Solid-State Optics

Winter term 2022/23

Department of Physics / Karlsruhe School of Optics and Photonics

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General Course Info

- General topic: solid-state optics (with some emphasis on semiconductor optics)

- Class jointly offered by Department of Physics and
  Karlsruhe School of Optics and Photonics (KSOP)

- Lectures: Thursday 15:45 – 17:15, Friday 14:00 – 15:30, Kl. HS B, building 30.22
- All slides on ILIAS:
  Repository > Organisationseinheiten > KIT-Fakultät für Physik > WS 22/23
  4020011 – Solid-State Optics

Overview

I. Motivation and introduction

II. Maxwell equations and light propagation in vacuum

- Maxwell equations
- Waves in vacuum

III. Light propagation in media

- Wave equation and dispersion
- Optical functions, extinction, absorption
- Boundary conditions at interfaces
- Anisotropic media

Overview

IV. Interaction of light with matter – classical models
- Drude–Lorentz model
- Optical properties of solids in the Lorentz model
- Optical properties of metals
- Spectroscopy

V. Interaction of light with matter – quantum mechanical models
- Electrons in periodical lattices
- Descriptive interpretation of optical transitions
- Treatment using perturbation theory
- Calculation of transition probabilities

VI. Band to band transitions
- Perturbative treatment
- Joint density of states
- van Hove singularities
- Measurement of optical functions
(Absorption, Reflectance, Ellipsometry, Fourier spectroscopy, modulation spectroscopy, …)

Overview

VII. Excitons

- Optical properties, binding energy and radius
- Exciton wavefunction
- Exciton polaritons
- Spectroscopy

VIII. Nonlinear optics

- Nonlinear processes (SHG, 3-wave mixing, parametric processes, …)
- High excitation effects in semiconductors
  (Burstein-Moss shift, band-gap renormalization, electron–hole plasma, applications, …)

IX. Group theory

- Motivation
- Basics
- Symmetry of eigenfunctions of the Hamiltonian
- Applications

Info for Physics Students

- Suitable as “Schwerpunktfach”, “Ergänzungsfach”, “Nebenfach”
- Up to 8 ECTS points (depending on agreed coverage)
- Combination with other classes (e.g., “Halbleiterphysik”)
- No exercises but discussions on demand
- Credits based on oral exam
  (individual agreement + registration at *Prüfungssekretariat*, *Zulassung* needed)

Info for KSOP students

- Oral exam (individual agreement, register in CAS system before exam)

- Exercises:

  No exercises, but possibility to discuss problems / questions individually
  (after lecture or make appointment via e-mail before)

Literature

- H. Kalt, C.F. Klingshirn, Semiconductor optics 1 – Linear optical properties of semiconductors, fifth edition, Springer 2019 (or older versions by C.F. Klingshirn)

- P.Y. Yu and M. Cardona, Fundamentals of semiconductors, Springer, 1995

- F. Wooten, Optical properties of solids, Academic Press, 1972

- P.K. Basu, Theory of optical processes in semiconductors, Oxford Science Publications, 1997

Overview

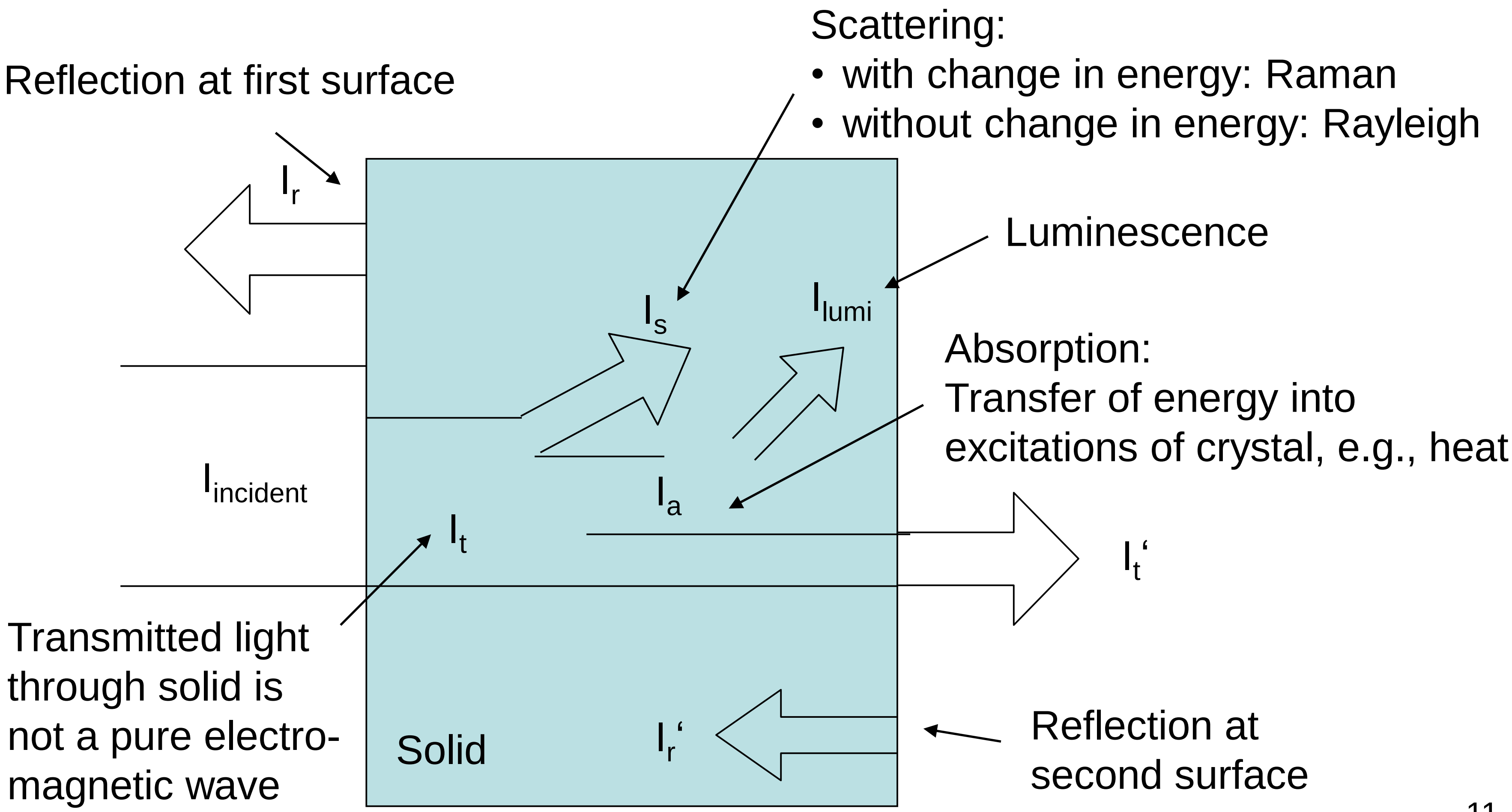
1. **Motivation and introduction**
2. Maxwell equations and light propagation in vacuum
3. Light propagation in media
4. Interaction of light with matter – classical models
5. Interaction of light with matter – quantum mechanical models
6. Group theory
7. Band to band transitions
8. Excitons
9. Nonlinear optics

I. Motivation and introduction – Why solid state optics?

- Understand optical properties of solids relevant for basic physics and applications (e.g., LEDs, lasers, optoelectronics)
- Different types of materials are relevant:
  - Insulators (amorphous, crystalline):
    - (Quartz) glass
    - Colored glass (insulators with dopand atoms, defects)
  - Semiconductors
    - Elementary semiconductors, e.g., Si, Ge
    - Compound semiconductors with small band gaps, e.g., InAs, GaAs
    - Compound semiconductors with large band gaps, e.g., GaN, ZnO
    - Compound semiconductor heterostructures (quantum structures)
  - Metals / doped semiconductors

I. Motivation and introduction – Light and solids

- Important topics:
  - Processes during light propagation through materials
  - Generation of light in materials



Overview

I. Motivation and introduction
II. Maxwell equations and light propagation in vacuum
III. Light propagation in media
IV. Interaction of light with matter – introduction
V. Interaction of light with matter – quantum mechanical models
VI. Group theory
VII. Interaction of light with matter – classical models
VIII. Band to band transitions
IX. Excitons
X. Nonlinear optics

Overview

I. Motivation and introduction

II. Maxwell equations and light propagation in vacuum

- **Maxwell equations**
- **Waves in vacuum**

III. Light propagation in media

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VIII. Excitons

IX. Nonlinear optics

III. Maxwell equations and light propagation in vacuum

Maxwell equations

Maxwell-Faraday equation: $\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$

Ampère-Maxwell equation: $\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} + \boldsymbol{j}$

Laws of Gauss: $\nabla \cdot \boldsymbol{D} = \rho$ $\quad \nabla \cdot \boldsymbol{B} = 0$

with:

$\boldsymbol{E}$: electric field, units: $\frac{\mathrm{V}}{\mathrm{m}} = \frac{\mathrm{N}}{\mathrm{As}}$

$\boldsymbol{B}$: magnetic induction, units: $\mathrm{T} = \frac{\mathrm{Vs}}{\mathrm{m}^2} = \frac{\mathrm{N}}{\mathrm{Am}}$

$\boldsymbol{H}$: magnetic field, units: $\frac{\mathrm{A}}{\mathrm{m}}$

$\boldsymbol{D}$: electric displacement field, units: $\frac{\mathrm{As}}{\mathrm{m}^2}$

$\boldsymbol{j}$: current density, units: $\frac{\mathrm{A}}{\mathrm{m}^2}$

ρ : charge density, units: $\frac{\mathrm{As}}{\mathrm{m}^3}$

III. Maxwell equations and light propagation in vacuum

Material equations

$$\boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P} = \varepsilon \varepsilon_0 \boldsymbol{E}$$

$$\boldsymbol{B} = \mu_0 (\boldsymbol{H} + \boldsymbol{M}) = \mu \mu_0 \boldsymbol{H}$$

with:

$\varepsilon_0 = 8.859 \cdot 10^{-12} \dfrac{\mathrm{As}}{\mathrm{Vm}}$: permittivity in free space

ε : relative permittivi ty

$\boldsymbol{P}$: dielectric polarization, units : $\dfrac{\mathrm{As}}{\mathrm{m}^2}$

$\boldsymbol{M}$: magnetization, units : $\dfrac{\mathrm{A}}{\mathrm{m}}$

$\mu_0 = 4\pi \cdot 10^{-7} \dfrac{\mathrm{Vs}}{\mathrm{Am}}$: permeability of free space

μ : relative permeabili ty

III. Maxwell equations and light propagation in vacuum

Wave propagation in vacuum

In vacuum: $\boldsymbol{P} = 0 \quad \Rightarrow \quad \varepsilon = 1$; $\boldsymbol{M} = 0 \quad \Rightarrow \quad \mu = 1$; $\boldsymbol{j} = 0$; $\rho = 0$

Resulting Maxwell equations in vacuum: $\nabla \times \boldsymbol{E} = -\mu_0 \dfrac{\partial \boldsymbol{H}}{\partial t}$ (1) and

$$\nabla \times \boldsymbol{H} = \varepsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} \qquad (2)$$

Application of $\nabla \times$ on (1) and $\dfrac{\partial}{\partial t}$ on (2) leads to:

$$-\mu_0 \varepsilon_0 \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = \nabla \times \left(\nabla \times \boldsymbol{E} \right)$$

Using the identity $\nabla \times \left(\nabla \times \boldsymbol{E} \right) = \nabla \left(\nabla \cdot \boldsymbol{E} \right) - \left(\nabla \cdot \nabla \right) \boldsymbol{E}$ we get:

$$-\mu_0 \varepsilon_0 \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = \nabla \cdot \left(\nabla \cdot \boldsymbol{E} \right) - \nabla^2 \boldsymbol{E}$$

III. Maxwell equations and light propagation in vacuum

With $\nabla \cdot \boldsymbol{E} = \frac{\rho}{\varepsilon_0} = 0$ and $\mu_0 \varepsilon_0 = \frac{1}{c^2}$ we get the wave equation:

$$\nabla^2 \boldsymbol{E} - \frac{1}{c^2} \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = 0$$

Simplest solution: *Transverse* electromagnetic plane wave: $\boldsymbol{E}(\boldsymbol{r}, t) = \boldsymbol{E}_0 e^{i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)}$

with wave vector $\boldsymbol{k}$ and angular frequency ω

Plug solution into wave equation $\Rightarrow \quad k^2 = \frac{\omega^2}{c^2}$

$\Rightarrow \quad \omega(k) = c \cdot k$ Dispersion relation

Phase velocity: $v_p = \frac{\omega}{k} = c = const.!$ Group velocity: $v_g = \frac{\partial \omega}{\partial k} = c = \frac{1}{\varepsilon_0 \mu_0} = const.!$

If no interaction with matter (!) : *Linear* dispersion, phase & group velocity const. !

III. Maxwell equations and light propagation in vacuum

Direction of vectors $\boldsymbol{k}, \boldsymbol{E}$ and $\boldsymbol{H}$:

$$\nabla \times \boldsymbol{E} = i\,\boldsymbol{k} \times \boldsymbol{E} = -\mu_0 \frac{\partial \boldsymbol{H}}{\partial t} = i\mu_0 \omega \boldsymbol{H} \quad \Rightarrow \quad \boldsymbol{H} = \frac{1}{\mu_0 \omega_0} \boldsymbol{k} \times \boldsymbol{E} \;: \quad \boldsymbol{k} \perp \boldsymbol{E} \perp \boldsymbol{H}$$

Energy flux density: Pointing vector $\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}$ in vacuum parallel to $\boldsymbol{k}$

Average over time $\Rightarrow$ light intensity
$$I = \frac{1}{2}\left|\boldsymbol{E}_0 \times \boldsymbol{H}_0\right| = \frac{1}{2}\left|\boldsymbol{E}_0 \times \left(\frac{1}{\mu_0 \omega} \boldsymbol{k} \times \boldsymbol{E}_0\right)\right|$$

With $\boldsymbol{a} \times (\boldsymbol{b} \times c) = \boldsymbol{b}(\boldsymbol{a} \cdot \boldsymbol{c}) - \boldsymbol{c}(\boldsymbol{a} \cdot \boldsymbol{b})$:
$$I = \frac{E_0^{\;2}}{2\mu_0 \omega} |\boldsymbol{k}| = \frac{1}{Z_0} E_0^{\;2}$$

With wave impedance in vacuum:
$$Z_0 = \sqrt{\frac{\mu_0}{\varepsilon_0}} \approx 377\,\Omega$$

III. Maxwell equations and light propagation in vacuum

Longitudinal modes in vacuum?

Split electric field into longitudinal and transverse components:

$$\boldsymbol{E} = \boldsymbol{E}_L + \boldsymbol{E}_T \quad \text{with} \quad \boldsymbol{E}_L \parallel \boldsymbol{k} \quad \text{and} \quad \boldsymbol{E}_T \perp \boldsymbol{k}$$

From this follows:

$$\nabla \times \boldsymbol{E} = i\,\boldsymbol{k} \times \boldsymbol{E} = i\,\boldsymbol{k} \times \boldsymbol{E}_T \quad \Rightarrow \quad \boldsymbol{H}$$

$$\nabla \cdot \boldsymbol{E} = i\,\boldsymbol{k} \cdot \boldsymbol{E} = i\,\boldsymbol{k} \cdot \boldsymbol{E}_L \equiv 0 \ \text{due to} \ \nabla \cdot \boldsymbol{D} = 0 \quad \Rightarrow \quad \boldsymbol{k} = 0 \quad \text{or} \quad \boldsymbol{E}_L = 0$$

However, $k \neq 0$, otherwise static field, not possible due to $\rho = 0$

$\Rightarrow \quad \boldsymbol{E}_L = 0$, i. e., *no longitudinal modes in vacuum !*

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III. Light propagation in media

- **Wave equation and dispersion**
- **Optical functions, extinction, absorption**
- **Boundary conditions at interfaces**
- **Anisotropic media**

IV. Interaction of light with matter – classical models

V. Interaction of light with matter – quantum mechanical models

VI. Group theory

VII. Band to band transitions

VIII. Excitons

IX. Nonlinear optics

IV. Light propagation through media – wave equation

Wave equation and dispersion

Aim: derive wave equation and general dispersion relation using Maxwell's equations

Assumptions:

- Material is semiconductor or insulator, not magnetic, i.e., $\mu = 1, \ \boldsymbol{M} = 0$
- No space charges: $\rho = 0 \quad \Rightarrow \quad \nabla \cdot \boldsymbol{D} = 0$
- No free charges / currents: $\boldsymbol{j} = 0 \quad \Rightarrow \quad \nabla \times \boldsymbol{H} = \partial \mathbf{D} / \partial t$

Analogous to wave equation in vacuum:

$$\nabla \times \left(\nabla \times \boldsymbol{E} \right) = -\mu_0 \nabla \times \partial \boldsymbol{H} / \partial t = -\mu_0 \, \partial^2 \mathbf{D} / \partial t^2 = -\mu_0 \varepsilon_0 \, \partial^2 \mathbf{E} / \partial t^2 - \mu_0 \, \partial^2 \mathbf{P} / \partial t^2$$

$$\Rightarrow \quad \Delta \boldsymbol{E} - \frac{1}{c^2} \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = +\mu_0 \frac{\partial^2 \boldsymbol{P}}{\partial t^2}$$

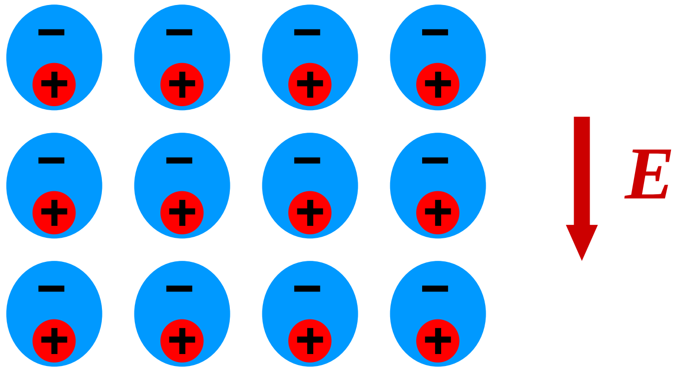
$\Rightarrow$ A time-dependent polarization with $\partial^2 \boldsymbol{P} / \partial t^2 \neq 0$ (e.g., an oscillating dipole) acts as a source for electromagnetic waves

IV. Light propagation through media – dielectric function

We need: relation between $\boldsymbol{P}$ and $\boldsymbol{E}$!

Question: How does material react to applied electric (electro-magnetic) field?

Answer to this question ($\mathbf{P}(\mathbf{E})$) provides all optical properties of material !



In general (→ section on non-linear optics): Taylor series

$$\frac{P_i}{\varepsilon_0} = \sum_j \chi_{ij}{}^{(1)} E_j + \sum_{j,k} \chi_{ijk}{}^{(2)} E_j E_k + \sum_{j,k,l} \chi_{ijkl}{}^{(3)} E_j E_k E_l + \ldots$$

χ : susceptibility tensor

- Only "linear optics", i.e., $\chi^{(>1)} = \mathbf{O}$
- Assume isotropic media (susceptibility scalar)

$$\Rightarrow \quad \boldsymbol{P} = \varepsilon_0 \chi \boldsymbol{E}$$

$$\boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P} = \varepsilon_0 \boldsymbol{E} + \varepsilon_0 \chi \boldsymbol{E} = \varepsilon_0 (1 + \chi) \boldsymbol{E} = \varepsilon_0 \ \varepsilon \ \boldsymbol{E}$$

All optical properties of the medium are given by knowledge of permittivity ε

IV. Light propagation through media – dielectric function

In general: $\varepsilon(\boldsymbol{r},t)$ or $\varepsilon(\boldsymbol{k},\omega)$

Remarks:

- ε is a linear response function, i.e., ε connects $\boldsymbol{D}(\boldsymbol{r},t)$ with $\boldsymbol{E}(\boldsymbol{r}',t')$ at all positions and previous times (causality must be fulfilled):

$$D_i(\boldsymbol{r},t) = \sum_j \int \int_{-\infty}^{t} \varepsilon_{ij}(\boldsymbol{r},\boldsymbol{r}',t,t')\varepsilon_0 E_j(\boldsymbol{r}',t')dt'd^3\boldsymbol{r}'$$

Without time-dependent perturbations and assuming a homogeneous material (or suitably averaged material properties) this can be rewritten as:

$$D_i(\boldsymbol{r},t) = \sum_j \int \int_{-\infty}^{t} \varepsilon_{ij}(|\boldsymbol{r}-\boldsymbol{r}'|,|t-t'|)\varepsilon_0 E_j(\boldsymbol{r}',t')dt'd^3\boldsymbol{r}'$$

In Fourier space (mostly used in this lecture): $D_i(\boldsymbol{k},\omega) = \sum_j \varepsilon_{ij}(\boldsymbol{k},\omega)\varepsilon_0 E_j(\boldsymbol{k},\omega)$

- Often, k ~ 0 is a good approximation (wave vector of light negligible → later):

$\varepsilon = \varepsilon(\omega)$ with Fourier transform $\varepsilon(\boldsymbol{r},t)\delta(\boldsymbol{r})$

i.e., local response $\boldsymbol{D}(\boldsymbol{r},t)$ depends only on the field $\boldsymbol{E}(\boldsymbol{r},t)$ at the same position

IV. Light propagation through media – dielectric function

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i \cdot \varepsilon_2(\omega)$$

Ask yourself: Why is ε complex ?

real part imaginary part

Due to restrictions implied by causality, there is a connection between

ε_1 and ε_2 , given by the Kramers–Kronig relations:

$$\varepsilon_1(\omega) = \varepsilon_1(\infty) + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega' \quad \text{and} \quad \varepsilon_2(\omega) = -\frac{2\omega}{\pi} P \int_0^\infty \frac{\varepsilon_1(\omega')}{\omega'^2 - \omega^2} d\omega'$$

where P is the Cauchy principal value:

$$P \int_0^\infty \frac{\varepsilon_{1,2}(\omega')}{\omega'^2 - \omega^2} d\omega' = \lim_{\alpha \to 0^+} \left(\int_0^{\omega - \alpha} \ldots d\omega' + \int_{\omega + \alpha}^\infty \ldots d\omega' \right)$$

IV. Light propagation through media – dispersion

Consider again the wave equation: $\Delta \boldsymbol{E} - \mu_0 \varepsilon_0 \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = +\mu_0 \frac{\partial^2 \boldsymbol{P}}{\partial t^2}$ with $\boldsymbol{P} = \varepsilon_0 \chi \boldsymbol{E}$

$$\Delta \boldsymbol{E} - \mu_0 \varepsilon_0 \frac{\partial^2 \boldsymbol{E}}{\partial t^2} - \mu_0 \chi \varepsilon_0 \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = 0 \Leftrightarrow \Delta \boldsymbol{E} - \mu_0 \varepsilon_0 (1+\chi) \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = 0 \Leftrightarrow \Delta \boldsymbol{E} - \mu_0 \varepsilon_0 \varepsilon \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = 0$$

Simplest solution in medium: Again $\boldsymbol{E} = \boldsymbol{E}_0 \cdot e^{i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)}$

Into wave eq. $\Rightarrow$ In general, *non-linear* dispersion rel.: $k^2 - \varepsilon(\omega, k)\mu_0 \varepsilon_0 \omega(k)^2 = 0$

$\Rightarrow$ Polariton Equation: $\varepsilon(k,\omega) = \frac{k^2 c^2}{\omega^2}$

Since ε is complex, $\boldsymbol{k}$ is complex, too: $\boldsymbol{k} = \boldsymbol{k}_1 + i\,\boldsymbol{k}_2$

real part: dispersion

imaginary part: extinction (spatial decrease in amplitude, not necessarily absorption!)

$$\Rightarrow \boldsymbol{E} = \boldsymbol{E}_0 \cdot e^{i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)} = \boldsymbol{E}_0 \cdot \underbrace{e^{-\boldsymbol{k}_2\cdot\boldsymbol{r}}}_{\text{Exponential decrease in amplitude}} \cdot \underbrace{e^{i(\boldsymbol{k}_1\cdot\boldsymbol{r} - \omega t)}}_{\text{wave with phase velocity } v_p = \omega/k_1}$$

IV. Light propagation through media – optical functions

Optical functions, extinction and absorption

Consider complex index of refraction (refractive index): $\tilde{n}(\omega)$ with $\tilde{n}^2(\omega) = \varepsilon$

For wave vector in medium: $k = k_{vacuum}\tilde{n}(\omega) = \frac{\omega}{c}\tilde{n}(\omega) = \frac{\omega}{c}(n + i\kappa)$

with
- n : real part of refractive index
  (usually > 0 but can be negative $\rightarrow$ meta-materials)
- κ : extinction coefficient

Wavelength in medium: $\lambda = \frac{\lambda_{vacuum}}{|n(\lambda)|}$

Light wave in isotropic medium:

$$\mathbf{E} = \mathbf{E}_0 \cdot e^{i\left(\tilde{n}\mathbf{k}_{vacuum}\cdot\mathbf{r} - \omega t\right)} = \underbrace{\mathbf{E}_0 \cdot e^{-\kappa(\omega)\mathbf{k}_{vacuum}\cdot\mathbf{r}}} \cdot \underbrace{e^{i\left(n(\omega)\mathbf{k}_{vacuum}\cdot\mathbf{r} - \omega t\right)}}$$

$I(z) = I_0 e^{-\alpha z}$

Beer's law
with $\alpha = 2k_2$

Wave with phase velocity

$$v_p = \frac{\omega}{k_1} = \frac{\omega}{nk_{vacuum}} = \frac{c}{n}$$

IV. Light propagation through media – optical functions

Connection between ε_1, ε_2 and n, κ as well as α

Complex permittivity: consider polariton equation $k^2 = \dfrac{\omega^2}{c^2}\varepsilon(\omega) = \dfrac{\omega^2}{c^2}\tilde{n}^2(\omega)$

$$\Rightarrow \quad \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) = \tilde{n}^2(\omega) = n^2(\omega) - \kappa^2(\omega) + i\,2n(\omega)\kappa(\omega)$$

$$\Rightarrow \quad \varepsilon_1(\omega) = n^2(\omega) - \kappa^2(\omega) \quad \text{and} \quad \varepsilon_2(\omega) = 2n(\omega)\kappa(\omega)$$

$$n(\omega) = \sqrt{\frac{1}{2}\left(\sqrt{\varepsilon_1{}^2(\omega) + \varepsilon_2{}^2(\omega)} + \varepsilon_1(\omega)\right)} \quad \text{and} \quad \kappa(\omega) = \sqrt{\frac{1}{2}\left(\sqrt{\varepsilon_1{}^2(\omega) + \varepsilon_2{}^2(\omega)} - \varepsilon_1(\omega)\right)}$$

$$\alpha(\omega) = \frac{\omega}{c}\frac{\varepsilon_2(\omega)}{n(\omega)} = k_{vacuum}\frac{\varepsilon_2(\omega)}{n(\omega)}$$

Remarks:

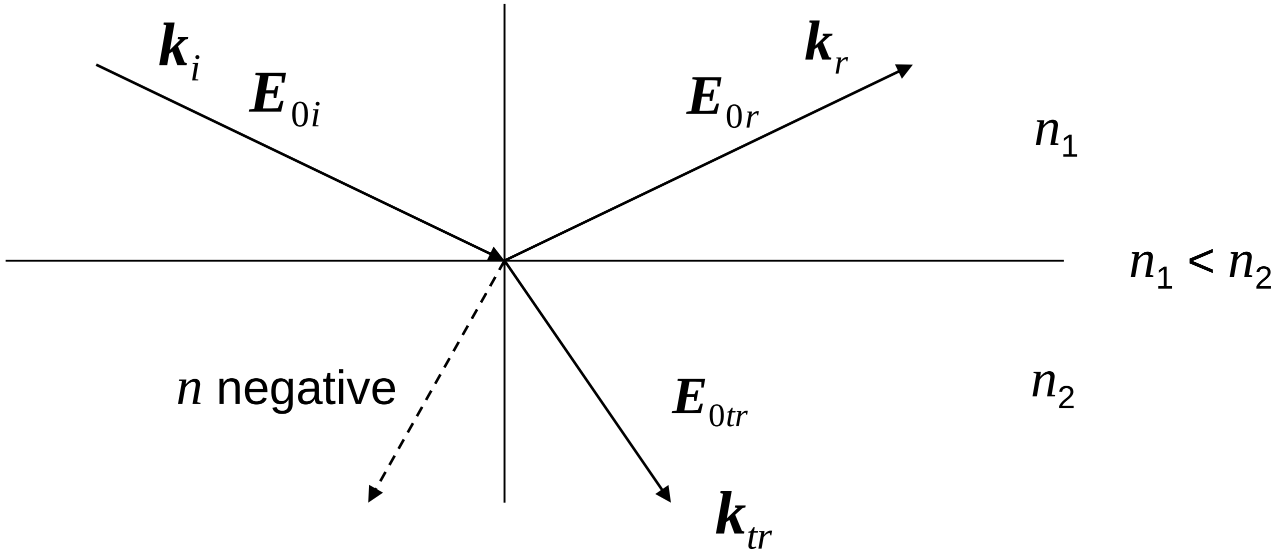
- All optical functions (n, κ, ε_1 and ε_2) depend on frequency ω
- One pair of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ or $n(\omega)$ and $\kappa(\omega)$ is sufficient to describe *all optical properties*
- Real and imaginary parts of these functions are connected through Kramers–Kronig relations: $\varepsilon_1 \leftrightarrow \varepsilon_2$, $n \leftrightarrow \kappa$

IV. Light propagation through media – boundary conditions

Boundary conditions, energy and momentum conservation at interfaces

In a typical experiment in solid state optics, we measure the reflectivity R and transmittivity T of a sample $\Rightarrow$ Find appropriate equations !

Def.: reflection coefficient: $r = \frac{E_{0r}}{E_{0i}}$ transmission coefficient: $t = \frac{E_{0tr}}{E_{0i}}$



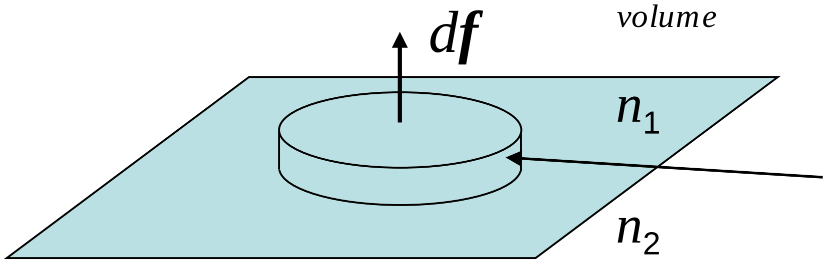
Measured values: $R = |r|^2$ and $T = |t|^2$

IV. Light propagation through media – boundary conditions

Derivation of Snell‘s law from Maxwell‘s equations

Gauss law: $\int_{volume} \nabla \cdot \boldsymbol{A}\, d\tau = \oint_{surface} \boldsymbol{A} \cdot d\boldsymbol{f}$ Stokes: $\oint_{surface} (\nabla \times \boldsymbol{A}) \cdot d\boldsymbol{f} = \oint_{boundary} \boldsymbol{A} \cdot d\boldsymbol{s}$

With $\nabla \cdot \boldsymbol{D} = \rho \quad \Rightarrow \quad \int_{volume} \nabla \cdot \boldsymbol{D}\, d\tau = \oint_{surface} \boldsymbol{D} \cdot d\boldsymbol{f} = \int_{volume} \rho\, d\tau$



Assumption: ratio height to radius is infinitesimally small
$\Rightarrow$ ignore side area

$$\Rightarrow (\boldsymbol{D}_1 - \boldsymbol{D}_2) \cdot d\boldsymbol{f} = (D_{n,1} - D_{n,2}) df = \rho_S\, df$$

normal components only   surface charge density

For $\rho_S = 0$: $D_{n,1} = D_{n,2}$

Normal component of $\boldsymbol{D}$ continuous!

Analogous for $\nabla \cdot \boldsymbol{B} = 0 \quad \Rightarrow \quad B_{n,1} = B_{n,2}$ Normal component of $\boldsymbol{B}$ continuous!

Using the Maxwell equations for curl $\boldsymbol{E}$, $\boldsymbol{H}$ and a closed path with infinitely small height through the surface we get:

$E_{t,1} = E_{t,2}$ and $H_{t,1} = H_{t,2}$ Tangential components of $\boldsymbol{E}$, $\boldsymbol{H}$ cont. !

IV. Light propagation through media – boundary conditions

Now consider Noether‘s theorem:

From every invariant transformation of the Hamilton / Lagrange density follows a conservation law, e.g.:

a) H invariant with respect to infinitesimal shifts in time: $H(t) = H(t + dt)$

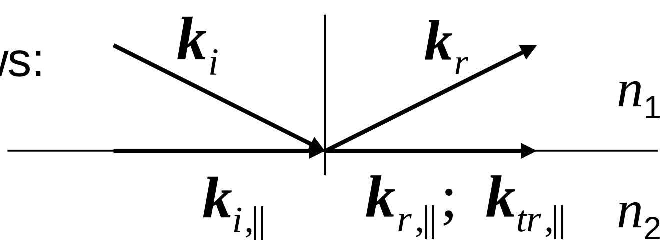
$\Rightarrow$ Total energy is conserved: E_{total} = const.

b) H invariant with respect to infinitesimal shifts in space: $H(x) = H(x + dx)$

$\Rightarrow$ Momentum is conserved: p_x = const.

From a) / continuity cond. for each time t follows: $\hbar\omega = \text{const.} \quad \Rightarrow \quad \omega_i = \omega_r = \omega_{tr}$

From b) follows:



Translational invariance only in direction parallel to surface

$\downarrow$

Conservation of momentum only in component parallel to surface

with momentum $\hbar\boldsymbol{k}$ $\Rightarrow$ $\boldsymbol{k}_{i,\parallel} = \boldsymbol{k}_{r,\parallel} = \boldsymbol{k}_{tr,\parallel}$ $(*)$

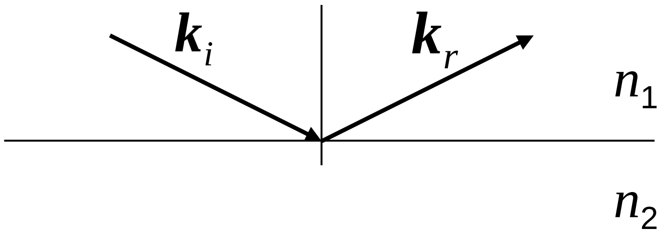
Since incident and reflected wave propagate in the same medium: $|\boldsymbol{k}_i| = |\boldsymbol{k}_r|$ $(**)$

IV. Light propagation through media – boundary conditions

Using (∗) and (∗∗), we get the law of reflection: $\alpha_i = \alpha_r$

and with $|\boldsymbol{k}_1| = n_1\, |\boldsymbol{k}_{vacuum}|$ and $|\boldsymbol{k}_2| = n_2\, |\boldsymbol{k}_{vacuum}|$ also Snell's law: $\dfrac{\sin\alpha_i}{\sin\alpha_{tr}} = \dfrac{n_2}{n_1}$

Total internal reflection



with $n_1 > n_2$

total reflection:

if $\alpha_i > \alpha_t$ with $\alpha_t = \arcsin(n_2 / n_1)$

Derivation: $\alpha_i = \arcsin(n_2 / n_1 \cdot \sin\alpha_{tr})$, assume $\alpha_{tr} = 90° \Rightarrow \sin\alpha_{tr} = 1$
(limit for no transmitted beam)

However, boundary conditions still require a finite amplitude in medium 2

⇒ evanescent wave parallel to interface

Frustrated total internal reflection

Consider another medium 3 with distance < λ and $n_3 > n_2$ below medium 2

⇒ evanescent wave reaches medium 3 and can escape, application as beam splitter

IV. Light propagation through media – boundary conditions

Fresnel formulas for angle-dependent reflection / transmission at interface

Consider *polarization* of light: $\perp$ (s polar.) and || (p polar.) to plane of incidence

Calculate r and t for two transparent media (ignore κ, i.e., weak extinction : $|\kappa| < |n|$)

$$r_\perp = \frac{n_1 \cos\alpha_i - n_2 \cos\alpha_{tr}}{n_1 \cos\alpha_i + n_2 \cos\alpha_{tr}} = -\frac{\sin(\alpha_i - \alpha_{tr})}{\sin(\alpha_i + \alpha_{tr})} \qquad r_{||} = \frac{-n_2 \cos\alpha_i + n_1 \cos\alpha_{tr}}{n_1 \cos\alpha_{tr} + n_2 \cos\alpha_i} = -\frac{\tan(\alpha_i - \alpha_{tr})}{\tan(\alpha_i + \alpha_{tr})}$$

$$t_\perp = \frac{2\sin\alpha_{tr}\cos\alpha_i}{\sin(\alpha_i + \alpha_{tr})} \qquad t_{||} = \frac{2\sin\alpha_{tr}\cos\alpha_i}{\sin(\alpha_i + \alpha_{tr})\cos(\alpha_i - \alpha_{tr})}$$

with $R_{\perp,||} = (r_{\perp,||})^2$ and $T_{\perp,||} = (t_{\perp,||})^2$

Special case: $\alpha_i = 0$ (polarization does not matter)

Weak extinction: $$R = \frac{(n_2 - n_1)^2}{(n_2 + n_1)^2}$$

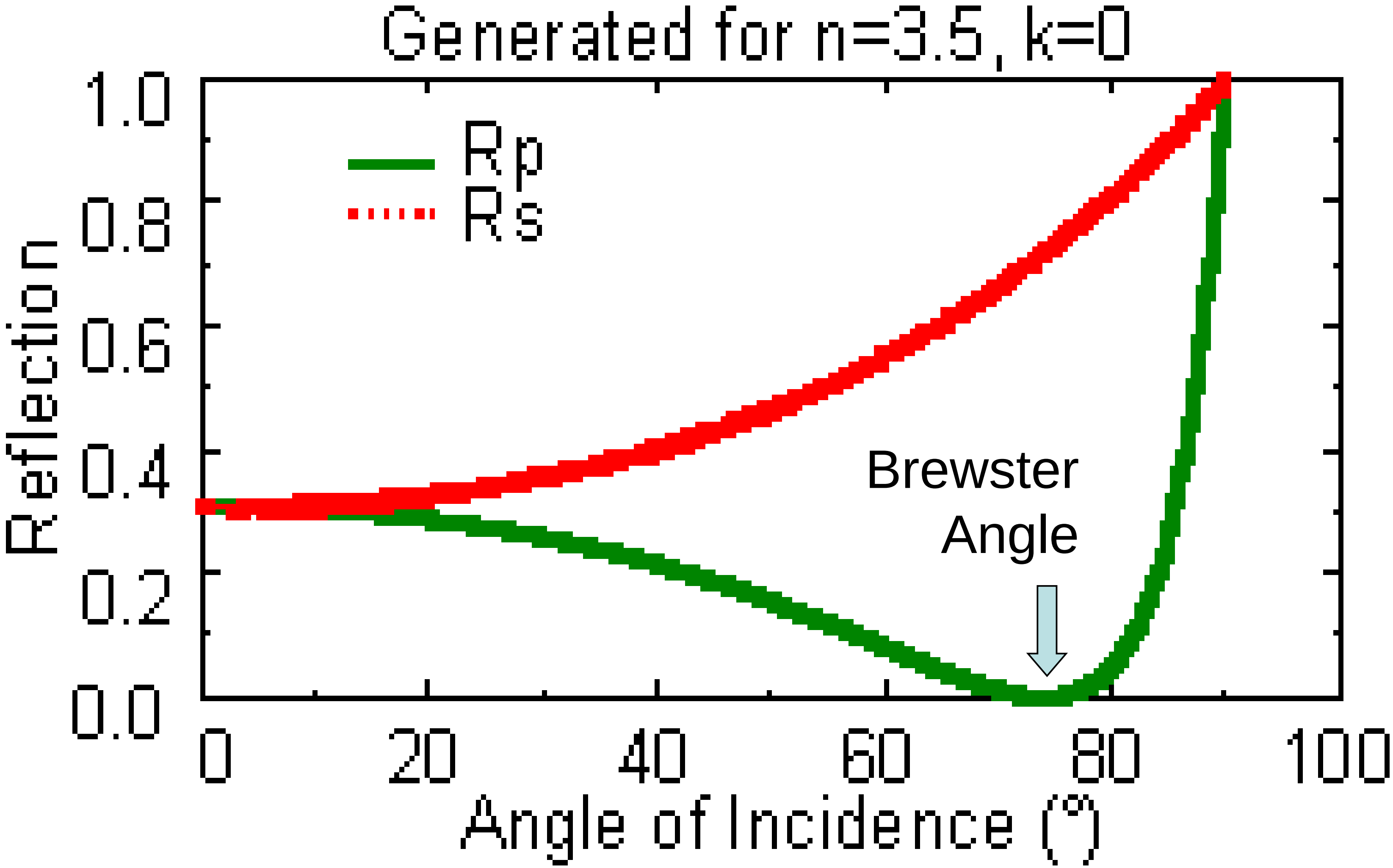
Strong extinction: $n_1 = 1$ $$R = \frac{(n_2 - 1)^2 + \kappa_2^2}{(n_2 + 1)^2 + \kappa_2^2}$$

leads to high reflectivity!

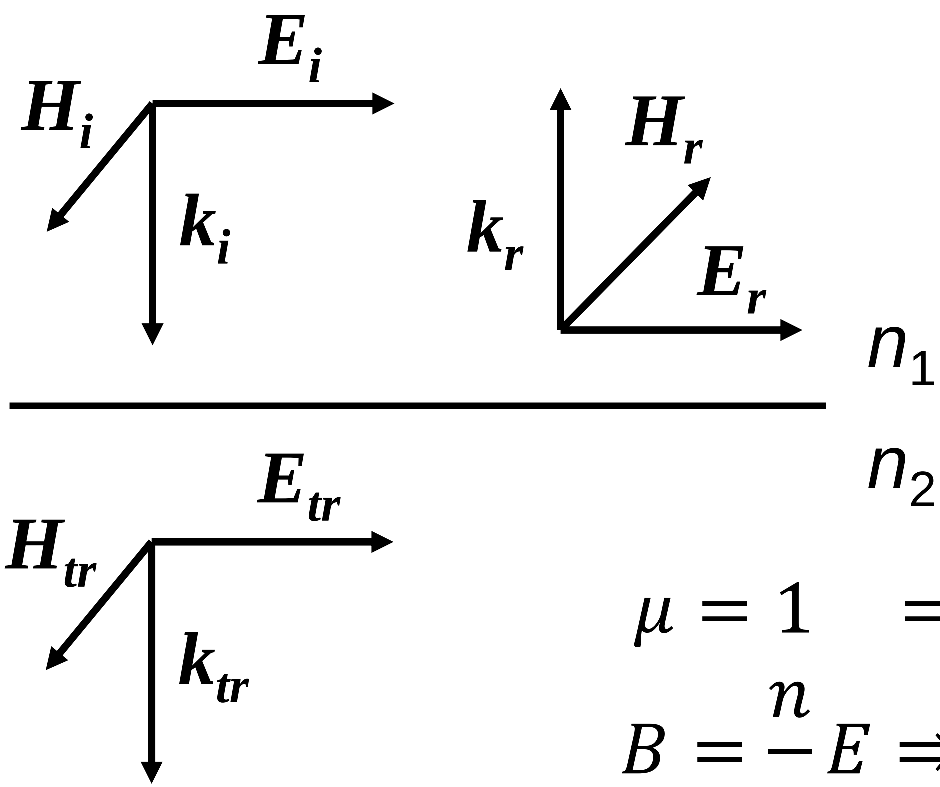
Remarks:

- R and T are related to energy flux densities
- $R + T = 1$ (without absorption)

Angular dependence of R, calculated for GaAs



Reflection coefficient for perpendicular incidence



Continuity of tangential fields

$$E_i + E_r = E_{tr} \ (*)$$

$$H_i - H_r = H_{tr}$$

$$\mu = 1 \quad \Rightarrow \quad B_i - B_r = B_{tr}$$

$$B = \frac{n}{c} E \Rightarrow \quad n_1 E_i - n_1 E_r = n_2 E_{tr}$$

$$(*) \cdot n_2 \Rightarrow \quad n_2 E_i + n_2 E_r = n_2 E_{tr}$$

$$\Rightarrow r = \frac{E_r}{E_i} = \frac{n_1 - n_2}{n_1 + n_2}$$

$r < 0 \quad \text{for } n_2 > n_1 \Rightarrow$

Phase jump for reflection on optically denser material !

IV. Light propagation through media – anisotropic media

Anisotropic media

Crystalline materials are generally anisotropic $\Rightarrow$ ε is a tensor

Typical examples:

- Crystals with uniaxial symmetry, e.g., wurtzite structure: ZnO, CdS, GaN
- Biaxial crystals
- Cubic crystals for $k \neq 0$ (however, only small effect)
- Materials under strain, application of external fields etc. (symmetry reduction)

Choice of coordinate system: $\boldsymbol{z}$-axis corresponds to symmetry axis $\boldsymbol{c}$

$\Rightarrow$ in *uniaxial* materials:

$$\varepsilon_{xx}(\omega) = \varepsilon_{yy}(\omega) \neq \varepsilon_{zz}(\omega),\ \varepsilon_{ij}(\omega) = 0 \ \text{ for } \ i \neq j$$

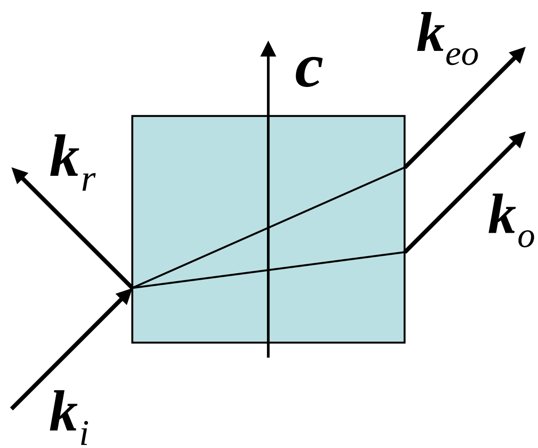
$\Rightarrow$ in *biaxial* materials:

$$\varepsilon_{xx}(\omega) \neq \varepsilon_{yy}(\omega) \neq \varepsilon_{zz}(\omega)$$

IV. Light propagation through media – anisotropic media

Birefringence

- $n(\omega)$ is polarization-dependent
- For uniaxial materials
  $\rightarrow$ two beams



extra-ordinary beam

polarization || $\boldsymbol{c}$
does not follow
Snell's law of refraction

ordinary beam

polarization $\perp$ $\boldsymbol{c}$

Example:
calcite

[wikipedia]

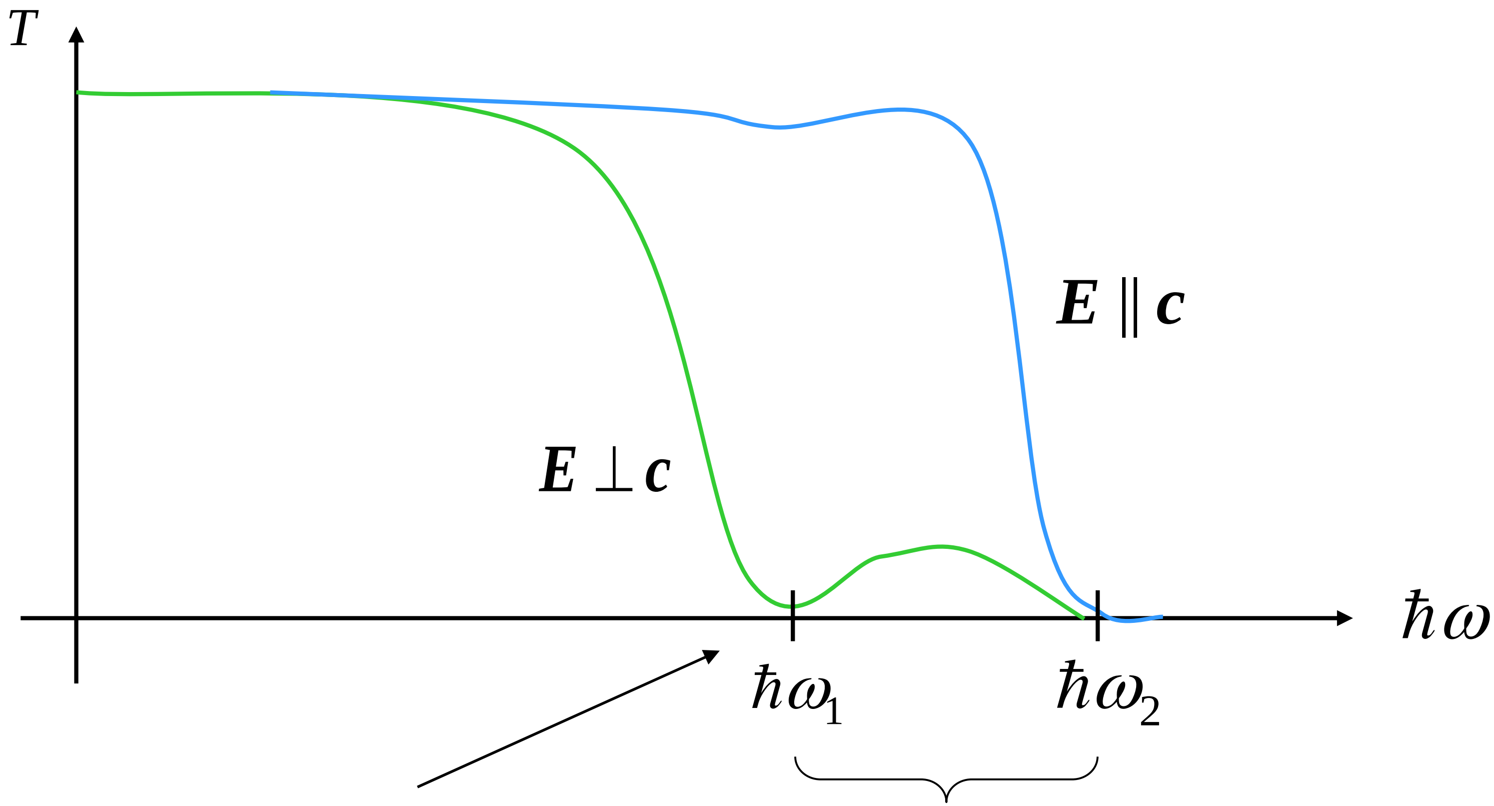
Applications:

crystal polarizers (large wavelength range, low absorption),
wave plates, non-linear optics (frequency doubling, see later)

IV. Light propagation through media – anisotropic media

Dichroism

- Transmission depends on polarization of incident light



Some resonance couples strongly
to perpendicular polarization

region of dichroism