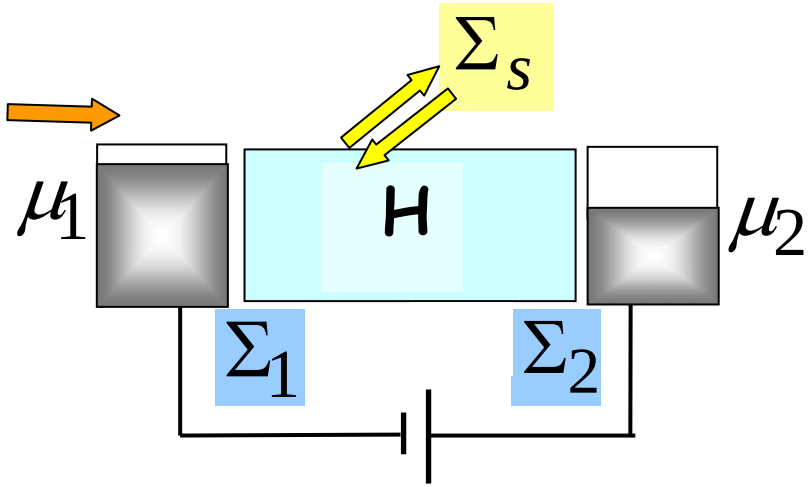
CQT, Lecture#3:
Probabilities, Wavefunctions and Green Functions

Unified Model for Quantum Transport Far from Equilibrium

Objectives:
To extend the simple model from Lecture 2 into the full-blown model shown opposite that combines the NEGF (Non-Equilibrium Green Function) method with the Landauer approach.



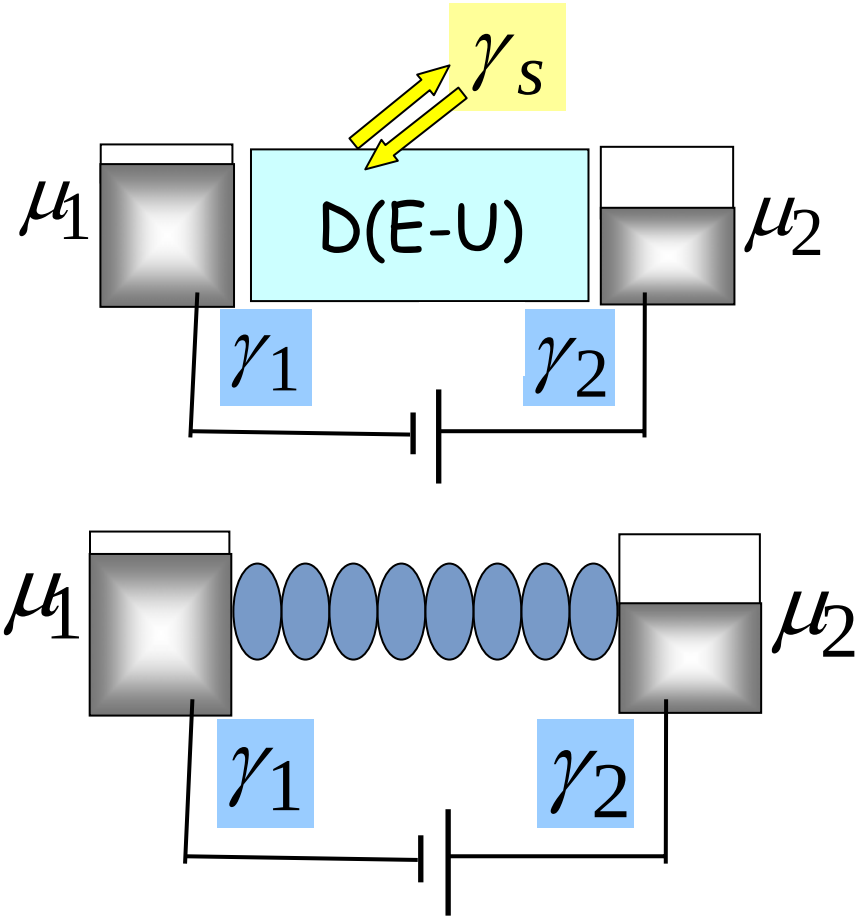
Model based on
(1)Datta, Phys.Rev.B40, 5830 (1989);J.Phys.Cond.Matt.2, 8023(1990).
(2)Meir and Wingreen, Phys.Rev.Lett.68, 2512(1992).

Reference: QTAT, Chapters 8-11.

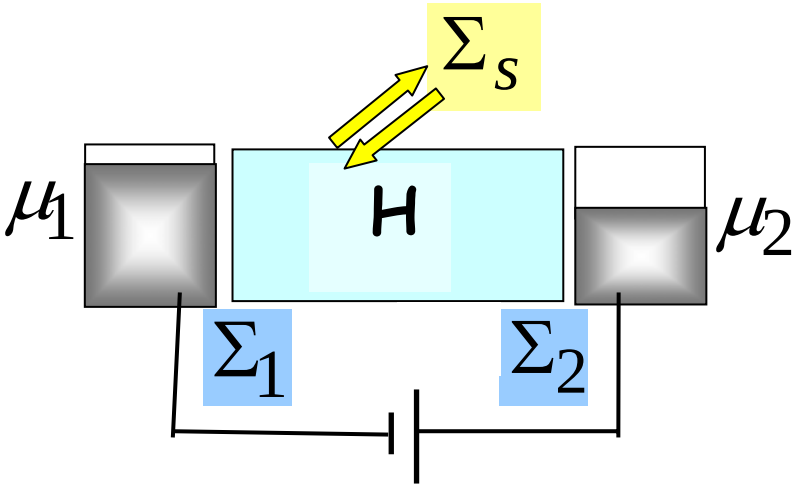
"QTAT"
Datta, Quantum Transport: Atom to Transistor, Cambridge (2005)

Probabilities, wavefunctions, Green functions

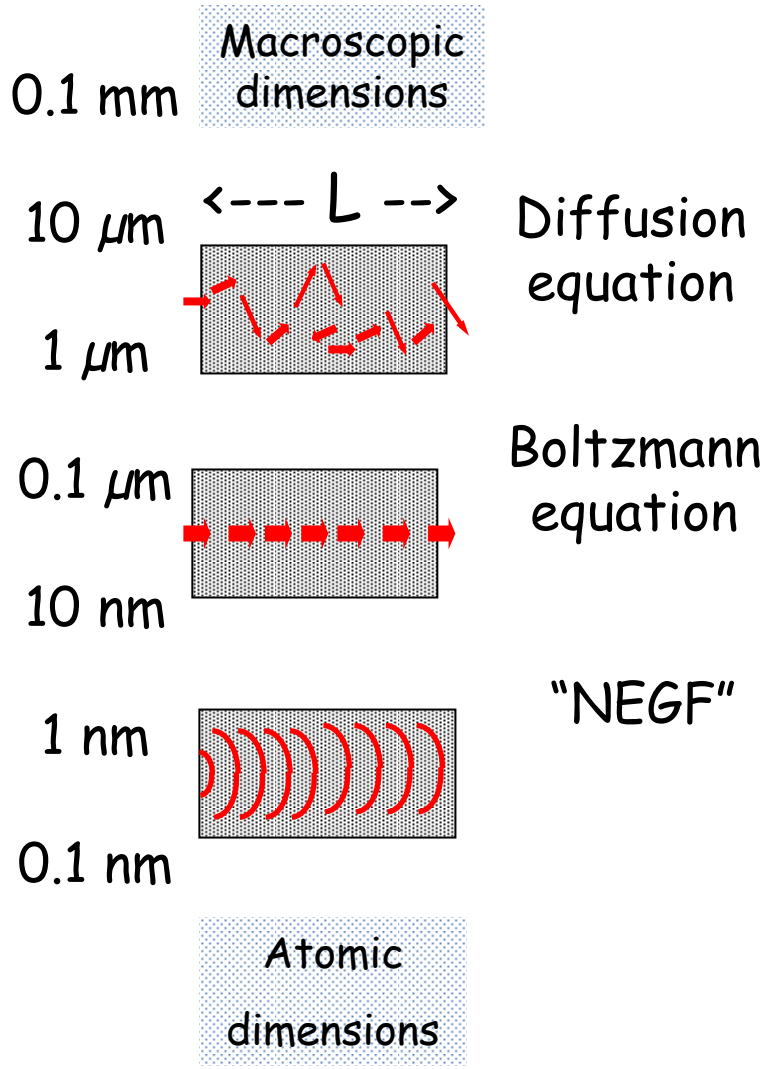
Simple quantitative model
For Transport
Far from Equilibrium



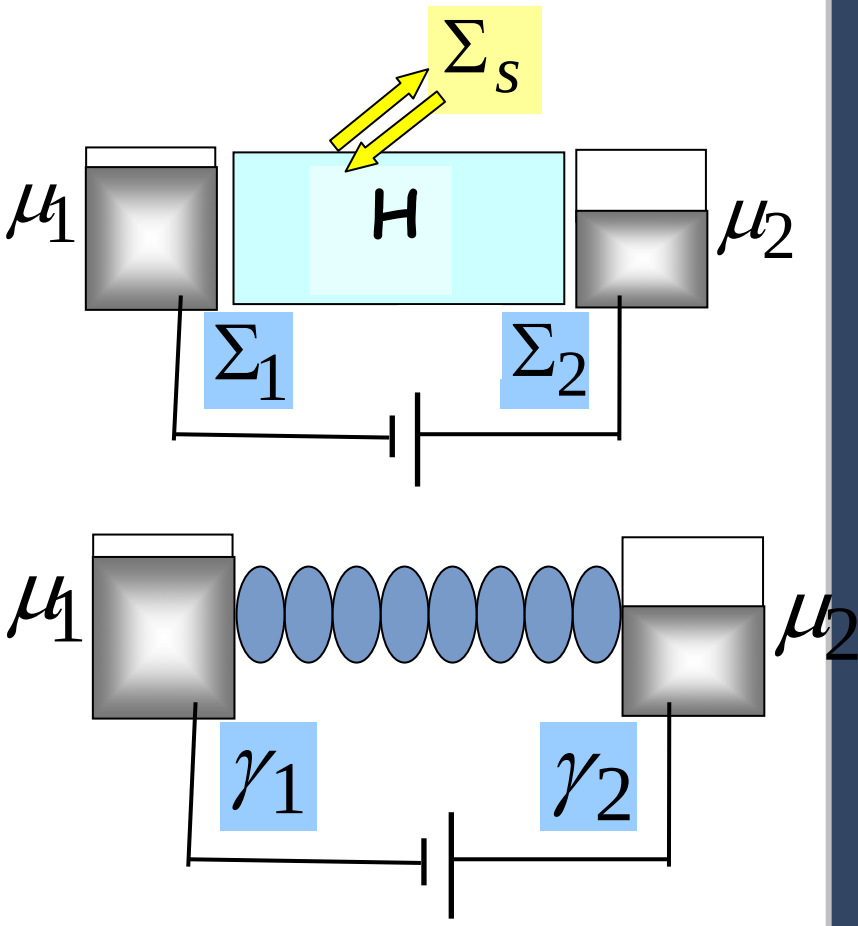
Unified Model for
Quantum Transport
Far from Equilibrium



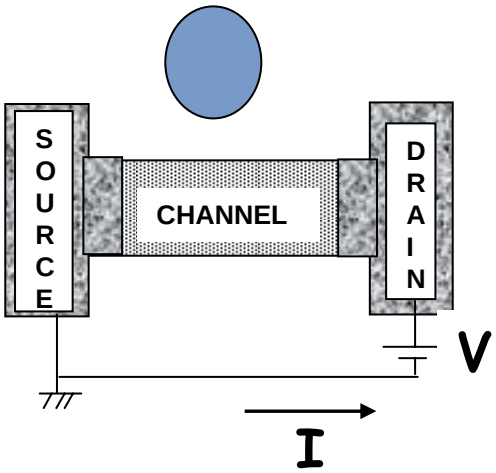
Probabilities, wavefunctions, Green functions

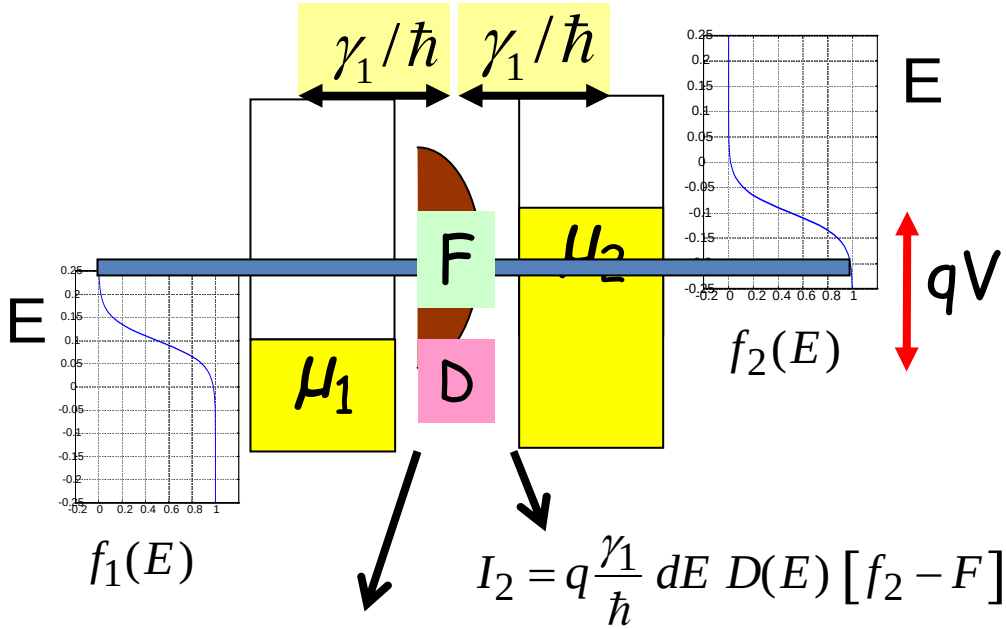


Unified Model for Quantum Transport Far from Equilibrium



Summary: 1-grid point model





$$I_2 = q\frac{\gamma_1}{\hbar}\, dE\; D(E)\,[f_2 - F]$$

$$I_1 = q\frac{\gamma_1}{\hbar}\, dE\; D(E)\,[F - f_1]$$

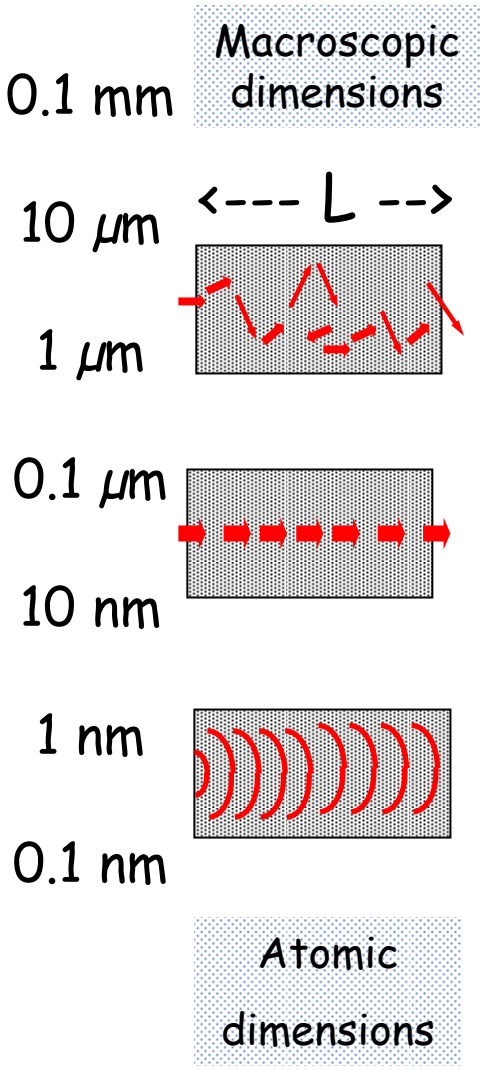
$$F - f_1 = f_2 - F$$

$$\Rightarrow \quad F - f_1 = \frac{f_2 - f_1}{2} \quad \Rightarrow I = \frac{q}{h}\int dE\; \frac{K(E)}{2}\,[f_2 - f_1]$$

Transmission

$$K(E) \equiv 2\pi D(E)\gamma_1$$

Introducing a Grid

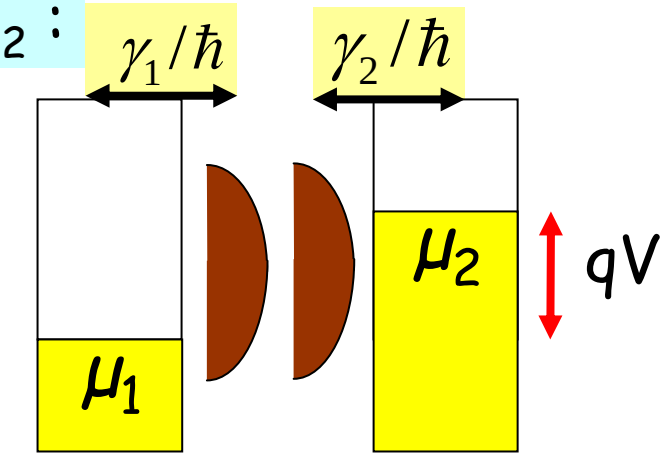


$R_2 > R_1$

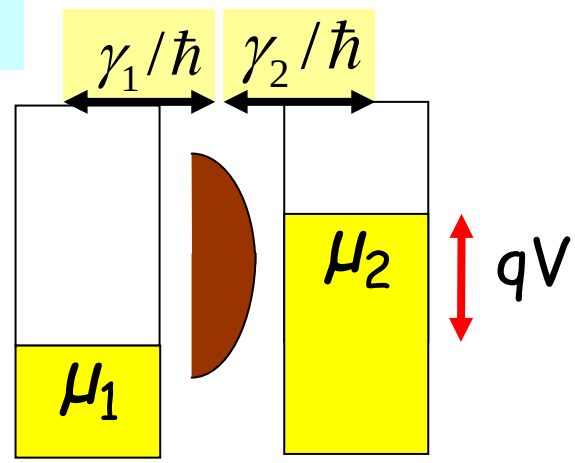
$R_2 = R_1$

R_2 can even be less than R_1

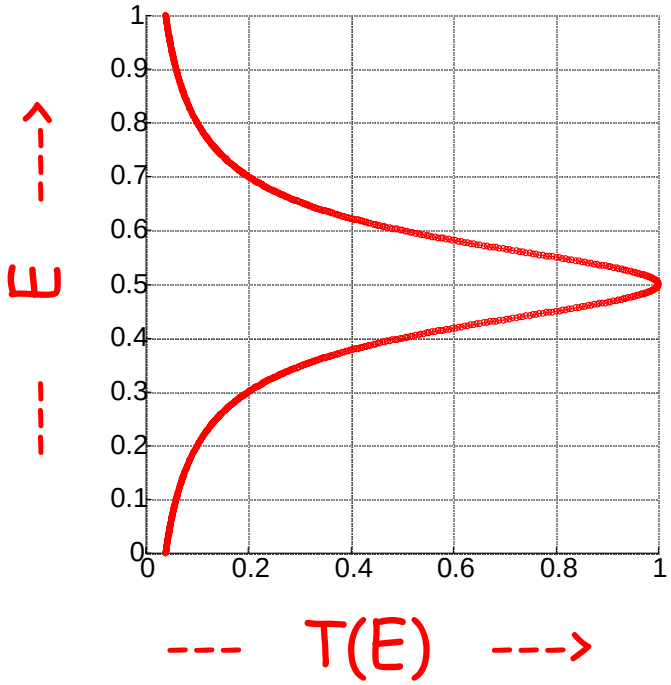
R_2 :

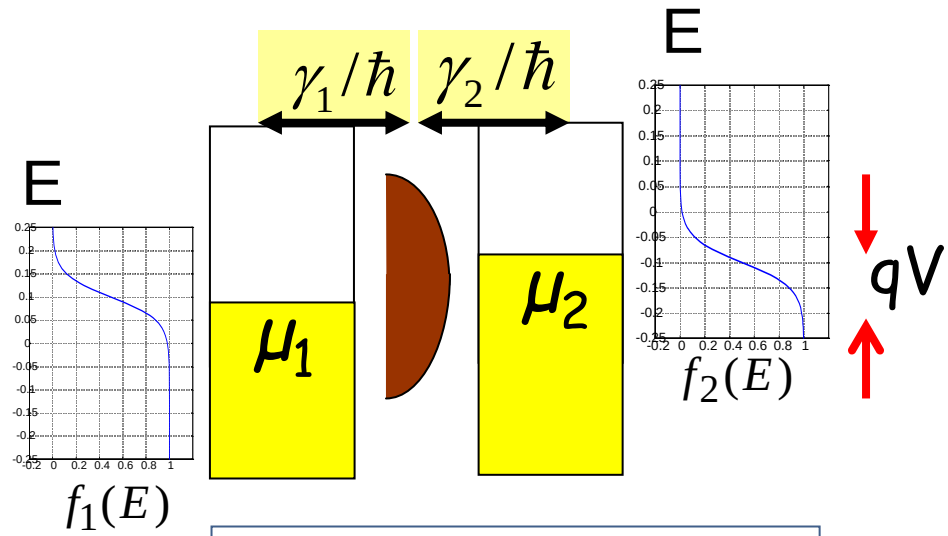


R_1 :



Energy -resolved current





1-grid point model

$$T(E) = K(E)/2$$

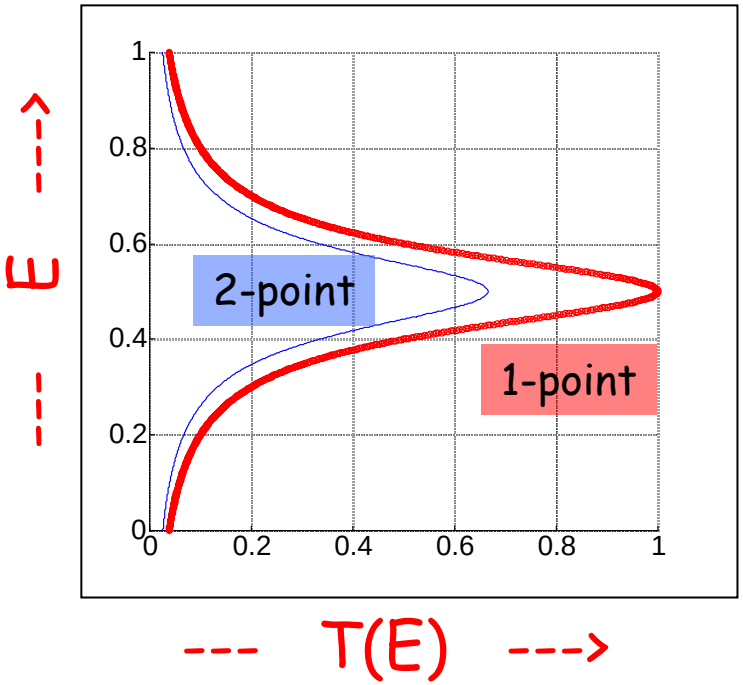
$$K(E) \equiv 2\pi D(E)\gamma_1$$

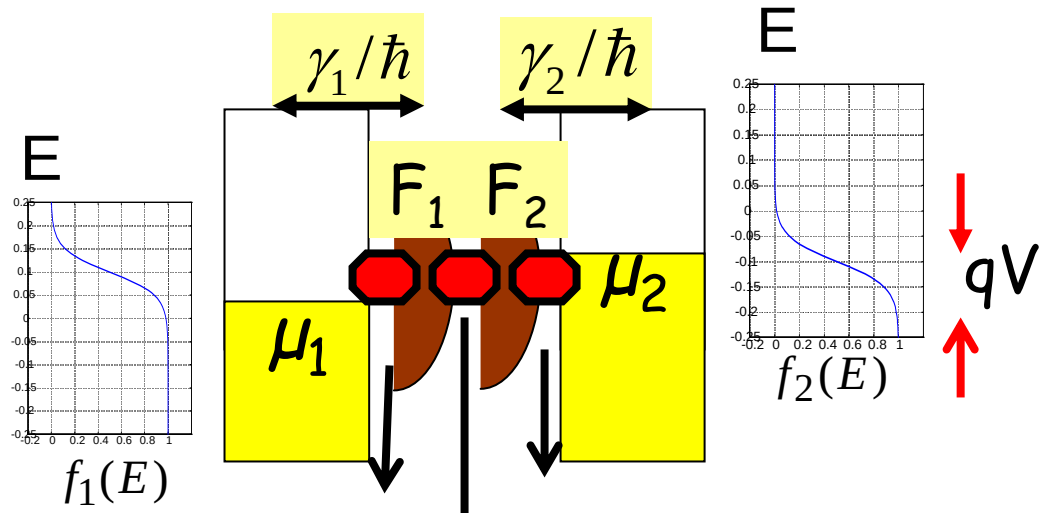
$$I = \frac{q}{h}\int dE \, \frac{K(E)}{2}\left[f_1 - f_2\right]$$

Transmission

$$\approx \frac{q}{h} qV \quad T$$

2-grid point diffusive model





$$I_1 = K(E)\,[F_1 - f_1] \qquad I_2 = K(E)\,[f_2 - F_2]$$

$$I_{12} = K(E)\,[F_1 - F_2]$$

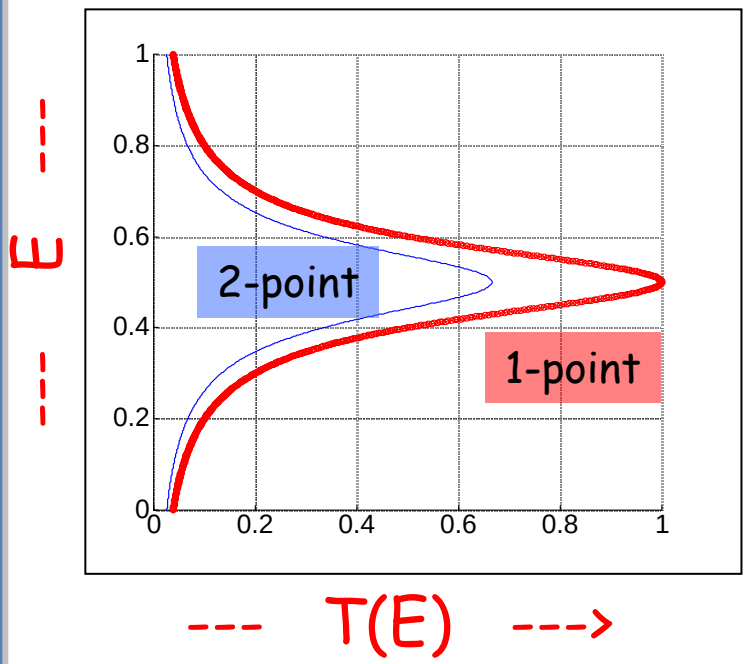
$$F_1 - f_1 = F_2 - F_1 = f_2 - F_2$$

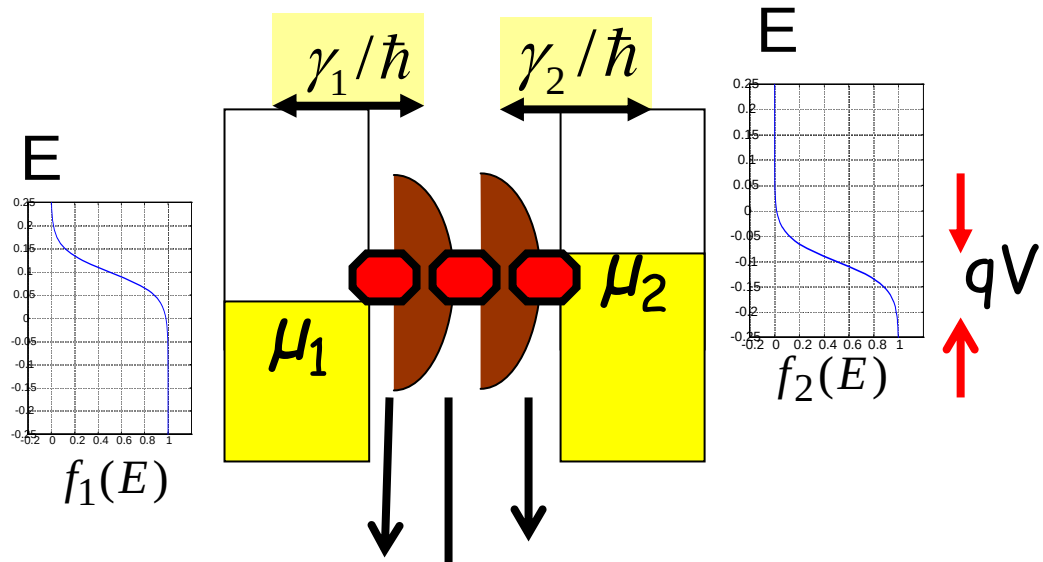
$$\Rightarrow \quad F_1 - f_1 = \frac{f_2 - f_1}{3} \qquad \Rightarrow I = \frac{K(E)}{3}\,[f_1 - f_2]$$

$$K(E) \equiv 2\pi\gamma_1 D(E)$$

(Currents normalized to q dE/h)

Equivalent circuit

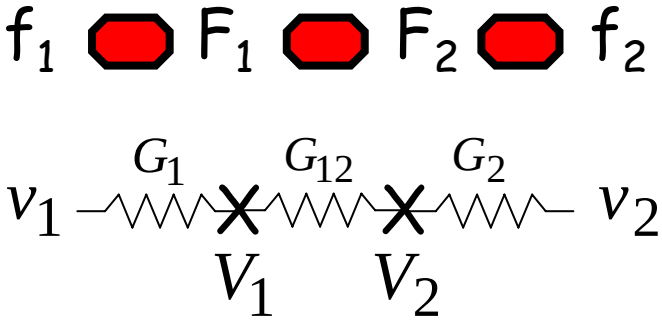




$$I_1 = K(E)\,[F_1 - f_1]$$

$$I_2 = K(E)\,[f_2 - F_2]$$

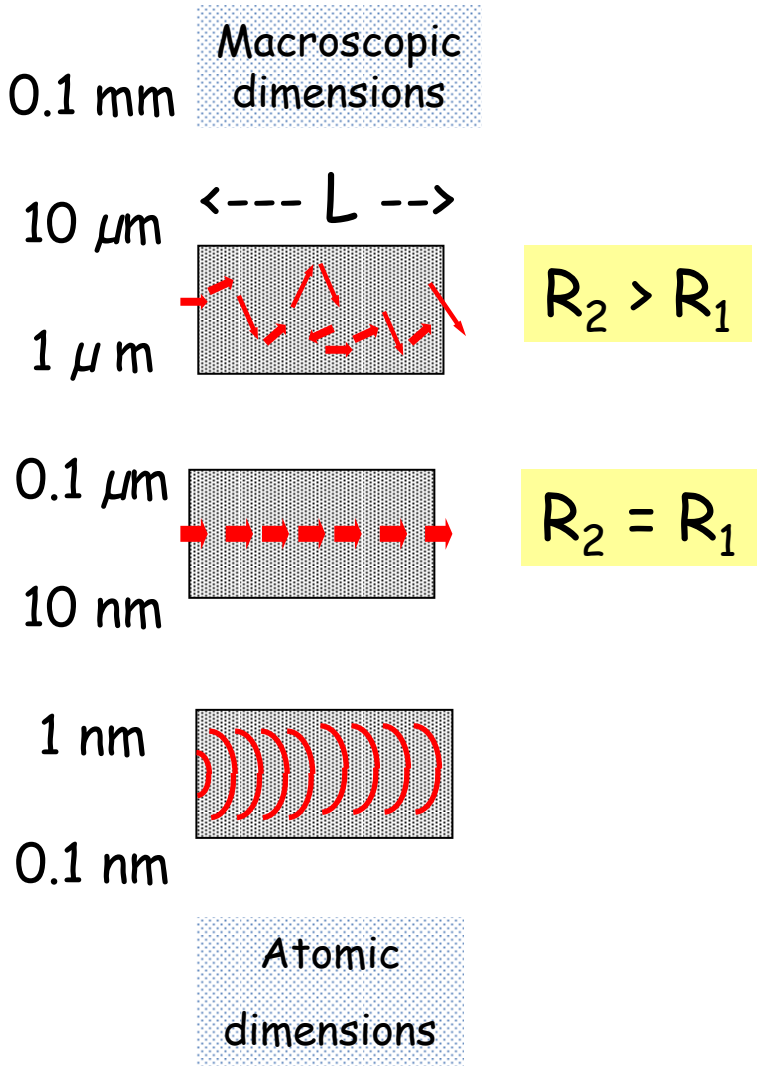
$$I_{12} = K(E)\,[F_1 - F_2]$$

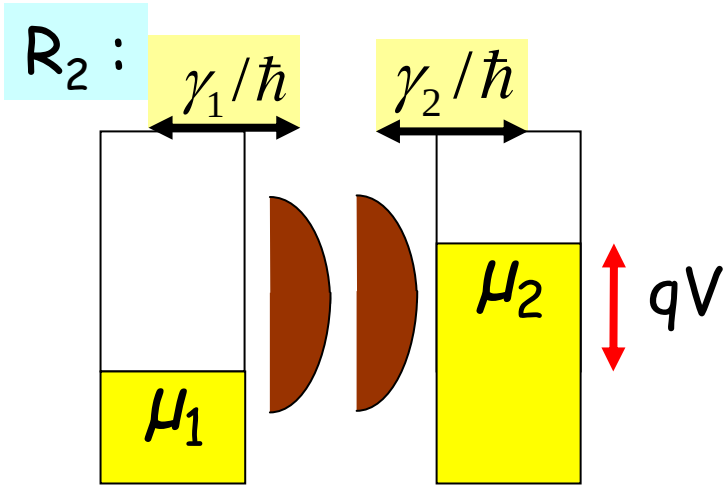


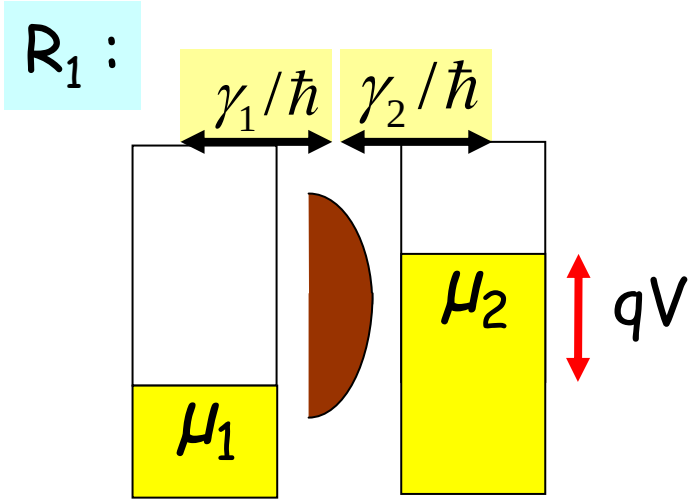
Discretized version of $I \sim \partial F / \partial z$

Diffusion equation

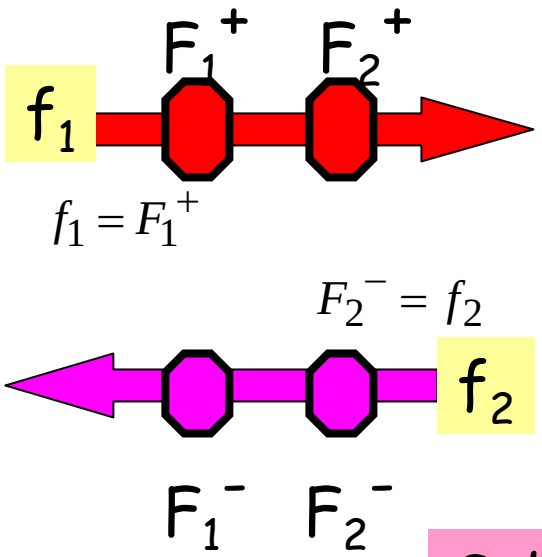
Introducing a Grid

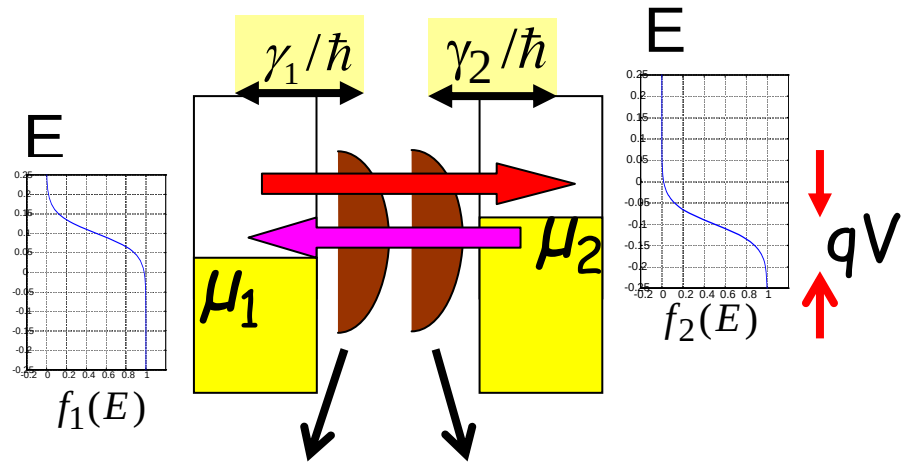






2-grid point ballistic model





$$I_1^+ = \frac{K(E)}{2} F_1^+ \qquad I_2^+ = \frac{K(E)}{2} F_2^+$$

Subtract →

$$I_1^- = \frac{K(E)}{2} F_1^- \qquad I_2^- = \frac{K(E)}{2} F_2^-$$

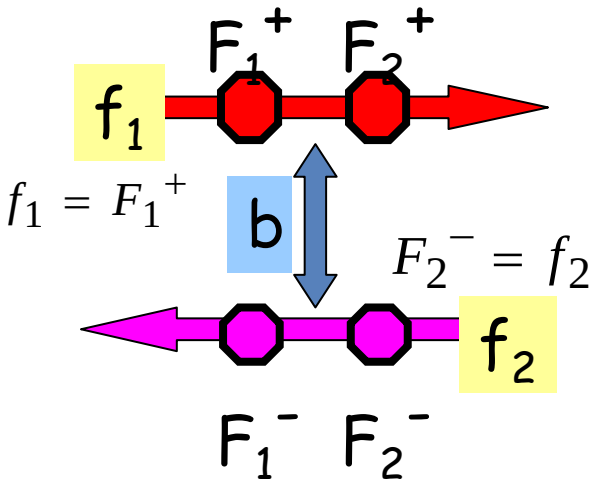
$$f_1 = F_1^+ = F_2^+$$

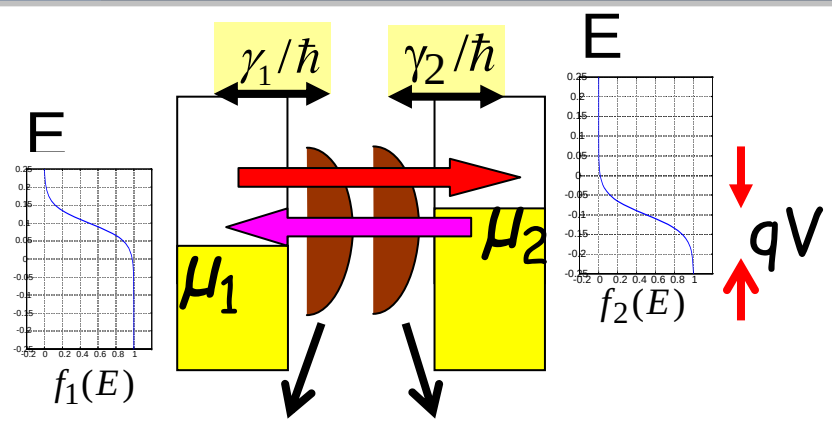
$$F_1^- = F_2^- = f_2$$

$$I = \frac{q}{h}\int dE \frac{K(E)}{2}[f_1 - f_2]$$

Current is same as in 1-point model: Ballistic transport

2-grid point, 2-flux model





$$I_1^+ = \frac{K(E)}{2} F_1^+ \qquad I_2^+ = \frac{K(E)}{2} F_2^+$$

$$I_1^- = \frac{K(E)}{2} F_1^- \qquad I_2^- = \frac{K(E)}{2} F_2^-$$

$$I_2^+ = (1-b)\, I_1^+ + b\, I_2^-$$

$$\Rightarrow \quad F_2^+ = (1-b)\, f_1 + b\, f_2$$

$$I_1^- = (1-b)\, I_2^- + b\, I_1^+$$

$$\Rightarrow \quad F_1^- = (1-b)\, f_2 + b\, f_1$$

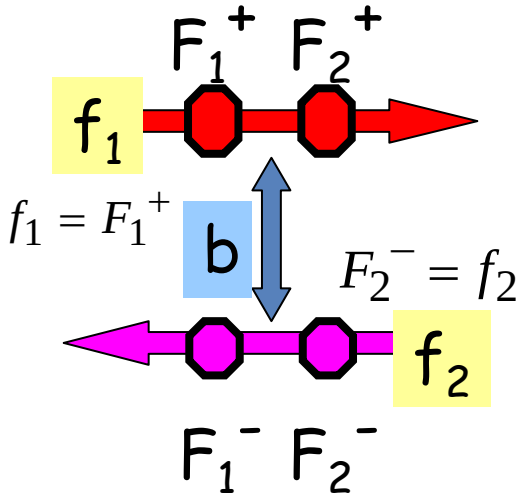
$$I = \frac{K(E)}{2}(1-b)\,[f_2 - f_1]$$

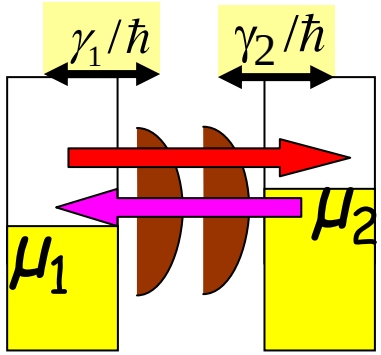
Can show that for 'n+1' sections each having a small 'b' :

$$I = \frac{K(E)}{2}\frac{1}{1+nb}\,[f_2 - f_1]$$

Interpolates smoothly from ballistic to diffusive transport

Boltzmann equation





$$I_1^- = (1-b)I_2^- + bI_1^+$$

$$\Rightarrow \quad F_1^- = (1-b)\, f_2 + b\, f_1$$

$$I_2^+ = (1-b)\, I_1^+ + bI_2^-$$

$$\Rightarrow \quad F_2^+ = (1-b)\, f_1 + b\, f_2$$

Discrete version of

$$\frac{\partial I^+}{\partial z} = -\beta I^+ - \beta I^-$$

$$\frac{\partial I^-}{\partial z} = \beta I^+ + \beta I^-$$

More generally

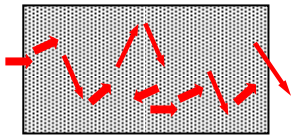
$$\frac{\partial I(\vec{k})}{\partial z} = \int d\vec{k}' \left(S(\vec{k},\vec{k}')I(\vec{k}') - S(\vec{k}',\vec{k})I(\vec{k}) \right)$$

Ref . Mark Lundstrom, Fundamentals of Carrier Transport, Cambridge (2000)

Introducing a Grid

0.1 mm — Macroscopic dimensions

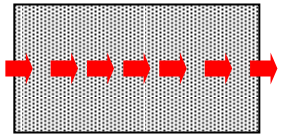
10 μm — <--- L --->



1 μm

$R_2 > R_1$

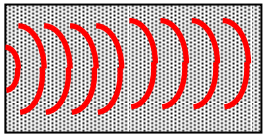
0.1 μm



10 nm

$R_2 = R_1$

1 nm

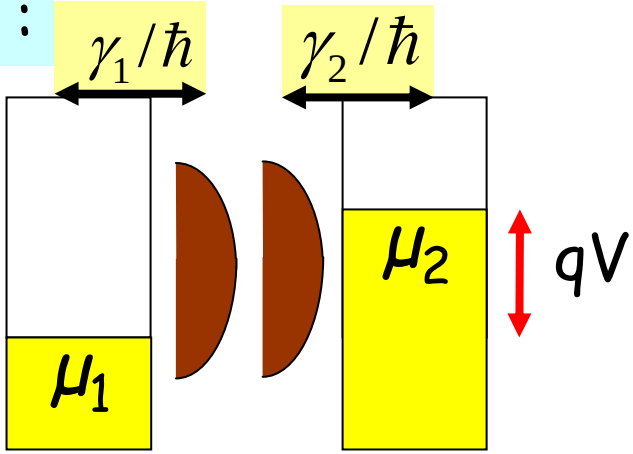


0.1 nm

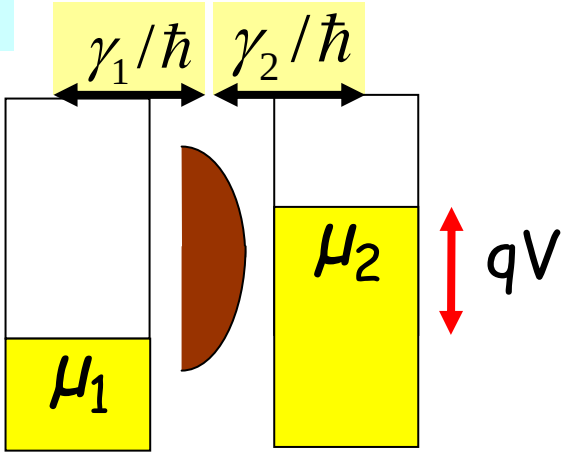
R_2 can even be less than R_1

Atomic dimensions

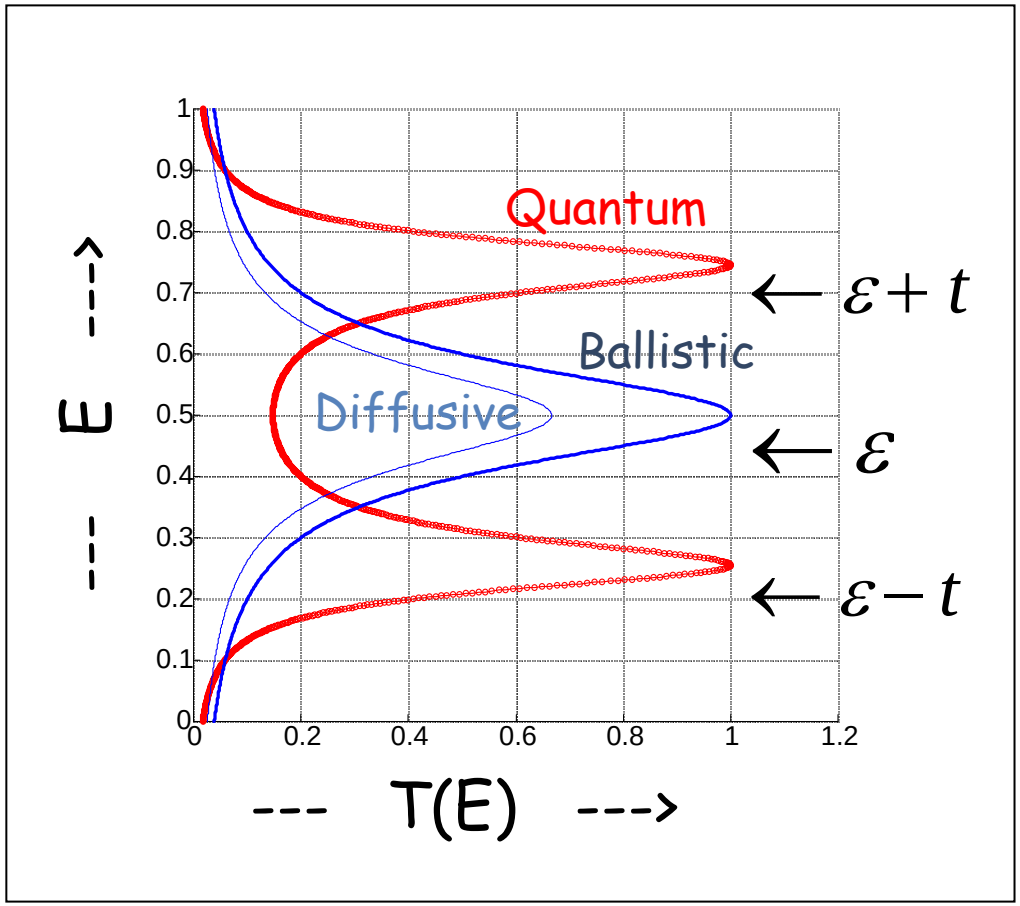
R_2 :

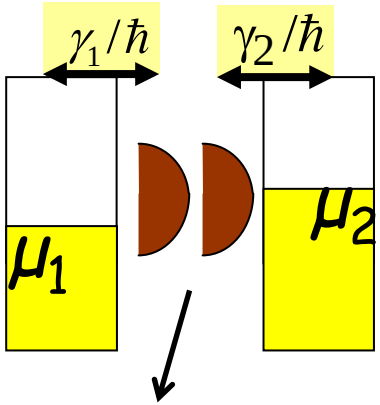


R_1 :



From particles to waves ..





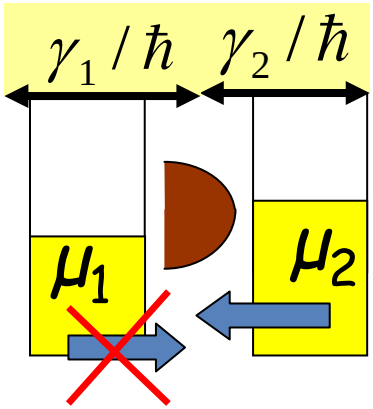
$$H = \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}$$

$$\begin{bmatrix} \varepsilon + t & 0 \\ 0 & \varepsilon - t \end{bmatrix} \rightarrow \begin{Bmatrix} +1 \\ +1 \end{Bmatrix}, \quad \begin{bmatrix} \varepsilon + t & 0 \\ 0 & \varepsilon - t \end{bmatrix} \rightarrow \begin{Bmatrix} +1 \\ -1 \end{Bmatrix}$$

Introducing the "wavefunction"

$$n_1 = \psi_1 \psi_1^*$$

1 grid point



$$\left[E - \varepsilon + \frac{i\gamma_1}{2} + \frac{i\gamma_2}{2}\right]\psi_1 = s_2$$

Source

$$s_2 s_2^* = \gamma_2 f_2$$

$$E\psi_1 = \varepsilon\psi_1 \longrightarrow [E - \varepsilon]\psi_1 = 0$$

$$\left[E - \varepsilon + \frac{i\gamma_1}{2} + \frac{i\gamma_2}{2}\right]\psi_1 = 0$$

$$\left[i\hbar\frac{d}{dt} - \varepsilon + \frac{i\gamma_1}{2} + \frac{i\gamma_2}{2}\right]\psi_1 = 0$$

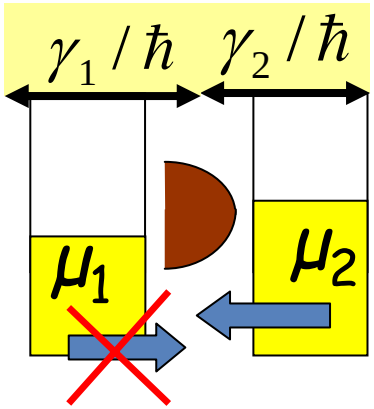
$$\psi_1 = \exp\left[\frac{-i\varepsilon t}{\hbar}\right]\exp\left[-\frac{\gamma_1 t}{2\hbar}\right]\exp\left[-\frac{\gamma_2 t}{2\hbar}\right]$$

$$\psi_1 \psi_1^* = \exp\left[-\frac{\gamma_1 t}{\hbar}\right]\exp\left[-\frac{\gamma_2 t}{\hbar}\right]$$

Introducing the "wavefunction"

$$n_1 = \psi_1 \psi_1^*$$

1 grid point



$$\left[E - \varepsilon + \frac{i\gamma_1}{2} + \frac{i\gamma_2}{2}\right]\psi_1 = s_2$$

Source

$$s_2 s_2^* = \gamma_2 f_2$$

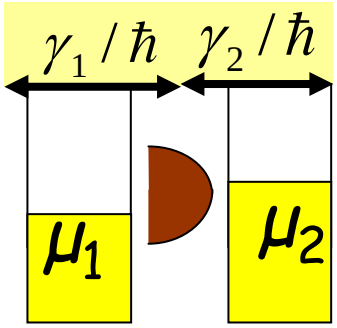
$$\psi_1 = \frac{s_2}{E - \varepsilon + \frac{i\gamma_1}{2} + \frac{i\gamma_2}{2}}$$

$$n_1(E) = \frac{\gamma_2 f_2}{(E-\varepsilon)^2 + \left(\frac{\gamma_1}{2} + \frac{\gamma_2}{2}\right)^2}$$

$$N_1 = \int \frac{dE}{2\pi} n_1(E) = \frac{\gamma_2 f_2}{\gamma_1 + \gamma_2}$$

The "wavefunction" with 2 grid points

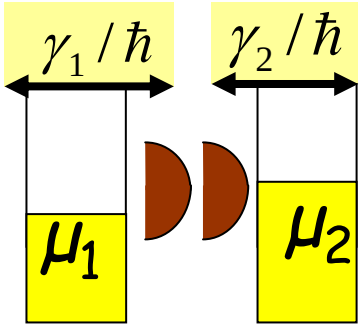
1 grid point



$$\left[E-\varepsilon+\frac{i\gamma_1}{2}+\frac{i\gamma_2}{2}\right]\psi_1 = s_2$$

$$s_2 s_2^* = \gamma_2 f_2$$

2 grid points



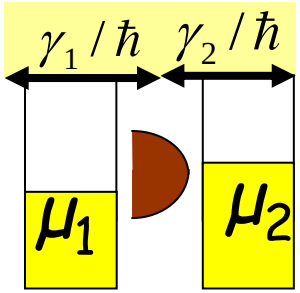
$$E\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \begin{bmatrix}\varepsilon_1 & t\\ t & \varepsilon_2\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

$$\begin{bmatrix}E-\varepsilon_1 & -t\\ -t & E-\varepsilon_2\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \begin{Bmatrix}0\\ 0\end{Bmatrix}$$

$$\begin{bmatrix}E-\varepsilon_1+\frac{i\gamma_1}{2} & -t\\ -t & E-\varepsilon_2+\frac{i\gamma_2}{2}\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \begin{Bmatrix}0\\ s_2\end{Bmatrix}$$

The "wavefunction" with multiple grid points

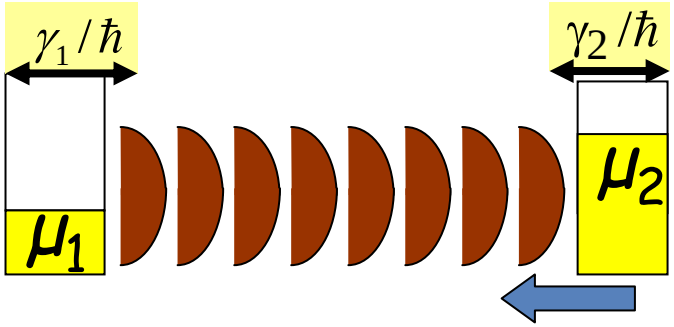
1 grid point



$$\left[E-\varepsilon+\frac{i\gamma_1}{2}+\frac{i\gamma_2}{2}\right]\psi_1 = s_2$$

$$s_2 s_2^* = \gamma_2 f_2$$

Multiple grid points



$$E\{\psi\} = [H]\{\psi\}$$

$$[EI-H]\{\psi\} = \{0\}$$

$$[EI-H-\Sigma_1-\Sigma_2]\{\psi\} = \{S_2\}$$

$$\begin{bmatrix} -i\gamma_1/2 & 0 & \cdots \\ \vdots & \vdots & \vdots \\ 0 & 0 & \cdots \end{bmatrix} \begin{bmatrix} 0 & 0 & \cdots & \cdots \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & -i\gamma_2/2 \end{bmatrix} \begin{Bmatrix} 0 \\ \vdots \\ s_2 \end{Bmatrix}$$

"Self-energy" matrices

Broadening matrices

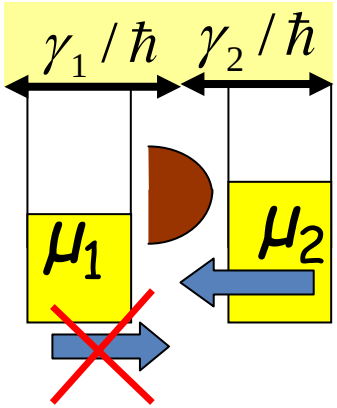
$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+]$$

$$\Gamma_2 = i[\Sigma_2 - \Sigma_2^+]$$

Multiple sources

$$n_1 = \psi_1 \psi_1^*$$

1 grid point



$$s_1 s_1^* = \gamma_1 f_1$$

$$s_2 s_2^* = \gamma_2 f_2$$

$$\left[E - \varepsilon + \frac{i\gamma_1}{2} + \frac{i\gamma_2}{2}\right]\psi_1 = s_2 + s_1$$

Source

$$\psi_1 = \frac{s_2}{E - \varepsilon + \frac{i\gamma_1}{2} + \frac{i\gamma_2}{2}}$$

$$n_1(E) = \frac{s_2 s_2^* + s_1 s_1^* + s_2 s_1^* + s_1 s_2^*}{(E-\varepsilon)^2 + \left(\frac{\gamma_1}{2} + \frac{\gamma_2}{2}\right)^2}$$

$$n_1(E) = \frac{s_2 s_2^* + s_1 s_1^*}{(E-\varepsilon)^2 + \left(\frac{\gamma_1}{2} + \frac{\gamma_2}{2}\right)^2}$$

$$N_1 = \int \frac{dE}{2\pi} n_1(E) = \frac{\gamma_2 f_2 + \gamma_1 f_1}{\gamma_1 + \gamma_2}$$

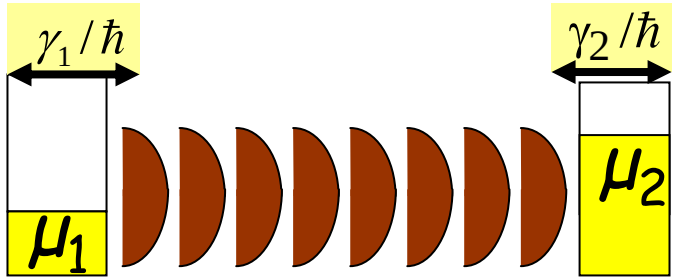
Wavefunctions excited by uncorrelated sources cannot be added … but wavefunction correlations can be ..

From "wavefunction" to Green function

Correlation function

$$G^n (\equiv -iG^<) = \{\psi\}\{\psi\}^+$$

$$\begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_N \end{Bmatrix} \begin{Bmatrix} \psi_1^* & \cdots & \psi_N^* \end{Bmatrix}$$



$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+]$$

$$\Gamma_2 = i[\Sigma_2 - \Sigma_2^+]$$

$$[EI - H - \Sigma_1 - \Sigma_2]\{\psi\} = \{S_2\}$$

Define Green function $[G] = [EI - H - \Sigma_1 - \Sigma_2]^{-1}$

$$\{\psi\} = [G]\{S_2\}$$

$$G^n = \{\psi\}\{\psi\}^+ = [G]\overbrace{\{S_2\}\{S_2^+\}}^{[\Gamma_2]\, f_2}[G]^+$$

Superpose contributions to correlation function from different sources

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1$$

Spectral function

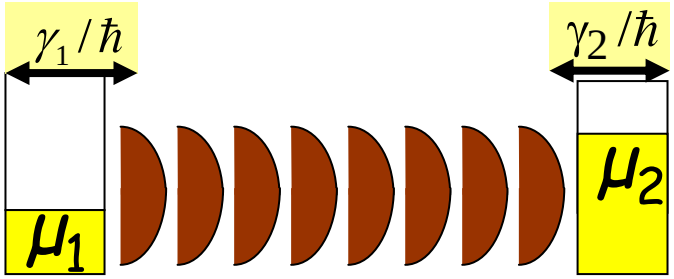
Correlation function

$$G^n (\equiv -iG^<) = \{\psi\}\{\psi\}^+$$

$$\begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_N \end{Bmatrix} \begin{Bmatrix} \psi_1^* & \cdots & \psi_N^* \end{Bmatrix} = \begin{bmatrix} \psi_1\psi_1^* & \cdots & \psi_1\psi_N^* \\ \vdots & \cdots & \vdots \\ \psi_N\psi_1^* & \cdots & \psi_N\psi_N^* \end{bmatrix}$$

Can show from (1) and (3):

$$A = i[G - G^+]$$



$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+]$$

$$\Gamma_2 = i[\Sigma_2 - \Sigma_2^+]$$

(1) $[G] = [EI - H - \Sigma_1 - \Sigma_2]^{-1}$

"Electron density"

(2) $G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1$

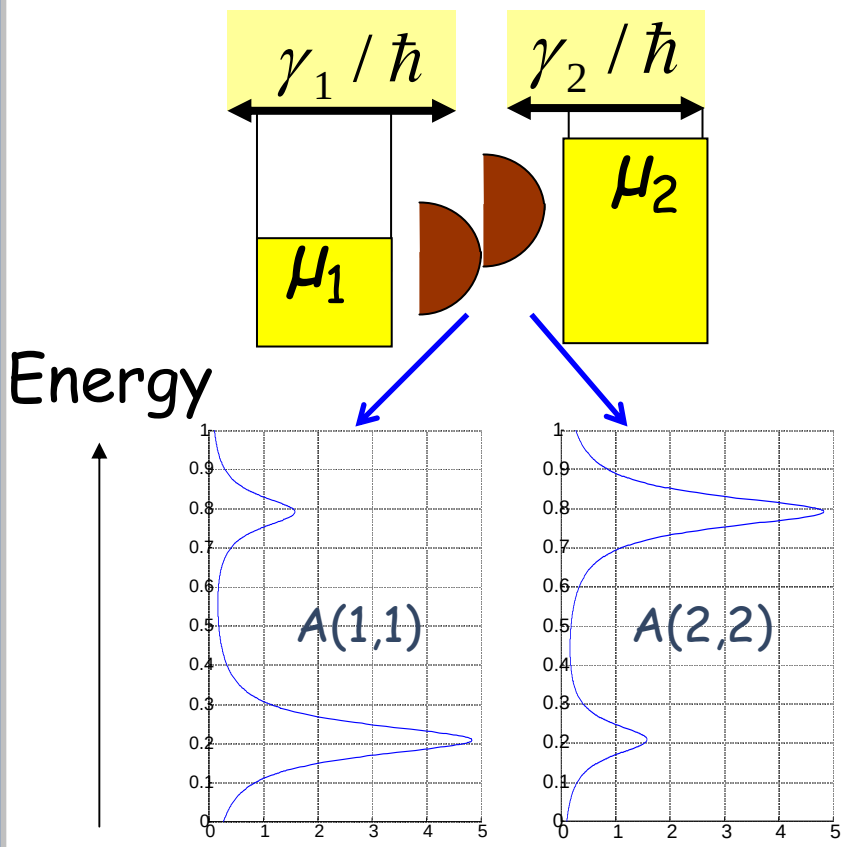
"Density of states"

(3) $A = G\Gamma_2 G^+ + G\Gamma_1 G^+$

2 grid points: LDOS

$$\Sigma_1 = \begin{bmatrix} -i\gamma_1/2 & 0 \\ 0 & 0 \end{bmatrix} \qquad \Sigma_2 = \begin{bmatrix} 0 & 0 \\ 0 & -i\gamma_2/2 \end{bmatrix}$$

$$H = \begin{bmatrix} \varepsilon_1 & t \\ t & \varepsilon_2 \end{bmatrix}$$



$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+] \qquad \Gamma_2 = i[\Sigma_2 - \Sigma_2^+]$$

$$[G] = [EI - H - \Sigma_1 - \Sigma_2]^{-1}$$

"Electron density"

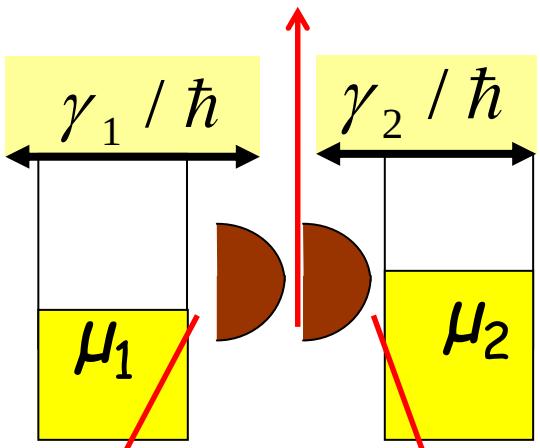
$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1$$

"Density of states"

$$A = i[G - G^+]$$

Calculating the current

$$\frac{I_{12}}{q/\hbar} = Trace\left([G^n_{12}H_{21}] - [H_{12}G^n_{21}]\right)$$



$$\frac{I_1}{q/\hbar} = Trace\begin{pmatrix}[\Gamma_1 A]\, f_1 \\ -[\Gamma_1 G^n]\end{pmatrix}$$

cf.

$$\gamma_1 D\, f_1 - \gamma_1 n$$

$$\frac{I_2}{q/\hbar} = Trace\begin{pmatrix}[\Gamma_2 A]\, f_2 \\ -[\Gamma_2 G^n]\end{pmatrix}$$

cf.

$$\gamma_2 D\, f_2 - \gamma_2 n$$

$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+] \qquad \Gamma_2 = i[\Sigma_2 - \Sigma_2^+]$$

$$[G] = \left[EI - H - \Sigma_1 - \Sigma_2\right]^{-1}$$

"Electron density"

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1$$

"Density of states"

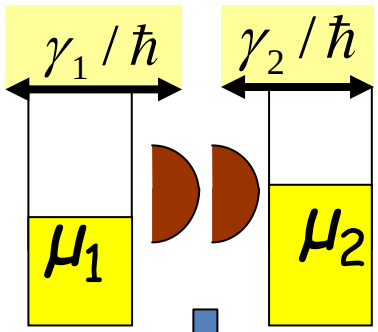
$$A = i[G - G^+]$$

Coherent transport

$$I = \frac{q}{h}\int dE\; T(E)\left[f_2 - f_1\right]$$

$$T(E) = Trace[\Gamma_1 G \Gamma_2 G^+]$$

Basis transformation

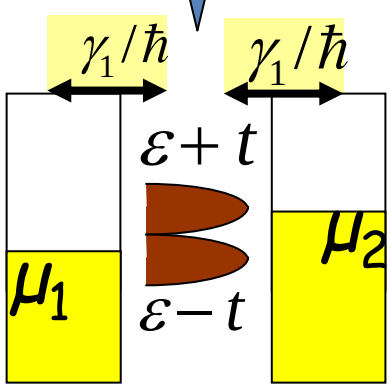


$$H = \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}$$

$$\Sigma_1 = -i\gamma_1/2 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\Sigma_2 = -i\gamma_2/2 \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Basis Transformation:
new H = U' * old H * U



$$H = \begin{bmatrix} \varepsilon + t & 0 \\ 0 & \varepsilon - t \end{bmatrix}$$

$$\Sigma_1 = -i\gamma_1/2 \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}$$

$$\Sigma_2 = -i\gamma_2/2 \begin{bmatrix} 0.5 & -0.5 \\ -0.5 & 0.5 \end{bmatrix}$$

$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+] \qquad \Gamma_2 = i[\Sigma_2 - \Sigma_2^+]$$

$$[G] = \left[EI - H - \Sigma_1 - \Sigma_2\right]^{-1}$$

"Electron density"

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1$$

"Density of states"

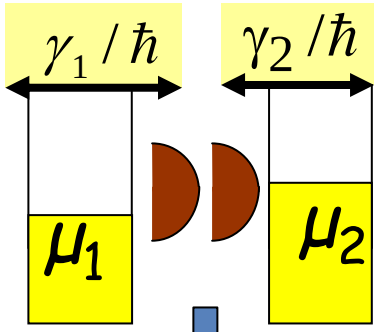
$$A = i[G - G^+]$$

Current

$$\frac{I_1}{q/\hbar} = Trace\left([\Gamma_1 A]\, f_1 - [\Gamma_1 G^n]\right)$$

Trace is invariant with basis transformation

Choice of basis

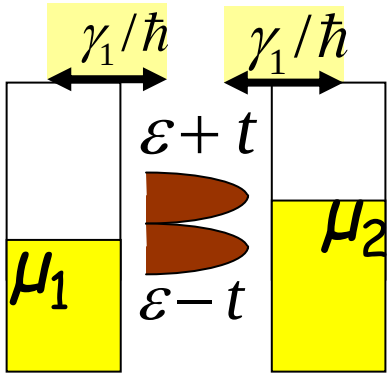


$$H = \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}$$

$$\Sigma_1 = -i\gamma_1/2 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\Sigma_2 = -i\gamma_2/2 \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Basis Transformation:
new H = U' * old H * U

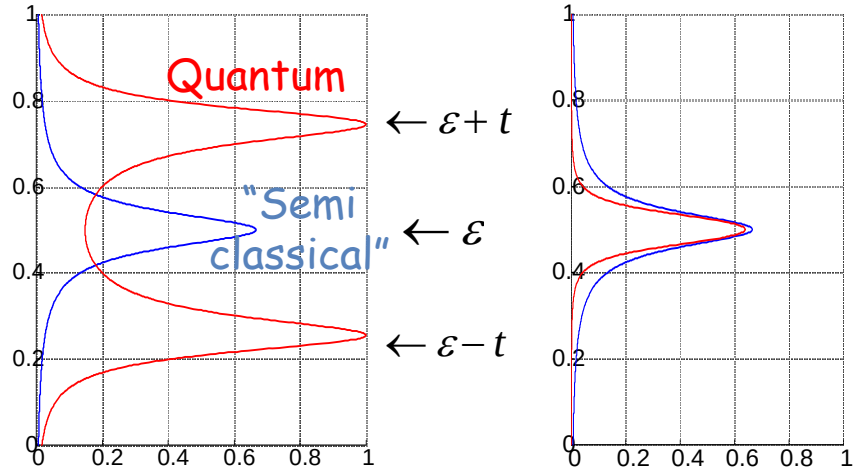


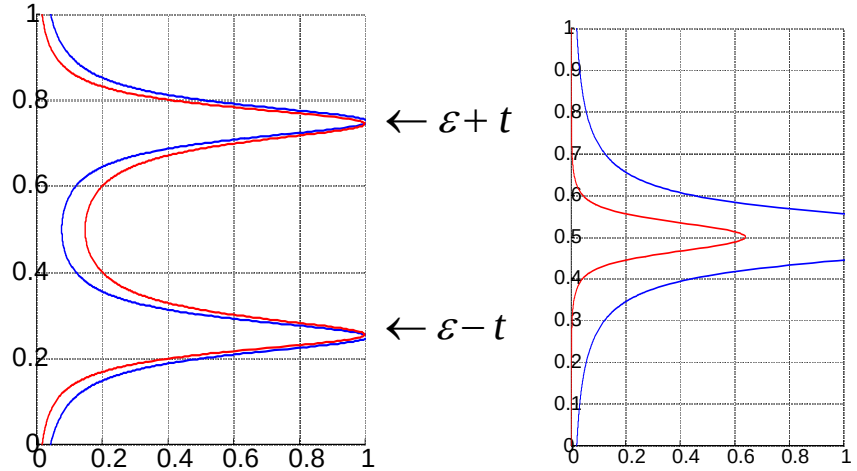
$$H = \begin{bmatrix} \varepsilon+t & 0 \\ 0 & \varepsilon-t \end{bmatrix}$$

$$\Sigma_1 = -i\gamma_1/2 \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}$$

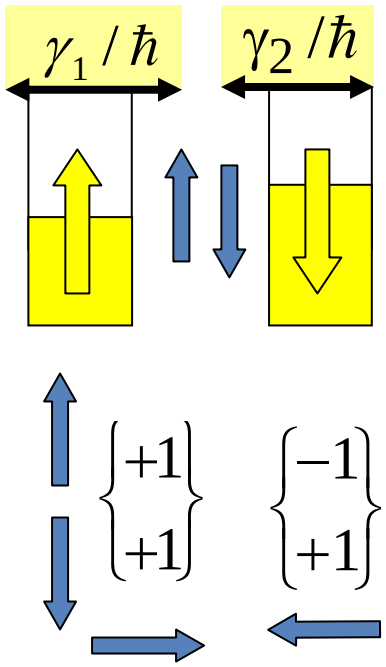
$$\Sigma_2 = -i\gamma_2/2 \begin{bmatrix} 0.5 & -0.5 \\ -0.5 & 0.5 \end{bmatrix}$$

$t = 0.25$ $\qquad$ $t = 0.025$





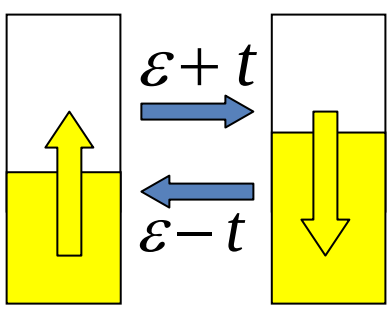
Spin as a "grid point"



$$H = \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}$$

$$\Sigma_1 = -i\gamma_1/2 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

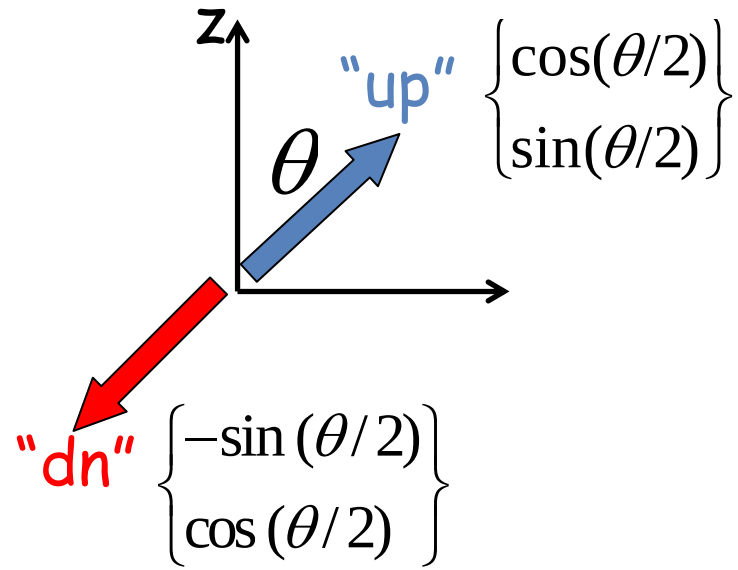
$$\Sigma_2 = -i\gamma_2/2 \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$



$$H = \begin{bmatrix} \varepsilon + t & 0 \\ 0 & \varepsilon - t \end{bmatrix}$$

$$\Sigma_1 = -i\gamma_1/2 \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}$$

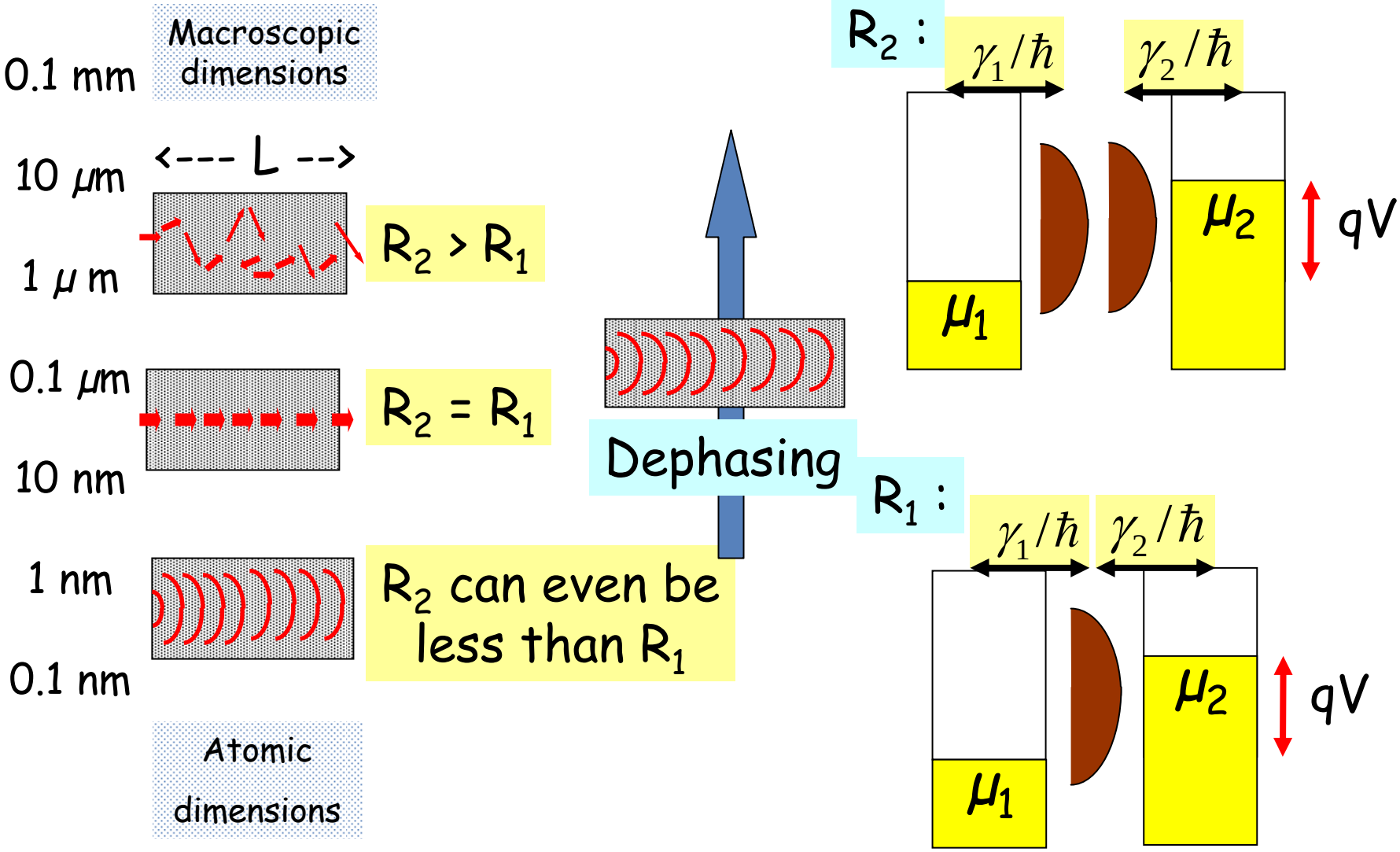
$$\Sigma_2 = -i\gamma_2/2 \begin{bmatrix} 0.5 & -0.5 \\ -0.5 & 0.5 \end{bmatrix}$$



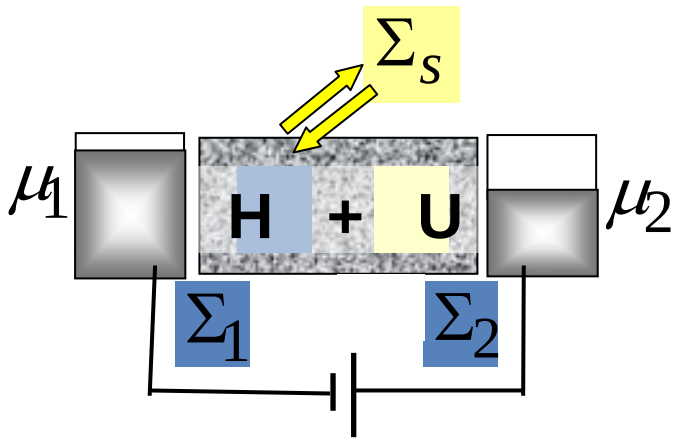
$$\theta = 0: \quad \begin{Bmatrix}1\\0\end{Bmatrix} \text{ and } \begin{Bmatrix}0\\1\end{Bmatrix}$$

$$\theta = \frac{\pi}{2}: \quad \begin{Bmatrix}+1\\+1\end{Bmatrix} \text{ and } \begin{Bmatrix}+1\\-1\end{Bmatrix}$$

Introducing a Grid



From coherent to incoherent transport



$$[G] = [EI - H - \Sigma_1 - \Sigma_2]^{-1}$$

$$[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$$

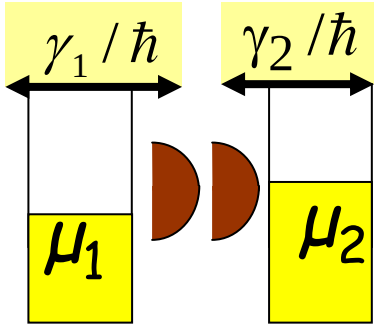
$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1 + G\Sigma_s^{in} G^+$$

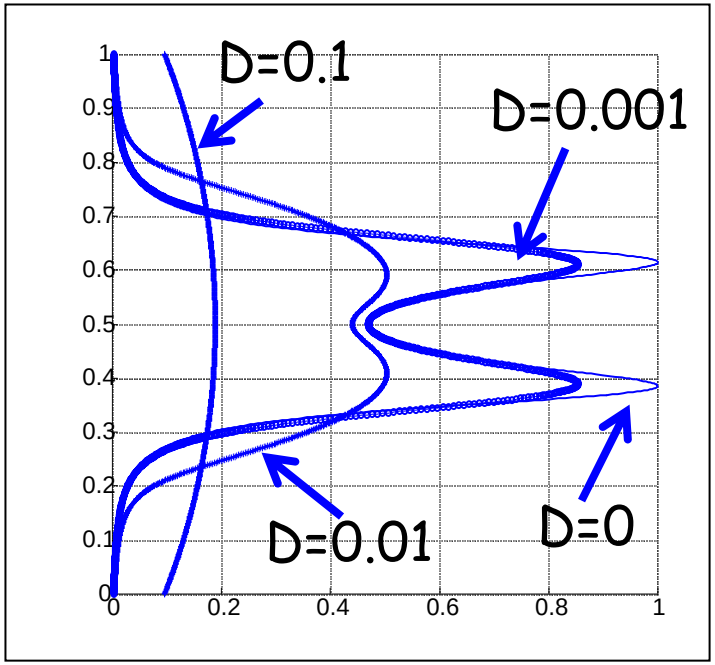
$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1$$

Simplest dephasing model

$$[\Sigma_s] = D[G]$$

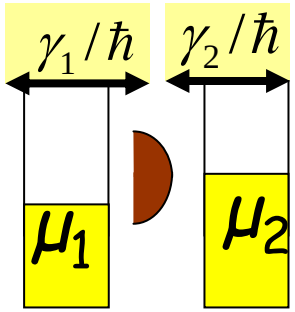
$$[\Sigma_s^{in}] = D[G^n]$$





Equations for Quantum Transport

1-point:



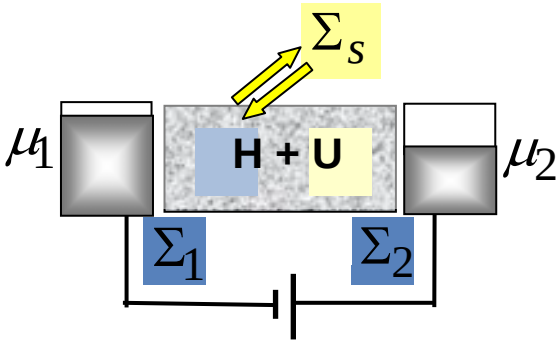
$$n = \int dE\, D(E-U)\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1+\gamma_2}\right]$$

$$I = \frac{q}{\hbar}\int dE\, D(E-U)\,\gamma_1\,[f_1 - F]$$

N points, quantum

$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+]$$

$$\Gamma_2 = i[\Sigma_2 - \Sigma_2^+]$$



$$\varepsilon \rightarrow [H]$$

$$\gamma \rightarrow [\Gamma],[\Sigma]$$

$$U \rightarrow [U]$$

$$n \rightarrow [\rho]$$

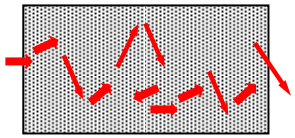
$$n(E) \rightarrow [G^n(E)] \equiv -iG^<(E)$$

$$D(E) \rightarrow [A(E)]$$

Unified view of nanodevices

0.1 mm — Macroscopic dimensions

10 μm — <--- L -->

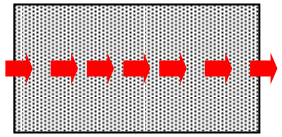


1 μm — $R_2 > R_1$

Diffusion equation

Boltzmann equation

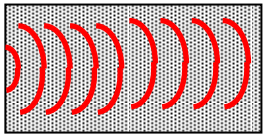
0.1 μm



10 nm — $R_2 = R_1$

"NEGF"

1 nm



0.1 nm — R_2 can even be less than R_1

Atomic dimensions