

NCN@Purdue - Intel Summer School: July 14-25, 2008

Physics of Nanoscale Transistors: Lecture 7:

Connection to the Bottom Up Approach

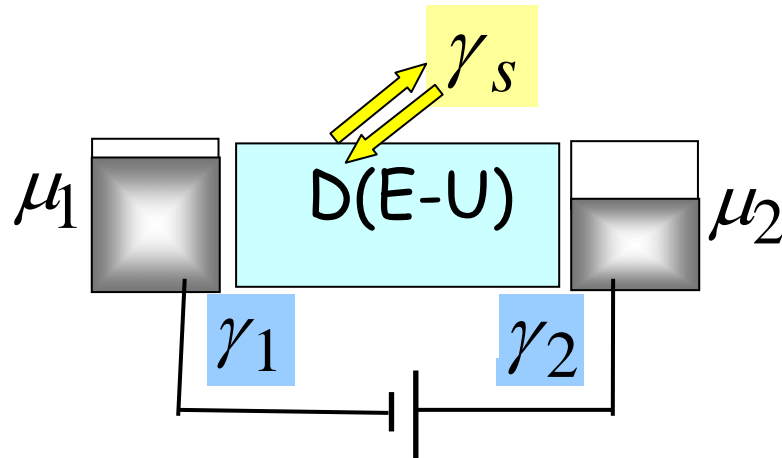
Mark Lundstrom

Network for Computational Nanotechnology

Purdue University

West Lafayette, Indiana USA

Datta's generic model for a nanodevice



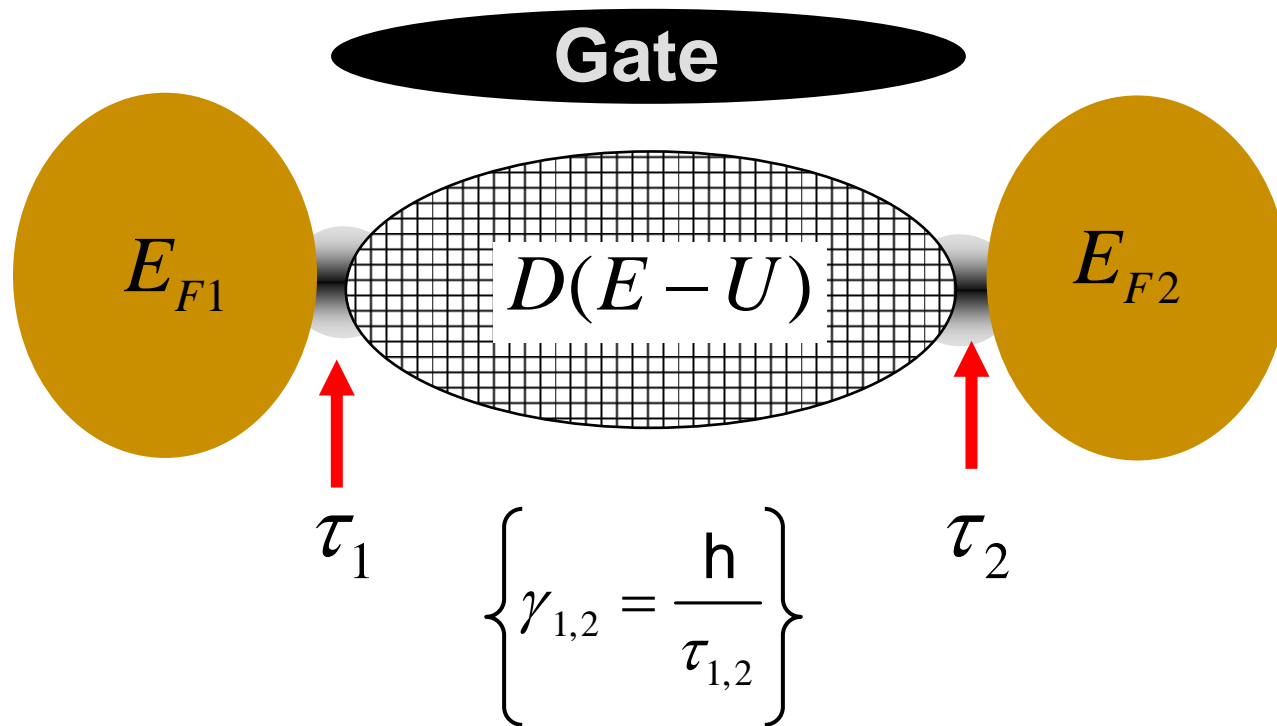
$$N = D(E - U) \left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \right]$$

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

outline

- 1) Introduction
- 2) Bottom-up approach**
- 3) The ballistic MOSFET
- 4) Treatment of scattering
- 5) Summary

generic model



S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
("Concepts of Quantum Transport" nanohub.org)

filling states from the left contact

Gate

Assumption:

Each energy channel is independent

E_{F1}

$D(E - U)$

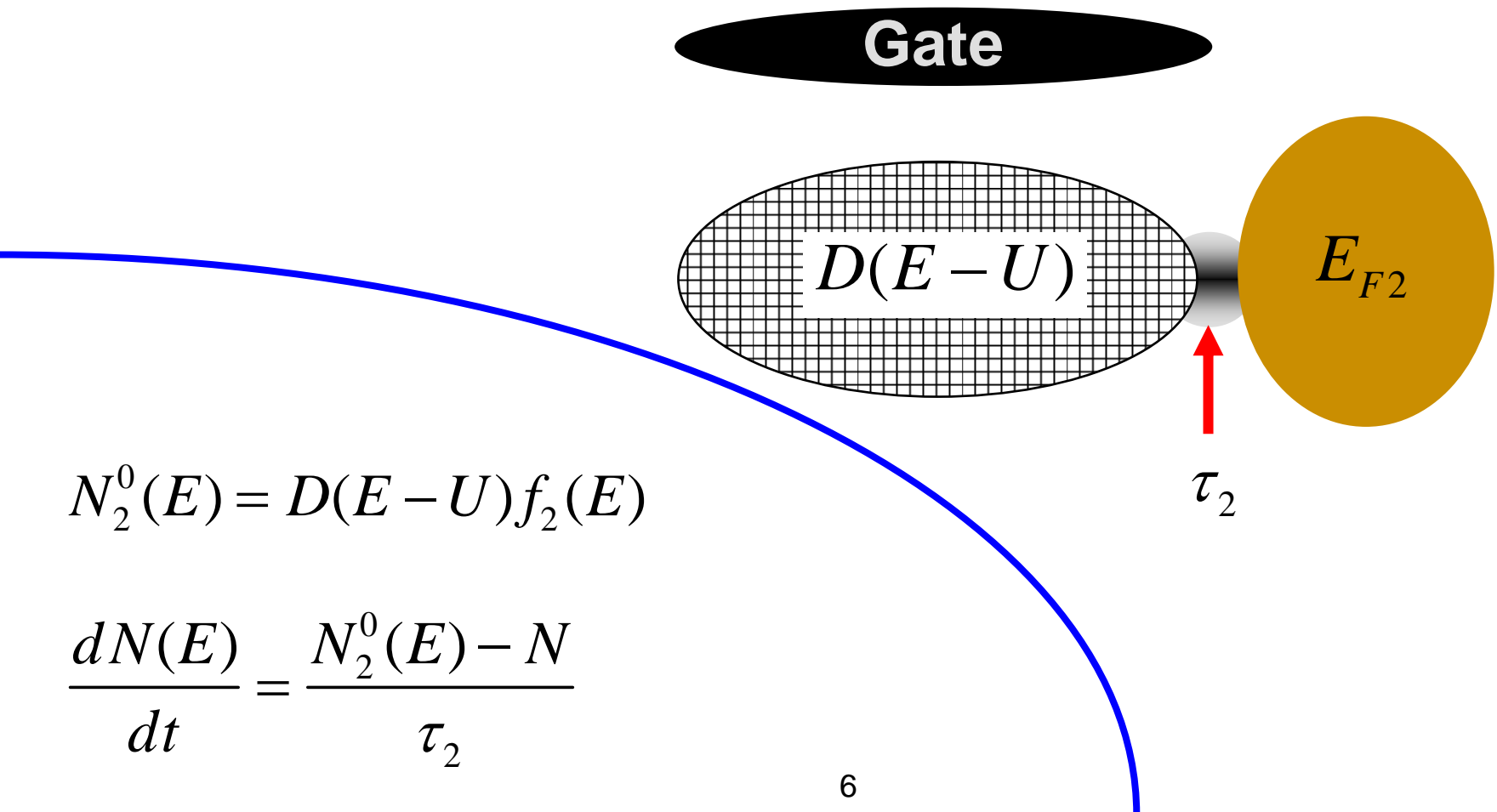
includes spin

τ_1

$$N_1^0(E) = D(E - U) f_1(E)$$

$$\frac{dN(E)}{dt} = \frac{N_1^0(E) - N}{\tau_1}$$

filling states from the right contact



$$N_2^0(E) = D(E - U)f_2(E)$$

$$\frac{dN(E)}{dt} = \frac{N_2^0(E) - N}{\tau_2}$$

steady-state

$$\frac{dN(E)}{dt} = \frac{N_1^0 - N}{\tau_1} + \frac{N_2^0 - N}{\tau_2} = 0$$

$$(1/\tau_1)N_1^0 - (1/\tau_1)N + (1/\tau_2)N_2^0 - (1/\tau_2)N = 0$$

$$N(E) = \frac{(1/\tau_1)}{(1/\tau_1) + (1/\tau_2)} N_1^0(E) + \frac{(1/\tau_2)}{(1/\tau_1) + (1/\tau_2)} N_2^0(E)$$

$$\left\{ \begin{array}{ll} N_1^0(E) \equiv D(E-U)f_1(E) & \gamma_1 = \hbar/\tau_1 \\ N_2^0(E) \equiv D(E-U)f_2(E) & \gamma_1 = \hbar/\tau_2 \end{array} \right\}$$

steady-state electron number, $N(E)$

$$N(E) = \frac{\gamma_1}{\gamma_1 + \gamma_2} D(E - U) f_1(E) + \frac{\gamma_2}{\gamma_1 + \gamma_2} D(E - U) f_2(E)$$

$$N(E) = D_1(E - U) f_1(E) + D_2(E - U) f_2(E)$$

$$D_1(E - U_{SCF}) = \frac{\gamma_1}{\gamma_1 + \gamma_2} D(E - U_{SCF}) \quad \text{DOS that can be filled by contact 1}$$

$$D_2(E - U_{SCF}) = \frac{\gamma_2}{\gamma_1 + \gamma_2} D(E - U_{SCF}) \quad \text{DOS that can be filled by contact 2}$$

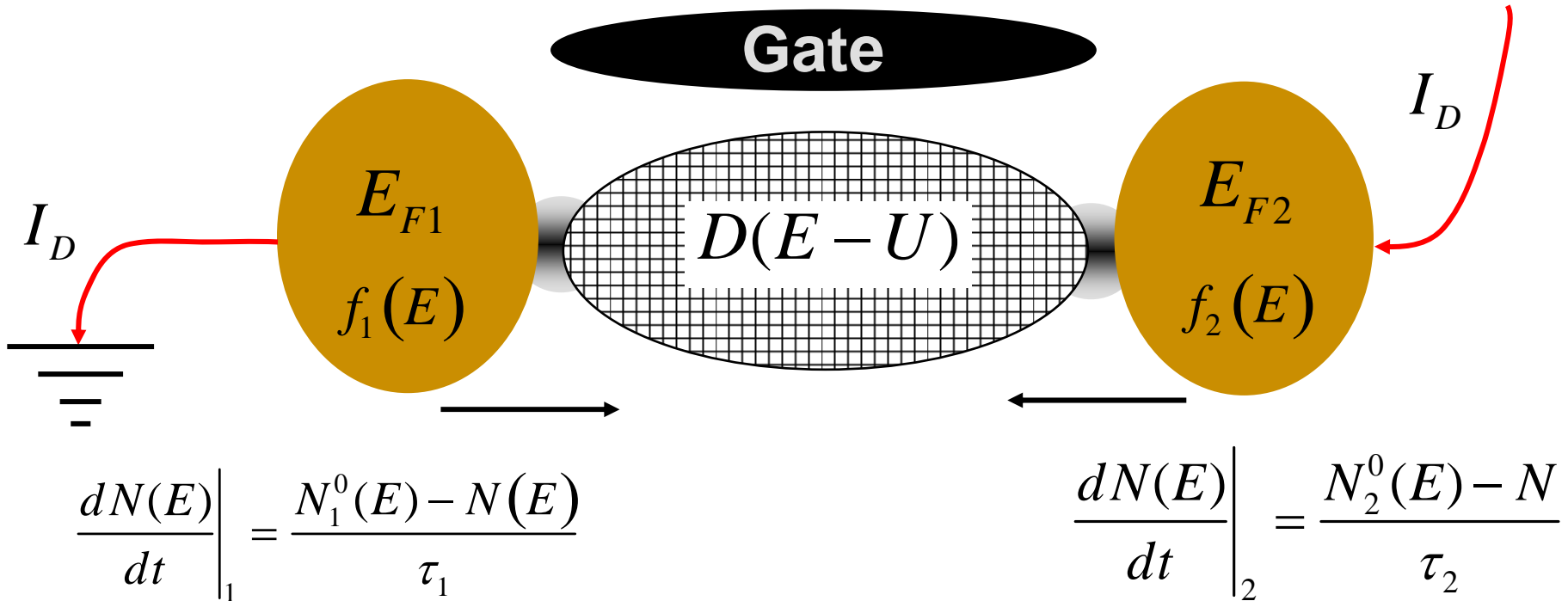
steady-state electron number, N

$$N = \int [D_1(E - U)f_1(E) + D_2(E - U)f_2(E)] dE$$

in equilibrium, we use:

$$N = \int D(E - U)f_0(E) dE$$

steady-state current, I



$$I_D(E) = +q \left. \frac{dN(E)}{dt} \right|_1 = -q \left. \frac{dN(E)}{dt} \right|_2$$

results

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

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

$$I_D = \int I(E) dE = \frac{2q}{h} \int \left(\frac{\gamma}{2} \right) \pi D(E - U) (f_1 - f_2) dE$$

$$N = \int N(E) dE = \int \left[\frac{D(E - U)}{2} (f_1(E) + f_2(E)) \right] dE$$

final results

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

$$I_D = \frac{2q}{h} \int \gamma \pi D'(E - U)(f_1 - f_2) dE$$

$$N = \int D'(E - U)[f_1(E) + f_2(E)] dE$$

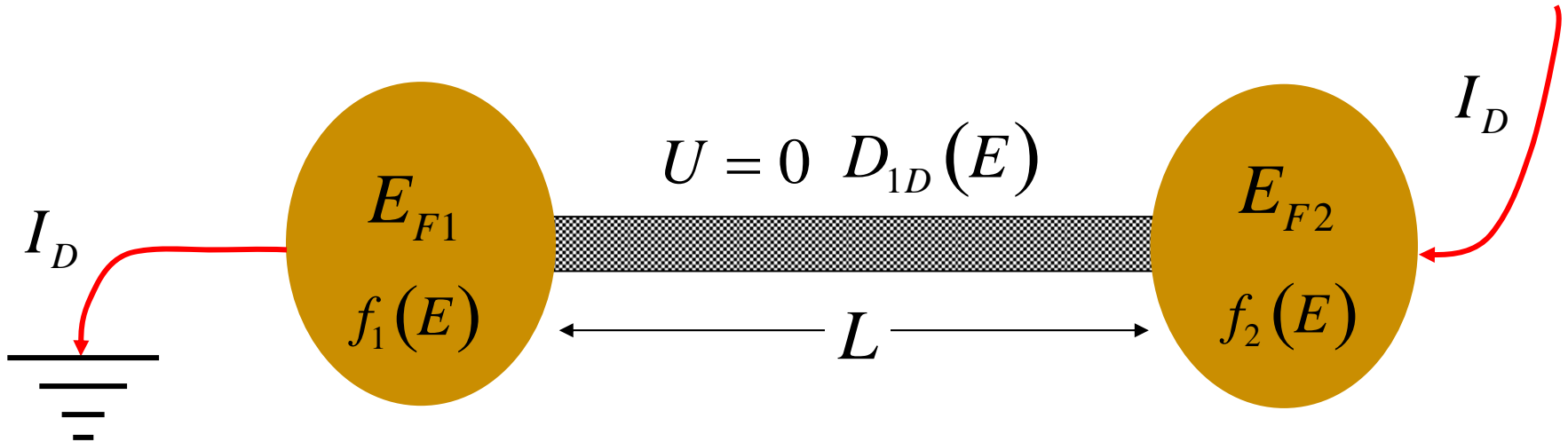
$$D'(E - U) = \frac{D(E - U)}{2}$$

density-of-states per spin

outline

- 1) Introduction
- 2) Bottom-up approach
- 3) Applications**
- 4) The ballistic MOSFET
- 5) Summary

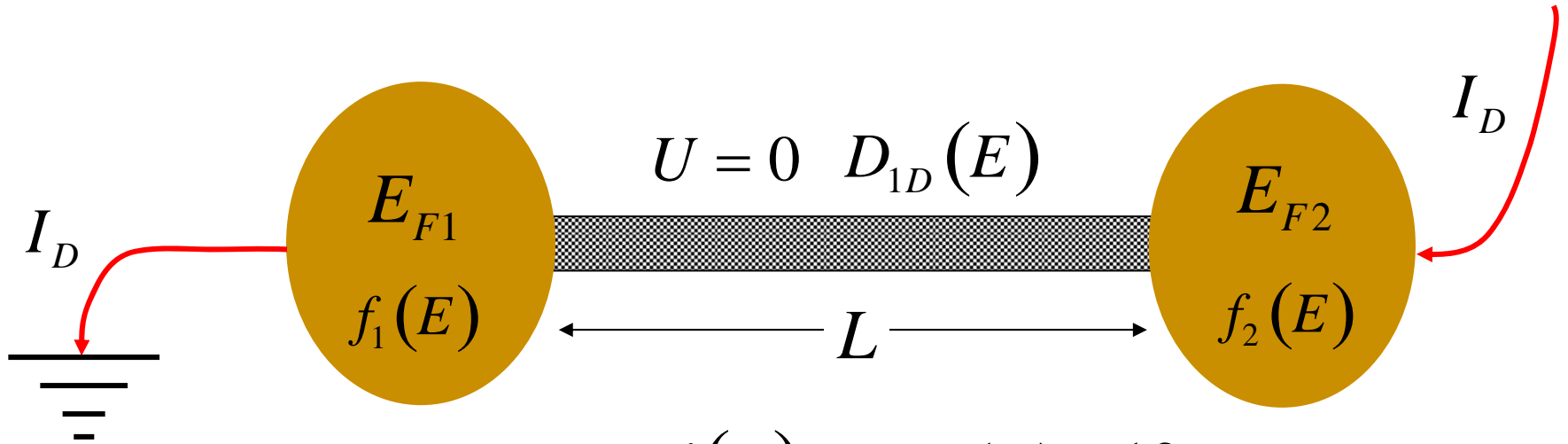
current in 1D



$$I_D = \frac{2q}{h} \int \gamma \pi D'(E - U)(f_1 - f_2) dE$$

$$I_D = \frac{2q}{h} \int M(E)(f_1 - f_2) dE \quad (\text{ballistic})$$

modes in 1D



$$\gamma \pi D'(E) = M_{1D}(E) = 1?$$

$$\gamma \pi D'(E) = \frac{\hbar v_x}{L} \pi \frac{1}{\pi \hbar v_x} = 1 \quad 4$$

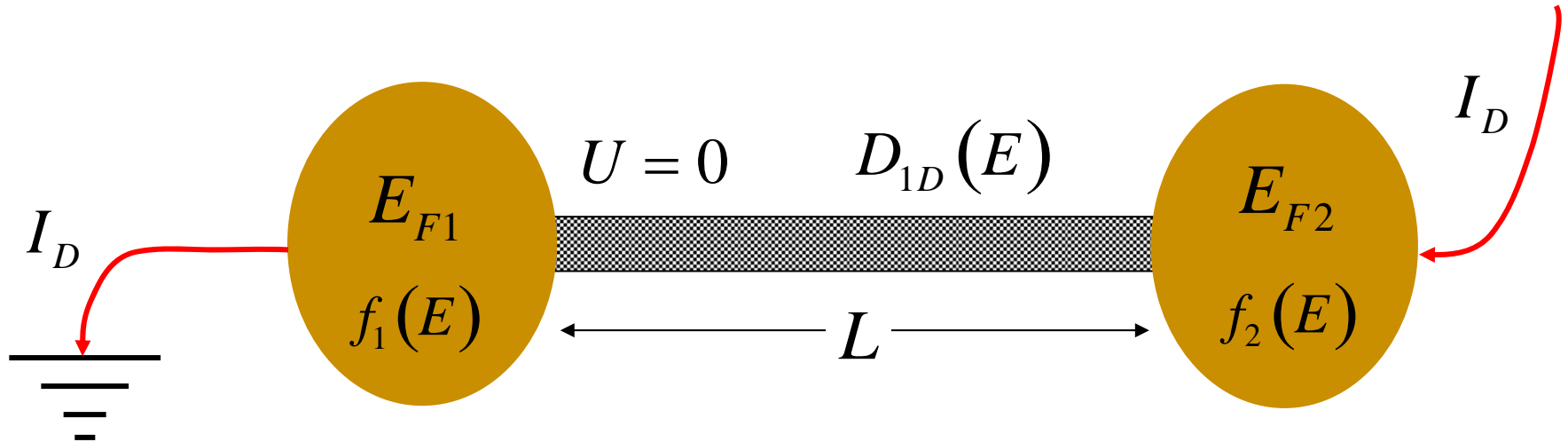
$$D'_{1D}(E) = \frac{1}{\pi \hbar v_x} L$$

$$\gamma = \frac{\hbar}{\tau}$$

$$\gamma = \frac{\hbar v_x}{L}$$

$$\left\{ I_D = \frac{qN}{L} v_x = \frac{qN}{\tau} \right.$$

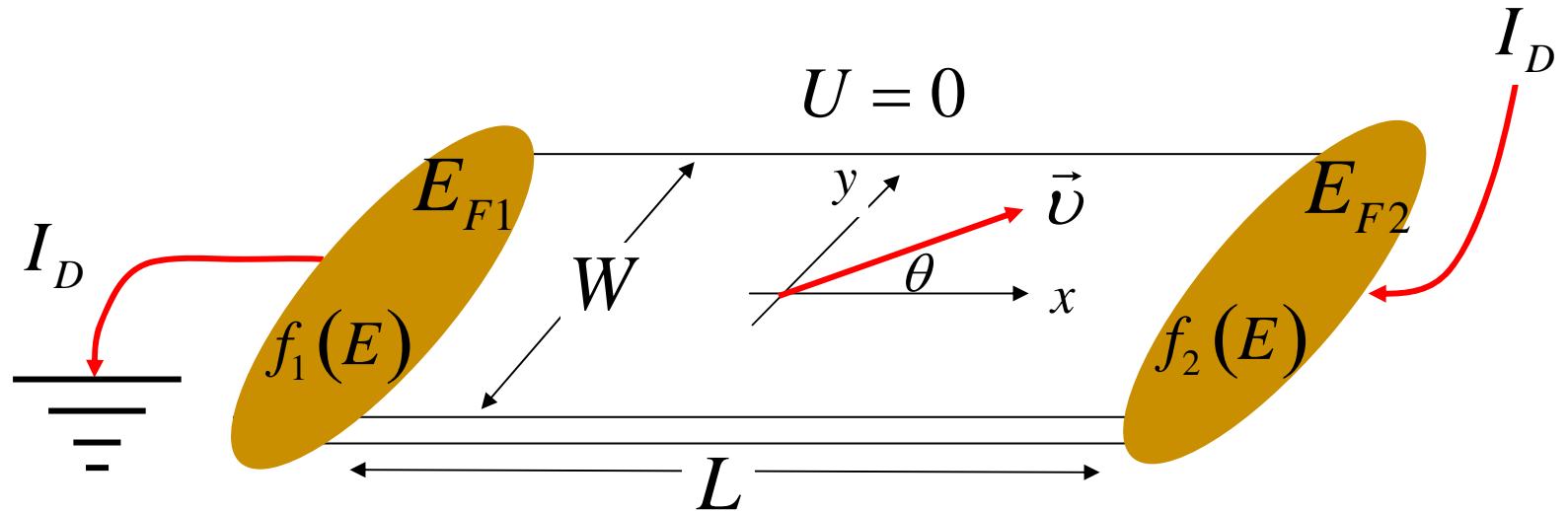
conductance in 1D



$$I_D = \frac{2q}{h} \int \gamma \pi D'(E) (f_1 - f_2) dE$$

$$I_D = \frac{2q}{h} \int (f_1 - f_2) dE = \frac{2q}{h} V_D \quad (T = 0K) \quad 4$$

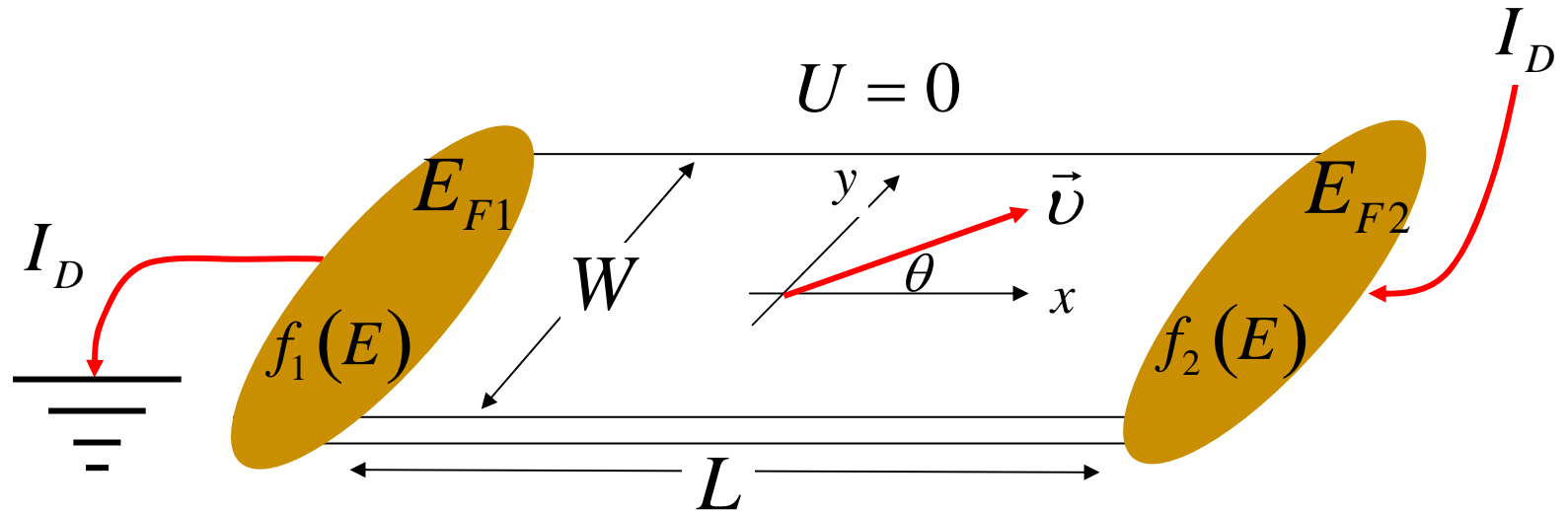
current in 2D



$$I_D = \frac{2q}{h} \int \gamma \pi D'(E) (f_1 - f_2) dE$$

$$\gamma \pi D'(E) = M_{2D}(E) = \frac{\sqrt{2m^* E}}{\pi \hbar} \quad ?$$

current in 2D



$$D'_{2D}(E) = \frac{m^*}{2\pi\hbar^2} WL$$

$$\gamma = \frac{\hbar}{\langle \tau \rangle} \quad \gamma = \frac{\hbar \langle v_x \rangle}{L} = \frac{\hbar \langle v \cos \theta \rangle}{L} = \frac{\hbar v}{L} \left(\frac{2}{\pi} \right) \quad v = \sqrt{2E/m^*}$$

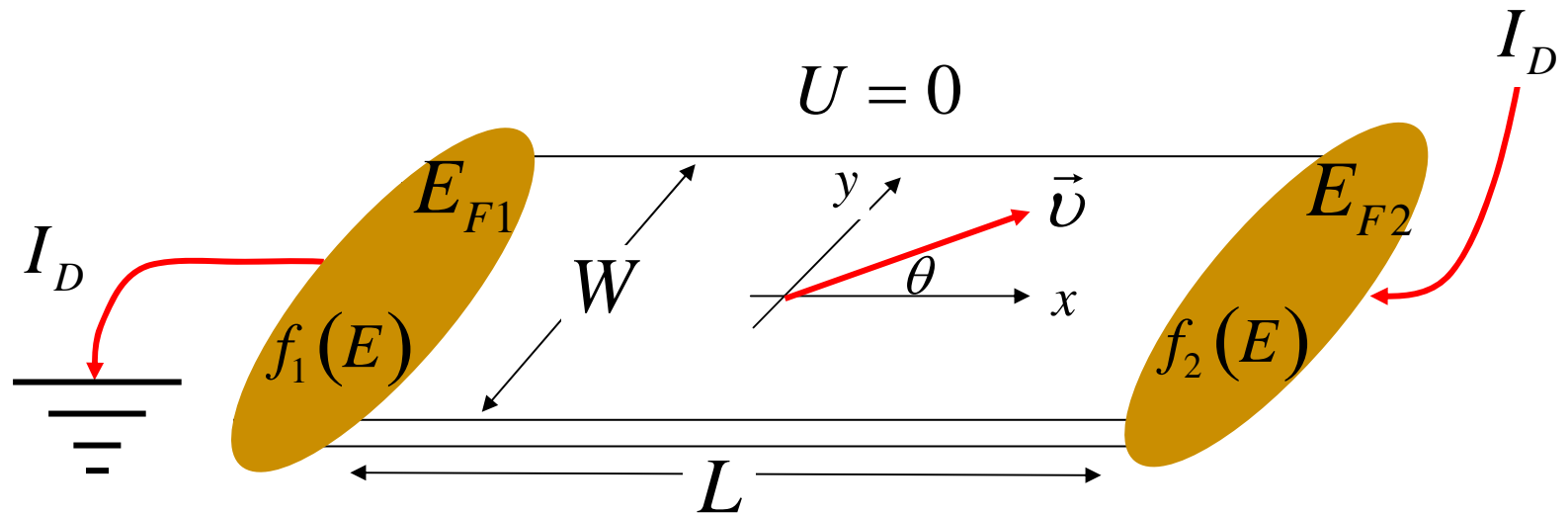
current in 2D

$$I_D = \frac{2q}{h} \int \gamma \pi D'_{2D}(E) (f_1 - f_2) dE \quad \left\{ \begin{array}{l} \gamma = \frac{h\nu}{L} \left(\frac{2}{\pi} \right) = \frac{h\sqrt{2E/m^*}}{L} \left(\frac{2}{\pi} \right) \\ D'_{2D}(E) = \frac{m^*}{2\pi\hbar^2} WL \end{array} \right.$$

$$\gamma \pi D'_{2D} = \frac{h}{L} \sqrt{\frac{2E}{m^*}} \left(\frac{2}{\pi} \right) \pi \frac{m^*}{2\pi\hbar^2} WL = W \frac{\sqrt{2m^*E}}{\pi\hbar} = M_{2D}(E) \quad 4$$

$$I_D = \frac{2q}{h} \int M_{2D}(E) (f_1 - f_2) dE$$

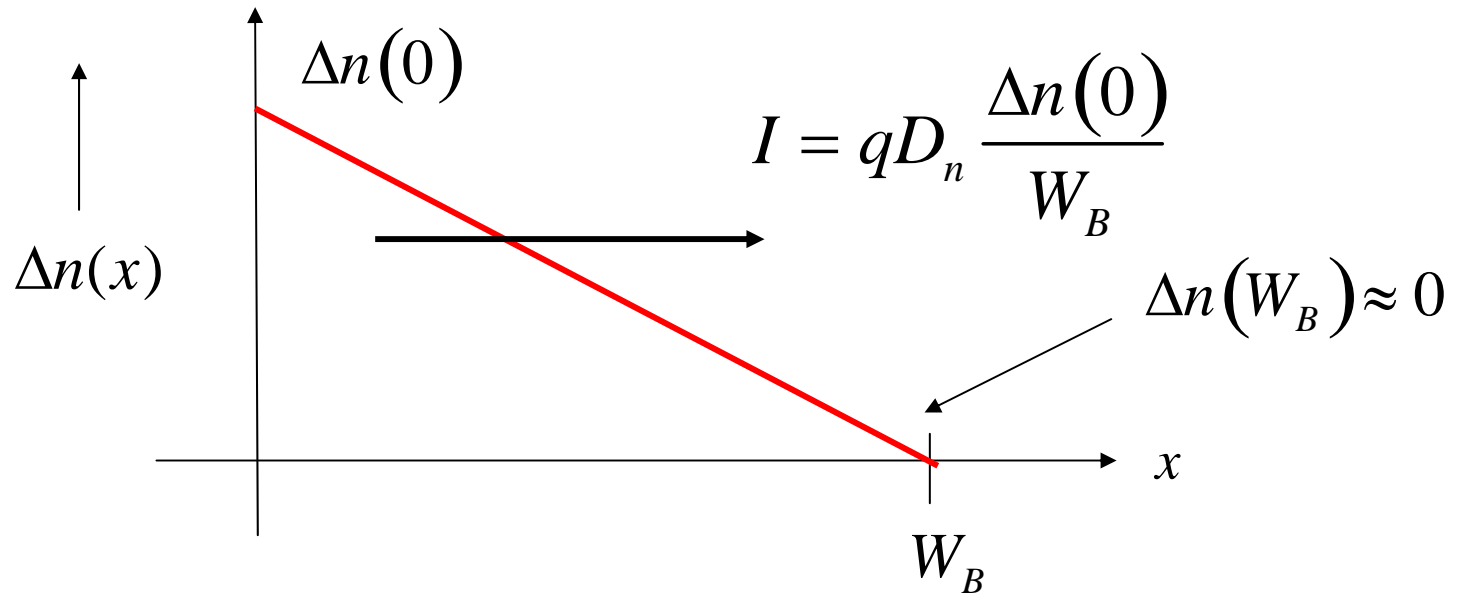
diffusive current in 2D



$$I_D = \frac{2q}{h} \int \gamma \pi D'(E) (f_1 - f_2) dE$$

$$\gamma = \frac{\hbar}{\langle \tau \rangle} \quad \langle \tau \rangle = ?$$

base transit time



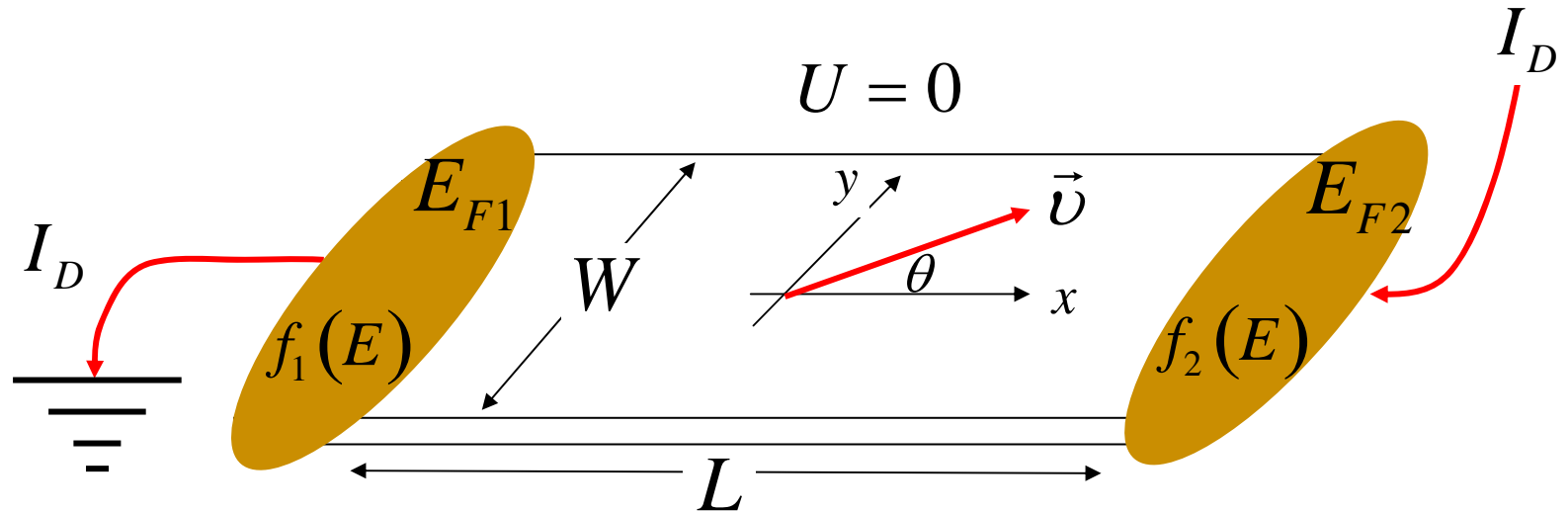
$$I = \frac{qN}{\tau}$$

$$\frac{qN}{\tau} = qD_n \frac{\Delta n(0)}{W_B}$$

$$N = \frac{1}{2} \Delta n(0) W_B$$

$$\tau = \frac{W_B^2}{2D_n}$$

diffusive current in 2D



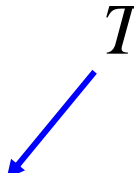
$$I_D = \frac{2q}{h} \int \gamma \pi D'(E) (f_1 - f_2) dE$$

$$\gamma = \frac{\hbar}{\langle \tau \rangle} \quad \langle \tau \rangle = \frac{L^2}{2D_n}$$

diffusive current in 2D

$$I_D = \frac{2q}{h} \int \gamma \pi D'(E) (f_1 - f_2) dE$$

$$\left. \begin{aligned} \gamma &= \frac{\hbar}{\langle \tau \rangle} \\ \langle \tau \rangle &= \frac{L^2}{2D_n} \\ D_n &= \frac{v(2/\pi)\lambda}{2} \end{aligned} \right\} \gamma = \frac{2D_n \hbar}{L^2} \rightarrow \gamma = \frac{v(2/\pi)\lambda \hbar}{L^2} = \frac{\lambda}{L} \frac{\hbar v}{L} \underbrace{\left(\frac{2}{\pi} \right)}_{\gamma_B}$$

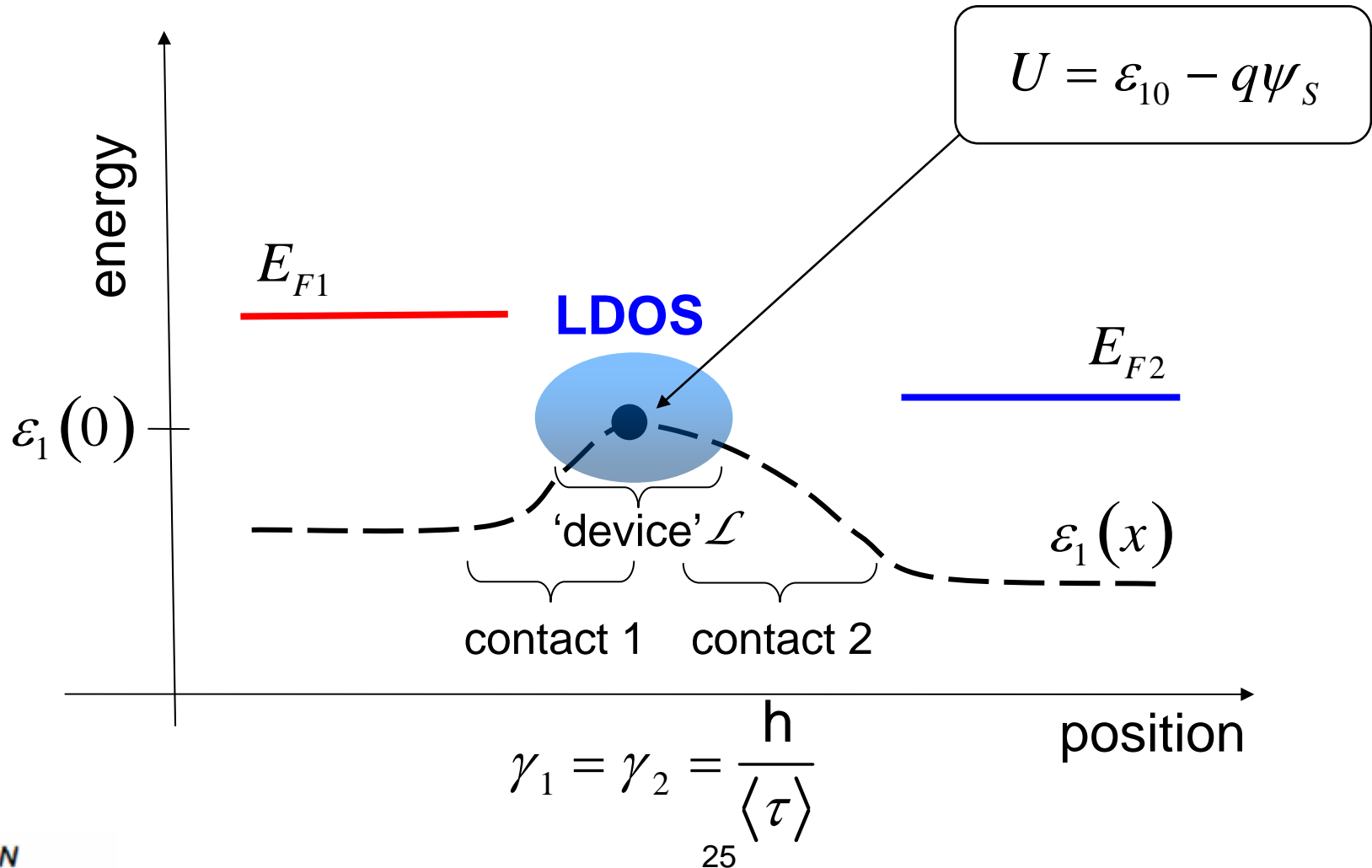


$$I_D = \frac{2q}{h} \int TM_{2D}(E) (f_1 - f_2) dE \quad \mathbf{4}$$

outline

- 1) Introduction
- 2) Bottom-up approach
- 3) Applications
- 4) The ballistic MOSFET**
- 5) Summary

“top of the barrier model”



MOSFET current

$$I_D = \frac{2q}{h} \int \gamma \pi D'(E) (f_1 - f_2) dE$$

$$\gamma_B \pi D'_{2D}(E) = M_{2D}(E)$$

$$\gamma = \frac{\gamma_D \gamma_B}{\gamma_D + \gamma_B}$$

$$I_D = \frac{2q}{h} \int T(E) M_{2D}(E) (f_1 - f_2) dE$$

$$\frac{\gamma_D}{\gamma_D + \gamma_B} \gamma_B \pi D'_{2D}(E) = T(E) M_{2D}(E)$$

$$T(E) = \frac{\gamma_D}{\gamma_D + \gamma_B} = \frac{\lambda(E)}{\lambda(E) + L}$$

outline

- 1) Introduction
- 2) Bottom-up approach
- 3) Applications
- 4) The ballistic MOSFET
- 5) **Summary**

summary

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

$$I_D = \frac{2q}{h} \int \gamma \pi D'(E - U)(f_1 - f_2) dE$$

$$N = \int \frac{D(E - U)}{2} [f_1(E) + f_2(E)] dE$$

$$\gamma = \frac{h}{\langle \tau \rangle} = \frac{\gamma_D \gamma_B}{\gamma_D + \gamma_B}$$

$$\gamma \pi D'(E - U) = T(E)M(E)$$

$$T(E) = \frac{\gamma_D}{\gamma_D + \gamma_B} \quad M(E) = \gamma_B \pi D'(U)$$

summary

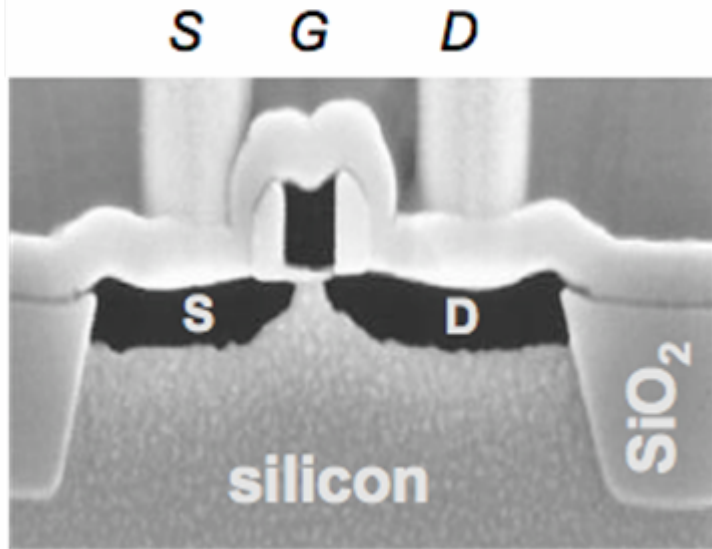
$$I_D = \frac{2q}{h} \int \gamma \pi D' (E - U) (f_1 - f_2) dE$$

or

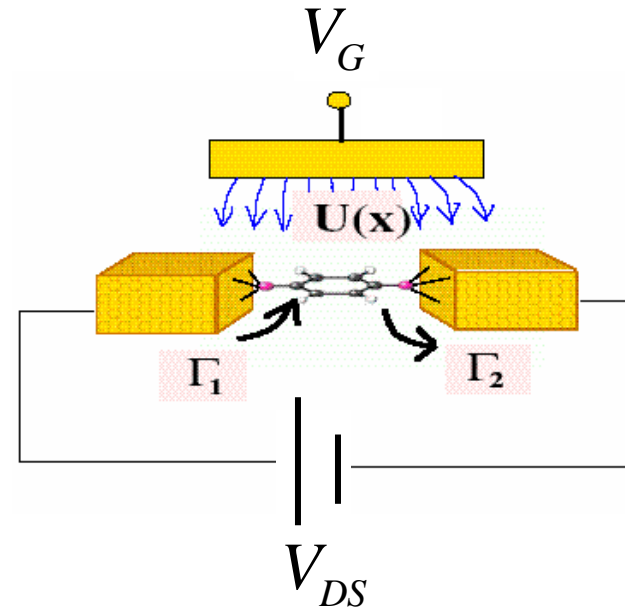
$$I_D = \frac{2q}{h} \int T(E) M(E) (f_1 - f_2) dE$$

?

molecular-scale MOSFETs



(Texas Instruments, 1997)



Avik W. Ghosh, Titash Rakshit, and Supriyo Datta, "Gating of a Molecular Transistor: Electrostatic and Conformational," *Nano Lett.*, **4**, 565-568, (2004).