3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

Homework # 8 - Solutions

Nicolas Poilvert & Nicola Marzari

November 18, 2007

1   Propagation equation in a non-dispersive medium.

a) Defining $\alpha = x + vt$ and $\beta = x - vt$, we have,

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial \alpha}\frac{\partial \alpha}{\partial x} + \frac{\partial}{\partial \beta}\frac{\partial \beta}{\partial x} = \frac{\partial}{\partial \alpha} + \frac{\partial}{\partial \beta}$$

so, taking the square,

$$\frac{\partial^2}{\partial x^2} = \left[\frac{\partial}{\partial \alpha} + \frac{\partial}{\partial \beta}\right]^2 = \frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \beta^2} + 2\frac{\partial^2}{\partial \alpha \partial \beta}$$

Proceeding likewise for the time derivative, we find,

$$\frac{\partial^2}{\partial t^2} = v^2\left[\frac{\partial}{\partial \alpha} - \frac{\partial}{\partial \beta}\right]^2 = v^2\left[\frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \beta^2} - 2\frac{\partial^2}{\partial \alpha \partial \beta}\right]$$

It implies, after substitution in the original wave equation, that,

$$\frac{\partial^2 y}{\partial \alpha \partial \beta} = 0$$

Integrating over α, we get,

$$\frac{\partial y}{\partial \beta} = g(\beta)$$

where the function $g(\beta)$ is arbitrary since in any case it does act as a constant with respect to the α dependence. By the same token, the second integration introduces a function $f(\alpha)$,

$$y = f(\alpha) + g(\beta) = f(x + vt) + g(x - vt)$$

The general solution is the sum of two waves propagating in opposite directions at the same speed v.

Note: Many of you say that $\frac{\partial^2 y}{\partial \alpha \partial \beta} = 0$ implies $\frac{\partial y}{\partial \alpha} = 0$ or $\frac{\partial y}{\partial \beta} = 0$. That is wrong. The second statement is a *sufficient* condition but is not *necessary*.

b) The previous result shows that, in a non-dispersive medium, any wave shape will propagate without any deformation.

c) Now we look for solutions of the form $y = f(x)g(t)$. Substituting in the equation, we have,

$$f''(x)g(t) - \frac{1}{v^2}f(x)g''(t) = 0$$

implying,

$$\frac{f''(x)}{f(x)} = \frac{1}{v^2}\frac{g''(t)}{g(t)}$$

This relation is true for any pair (x, t). So, for example, if you fix x but let t vary, you see that the function of t defined by the right-hand side is actually a constant. Same reasoning for the left-hand side. Therefore, we can write,

$$\frac{f''(x)}{f(x)} = \frac{1}{v^2}\frac{g''(t)}{g(t)} = C$$

where C is a constant. C positive would mean that f and g are linear combinations of real exponentials, which would imply a divergence at infinity. We then only consider the case of C being negative, leading us to introduce a wave-number k such that $C = -k^2$. f and g can therefore be written in terms of the cos function, and we have,

$$y = f(x)g(t) = A cos(kx + \phi_x)cos(\omega t + \phi_t)$$

where $\omega = kv$ and A, ϕ_x, ϕ_t are constants, determined by initial conditions and a normalization constraint. Furthermore, if the medium is finite, boundary conditions - for example y = 0 at extremities - will introduce quantization of k. We have already seen this phenomenon when studying the infinite well in quantum mechanics.

d) Using a trigonometry formula,

$$A cos(kx+\phi_x)cos(\omega t+\phi_t) = \frac{A}{2}\left[cos(kx + \omega t + \phi_x + \phi_t) + cos(kx - \omega t + \phi_x - \phi_t)\right]$$

This proves that a stationary wave is the superposition of two waves propagating in opposite directions. In the electronic band structure of an infinite crystal, this happens at the boundaries of the first Brillouin zone and at the Γ point.

2   Propagation in a dispersive medium.

a) Plugging the relation $y = e^{-i\omega t}g(x)$ into the wave equation, we get,

$$g''(x) + \frac{\omega^2}{v^2}g(x) = 0$$

The wave-number k appears naturally as holding the dispersion relation $\frac{\omega}{k} = v(\omega)$, and the general solution is,

$$g(x) = Ae^{ikx} + Be^{-ikx}$$

A, B are constants. The solution is a de Broglie wave when either A or B is equal to zero.

b) The wave equation is defined for a given angular frequency ω or, equivalently, for a given wave-number k. So, the idea is to decompose $f(x)$ into an infinite number of de Broglie waves (this is a Fourier transform). Taking advantage of the linearity of the wave function, we can say that at any time, the wave is the sum of the contributions by each harmonic component propagating with its own phase velocity along the medium.

c) We apply this method to a simple case, in which the Fourier transform of f is a constant function between $k_0 - \Delta k$ and $k_0 + \Delta k$, and zero anywhere else. Initially,

$$f(x) = A \int_{k_0 - \Delta k}^{k_0 + \Delta k} e^{ikx} dk = Ae^{ik_0 x} \left[\frac{e^{ikx}}{ix} \right]_{-\Delta k}^{\Delta k} = 2A\Delta k e^{ik_0 x} sinc(x\Delta k)$$

The first zero of the sinus cardinal function is for $x\Delta k = \pi$, so we see that the size of the wave packet in real space is inversely proportional to its size in reciprocal space,

$$\Delta x \sim \frac{1}{\Delta k}$$

d) After a certain time t, each harmonic component has propagated at its own speed, and the wave can be reconstructed by adding them all,

$$y(x,t) = A \int_{k_0 - \Delta k}^{k_0 + \Delta k} e^{i(kx - \omega t)} dk$$

e) If ω is a linear function of k, only the first two terms of the Taylor expansion remain, and we have,

$$y(x,t) = A \int_{k_0 - \Delta k}^{k_0 + \Delta k} e^{ikx} e^{-i\left(\omega_0 + \frac{d\omega}{dk}(k - k_0)\right)t} dk$$

and introducing the notation $v_g = \dfrac{d\omega}{dk}$,

$$y(x,t) = Ae^{i(k_0 x - \omega_0 t)} \left[\frac{e^{ik(x - v_g t)}}{i(x - v_g t)} \right]_{-\Delta k}^{\Delta k} = 2A\Delta k e^{i(k_0 x - \omega_0 t)} sinc\left[k(x - v_g t) \right]$$

We see that the de Broglie wave $e^{i(k_0 x - \omega_0 t)}$ is modulated by the sinus cardinal propagating at v_g, which justifies the name *group velocity*.

f) Distortion.

3   Propagation of light in a conducting medium.

a) The electron feels an electric force $-e\mathbf{E}$ and a magnetic force $-e\mathbf{v} \times \mathbf{B}$. For a plane wave, we have $|\mathbf{B}| = \dfrac{|\mathbf{E}|}{c}$. So the ratio of the magnetic force over the electric force is equal to $\dfrac{|\mathbf{v}|}{c}$, which is very small for an electron in a crystal. We

can therefore neglect the magnetic force.

b) The damping process has a typical time of τ. If this is much smaller than the typical time ω^{-1} over which the electric field varies, then the electron reaches a steady state velocity proportional to the electric force almost immediately after the electric field has been set to a new value. This absence of phase lag leads us to drop the $\frac{d\mathbf{p}}{dt}$ term. The condition we are looking for is then $\omega\tau \ll 1$. For $\tau \sim 1 - 10$ fs, we find that the wave-length must be at least of the order of several hundreds of microns.

c) Since we are in the right spectral range, we obtain the electron velocity by saying,
$$\mathbf{v} = \frac{\mathbf{p}}{m} = \frac{\tau}{m}\mathbf{f(t)} = -\frac{e\tau}{m}\mathbf{E}$$
where m is the mass of the electron. The current density is then,
$$\mathbf{J} = -ne\mathbf{v} = \frac{ne^2\tau}{m}\mathbf{E}$$
where n is the electron density. We identify the conductivity,
$$\sigma = \frac{ne^2\tau}{m}$$

d) We start with the mathematical identity,
$$\nabla \times (\nabla \times \mathbf{E}) = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2\mathbf{E} \tag{1}$$
Using the two Maxwell *curl* equations, we say that,
$$\nabla \times (\nabla \times \mathbf{E}) = -\frac{\partial}{\partial t}[\nabla \times \mathbf{B}] = -\frac{\partial}{\partial t}\left[\mu_0\mathbf{J} + \epsilon_0\mu_0\frac{\partial\mathbf{E}}{\partial t}\right]$$
$$\nabla \times (\nabla \times \mathbf{E}) = -\mu_0\sigma\frac{\partial\mathbf{E}}{\partial t} - \epsilon_0\mu_0\frac{\partial^2\mathbf{E}}{\partial t^2} \tag{2}$$

Now, what about the term $\nabla(\nabla \cdot \mathbf{E})$ in Equation (1)? We need to know more about the free charge density. For that, we express the law of charge conservation,
$$-\frac{\partial\rho}{\partial t} = \nabla \cdot \mathbf{J}$$
We substitute $\mathbf{E}$ for $\mathbf{J}$ using Ohm's law (that we derived earlier), and then we use Gauss' law,
$$-\frac{\partial\rho}{\partial t} = \sigma\nabla \cdot \mathbf{E} = \frac{\sigma}{\epsilon_0}\rho$$
We conclude that the charge density follows an exponential decay,
$$\rho = \rho_0 e^{-\frac{t}{t_1}}$$

where $t_1 = \dfrac{\epsilon_0}{\sigma}$. For a typical conductivity of 10^6 $\Omega^{-1}{\cdot}m^{-1}$, this yields $t_1 \sim 10^{-17}$ s. In practice, we can then write $\rho = 0$. So now, if we reapply Gauss' law, we find,

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} = 0 \tag{3}$$

Combining Equations (1), (2) and (3), we get,

$$\nabla^2 \mathbf{E} - \mu_0 \sigma \frac{\partial \mathbf{E}}{\partial t} - \epsilon_0 \mu_0 \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0 \tag{4}$$

e) We look for a solution of the form $e^{-i(\omega t - kx)}$ (congratulations to those who found out that the inverse, $e^{i(\omega t - kx)}$, does not work well. This is because time is not reversible...). Plugging that into the wave equation, we find,

$$-k^2 + \mu_0 \sigma i \omega + \frac{\omega^2}{c^2} = 0$$

and rearranging to find the complex refractive index,

$$n^2 = \left(c \frac{k}{\omega} \right)^2 = 1 + \frac{\mu_0 \sigma i \omega c^2}{\omega^2} = 1 + i \frac{\sigma}{\omega \epsilon_0}$$

f) $\dfrac{\sigma}{\omega \epsilon_0} \gg \dfrac{\sigma \tau}{\epsilon_0} \sim 100$ assuming $\tau \sim 1$ fs and σ of the order of 10^6 $\Omega^{-1} \cdot m^{-1}$. Therefore, we can neglect the 1 in the expression of n^2,

$$n^2 = i \frac{\sigma}{\omega \epsilon_0}$$

Taking the right square root so that the wave will propagate along increasing x, we find,

$$n = \sqrt{\frac{\sigma}{2\omega \epsilon_0}} (1 + i)$$

g) The presence of an imaginary part in the refractive index causes an exponential decay of the light wave amplitude along the x-axis. The light intensity is proportional to the square of the wave amplitude. Therefore, taking the time-average of the intensity, we find,

$$I(x) = I_0 e^{-x/\delta(\omega)}$$

where,

$$1/\delta(\omega) = \frac{2\omega}{c} Im(n) = \frac{2\omega}{c} \sqrt{\frac{\sigma}{2\omega \epsilon_0}} = \sqrt{2\sigma \omega \mu_0}$$

$$\delta(\omega) = \sqrt{\frac{1}{2\sigma \omega \mu_0}}$$

4 Interband absorption.

a) GaAs is a direct-gap semiconductor. Si is not.

b) Rigorously speaking, yes, k change by the amount of the photon momentum (by application of the law of momentum conservation). However, optical frequency photons have k values of about 10^7 m^{-1} when the size of the first Brillouin zone of a crystal is given by $\pi/a \sim 10^{10}$ m^{-1}, if one assumes a typical crystal parameter a of the order of one angstrom. Therefore, in practice, when no phonon is involved, k remains unchanged after the transition.

c) If a transition occurs between states i and f, it means that they are not eigenstates of the total hamiltonian.

d) Hybridization.

e) In order to know whether a transition is allowed, one has to calculate the energy matrix element between the two states involved. This is exactly what Fermi's golden rule expresses since the transition rate is written in terms of the square of the perturbing hamiltonian element between the initial state Ψ_i and the final state Ψ_f. In the framework of the electric dipole approximation, the perturbing hamiltonian is $-\mathbf{p} \cdot \mathbf{E}$, where $\mathbf{p}$ is the dipole moment of the electron. The matrix element we are interested in is then,

$$M = \langle \Psi_f | -\mathbf{p} \cdot \mathbf{E} | \Psi_i \rangle = \langle \Psi_f | e\mathbf{r} \cdot \mathbf{E} | \Psi_i \rangle$$

$$M = e\mathbf{E} \cdot \int_{space} \Psi_f^* \mathbf{r} \Psi_i d\mathbf{r}$$

If Ψ_i and Ψ_f have the same quantum number l, the product $\Psi_f^* \Psi_i$ is even (either as the product of two positive parities or as the product of two negative parities), which makes the function $\Psi_f^* \mathbf{r} \Psi_i$ odd. The integral over space of an odd function is zero, which implies $M = 0$. We conclude that no transition is allowed between these two states through the electric dipole interaction.

f) Refer to Optical Properties of Solids by Mark Fox, p. 58.

g) The lower the curvature, the higher the joint density of states, therefore the higher the absorption coefficient.