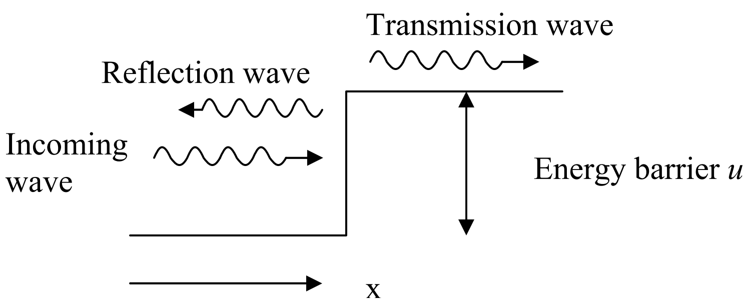
2.57 Nano-to-Macro Transport Processes
Fall 2004
Lecture 12

5.1 Plane waves & their interface reflection (continue)



For the above problem, we have obtained

$\Psi_i = Ae^{-i(\omega t - k_1 x)}$ (incoming wave),

$\Psi_r = Be^{-i(\omega t + k_1 x)}$ (reflected wave), $k_1 = \sqrt{\dfrac{2mE}{\hbar^2}}$

$\Psi_t = Ce^{-i(\omega t - k_2 x)}$ (transmitted wave), $k_2 = \sqrt{\dfrac{2m(E-u)}{\hbar^2}}$.

The boundary conditions are applied

$(\Psi_i + \Psi_r)_{x=0^-} = \Psi_t|_{x=0^+}$, $(\Psi_i' + \Psi_r')_{x=0^-} = \Psi_t'|_{x=0^+}$,

which yields

$A + B = C; k_1(A - B) = k_2 C$

or $\dfrac{B}{A} = \dfrac{k_1 - k_2}{k_1 + k_2}; \dfrac{C}{A} = \dfrac{2k_1}{k_1 + k_2}$.

The incoming flux term is (note A and k_1 can be complex)

$$J_i = \mathrm{Re}\left(\frac{i\hbar}{m}\Psi_i \nabla \Psi_i^*\right)$$

$$= \mathrm{Re}\left(\frac{i\hbar}{m} Ae^{-i(\omega t - k_1 x)} A^* (-ik_1^*) e^{i(\omega t - k_1^* x)}|_{x=0}\right)$$

$$= \frac{\hbar}{m}|A|^2 \,\mathrm{Re}\left(k_1^* e^{i(k_1 - k_1^*)x}|_{x=0}\right)$$

$$= \frac{\hbar}{m}|A|^2 \,\mathrm{Re}\left(k_1^*\right)$$

$$= \frac{\hbar}{m}|A|^2 k_1 ,$$

where we use the fact that k_1 is a real number in the last step. Similarly, we have

$J_r = -\frac{\hbar}{m}|B|^2 k_1$ (negative sign indicating the direction of reflection),

$J_t = \frac{\hbar}{m}|C|^2 \operatorname{Re}\left(k_2^*\right)$.

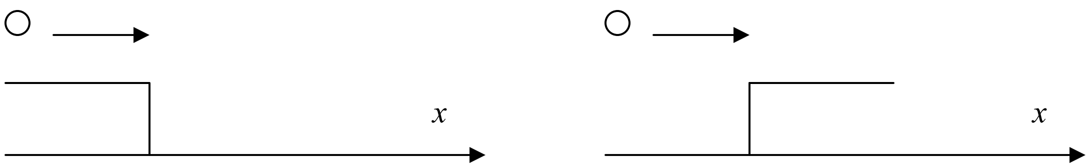
The reflectivity is

$$R = -J_r / J_i = \left|\frac{B}{A}\right|^2 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2 = \left|\frac{\sqrt{E} - \sqrt{E-u}}{\sqrt{E} + \sqrt{E-u}}\right|^2,$$

and transmittivity is

$$T = J_t / J_i = \left|\frac{C}{A}\right|^2 \frac{\operatorname{Re}\left(k_2^*\right)}{k_1}.$$

For E>u, the equation gives reflectivity $R \neq 0$ in both cases shown below, which is inconsistent with classical mechanics.

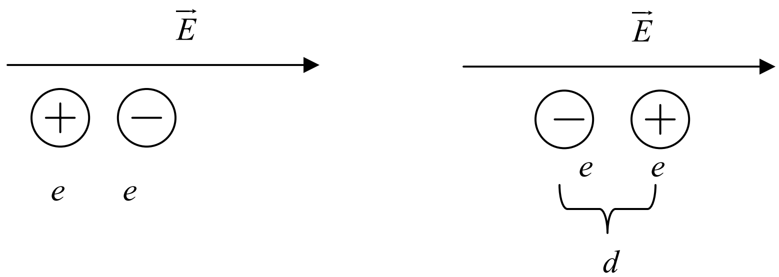


When E<u, the equations yield R=1, T=0, which is reasonable from classical viewpoint. However, the wavefunction is $\Psi_t = Ce^{-i\omega t - \sqrt{\frac{2m(u-E)}{\hbar^2}}x} \neq 0$ in this case. The wave will decay rapidly from the barrier and is thus called "evanescent wave."

Electromagnetic (EM) waves

In this chapter, we will see that the wave reflection, interference, and tunneling phenomena can occur for all the three types of carriers (phonons, electrons, photons) and the descriptions of these phenomena are also similar.

An electromagnetic wave in vacuum is characterized by an **electric field vector**, $\vec{E}$, and a **magnetic field vector**, $\vec{H}$. Consider a pair of charged particles placed in an electrical field. The field will attract the positively charged particle in one direction and repel the other particle in the same direction. Consequently, the particles are distorted and form an electrical dipole, whose moment is $p = e \cdot d$ (d is the separation distance).



A measure of the capability of the material responding to incoming electric field is the electric polarization per unit volume, or the **dipole moment** per unit volume, **P** [C m^{-2}], which is related to the electric field through the electric susceptibility, χ,

$\mathbf{P}=\varepsilon_0\chi\mathbf{E}$,

where ε_0 is the vacuum electric permittivity, ε_o=8.85x10^{-12} [C^2 N^{-1}m^{-2}], and the electric susceptibility is nondimensional. The electric susceptibility χ describes the extent to which positive and negative charges are displaced in a dielectric material under an applied electric field.

The total field inside the medium is measured by the **electric displacement**, D [Cm^{-2}], which is a superposition of the contributions from the external electric field and the electric polarization,

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

where ε is called the electrical **permittivity** of the medium.

The electron and ion motion in a medium also induces a magnetic field, which is superimposed onto the external magnetic field. A measure of the total magnetic field inside the medium is called magnetic induction, **B** (N.s m^{-1}.C^{-1}),

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

where μ is the magnetic **permeability**.

The propagation of an electromagnetic wave is governed by the following **Maxwell equations**:

(1) $\nabla\times\mathbf{E}=-\dfrac{\partial\mathbf{B}}{\partial t}$

This is the Farady law, which states that a changing magnetic field induces an electric field.

(2) $\nabla\times\mathbf{H}=\dfrac{\partial\mathbf{D}}{\partial t}+\mathbf{J_e}$

Without the $\dfrac{\partial\mathbf{D}}{\partial t}$ term, the above equation is the Ampere law, which says an electric current induces a magnetic field. The term $\dfrac{\partial\mathbf{D}}{\partial t}$ is the current due to the electron oscillation around the ion even though they are not free to move. It is also called displace current. This term is Maxwell's contribution. The current density term on the RHS is determined by $\mathbf{J_e}=\sigma\mathbf{E}$, in which σ is electrical conductivity.

(3) $\nabla\bullet\mathbf{D}=\rho_e$

Here ρ_e is the net charge per unit volume (C m^{-3}).

(4) $\nabla\bullet\mathbf{B}=0$

It states that there is no magnetic analog of an electric charge as in (3).

Rearranging the Maxwell equations yields $\nabla^2\mathbf{E}=\mu\varepsilon\frac{\partial^2\mathbf{E}}{\partial t^2}+\mu\sigma\frac{\partial\mathbf{E}}{\partial t}$, where the term $\mu\varepsilon\frac{\partial^2\mathbf{E}}{\partial t^2}$ denotes displacement, while $\mu\sigma\frac{\partial\mathbf{E}}{\partial t}$ denotes the current. Without $\mu\sigma\frac{\partial\mathbf{E}}{\partial t}$, the equation $\nabla^2\mathbf{E}=\mu\varepsilon\frac{\partial^2\mathbf{E}}{\partial t^2}$ is just a regular wave function. The additional term $\mu\sigma\frac{\partial\mathbf{E}}{\partial t}$ corresponds to damping and is also called dissipation term.

By solving equations (1)-(5), we obtain the following results for EM waves

$\mathbf{E}(\mathbf{r},t) = \mathbf{E_o}\exp[-i(\omega t- \mathbf{k}\bullet\mathbf{r})]$,

$\mathbf{k}\bullet\mathbf{k} = \mu\omega^2[\varepsilon_o(1+\chi)+i\sigma_e/\omega] = \mu\varepsilon\omega^2$,

where the first equation has the same form as the foregoing transmitted wave. In vacuum $\sigma_e=\chi=0$, the second equation yields

$$|\mathbf{k}|^2=\varepsilon_0\mu_0\omega^2,$$

or

$$\omega=\frac{|\mathbf{k}|}{\sqrt{\varepsilon_0\mu_0}}=c_0\,|\mathbf{k}|,$$

in which c_0 is the light speed in vacuum. This is familiar energy dispersion relationship for photons. Compared with photons, Maxwell concluded that EM waves were the same kind of wave as light. Here we also define the **complex reflective index** *N* as

$$N=\frac{c_0}{c}=\sqrt{\frac{\varepsilon\mu}{\varepsilon_0\mu_0}}\approx\sqrt{\frac{\varepsilon}{\varepsilon_0}}=\sqrt{\varepsilon_r}=n+ik,$$

where $\varepsilon_r = \varepsilon/\varepsilon_o$ is called the **dielectric constant** or dielectric function, the real part of N, n, is the usual refractive index of materials. The imaginary part of N, k, is called the **extinction coefficient**, measures the damping of the electromagnetic field, which not only arises from the free electrons absorption, but also from the dipole oscillation of bounded electrons and other mechanisms.

Note: The ε_r value depends on the wave frequency and is not a constant.

Based on N, $|\mathbf{k}|^2=\varepsilon\mu\omega^2$ can be rewritten as

$$|\mathbf{k}|^2=\frac{\omega^2}{c^2}=\frac{\omega^2}{c_0^{\,2}}\frac{c_0^{\,2}}{c^2}=\frac{\omega^2}{c_0^{\,2}}N^2,$$

or

$$|\mathbf{k}|=\frac{N\omega}{c_o}.$$

One can prove that the electromagnetic wave is a transverse wave, and that the electrical and magnetic fields are perpendicular to each other, i.e.,

$\mathbf{E}\perp\mathbf{H}\perp\mathbf{k}$

In the special case that a plane wave is traveling along the x-direction with the electric and magnetic fields pointing to the y- and z-direction, respectively.

We also define the **Poynting vector S** (W/m^2) as

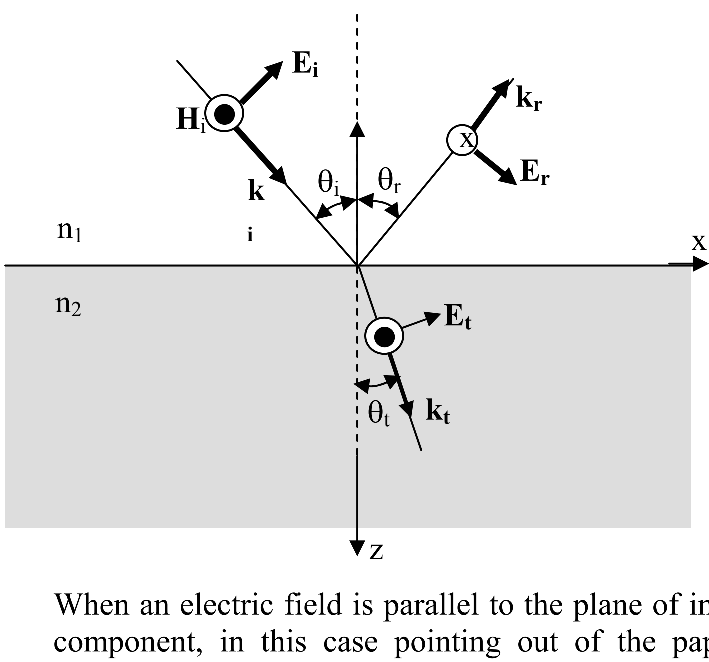
$$\mathbf{S}=\mathbf{E}\times\mathbf{H},$$

which represents the instantaneous energy flux. It oscillates at twice frequency of the electromagnetic field. No electronic devices can measure such a fast signal. What can be measured is the time-averaged Poynting vector that is further expressed as

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

Note: Normally we have μ, $\varepsilon>0$, and thus $n>0$ and the vector **S** is parallel to the wavevector **k**, which indicates the energy flows in the propagation direction of the wave. When μ, $\varepsilon<0$, the refractive index n should take a negative value. Such media do not exist in nature but has recently been demonstrated in laboratories, are called negative index materials or left handed materials. In these materials, the energy propagation direct is opposite to the phase propagation direction.

Here we will consider the more general case of oblique incidence of an electromagnetic wave onto an interface. As shown in the following figure, a plane electromagnetic wave propagates along direction $\mathbf{k_i}$ (wave vector direction) and meets an interface with norm $\hat{\mathbf{n}}$. The reflected wave and refracted wave propagates along the $\mathbf{k_r}$ and $\mathbf{k_t}$ directions, respectively. We call the plane formed by $\mathbf{k_i}$ and $\hat{\mathbf{n}}$ as the plane of incidence, and the angle formed between $\hat{\mathbf{n}}$ and $\mathbf{k_i}$ as the angle of incidence.



When an electric field is parallel to the plane of incidence, its conjugated magnetic field component, in this case pointing out of the paper, is perpendicular to the plane of incidence and is thus always parallel to the interface (refer to the figure).

In the plane wave expression obtained earlier in this lecture, we have

$\mathbf{k}\cdot\mathbf{r} = (k\sin\theta_i, 0, k\cos\theta_i)\cdot(x, y, z) = k(x\sin\theta_i + z\cos\theta_i)$,

$k = \frac{N\omega}{c_0} = N\frac{2\pi}{\lambda_0}$.

Thus the incident, reflected, and transmitted electric fields can be expressed as,

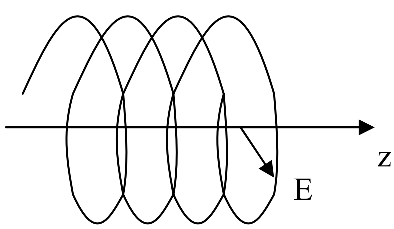
$$E_{//i}\exp\left[-i\left(\omega t - n_1 2\pi\frac{x\sin\theta_i + z\cos\theta_i}{\lambda_0}\right)\right],$$

$$E_{//r}\exp\left[-i\left(\omega t - n_1 2\pi\frac{x\sin\theta_r - z\cos\theta_r}{\lambda_o}\right)\right],$$

$$E_{//t}\exp\left[-i\left(\omega t - n_2 2\pi\frac{x\sin\theta_t + z\cos\theta_t}{\lambda_o}\right)\right],$$

where in the second equation the negative sign before $z\cos\theta_r$ indicates different propagation direction (upward in the z direction) from the incoming and refraction waves. The subscript "//" means that the electric field is polarized parallel to the plane of incidence for the sketched TM transverse wave.

Note: For EM waves, two transverse vibrating directions exist. In general, the resultant electric field vector will moves around in an ellipse instead of pointing in the same direction all the time. The path of the E vector is like a spiral in this situation.



Assuming there is no net surface charge or current on the interface (z=0), we can apply the continuity boundary condition to the vertical and tangential electric fields, respectively. In the x-direction, the tangential fields give

$$\cos\theta_i E_{//i}\exp\left[-i\omega\left(t - \frac{n_1 x\sin\theta_i}{c_o}\right)\right] + \cos\theta_r E_{//r}\exp\left[-i\omega\left(t - \frac{n_1 x\sin\theta_{rr}}{c_o}\right)\right]$$

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

where the above equation is valid only when the exponents are equal because x can take any value. Thus we have

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

which leads to the **Snell law** for reflection and refraction

$\theta_i=\theta_r$ and $n_1\sin\theta_i=n_2\sin\theta_t$,

which yield

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

The magnitude of the magnetic field, which is pointing out of the paper, is related to the electric field by

$$H_y = \frac{n}{\mu c_o} E_{//}.$$

We can write the continuity of the tangential component of the magnetic field as

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

Based on the equations for electric and magnetic fields, we obtain the reflection coefficient, $r_{//}$, and transmission coefficient, $t_{//}$, for a TM wave as

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

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

Note: (1) For an incident light shown as below (e.g. from air to water), in this case the refraction light will be bended and the object in the second media will looks higher if the observer is in the first media. (2) If $n_2<0$, $n_1>0$, the refraction light will be bended as the right figure. However, in nature no negative-*n* materials exist.