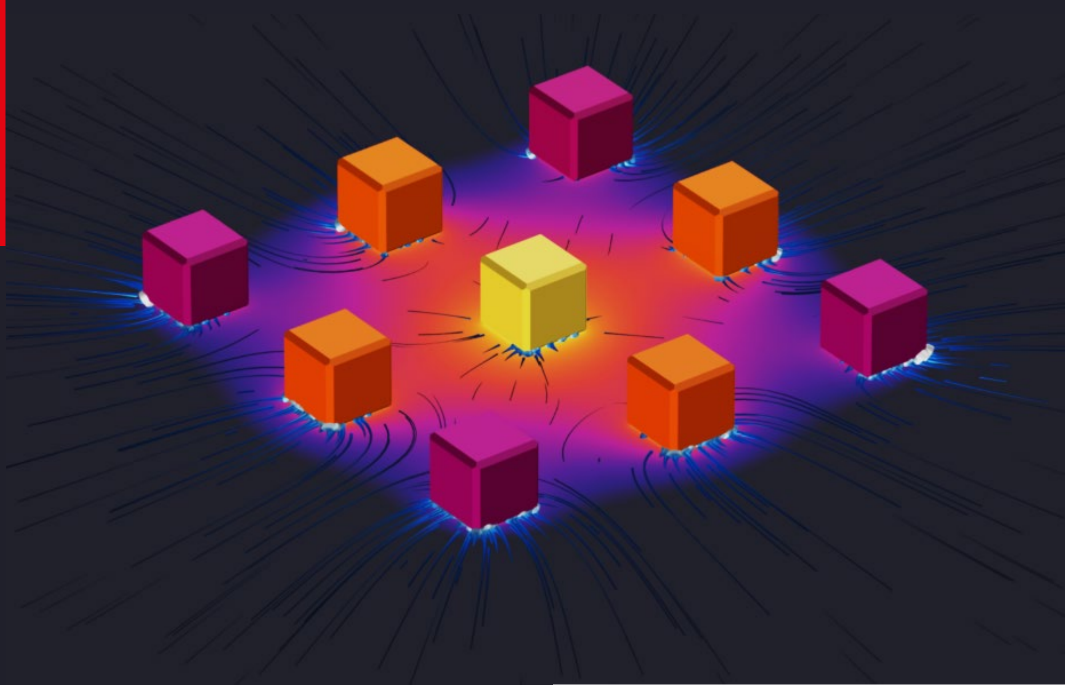
Nanoscale Heat Transfer (and Energy Conversion) ME469

Instructor: Giulia Tagliabue



École polytechnique fédérale de Lausanne

Spring Semester 2020

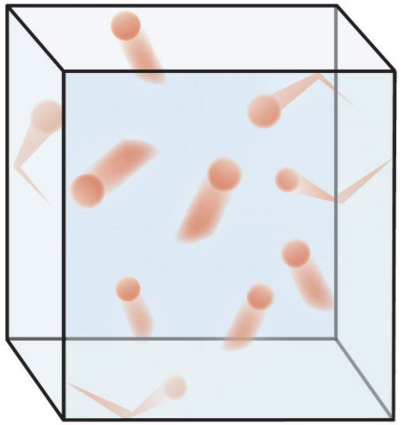
What we covered so far…

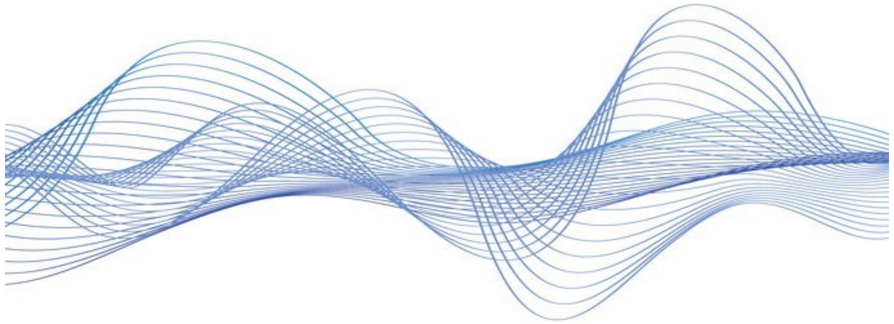
Nanoscale Heat Transfer (and Energy Conversion)

- **Energy States**
  - Introduction to Quantum Mechanics (Ch. 2)
  - Introduction to Solid State Physics (Ch. 3)
- **Thermal Energy Storage**
  - Introduction to Statistical Thermodynamics (Ch. 4)
- **Thermal Energy Transport**
  - Energy Transport by Waves (Ch. 5)
  - Energy Transport by Particles (Ch. 6 -7)
    - Classical Laws
    - Classical Size Effects
  - Energy Transport in Liquids (Ch. 9)
- **Thermal Energy Conversion**
  - Energy Conversion Mechanisms (Ch. 8)

Wave-particle Duality

The wave nature of material particles gives rise to quantum mechanical effects!





Particle View

Wave View

Energy ← $\boldsymbol{E = h\nu = \hbar\omega}$ → **Frequency, Amplitude**

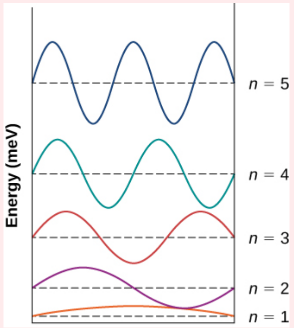
Momentum ← $\boldsymbol{p = \hbar k = \frac{h}{\lambda}}$ → **Wavevector**

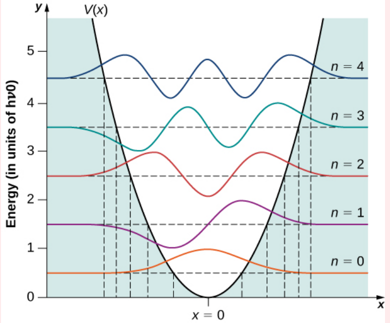
$$h = 6.6 \cdot 10^{-34} Js$$
$$\hbar = h/2\pi$$

From Quantum States to Macroscopic Properties

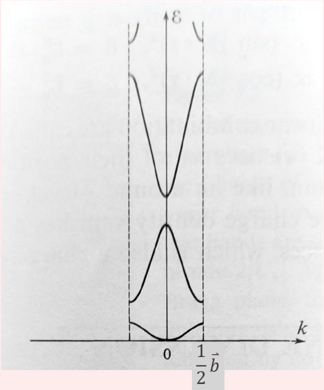
EPFL

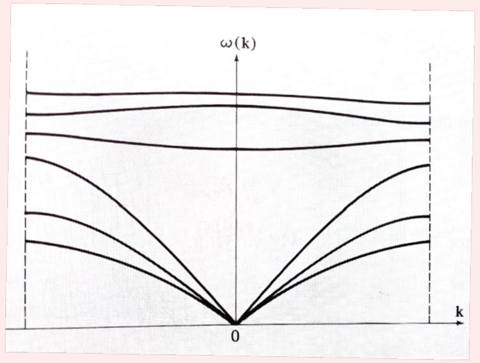
Localized potential



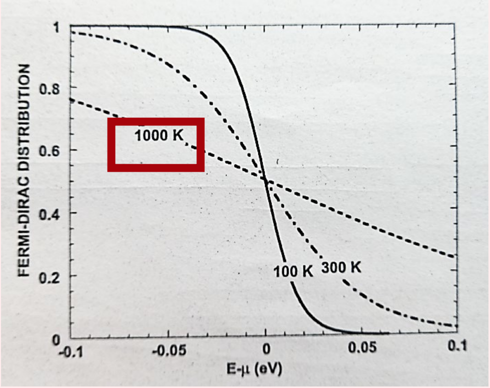


Periodic potential

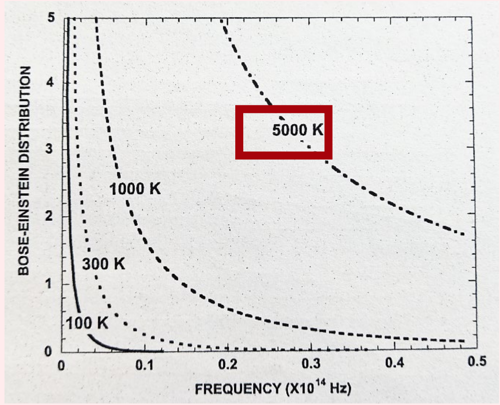


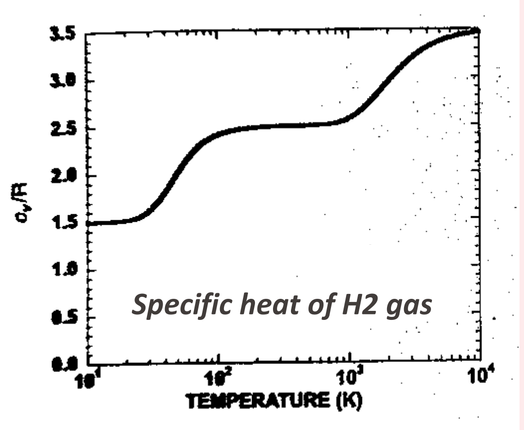


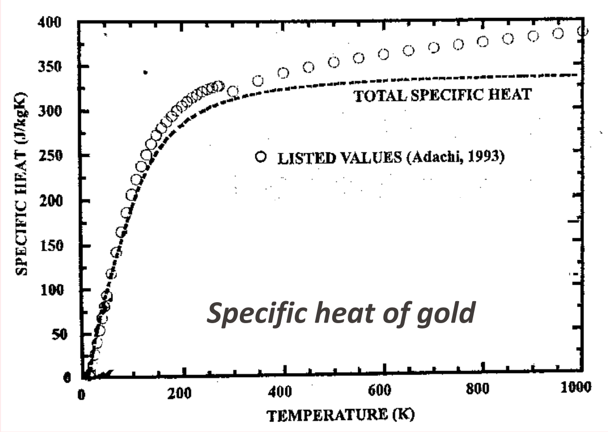
Fermi Dirac Distribution



Bose Einstein Distribution







Allowed quantum states (steady-state Schrodinger eqn)

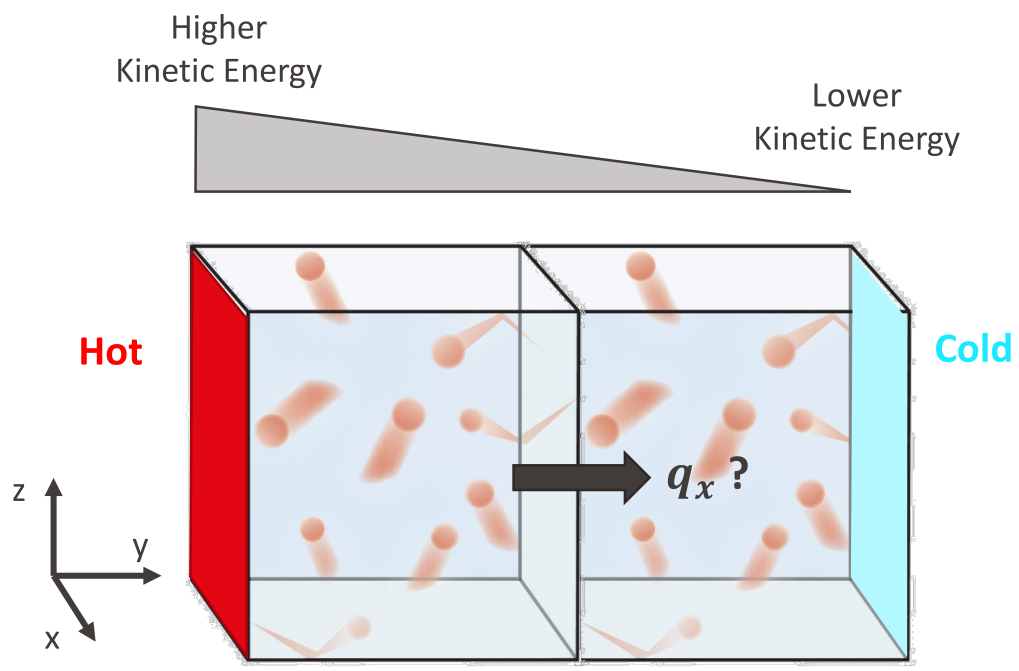
Connect quantum states and energy levels with the temperature

Probability that matter will be in a given quantum state when it is at equilibrium. (Statistical Thermodynamics)

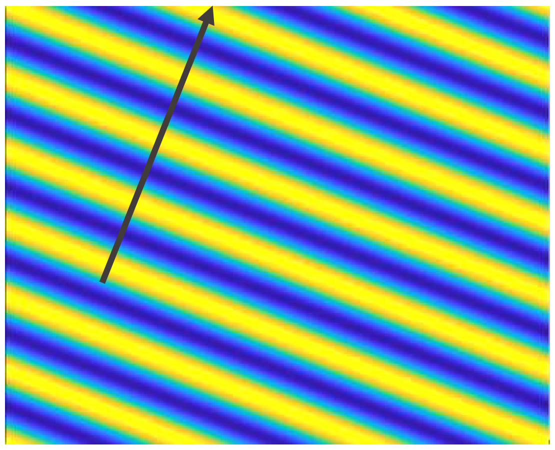
Investigate the properties of matter at finite temperatures

Macroscopic properties and their dependence on temperature

Energy Transport



Particle View



Wave View

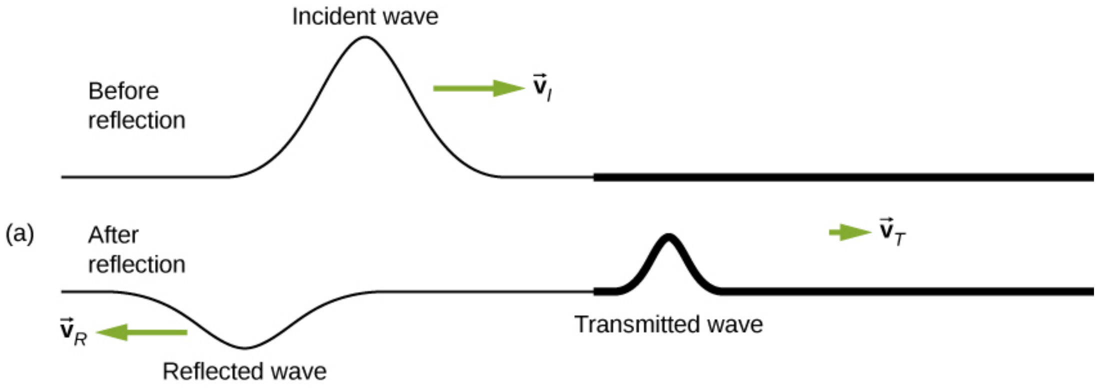
What are the peculiarities of energy transport by waves?

Energy Transport by Waves

It can be always demonstrated that the energy U transported by a wave is proportional to the square of its amplitude:

$$U \propto \left|\vec{\Phi}\right|^2$$

Contrary to classical particles, waves can be transmitted or reflected across an interface. Therefore, the energy transported on either side will depend on the amplitude of the transmitted and reflected component.



Furthermore precise phase relationship between different waves can lead to constructive or destructive interference phenomena that results in a maximization or minimization of the transported energy.

The wave nature of material particles give also rise to unique effects such as tunneling.

This Lecture

EPFL

Nanoscale Heat Transfer (and Energy Conversion)

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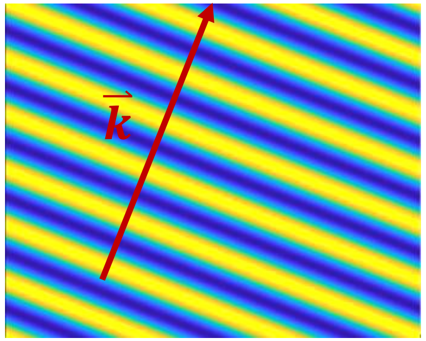
  - Energy Conversion Mechanisms (Ch. 8)

In This Lecture …

- **Plane Waves and Energy Transport***
  - **EM waves and Poynting vector**
  - **Electron Flux**
- Plane waves at an interface
  - Fresnel coefficients
  - Electron transport at an interface
- Plane waves propagating in a multilayer structure (multiple interfaces and periodicity)
- Evanescent waves and tunneling

*We will focus on photons and electrons. The detailed analysis for phonons can be found in the book (Ch. 5) and in a short version, in the supplementary slides. Indeed, as we will see, due to the very short wavelength of phonons it is very difficult to observe their wave nature.

Plane Waves and Energy Transport

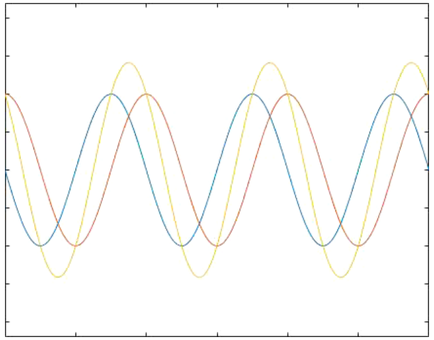


$$\vec{\Phi} = \vec{A}cos(\omega t - \vec{k}\cdot\vec{r})$$

$$\vec{k} = \frac{2\pi}{\lambda}$$

$$\Rightarrow \overrightarrow{\Phi_c} = \vec{A}e^{i\vec{k}\cdot\vec{r}}e^{-i(\omega t)} = \overrightarrow{A_c}e^{-i(\omega t)}$$

$$\Rightarrow \vec{\Phi} = \mathrm{Re}\left\{\vec{A}e^{-i(\omega t-\vec{k}\cdot\vec{r})}\right\}$$



$$\vec{\Phi} = \vec{A}cos(\omega t - \vec{k}\cdot\vec{r}) + \vec{B}sin(\omega t - \vec{k}\cdot\vec{r})$$

$$\Rightarrow \overrightarrow{\Phi_c} = \vec{C}(\vec{r})e^{-i(\omega t)}$$

$$\vec{C}(\vec{r}) = \overrightarrow{A_c} + i\overrightarrow{B_c}$$

How do we calculate the wave equation associated with different types of (material) waves?

What is the energy flux associated with different types of (material) waves?

Wave Energy Transport - Photons

The transport of photons is governed by Maxwell's equations, i.e. the propagation equations of the electromagnetic waves. There are four *fields* to consider:

$\vec{E} = electric\ field\ vector\ [V/m]$

$\vec{H} = magnetic\ field\ vector\ [A/m]$

$\vec{D} = electric\ displacement\ [C/m^2]$

$\vec{B} = magnetic\ induction\ [N/Am]$

Fields generated by the motion of ions and electrons under the force of the electric and magnetic fields.

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Fields generated by the motion of ions and electrons under the force of the electric and magnetic fields.

$$\begin{cases} \nabla \times \vec{E} = -\dfrac{\partial \vec{B}}{\partial t} \\ \nabla \times \vec{H} = \dfrac{\partial \vec{D}}{\partial t} + \vec{J_e} \\ \nabla \cdot \vec{D} = \rho_e \\ \nabla \cdot \vec{B} = 0 \end{cases}$$

$\rho_e = net\ charge\ density\ [C/m^3]$

To connect the $\vec{E}$, $\vec{H}$ to $\vec{D}$ and $\vec{B}$ we need to introduce the physical properties of the material through the constitutive equations. We have:

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P} \qquad \vec{P} = \varepsilon_0 \chi \vec{E}$$

where

$\varepsilon_0 =$ vacuum permittivity $= 8.85 \cdot 10^{-12} [F/m]$

$\vec{P} = polarizability\ [C/m^2]$

$\chi =$ susceptibility

$$\vec{B} = \mu \vec{H}$$

where

$\mu = magnetic\ permeability$

Non-magnetic materials: $\mu = \mu_0 = 4\pi \cdot 10^{-7} [H/m]$

Diamagnetic materials: $\mu < \mu_0$

Paramagnetic materials: $\mu > \mu_0$

$$\vec{J_e} = \sigma_e \vec{E}$$

where

$\sigma_e = electrical\ conductivity\ [1/\Omega m]$

Wave Energy Transport - Photons

EPFL

To identify the form of the solution to Maxwell's equation we calculate: $\nabla \times \nabla \times \vec{E} = -\frac{\partial(\nabla \times \vec{B})}{\partial t}$

For $\rho_e = 0$ (no net charge) and ε independent of space $\nabla \times \nabla \times \vec{E} = \nabla(\nabla \cdot \vec{E}) - \nabla^2 \vec{E} = \frac{1}{\varepsilon}\nabla(\nabla \cdot \vec{D}) - \nabla^2 \vec{E} = -\nabla^2 \vec{E}$

$$-\frac{\partial(\nabla \times \vec{B})}{\partial t} = -\mu \frac{\partial(\nabla \times \vec{H})}{\partial t} = -\mu \frac{\partial^2 \vec{D}}{\partial t^2} - \mu \frac{\partial \vec{J_e}}{\partial t} = -\mu\varepsilon \frac{\partial^2 \vec{E}}{\partial t^2} - \mu\sigma_e \frac{\partial \vec{E}}{\partial t}$$

$$\Rightarrow \quad \nabla^2 \vec{E} = \mu\varepsilon \frac{\partial^2 \vec{E}}{\partial t^2} + \mu\sigma_e \frac{\partial \vec{E}}{\partial t}$$

Wave-equation
Damping term determined by the absorption by free-electrons.
If $\sigma_e = 0$ no damping

We guess: $\overrightarrow{E_c}(\vec{r}, t) = \overrightarrow{E_0} e^{-i(\omega t - \vec{k}\cdot\vec{r})}$ $\Rightarrow$ $\vec{k} \cdot \vec{k} = \mu\omega^2 \left[\varepsilon_0(1+\chi) + i\frac{\sigma_e}{\omega}\right]$ $\Rightarrow$ $\left|\vec{\boldsymbol{k}}\right| = \sqrt{\boldsymbol{\mu\varepsilon_c}}\boldsymbol{\omega} = \frac{\boldsymbol{N}}{\boldsymbol{c_0}}\boldsymbol{\omega}$

where $\varepsilon_c = \varepsilon_0(1+\chi) + i\frac{\sigma_e}{\omega} = \varepsilon_0\left[(1+\chi) + i\frac{\sigma_e}{\varepsilon_0\omega}\right] = \varepsilon_0\varepsilon_r$ $\quad \varepsilon_r = (1+\chi) + i\frac{\sigma_e}{\varepsilon_0\omega}$

$\varepsilon_c =$ *complex permittivity* $[F/m]$
$\varepsilon_r =$ *complex relative permittivity*

$c_0 = \frac{1}{\sqrt{\mu_0\varepsilon_0}}$ $\quad c = c_0/N$

$N = \sqrt{\frac{\mu\varepsilon_c}{\mu_0\varepsilon_0}} = n + i\kappa$ $\quad N =$ *complex refractive index*

$n =$ *(real part) refractive index*

$\kappa =$ *(imaginary part) refreactive index*
= extinction coefficient

It can be shown that **an electromagnetic wave in vacuum must be a transverse wave**, i.e. $\vec{E} \perp \vec{H} \perp \vec{k}$

Wave Energy Transport - Photons

EPFL

We now consider an electromagnetic wave traveling along x $(\vec{k} = \pm k_x)$ with electric field polarized along y and magnetic field along z, we have:

$$\overrightarrow{E_c}(y,t) = E_{y0} e^{-i\omega\left(t \mp \frac{N}{c_0}x\right)} \hat{y}$$

$$\overrightarrow{H_c}(y,t) = H_{z0} e^{-i\omega\left(t \mp \frac{N}{c_0}x\right)} \hat{z}$$

$$H_{z0} = \pm \frac{N}{\mu c_0} E_{y0}$$

We now want to find an expression for the energy flow associated with an electromagnetic wave. Again we need to manipulate the Maxwell equations:

$$\vec{H} \cdot (\nabla \times \vec{E}) = -\frac{\partial}{\partial t}(\vec{H} \cdot \vec{B})$$

$$\vec{E} \cdot (\nabla \times \vec{H}) = \frac{\partial \vec{D}}{\partial t}(\vec{E} \cdot \vec{D}) + \vec{E} \cdot \vec{J_e}$$

$$-\nabla \cdot (\vec{E} \times \vec{H}) = \frac{\partial}{\partial t}\left[\frac{1}{2}\mu \vec{H} \cdot \vec{H} + \frac{1}{2}\varepsilon \vec{E} \cdot \vec{E}\right] + \vec{E} \cdot \vec{J_e}$$

$$\Rightarrow \quad -\iiint \nabla \cdot (\vec{E} \times \vec{H}) dV = \iiint \left\{\frac{\partial}{\partial t}\left[\frac{1}{2}\mu \vec{H} \cdot \vec{H} + \frac{1}{2}\varepsilon \vec{E} \cdot \vec{E}\right] + \vec{E} \cdot \vec{J_e}\right\} dV$$

$$\Rightarrow \quad -\oiint (\vec{E} \times \vec{H}) \cdot \hat{n} dA = \iiint \left\{\frac{\partial}{\partial t}\left[\frac{1}{2}\mu \vec{H} \cdot \vec{H} + \frac{1}{2}\varepsilon \vec{E} \cdot \vec{E}\right] + \vec{E} \cdot \vec{J_e}\right\} dV$$

- Instantaneous energy flux INTO the control volume $[W/m^2]$
- Magnetic energy density $[J/m^3]$
- Electric energy density $[J/m^3]$
- Dissipation (joule heating) $[W/m^3]$

$\Rightarrow$ $\vec{\boldsymbol{S}} = \vec{\boldsymbol{E}} \times \vec{\boldsymbol{H}}$ **Poynting vector**

$\Rightarrow$ $\langle \vec{S} \rangle = \frac{1}{T}\int_t^{t+T} \vec{S} dt' = \frac{\boldsymbol{1}}{\boldsymbol{2}} \boldsymbol{Re}\left\{\overrightarrow{\boldsymbol{E_c}} \times \overrightarrow{\boldsymbol{H_c^*}}\right\}$ **Time averaged Poynting vector**

Wave Energy Transport - Photons

We now want to calculate the time average Poynting vector for a plane electromagnetic wave travelling in a material with complex refractive index N.

$$\overrightarrow{E_c}(y,t) = E_{y0}e^{-i\omega\left(t-\frac{N}{c_0}x\right)}\hat{y}$$

$$\overrightarrow{H_c}(y,t) = H_{z0}e^{-i\omega\left(t-\frac{N}{c_0}x\right)}\hat{z} = \frac{N}{\mu c_0}E_{y0}e^{-i\omega\left(t-\frac{N}{c_0}x\right)}\hat{z} \qquad N = \sqrt{\varepsilon_r} = n + i\kappa$$

$$\Rightarrow \overrightarrow{H_c^*}(y,t) = H_{z0}e^{i\omega\left(t-\frac{N^*}{c_0}x\right)}\hat{z} = \frac{N^*}{\mu c_0}E_{y0}^*e^{i\omega\left(t-\frac{N^*}{c_0}x\right)}\hat{z} \qquad N^* = n - i\kappa$$

$$\Rightarrow \langle\vec{S}\rangle = \frac{1}{2}Re\left\{\overrightarrow{E_c}\times\overrightarrow{H_c^*}\right\} = \frac{1}{2}Re\left\{E_{y0}\frac{N^*}{\mu c_0}E_{y0}^*e^{-i\omega\left(t-\frac{N}{c_0}x\right)}e^{i\omega\left(t-\frac{N^*}{c_0}x\right)}\right\}(\hat{y}\times\hat{z}) = \frac{1}{2}Re\left\{\frac{n-i\kappa}{\mu c_0}e^{\left(-\frac{2\omega\kappa}{c_0}x\right)}\right\}E_{y0}^2\hat{x}$$

$$\Rightarrow \langle\vec{S}\rangle = \frac{1}{2}\frac{n}{\mu c_0}e^{\left(-\frac{2\omega\kappa}{c_0}x\right)}E_{y0}^2\hat{x} = \frac{1}{2}\frac{n}{\mu c_0}e^{\left(-\frac{4\pi\kappa}{\lambda_0}x\right)}E_{y0}^2\hat{x}$$

where $\omega = kc = \frac{2\pi}{\lambda}c$

$$\Rightarrow \langle\vec{S}\rangle = \frac{1}{2}\frac{n}{\mu c_0}e^{(-\alpha x)}E_{y0}^2\hat{x}$$

where $\alpha = \frac{4\pi\kappa}{\lambda_0} = absorption\ coefficient$

The energy decreases exponentially

The energy is proportional to the square of the amplitude

Wave Energy Transport - Electrons

For a free electron ($U = const$) we can show that the wavefunction is a plane wave*****:

$$\Psi_t = Y(t)\Psi(x) = Ae^{-i(\omega t + kx)} + Be^{-i(\omega t - kx)} \qquad k = \sqrt{\frac{2m(E-U)}{\hbar^2}}$$

Furthermore we have seen that from the Schrodinger equation we can derive a continuity equation from which the particle current (or flux) can be calculated as******:

$$\vec{J}(\vec{r},t) = \frac{i\hbar}{2m}\left[\Psi_t \nabla \Psi_t^{\,*} - \Psi_t^{\,*} \nabla \Psi_t\right] = Re\left[\frac{i\hbar}{m}\Psi_t \nabla \Psi_t^{\,*}\right]$$

*see Lecture L3, slide 12 for the case U=0 **see Lecture L3, slide 10

Plane Waves and Energy Transport - Summary

Wave type	Wave Equation	Energy Flux
Photons	$\overrightarrow{E_c}(\vec{r},t) = \overrightarrow{E_0} e^{-i\omega\left(t-\frac{N}{c_0}\hat{k}\cdot\vec{r}\right)}$ $c_0 = 1/\sqrt{\mu_0\varepsilon_0}$ $N = n + i\kappa$	$\langle\vec{S}\rangle = \frac{1}{2} Re\left\{\overrightarrow{E_c} \times \overrightarrow{H_c^*}\right\}$
Electrons	$\Psi_t = Ae^{-i(\omega t+kx)} + Be^{-i(\omega t-kx)}$ $k = \sqrt{(2m(E-U))/\hbar\text{^}2}$	$\vec{J}(\vec{r},t) = Re\left[\frac{i\hbar}{m}\Psi_t\nabla\Psi_t{}^*\right]$
Phonons	$\overrightarrow{v_{T1}} = \hat{a}A_{T1}e^{-i(\omega t-k_T\hat{k}\cdot\vec{r})}$ $\overrightarrow{v_{T2}} = \hat{a}\times\hat{k}A_{T2}e^{-i(\omega t-k_T\hat{k}\cdot\vec{r})}$ $\overrightarrow{v_L} = \hat{k}A_L e^{-i(\omega t-k_L\hat{k}\cdot\vec{r})}$	$\vec{J}_{ac} = -\frac{1}{2} Re\left[\overrightarrow{v^*}\cdot\bar{\bar{\sigma}}\right]$

How do waves transfer energy across an interface?

In This Lecture …

- Plane Waves and Energy Transport*
  - EM waves and Poynting vector
  - Electron Flux
- **Plane waves at an interface**
  - **Fresnel coefficients**
  - **Electron transport at an interface**
- Plane waves propagating in a multilayer structure (multiple interfaces and periodicity)
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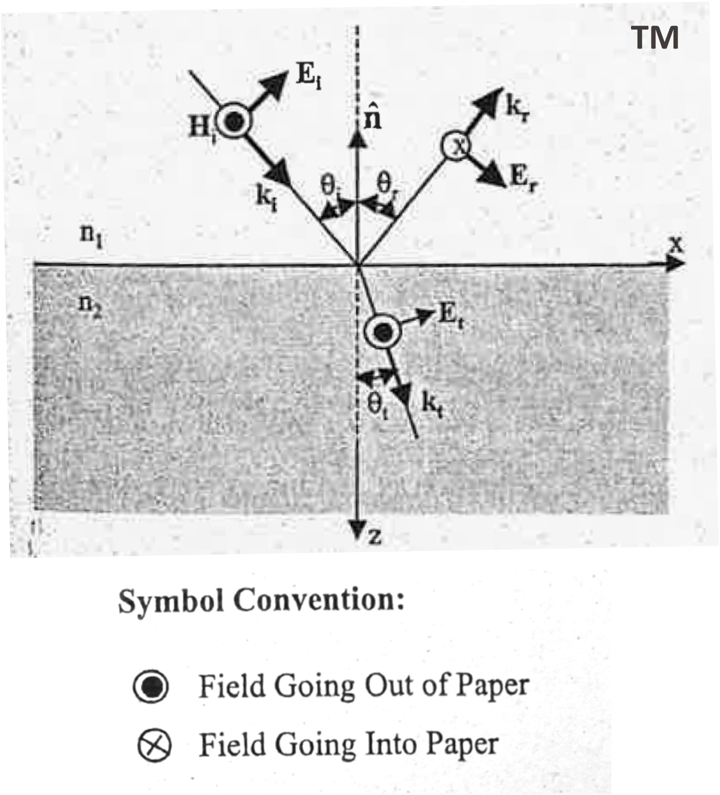
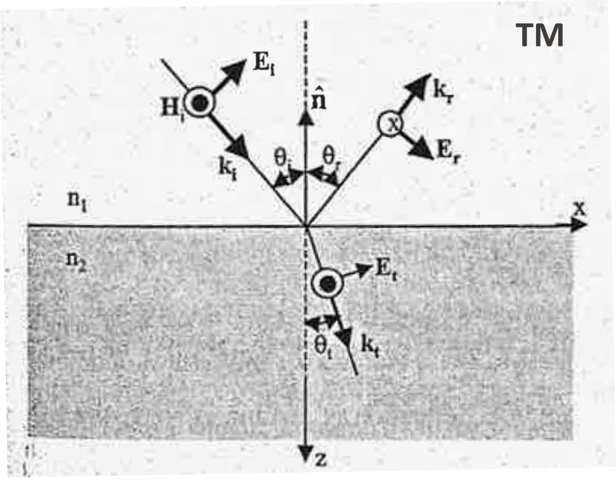
Plane Waves at an Interface - Photons



When an electromagnetic waves reaches an interfaces it can be reflected or refracted.
We need to take into account the **polarization** of the wave with respect to the interface.

- **Transverse Magnetic** (TM) wave (also called p-wave or // wave)
  - ➢ The electric field lies in the plane of incidence
  - ➢ The component of the electric field perpendicular to the interface changes with the angle of incidence
- **Transverse Electric** (TE) wave (also called s-wave or ⊥ wave)
  - ➢ The electric field is perpendicular to the plane of incidence
  - ➢ The electric field is only parallel to the interface and its magnitude does not change with the angle of incidence

Plane Waves at an Interface - Photons



To solve the problem we need to define appropriate boundary conditions at the interface.
It can be shown from Maxwell equations that the following conditions must be satisfied at the interface*:

$$\hat{\mathbf{n}} \bullet (\mathbf{D}_2 - \mathbf{D}_1) = \rho_s$$

The difference of the normal components of the displacement fields is related to the net surface charge density ρ_s

$$\hat{\mathbf{n}} \times (\mathbf{E}_2 - \mathbf{E}_1) = 0$$

The tangential components of the electric field must be continuous

$$\hat{\mathbf{n}} \bullet (\mathbf{B}_2 - \mathbf{B}_1) = 0$$

The normal components of the magnetic induction field must be continuous

$$\hat{\mathbf{n}} \times (\mathbf{H}_2 - \mathbf{H}_1) = J_s$$

The difference of the tangential components of the magnetic field is related to the net surface current density J_s

We consider a plane **TM wave** (shown in the picture) propagating from the lossless medium 1 to lossless medium 2 with an incidence angle θ_i.
The incident, reflected and transmitted electric fields can be written as:

$$\mathbf{E}_{//i} \exp\left[-i\omega\left(t - \frac{n_1 x \sin\theta_i + n_1 z \cos\theta_i}{c_0}\right)\right]$$

$$\mathbf{E}_{//r} \exp\left[-i\omega\left(t - \frac{n_1 x \sin\theta_r - n_1 z \cos\theta_r}{c_0}\right)\right]$$

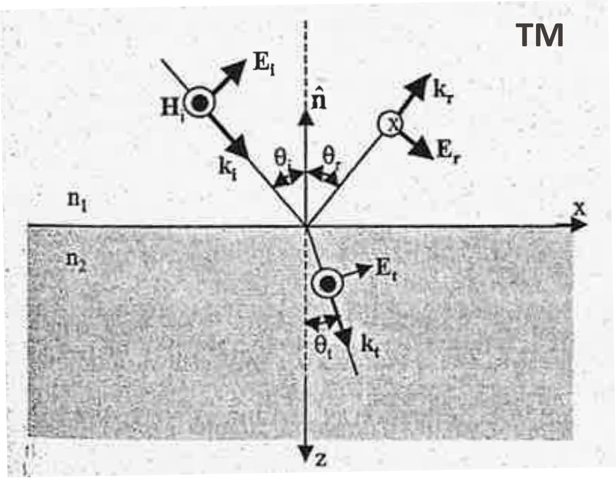
$$\mathbf{E}_{//t} \exp\left[-i\omega\left(t - \frac{n_2 x \sin\theta_t - n_2 z \cos\theta_t}{c_0}\right)\right]$$

$$H_y = \frac{n}{\mu c_0} E_{//} (\text{forward}), \quad H_y = -\frac{n}{\mu c_0} E_{//} (\text{backward})$$

*see Griffith, Ch. 7

Plane Waves at an Interface - Photons

EPFL



$$\mathbf{E}_{//i} \exp\left[-i\omega\left(t - \frac{n_1 x \sin\theta_i + n_1 z \cos\theta_i}{c_0}\right)\right]$$

$$\mathbf{E}_{//r} \exp\left[-i\omega\left(t - \frac{n_1 x \sin\theta_r - n_1 z \cos\theta_r}{c_0}\right)\right]$$

$$\mathbf{E}_{//t} \exp\left[-i\omega\left(t - \frac{n_2 x \sin\theta_t - n_2 z \cos\theta_t}{c_0}\right)\right]$$

$$H_y = \frac{n}{\mu c_0} E_{//}(\text{forward}), \quad H_y = -\frac{n}{\mu c_0} E_{//}(\text{backward})$$

For an interface free of charge we get:

$$\cos\theta_i E_{//i} \exp\left[i\omega \frac{n_1 x \sin\theta_i}{c_0}\right] + \cos\theta_r E_{//r} \exp\left[i\omega \frac{n_1 x \sin\theta_r}{c_0}\right] = \cos\theta_t E_{//t} \exp\left[i\omega \frac{n_2 x \sin\theta_t}{c_0}\right]$$

➡ $n_1 sin\theta_i = n_1 sin\theta_r = n_2 sin\theta_t$

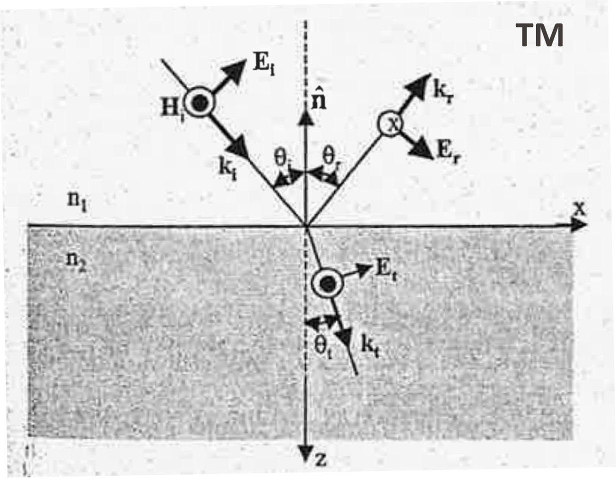
➡ $\boldsymbol{n_1 sin\theta_i = n_2 sin\theta_t}$ $\quad$ $\boldsymbol{\theta_i = \theta_r}$ $\quad$ **Snell's law**

Additionally we obtain the following expressions for the fields:

$$\cos\theta_i E_{//i} + \cos\theta_i E_{//r} = \cos\theta_t E_{//t}$$

$$n_1 E_{//i} - n_1 E_{//r} = n_2 E_{//t}$$

Plane Waves at an Interface - Photons



$$\mathbf{E}_{//i} \exp\left[-i\omega\left(t - \frac{n_1 x \sin\theta_i + n_1 z \cos\theta_i}{c_0}\right)\right]$$

$$\mathbf{E}_{//r} \exp\left[-i\omega\left(t - \frac{n_1 x \sin\theta_r - n_1 z \cos\theta_r}{c_0}\right)\right]$$

$$\mathbf{E}_{//t} \exp\left[-i\omega\left(t - \frac{n_2 x \sin\theta_t - n_2 z \cos\theta_t}{c_0}\right)\right]$$

$$\cos\theta_i E_{//i} + \cos\theta_i E_{//r} = \cos\theta_t E_{//t}$$

$$n_1 E_{//i} - n_1 E_{//r} = n_2 E_{//t}$$

We define a reflection and a transmission coefficient as the ratio of the amplitudes of the electric fields. These are also called **Fresnel coefficients**.

TM wave:

$$r_{//} = \frac{E_{//r}}{E_{//i}} = \frac{-n_2 \cos\theta_i + n_1 \cos\theta_t}{n_2 \cos\theta_i + n_1 \cos\theta_t}$$

$$t_{//} = \frac{E_{//t}}{E_{//i}} = \frac{2n_1 \cos\theta_i}{n_2 \cos\theta_i + n_1 \cos\theta_t}$$

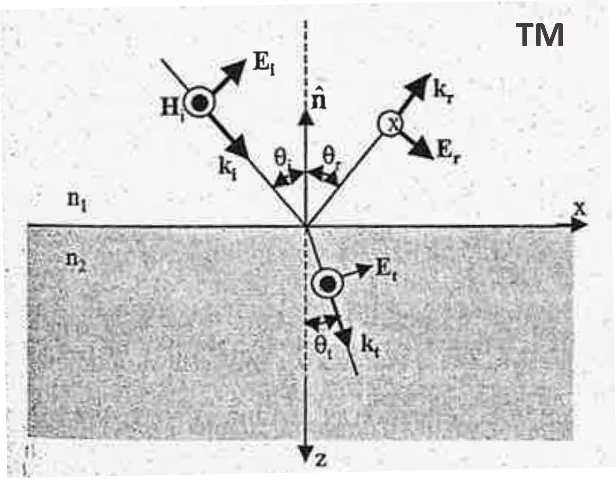
TE wave:

$$r_{\perp} = \frac{n_1 \cos\theta_i - n_2 \cos\theta_t}{n_1 \cos\theta_i + n_2 \cos\theta_t}$$

$$t_{\perp} = \frac{2n_1 \cos\theta_i}{n_1 \cos\theta_i + n_2 \cos\theta_t}$$

Note: For an absorbing medium, we need to use the complex N instead of the real n. If N_2 is complex we obtain a complex refraction angle θ_t which corresponds to an inhomogeneous wave, i.e. where constant amplitude and constant phase surfaces do not coincide.

Plane Waves at an Interface - Photons



Once the fields are known we can calculate the energy fluxes. For a TM wave we have:

$$\langle \mathbf{S} \rangle = \frac{1}{2}\mathrm{Re}(\mathbf{E} \times \mathbf{H}^*) = -\frac{1}{2}\mathrm{Re}(E_z H_y^*)\hat{\mathbf{x}} + \frac{1}{2}\mathrm{Re}(E_x H_y^*)\hat{\mathbf{z}}$$

$$= \frac{n}{2\mu c_0} E_{//}^2 \sin\theta \,\hat{\mathbf{x}} + \frac{n}{2\mu c_0} E_{//}^2 \cos\theta \,\hat{\mathbf{z}}$$

$$= \langle S_x \rangle \hat{\mathbf{x}} + \langle S_z \rangle \hat{\mathbf{z}}$$

Parallel to the interface ($\langle S_x \rangle \hat{\mathbf{x}}$) — *Across the interface* ($\langle S_z \rangle \hat{\mathbf{z}}$)

We thus define the reflectivity and the transmissivity by calculating the ratio of the power normal to the interface $S_{i,z}$:

TM wave:

$$R_{//} = \frac{S_{//r,z}}{S_{//i,z}} = \frac{S_{//r}}{S_{//i}} = |r_{//}|^2$$

$$\tau_{//} = \frac{S_{//t,z}}{S_{//i,z}} = \frac{S_{//t}}{S_{//i}} = \frac{\mathrm{Re}(N_2^* \cos\theta_t)}{\mathrm{Re}(N_1^* \cos\theta_i)} |t_{//}|^2$$

TE wave:

$$R_\perp = |r_\perp|^2$$

$$\tau_\perp = \frac{\mathrm{Re}(N_2 \cos\theta_t)}{\mathrm{Re}(N_1 \cos\theta_i)} |t_\perp|^2$$

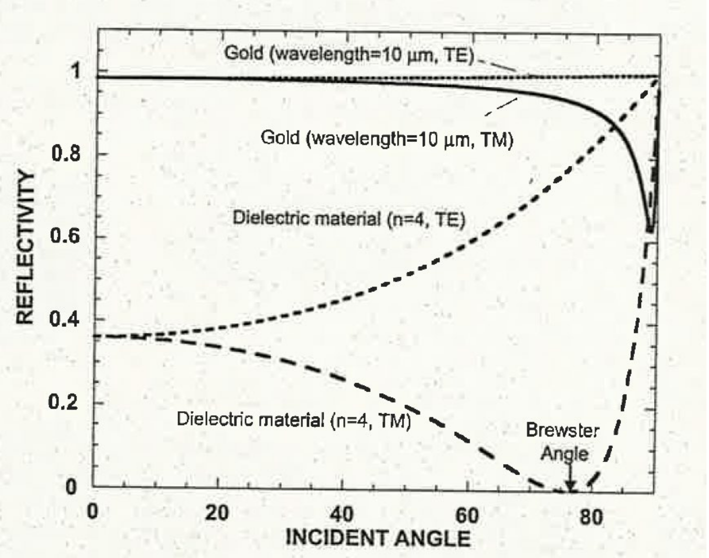
For a non-absorbing medium: $R + \tau = 1$

At normal incidence:

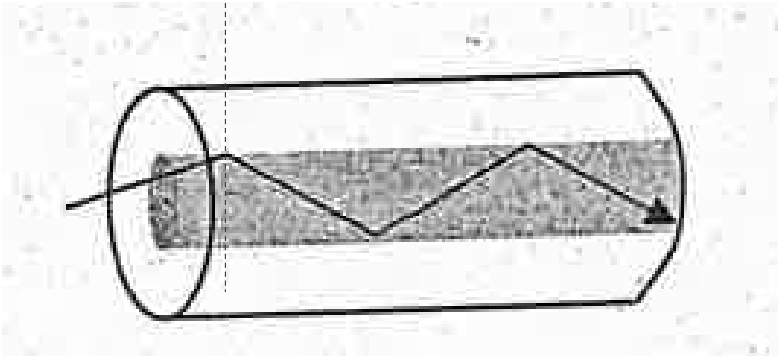
$$R = R_{//} = R_\perp = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2 = \left|\frac{N_2 - n_1}{N_2 + n_1}\right|^2 = \frac{(n_2 - n_1)^2 + (\kappa_2 - \kappa_1)^2}{(n_2 + n_1)^2 + (\kappa_2 + \kappa_1)^2}$$

Plane Waves at an Interface - Photons

We observe two interesting conditions:



When $tan\theta_B = n_2/n_1$ then the reflectivity of a TM wave, $r_{||} = 0$ and therefore only the TE component is reflected.
This angle is called **Brewster angle**.



When $n_1 > n_2$ there exist a critical angle θ_c above which no real solution for θ_t exists:

$$n_1 sin\theta_c = n_2 \sin(\pi/2) \quad \Rightarrow \quad \theta_c = \arcsin(n_2/n_1)$$

This is the condition of **total internal reflection**. We will see later what it means

Plane Waves at an Interface - Photons

Let's now briefly consider the dissipation. For example, let's consider a laser beam incident on a metallic film (normal incidence). Knowing the complex refractive index of the metal at the laser wavelength, we want to determine the energy dissipation profile.

From the Poynting vector expression we know that the energy flux decreases exponentially inside the metal, thus the intensity will be equal to:

$$I = (1 - R) I_i e^{-\alpha x} \ [\mathrm{W\,m^{-2}}]$$

where

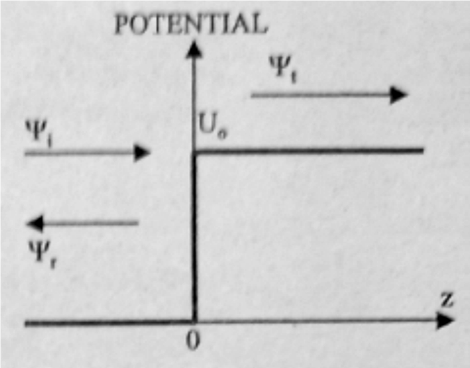
$$R = \left| \frac{1 - N}{1 + N} \right|^2 \qquad \alpha = \frac{4\pi\kappa}{\lambda}$$

Thus the heat dissipation will be :

$$\dot{q} = -\frac{dI}{dx} = (1 - R)\alpha I_i e^{-\alpha x} \ [\mathrm{W\,m^{-3}}]$$

We observe that, is the medium is infinite the energy transmitted into the medium will be eventually absorbed, hence the transmittivity equals the absorptivity. We remind that based on Kirchoff's laws, the emissivity is equal to the absorptivity at the same incident direction and wavelength.

Plane Waves at an Interface - Electrons



When an electron reaches the interface between two materials we expect it will be subject to a different potential.
We can thus understand what will happen by calculating the transmission and reflection of an electron wave at a potential step.

Incident wave: $\Psi_i = A_i e^{-i(\omega t - k_1 x)}$

Reflected wave: $\Psi_r = A_r e^{-i(\omega t + k_1 x)}$

Transmitted wave: $\Psi_t = A_t e^{-i(\omega t - k_2 x)}$

$$\omega = \frac{E}{\hbar},\ k_1 = \sqrt{\frac{2mE}{\hbar^2}},\ k_2 = \sqrt{\frac{2m(E-U_0)}{\hbar^2}}$$

To find the amplitudes of these three waves we need to apply continuity of the function and its first-derivative at the interface. We obtain the reflection and transmission coefficients:

$$r = \frac{A_r}{A_i} = \frac{k_1 - k_2}{k_1 + k_2} \text{ and } t = \frac{A_t}{A_i} = \frac{2k_1}{k_1 + k_2}$$

We then know that to each wave we have an associated flux of particles $\vec{J}$. We can thus calculate the reflectivity and transmissivity of the electron flux:

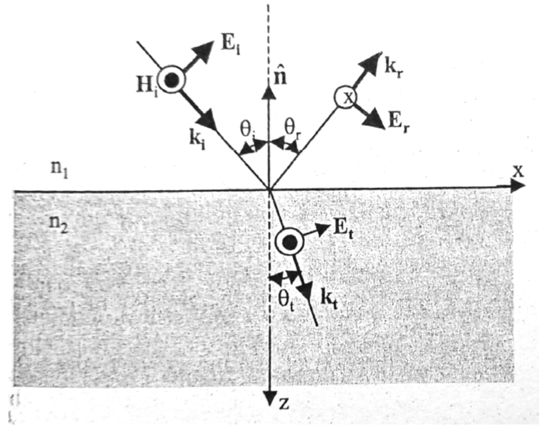
$$R = \frac{J_r}{J_i} = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2$$

$$\tau = \frac{J_t}{J_i} = \frac{\mathrm{Re}\left[k_2^* A_t A_t^*\right]}{\mathrm{Re}\left[k_1^* A_i A_i^*\right]} = \frac{4\,\mathrm{Re}(k_1 k_2^*)}{|k_1 + k_2|^2} = 1 - R$$

- For $E > U_0$, the wave will be partially transmitted and partially reflected. This is contrary to the common experience of classical mechanics and it is a quantum effect dictated by the wave nature of the particle.
- For $E < U_0$, k_2 is imaginary. Therefore Ψ_t is an **evanescent wave** (exponential decay). It can be shown that $R = 1$ and $\tau = 0$.

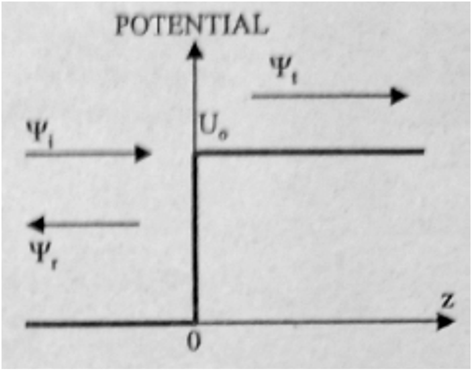
Plane Waves at an Interface

Photons



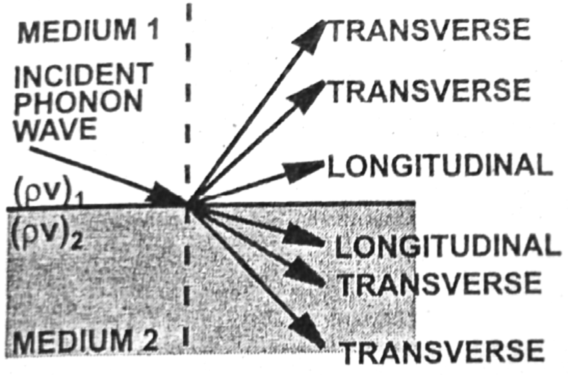
Reflection and Refraction
TM and TE waves
Brewster Angle & Total Internal reflection

Electrons



Reflection and Transmission
Evanescent Wave for E<U
Reflection even for E>U

Phonons



Reflection and Refraction
Coupling between different polarizations

How do we describe wave propagation across multiple interfaces?

What happens in periodic structures?

How does the thickness of a layer impact the propagation?

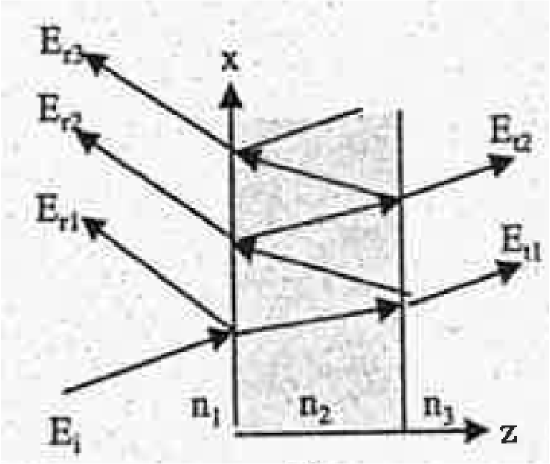
In This Lecture ...

- Plane Waves and Energy Transport*
  - EM waves and Poynting vector
  - Electron Flux
- Plane waves at an interface
  - Fresnel coefficients
  - Electron transport at an interface
- **Plane waves propagating in a multilayer structure (multiple interfaces and periodicity)**
- Evanescent waves and tunneling

*We will focus on photons and electrons. The detailed analysis for phonons can be found in the book (Ch. 5) and in a short version, in the supplementary slides. Indeed, as we will see, due to the very short wavelength of phonons it is very difficult to observe their wave nature.

Wave Propagation in Thin Films

EPFL



When multiple interfaces are present, there will be a superposition between reflected and transmitted waves at every interface:

- Depending on the thickness of the layer, the reflected and transmitted waves can interfere constructively or destructively.
- The observed reflection and transmission will depend on the thickness of the layer.

For a thin film of thickness *d* it is possible to demonstrate that :

$$r = \frac{r_{12} + r_{23} e^{2i\varphi_2}}{1 + r_{12} r_{23} e^{2i\varphi_2}} \qquad t = \frac{t_{12} t_{23} e^{i\varphi_2}}{1 + r_{12} r_{23} e^{2i\varphi_2}}$$

where r_{ij}, t_{ij} are the Fresnel coefficient of the interface between material *i* and *j* and $\varphi_2 = \frac{\omega n_2 d cos\theta_2}{c_0} = spatial\ phase$

For a non-absorbing thin film it is then straightforward to obtain:

$$R = |r|^2 = \frac{r_{12}^2 + r_{23}^2 + 2r_{12}r_{23}\cos 2\varphi_2}{1 + 2r_{12}r_{23}\cos 2\varphi_2 + r_{12}^2 r_{23}^2}$$

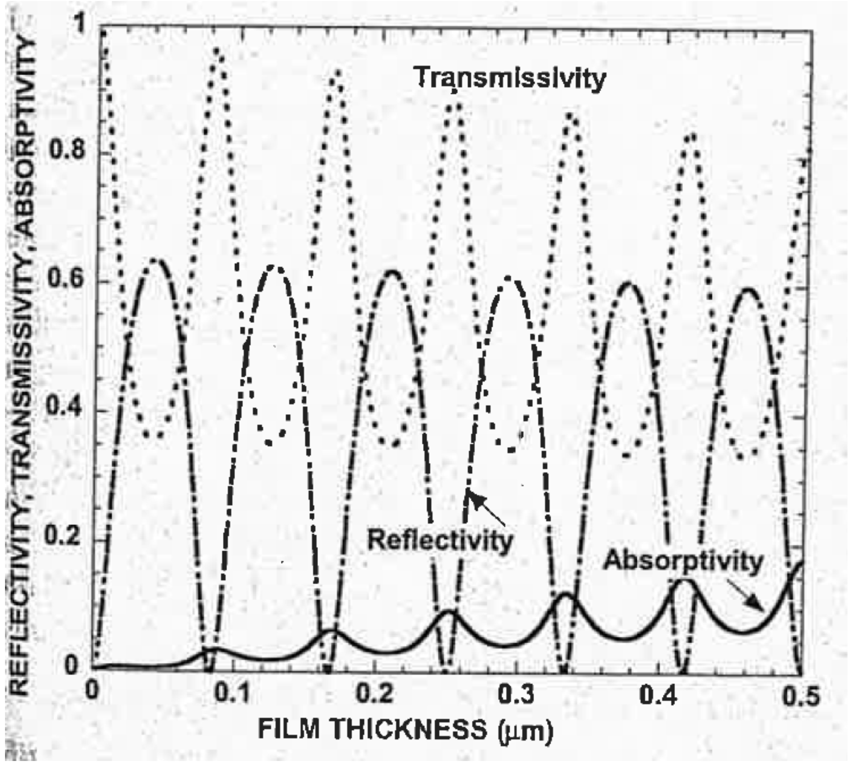
Oscillates with the thickness

$$\tau = \frac{n_3 \cos\theta_t}{n_1 \cos\theta_i} |t|^2 = \frac{(1 - r_{12}^2)(1 - r_{23}^2)}{1 + 2r_{12}r_{23}\cos 2\varphi_2 + r_{12}^2 r_{23}^2}$$

For an absorbing thin film, instead, we should use the complex refractive indices: $R = rr^*$ $\qquad \tau_{\parallel} = \frac{Re(N_3^* cos\theta_t)}{Re(N_1^* cos\theta_t)} t_{\parallel} t_{\parallel}^*$ $\qquad \tau_{\perp} = \frac{Re(N_3\ cos\theta_t)}{Re(N_1\ cos\theta_t)} t_{\perp} t_{\perp}^*$

Wave Propagation in Thin Films – Photons

EPFL



Oscillatory behavior of transmission and reflection as a function of the thickness of the thin film

- **Interference phenomenon characteristic of wave behavior**

The peaks appear for thicknesses d such as: $sin2\varphi_2 = 0 \;\Rightarrow\; d = \frac{m\lambda_0}{4n_2 cos\theta_2}$

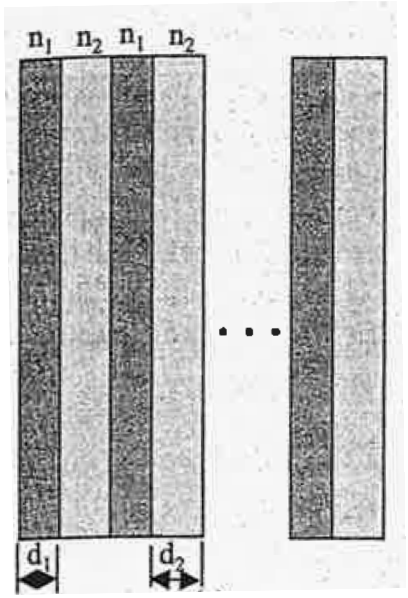
And the reflectivity is:

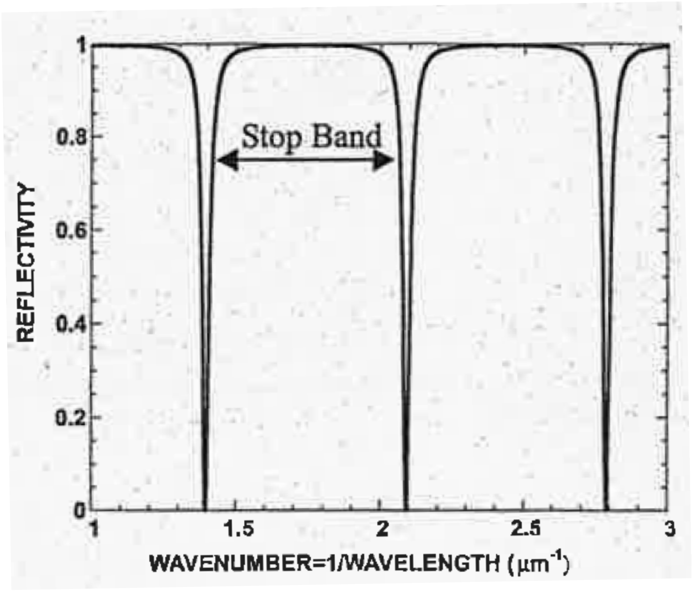
$$R = \left(\frac{r_{12} - r_{23}}{1 - r_{12}r_{23}}\right)^2 = \left(\frac{n_1 n_3 - n_2^2}{n_1 n_3 + n_2^2}\right)^2 \quad \text{(for odd m} = 2l + 1)$$

$$R = \left(\frac{r_{12} + r_{23}}{1 + r_{12}r_{23}}\right)^2 = \left(\frac{n_1 - n_3}{n_1 + n_3}\right)^2 \quad \text{(for even } m = 2l)$$

We observe that it is possible to minimize R by appropriate choice of n_2, n_3 and this constitute the basis of anti-reflection coatings.
Further manipulations of the reflectivity and transmissivity are possible using multiple layers.

Wave Propagation in Thin Films – Photons





A special case of multilayer films consist in a periodic arrangement of two thin layers with different refractive indices. Each layer has a thickness equal to a quarter of the light wavelength inside the film.
This structure is called a *Bragg reflector*. Indeed the coherent superposition of all the reflected fields can generate a reflectivity of 100% . The spectral range for which this occurs is called *stop band* .

The condition for 100% reflectivity is that in one period of the structure the total phase accumulation is a multiple of 2π

$$\frac{4\pi n_1 d_1 \cos\theta_1}{\lambda_0} + \frac{4\pi n_2 d_2 \cos\theta_2}{\lambda_0} = 2\ell\pi$$

This can be re-written as

$ka = l\pi$ where $a = n_1 d_1 cos\theta_1 + n_2 d_2 cos\theta_2$

We observe that this is identical to the condition for the formation of an electronic bandgap in a crystal!!
We thus see that it is the wave nature of the electrons combined with the periodicity of the crystal to give rise to destructive interference effects that result in the absence of propagation of the wave in the material. Similarly to natural crystals, we can create photonic crystal and phononic crystals by engineering the periodicity.

In This Lecture …

- Plane Waves and Energy Transport*
  - EM waves and Poynting vector
  - Electron Flux
- Plane waves at an interface
  - Fresnel coefficients
  - Electron transport at an interface
- Plane waves propagating in a multilayer structure (multiple interfaces and periodicity)
- **Evanescent waves and tunneling**

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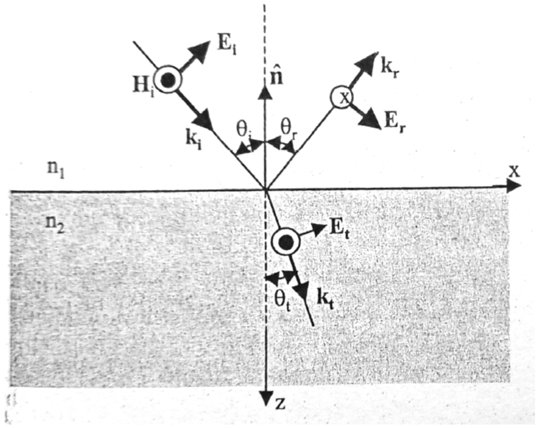
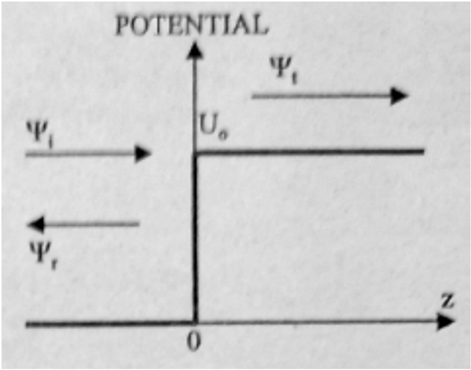
Plane Waves at an Interface

Photons



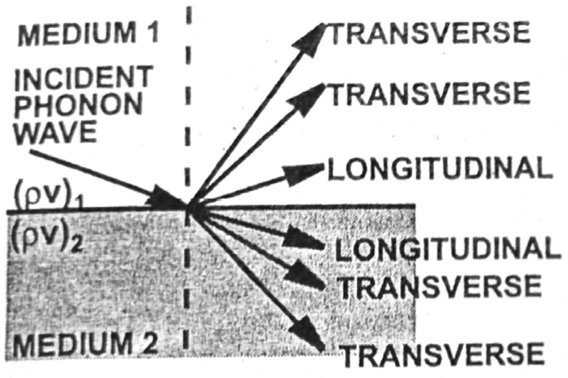
Reflection and Refraction
TM and TE waves
Brewster Angle & **Total Internal reflection**

Electrons



Reflection and Transmission
Evanescent Wave for E<U
Reflection even for E>U

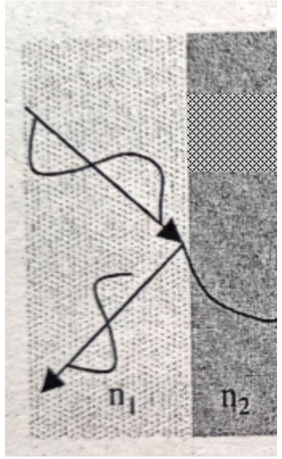
Phonons



Reflection and Refraction
Coupling between different polarizations

Let’s focus briefly on the evanescent waves and their physical implications for transport across multiple interfaces

Evanescent Waves and Tunneling - Photons



Snell's law tells us that: $\sin\theta_t = \frac{n_1 \sin\theta_i}{n_2}$

Thus if $n_1 > n_2$ we can have: $\sin\theta_t = \frac{n_1 \sin\theta_i}{n_2} > 1$

$$\Rightarrow \cos\theta_t = \sqrt{1-\sin^2\theta_t} = i\sqrt{\left(\frac{n_1 \sin\theta_i}{n_2}\right)^2 - 1} = i|\cos\theta_t|$$

We now consider a TM wave such that: $\mathbf{E}_{//t} \exp\left[-i\omega\left(t - \frac{n_2 x \sin\theta_t - n_2 z \cos\theta_t}{c_0}\right)\right]$ $\quad t_{//} = \frac{E_{//t}}{E_{//i}} = \frac{2n_1\cos\theta_i}{n_2\cos\theta_i + n_1\cos\theta_t}$

$$\Rightarrow \frac{2n_1\cos\theta_i(\hat{\mathbf{x}}\cos\theta_t - \hat{\mathbf{z}}\sin\theta_t)}{n_2\cos\theta_i + n_1|\cos\theta_t|i}|\mathbf{E}_{i//}|\exp\left[-i\omega\left(t - \frac{n_2 x\sin\theta_t}{c_0}\right)\right]\exp\left(-z\frac{n_2\omega}{c_0}|\cos\theta_t|\right)$$

Exponentially decaying wave

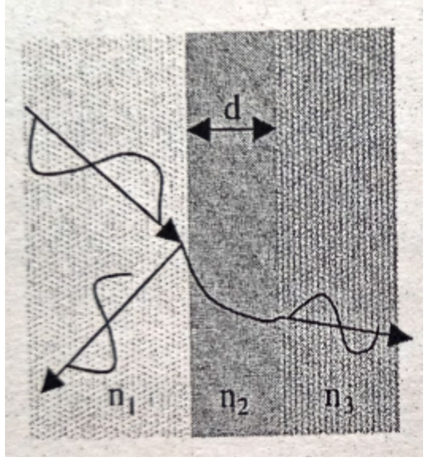
$$\Rightarrow \delta = \frac{\lambda_0}{2\pi n_2|\cos\theta_t|}$$

$$\Rightarrow \langle \mathbf{S}_z \rangle = \frac{1}{2}\mathrm{Re}(\mathbf{E}\times\mathbf{H}^*)_z = \frac{1}{2}\mathrm{Re}(E_x H_y)\hat{\mathbf{z}} = 0$$

Instantaneously there is an energy flux across the interface but the time average is zero when we have an evanescent wave.

This condition corresponds to **total internal reflection**.

Evanescent Waves and Tunneling - Photons



If the material with n_2 is sufficiently thin and is followed by a material where the wave can become again propagating, we will have tunneling of photons across the layer. For a thin layer of thickness *d* (see transfer matrix method in SI):

$$t = \frac{t_{12}t_{23}\exp\left[-\frac{2\pi n_2 d|\cos\theta_2|}{\lambda_0}\right]}{1 + r_{12}r_{23}\exp\left[-\frac{4\pi n_2 d|\cos\theta_2|}{\lambda_0}\right]}$$

$$\tau = \frac{Re(n_3\cos\theta_t)}{n_1\cos\theta_1}|t|^2$$

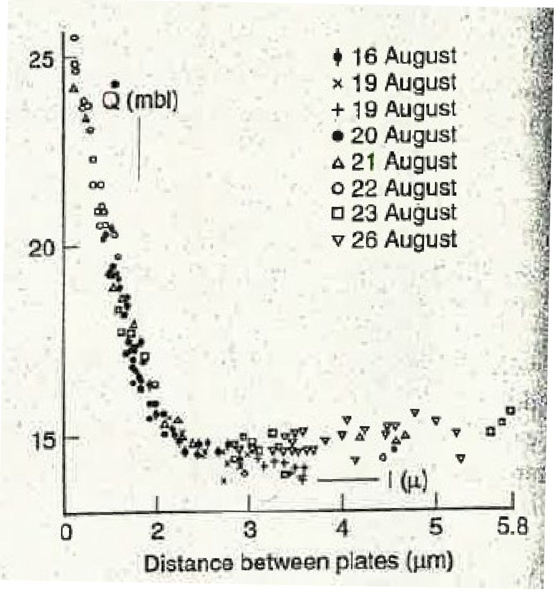
For $n_2 > n_3$ we can find the angles θ_i for which a real θ_t can be obtained:

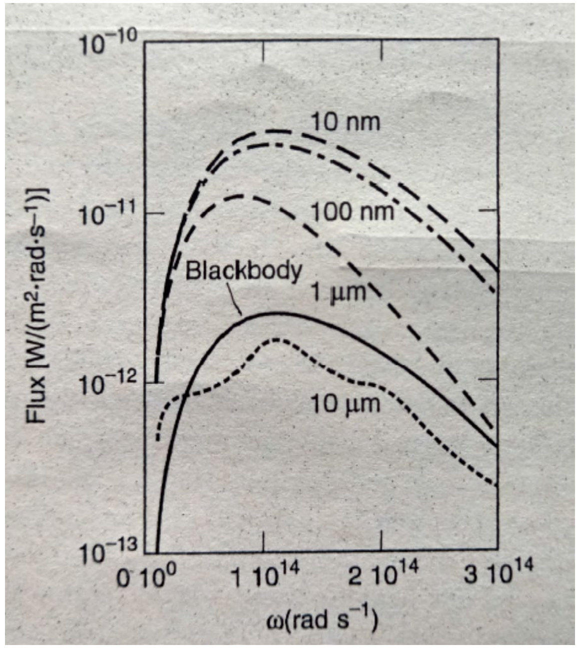
$$\sin^{-1}\left(\frac{n_2}{n_1}\right) \leq \theta_i \leq \sin^{-1}\left(\frac{n_3}{n_1}\right)$$

If the tunneling medium is non-absorbing, we will have: $R = 1 - \tau < 1$

An analogous behavior can be obtained also for phonons.

Near-field Radiative Heat Transfer





In Lecture 10, slide 24 we demonstrated how the Planck's blackbody radiation law can be obtained once the statistical distribution of the photons is known.
However, in obtaining such expression we have implicitly assumed that all photons are associated with a propagating wave.

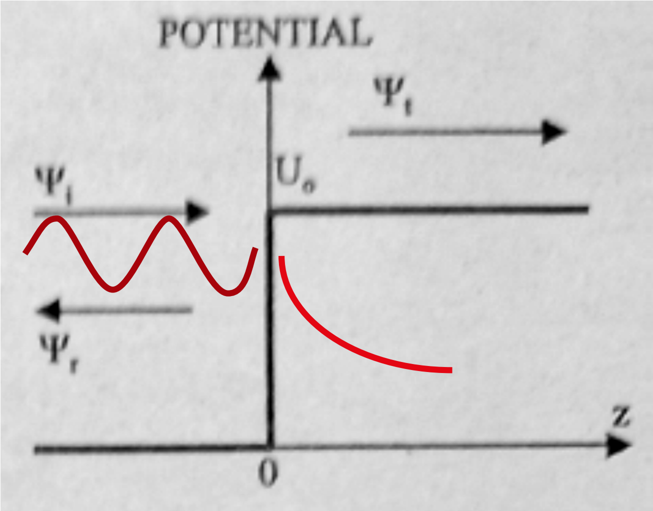
When two plates are brought in close proximity and the radiative heat transfer is dominant (vacuum), tunneling through the small gap modifies the heat transfer compared to the Plank's law. In particular, **the radiation flux increases as the vacuum gap decreases**. This can become important for applications such as **thermophotovoltaics**.

When two identical objects are separated by a small gap with refractive index n, it can be shown that the maximum radiative heat transfer can be increased by n^2 times the blackbody radiation heat transfer thanks to the tunneling of an internally reflected wave.

Surface waves, such as surface plasmon or surface phonon polariton, can also tunnel across the gap, further enhancing the near-field radiative heat transfer.

Finally, we note that interference and tunneling effects will also alter the radiative properties of thin films grown on substrates. In particular the emissivity will change with the film thickness.

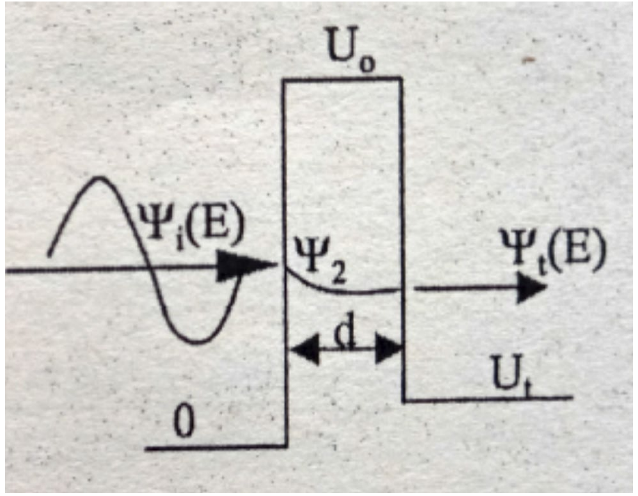
Evanescent Waves and Tunneling - Electrons



For $E < U_0$, k_2 is imaginary. Therefore Ψ_t is an **evanescent wave**

$$\Psi_t = \frac{2i|k_2|e^{-|k_2|z}}{k_1 + i|k_2|}\Psi_i \qquad |k_2| = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

$$\delta = \frac{1}{|k_2|} \qquad U_0 - E = 1\ \mathrm{eV}, \qquad \delta \approx 2\ \text{Å},$$



If the barrier is sufficiently thin, the wave can become again oscillatory beyond the barrier $k_t \in Re$ and therefore overall we have a net transmission of the electron across the barrier even if initially $E < U_0$.

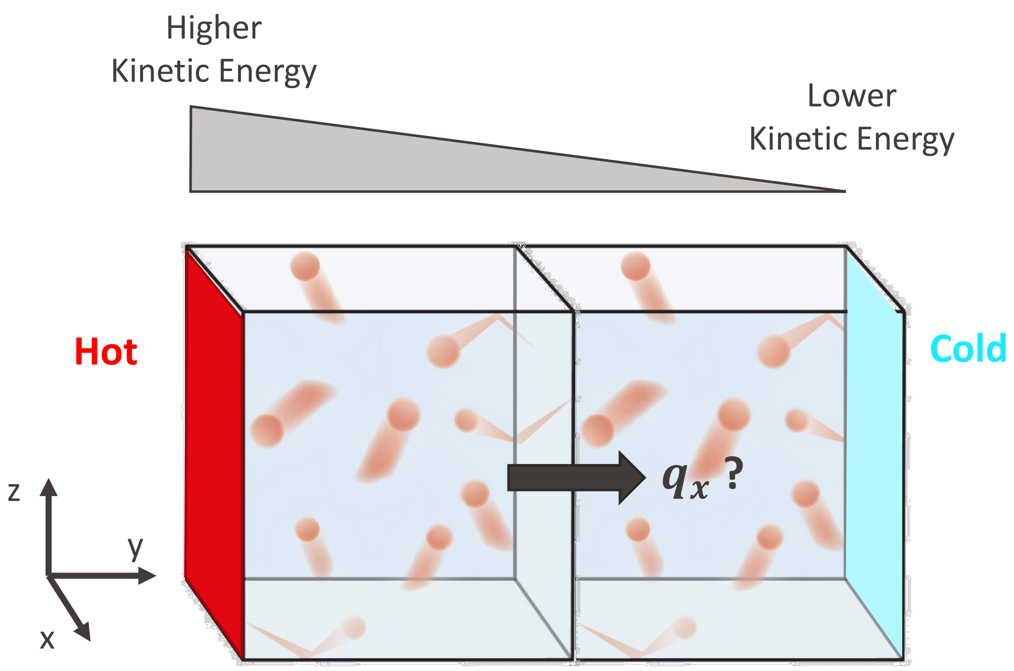
This process is called **tunneling** and it is a clear manifestation of the wave nature of electrons. The tunneling transmissivity through a potential barrier of height U_0 and width *d* is:

$$\tau = \frac{4E(U_0 - E)}{4E(U_0 - E) + U_0^2 \sinh^2[\sqrt{2m(U_0 - E)}d/\hbar]}$$

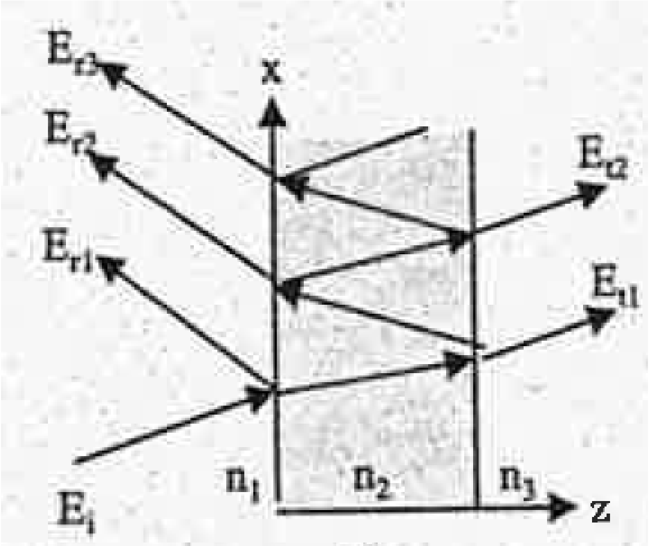
$$\tau \approx \frac{16E(U_0 - E)}{U_0^2}\exp[-2\sqrt{2m\,(U_0 - E)}d/\hbar] = \frac{16E\,(U_0 - E)}{U_0^2}e^{-2|k_2|d}$$

Important instruments such as the scanning tunneling microscope are based on this phenomenon!!

Next Week



Particle View



Wave View

How can we describe transport in a particle view accounting for the wave nature?
When and how does the wave-behavior affects energy transport?

Next Week

EPFL

Nanoscale Heat Transfer (and Energy Conversion)

- **Energy States**
  - Introduction to Quantum Mechanics (Ch. 2)
  - Introduction to Solid State Physics (Ch. 3)
- **Thermal Energy Storage**
  - Introduction to Statistical Thermodynamics (Ch. 4)
- **Thermal Energy Transport**
  - Energy Transport by Waves (Ch. 5)
  - Energy Transport by Particles (Ch. 6 -7)
    - Classical Laws
    - Classical Size Effects
  - Energy Transport in Liquids (Ch. 9)
- **Thermal Energy Conversion**
  - Energy Conversion Mechanisms (Ch. 8)

Wave Energy Transport – Phonons

In order to analyze energy transport by phonons we consider the long wavelength limit ($\lambda \gg a, k \ll a$) in which the atomic structure can be neglected (continuum). Under this assumption, we can use the **acoustic wave equation**.

An acoustic wave propagation is defined as a function of the local medium displacement $\vec{u}$ from the equilibrium position. The velocity of the displacement is: $\vec{v} = \frac{d\vec{u}}{dt}$

Two third-rank tensor can be defined :

$$\bar{\bar{S}} = S_{ij}(\vec{r}, t) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = strain\ tensor$$

$$\bar{\bar{\sigma}} = stress\ tensor \quad \Rightarrow \quad \vec{F} = \bar{\bar{\sigma}} \cdot \hat{n}$$

$$\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$$

For an isotropic medium with no damping (no viscosity), it is possible to obtain a stiffness tensor as a function of only two constants (Lame constants, λ_L, μ_L). Considering a plane elastic wave of the form $\vec{v}\exp(-i(\omega t - k\hat{k} \cdot \vec{r})$ it is possible to obtain an eigenvalue equation :

$$k^2 \begin{bmatrix} c_{11}\hat{k}_x^2 + \mu_L(1-\hat{k}_x^2) & (\lambda_L + \mu_L)\hat{k}_x\hat{k}_y & (\lambda_L + \mu_L)\hat{k}_x\hat{k}_z \\ (\lambda_L + \mu_L)\hat{k}_y\hat{k}_x & c_{11}k_y^2 + \mu_L(1-\hat{k}_y^2) & (\lambda_L + \mu_L)\hat{k}_y\hat{k}_z \\ (\lambda_L + \mu_L)\hat{k}_z\hat{k}_x & (\lambda_L + \mu_L)\hat{k}_z\hat{k}_y & c_{11}\hat{k}_z^2 + \mu_L(1-k_z^2) \end{bmatrix} \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = \rho\omega^2 \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix}$$

$$c_{11} = \lambda_L + 2\mu_L$$

From this one can obtain the dispersion relation for different acoustic waves:

- plane **transverse** acoustic wave: $\mathbf{v}_T = A_T e^{-i(\omega t - k_T z)}\hat{\mathbf{x}}$ ➡ $\mu_L k_T^2 = \rho\omega^2$ or $\omega = v_T k_T$ $\quad v_T = (\mu_L/\rho)^{1/2}$
- plane **longitudinal** acoustic wave: $\mathbf{v}_L = A_L e^{-i(\omega t - k_L z)}\hat{\mathbf{z}}$ ➡ $k_L^2 c_{11} = \rho\omega^2$ or $\omega = v_L k_L$ $\quad v_L = (c_{11}/\rho)^{1/2} = [(\lambda_L + 2\mu_L)/\rho]^{1/2}$

Plane Waves and Energy Transport - Phonons

Therefore, acoustic wave can be both transversal and longitudinal and for an arbitrary propagation direction $\hat{k}$ we can write:

$$\overrightarrow{v_{T1}} = \hat{a}A_{T1}e^{-i(\omega t - k_T\hat{k}\cdot\vec{r})} \quad \hat{a}\cdot\hat{k} = 0$$

$$\overrightarrow{v_{T2}} = \hat{a}\times\hat{k}A_{T2}e^{-i(\omega t - k_T\hat{k}\cdot\vec{r})}$$

$$\overrightarrow{v_L} = \hat{k}A_L e^{-i(\omega t - k_L\hat{k}\cdot\vec{r})}$$

Once the displacement velocity is known, it is possible to obtain the stress tensor:

$$\frac{\partial}{\partial t}\begin{bmatrix}\sigma_{xx}\\ \sigma_{yy}\\ \sigma_{zz}\\ \sigma_{yz}\\ \sigma_{xz}\\ \sigma_{xy}\end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & c_{44}\end{bmatrix}\begin{bmatrix}\partial v_x/\partial x\\ \partial v_y/\partial y\\ \partial v_z/\partial z\\ \partial v_y/\partial z + \partial v_z/\partial y\\ \partial v_x/\partial z + \partial v_z/\partial x\\ \partial v_x/\partial y + \partial v_y/\partial x\end{bmatrix}$$

$$c_{12} = \lambda_L$$
$$c_{44} = \mu_L$$

Finally the time-averaged power carried by the acoustic wave can be calculated from the acoustic Poynting vector as:

$$\vec{J}_{ac} = -\frac{1}{2}Re\left[\overrightarrow{v^*}\cdot\bar{\bar{\sigma}}\right]$$

Plane Waves at an Interface - Phonons

EPFL

For an acoustic wave we also have to apply boundary conditions. In particular, we need force to be continuous at the interface. Furthermore, in the long wavelength limit we require also continuity for the displacement velocity (atomic motion can be discontinuous):

$$\sum \mathbf{v}_1 = \sum \mathbf{v}_2 \text{ and } \sum \bar{\bar{\sigma}}_1 \bullet \hat{\mathbf{n}} = \sum \bar{\bar{\sigma}}_2 \bullet \hat{\mathbf{n}}$$

The derivations of the reflection/transmission coefficients is much more complicated than for an electromagnetic wave. For the simple case of an isotropic medium and considering a transverse wave polarized with the displacement perpendicular to the plane of incidence (horizontally polarized shear wave), we have:

$$r_s = \frac{v_r}{v_i} = \frac{Z_1 \cos\theta_i - Z_2 \cos\theta_t}{Z_1 \cos\theta_i + Z_2 \cos\theta_t}$$

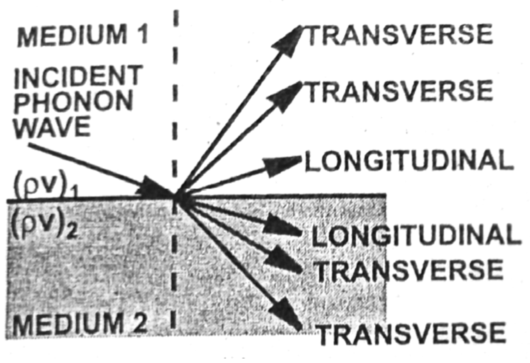
$$t_s = \frac{v_t}{v_i} = \frac{2Z_1 \cos\theta_i}{Z_1 \cos\theta_i + Z_2 \cos\theta_t}$$

where $Z = \sqrt{\rho c_{44}} = \rho v_T$

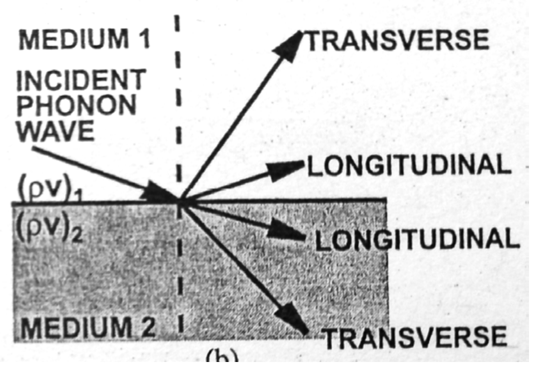
We can also obtain an equivalent of Snell's law: $$\frac{\sin\theta_i}{v_{T1}} = \frac{\sin\theta_t}{v_{T2}}$$

And from the Poynting vector the reflectivity: $$R_s = \left|\frac{Z_1 - Z_2}{Z_1 + Z_2}\right|^2$$

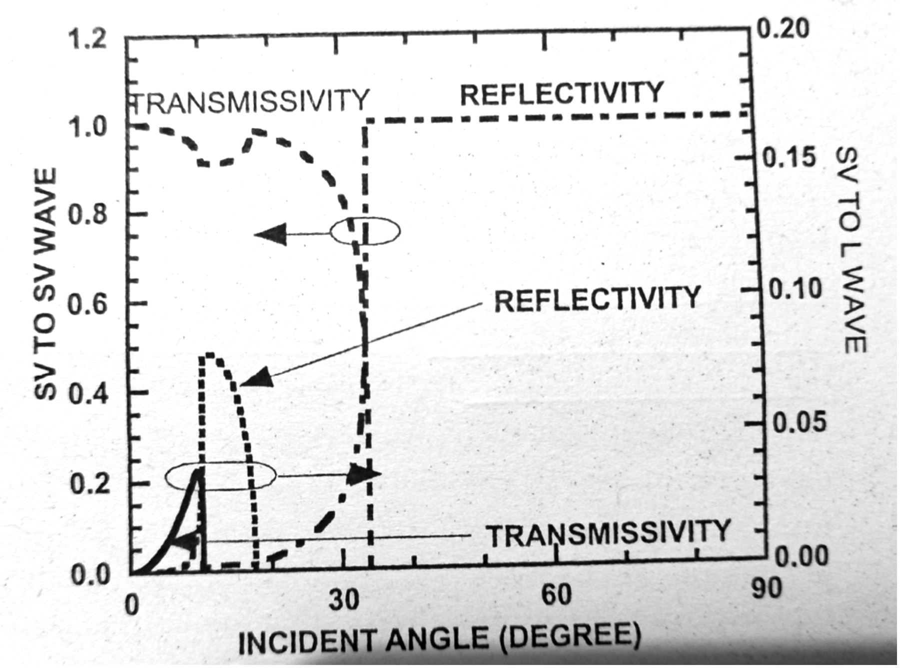
Plane Waves at an Interface - Phonons



Anisotropic Medium



Isotropic Medium



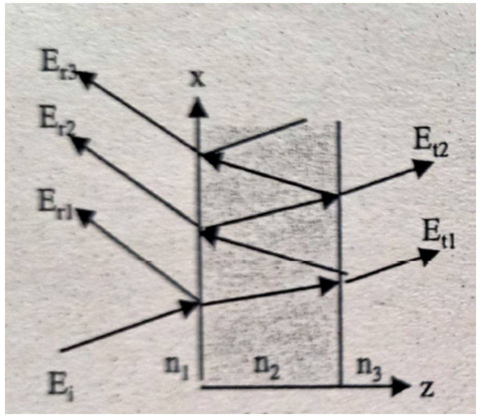
For a transverse acoustic wave polarized in the plane of incidence (vertically polarized shear wave, SV) and for a longitudinally polarized acoustic wave, coupling between different polarizations can occur. In particular, one wave can excited three reflected and three transmitted waves and Snells' law becomes:

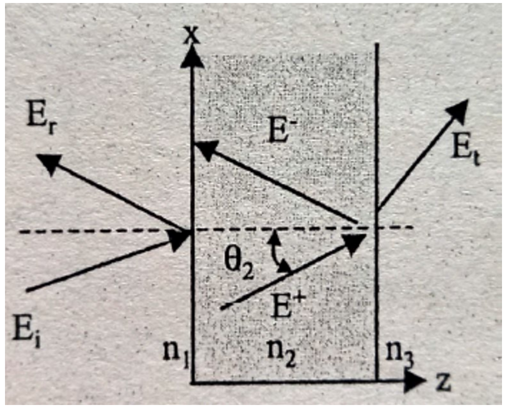
$$\frac{\sin\theta_i}{v_i} = \frac{\sin\theta_{rL}}{v_{L1}} = \frac{\sin\theta_{rT}}{v_{T1}} = \frac{\sin\theta_{tL}}{v_{L2}} = \frac{\sin\theta_{tT}}{v_{T2}}$$

In an isotropic medium the two transverse reflected and the two transverse transmitted waves are degenerate.

Wave Propagation in Thin Films – Photons

EPFL





We consider a **TM wave propagating in the z-direction** with E_x, H_y components. We simplify the picture by considering for each layer just the forward and backward propagating waves, each resulting from the superposition of the multiple transmitted and reflected waves). For convenience we drop the time and space phases:

$$E_x(z) = \cos\theta_2 E^+ e^{i\varphi(z)} + \cos\theta_2 E^- e^{-i\varphi(z)}$$

$$H_y(z) = \frac{n_2}{\mu c_0}[E^+ e^{i\varphi(z)} - E^- e^{i\varphi(z)}]$$

where $E^+, E^- = amplitudes$ $\quad \varphi_{(z)} = \frac{\omega n_2 z \cos\theta_2}{c_0} = spatial\ phase$

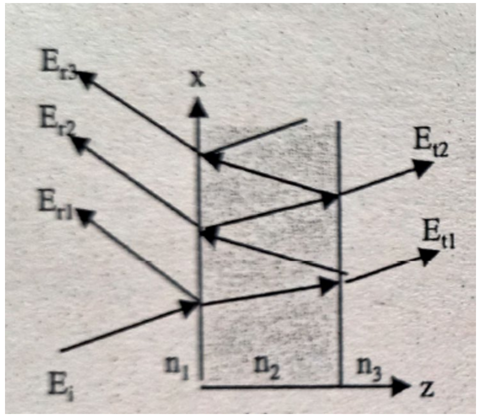
We observe that at $z = 0$ we have:

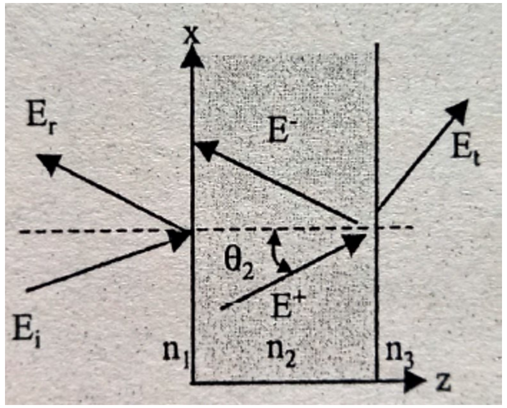
$$\begin{cases} E_x(0) = \cos\theta_2 E^+ + \cos\theta_2 E^- \\ H_y(0) = \frac{n_2}{\mu c_0}[E^+ - E^-] \end{cases} \Rightarrow \begin{cases} E_x(z) = E_x(0)\cos\varphi(z) + ip_2 H_y(0)\sin\varphi(z) \\ H_y(z) = \frac{i}{p_2}E_x(0)\sin\varphi(z) + H_y(0)\cos\varphi(z) \end{cases}$$

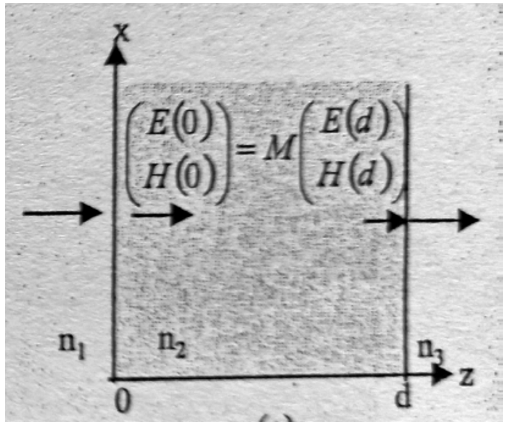
$$p_2 = \frac{\cos\theta_2}{n_2/\mu c_0} = surface\ impedance$$

➡ We can express the field in the thin layer as a function of the field at the front interface.

Wave Propagation in Thin Films – Photons







We can re-write in matrix form:

$$\begin{pmatrix} E_x(z) \\ H_y(z) \end{pmatrix} = \begin{pmatrix} \cos\varphi(z) & ip_2 \sin\varphi(z) \\ \frac{i}{p_2}\sin\varphi(z) & \cos\varphi(z) \end{pmatrix} \begin{pmatrix} E_x(0) \\ H_y(0) \end{pmatrix}$$

Further, we can now invert this expression to calculate the field at $z = 0$ as a function of the field at $z = d$:

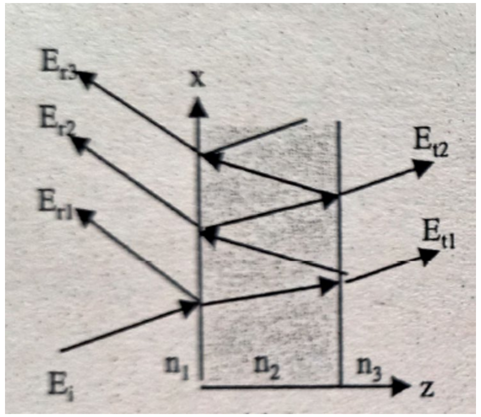
$$\begin{pmatrix} E_x(0) \\ H_x(0) \end{pmatrix} = \begin{pmatrix} \cos\varphi_2 & -ip_2 \sin\varphi_2 \\ -\frac{i}{p_2}\sin\varphi_2 & \cos\varphi_2 \end{pmatrix} \begin{pmatrix} E_x(d) \\ H_y(d) \end{pmatrix} = M \begin{pmatrix} E_x(d) \\ H_y(d) \end{pmatrix}$$

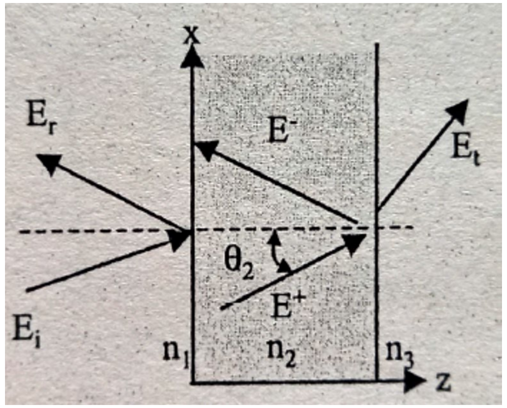
where $\varphi_2 = \varphi(d)$

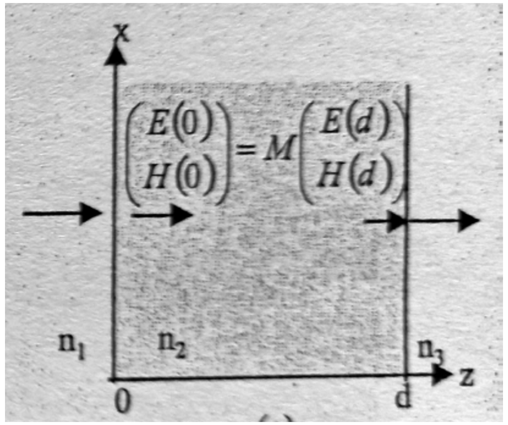
We call M the **interference matrix** and it can be shown that $|M| = 1$

We can now easily describe the field in the thin film with a matrix. The next step is to describe the change of the field across an interface.

Wave Propagation in Thin Films – Photons







Considering an interface without surface charges nor currents, we have to apply the boundary conditions. In particular, the continuity of the fields gives:

At $z = 0$:

$$E_x(0) = E_i \cos\theta_i + E_r \cos\theta_r = E_{ix} + E_{rx}$$

$$H_y(0) = \frac{n_1}{\mu c_0}(E_i - E_r) = \frac{1}{p_1}(E_{ix} - E_{rx})$$

$$p_1 = \frac{\cos\theta_1}{n_1/\mu c_0}$$

At $z = d$:

$$E_x(d) = E_t \cos\theta_t = E_{tx}$$

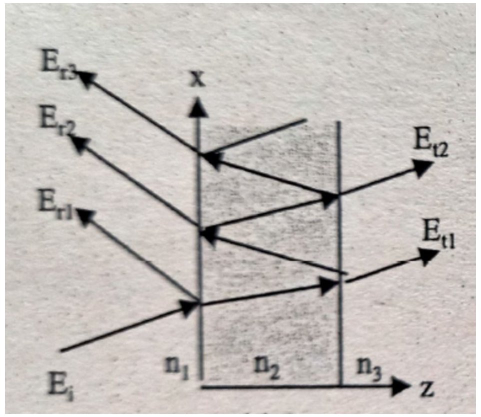
$$H_y(d) = \frac{n_3}{\mu c_0} E_t = \frac{1}{p_3} E_{tx}$$

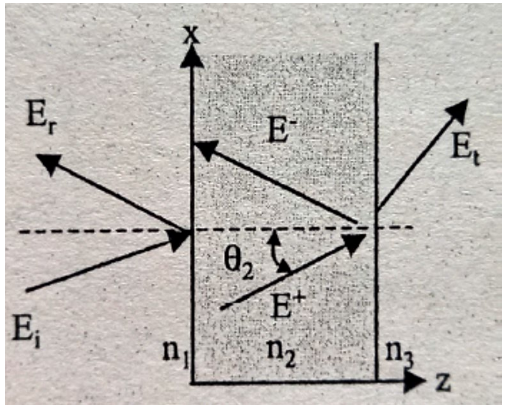
$$p_3 = \frac{\cos\theta_3}{n_3/\mu c_0}$$

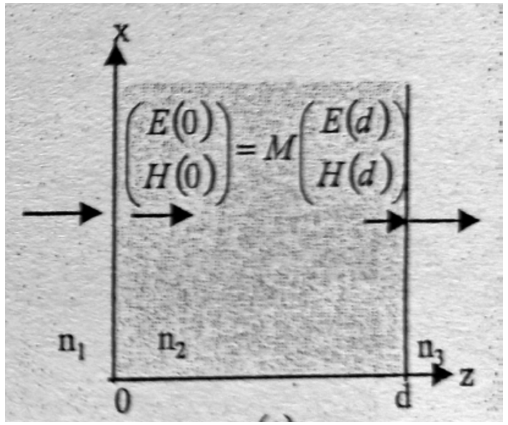
$$\begin{pmatrix} E_x(0) \\ H_y(0) \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \frac{1}{p_1} & -\frac{1}{p_1} \end{pmatrix} \begin{pmatrix} E_{ix} \\ E_{rx} \end{pmatrix}$$

$$\begin{pmatrix} E_x(d) \\ H_y(d) \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{p_3} \end{pmatrix} E_{tx}$$

Wave Propagation in Thin Films – Photons







We can now combine the results of the previous two slides:

$$\begin{pmatrix} E_x(0) \\ H_x(0) \end{pmatrix} = \begin{pmatrix} \cos\varphi_2 & -ip_2 \sin\varphi_2 \\ -\frac{i}{p_2}\sin\varphi_2 & \cos\varphi_2 \end{pmatrix} \begin{pmatrix} E_x(d) \\ H_y(d) \end{pmatrix} = M \begin{pmatrix} E_x(d) \\ H_y(d) \end{pmatrix}$$

$$\begin{pmatrix} E_x(0) \\ H_y(0) \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \frac{1}{p_1} & -\frac{1}{p_1} \end{pmatrix} \begin{pmatrix} E_{ix} \\ E_{rx} \end{pmatrix}$$

$$\begin{pmatrix} E_x(d) \\ H_y(d) \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{p_3} \end{pmatrix} E_{tx}$$

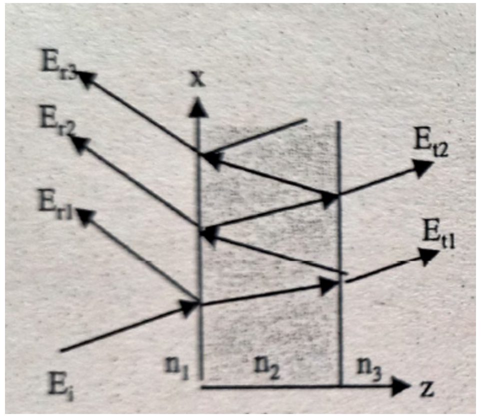
$$\begin{pmatrix} 1 & 1 \\ \frac{1}{p_1} & -\frac{1}{p_1} \end{pmatrix} \begin{pmatrix} E_{ix} \\ E_{rx} \end{pmatrix} = \underbrace{\begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}}_{M} \begin{pmatrix} 1 \\ \frac{1}{p_3} \end{pmatrix} E_{tx}$$

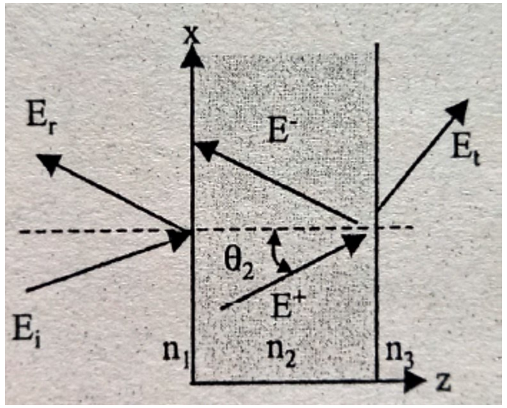
$$\begin{pmatrix} E_{ix} \\ E_{rx} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} (m_{11} + \frac{1}{p_3} m_{12}) + (m_{21} + \frac{1}{p_3} m_{22}) p_1 \\ (m_{11} + \frac{1}{p_3} m_{12}) - (m_{21} + \frac{1}{p_3} m_{22}) p_1 \end{pmatrix} E_{tx}$$

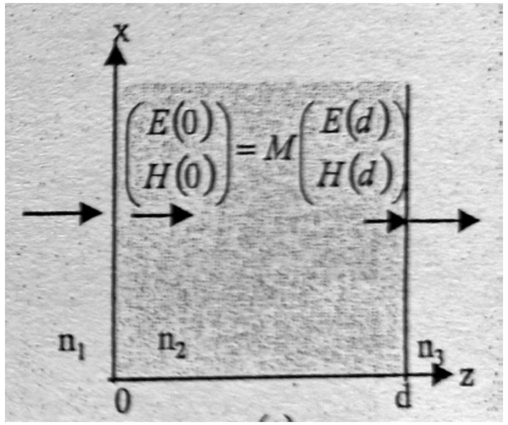
This approach is called **transfer matrix method** or TMM.

Wave Propagation in Thin Films – Photons

EPFL







From these we can then easily compute the reflection and transmission coefficients as the ratios of the intensities of the electric fields:

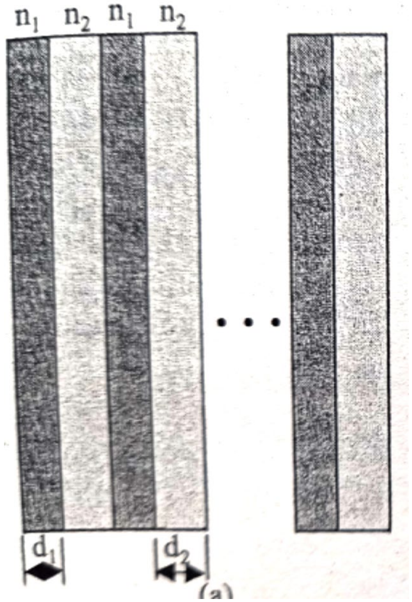
$$r = \frac{E_r}{E_i} = \frac{E_{rx}}{E_{ix}} = \frac{(m_{11} + \frac{1}{p_3}m_{12}) - (m_{21} + \frac{1}{p_3}m_{22})p_1}{(m_{11} + \frac{1}{p_3}m_{12}) + (m_{21} + \frac{1}{p_3}m_{22})p_1}$$

$$c_{tm} = \cos\theta_i / \cos\theta_t$$

$$t = \frac{E_t}{E_i} = \frac{E_{tx}/\cos\theta_t}{E_{ix}/\cos\theta_i} = \frac{2c_{tm}}{(m_{11} + \frac{1}{p_3}m_{12}) + (m_{21} + \frac{1}{p_3}m_{22})p_1}$$

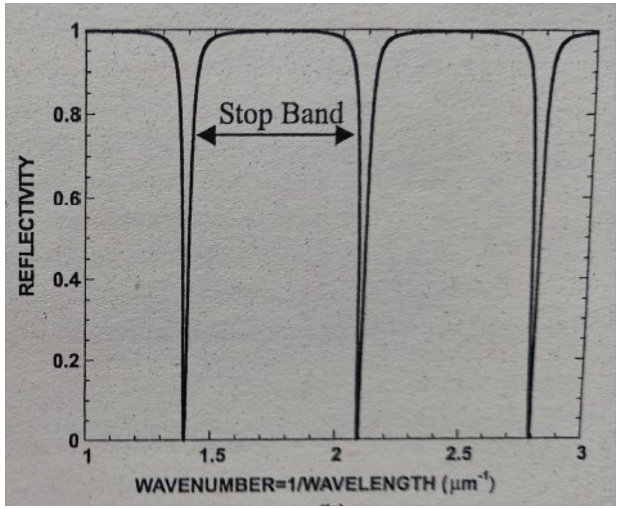
For a **TE wave** we would get analogous expressions only with $p = -\frac{n\cos\theta}{\mu c_0}$ and $c_{te} = 1$

Wave Propagation in Thin Films – Photons



The TMM method is particularly convenient to deal with multi-layer structures.
In fact, we can calculate the total interference matrix as:

$$M = M_1 M_2 M_3 \ldots M_n \quad \Rightarrow \quad \begin{pmatrix} E_{ix} \\ E_{rx} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} (m_{11} + \frac{1}{p_3} m_{12}) + (m_{21} + \frac{1}{p_3} m_{22}) p_1 \\ (m_{11} + \frac{1}{p_3} m_{12}) - (m_{21} + \frac{1}{p_3} m_{22}) p_1 \end{pmatrix} E_{tx}$$



A special case of multilayer films consist in a periodic arrangement of two thin layers with different refractive indices. Each layer has a thickness equal to a quarter of the light wavelength inside the film.
This structure is called a *Bragg reflector*. Indeed the coherent superposition of all the reflected fields can generate a reflectivity of 100% . The spectral range for which this occurs is called *stop band .*

The condition for 100% reflectivity is that in one period of the structure the total phase accumulation is a multiple of 2π

$$\frac{4\pi n_1 d_1 \cos\theta_1}{\lambda_0} + \frac{4\pi n_2 d_2 \cos\theta_2}{\lambda_0} = 2\ell\pi$$

This can be re-written as

$$ka = l\pi \qquad \text{where} \qquad a = n_1 d_1 cos\theta_1 + n_2 d_2 cos\theta_2$$

We observe that this is identical to the condition for the formation of an electronic bandgap in a crystal!!
We thus see that it is the wave nature of the electrons combined with the periodicity of the crystal to give rise to destructive intereference effects that result in the absence of propagation of the wave in the material. Similarly to natural crystals, we can create photonic crystal and phononic crystals by engineering the periodicity.

Wave Propagation in Thin Films – Phonons

For an SH wave propagating through a film with thickness d, the reflectivity and transmissivity are: $r = v_r(0)/v_i(0) \quad t = v_t(d)/v_i(0)$

The transfer matrix method concept can be applied also for an elastic waves:

$$\begin{pmatrix} 1 \\ r \end{pmatrix} = A_i^{-1} M A_t \begin{pmatrix} t \\ 0 \end{pmatrix} \qquad M = \begin{pmatrix} \cos\varphi_{T2} & i\sin\varphi_{T2}/Y_2 \\ iY_2\sin\varphi_{T2} & \cos\varphi_{T2} \end{pmatrix} \qquad A_i = \begin{pmatrix} 1 & 1 \\ -Z_{Ti}\cos\theta_{Ti} & Z_{Ti}\cos\theta_{Ti} \end{pmatrix}$$

$$\varphi_{T2} = \omega d \cos\theta_2 / v_{T2}, \quad Y_2 = -Z_{T2}\cos\theta_2$$

where the subscript T indicates the transverse wave.

For a longitudinal (L) and vertically polarized transverse wave (SV), i.e. displacement polarized in the plane of incidence, the velocities of the incident, reflected and transmitted waves are:

$$\begin{pmatrix} v_{Ti}(0) \\ v_{Li}(0) \\ v_{Tr}(0) \\ v_{Lr}(0) \end{pmatrix} = B_i^{-1} M B_t \begin{pmatrix} v_{Tt}(d) \\ v_{Lt}(d) \\ 0 \\ 0 \end{pmatrix}$$

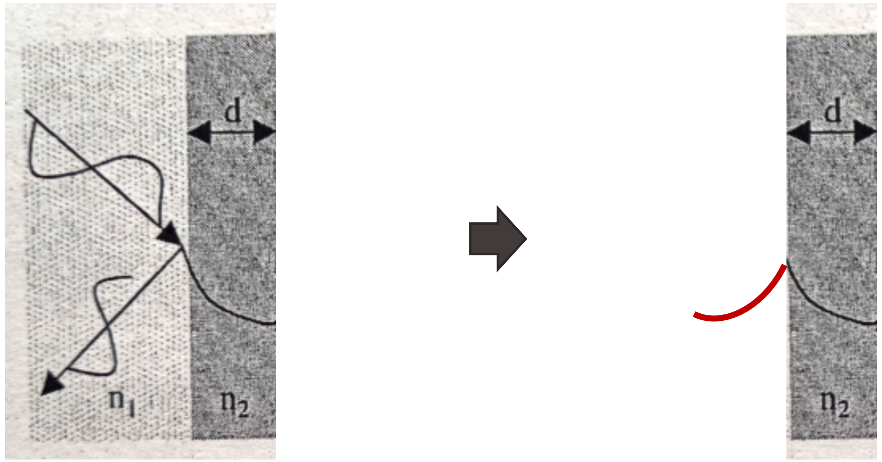
$$B_i = \begin{pmatrix} -\sin\theta_{Ti} & \cos\theta_{Li} & \sin\theta_{Ti} & -\cos\theta_{Li} \\ \cos\theta_{Ti} & \sin\theta_{Li} & \cos\theta_{Ti} & \sin\theta_{Li} \\ -\mu_1 k_{Ti}\sin 2\theta_{Ti} & (\lambda_1 + 2\mu_1\cos^2\theta_{Li})k_{Li} & -\mu_1 k_{Ti}\sin 2\theta_{Ti} & (\lambda_1 + 2\mu_1\cos^2\theta_{Li})k_{Li} \\ \mu_1 k_{Ti}\cos 2\theta_{Ti} & \mu_1 k_{Li}\sin 2\theta_{Li} & -\mu_1 k_{Ti}\cos 2\theta_{Ti} & -\mu_1 k_{Li}\sin 2\theta_{Li} \end{pmatrix}$$

where $k_i(=\omega/v_i)$ $\quad M = B_2^{-1} N_2 B_2,$

$$N_2 = \begin{pmatrix} e^{i\varphi_{T2}} & 0 & 0 & 0 \\ 0 & e^{i\varphi_{L2}} & 0 & 0 \\ 0 & 0 & e^{-i\varphi_{T2}} & 0 \\ 0 & 0 & 0 & e^{-i\varphi_{L2}} \end{pmatrix}$$

For a multilayer system it is then sufficient to calculate the compounded interference matrix: $M = M_1 M_2 \ldots M_{2n-1}$

Evanescent Waves – Surface Plasmon/Phonon Polaritons



A surface plasmon/phonon polariton is a wave that propagates along an interface but is exponentially decaying on BOTH sides of the interface

Energy is bound to the interface and cannot be transported away from it

A **plasmon polariton** can exist at the interface of a metallic-like material and a dielectric and it is mixture of an electron wave and a photon.
A **phonon polariton** can exist at the interface between a polar material (e.g. SiC) and a dielectric and it is a mixture of an optical phonon and a photon.