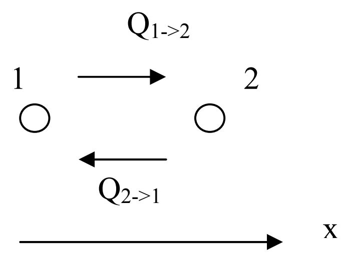
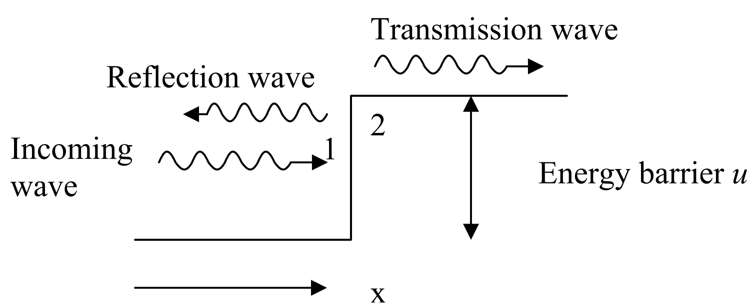
2.57 Nano-to-Macro Transport Processes
Fall 2004
Lecture 13

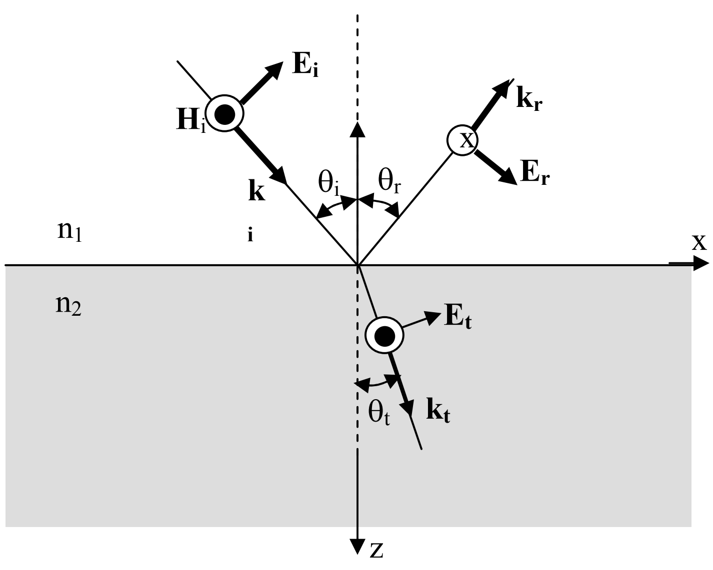
Review of previous lectures
1. Energy transport between two points



2. Plane waves & their interface reflection
We are interested in the wave energy at points 1 and 2 on two sides of the interface.



3. Oblique incidence of an electromagnetic wave onto an interface



Assuming flat interface, we have $\theta_i = \theta_r$. In last lecture, we have derived

$$r_{//} = \frac{E_{//r}}{E_{//i}} = \frac{-n_2 \cos\theta_i + n_1 \cos\theta_t}{n_2 \cos\theta_i + n_1 \cos\theta_t}, \quad t_{//} = \frac{E_{//t}}{E_{//i}} = \frac{2n_1 \cos\theta_i}{n_2 \cos\theta_i + n_1 \cos\theta_t},$$

which are known as the **Fresnel coefficients** of reflection and transmission. For normal incidence ($\theta_i = 0$), similarity exists between case 2 and case 3 (see the following table).

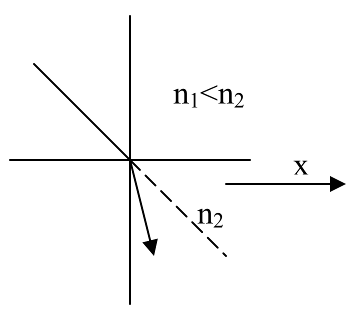
Electron propagation across a barrier	Normal incidence onto an interface
$r = -\frac{\Psi_r}{\Psi_i} = \frac{k_1 - k_2}{k_1 + k_2}$	$r_{//} = \frac{E_{//r}}{E_{//i}} = \frac{-n_2 + n_1}{n_2 + n_1}$
$t = \frac{2k_1}{k_1 + k_2}$	$t_{//} = \frac{2n_1}{n_2 + n_1}$
$R = -J_r / J_i = \left\lvert \frac{B}{A} \right\rvert^2 = \left\lvert \frac{k_1 - k_2}{k_1 + k_2} \right\rvert^2$	$R_{//} = \frac{S_{r,z}}{S_{i,z}} = \frac{S_r}{S_i} = \lvert r_{//} \rvert^2$
$T = \frac{J_t}{J_i} = \frac{\mathrm{Re}\left(k_2^*\right)}{\mathrm{Re}\left(k_1^*\right)} \lvert t \rvert^2$	$T_{//} = \frac{S_{t,z}}{S_{i,z}} = \mathrm{Re}\left(\frac{n_2 \cos\theta_t}{n_1 \cos\theta_i}\right) \lvert t_{//} \rvert^2$

Discussions

1) Critical & total internal reflection

A) $n_1 < n_2$

The Snell law is applied, $n_1 \sin\theta_i = n_2 \sin\theta_t$.



Note: The Snell law indicates the momentum conservation, or wavevector $k_{x1} = k_{x2}$ on the interface.

B) $n_1 > n_2$

Because the maximum angle of the refracted wave is $\theta_t = 90^o$, there exists an angle of incidence above which no real solution for θ_t exists. This **critical angle** happens when, according to the Snell law,

$$n_1 \sin\theta_c = n_2 \sin 90^o \text{ or } \sin\theta_c = \frac{n_2}{n_1}$$

Above this angle, the reflectivity equals one, i.e., all the incident energy is reflected (T=0, R=1).

For an electromagnetic wave incident above the critical angle, the Snell law gives,

$$\sin\theta_t = \frac{n_1 \sin\theta_i}{n_2} > 1,$$

and thus,

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

In the wave function of the transmitted wave, the imaginary $\cos\theta_t$ leads to an exponential decay wave

$$E_{//t}\exp\left[-i\omega\left(t-\frac{n_2 x\sin\theta_t + n_2 z\cos\theta_t}{c_o}\right)\right]$$

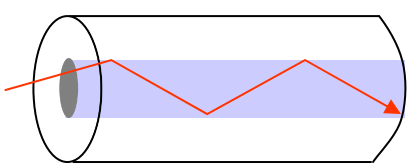
$$= E_{//t}\exp\left[-i\omega\left(t-\frac{n_2 x\sin\theta_t}{c_o}\right)-\frac{n_2 z\omega a}{c_o}\right],$$

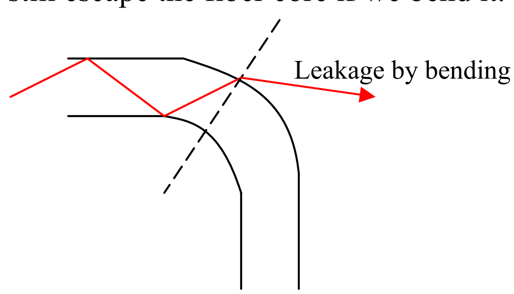
which is similar to the encountered evanescent wave.

Two applications:

a) Optical fiber

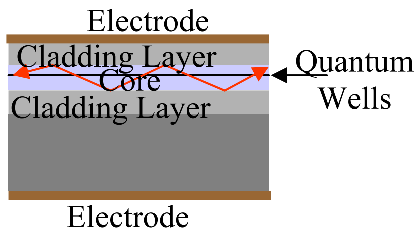
An optical fiber has a core region and a cladding layer. The refractive index in the core region is higher than in the cladding layer. If light is launched into the fiber at an angle larger than the critical angle, the light will be bounced inside the core only without leakage, thus traveling a long distance along the fiber if the absorption coefficient of the core is small. However, the light can still escape the fiber core if we bend it.





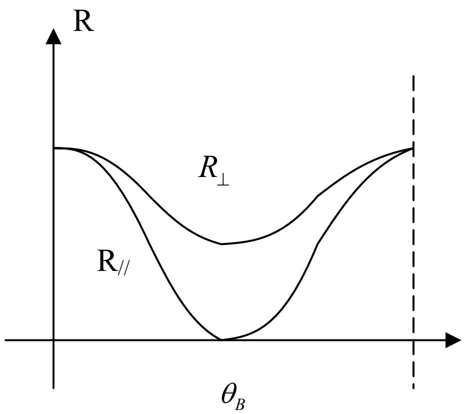
b) Semiconductor laser

In a semiconductor laser, light is emitted through electron-hole recombination inside the quantum well. The emitted light spreads over the core region and is confined by cladding layers that have a low refractive index than the core.



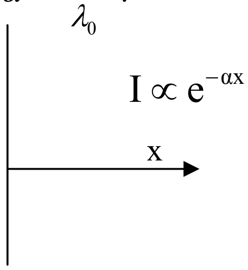
2) Brewster angle

When $\theta_t + \theta_i = \frac{\pi}{2}$, we have the electric wave $r_{//} = 0$, but the magnetic wave $r_{\perp} \neq 0$. This incident angle θ_B is called the **Brewster angle**. The corresponding reflectivity is drawn in the following figure.



3) Complex refractive index

For a complex refractive index $N = n + i\kappa$, the intensity of the wave decay as $I \propto e^{-\alpha x}$, where $\alpha = \frac{4\pi\kappa}{\lambda_0}$.



For real n_1 and complex N_2, from $n_1 \sin\theta_i = N_2 \sin\theta_t$, we obtain complex θ_t and

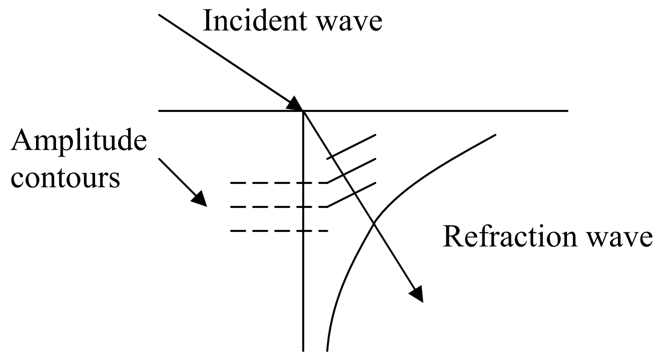
$\sin\theta_t = \frac{n_2 \sin\theta_i}{n_1} = a + bi$, $\cos\theta_t = \sqrt{1 - \sin^2\theta_t} = c + di$.

Thus the transmission wave is

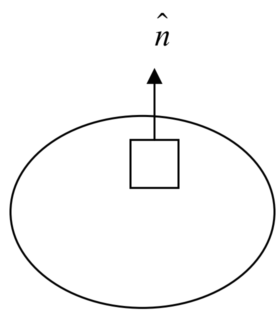
$$E_{//t} \exp\left[-i\omega\left(t - \frac{n_2 x \sin\theta_t + (n_2 + i\kappa_2)(c + di) z}{c_o}\right)\right].$$

Let $c_1 + d_1 i = (n_2 + i\kappa_2)(c + di)$. Similar to the evanescent wave, the imaginary component of the product leads to a decaying amplitude, while the real part contributes to the phase factor. The energy flow is still

$$\langle S \rangle = \frac{1}{2}\mathrm{Re}\left(\vec{E}\times\vec{H}^*\right).$$



4) Acoustic waves



Recall the Newton's law

$$\vec{F} = m\vec{a},$$

where the force is $\vec{F} = \hat{n}\cdot\overline{\overline{\sigma}}$, acceleration is $\vec{a} = \frac{d\vec{v}}{dt}$. Denote u as the displacement, i.e., $\vec{u} = \vec{x} - \vec{x}_0$. We have

$$\vec{v} = \frac{d\vec{x}}{dt} = \frac{d\vec{u}}{dt}.$$

In mechanics, we define the strain as

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right),$$

and the stress is

$$\overline{\overline{\sigma}} = \overline{\overline{\overline{\overline{c}}}}\cdot\overline{\overline{S}}.$$

Note: $\overline{\overline{\overline{\overline{c}}}}$ is a fourth-order tensor and has 81 components.

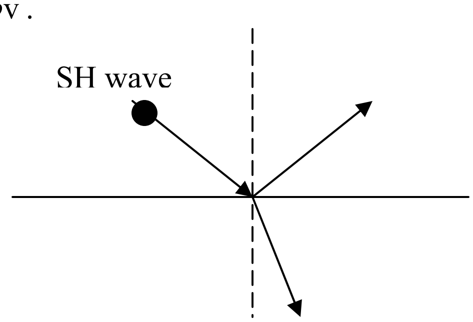
For phonons, we have two transverse waves and one longitudinal wave. The poynting vector for acoustic waves is

$$\langle \overline{p} \rangle = -\frac{1}{2}\mathrm{Re}\left(\overline{v}^{*} \cdot \overline{\overline{\sigma}}\right).$$

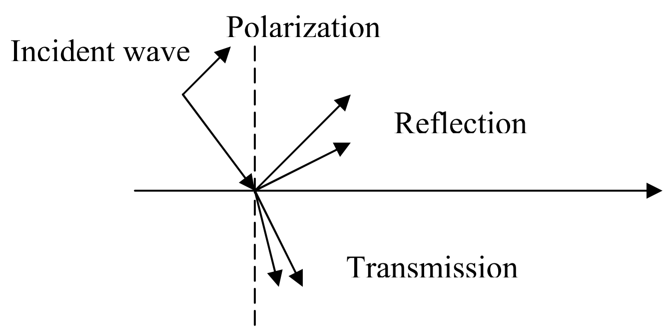
When the media is isotropic and the incident wave is a transverse wave with displacement polarized in the direction perpendicular to the plane of incidence (called a shear wave or SH wave), only one SH reflected and one SH transmitted wave are excited. At normal incidence, the acoustic reflectivity for a SH wave is

$$R_s = \left|\frac{Z_1 - Z_2}{Z_1 + Z_2}\right|^2,$$

in which the acoustic impedance Z (similar to refractive index in optics) is defined as $Z=\rho v$.



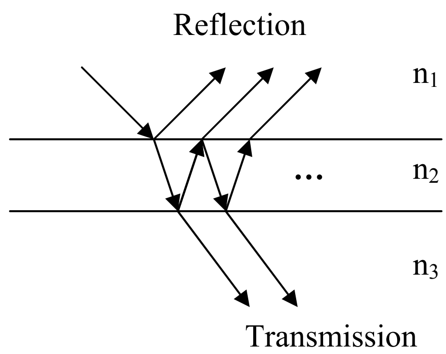
When the incident wave is polarized in the direction parallel to the plane of incidence, one longitudinal wave and one transverse wave are excited for both reflection and transmission waves. If the materials are anisotropic, one more transverse is excited for both reflection and transmission waves.



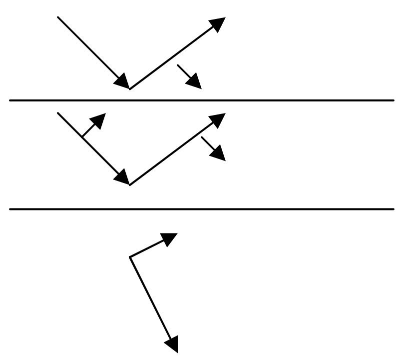
Note: The thermal resistance on the interface is very important for nanomaterials. Acoustic waves (or heat propagation) can be cut off by the interface, just as using a foil to cut off the radiation between two surfaces.

5.3 Wave propagation in thin films

First let us consider the following structure. Many reflections and transmissions exist in this case. Summation is required to calculate the total reflection and transmission.



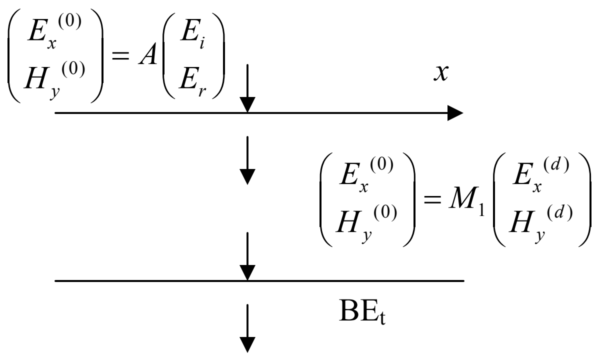
To avoid the summation of infinite series, two other methods are utilized:
1) Resultant wave method
In this method, the multiple reflection or transmission waves are combined into one in every material. In the following figure, we have four unknowns and four interfacial boundary conditions. The reflectivity and transmissivity can be determined on each interface.



2) Transfer matrix method
The transfer matrix method combines all the waves (both forward and backward ones) in each medium into one wave, and uses a matrix to relate the electric and the magnetic fields between two different points inside a medium. Because the tangential components of the electric and the magnetic fields are continuous across the interface when there is no interface charge and interface current, the transfer matrix method can be easily extended to multilayers.

In the following figure, the x-component of the electric field $E_x^{(z)}$ and y-component of the magnetic field $H_y^{(z)}$ on the interface are related by 2×2 matrix A, 2×2 matrix M_1, 2×1 matrix B. And we obtain

$$\begin{pmatrix} E_i \\ E_r \end{pmatrix} = A^{-1} M_1 B E_t .$$



For multilayers, M is determined by the chain rule as
$M = M_1 M_2 \cdots M_n$,
where n is the number of layers.

For a single layer of film, $\begin{pmatrix} E_i \\ E_r \end{pmatrix} = A^{-1} M_1 B E_t$ yields

$$r = \frac{E_r}{E_i} = \frac{r_{12} + r_{23} \exp[2i\varphi_2]}{1 + r_{12} r_{23} \exp[2i\varphi_2]},$$

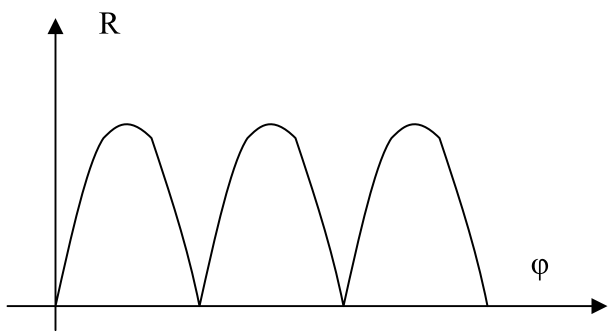
$$\varphi = \frac{2\pi n_2 d \cos\theta_2}{\lambda_0}.$$

Thus for a nonabsorbing film, we obtain

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

in which the cosine function indicates periodicity of R. This is just the interference effect.

Discussions:
(1) Periodic variation in R



Note: In microfabrication, the color of a thin film will change periodically according to the thickness, which is used to estimate the film thickness by eyes.

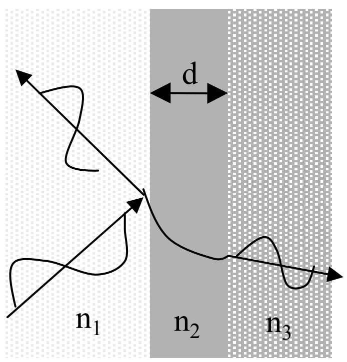
(2) Tunneling

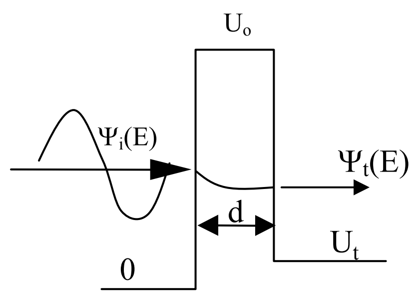
Back to the case in which $\theta_i > \theta_{cr}$. We have

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

which causes decay in the second medium. If the second medium is very thin, a third medium attached to the second medium will have tunneling effects. The wave will be partly transmitted into the third medium before decaying off and the reflectivity $R \neq 1$ in this case.

Note: From $n_1\sin\theta_i = n_2\sin\theta_2 = n_3\sin\theta_3$, in this case θ_i, θ_3 are real numbers, while θ_2 is imaginary number.





Similar phenomena happen to the electron propagation across a barrier. In the right figure, we can see tunneling happens when the barrier is thin. The transmissivity is

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

or

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