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Near-equilibrium Transport:
Fundamentals and Applications

Lecture 2: General model for transport

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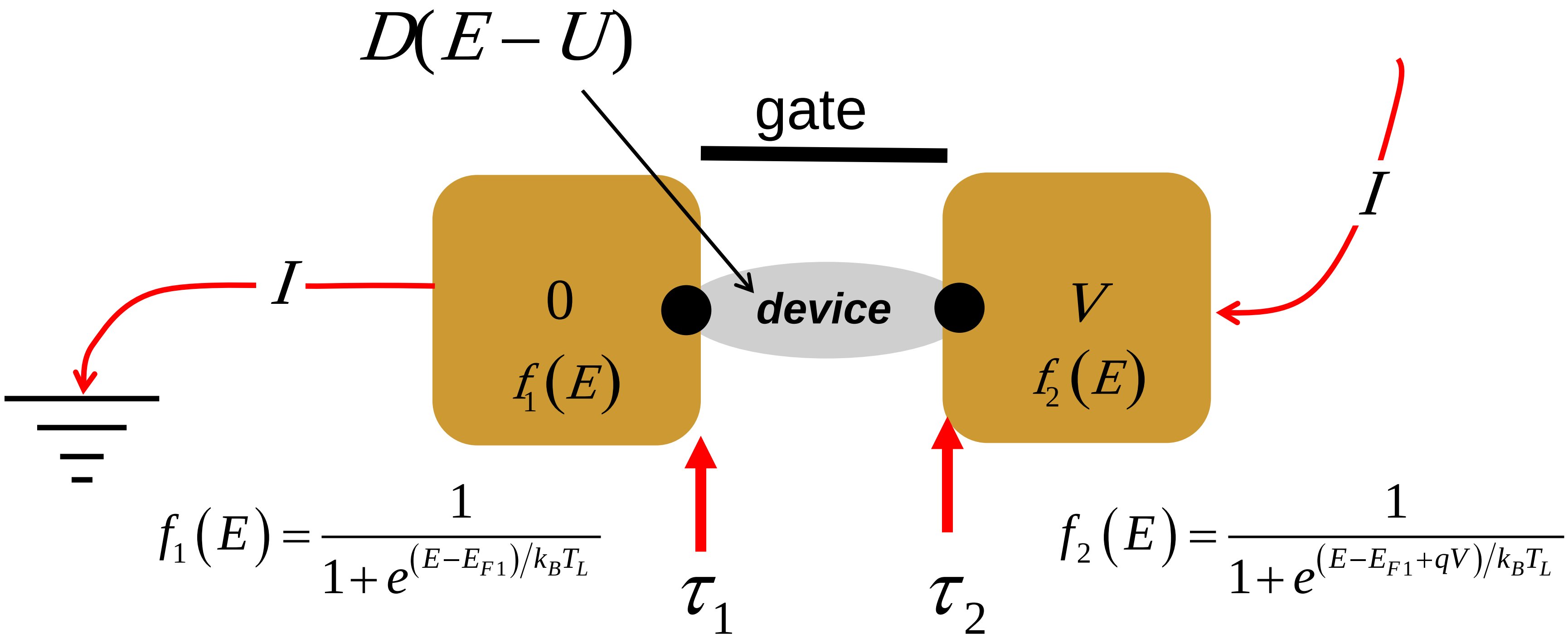
outline

1) **The model device**
2) The mathematical model
3) Modes
4) Transmission
5) Near-equilibrium (linear) transport
6) Transport in the bulk
7) Summary
8) References

Landauer-Datta model for a nano-device



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

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

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

For a fuller discussion about the model to be presented, see S. Datta in the references at the end of this lecture.

questions

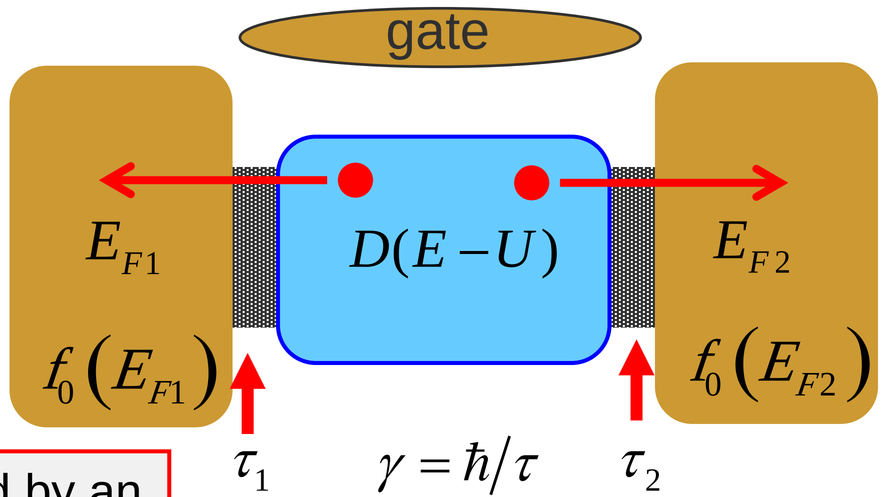
1) How is the **number of electrons** in the device related to the Fermi levels in the contacts, to the density of states, and to the characteristic times?

2) How is the **electron current** through the device related to the same parameters?

assumptions

2) **Contacts** are large with strong inelastic scattering, always near equilibrium

3) *U* is the self-consistent (mean-field) potential. (For "strongly correlated" transport, see Datta.)



5) ***Reflectionless*** ("absorbing") contacts.

1) Device is described by an *E*(*k*). For the more general case, see Datta.

4) All **inelastic scattering** takes place in the contacts. Electrons flow from left to right (or right to left) in **independent** energy channels.

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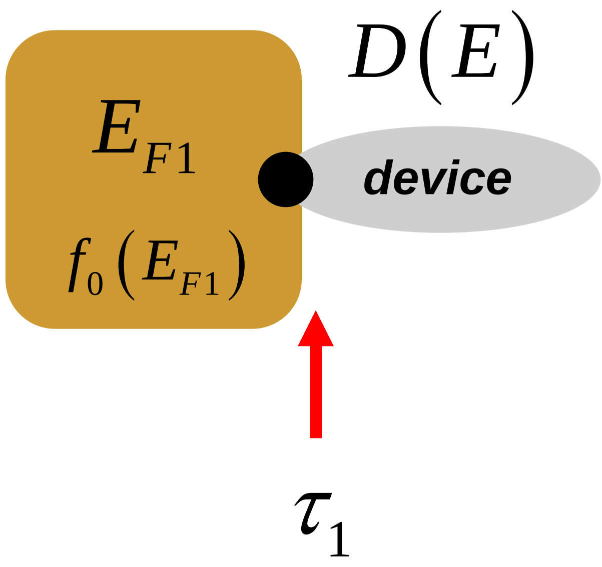
filling states from the left contact

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

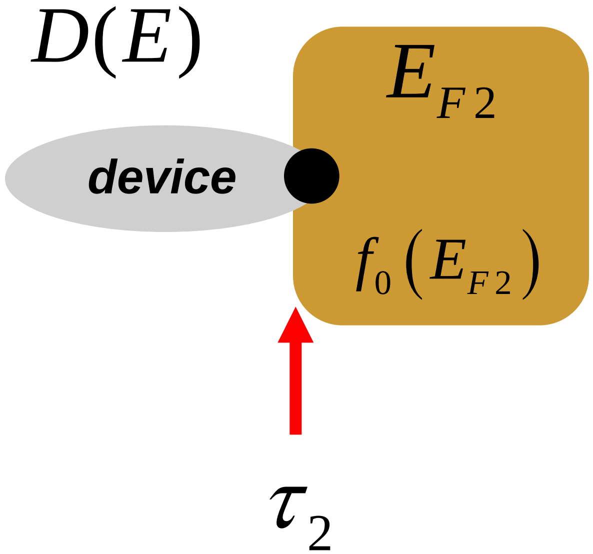


includes spin

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

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

filling states from the right contact



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

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

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steady-state

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

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

$$\left\{ \begin{aligned} N_1^0(E) &\equiv D(E) f_1(E) \\ N_2^0(E) &\equiv D(E) f_2(E) \end{aligned} \right\}$$

To keep things simple, assume:

$$\tau_1 = \tau_2$$

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

$$N(E) = \frac{D(E)}{2} f_1(E) + \frac{D(E)}{2} f_2(E)$$

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

Recall that in equilibrium, we use:

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

steady-state electron number, *N*

Remember that *N* is the total **number** of electrons and that *D* is the total DOS - #/J

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

$$n_L = \frac{N}{L} \text{ cm}^{-1} \qquad n_S = \frac{N}{A} \text{ cm}^{-2} \qquad n = \frac{N}{\Omega} \text{ cm}^{-3}$$

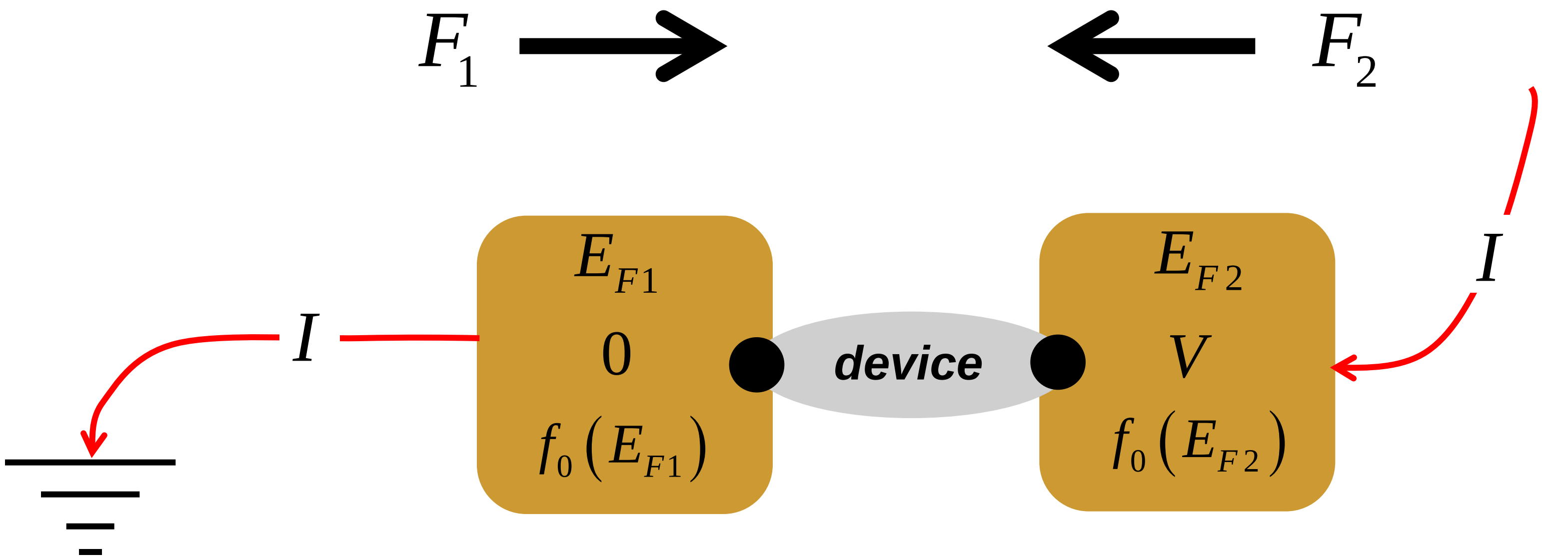
questions

1) How is the **electron density** in the device related to the Fermi levels in the contacts, the density of states, and the characteristic times?

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

2) How is the **electron current** through the device related to the same parameters?

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*

$$I(E) = +qF_1 = -qF_2$$

$$I(E) = +\frac{q}{2}\left(F_1 - F_2\right)$$

$$I(E) = +\frac{q}{2\tau(E)}\left(N_1^0 - N_2^0\right)$$

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

$$F_1 = \frac{N_1^0(E) - N(E)}{\tau(E)}$$

$$F_2 = \frac{N_2^0(E) - N(E)}{\tau(E)}$$

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

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

$$\gamma(E) \equiv \frac{\hbar}{\tau(E)}$$

questions

1) How is the **electron density** in the device related to the Fermi levels in the contacts, the density of states, and the characteristic times?

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

2) How is the **electron current** through the device related to the same parameters?

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

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modes or conducting channels

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

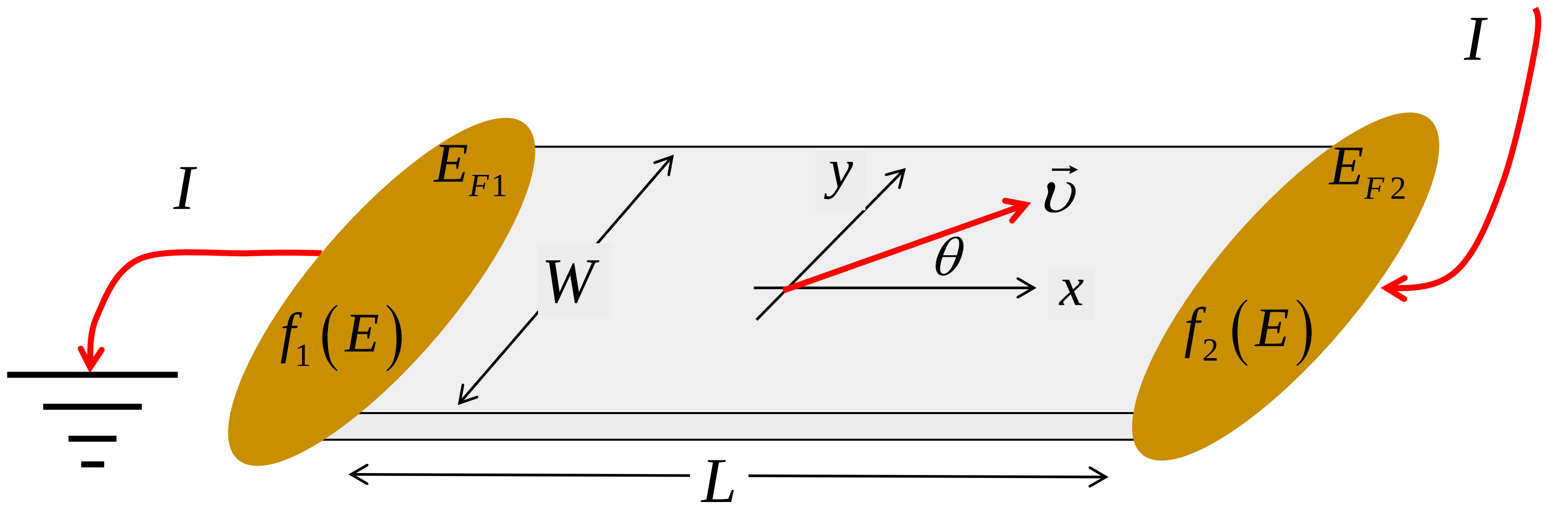
$$\gamma(E)\pi D(E)/2 = ?$$

$$\gamma(E) = \frac{\hbar}{\tau(E)}$$ 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 2D ballistic channel



$$M(E) = \gamma \pi D(E)/2 = ? \qquad D(E) = D_{2D}(E)WL \quad D_{2D}(E) = \frac{m^*}{\pi \hbar^2}$$

(parabolic bands)

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

the "experiment"

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

(energy channels are independent)

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

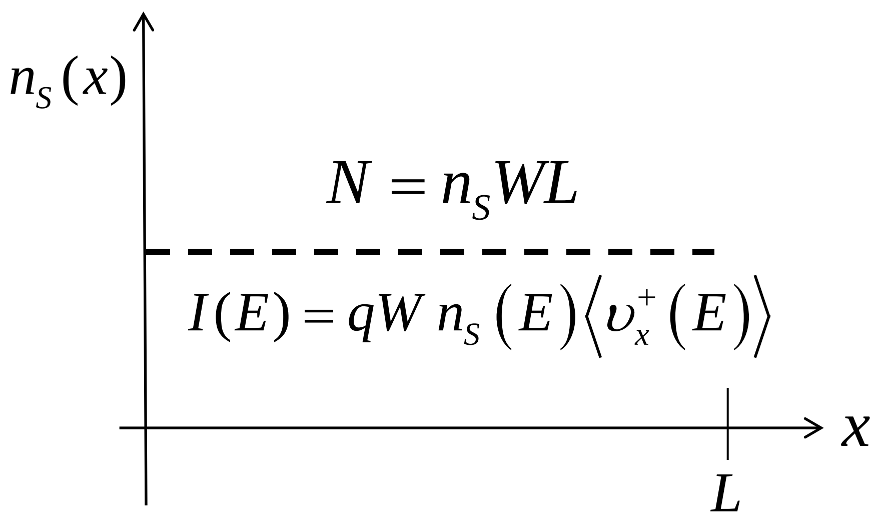
$$\frac{qN}{I} = \frac{\hbar}{\gamma} \frac{(f_1 + f_2)}{(f_1 - f_2)}$$

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

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

transit time

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

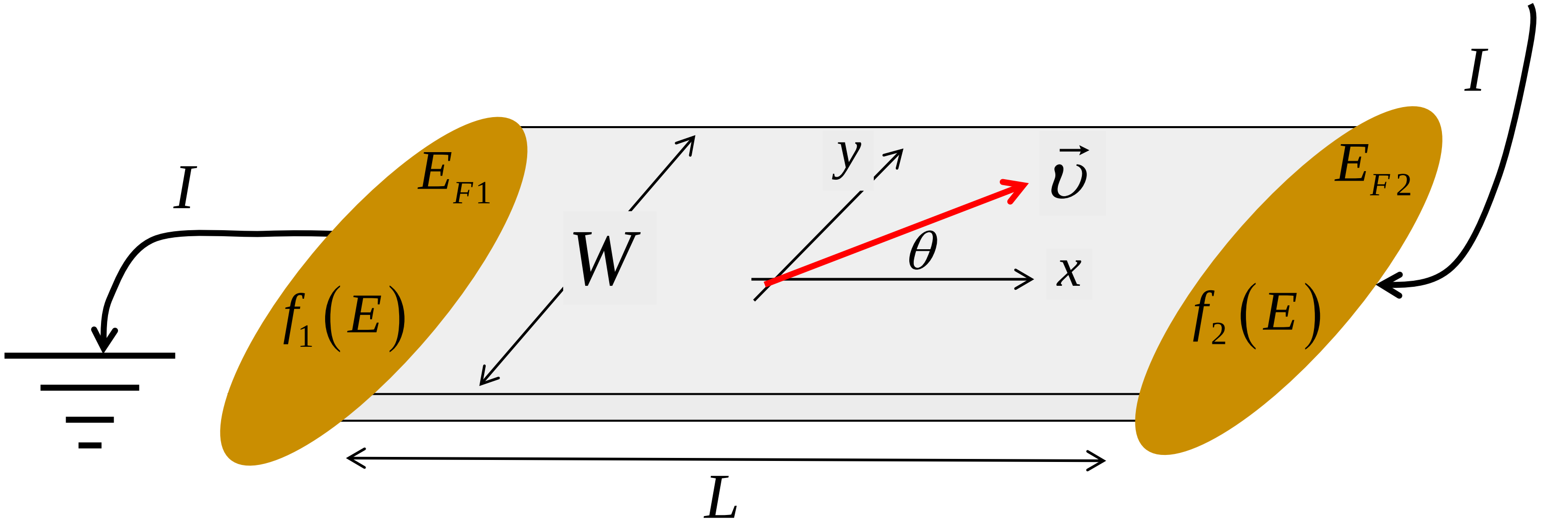


(ballistic transport)

$$\tau(E) = \frac{qN(E)}{I(E)} = \frac{L}{\left\langle \upsilon_x^+(E) \right\rangle}$$

"transit time"

modes (conducting channels) in 2D



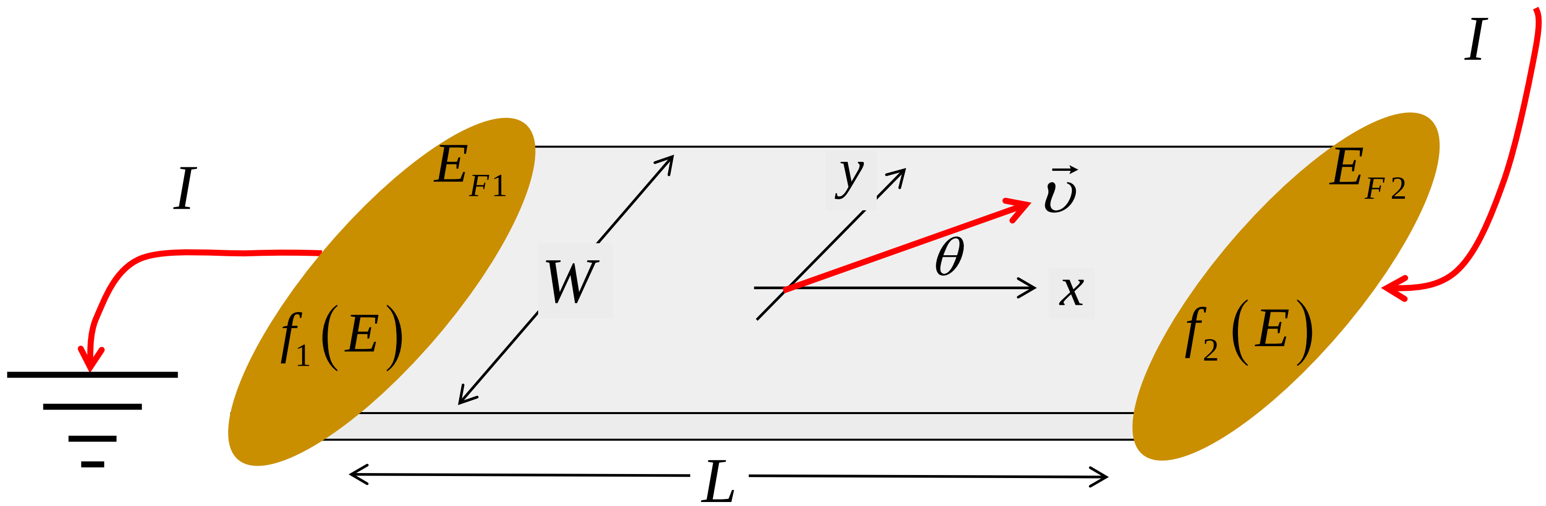
$$\langle \upsilon_x^+ \rangle = \upsilon \langle \cos\theta \rangle$$

$$\langle \cos\theta \rangle = \frac{\int_{-\pi/2}^{+\pi/2} \cos\theta d\theta}{\pi} = \frac{2}{\pi}$$

$$\langle \upsilon_x^+ \rangle = \frac{2}{\pi} \upsilon$$

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

a 2D ballistic channel



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

modes in 2D

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

$$\gamma(E) = \frac{\hbar}{\tau} = \frac{\hbar}{L/\langle \upsilon_x^+ \rangle}$$

$$M(E) = \frac{\hbar}{L}\langle \upsilon_x^+ \rangle \pi \frac{D_{2D}(E)WL}{2}$$

$$M(E) = W\frac{h}{4}\langle \upsilon_x^+ \rangle D_{2D}(E)$$

$$M_{1D}(E) = \frac{h}{4}\langle \upsilon_x^+ \rangle D_{1D}(E)$$

$$M_{2D}(E)W = W\frac{h}{4}\langle \upsilon_x^+ \rangle D_{2D}(E)$$

$$M_{3D}(E)A = A\frac{h}{4}\langle \upsilon_x^+ \rangle D_{3D}(E)$$

But how do we interpret this result physically?

interpretation

$$M(E) = W\frac{h}{4}\langle \upsilon_x^+ \rangle D_{2D}(E)$$

$$M(E) = W\frac{\sqrt{2m^*(E-E_C)}}{\pi\hbar}$$

$$M(E) = \frac{Wk}{\pi} = \frac{W}{\lambda_B(E)/2}$$

M(*E*) is the number of electron half wavelengths that fit into the width, W, of the conductor.

$$\langle \upsilon_x^+ \rangle = \frac{2}{\pi}\upsilon$$

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

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

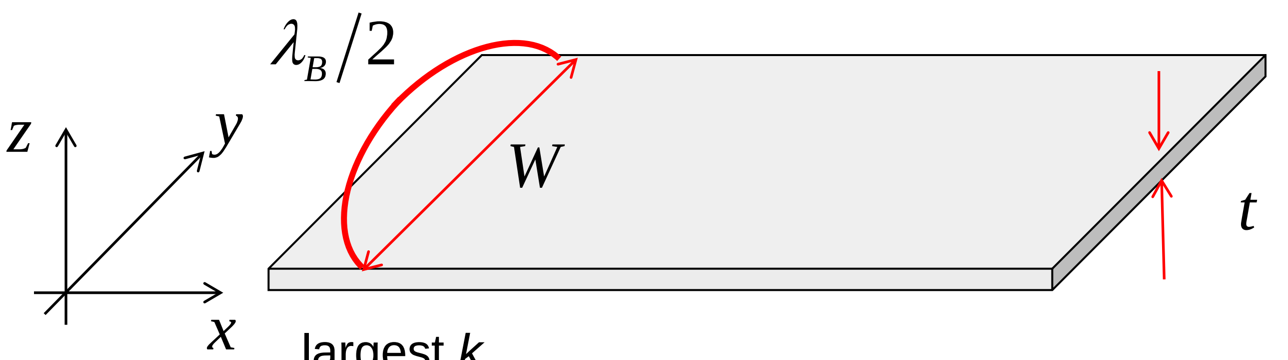
$$E(k) = E_C + \frac{\hbar^2 k^2}{2m^*}$$

waveguide modes

Assume that there is **one** subband associated with confinement in the z-direction. How many subbands (channels) are there associated with confinement in the y-direction?

$$M(E) = \frac{W}{\lambda_B(E)/2}$$

When $M(E) = 1 \rightarrow \lambda_B(E)/2 = W$



$$\psi(x,y) \propto e^{ik_x x} \sin k_y y$$

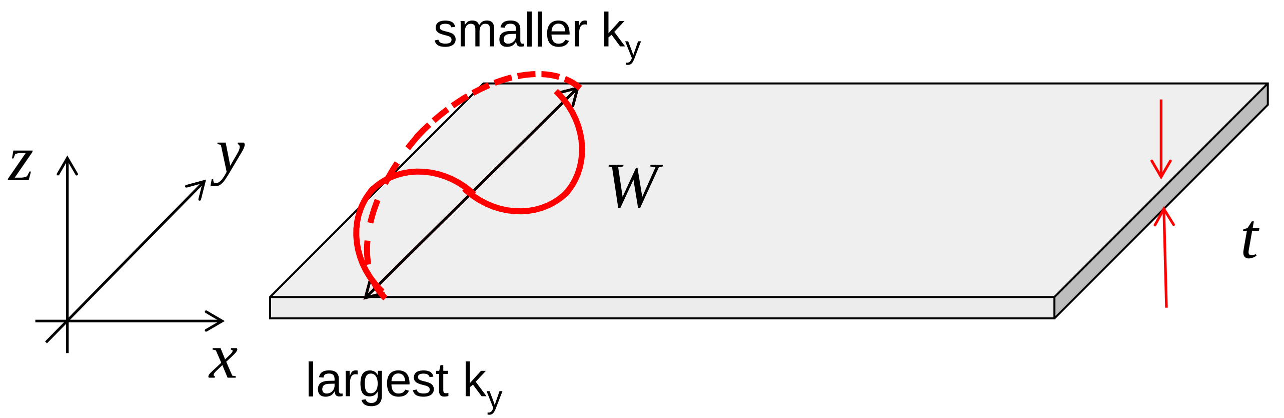
$$k_y = m\pi/W \quad m = 1, 2, \ldots$$

waveguide modes

$$M(E) = \frac{W}{\lambda_B(E)/2}$$

When

$$M(E) = 2 \rightarrow \lambda_B(E) = W$$



$$\psi(x,y) \propto e^{ik_x x} \sin k_y y$$

$$k_y = m\pi/W \quad m = 1, 2, \ldots$$

***M* = # of electron half wavelengths that fit into *W*.**

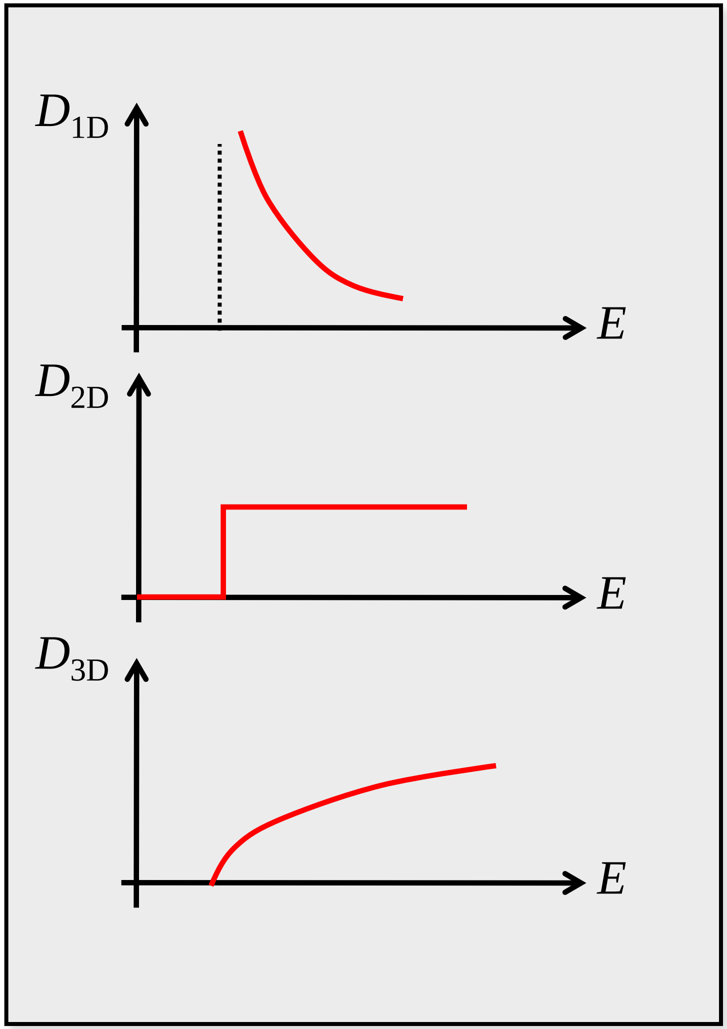
density of states (for parabolic energy bands)

$$D(E) = L\,D_{1D}(E) = \frac{L}{\pi\hbar}\sqrt{\frac{2m^*}{(E-\varepsilon_1)}}\,\Theta(E-\varepsilon_1)$$

$$D(E) = A D_{2D}(E) = A\frac{m^*}{\pi\hbar^2}\Theta(E-\varepsilon_1)$$

$$D(E) = \Omega\,D_{3D}(E) = \Omega\frac{m^*\sqrt{2m^*(E-E_C)}}{\pi^2\hbar^3}\Theta(E-E_C)$$

$$\left(E(k) = E_C + \hbar^2 k^2 / 2m^*\right)$$



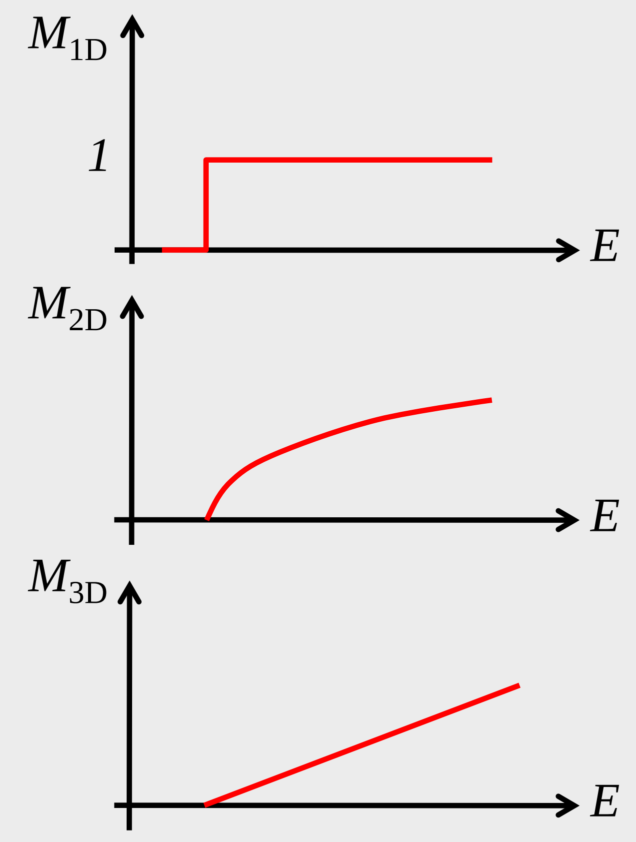
number of modes (for parabolic energy bands)

$$M(E) = M_{1D}(E) = H(E - E_C)$$

$$M(E) = W M_{2D}(E) = W \frac{\sqrt{2m^*(E - \varepsilon_1)}}{\pi\hbar} H(E - E_C)$$

$$M(E) = A M_{3D}(E) = A \frac{m^*}{2\pi\hbar^2}(E - E_C) H(E - E_C)$$

$$\left(E(k) = E_C + \hbar^2 k^2 / 2m^*\right)$$



summary

1) The density of states is used to compute carrier densities.

2) The number of modes (channels) is used to compute the current.

3) The number of modes at energy, *E*, is proportional to the average velocity (in the direction of transport) at energy, *E* times the DOS(*E*).

4) *M*(*E*) depends on the bandstructure ***and*** on dimensionality.

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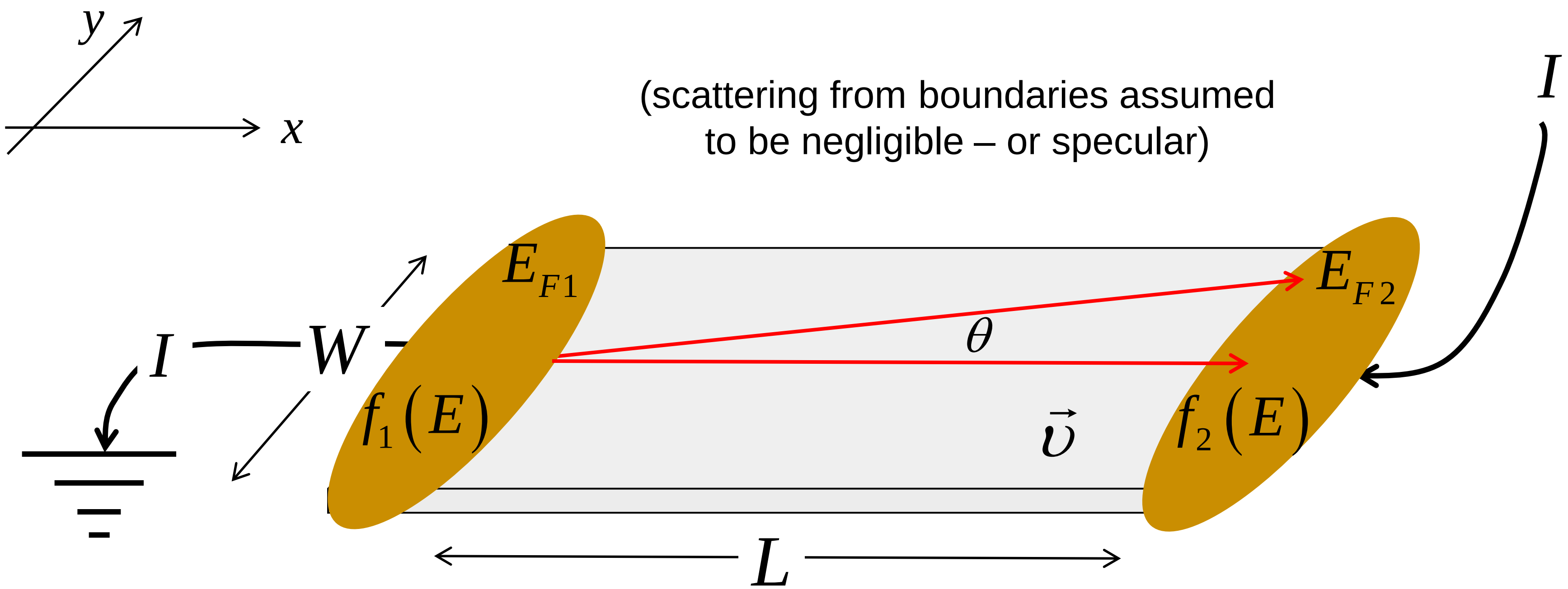
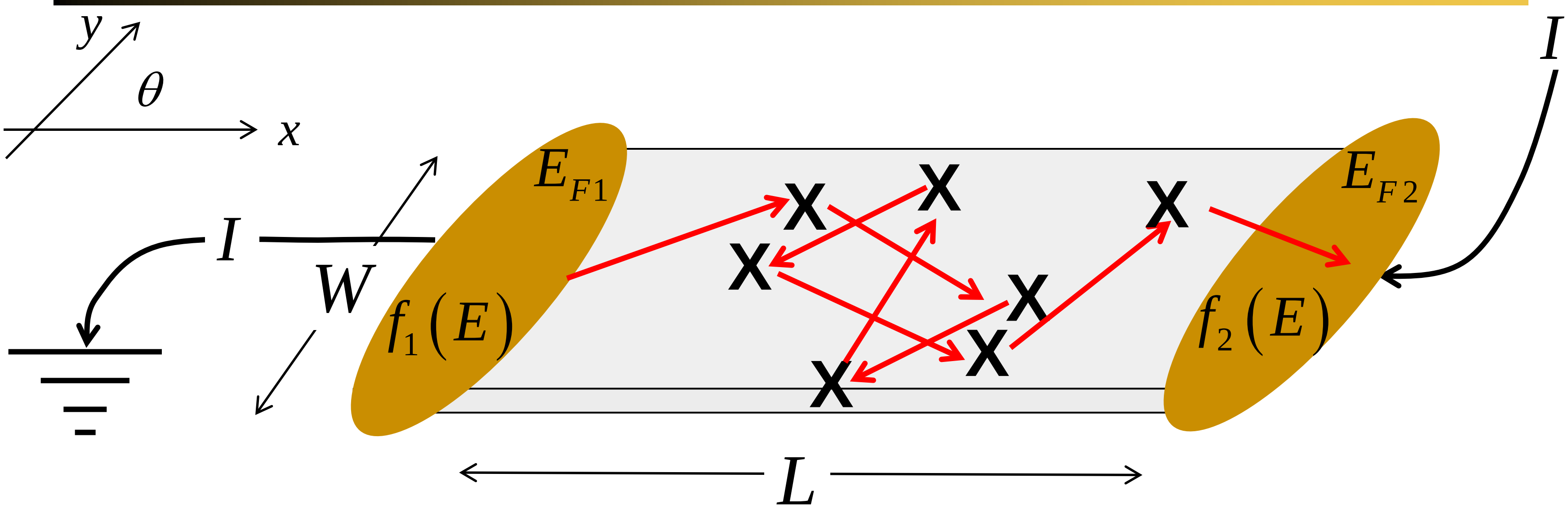
ballistic transport in 2D



diffusive transport in 2D



- Electrons undergo a **random walk** as they go from left to right contact.
- Some terminate at contact 1, and some at contact 2.
- The average distance between collisions is the mfp, ⌊
- "Diffusive" transport means $\Lambda >>$ ⌊
- The diffusive transit time will be much longer than the ballistic transit time.

ballistic vs. diffusive transport

1) Ballistic:

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

$$\langle \upsilon_x^+ \rangle = \frac{2}{\pi}\upsilon(E)$$

2) Diffusive:

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

$$\langle \upsilon_x^+ \rangle = ?$$

diffusive transport

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

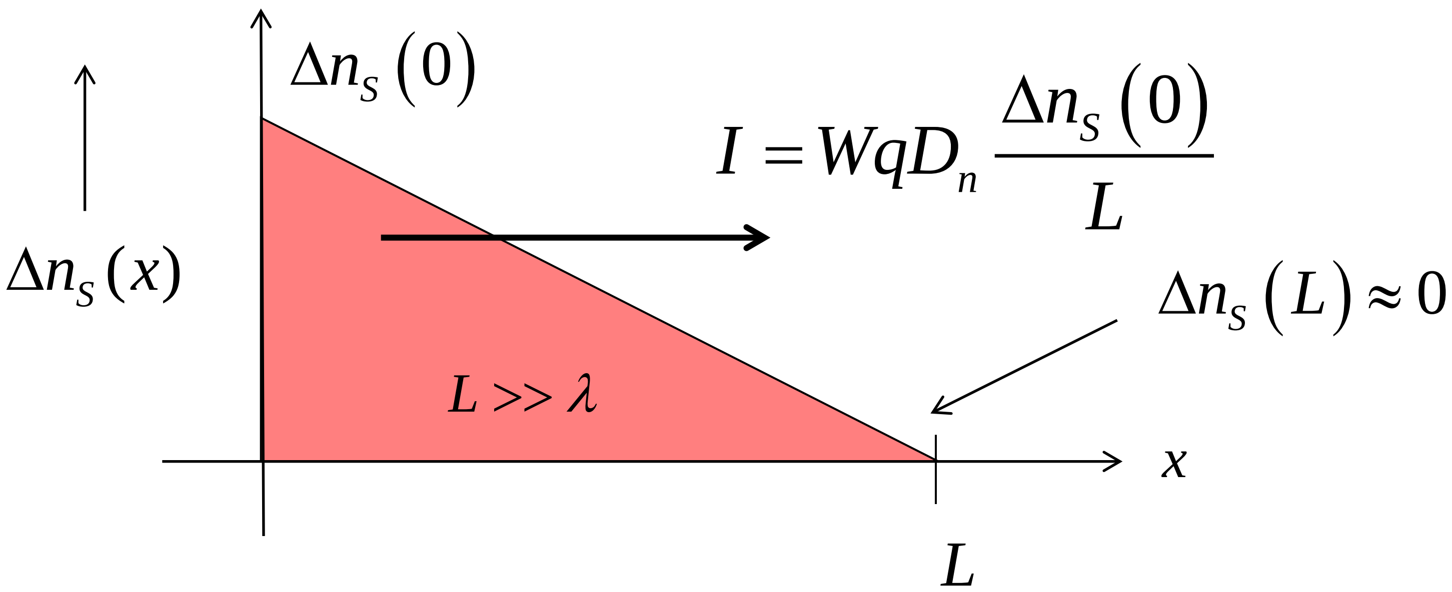
Assume a channel that is **much longer** than the mean-free-path for backscattering,

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

$$L >> \lambda \quad J = -qD_n \frac{dn_S}{dx} \ \text{A/cm} \quad \text{(2D)}$$

transit time

Inject from the left contact, and collect at the right contact.



$$\tau = \frac{qN}{I} = \frac{Wq\Delta n_S(0)L/2}{WqD_n\Delta n_S(0)/L} = \frac{L^2}{2D_n}$$

diffusive transport

$$\gamma_B = \frac{\hbar}{\tau_B} \qquad \gamma_D = \frac{\hbar}{\tau_D}$$

(ballistic) (diffusive)

$$\gamma_D = \frac{\hbar}{\tau_B}\frac{\tau_B}{\tau_D} = \frac{\tau_B}{\tau_D}\gamma_B$$

$$\gamma_D = \frac{\lambda}{L}\gamma_B << \gamma_B$$

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

$$\tau_B = \frac{L}{\langle \upsilon_x^+ \rangle} \qquad \tau_D = \frac{L^2}{2D_n}$$

$$D_n = \frac{\langle \upsilon_x^+ \rangle \lambda}{2}$$

$$M(E) \rightarrow T(E)M(E)$$

$$T(E) = \frac{\lambda(E)}{L} << 1$$

transmission

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

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.

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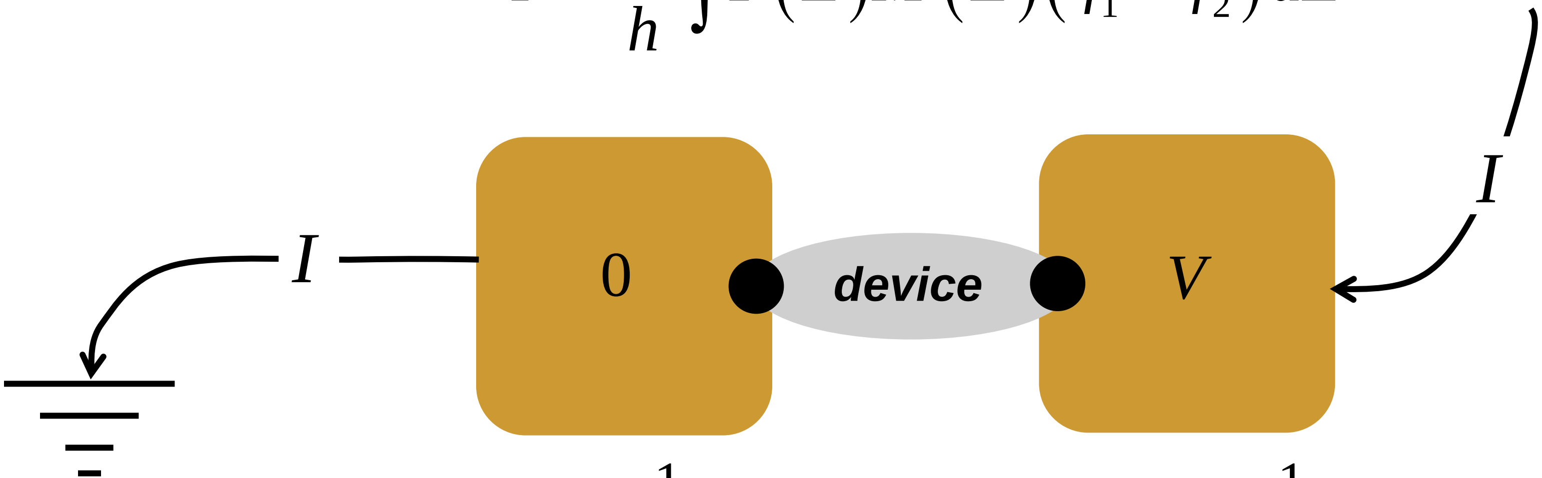
Landauer expression for current

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



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

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

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

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

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

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

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

(assume constant T_L)

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

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

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near-equilibrium, bulk transport

By "bulk" transport, we mean that the conductor is long enough so that contacts do not matter and transport is **diffusive.**

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

$$\gamma(E) = \frac{\hbar}{\tau} = \frac{\hbar}{L^2/2D_n} \quad D(E) = D_{2D}(E)WL \quad J_x = -I/W \quad (f_1 - f_2) \approx \left(-\frac{\partial f_0}{\partial E_F}\right)\Delta E_F$$

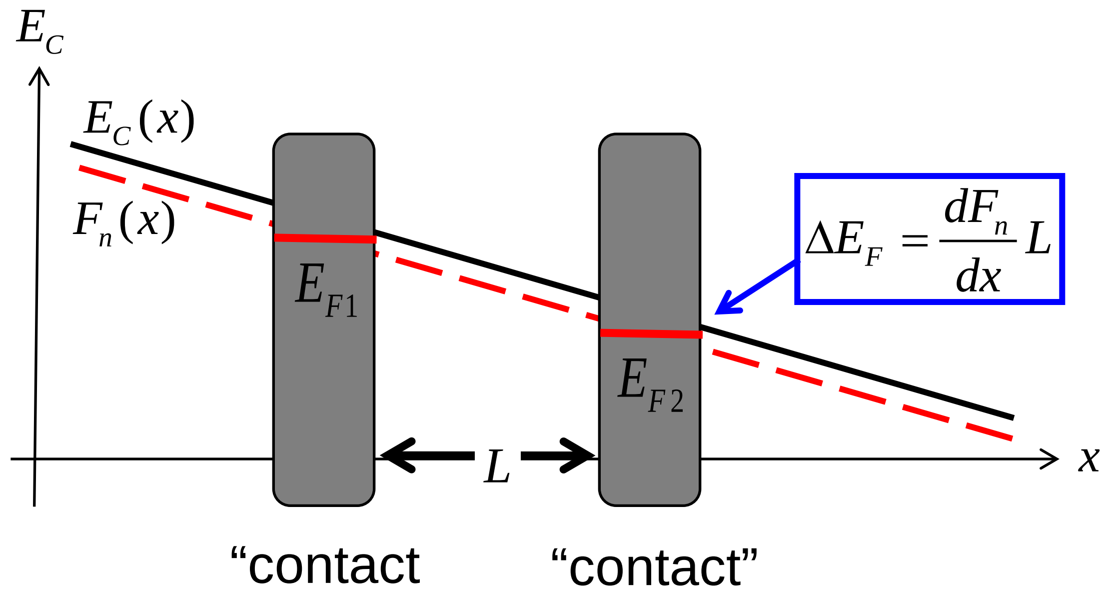
$$J_x = \left\{\int q D_n(E) D_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\right\}\frac{\Delta F_n}{L}$$

near-equilibrium, bulk transport

$$J_x = \sigma_n \frac{dF_n/q}{dx} \qquad \sigma_n = \int q^2 D_n(E) D_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$

Fundamental description of near-equilibrium transport.

F_n(x) is the *electrochemical potential* (or “quasi-Fermi level”) which we now regard as slowly varying across the sample.



the drift-diffusion equation

$$J_x = \sigma_n \frac{dF_n/q}{dx} \qquad \sigma_n = \int q^2 D_n(E) D_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$

conventional semiconductors:

$$n_S = N_{2D} e^{(F_n - E_C)/k_B T_L}$$

$$N_{2D} = \frac{m^* k_B T_L}{\pi \hbar^2}$$

$$F_n = E_C + k_B T_L \ln \frac{N_{2D}}{n_S}$$

$$\sigma_n = nq\mu_n$$

$\rightarrow$

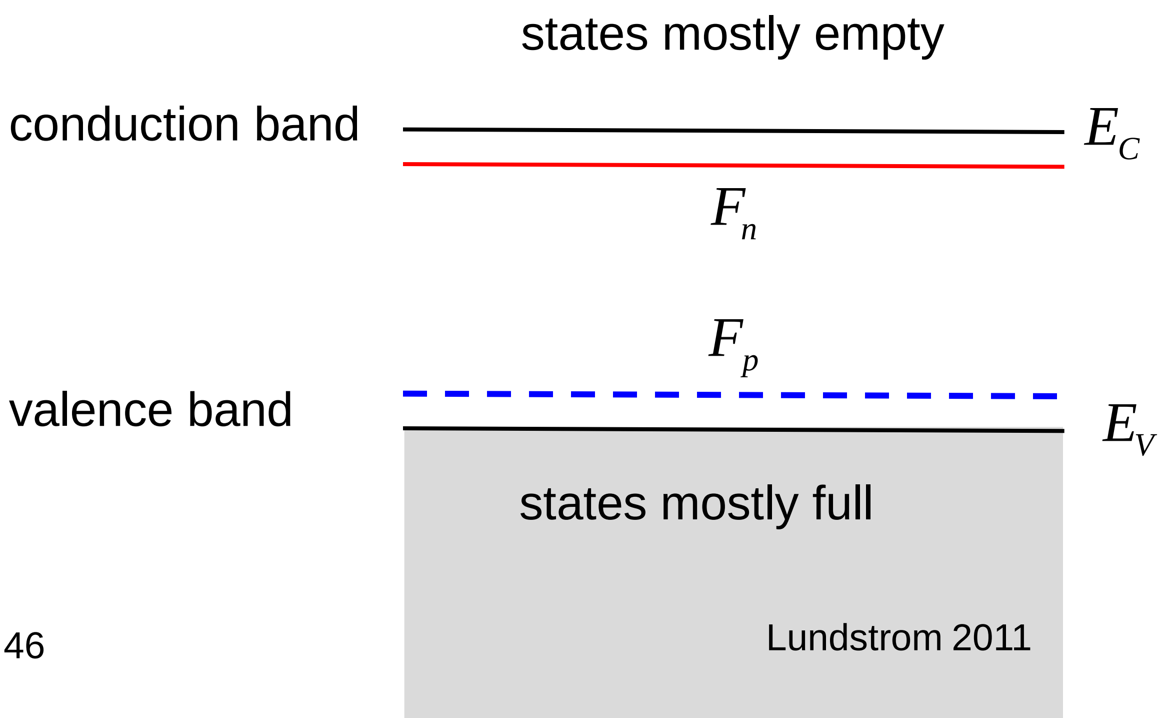
$$J_x = n_S q \mu_n \mathcal{E}_x + qD_n \frac{dn_S}{dx} \quad (A/m)$$

$$D_n = \frac{\upsilon_T \lambda_0}{2} \qquad \frac{D_n}{\mu_n} = \frac{k_B T_L}{q}$$

- near-equilibrium
- constant temperature
- MB statistics

what about holes?

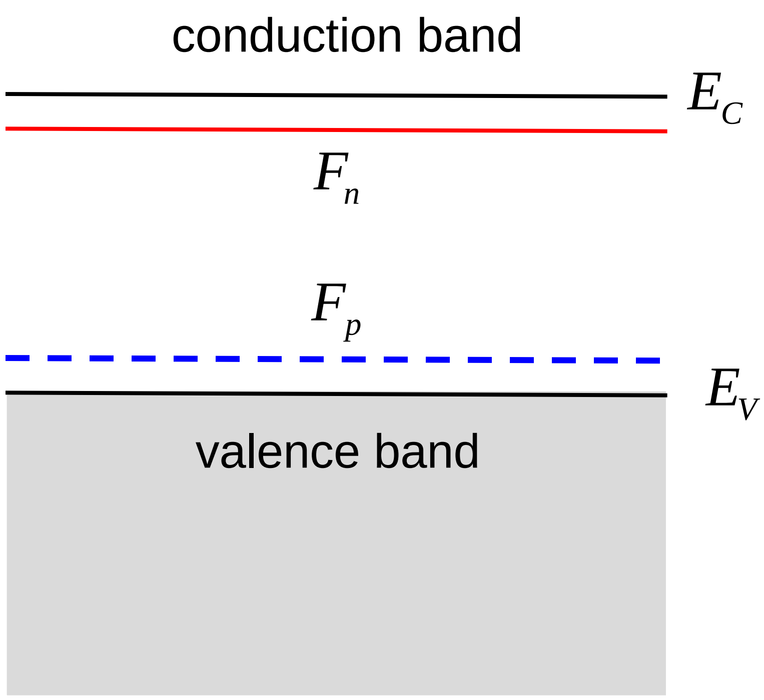
$$J_x = \sigma_n \frac{dF_n/q}{dx} \qquad \sigma_n = \int q^2 D_n(E) D_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$



Electrons in either band are in equilibrium with other electrons in that band but out of equilibrium with electrons in the other band.

So we need two QFL’s.

what about ~~holes~~?



All of these expressions refer to ***electrons*** in the conduction and valence bands

$$J_n = \sigma_n \frac{dF_n/q}{dx}$$

$$\sigma_n = \int q^2 D_n(E) D_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$

$$f_0(E) = \frac{1}{1 + e^{(E - F_n(x))/k_B T_L}}$$

$$J_p = \sigma_p \frac{dF_p/q}{dx}$$

$$\sigma_p = \int q^2 D_p(E) D_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$

$$f_0(E) = \frac{1}{1 + e^{(E - F_p(x))/k_B T_L}}$$

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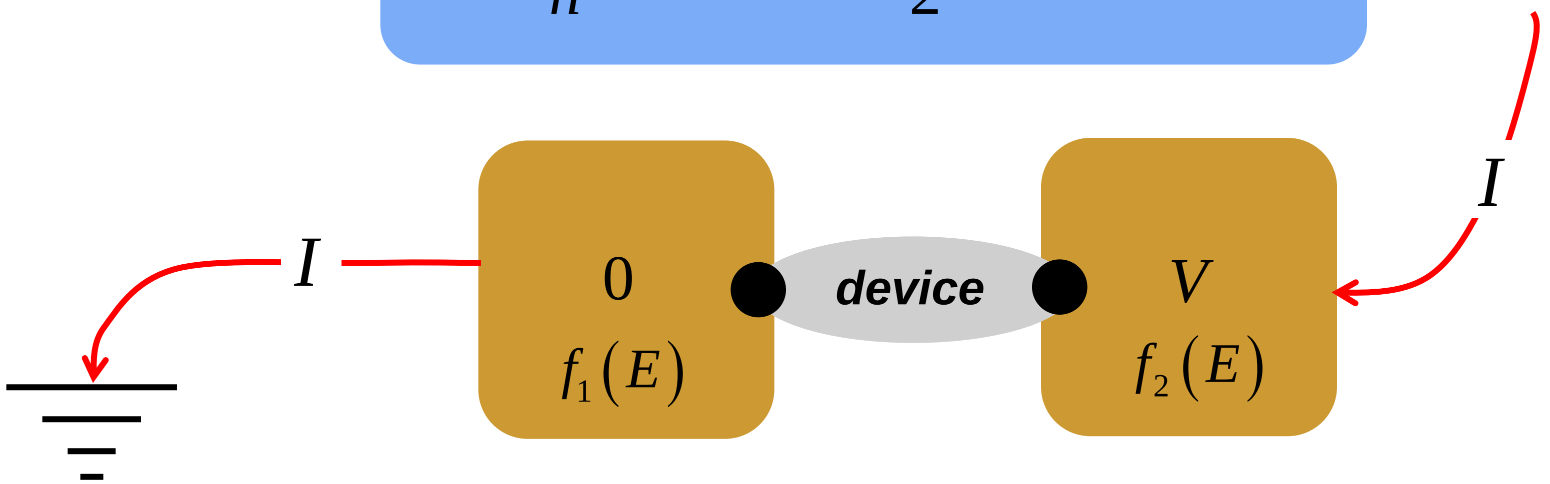
current flows when the Fermi-levels are different

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



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

near equilibrium

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

for small applied bias: $I = GV$

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

transport in the bulk

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

For long (diffusive) conductors near equilibrium:

$$J_x = \sigma_n \frac{dF_n/q}{dx} \qquad \sigma_n = \int q^2 D_n(E) D_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

outline

1) The model device
2) The mathematical model
3) Modes
4) Transmission
5) Near-equilibrium (linear) transport
6) Transport in the bulk
7) Summary
8) References

for more information

In this lecture, we have tried to present the general model as simply and clearly as possible. Now we are ready to use it to solve problems. But there is much more about the physics of transport that one can learn from simple models like this. For a concise introduction to fuamental concepts, see:

Supriyo Datta, *Lessons from Nanoelectronics: A New Approach to Transport Theory*, World Scientific Publishing Co., Singapore, 2011.

for even more information

Read Chapter 1 in *Quantum Transport: Atom to Transistor*, Supriyo Datta, Cambridge, 2005.

View Lectures 1-7 in ECE 495: *Fundamentals of Nanoelectronics*, Supriyo Datta, 2008.
http://nanohub.org/resources/5346

View: *Concepts of Quantum Transport*, Supriyo Datta, 2006.
http://nanohub.org/resources/2039

View: *Nanoelectronics and the Meaning of Resistance*, Supriyo Datta, 2008.
http://nanohub.org/resources/5279

View Lectures 1-4 in ECE 656: *Electronic Transport in Semiconductors*, Mark Lundstrom, 2009.
http://nanohub.org/resources/7281

questions

1) The model device
2) The mathematical model
3) Modes
4) Transmission
5) Near-equilibrium (linear) transport
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7) Summary
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