ECE-656: Fall 2009

Lecture 3: General model for transport

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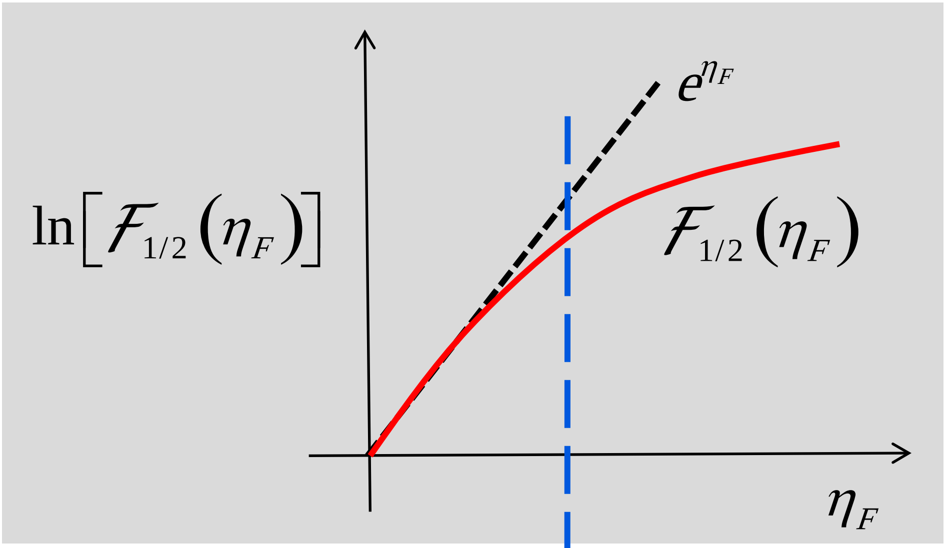
from lecture 2



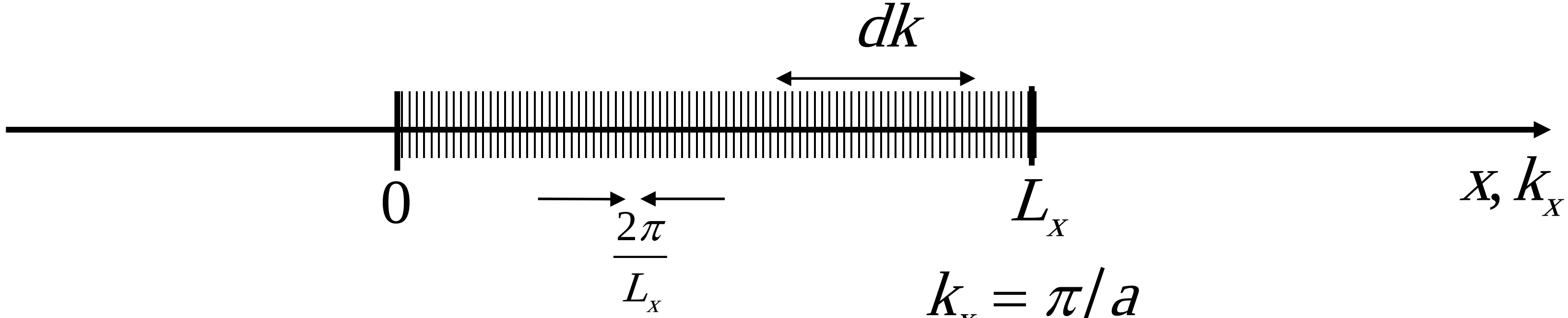
$\eta_F = 0 \quad (E_F = E_C)$

$$\mathcal{F}_{1/2}(\eta_F) = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{\eta^{1/2}\, d\eta}{1 + e^{\eta - \eta_F}}$$

$$\eta_F = (E_F - E_C)/k_B T$$

$$\mathcal{F}_{1/2}(0) = 0.7652$$

lecture 2: periodic boundary conditions



$$k_x = \pi / a$$

$$k_x = \frac{2\pi}{L_x} j \qquad L_x = N_A\, a \qquad k_x(\max) = \frac{2\pi}{a}$$

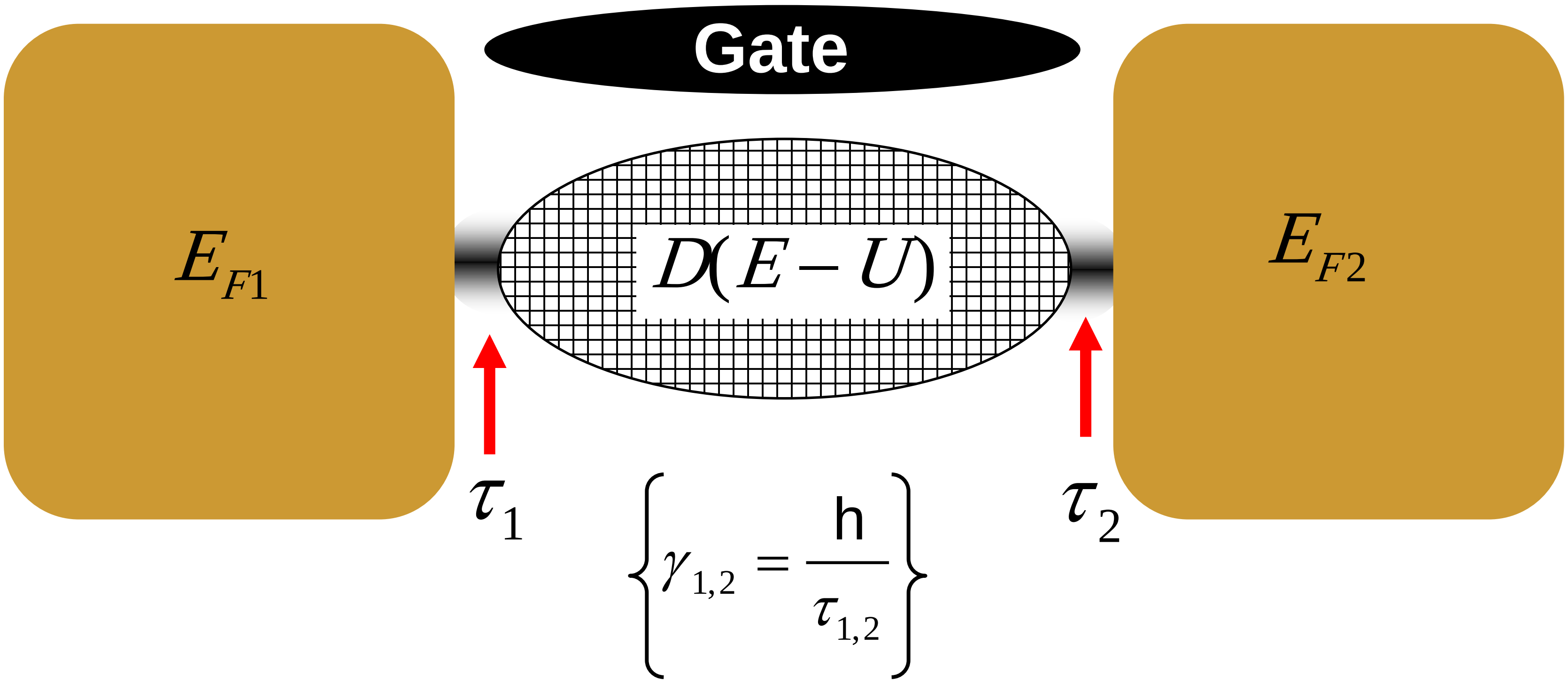
$$0 < k_x < \frac{2\pi}{a}$$

$$-\frac{\pi}{a} < k_x < +\frac{\pi}{a}$$

outline

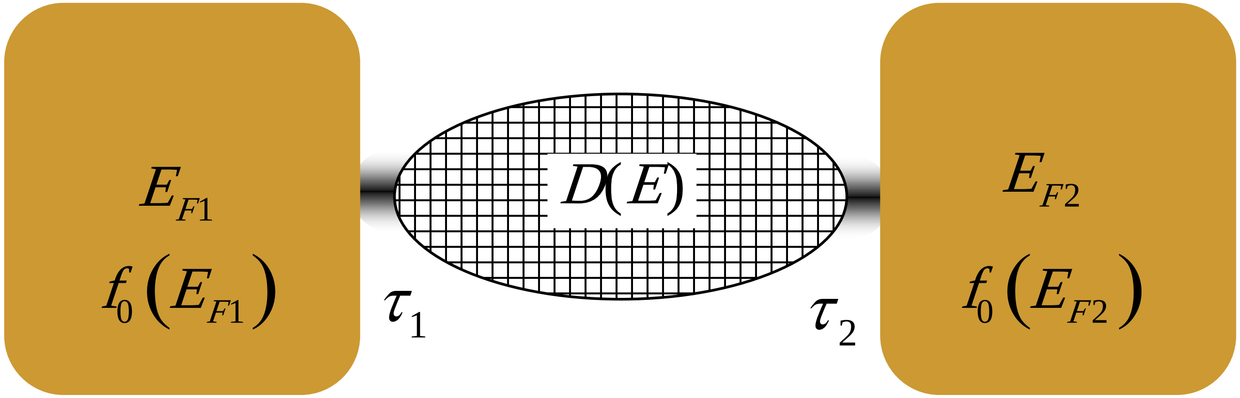
1) **General model for low-field transport**
2) Modes
3) Transmission
4) Linear (near equilibrium) transport
5) Summary

general model



S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
("Electronics from the Bottom Up" **nanohub.org**)

final result (near-equilibrium transport)



$$I = \frac{2q^2}{h}\left(\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right) dE\right) V$$

$$f_1(E) \approx f_2(E) \approx f_0(E)$$

$0 \leq T(E) \leq 1$ transmission

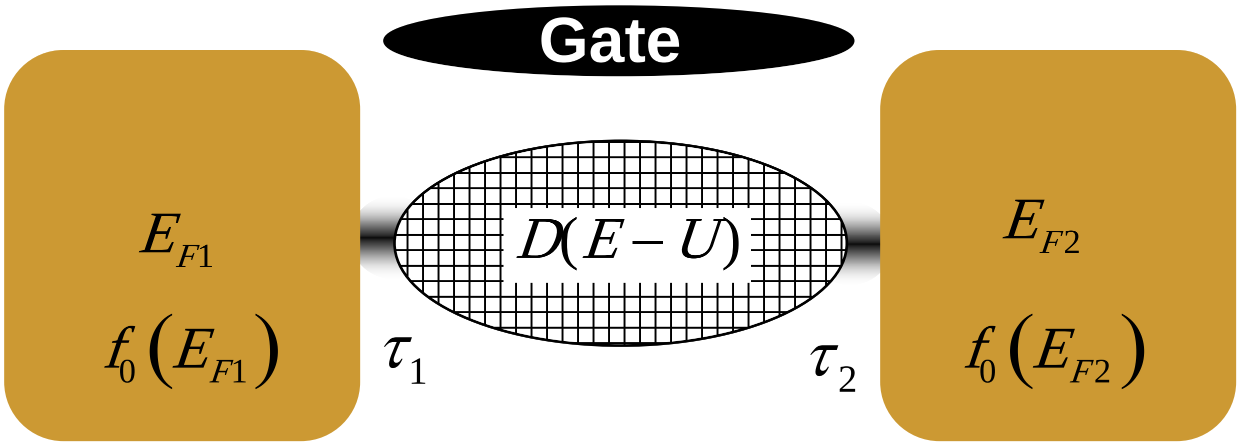
$M(E)$ number of conducting channels

assumptions

1) Contacts are large with strong scattering, always very near equilibrium

2) U, the self-consistent (mean-field) potential.

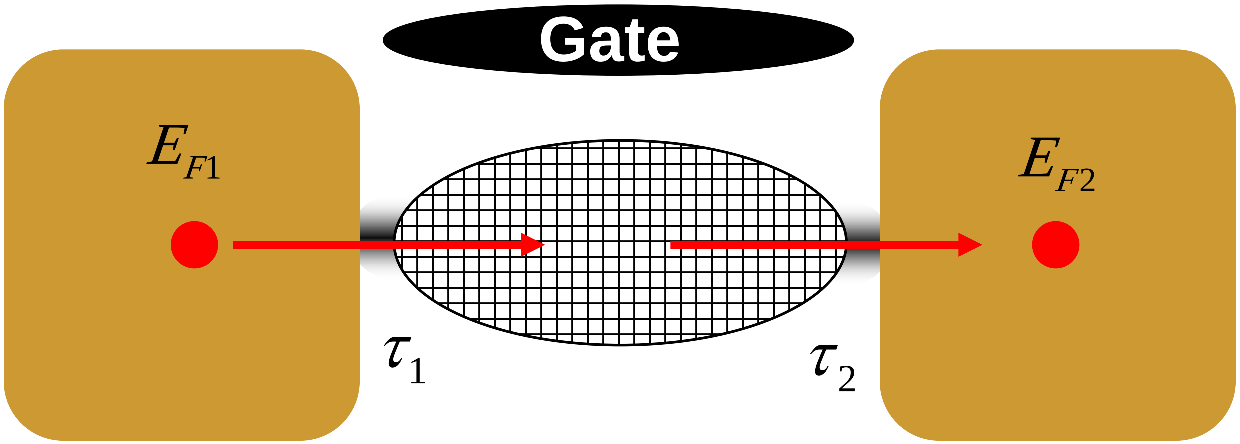
(For 'strongly correlated' transport, see Datta.)



3) In this class, we will assume that the device can be described by an $E(k)$.

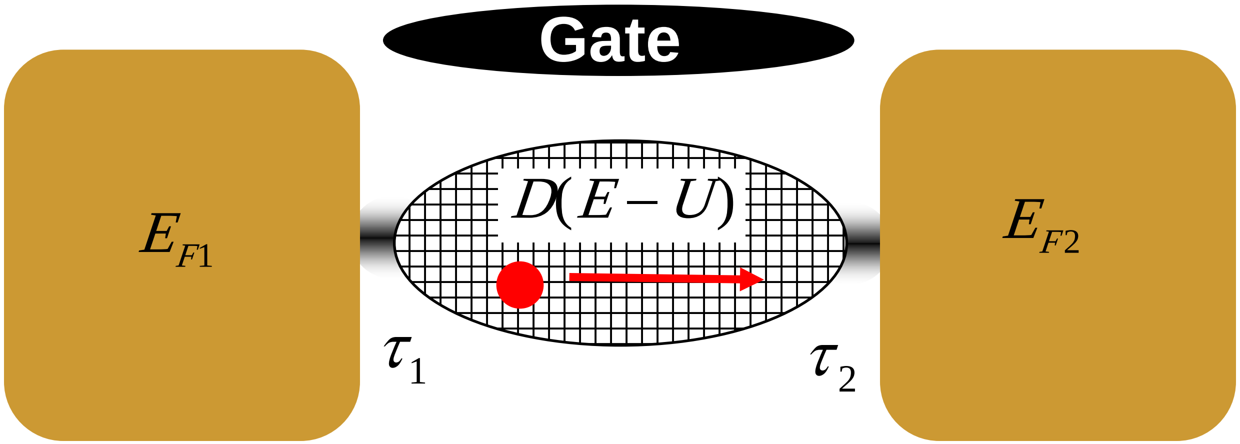
For the more general case, see Datta.

general model: contacts



4) Contacts are ***reflectionless*** (‘absorbing’). Any electron that enters from the device, stays in the contact and equilibriates with it.

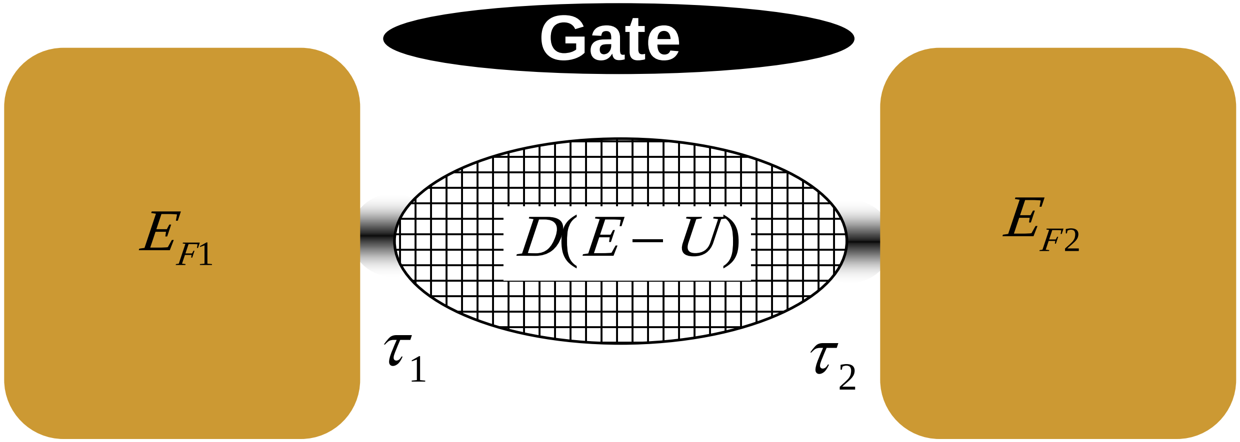
general model: energy channels



5) Electrons flow from left to right (or right to left) in different energy channels (modes). **Energy channels are independent**. Elastic scattering may occur in the device, but electrons do not change energy channels.

All inelastic scattering takes place in the contacts.

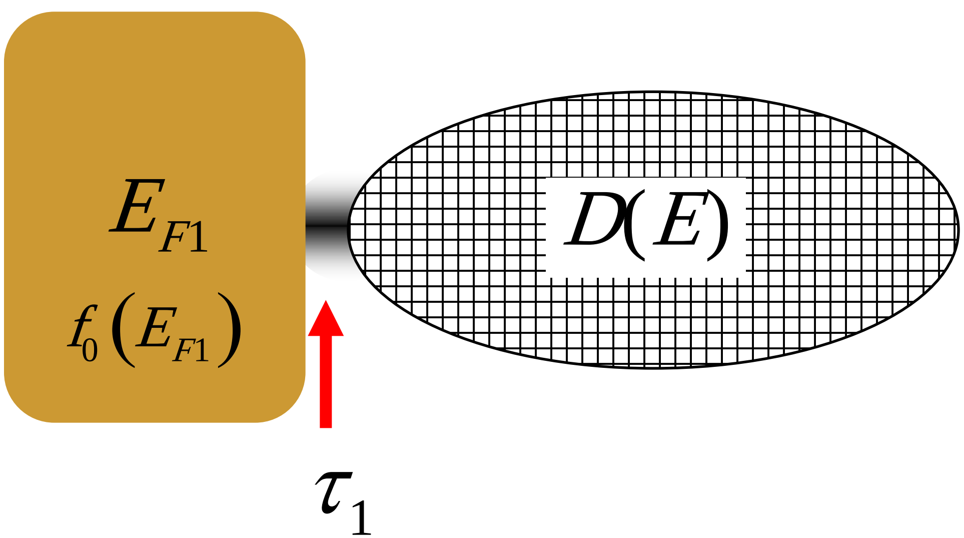
general model: summary



1) Contacts stay in equilibrium.
2) Electrons respond to the average potential, *U.*
3) Device is described by an *E*(*k*) from which we can determine *D*(*E*) (not a necessary assumption).
4) Contacts are reflectionless.
5) Independent energy channels in the device (if scattering occurs, it is elastic).

filling states from the left contact

(ignore electrostatics for now; $U = 0$)

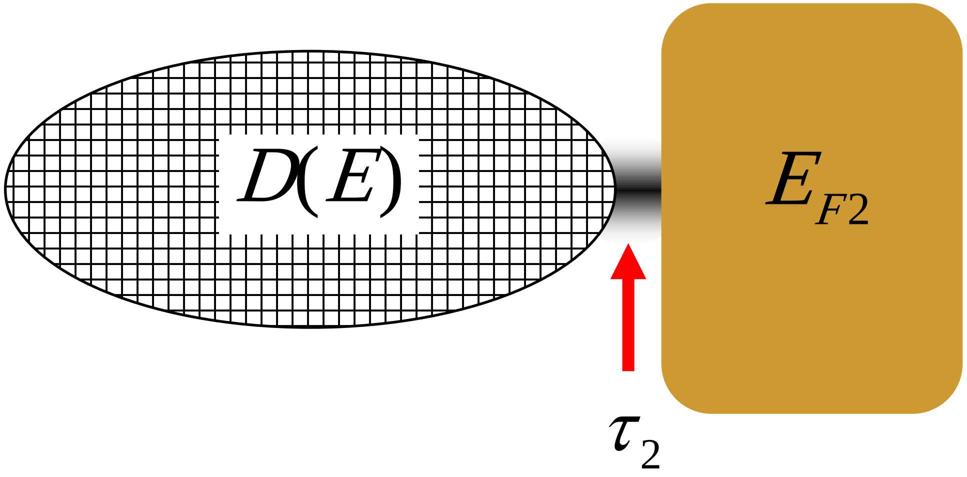


includes spin

$$N_1^0(E) = D(E)\, f_1(E)$$

$$\left.\frac{dN(E)}{dt}\right|_1 = \frac{N_1^0(E) - N(E)}{\tau_1}$$

filling states from the right contact



$$N_2^0(E) = D(E)\, f_2(E)$$

$$\left.\frac{dN(E)}{dt}\right|_2 = \frac{N_2^0(E) - N(E)}{\tau_2}$$

steady-state

$$\left.\frac{dN(E)}{dt}\right|_{tot} = \left.\frac{dN(E)}{dt}\right|_{1} + \left.\frac{dN(E)}{dt}\right|_{2} = \frac{N_1^0 - N}{\tau_1} + \frac{N_2^0 - N}{\tau_2} = 0$$

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

$$\left\{ \begin{array}{ll} N_1^0(E) \equiv D(E) f_1(E) & \gamma_1 = \hbar/\tau_1 \\ N_2^0(E) \equiv D(E) f_2(E) & \gamma_2 = \hbar/\tau_2 \end{array} \right\}$$

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

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

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

$$D_1(E) = \frac{\gamma_1}{\gamma_1 + \gamma_2} D(E)$$

DOS that can be filled by contact 1

$$D_2(E) = \frac{\gamma_2}{\gamma_1 + \gamma_2} D(E)$$

DOS that can be filled by contact 2

steady-state electron number, *N*

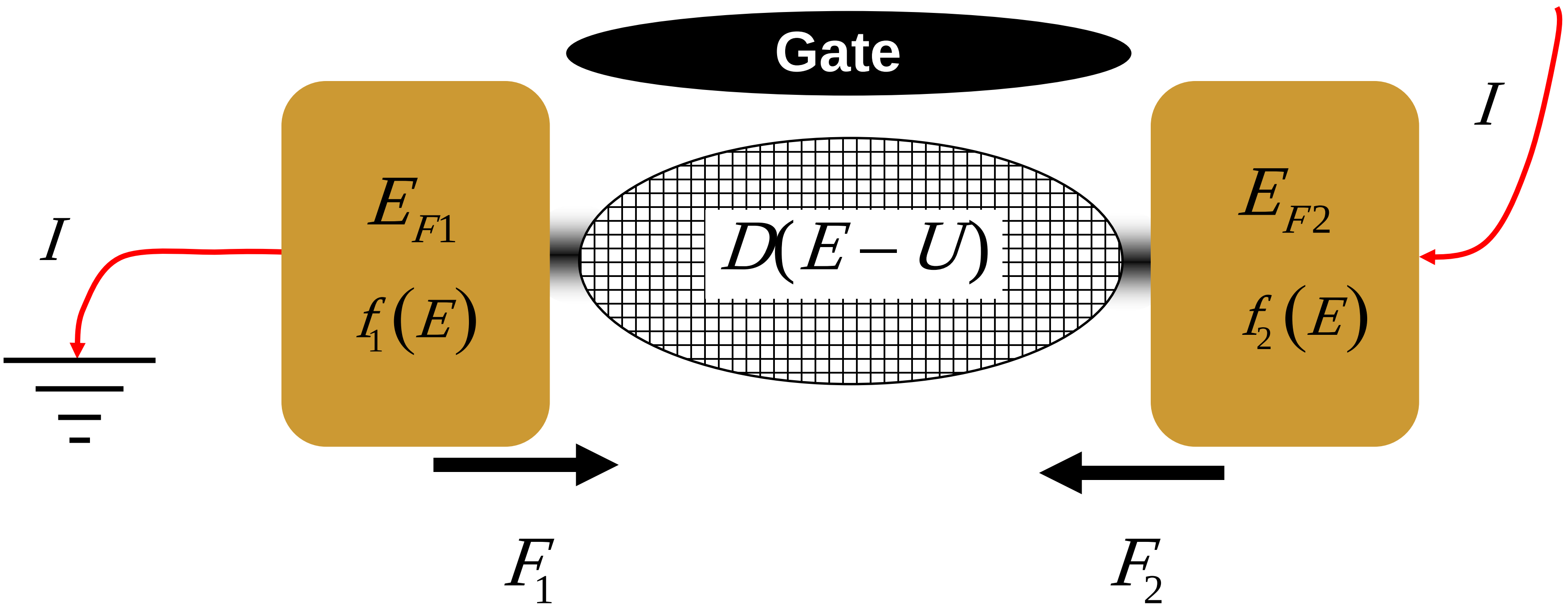
$$N = \int \left[D_1(E) f_1(E) + D_2(E) f_2(E) \right] dE$$

Recall that in equilibrium, we use:

$$N_0 = \int D(E) f_0(E) dE$$

$D(E) \propto L \text{ (1D)}$	$D(E) \propto A \text{ (2D)}$	$D(E) \propto \Omega \text{ (3D)}$
n_L	n_S	n

steady-state current, *I*



Contact 1 tries to fill up the device according to its Fermi level.

$$F_1 + F_2 = 0$$

$$I = qF_1 = -qF_2$$

Contact 2 tries to fill up the device according to its Fermi level.

steady-state current, *I*

$$F_1 = \left.\frac{dN(E)}{dt}\right|_1 = \frac{N_1^0(E) - N(E)}{\tau_1} \qquad F_2 = \left.\frac{dN(E)}{dt}\right|_2 = \frac{N_2^0(E) - N}{\tau_2}$$

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

$$N_1^0(E) \equiv D(E) f_1(E) \qquad N_2^0(E) \equiv D(E) f_2(E)$$

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

results

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

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

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

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

the current:

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

We will think of this "2" as representing the two degenerate spins.

When we compute the DOS, we usually include a factor of 2 for spin. *D*/2 is **the DOS per spin**.

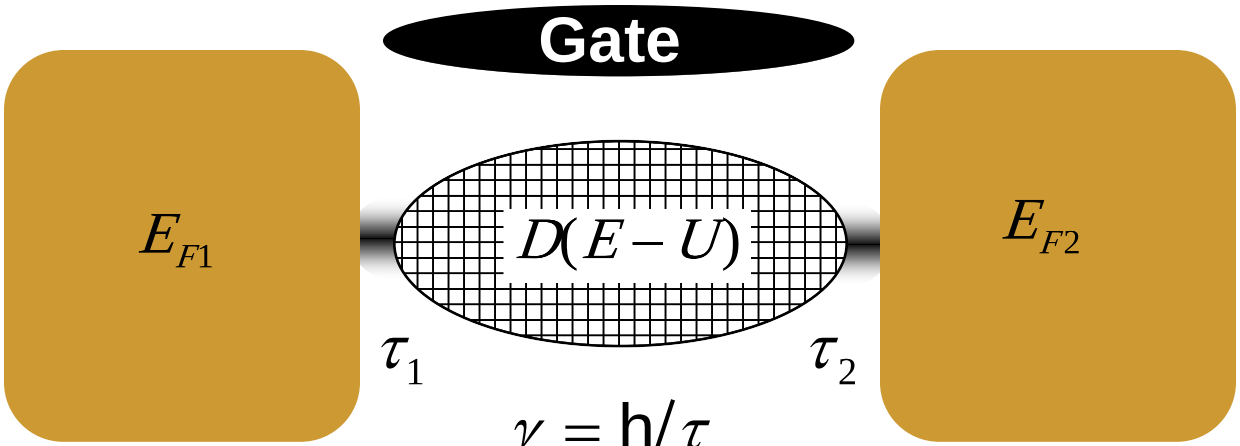
$$I = \frac{2q}{h}\int \gamma\pi\frac{D(E)}{2}(f_1 - f_2)dE$$

$$D(E)/2 = \text{density of states per spin}$$

general model for nanodevice

3) The device is described by some density-of-states.

5) For transistors, we use a gate to control the self-consistent potential, *U*.



$$\gamma = \hbar/\tau$$

1) Strong, inelastic scattering maintains equilibrium in the contacts.

2) Contacts are described by escape or transit times or by a 'broadening' energy.

4) Device may be ballistic, or there may be elastic scattering.

current and carrier density

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

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

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

$\frac{D(E)}{2}$: density-of-states per spin

outline

1) A general model for low-field transport
2) **Modes**
3) Transmission
4) Linear (near equilibrium) transport
5) Summary

conducting channels

$$I = \frac{2q}{h}\int \gamma\,\pi\,\frac{D}{2}\left(f_1 - f_2\right)dE \qquad U = 0$$

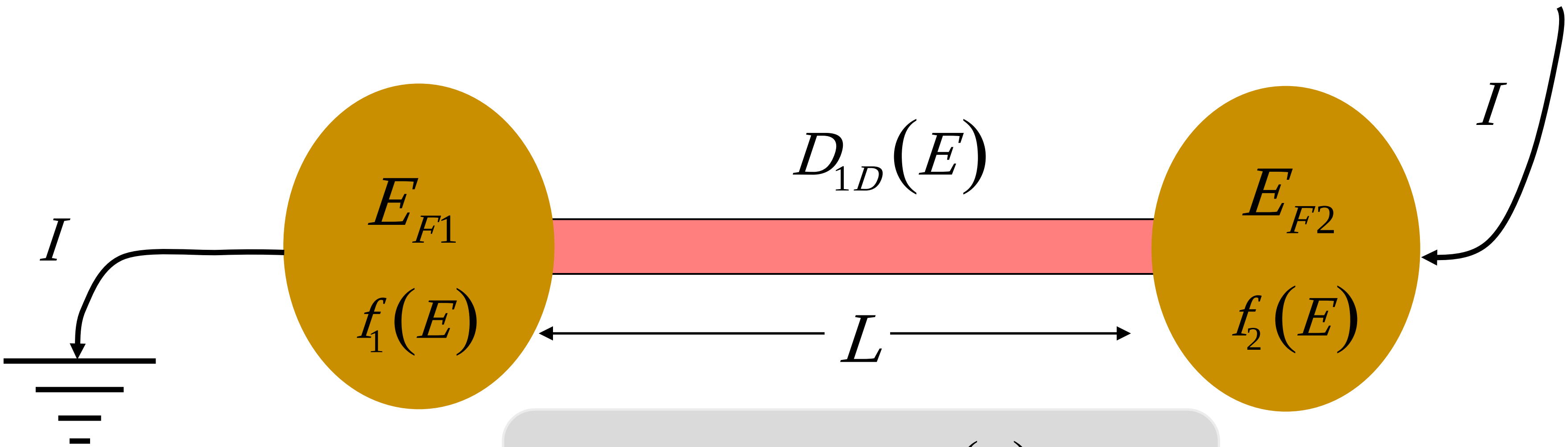
$$\gamma(E)\pi D(E)/2 = ?$$

$$\gamma(E) = \frac{\hbar}{\tau(E)}$$ is the 'broadening' and has units of energy.

$$D(E)$$ has units of 1/energy.

$$\gamma(E)\pi D(E)/2 = M(E)$$ is a **number**. We will show that *M* is the number of conducting channels at energy, *E*.

a 1D ballistic nanowire



$$I(E) = \frac{2q}{h}\gamma(E)\pi\frac{D_{1D}(E)}{2}\left(f_1 - f_2\right)$$

$$N(E) = \frac{D_{1D}(E)}{2}\left[f_1(E) + f_2(E)\right]$$

Let's do an "experiment" to determine what γ (or τ) is.

the "experiment"

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

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

(energy channels are independent)

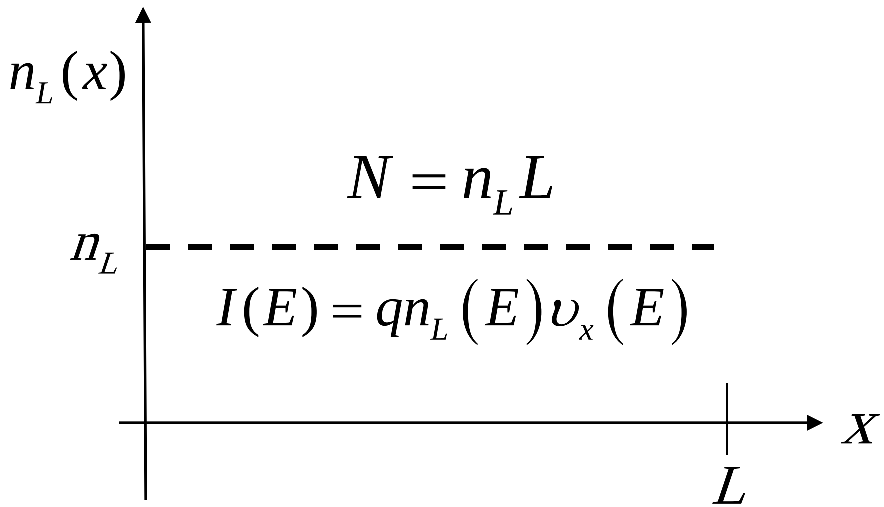
$$\frac{qN}{I} = \frac{\hbar}{\gamma}\frac{\left(f_1 + f_2\right)}{\left(f_1 - f_2\right)}$$

Apply V >> 0 to right contact, if $f_2 << f_1$ (injection from the source only), then:

$$\frac{qN}{I} = \frac{\text{stored charge}}{\text{current}} = \frac{\hbar}{\gamma} = \tau$$

transit time

$$\tau = \frac{\text{stored charge}}{\text{current}}$$



$$N = n_L L$$

$$I(E) = q n_L(E)\upsilon_x(E)$$

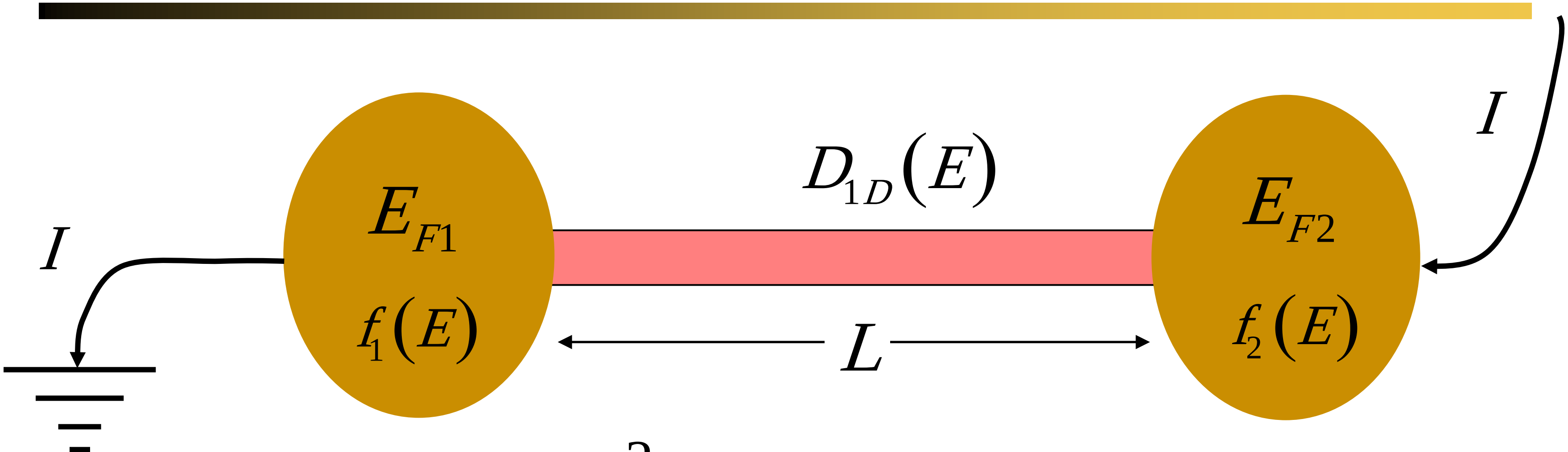
(ballistic transport)

$$\tau = \frac{q n_L L}{q n_L \upsilon_x} = \frac{L}{\upsilon_x}$$

'transit time'

$$(\gamma\tau = \hbar)$$

modes in 1D

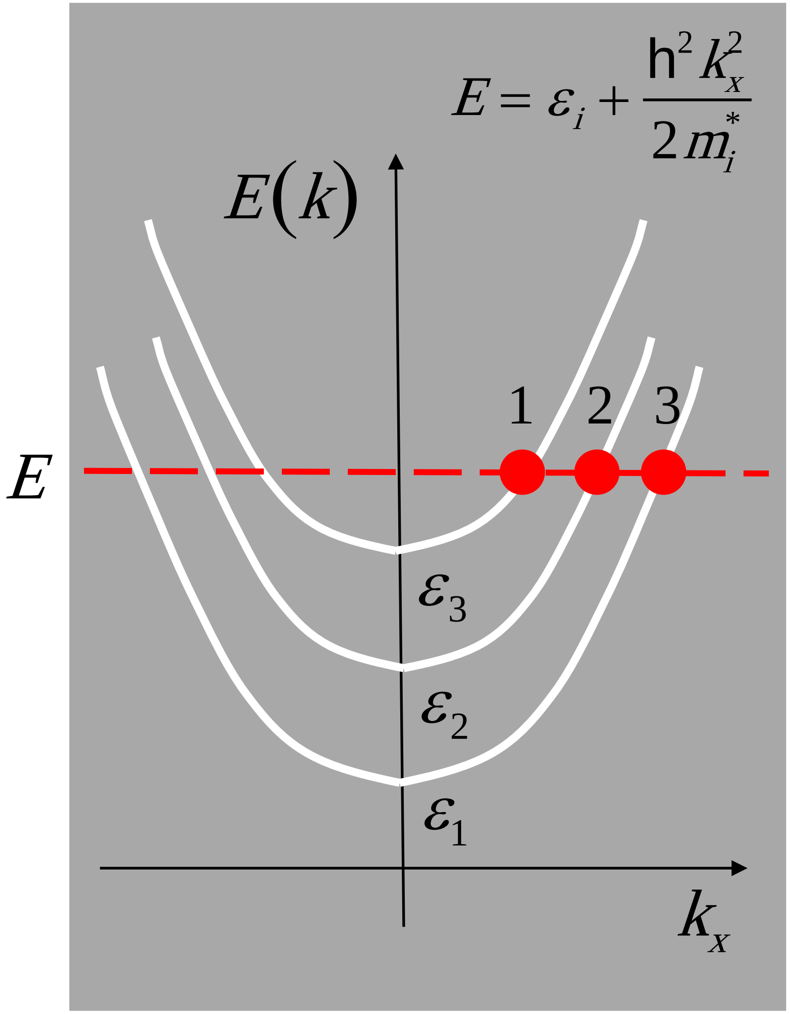


$$I = \frac{2q}{h}\int M(E)\left(f_1 - f_2\right)dE$$

$$M(E) = \gamma(E)\,\pi\,\frac{D(E)}{2}$$

$$\gamma\,\pi\frac{D(E)}{2} = \frac{h}{\left(L/\upsilon_x\right)}\pi\frac{L}{\pi h \upsilon_x} = 1$$

$M(E)$ in 1D



$M(E)$ is the number of subbands at energy, E.

outline

1) A general model for low-field transport
2) Modes
3) **Transmission**
4) Linear (near equilibrium)
5) Summary

ballistic vs. diffusive transport

1) Ballistic:

Electrons travel without scattering from the injecting contact to the absorbing contact.

$$\langle \upsilon \rangle = \upsilon(E) = \sqrt{2\left(E - \varepsilon_1\right)/m^*}$$

2) Diffusive:

Injected electrons undergo a random walk and leave the device either through the contact from which they were injected or the other one.

$$\langle \upsilon \rangle = ?$$

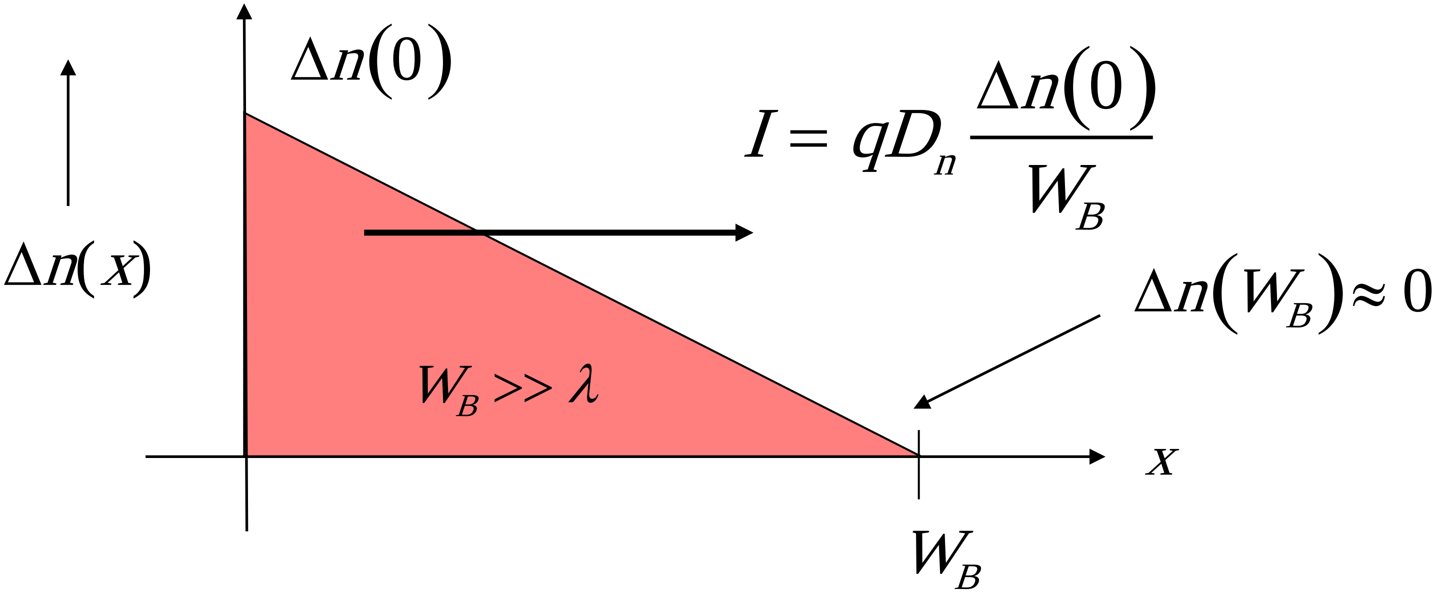
diffusive transport

$$\gamma = \frac{h}{\langle \tau \rangle} \qquad \langle \tau \rangle = ?$$

Assume a nanowire that is much longer than the mean-free-path for backscattering, $L >> \lambda$,

then, injected carriers diffuse to the other contact. Fick's Law of diffusion should apply.

recall: base transit time of a BJT



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

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

ballistic

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

$$\tau = \frac{L}{\upsilon}$$

$$\gamma_{ball} = \frac{\hbar}{L/\upsilon}$$

$$\upsilon = \sqrt{\frac{2\left(E - \varepsilon_1\right)}{m^*}}$$

transmission (diffusive)

$$\gamma = \frac{h}{\langle \tau \rangle}$$

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

$$\gamma_{Diff} = \frac{h}{L^2/2D_n} \rightarrow \gamma_{Diff} = \frac{h}{L^2/(\upsilon\lambda)} = \frac{\lambda}{L}\left(\frac{h}{L/\upsilon}\right)$$

$$D_n = \frac{\upsilon\lambda}{2}$$

$$\gamma_{Diff} = T \times \gamma_{Ball}$$

$$T = \frac{\lambda}{L} << 1$$

transmission

$$I=\frac{2q}{h}\int M(E)\left(f_1-f_2\right)dE \quad \Rightarrow \quad I=\frac{2q}{h}\int T\,M(E)\left(f_1-f_2\right)dE$$

1) Diffusive: $L >> \lambda \quad T=\frac{\lambda}{L}<<1$

2) Ballistic: $L << \lambda \quad T=1$

3) Quasi-ballistic: $L \approx \lambda \quad T<1$

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

λ is the ‘mean-free-path for backscattering’

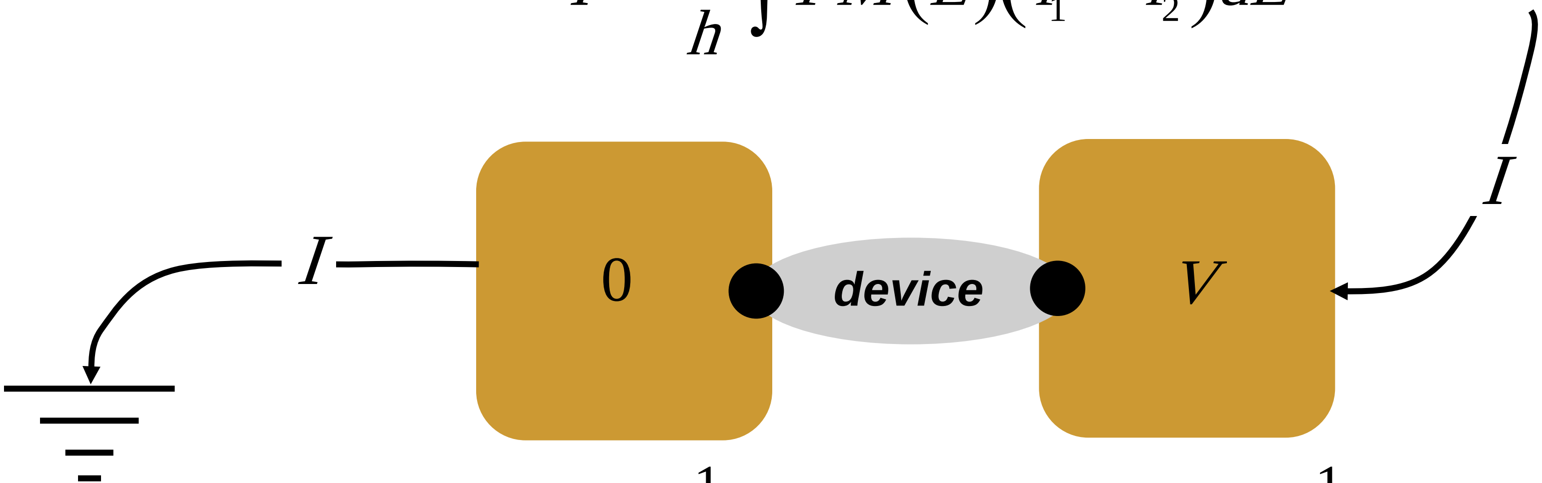
This expression can be derived with relatively few assumptions.

outline

1) A general model for low-field transport
2) Modes
3) Transmission
4) **Linear (near-equilibrium) transport**
5) Summary

Landauer expression for current

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



$$f_1(E) = \frac{1}{1 + e^{(E - E_{F1})/k_B T}} \qquad f_2(E) = \frac{1}{1 + e^{(E - E_{F1} + qV)/k_B T}}$$

For small bias, we can linearize (f_1 - f_2) and the current becomes proportional to V (linear, near-equilibrium, low-field response).

linear response

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

$$f_1(E) = \frac{1}{1 + e^{(E - E_{F1})/k_B T}}$$

$$f_2 = f_1 + \frac{\partial f_1}{\partial E_F}\Delta E_F = f_1 + \frac{\partial f_1}{\partial E_F}(-qV)$$

$$f_2(E) = \frac{1}{1 + e^{(E - E_{F1} + qV)/k_B T}}$$

$$f_1 - f_2 = \frac{\partial f_1}{\partial E_F}(qV)$$

$$\frac{\partial f_1}{\partial E_F} = -\frac{\partial f_1}{\partial E}$$

$$f_1 - f_2 = \left(-\frac{\partial f_1}{\partial E}\right)qV$$

$$I = \frac{2q^2}{h}\left(\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\right)V$$

$$f_1(E) \approx f_2(E) \approx f_0(E)$$

outline

1) A general model for low-field transport
2) Modes
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5) **Summary**

mathematics

This lecture has presented a lot of equations. Don't try to memorize them; try to understand the results.

"Mathematics is the language of clear thinking."

Richard W. Hamming in
The Art of Doing Science and Engineering: Learning to Learn,
Gordon and Breech Science Publishers, Amsterdam, 1997.

questions

1) A general model for low-field transport
2) Modes
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