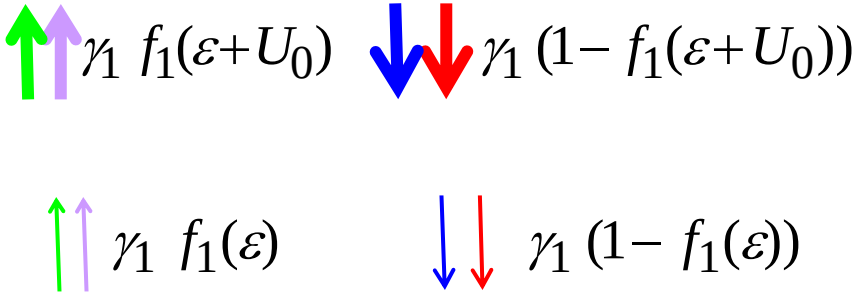


2^2 many-electron levels

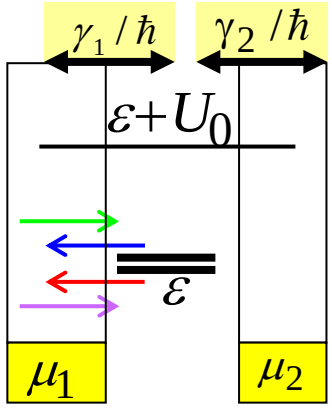


Equilibrium in "Fock space"





$$\frac{P_{N+1}}{P_N} = \frac{\Uparrow}{\Downarrow} = \frac{f_1(\Delta E)}{1 - f_1(\Delta E)} = e^{-(\Delta E - \mu)/k_B T}$$

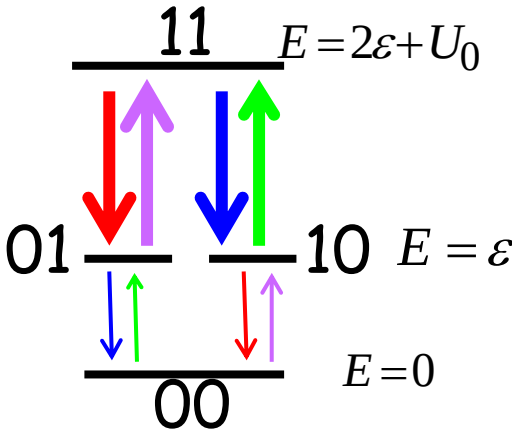


Law of Equilibrium

$$P_i = \frac{1}{Z} e^{-(E_i - \mu N_i)/k_B T}$$

No general solution out-of-equilibrium with $\mu_2 \neq \mu_1$

Rate equations in "Fock space"



$\gamma_1 \; f_1(\varepsilon + U_0)$
$+\gamma_2 \; f_2(\varepsilon + U_0)$

$\gamma_1 \; \bar{f}_1(\varepsilon + U_0)$
$+\gamma_2 \; \bar{f}_2(\varepsilon + U_0)$

$\gamma_1 \; f_1(\varepsilon)$
$+\gamma_2 \; f_2(\varepsilon)$

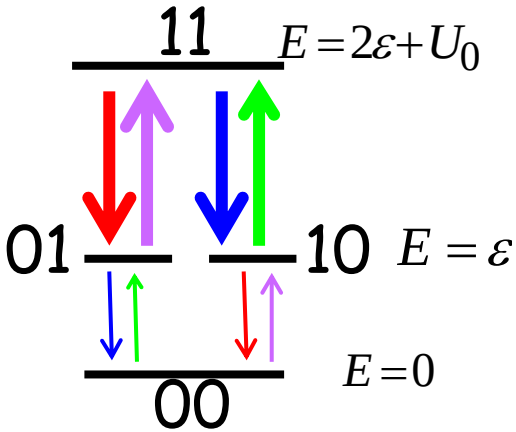
$\gamma_1 \; \bar{f}_1(\varepsilon)$
$+\gamma_2 \; \bar{f}_2(\varepsilon)$

$$\frac{d}{dt}\begin{Bmatrix} P_{00} \\ P_{01} \\ P_{10} \\ P_{11} \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} = \begin{bmatrix} * & \downarrow & \downarrow & 0 \\ \uparrow & * & 0 & \Downarrow \\ \uparrow & 0 & * & \Downarrow \\ 0 & \Uparrow & \Uparrow & * \end{bmatrix} \begin{Bmatrix} P_{00} \\ P_{01} \\ P_{10} \\ P_{11} \end{Bmatrix}$$

Each column adds to zero

$$\bar{0} \quad \bar{0} \quad \bar{0} \quad \bar{0}$$

Solving the rate equations

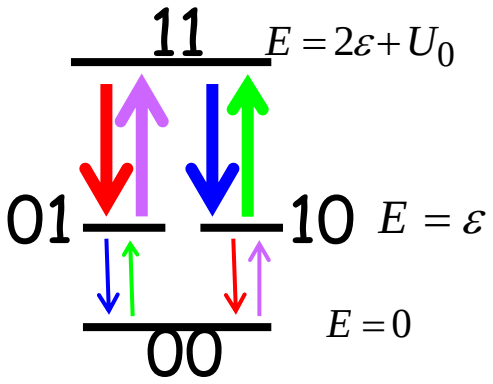


$$\begin{Bmatrix} P_{00} \\ P_{01} \\ P_{10} \\ P_{11} \end{Bmatrix} = \begin{bmatrix} * & \downarrow & \downarrow & 0 \\ \uparrow & * & 0 & \Downarrow \\ \uparrow & 0 & * & \Downarrow \\ 1 & 1 & 1 & 1 \end{bmatrix}^{-1} \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{Bmatrix}$$

$$\begin{Bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{Bmatrix} = \begin{bmatrix} * & \downarrow & \downarrow & 0 \\ \uparrow & * & 0 & \Downarrow \\ \uparrow & 0 & * & \Downarrow \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{Bmatrix} P_{00} \\ P_{01} \\ P_{10} \\ P_{11} \end{Bmatrix}$$

All probabilities add to ONE

Calculating current in "Fock space"



$\gamma_1 \; f_1(\varepsilon + U_0)$
$+\gamma_2 \; f_2(\varepsilon + U_0)$

$\gamma_1 \; \bar{f}_1(\varepsilon + U_0)$
$+\gamma_2 \; \bar{f}_2(\varepsilon + U_0)$

$\gamma_1 \; f_1(\varepsilon)$
$+\gamma_2 \; f_2(\varepsilon)$

$\gamma_1 \; \bar{f}_1(\varepsilon)$
$+\gamma_2 \; \bar{f}_2(\varepsilon)$

$$\{1 \quad 1 \quad 1 \quad 1\} \begin{bmatrix} 0 & -\downarrow & -\downarrow & 0 \\ \uparrow & 0 & 0 & -\Downarrow \\ \uparrow & 0 & 0 & -\Downarrow \\ 0 & \Uparrow & \Uparrow & 0 \end{bmatrix} \begin{Bmatrix} P_{00} \\ P_{01} \\ P_{10} \\ P_{11} \end{Bmatrix}$$

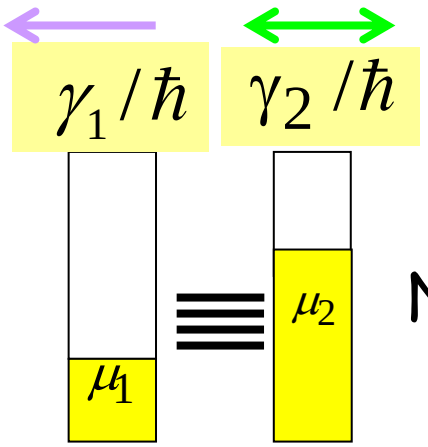
"Fock space" for 4 one-electron levels

Two problems: *Size

"Orthodox Theory"

N one-electron levels

2^N many-electron levels



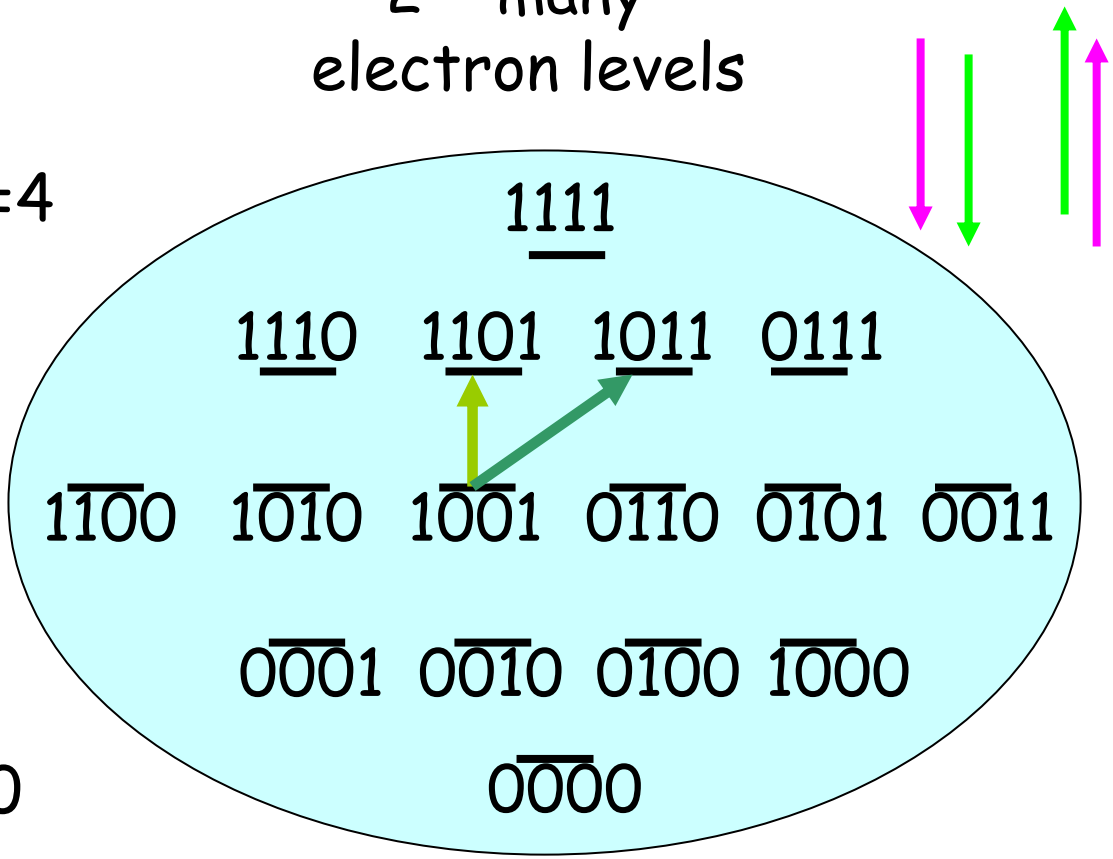
N=4

N=3

N=2

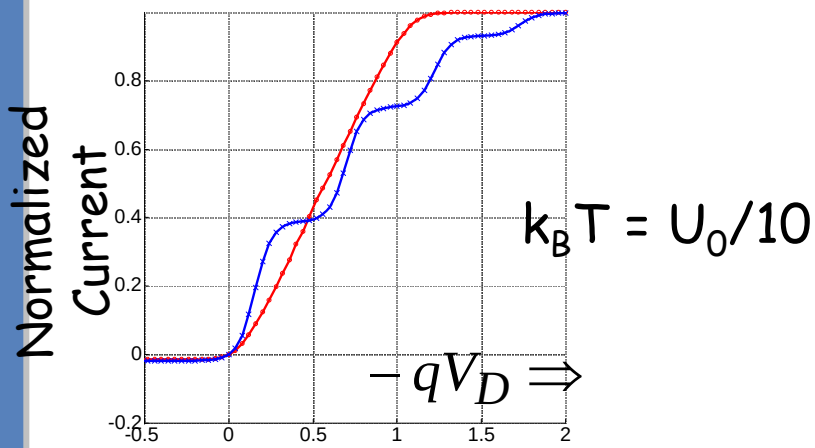
N=1

N=0



When is Fock space needed ?

If $k_B T$ + broadening << charging U_0

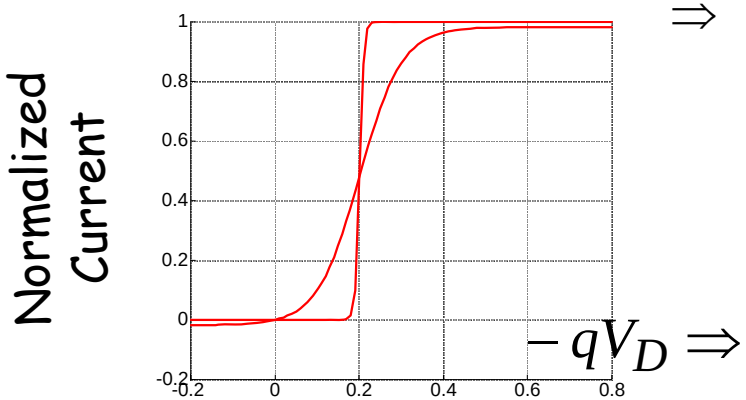


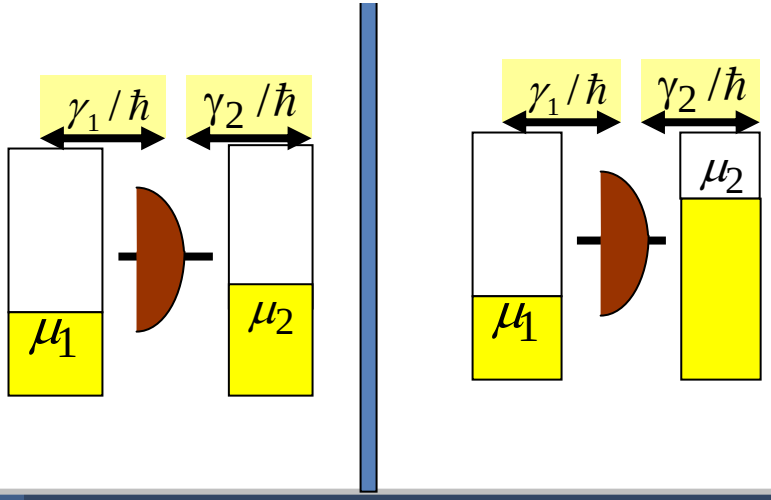
$$U_0 < k_B T, \underbrace{\gamma_1, \gamma_2}$$

Use SCF method

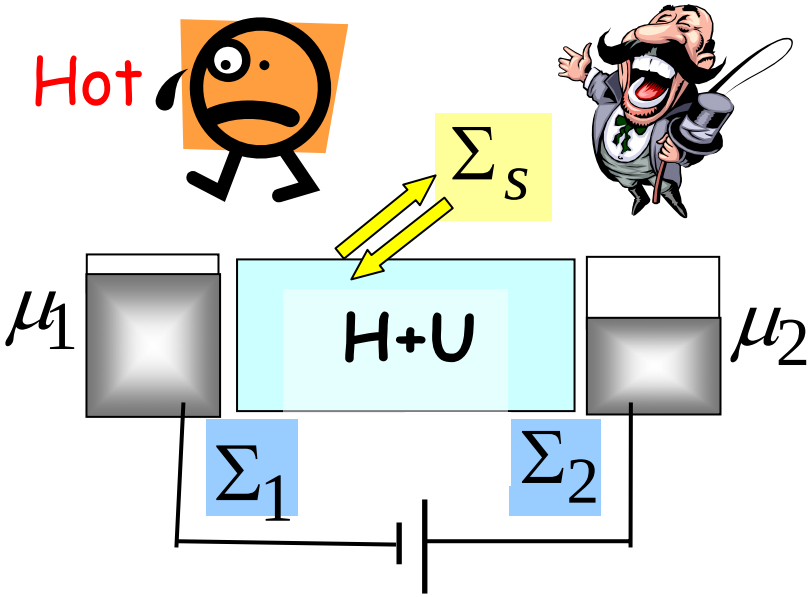
$$\text{Assume } \gamma_2 = \gamma_1$$

$$2\gamma_1 + 4k_B T \Rightarrow \frac{q\gamma_1}{2\hbar}$$





Concepts of Quantum Thermodynamics (QT)



Entangled!

Nanowires, nanotubes, molecules .....

Switches, energy conversion ...

Concepts of Quantum Transport (CQT)

Concepts of Quantum Transport

Introduction :

Lecture #1:

Nanodevices and Maxwell's demon

Lecture #2:

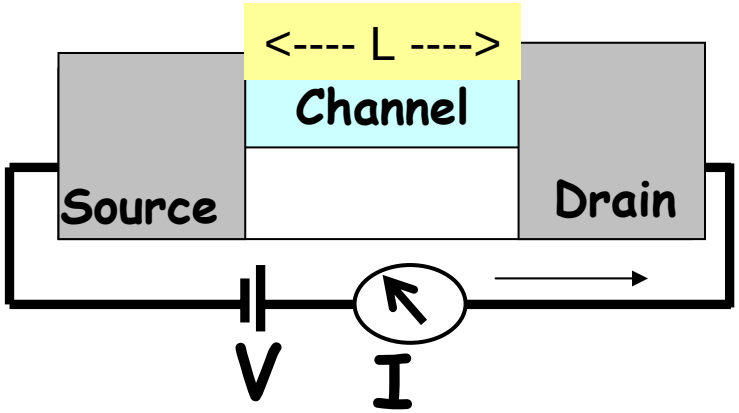
Electrical Resistance:A Simple Model

Lecture #3:

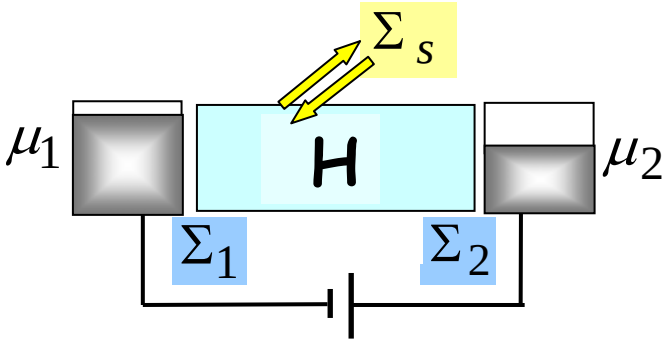
Probabilities, Wavefunctions and Green functions

Lecture #4:

Coulomb blockade and Fock space



Unified Model for Quantum Transport Far from Equilibrium



No advanced background required. Familiarity with linear algebra may be useful for some topics.

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Tehseen Raza and the NCN