Near-equilibrium Transport:
Fundamentals and Applications

Lecture 6: An Introduction to Scattering

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outline

1) **Introduction**
2) Physics of carrier scattering
3) Transmission and mfp
4) MFP and scattering
5) Discussion
6) Summary

introduction

We have argued that there is a simple connection between the mean-free-path and transmission:

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

Where does this expression come from?

The mean-free-path is expected to be the "average distance" between scattering events:

$$\lambda(E) \propto \upsilon(E)\tau(E)$$

Exactly what is the relation, and what determines the time between collisions, τ?

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characteristic times

1) single particle lifetime, τ :

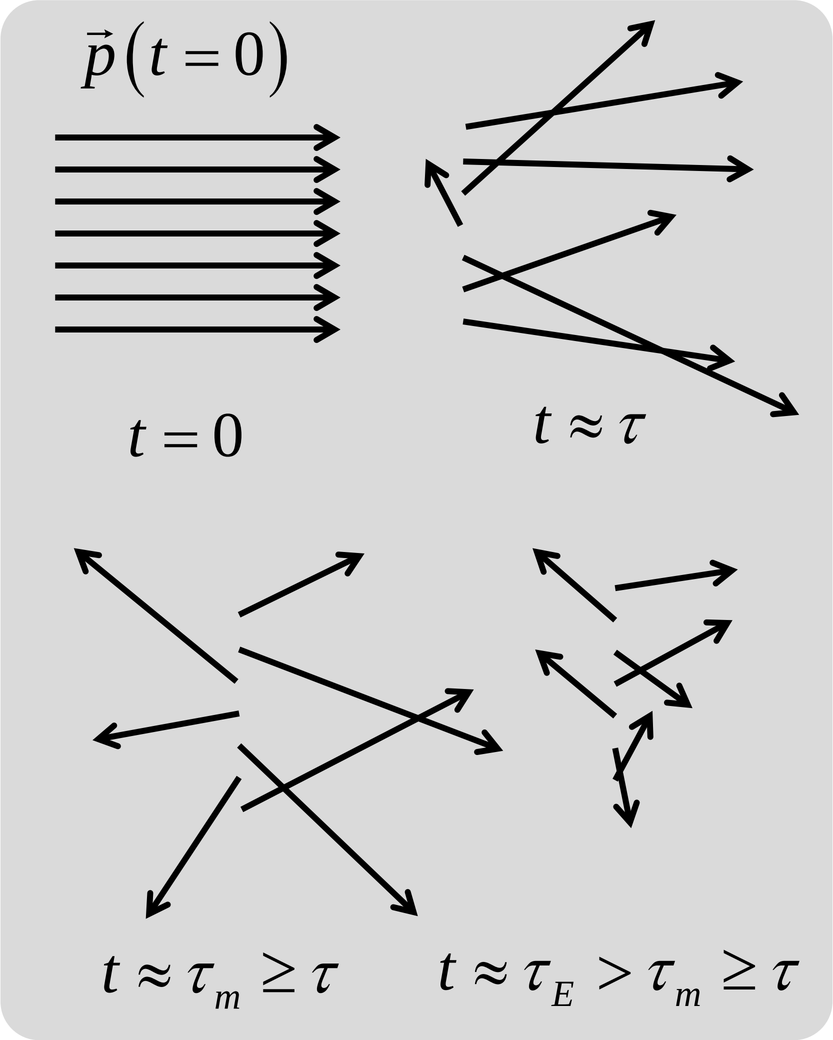
$$\tau(\vec{p})$$

2) momentum relaxation time, τ_m :

$$\tau_m(\vec{p})$$

3) energy relaxation time, τ_E :

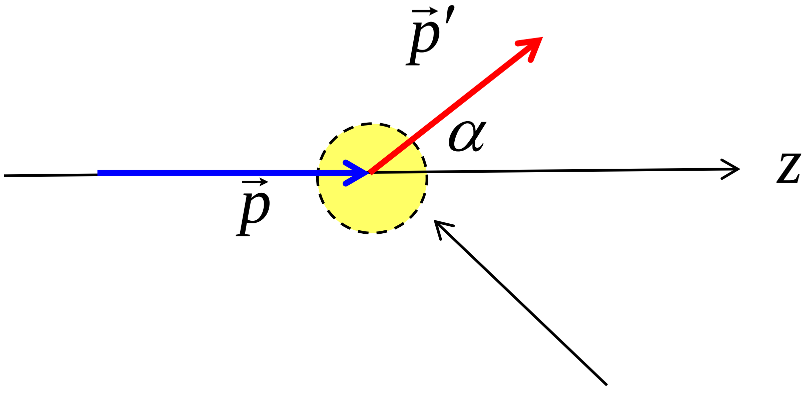
$$\tau_E(\vec{p})$$



transition rate

Transition rate from *p* to *p'* (probability per second)

$$S\left(\vec{p}, \vec{p}\,'\right)$$

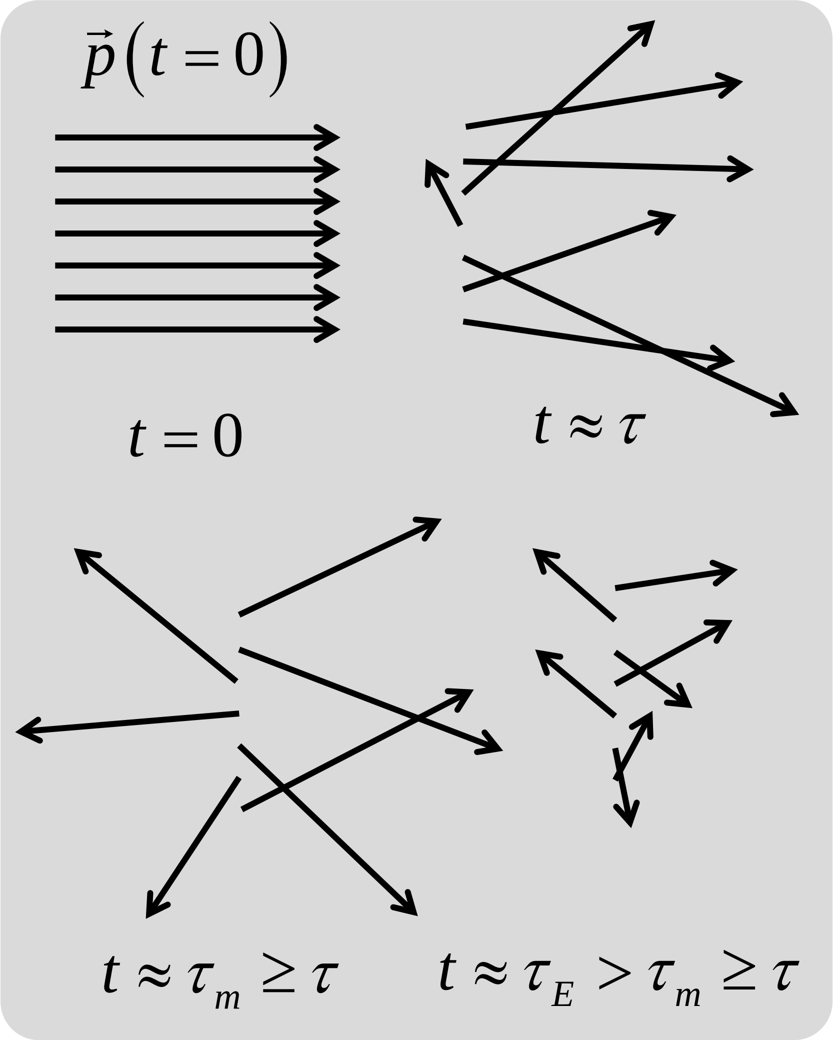


characteristic times

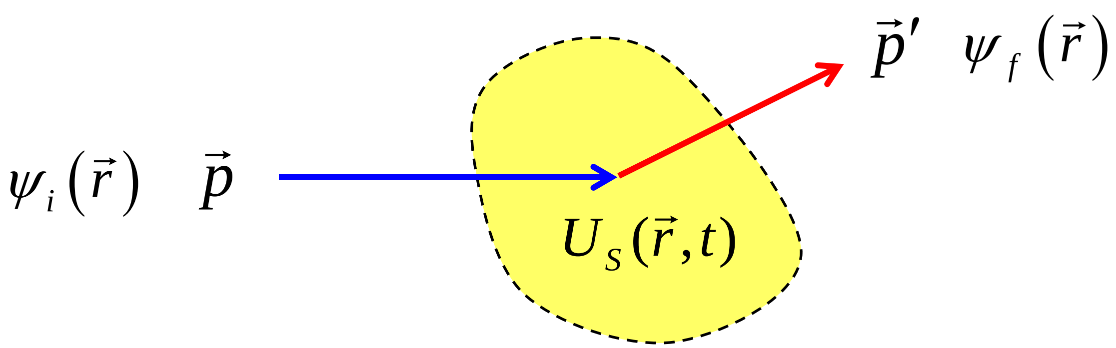
$$\frac{1}{\tau(\vec{p})} = \sum_{\vec{p}',\uparrow} S(\vec{p},\vec{p}')$$

$$\frac{1}{\tau_m(\vec{p})} = \sum_{\vec{p}',\uparrow} S(\vec{p},\vec{p}')\frac{\Delta p_z}{p_z}$$

$$\frac{1}{\tau_E(\vec{p})} = \sum_{\vec{p}',\uparrow} S(\vec{p},\vec{p}')\frac{\Delta E}{E_0}$$



Fermi's Golden Rule



$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|H_{p'p}\right|^2 \delta\left(E' - E - \Delta E\right)$$

$$H_{\vec{p}',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_S(\vec{r}) \psi_i \, d\vec{r}$$

$E' = E + \Delta E$ $\qquad$ $\Delta E = 0$ for a static U_S

$\Delta E = \pm\hbar\omega$ for an oscillating U_S

(See Sec.1.7 of Lundstrom for a derivation of FGR)

scattering

1) Identify the scattering potential (ionized impurity, lattice vibrations, surface roughness, etc.

2) Compute the transition rate from *p* to *p'*: $S(p \rightarrow p')$

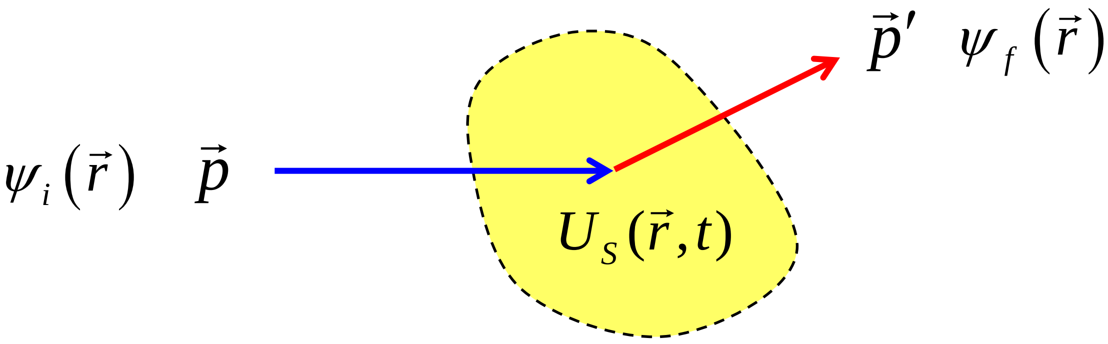
3) Compute the scattering time, and momentum relaxation time

$$1/\tau(\vec{p}) = 1/\tau_m(\vec{p})$$ for isotropic scattering

4) Compute the mean-free-path:

$$mfp = \upsilon(\vec{p})\tau_m(\vec{p})$$ **???**

scattering and DOS



The number of ways that an incident electron at energy, *E*, can scatter is expected to be proportional to the density of final states that conserve energy and momentum.

1) elastic scattering

$$\frac{1}{\tau(E)} \propto D_f(E)$$

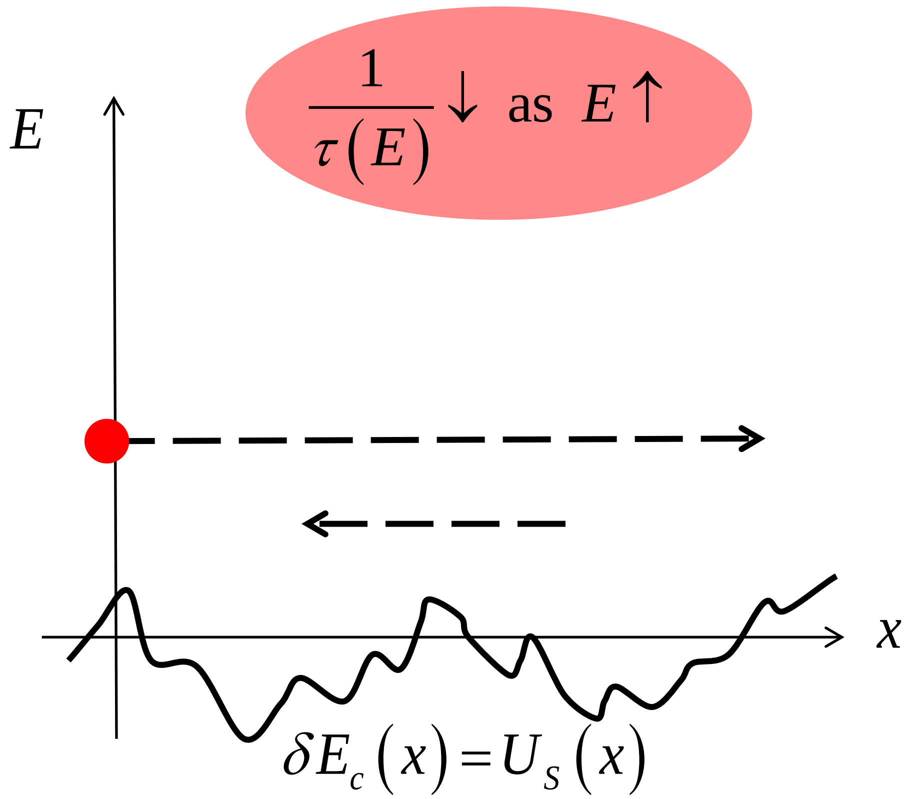
2) phonon absorption

$$\frac{1}{\tau(E)} \propto D_f(E+\hbar\omega)$$

3) phonon emission

$$\frac{1}{\tau(E)} \propto D_f(E-\hbar\omega)$$

II scattering



Random charges introduce random fluctuations in E_C, which act a scattering centers.

II scattering is anisotropic – it picks out final states with small angle deflections.

High energy electrons don't "see" these fluctuations and are not scattered as strongly.

“power law scattering”

For some common scattering mechanisms, the scattering time can be written as (or approximately as)

$$\tau(E) = \tau_0 \left(\frac{E - E_c}{k_B T_L} \right)^s$$

Where “*s*” is a characteristic exponent that describes the particular scattering mechanism. For example, in 3D,

s = -1/2 for acoustic phonon scattering
s = +3/2 for ionized impurity scattering

transmission and mean-free-path

- Transmission is a key parameter in the Landauer approach.

- Transmission is related to the mean-free-path *for back-scattering*.

- The mfp for backscattering is related to the microscopic scattering processes.

Questions:

1) Why is $T(E) = \lambda(E)/(\lambda(E)+L)$?

2) How is $\lambda(E)$ related to $S(p, p')$?

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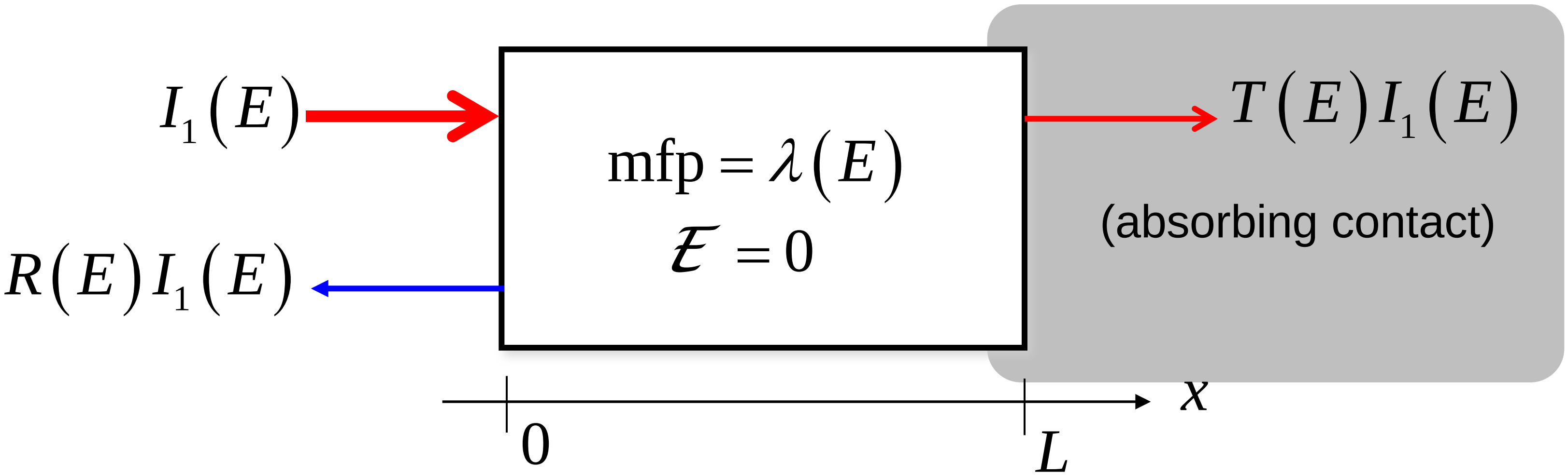
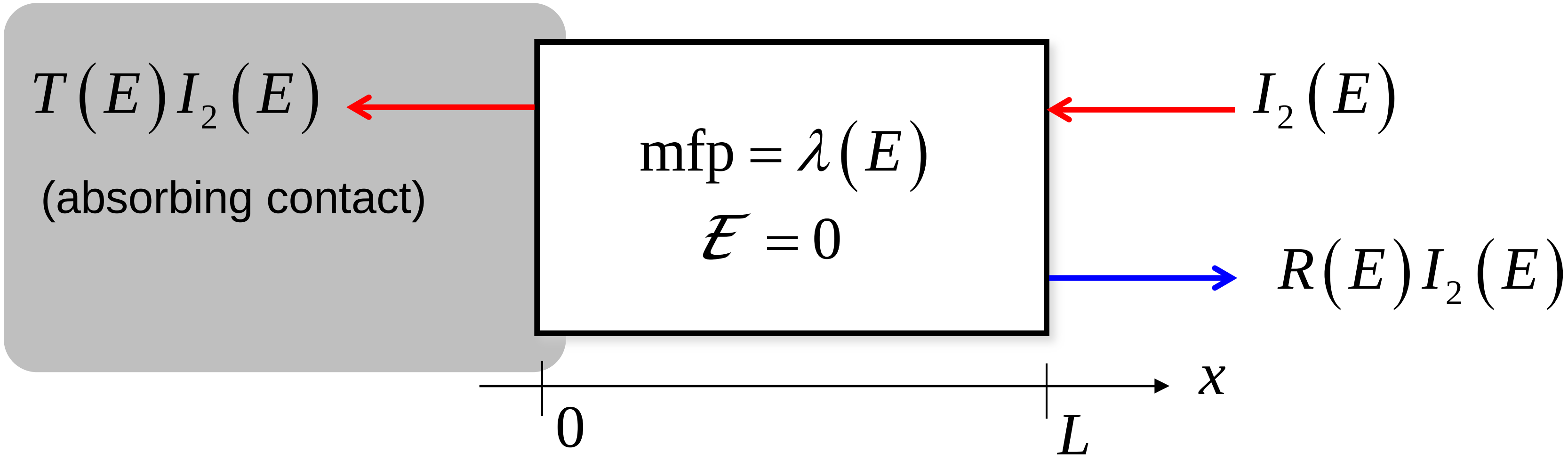
transmission across a field-free slab



Consider a flux of carriers injected from the left into a field-free slab of length, *L*. The flux that emerges at $x = L$ is *T* times the incident flux, where $0 < T < 1$. The flux that emerges from $x = 0$ is *R* times the incident flux, where $T + R = 1$, assuming no carrier recombination-generation.

How is *T* related to the mean-free-path for backscattering within the slab?

injection from the right

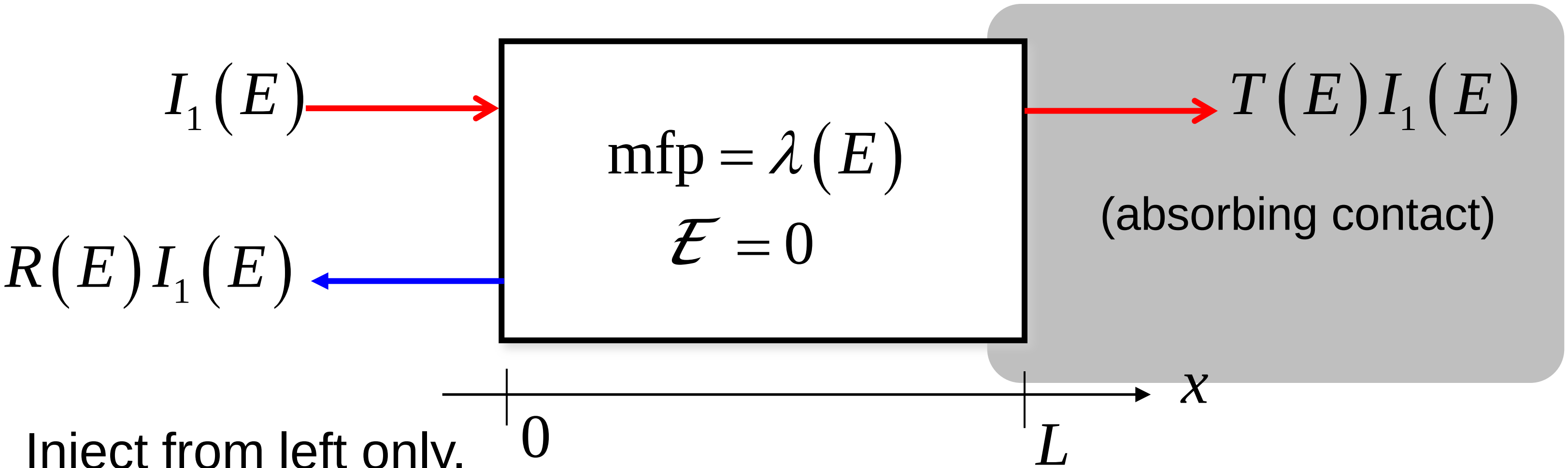


In general, there *could* be injection from both the left and the right contacts.

For elastic scattering: $T_{12}(E) = T_{21}(E) = T(E)$

Near equilibrium: $T_{12}(E) \approx T_{21}(E) \approx T(E)$ (no built-in fields)

problem specification

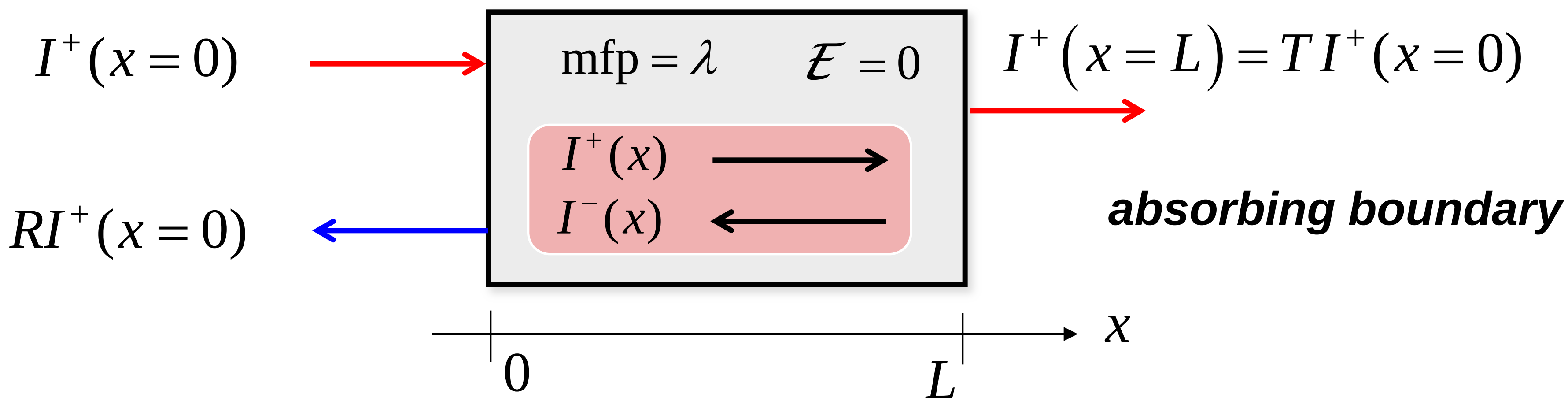


1) Inject from left only.

2) Ignore "vertical transport" (elastic scattering or near-equilibrium), so $T_{12}(E) = T_{21}(E) = T(E)$.

Then relate *T* to the mean-free-path for backscattering within the slab. (No assumption about whether the slab length, *L*, is long or short compared to the mfp, but we **do assume** that the mean-free-path is not position-dependent.)

transmission



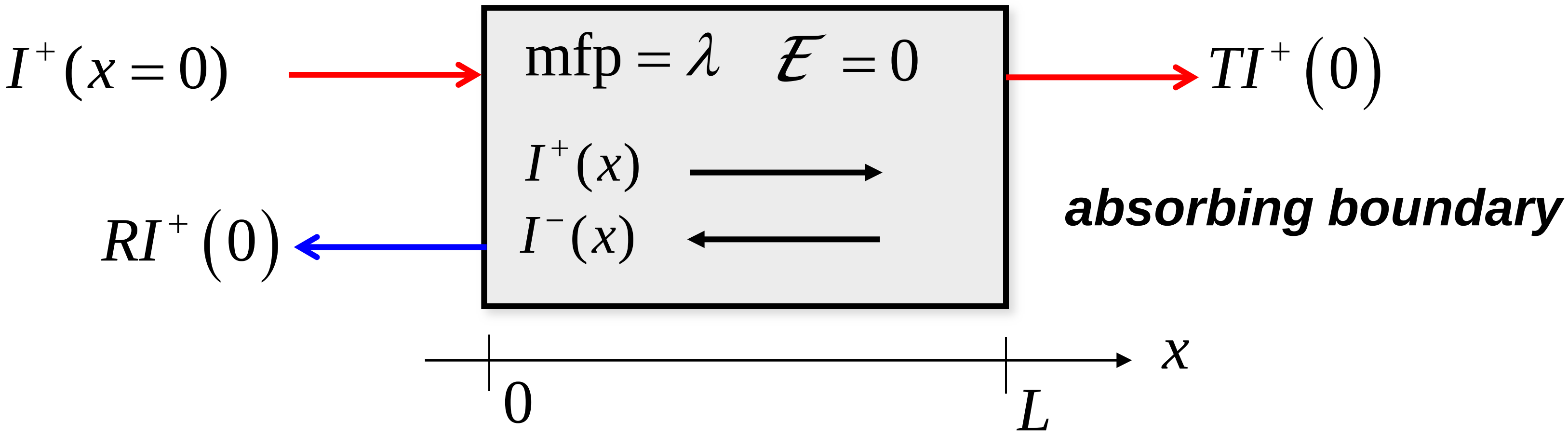
$$\frac{dI^+(x)}{dx} = -\frac{I^+(x)}{\lambda} + \frac{I^-(x)}{\lambda}$$

$$I = I^+(x) - I^-(x) \quad \text{(constant)}$$

$$I^-(x) = I^+(x) - I$$

$$\frac{dI^+(x)}{dx} = -\frac{I}{\lambda} =$$

transmission (ii)

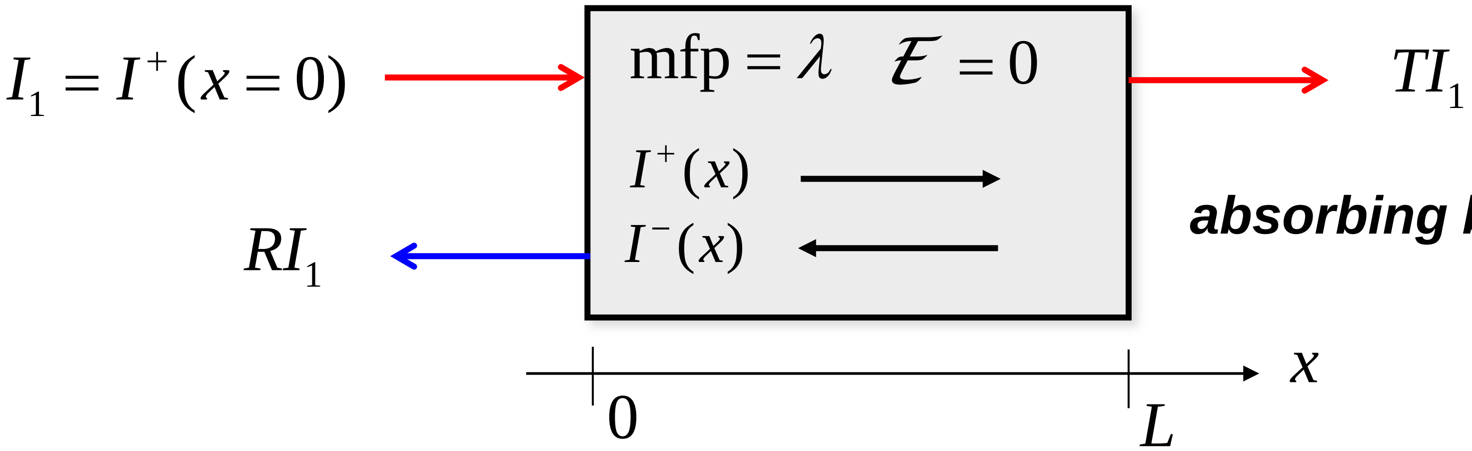


$$\frac{dI^+(x)}{dx} = -\frac{I}{\lambda}$$

$$\int_{I^+(0)}^{I^+(x)} dI^+ = -\frac{I}{\lambda}\int_0^x dx'$$

$$I^+(x) = I^+(0) - I\,\frac{x}{\lambda}$$

transmission (iii)



absorbing boundary

$$I^+(x) = I^+(0) - I\frac{x}{\lambda}$$

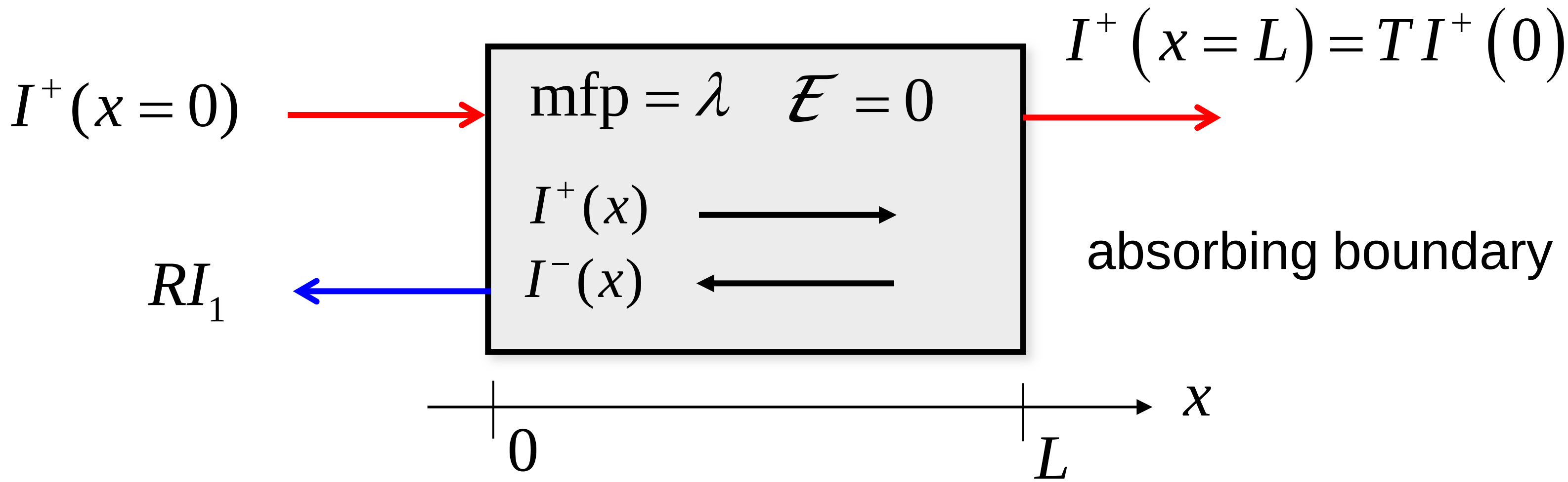
$$I^+(x) = I^+(0) + \left(I^+(x) - I^-(x)\right)\frac{x}{\lambda}$$

$$I^+(L) = I^+(0) + \left(I^+(L) - I^-(L)\right)\frac{L}{\lambda}$$

$$I^-(L) = 0$$

$$I^+(L) = I^+(0) + I^+(L)\frac{L}{\lambda}$$

transmission (iv)



$$I^+(L) = I^+(0) - I^+(L)\frac{L}{\lambda}$$

$$I^+(L) = \frac{I^+(0)}{1 + L/\lambda}$$

$$\frac{I^+(L)}{I^+(0)} = T = \frac{\lambda}{\lambda + L}$$

$$T(E) = \frac{\lambda(E)}{\lambda(E) + L} \qquad T(E) + R(E) = 1$$

$$T \rightarrow 0 \quad L >> \lambda$$

$$T \rightarrow 1 \quad L << \lambda$$

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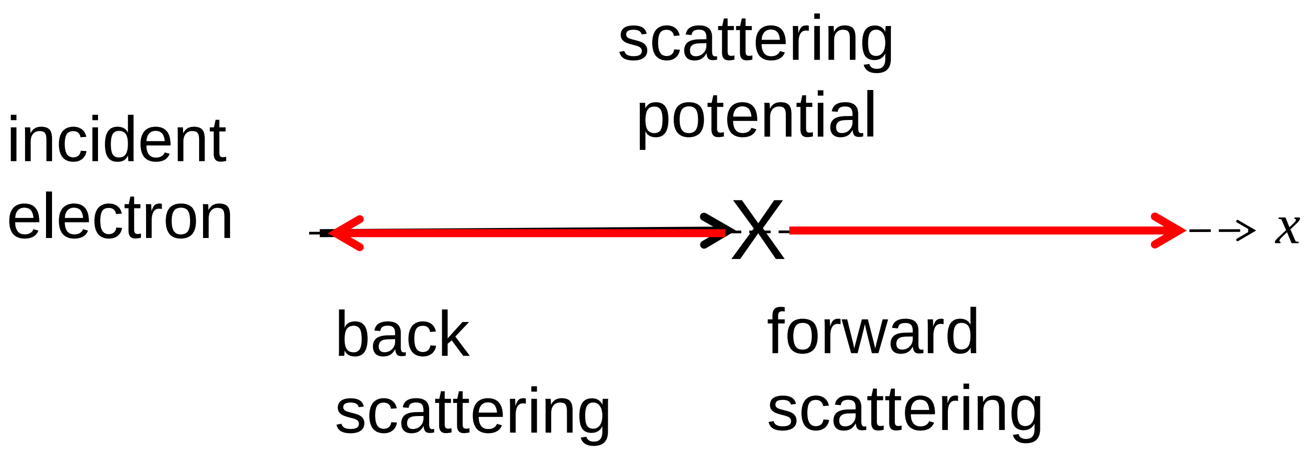
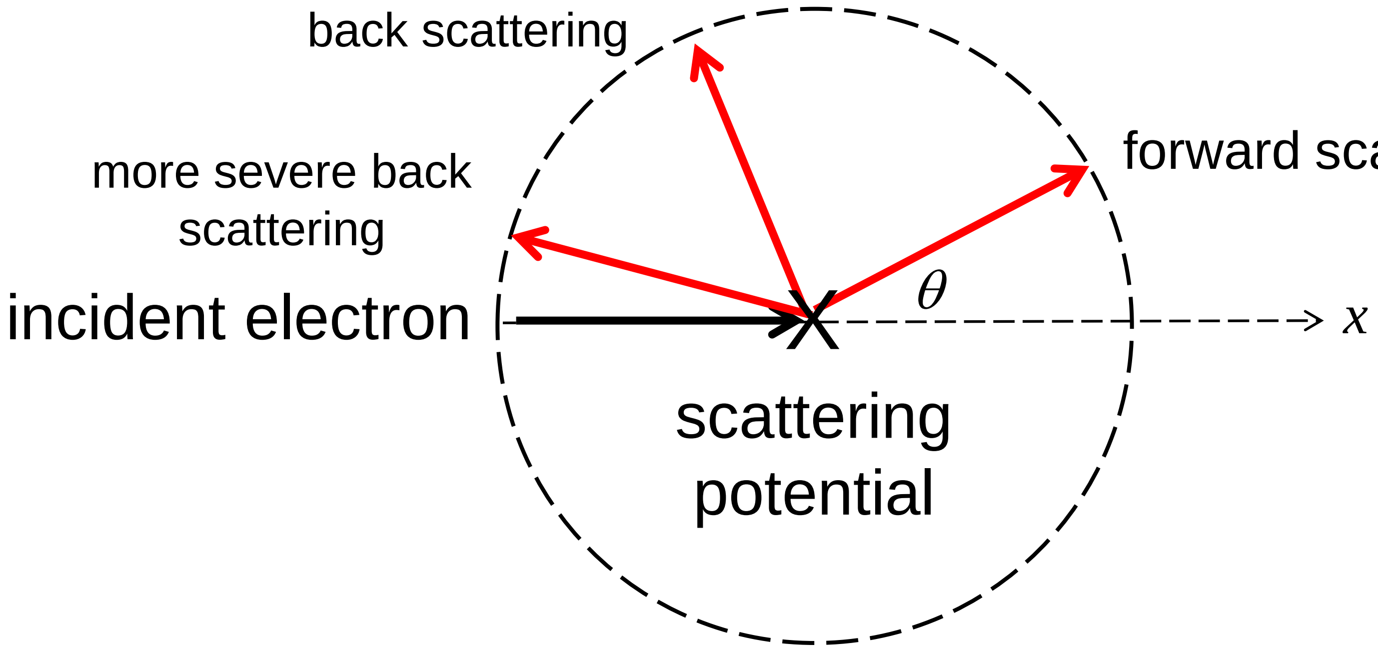
backscattering in 1D



If we assume that the scattering is ***isotropic*** (equal probability of scattering forward or back) then average time between backscattering events is 2|.

$$\lambda(E) = 2\upsilon(E)\tau_m(E)$$

backscattering in 2D



If we assume that the scattering is ***isotropic***:

$$\lambda(E) = \frac{\pi}{2}\upsilon(E)\tau_m(E)$$

mean-free-path for backscattering

$$\lambda(E) \equiv 2\frac{\langle \upsilon_x^2 \tau_m \rangle}{\langle |\upsilon_x| \rangle}$$

This is an average over angle at a specific energy, *E.*

$$\lambda(E) = 2\upsilon(E)\tau_m(E) \quad \text{1D}$$

$$\lambda(E) = \frac{\pi}{2}\upsilon(E)\tau_m(E) \quad \text{2D}$$

$$\lambda(E) = \frac{4}{3}\upsilon(E)\tau_m(E) \quad \text{3D}$$

ECE-656 Lecture 17. http://nanohub.org/resources/7281.

Changwook Jeong, et al. "On Landauer vs. Boltzmann and Full Band vs. Effective Mass Evaluation of Thermoelectric Trans-port Coefficients," *J. Appl. Phys*., **107**, 023707, 2010.

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discussion

i) estimating the mfp from measurements

ii) relating the mfp to the diffusion coefficient

iii) relating the mfp to the mobility

iv) average mfp for power law scattering

v) exercise: mfp for a Si MOSFET

i) estimating the mfp from measurements

Consider a 2D diffusive conductor

$$G_{2D} = \sigma_s \frac{W}{L}$$

Recall that the sheet conductance is given by:

$$\sigma_S = \frac{2q^2}{h} \int M_{2D}\left(E\right) \lambda\left(E\right) \left(-\frac{\partial f_0}{\partial E}\right) dE$$

Having measured σ_S, how can we estimate the average mfp?

average mfp

$$\sigma_S = \frac{2q^2}{h}\int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$ expression for sheet conductance

$$\sigma_S = \frac{2q^2}{h}\frac{\int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}\int M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$\langle M_{2D}\rangle \equiv \int M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$\langle\langle \lambda \rangle\rangle \equiv \frac{\int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

$$\sigma_S = \frac{2q^2}{h}\langle\langle \lambda(E) \rangle\rangle \langle M_{2D}\rangle$$

for 2D parabolic bands….

(single subband)

$$\left\langle M_{2D} \right\rangle = \int M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right) dE \qquad M_{2D}(E) = g_V \frac{\sqrt{2m^*(E-E_c)}}{\pi\hbar}$$

$$\left\langle M_{2D} \right\rangle = \frac{\sqrt{\pi}}{2} M_{2D}(k_B T_L)\mathcal{F}_{-1/2}(\eta_F) \qquad \eta_F = (E_F - E_c)/k_B T_L$$

$$n_S = \int D_{2D} f_0(E) dE \qquad D_{2D} = g_V \frac{m^*}{\pi\hbar^2}$$

$$n_S = g_v \frac{m^* k_B T}{\pi\hbar^2}\mathcal{F}_0(\eta_F) \qquad \mathcal{F}_0(\eta_F) = \ln\left(1+e^{\eta_F}\right)$$

the procedure….

1) Measure sheet conductance

$$\sigma_S = \frac{2q^2}{h}\left\langle\left\langle \lambda(E)\right\rangle\right\rangle\left\langle M_{2D}\right\rangle$$

2) Deduce average mfp

$$\left\langle\left\langle \lambda(E)\right\rangle\right\rangle = \frac{\sigma_S}{\left(2q^2/h\right)\left\langle M_{2D}\right\rangle} = \frac{\sigma_S}{\left(2q^2/h\right)M_{2D}\left(k_B T_L\right)}\frac{1}{\left(\sqrt{\pi}/2\right)\mathcal{F}_{-1/2}\left(\eta_F\right)}$$

3) Deduce η_F from the measured carrier density.

$$n_S = \frac{m^* k_B T}{\pi\hbar^2}\mathcal{F}_0\left(\eta_F\right)$$

the procedure….for a non-degenerate semiconductor

$$\langle\langle\lambda(E)\rangle\rangle = \frac{2(k_B T_L/q)}{q\upsilon_T}\left(\frac{\sigma_S}{n_S}\right) \qquad \upsilon_T = \sqrt{2k_B T_L/\pi m^*}$$

Key point: need to measure two quantities:

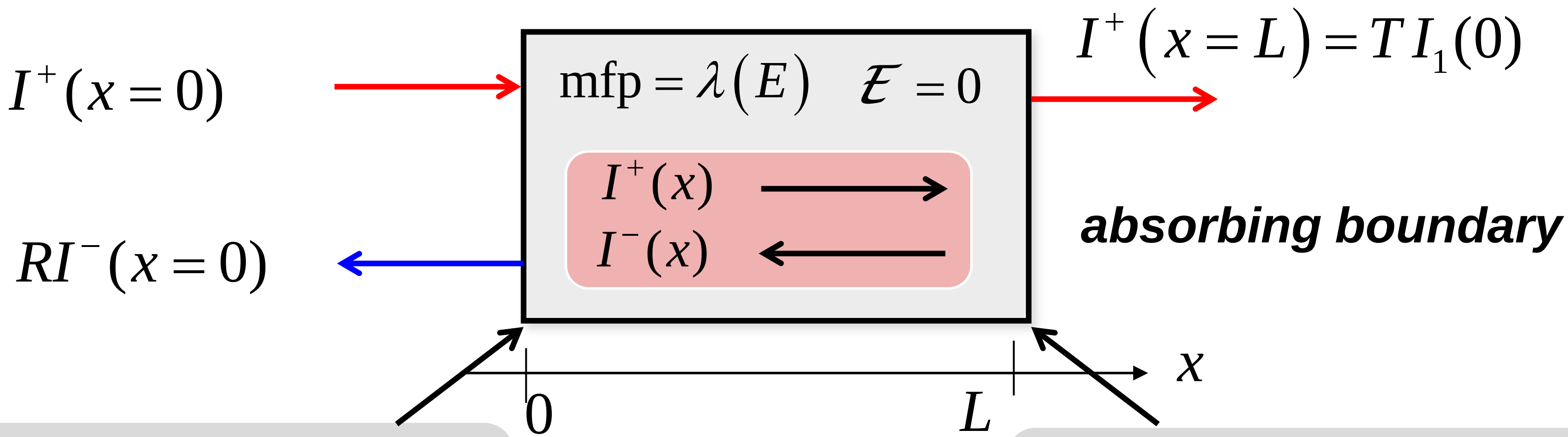
1) sheet conductance
2) sheet carrier density

$$\langle\langle\lambda(E)\rangle\rangle = \frac{2(k_B T_L/q)}{q\upsilon_T}\left(\frac{n_S q \mu_n}{n_S}\right)$$

$$\mu_n = \frac{\upsilon_T \langle\langle\lambda(E)\rangle\rangle/2}{(k_B T_L/q)}$$

$$D_n = \frac{\upsilon_T \langle\langle\lambda(E)\rangle\rangle}{2}$$

ii) mfp and diffusion coefficient



$$n^+(0) = I^+(0)\big/\langle \upsilon_x^+ \rangle$$

$$n^-(0) = I^-(0)\big/\langle \upsilon_x^+ \rangle$$

$$n(0) = (1+R)\,I^+(0)\big/\langle \upsilon_x^+ \rangle$$

$$n(0) = (2-T)\,I^+(0)\big/\langle \upsilon_x^+ \rangle$$

$$n^+(L) = I^+(L)\big/\langle \upsilon_x^+ \rangle$$

$$n^-(0) = 0$$

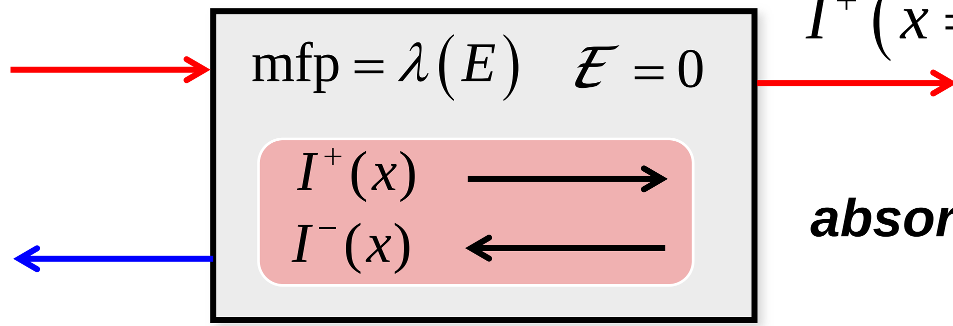
$$n(L) = I^+(L)\big/\langle \upsilon_x^+ \rangle$$

$$n(L) = TI^+(0)\big/\langle \upsilon_x^+ \rangle$$

carrier densities

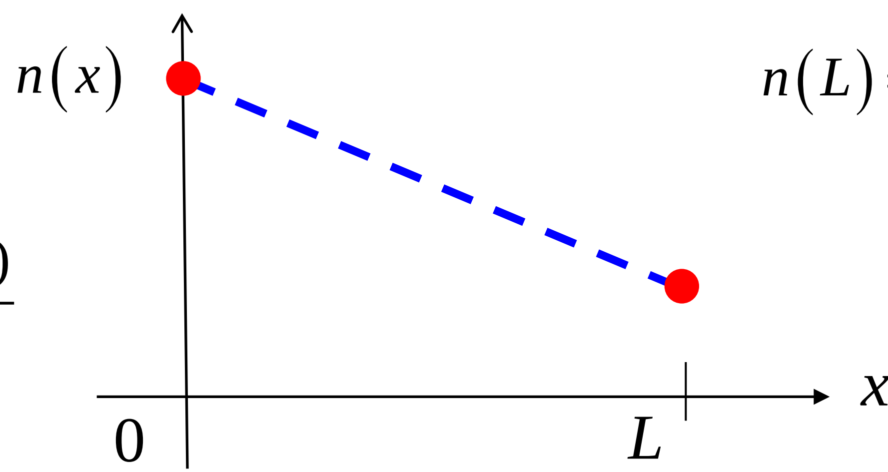
$$I^{+}(x=0)$$

$$RI^{-}(x=0)$$



$$I^{+}(x=L) = T I_1(0)$$

absorbing boundary



$$n(L) = \frac{TI^{+}(0)}{\langle \upsilon_x^{+} \rangle}$$

$$n(0) = \frac{(2-T)I^{+}(0)}{\langle \upsilon_x^{+} \rangle}$$

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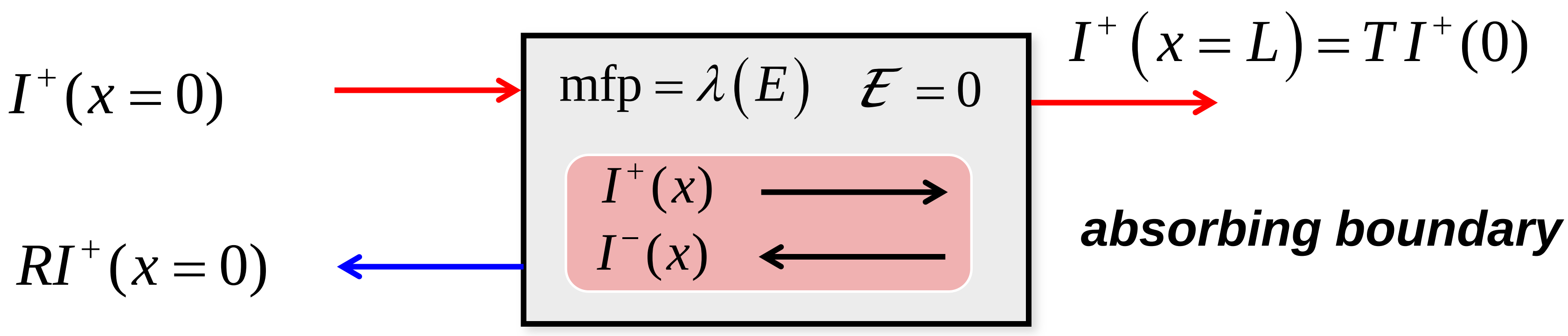
carrier densities



$$n(0) = \frac{(2-T)I^+(0)}{\langle \upsilon_x^+ \rangle}$$

$$n(L) = \frac{TI^+(0)}{\langle \upsilon_x^+ \rangle}$$

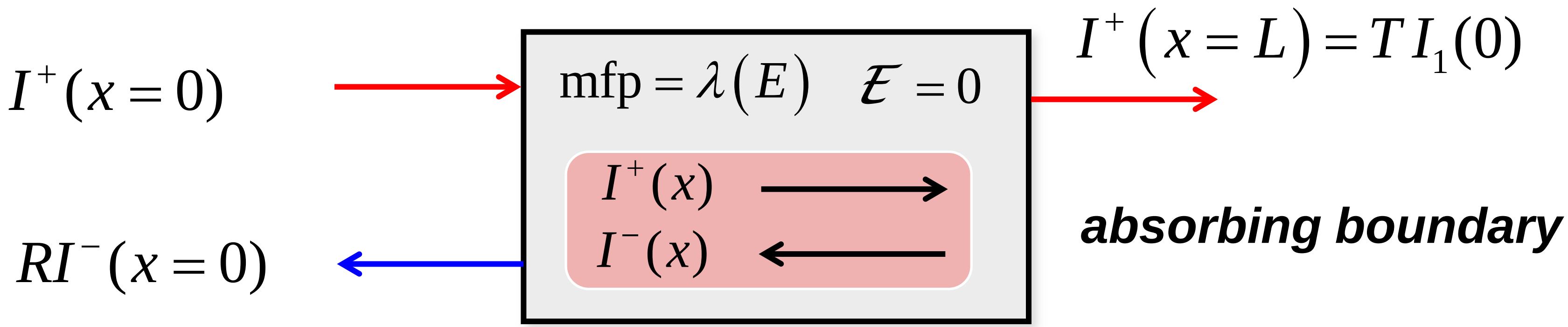
$$n(0) - n(L) = \frac{(2-T)I^+(0)}{\langle \upsilon_x^+ \rangle} - \frac{TI^+(0)}{\langle \upsilon_x^+ \rangle}$$

$$n(0) - n(L) = \frac{I^+(0)}{\langle \upsilon_x^+ \rangle} 2(1-T)$$

$$I = TI^+(0)$$

$$I = \frac{\langle \upsilon_x^+ \rangle}{2} \frac{TL}{1-T} \times \left[\frac{n(0)-n(L)}{L} \right]$$

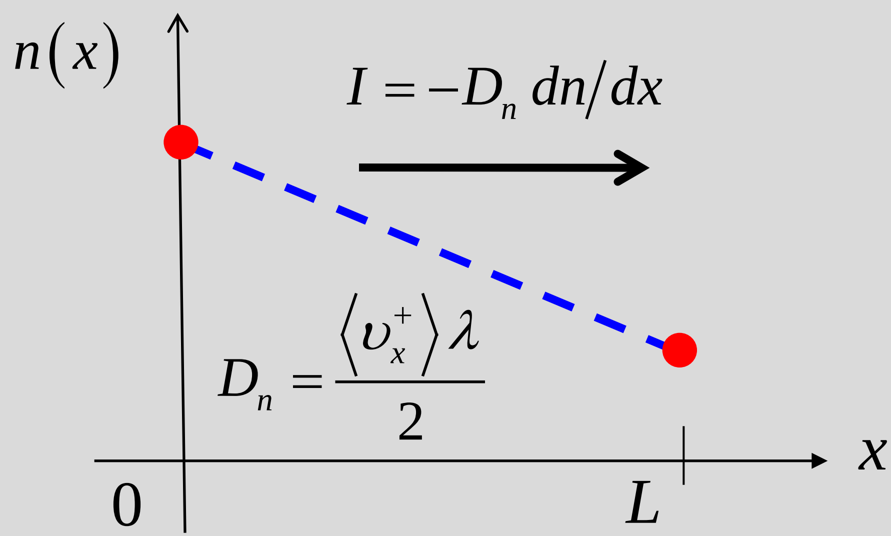
Fick's Law



$$I = \frac{\langle \upsilon_x^+ \rangle}{2} \frac{TL}{1-T} \times \left[\frac{n(0) - n(L)}{L} \right]$$

$$I = -D_n \frac{dn}{dx} \qquad D_n = \frac{\langle \upsilon_x^+ \rangle}{2} \frac{TL}{1-T}$$

$$T = \frac{\lambda}{\lambda + L}$$



diffusion coefficient

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

The average <•> is an average over angle at a given energy, *E*.

In 1D: $\langle \upsilon_x^+(E)\rangle = \upsilon(E)$

$$D_n(E) = \frac{\upsilon(E)\left[2\upsilon(E)\tau(E)\right]}{2} = \upsilon^2(E)\tau(E)$$

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

$$D_n(E) = \frac{\frac{2}{\pi}\upsilon(E)\left[\frac{\pi}{2}\upsilon(E)\tau(E)\right]}{2} = \frac{\upsilon^2(E)\tau(E)}{2}$$

In 3D: $\langle \upsilon_x^+(E)\rangle = \frac{1}{2}\upsilon(E)$

$$D_n(E) = \frac{\frac{1}{2}\upsilon(E)\left[\frac{4}{3}\upsilon(E)\tau(E)\right]}{2} = \frac{\upsilon^2(E)\tau(E)}{3}$$

iii) mobility

Frequently, we are given the measured mobility, not the measured sheet conductance. To estimate the average mfp, we must relate the mobility to the average mfp.

To measure the mobility, write the conductance as

$$G_{ch} = n_S q \mu_n \frac{W}{L}$$

We obtain the mobility from the two measured quantities, n_S and G_{CH}

$$\mu_n = \frac{L}{W} \frac{G_{ch}}{q n_S}$$

From the measured mobility, we can estimate the average mfp as follows.

mobility

The 2D conductance (in the diffusive limit) is given by the Landauer expression:

$$G_{ch} = \left[\frac{2q^2}{h} \int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right) dE \right] \frac{W}{L}$$

We can also write the 2D conductance as:

$$G_{ch} = n_S q \mu_n \frac{W}{L}$$

Equating the two expressions gives a formula for the mobility…

definition of mobility

$$G_{ch} = \left[\frac{2q^2}{h} \int M_{2D}(E) \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \right] \frac{W}{L} = n_S q \mu_n \frac{W}{L}$$

So the mobility is given by:

$$\mu_n = \frac{\frac{2q}{h} \int M_{2D}(E) \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) dE}{n_S}$$

How do we now relate this to the average mfp?

average mfp

$$\mu_n = \frac{1}{n_S}\frac{2q}{h}\int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

expression for mobility

$$\mu_n = \frac{1}{n_S}\frac{2q}{h}\frac{\int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}\int M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$\langle M_{2D}\rangle \equiv \int M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$\mu_n = \frac{1}{n_S}\frac{2q}{h}\langle\langle\lambda\rangle\rangle\langle M_{2D}\rangle$$

$$\langle\langle\lambda\rangle\rangle \equiv \frac{\int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

mfp from mobility

$$\mu_n = \frac{1}{n_S}\frac{2q}{h}\langle\langle\lambda\rangle\rangle\langle M_{2D}\rangle$$

$$\langle M_{2D}\rangle = \frac{g_V m^*}{2\hbar}\upsilon_T \mathcal{F}_{-1/2}(\eta_F)$$

$$n_S = \frac{m^* k_B T_L}{\pi\hbar^2}\mathcal{F}_0(\eta_F)$$

$$\eta_F = (E_F - E_c)/k_B T_L$$

$$\upsilon_T = \sqrt{2k_B T_L/\pi m^*}$$

$$\langle\langle\lambda\rangle\rangle = \frac{2(k_B T_L/q)\mu_n}{\upsilon_T}\frac{\mathcal{F}_0(\eta_F)}{\mathcal{F}_{-1/2}(\eta_F)}$$

$$\langle\langle\lambda\rangle\rangle = \frac{2(k_B T_L/q)\mu_n}{\upsilon_T}$$ (non-degenerate)

$$D_n = \frac{\upsilon_T\langle\langle\lambda\rangle\rangle}{2} \qquad \frac{D_n}{\mu_n} = \frac{k_B T}{q}$$

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iv) average mfp for power law scattering

$$\lambda(E) = \lambda_0 \left(\frac{E - E_c}{k_B T_L} \right)^r$$

$$\langle\langle \lambda \rangle\rangle = \frac{\int \lambda(E) M_{2D}(E) \left(-\frac{\partial f_0}{\partial E} \right) dE}{\int M_{2D}(E) \left(-\frac{\partial f_0}{\partial E} \right) dE}$$

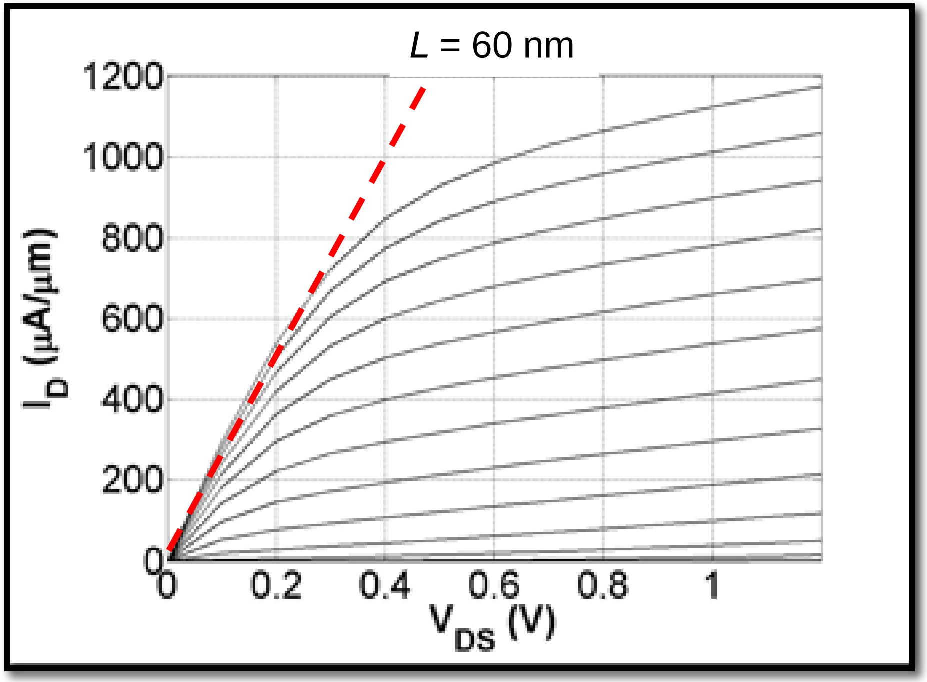
$$\langle\langle \lambda \rangle\rangle = \lambda_0 \frac{\Gamma(r + 3/2)}{\Gamma(3/2)} \frac{\mathcal{F}_{r-1/2}(\eta_F)}{\mathcal{F}_{1/2}(\eta_F)}$$

$$\langle\langle \lambda \rangle\rangle = \lambda_0 \frac{\Gamma(r + 3/2)}{\Gamma(3/2)}$$ (non-degenerate)

v) exercise: mfp in a Si N-MOSFET

2007 N-MOSFET

(unstrained Si technology)



(Courtesy, Shuji Ikeda, ATDF, Dec. 2007)

What is the mfp at high gate voltage?

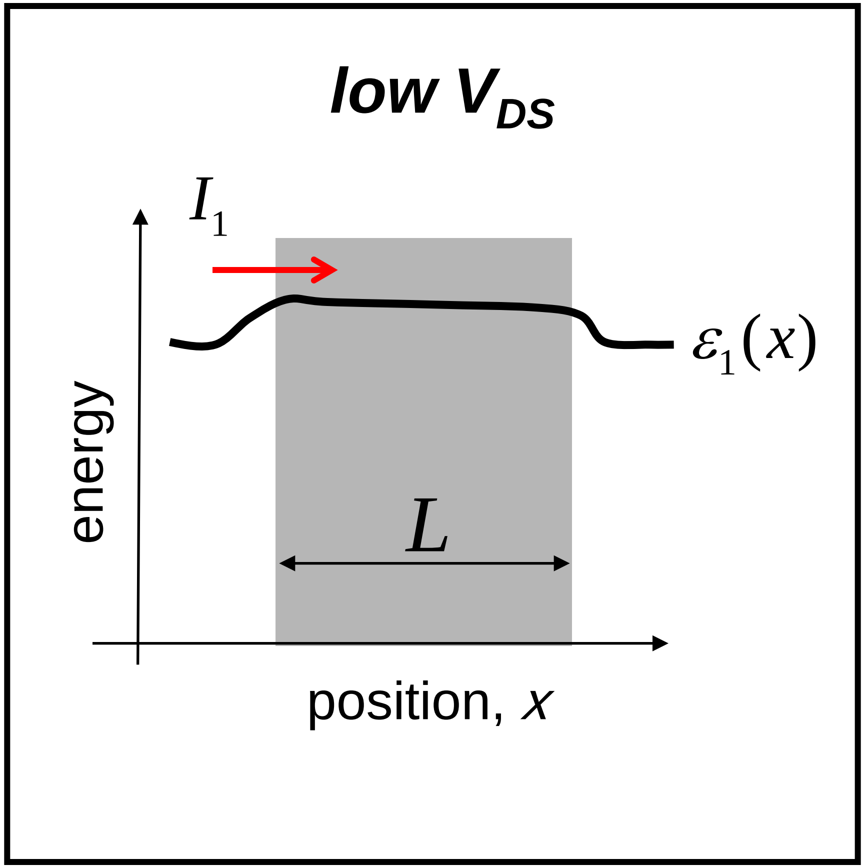
$$\mu_n\left(V_G = 1.2V\right) = 260 \text{ cm}^2/\text{V-s}$$

(measured for long channels)

$$n_S\left(V_G = 1.2V\right) = 7.9\times10^{12} \text{ cm}^{-2}$$

C. Jeong, et al., *IEEE Trans. Electron Dev.*, **56**, pp. 2762-2769, 2009.

example



$$\mu_n \approx 260 \text{ cm}^2/\text{V-s}$$

$$\langle\langle\lambda\rangle\rangle = \frac{2(k_B T_L/q)\mu_n}{\upsilon_T}\frac{\mathcal{F}_0(\eta_F)}{\mathcal{F}_{-1/2}(\eta_F)}$$

$$n_S \approx 7.9\times10^{12} \text{ cm}^{-2}$$

$$n_S = g_V \frac{m^* k_B T}{\pi\hbar^2}\ln\left(1+e^{\eta_F}\right) \text{ cm}^{-2}$$

$$\langle\langle\lambda\rangle\rangle \approx 7 \text{ nm} \approx 0.12L$$

outline

1) Physics of scattering

2) Transmission and mfp

3) MFP and scattering

4) Diffusion coefficient and MFP

5) Estimating mfp experimentally

6) Summary

summary

1) Transmission is related to the mean-free path for backscattering.

2) The mean-free-path for backscattering is longer than the mfp.

3) The mfp for backscattering can be related to microscopic scattering processes.

4) The mfp for backscattering can be estimated from the mobility.

questions

1) Physics of scattering

2) Transmission and mfp

3) MFP and scattering

4) Diffusion coefficient and MFP

5) Estimating mfp experimentally

6) Summary