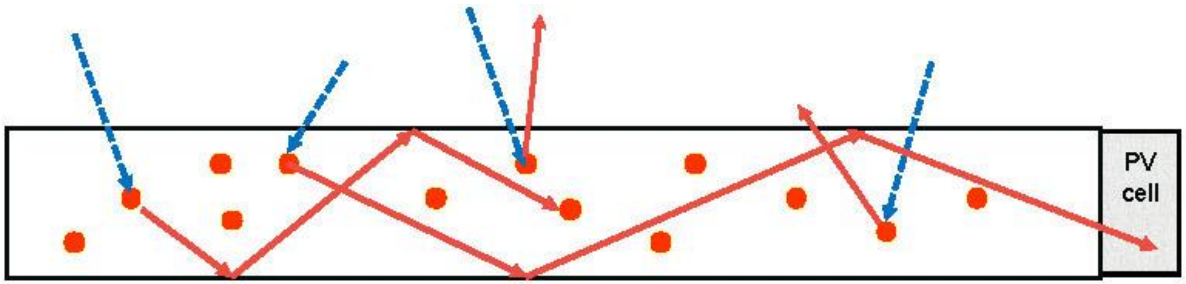
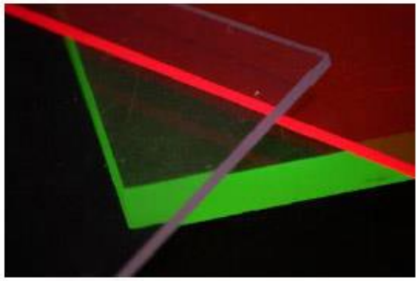
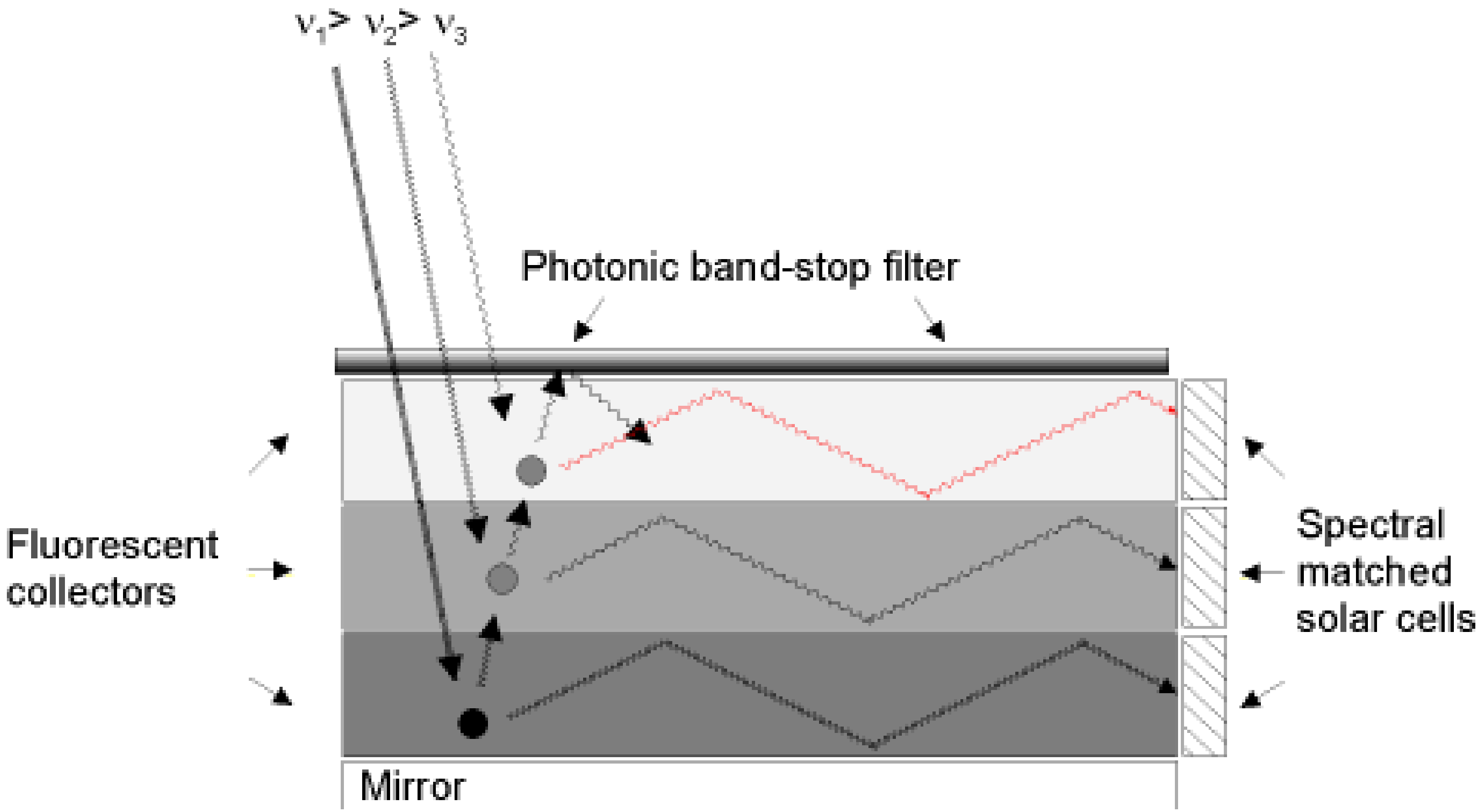
Cool concept of the week

Fluorescent concentrators

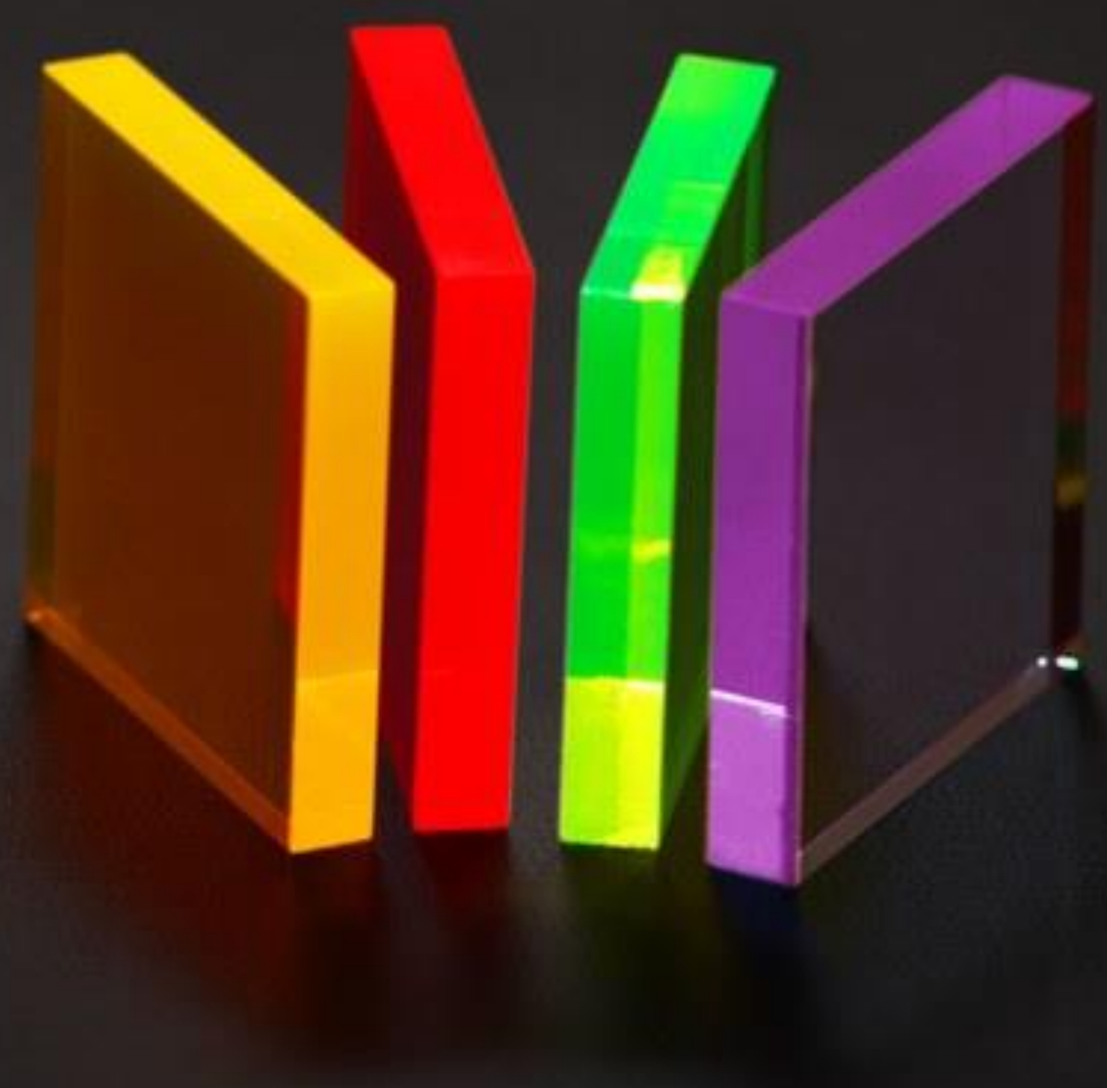




Fluorescent concentrators



Goldschmidt FhG ISE



FhG ISE

UNIK 4450/9450 – Schedule

- 30/8 Solar cell fundamentals
- 6/9 Solar cell efficiency
- 13/9 Semiconductor theory
- 20/9 Generation
- 27/9 Recombination and lifetime
- 4/10 Silicon
- 11/10 Junctions
- 18/10 Solar cells
- 25/10 Silicon solar cells I (@IFE)
- 1/11 Silicon solar cells II
- 8/11 Light management
- 15/11 Alternative solar cells
- 29/11 Solar modules & systems
- 6/12 Q&A

- Oral exam (Week 50)

Generation

Agenda

1. Where are we?
2. Formulation of the transport problem
3. Generation and recombination – fundamentals
4. Absorption – the macroscopic view
5. Absorption – the microscopic view

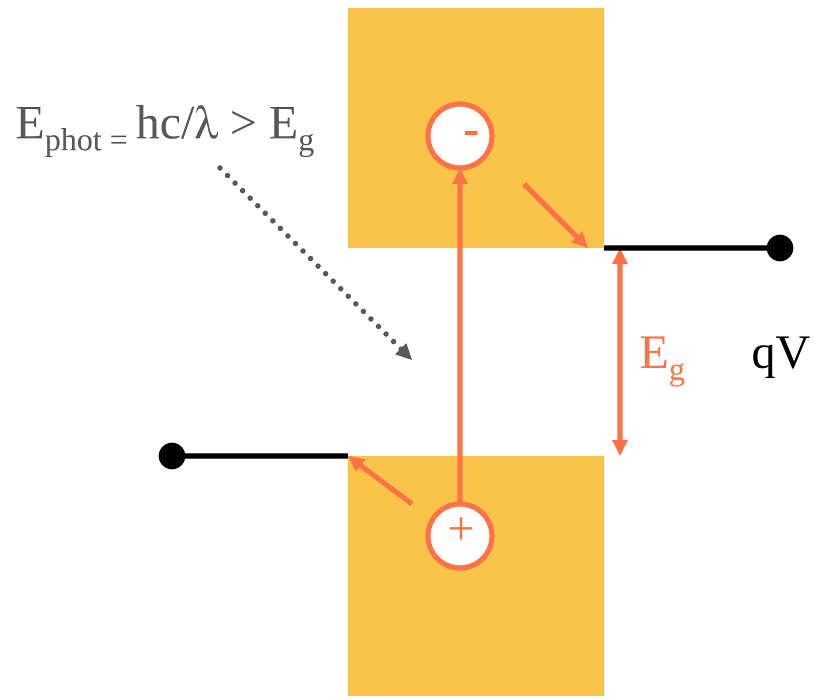
Where are we?

Main principle – solar cell operation

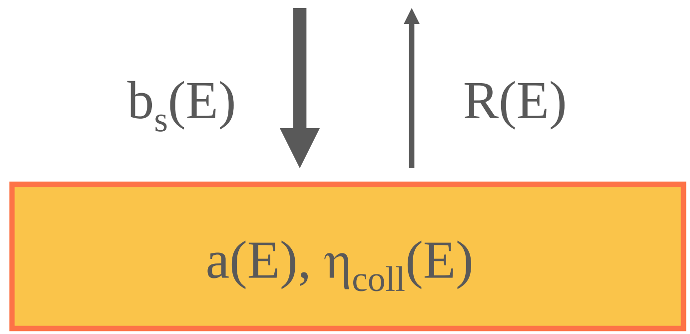
- The **short circuit current density** is directly proportional to the number of absorbed/generated and successfully collected charge carriers
  - Generation is the main topic of this lecture

- A junction is responsible for supplying a driving force for the photocurrent in a solar cell

- We want to be able to collect as many excited h^+ and e^- as possible while maintaining as big a voltage difference as possible between the contacts

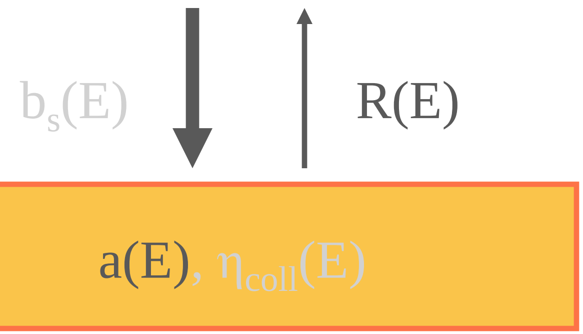


Photogenerated current



$$I_{SC}(E) = q \cdot A \cdot ([1 - R(E)] \cdot \eta_{coll}(E) \cdot a(E) \cdot b_s(E))$$

Today



$$I_{SC}(E) = q \cdot A \cdot ([1 - R(E)] \cdot \eta_{coll}(E) \cdot a(E) \cdot b_s(E))$$

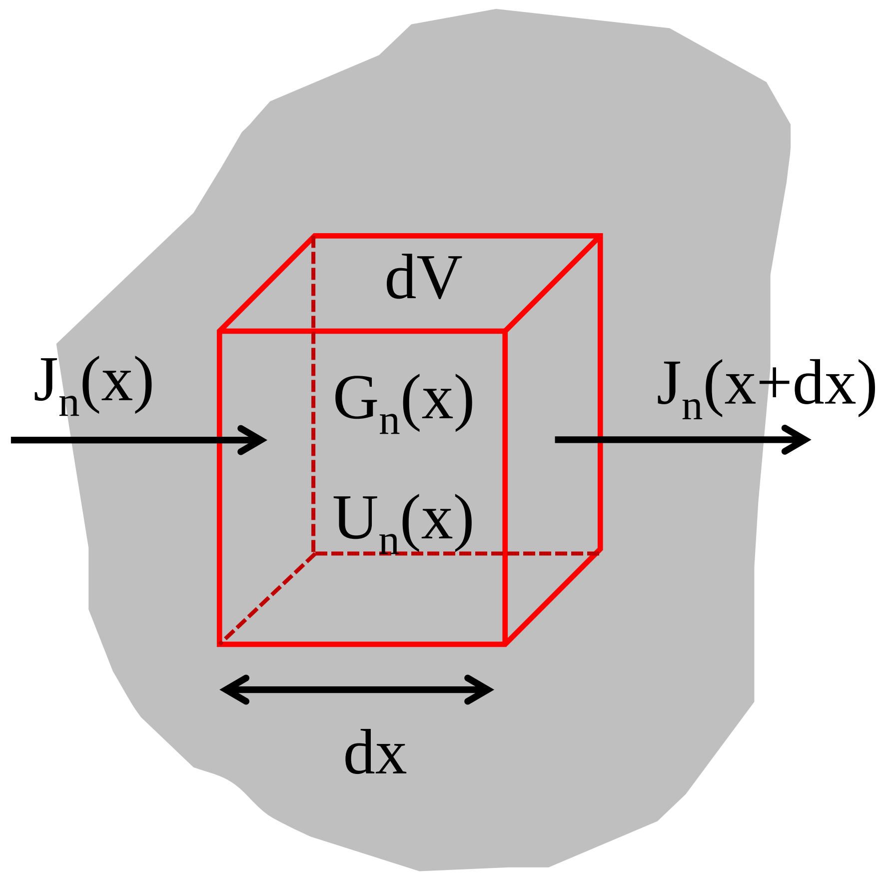
Nomenclature

- $G_n(x)$ generation rate of electrons
- $U_n(x)$ recombination rate of electrons

- $G_p(x)$ generation rate of holes
- $U_p(x)$ recombination rate of holes

Formulation of the transport problem

Transport in semiconductors



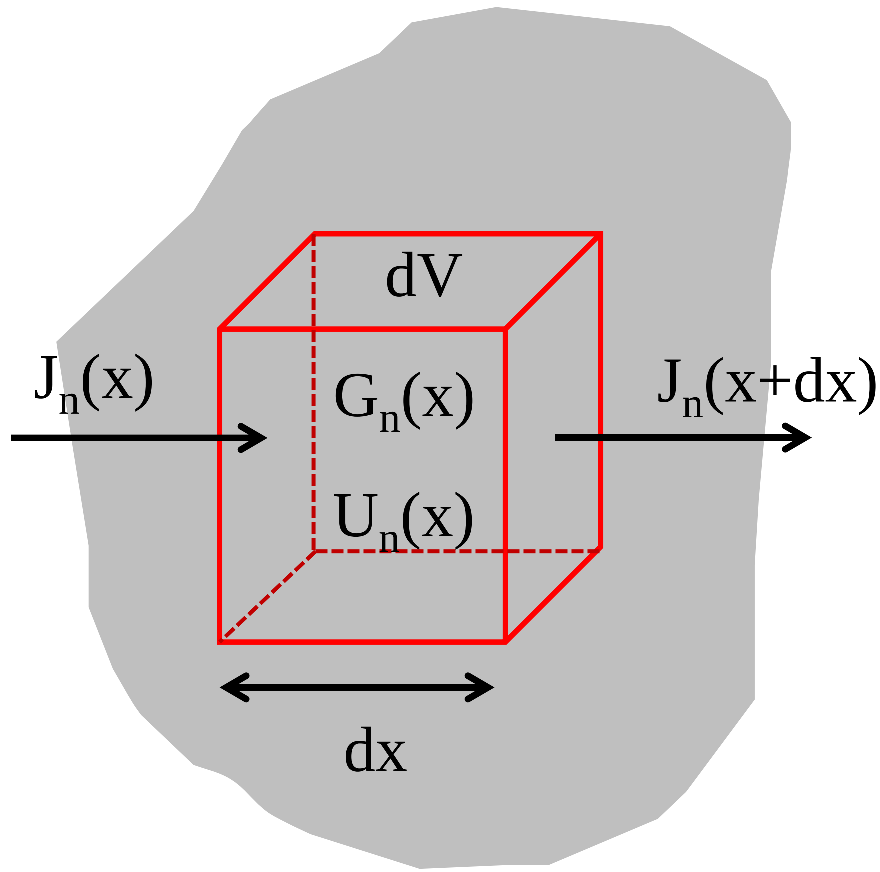
$$\delta n/\delta t = 1/q \cdot \delta/\delta x(J_n(x)) + G_n(x) - U_n(x)$$

Transport in semiconductors

- Solar cell device operation:

  1. The number of charge carriers must be conserved

  2. The electrostatic potential $\varphi(x)$ obeys Poisson's equation



Formulation of the transport problem

$$\delta n/\delta t = 1/q \cdot \delta/\delta x(J_n(x)) + G_n(x) - U_n(x)$$

$$\delta p/\delta t = 1/q \cdot \delta/\delta x(J_p(x)) + G_p(x) - U_p(x)$$

$$(\delta/\delta x)^2\varphi(x) = (q/\varepsilon_0\varepsilon_s)(-Q_{fixed} + n - p)$$

Steady state

$$\delta n/\delta t = 1/q \cdot \delta/\delta x(J_n(x)) + G_n(x) - U_n(x) = 0$$

$$\delta p/\delta t = 1/q \cdot \delta/\delta x(J_p(x)) + G_p(x) - U_p(x) = 0$$

$$(\delta/\delta x)^2\varphi(x) = (q/\varepsilon_0\varepsilon_s)(-Q_{fixed} + n - p)$$

Formulation of the transport problem

$$\delta n/\delta t = 1/q \cdot \delta/\delta x(J_n(x)) + G_n(x) - U_n(x)$$

$$\delta p/\delta t = 1/q \cdot \delta/\delta x(J_p(x)) + G_p(x) - U_p(x)$$

$$(\delta/\delta x)^2\varphi(x) = (q/\varepsilon_0\varepsilon_s)(-Q_{fixed} + n - p)$$

Formulation of the transport problem

$$J_n(x) = \mu_n n \cdot \delta/\delta x(E_{Fn}(x))$$

$$J_p(x) = \mu_p p \cdot \delta/\delta x(E_{Fp}(x))$$

Current densities

Total current density:

$$J_{TOT} = J_n + J_p$$

$$J_{TOT} = \mu_n n \nabla E_{Fn} + \mu_p p \nabla E_{Fp}$$

Electron current density:

$$J_n = \underbrace{+ q D_n \nabla n}_{\text{DIFFUSION}} + \underbrace{\mu_n n [qE - \nabla\chi - kT \nabla \ln(N_c)]}_{\text{DRIFT}}$$

Hole current density:

$$J_p = - q D_p \nabla p + \mu_p p[qE - \nabla\chi - \nabla E_g + kT \nabla \ln(N_c)]$$

- A net current density can be obtained in many ways!

Current densities in a homojunction

Total current density:

$$J_{TOT} = J_n + J_p$$

$$J_{TOT} = \mu_n n \nabla E_{Fn} + \mu_p p \nabla E_{Fp}$$

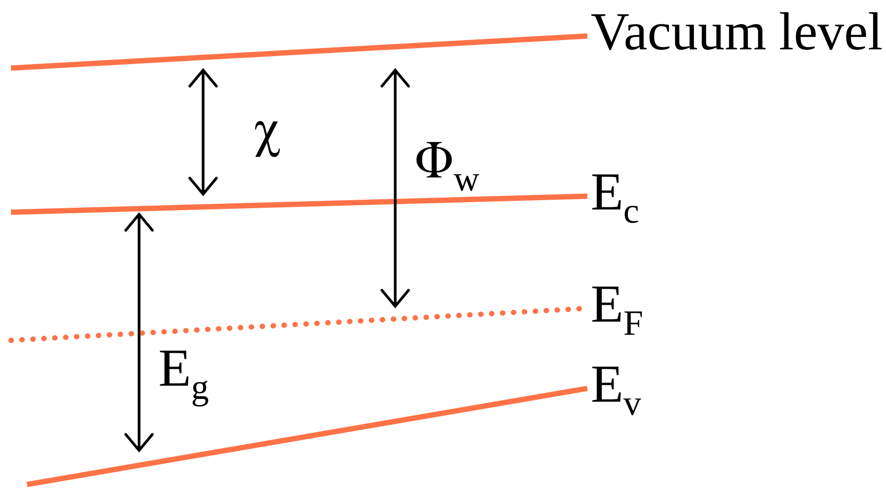
Electron current density:

$$J_n = + q D_n \nabla n + \mu_n nqE$$

Hole current density:

$$J_p = - q D_p \nabla p + \mu_p pqE$$

Driving forces



χ = electron affinity

E_g = band gap energy

E_F = Fermi level

E_c = conduction band energy

E_v = valence band energy

Φ_w = work function

Formulation of the transport problem

- The conservation equation for electrons then becomes

$$1/q \cdot \delta/\delta x(J_n(x)) + G_n(x) - U_n(x) = 0$$

- We then also recall the Einstein relation

$$\mu_n = qD_n/kT$$

Formulation of the transport problem

- We combine with the expression for $J_n(x)$

$$1/q \cdot \delta/\delta x(q\, D_n(\delta/\delta x)n + \mu_n nqE) + G_n(x) - U_n(x) = 0$$

- We rearrange terms and get the following equation

$$D_n(\delta^2/\delta x^2)n + \mu_n E(\delta/\delta x)n + \mu_n n(\delta/\delta x)E + G_n(x) - U_n(x) = 0$$

Formulation of the transport problem

- If E is 0 or constant we get

$$D_n(\delta^2/\delta x^2)n + \mu_n E(\delta/\delta x)n + G_n(x) - U_n(x) = 0$$

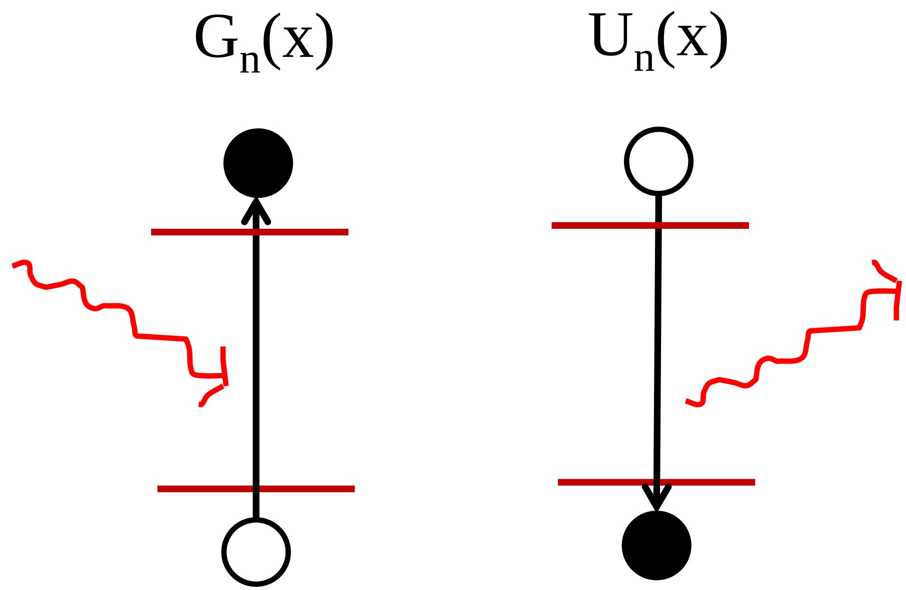
- With a final rearrangement, this finally becomes

$$(\delta^2/\delta x^2)n + (qE/kT)(\delta/\delta x)n + G_n(x)/D_n - U_n(x)/D_n = 0$$

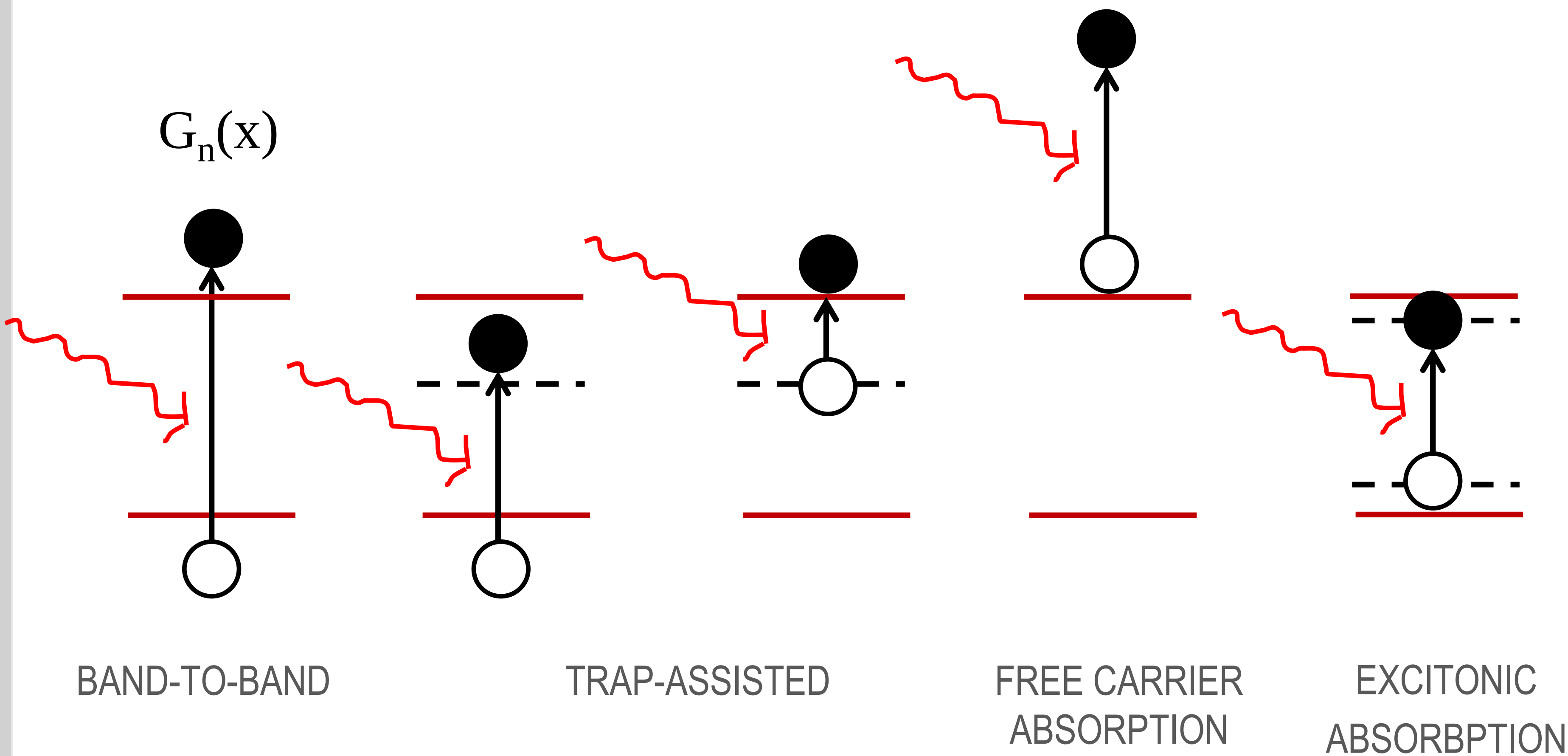
Recombination and generation – basics

Recombination and generation

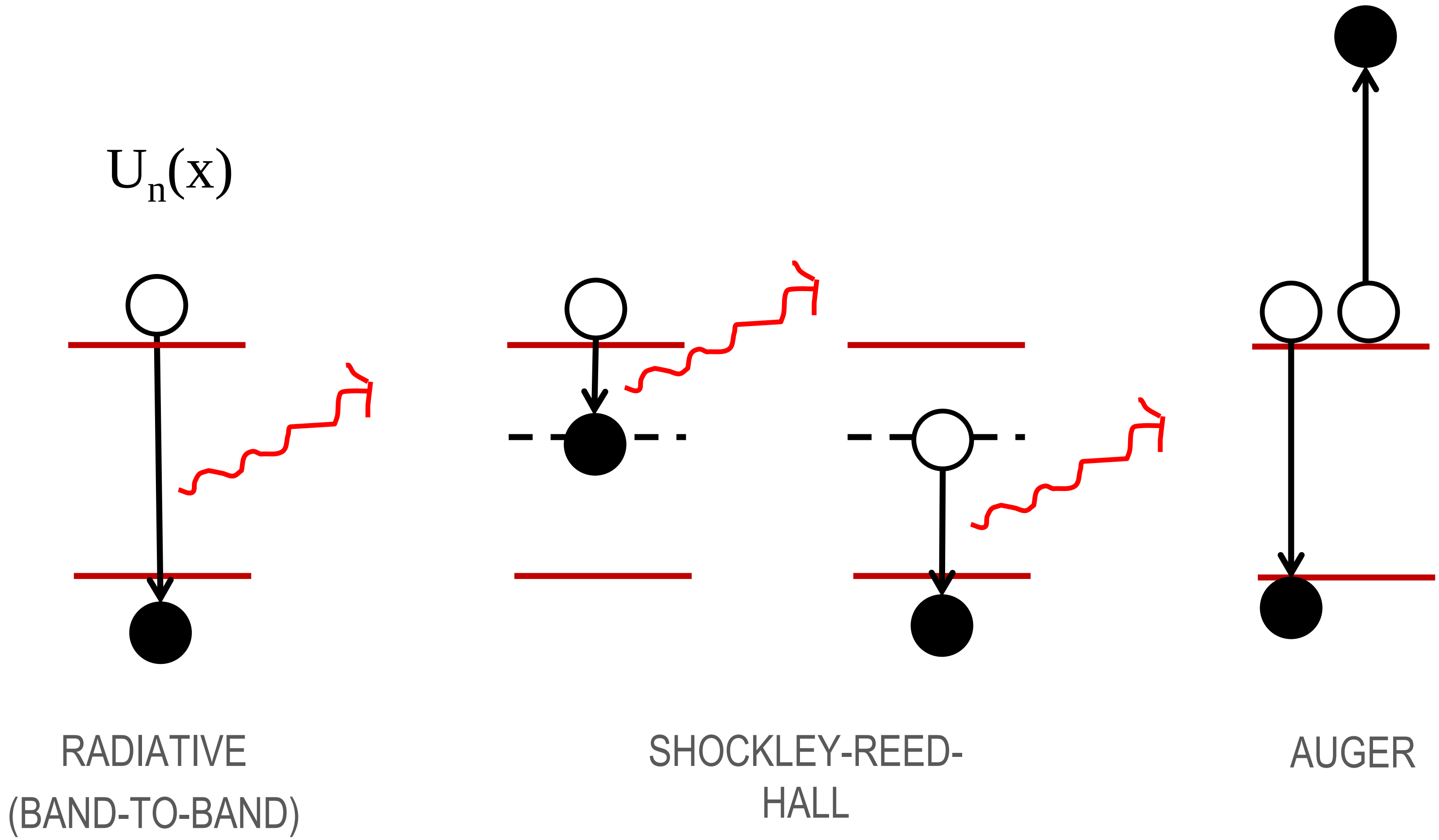
- Energy conservation
- Every generation process has an equivalent recombination process



Generation processes



Recombination processes



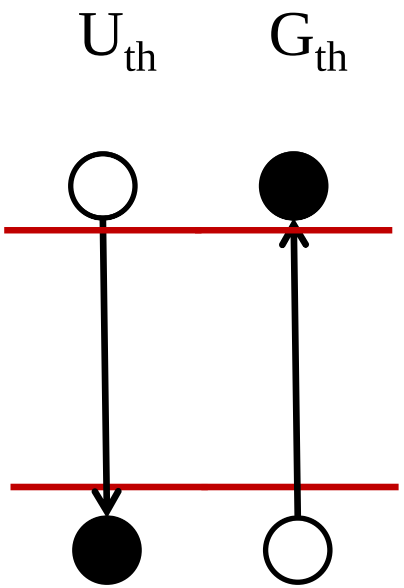
Thermal generation and recombination

- At $T = 0$:

$$G_{n,th} = U_{n,th} = G_{p,th} = U_{p,th} = 0$$

- At $T > 0$ and in equilibrium:

$$G_{n,th} = U_{n,th}$$
$$G_{p,th} = U_{p,th}$$



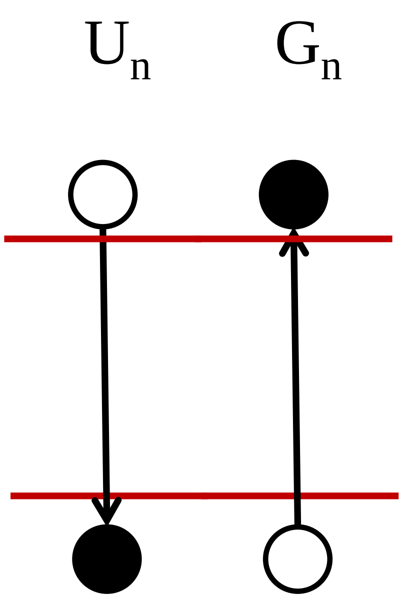
Net generation and recombination

- In the following, we will only be interested in additional generation and recombination
- We define net generation and recombination rates:

$$G_n = G_{n,tot} - G_{n,th}$$

$$U_n = U_{n,tot} - U_{n,th}$$

- …and similar for holes

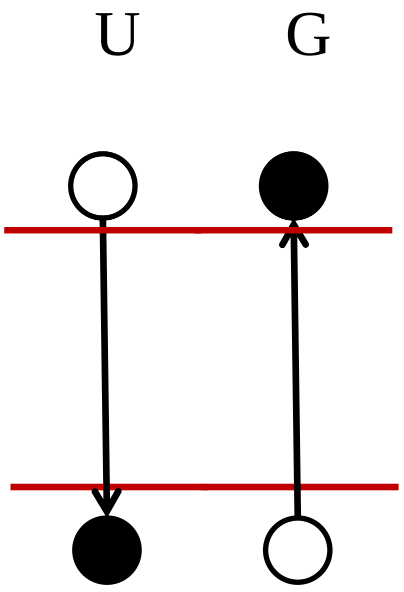


Band to band processes

- In our calculations, we will assume that band-to-band processes dominate.

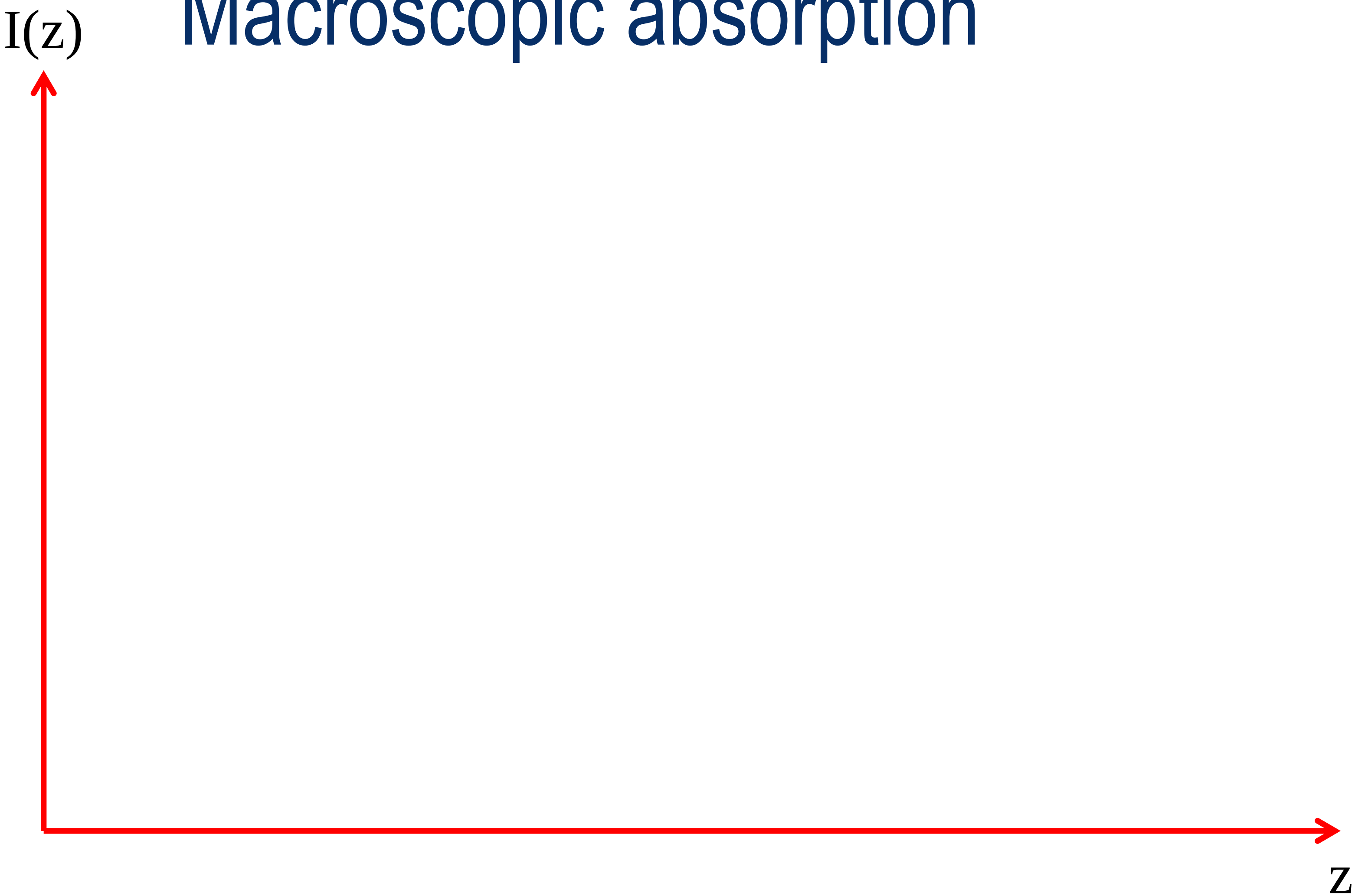
$$G_n = G_p = G$$

$$U_n = U_p = U$$

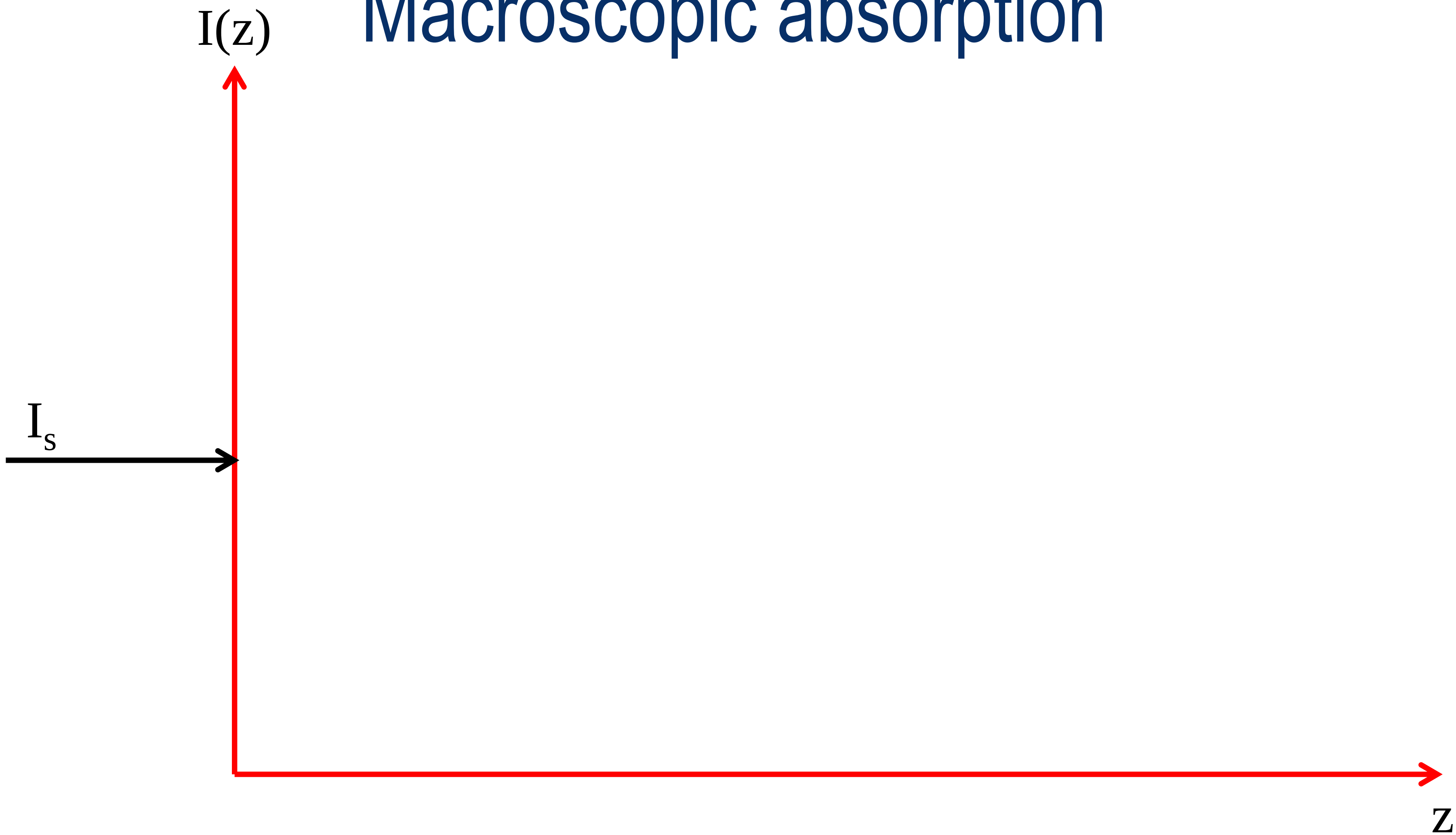


Absorption – the macroscopic view

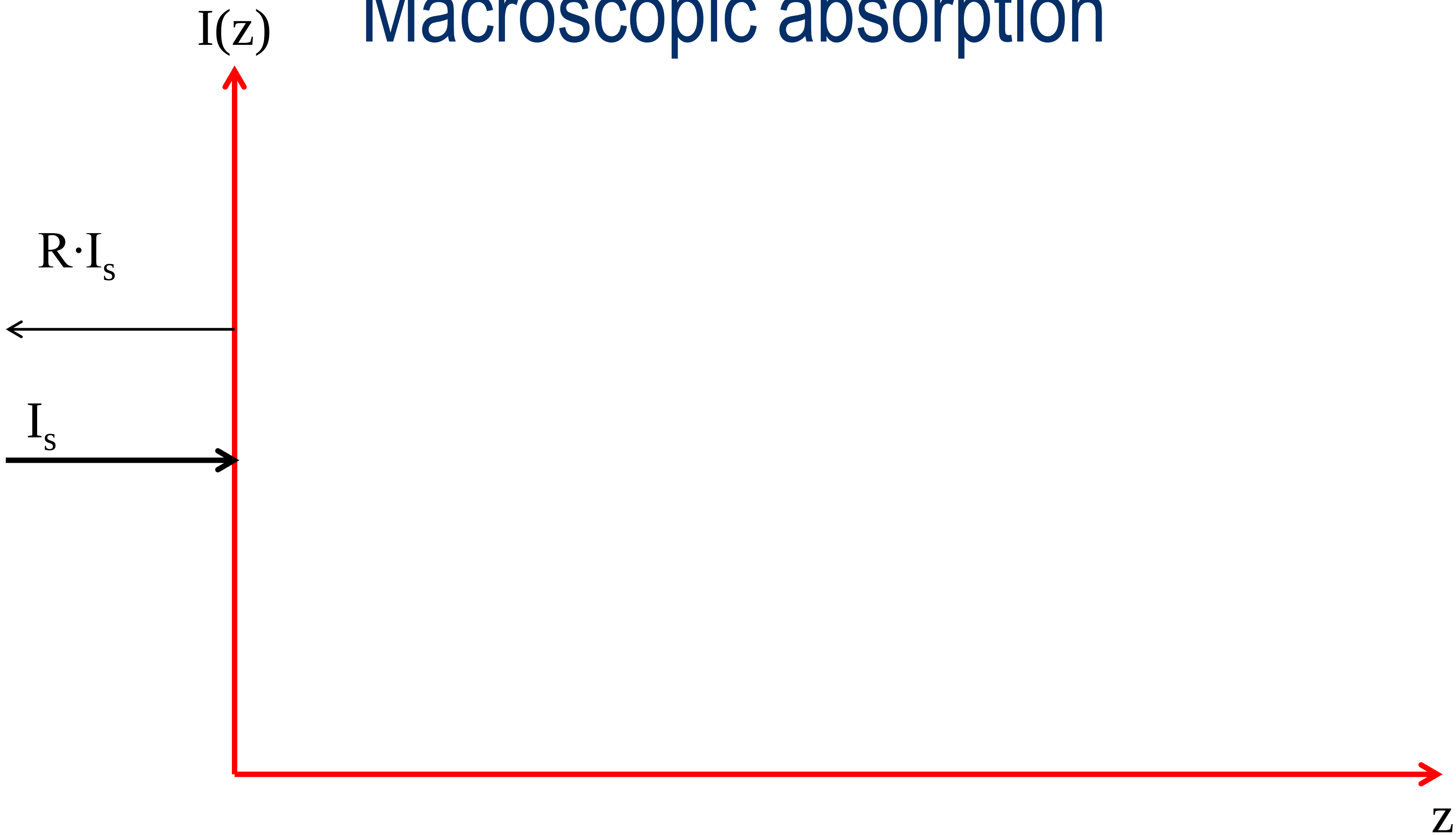
Macroscopic absorption



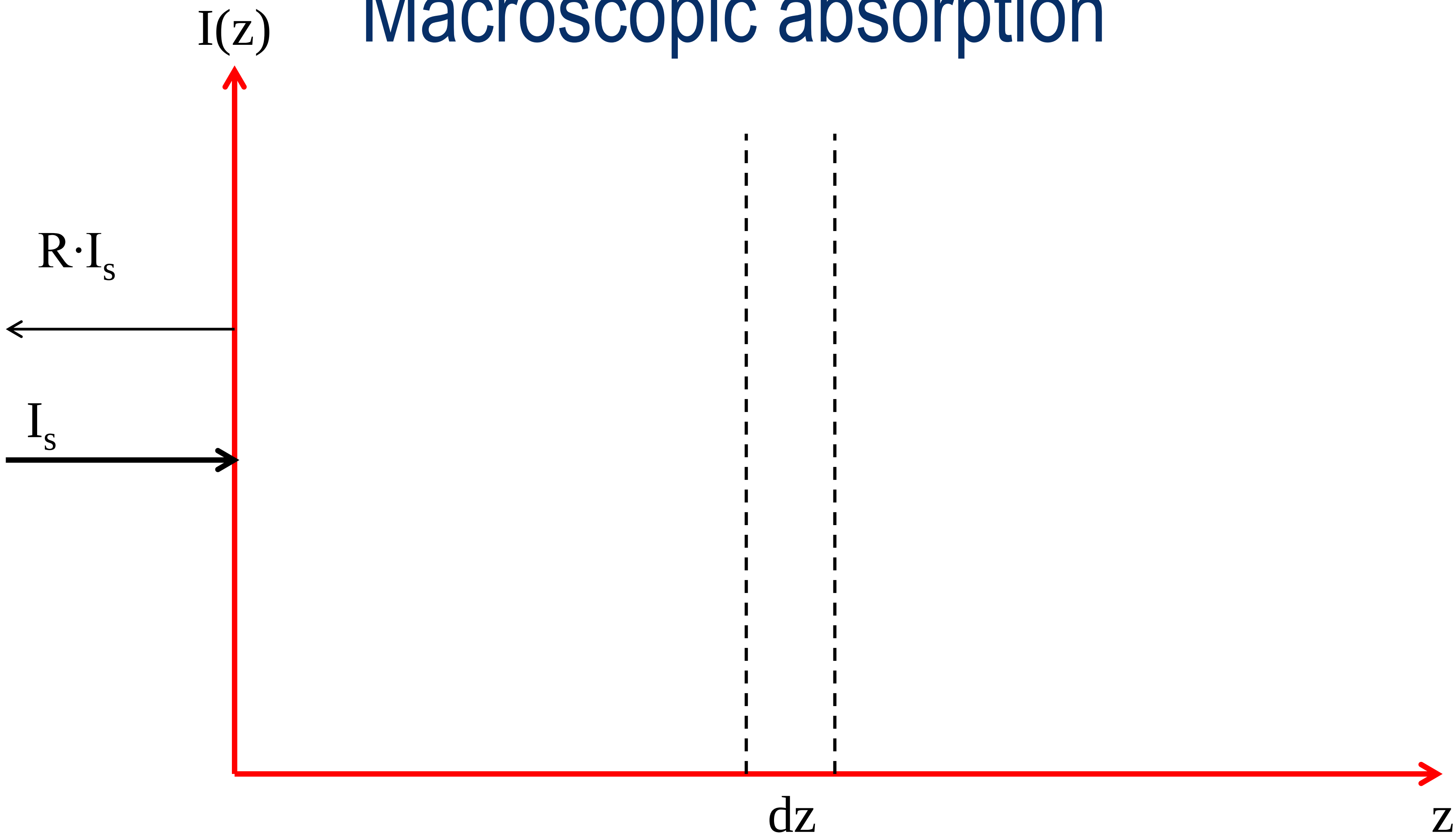
Macroscopic absorption



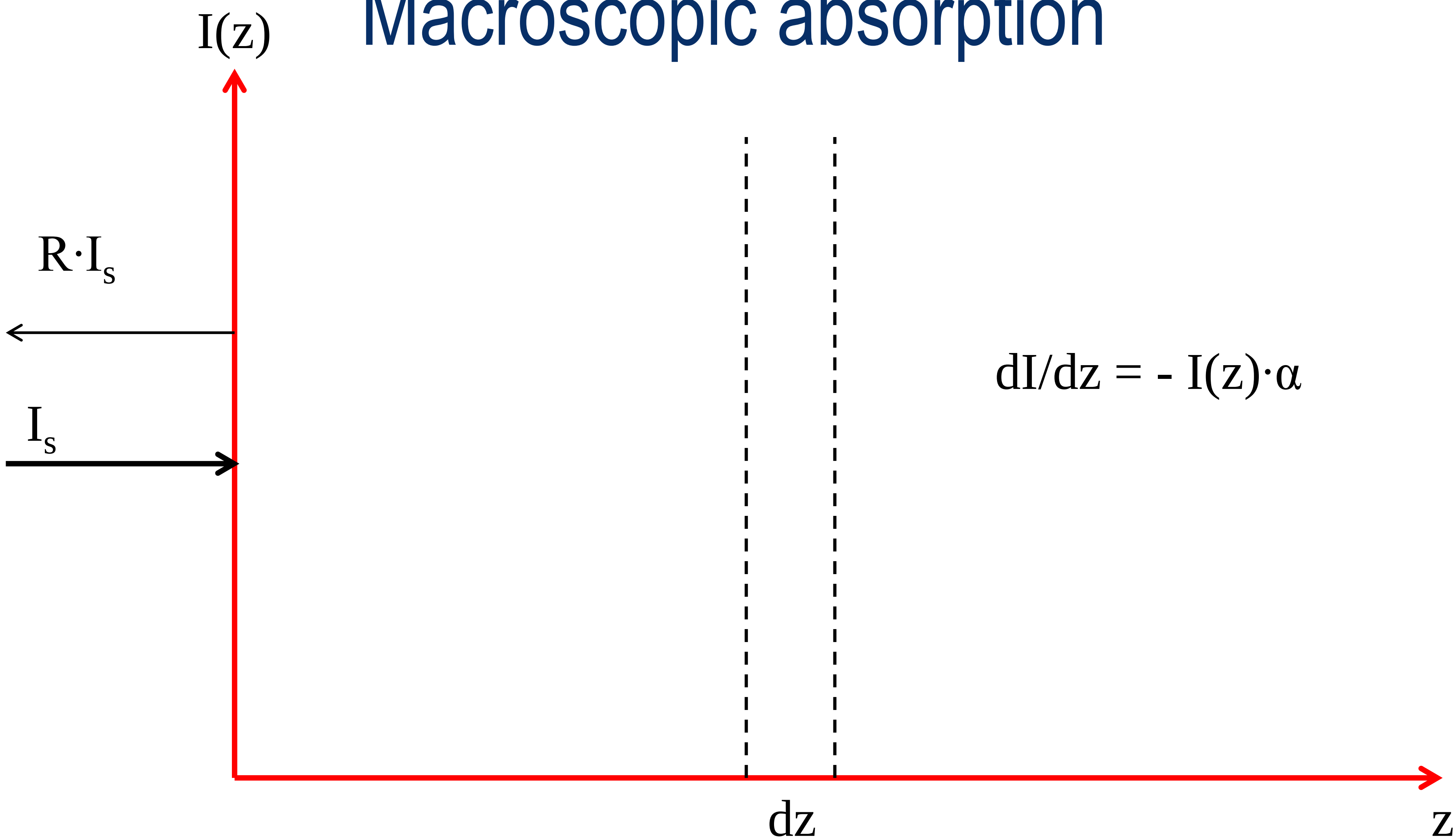
Macroscopic absorption



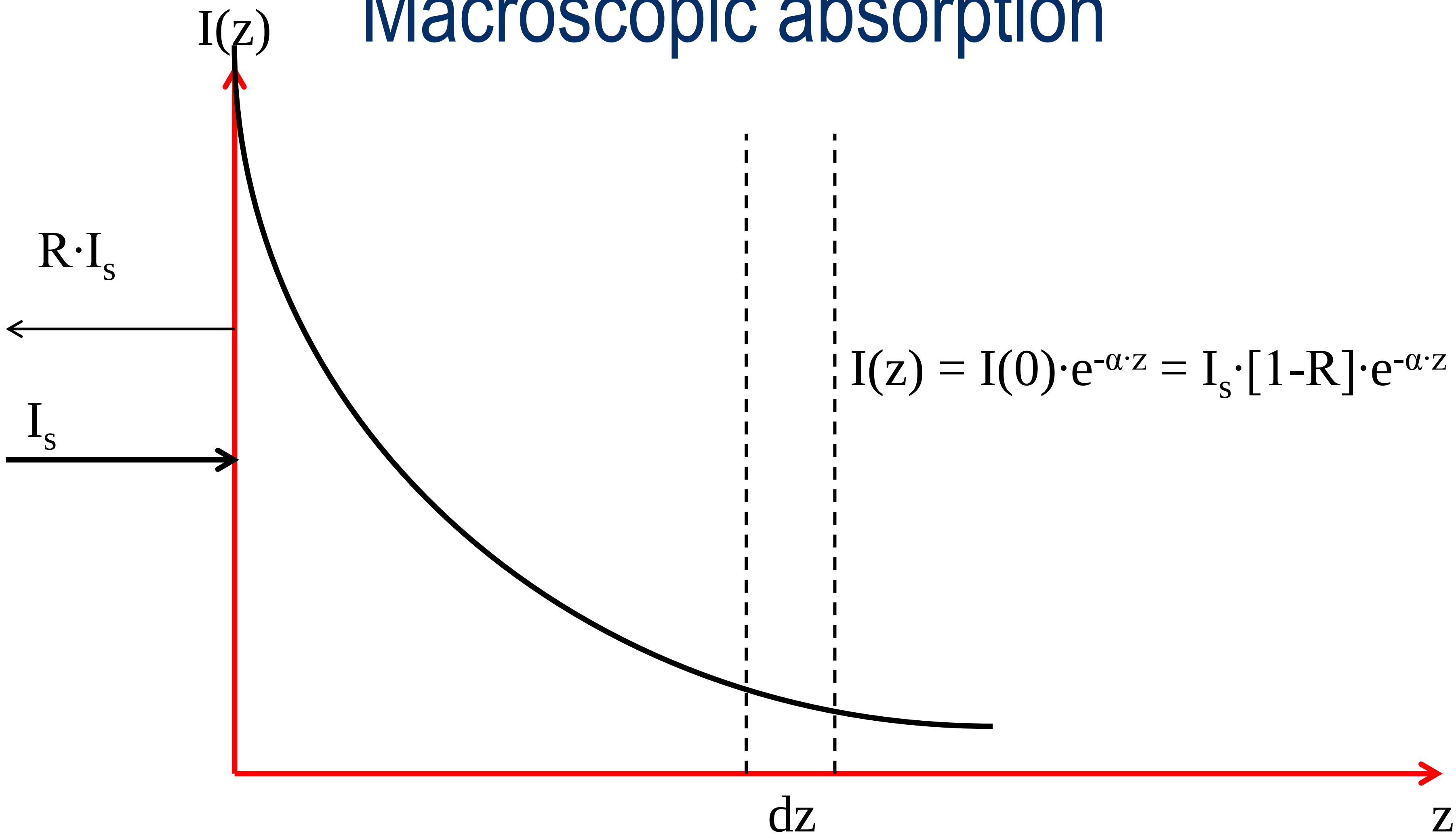
Macroscopic absorption



Macroscopic absorption



Macroscopic absorption



Energy and spatial dependence

- All important parameters are energy dependent

$$I(z,E) = I_s(E)\cdot[1\text{-}R(E)]\cdot e^{-\alpha(E)\cdot z}$$

- Variations in $\alpha(E)$ in space in real solar cells

$$I(z,E) = I_s(E)\cdot[1\text{-}R(E)]\cdot e^{-\int\alpha(E,z')\cdot dz'}$$

Generation current densities

- The rate of carrier generation at x per volume is given by

$$g(E,x) = b_s(E,x)\cdot\alpha[E,x]$$

- With respect to $b_s(E)$, this then becomes

$$g(E,x) = [1-R(E)]\cdot b_s(E)\cdot\alpha[E,x]\cdot e^{-\int\alpha(E,x')\cdot dx'}$$

Generation current densities

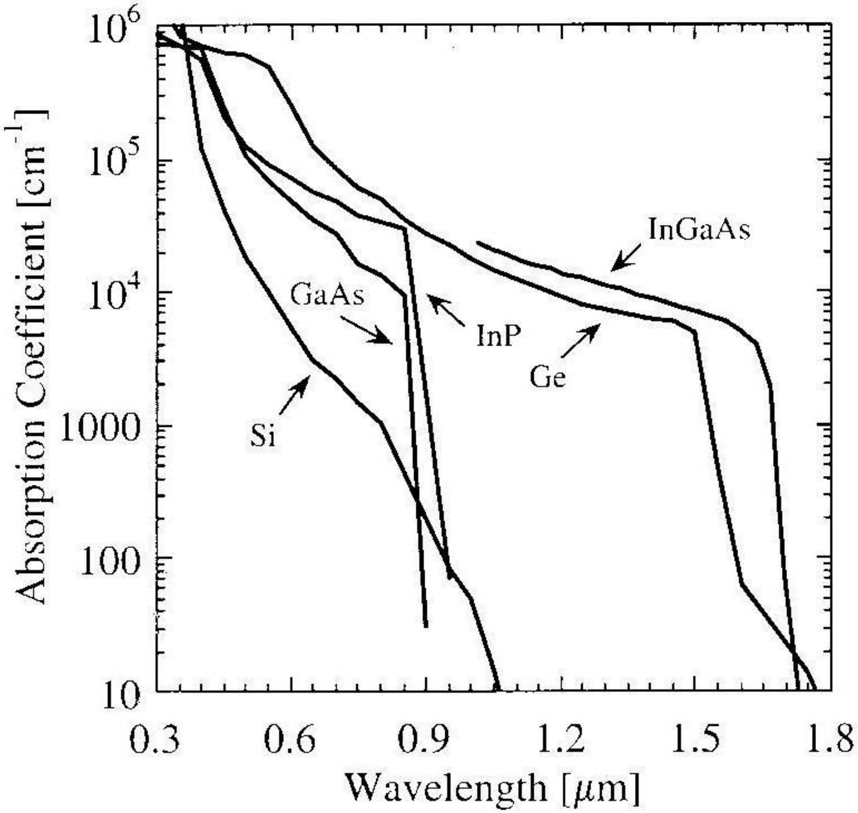
- The total generation current density is given by

$$G(x) = \int g(E,x)dE$$

- This term is then used to express the transport problem

$$D_n(\delta^2/\delta x^2)n + \mu_n E(\delta/\delta x)n + \mu_n n(\delta/\delta x)E + \mathbf{G_n(x)} - U_n(x) = 0$$

Material dependence



Handbook of Optical Constants of Solids, edited by Edward D. Palik, (1985), Academic Press NY.

Clever student question:

”Why?”

Clever student question (refined):

”Where does the material dependence come from?”

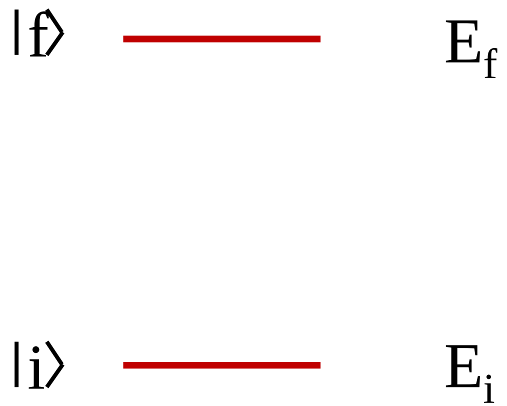
Absorption – the microscopic view

Microscopic absorption

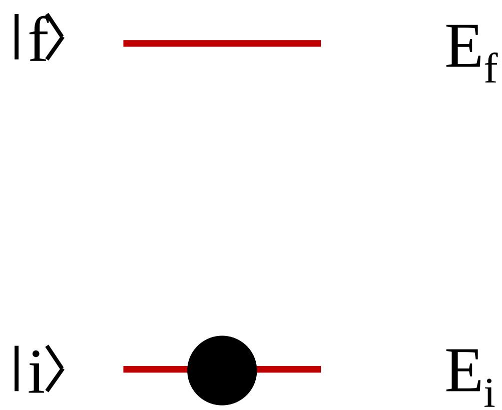
- $G(E,x)$ and $U(E,x)$ can be calculated from first principles

- The way ahead:
  - Definition of initial and final states $|i\rangle$ $|f\rangle$
  - Determining transition probabilities $w_{i\to f}$ $w_{f\to i}$
    - Fermi's golden rule
  - Determining transition rates $r_{i\to f}$ $r_{f\to i}$
  - Determining net transition rates r_{if}
  - Determining total, spectral transition rates $r(E)$

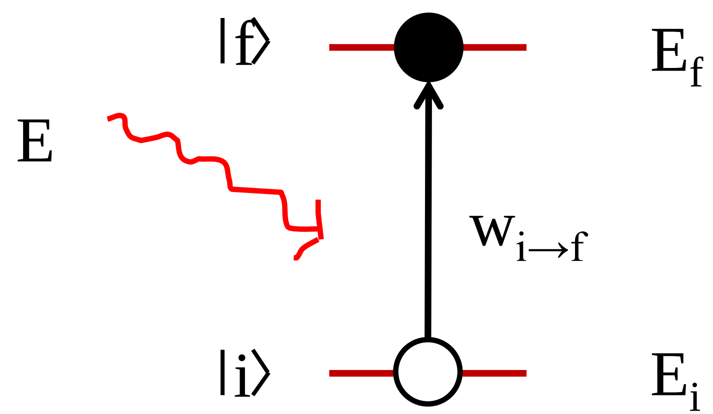
Our system



Our system



Our system



Transition probabilities
(Fermi's golden rule)

$$w_{i\to f} = 2\pi/h\,|\langle i|\mathbf{H}|f\rangle|^2\cdot\delta(E_f - E_i \pm E)$$

Transition probabilities
(Fermi's golden rule)

$$w_{i\rightarrow f} = 2\pi/h\ |\langle i|\mathbf{H}|f\rangle|^2\cdot\delta(E_f - E_i \pm E)$$

- Energy conservation
  - The energies must match precicely

- Matrix element
  - Quantifies the transition probability
  - Is what we will show how to calculate

Transition probability → Transition rate

$|f\rangle$ E_f f_f

$|i\rangle$ E_i f_i

Transition rates

- The transition rates take the distribution functions into account:

$$r_{i\rightarrow f} = 2\pi/h\ |\langle i|\mathbf{H}|f\rangle|^2 \cdot \delta(E_f - E_i \pm E)\cdot f_i \cdot (1\text{-}f_f)$$

$$r_{f\rightarrow i} = 2\pi/h\ |\langle i|\mathbf{H}|f\rangle|^2 \cdot \delta(E_f - E_i \pm E)\cdot f_f \cdot (1\text{-}f_i)$$

Net transition rates

- The net transition rate is the difference between $r_{i\rightarrow f}$ and $r_{f\rightarrow i}$

$$r_{if} = r_{i\rightarrow f} + r_{f\rightarrow i}$$

$$r_{if} = 2\pi/h \,|\langle i|\mathbf{H}|f\rangle|^2 \cdot \delta(E_f - E_i \pm E)\cdot[f_i\cdot(1-f_f) - f_f\cdot(1-f_i)]$$

- Which finally becomes for a single pair of states

$$r_{if} = 2\pi/h \,|\langle i|\mathbf{H}|f\rangle|^2 \cdot \delta(E_f - E_i \pm E)\cdot(f_i - f_f)$$

Total spectral transition rates

- To get to the total spectral transition rates, we must sum over all pairs of initial and final states:

$$r(E) = 2\pi/h \cdot \iint |\langle i|\mathbf{H}|f\rangle|^2 \cdot \delta(E_f - E_i \pm E) \cdot (f_i - f_f) \cdot g_i(E_i) \cdot g_f(E_f) dE_i dE_f$$

Generation rate

- The total rate of band to band transitions is finally found by also taking the density of available photons into account:

$$G = \int r(E) \cdot g_{photon}(E) \cdot dE$$

Microscopic description of absorption

- The net transition rate is given by

$$r(E) = 2\pi/h \cdot \iint |\langle i|\mathbf{H}|f\rangle|^2 \cdot \delta(E_f - E_i \pm E) \cdot (f_i - f_f) \cdot g_i(E_i) \cdot g_f(E_f) dE_i dE_f$$

Microscopic description of absorption

- For an electromagnetic field of strength E_0, a polarization vector ε and angular frequency ω, for wavelengths longer than interatomic distances H is given by the dipole approximation as

$$H = (iqE_0/2m_0\omega)\ \varepsilon \cdot p$$

- Here, p is the quantum mechanical momentum operator

Microscopic description of absorption

- We define $M_{cv} = |\langle v,i|\varepsilon\cdot p|c,f\rangle|$

- We then get the following expression:

$$r(E) = (2\pi/h) \cdot (q^2E_0{}^2h^2/2m_0E^2) \cdot$$
$$\iint M_{cv}{}^2\, \delta(E_c - E_v \pm E)\cdot(f_v - f_c)\cdot g_c\cdot g_v dE_c dE_v$$

Microscopic description of absorption

- The transition rate represents the net rate of photon absorption
- The electromagnetic field transfers energy to the semiconductor at a net rate

$$\delta U_E/\delta t = -E \cdot r(E)$$

- For a plane wave, this corresponds to the cycle-averaged rate of intensity loss, $\delta I/\delta x$

Microscopic description of absorption

- Since

$$\delta I/\delta x = \delta U_E/\delta t$$

- We get:

$$-\alpha I = \delta U_E/\delta t$$

Microscopic description of absorption

- Furthermore

$$I = U_e c / n_s$$

- and

$$U_E = n_s^2 E_0^2 / 8\pi$$

Microscopic description of absorption

- We finally get the following relation between the transition rate and the absorption coefficient:

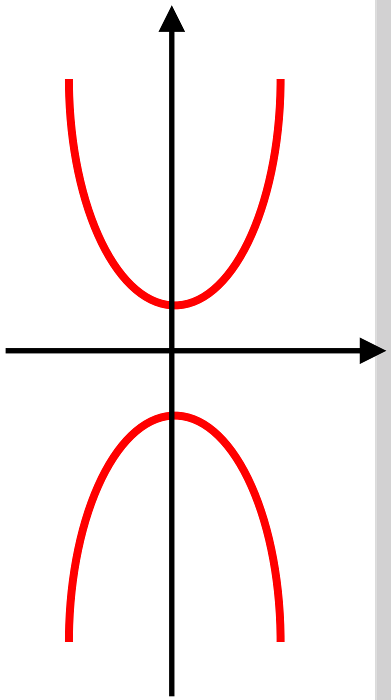
$$\alpha = (n_s E_0 / c U_E)\ r(E)$$

- This equation can now be used to calculate α for different materials

Direct band semiconductors

- For semiconductors with a direct band, the calculations yield:

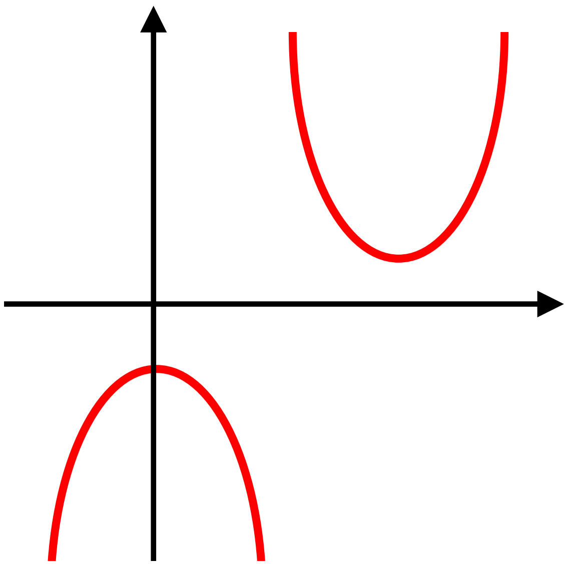
$$\alpha(E) = \alpha_0(E - E_g)^{1/2}$$



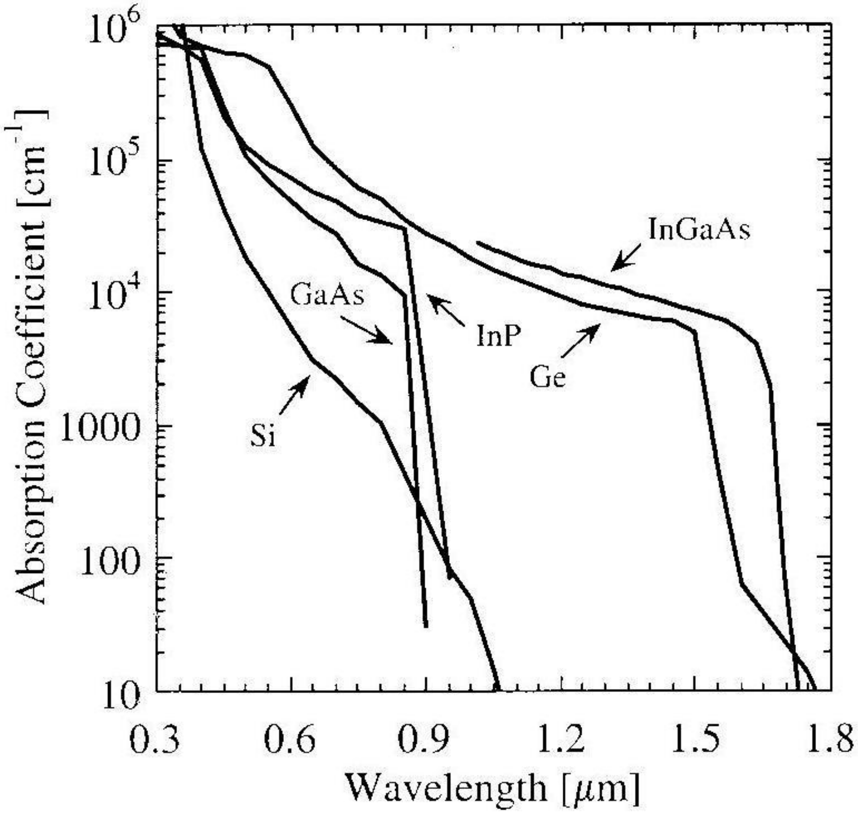
Indirect band semiconductors

- For semiconductors with an indirect band, the calculations yield:

$$\alpha(E) = \alpha_0(E - E_g)^2$$



Material dependence



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