3.23 Electrical, Optical, and Magnetic Properties of Materials
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Homework # 8

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1 Propagation equation in a non-dispersive medium.

Consider the following propagation equation in an infinite, one-dimension medium:

$$\frac{\partial^2 y}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2} = 0$$

where y is a real function and v is called the phase velocity.

a) Prove that any solution is the superposition of two waves propagating in opposite directions at the speed v, in other words any solution y can be written $y(x,t) = f(x + vt) + g(x - vt)$ where f and g can be of arbitrary shape (twice differentiable though). Show the details of the derivation.

Hint: You can define new variables $\alpha = x + vt$ and $\beta = x - vt$ and rewrite the differential equation with these new variables.

b) What can you conclude about the shape of a wave propagating in a non-dispersive medium?

Now, we look for stationary solutions, that is solutions for which space and time dependences can be separated: $y(x,t) = f(x)g(t)$, where f and g must be **real** functions.

c) Find equations for f and g, and solve them. Use physical arguments to eliminate some classes of solutions. For a finite medium, what else would you have to know to completely solve the equation? How does that introduce quantization? Give an example and draw a parallel with a quantum-mechanical system that you have studied.

d) Since the result of a) still holds, prove that any stationary solution is indeed the superposition of two waves propagating in opposite directions. Where does that happen in the first Brillouin zone of an infinite crystal?

2 Propagation in a dispersive medium.

For a dispersive medium, the phase velocity v must be defined as a function of an angular frequency ω. Therefore, we first consider waves whose time dependence

is imposed by an oscillatory source, leading us to write: $y(x,t) = Re\left(e^{-i\omega t}g(x)\right)$, or, to simplify the notation (provided we remember to take the real part at the end), $y(x,t) = e^{-i\omega t}g(x)$ (this is not *a priori* a stationary solution as we defined it earlier because taking the real part may have the effect of mixing time and space dependences). An example of such functions are the well-known de Broglie waves $e^{-i(\omega t - kx)}$, where k is called the wave number.

a) Derive an equation for $g(x)$, and introducing a wave number k, find the dispersion relation $\dfrac{\omega}{k} = v(\omega)$. When is the solution a de Broglie wave?

Now we want to study the propagation of any type of wave function. At t=0, the space dependence is not e^{ikx} anymore, but a more complicated function f(x).

b) How would you proceed to solve the problem by means of de Broglie waves only?

Let us take an example. Assume that the initial space dependence $f(x)$ can be decomposed into an infinite number of harmonics e^{ikx} with k spanning the $[k_0 - \Delta k; k_0 + \Delta k]$ interval with uniform spectral density A. In other words,

$$f(x) = A \int_{-\Delta k}^{\Delta k} e^{ikx} dx$$

c) Calculate f(x) explicitly. Can you comment on the space width of the wave with respect to the wave number domain width? This is a very general result, that gives rise, in quantum mechanics, to the Heisenberg uncertainty principle.

d) Now, at $t > 0$, express the solution in the form of an integral.

To calculate the integral that you found in d), we will consider the Taylor expansion,

$$\omega = \omega_0 + \frac{d\omega}{dk}(k - k_0) + \frac{1}{2}\frac{d^2\omega}{dk^2}(k - k_0)^2$$

where $\omega_0 = \omega(k_0)$.

e) Assuming that ω is a linear function of k, calculate the solution at any time t. Can you see why $\dfrac{d\omega}{dk}$ is called the group velocity?

f) If $\dfrac{d^2\omega}{dk^2}$ is not equal to zero, give a qualitative discussion of what will happen. Justify the expression *dispersive medium*.

3 Propagation of light in a conducting medium.

To solve Maxwell's equations, one has to know how to relate the charge density ρ and the current density **J** to the fields **E** and **B**. In this problem, we treat the case of an uncharged, non-polarizable metal. The latter assumption means that we neglect polarization due to bound electrons. The electrons of the conduction band, however, are free to move under the influence of an electromagnetic field.

In the classical Drude model, the movement of a conduction electron in a field $(\mathbf{E},\mathbf{B})$ is described by the equation,

$$\frac{d\mathbf{p}}{dt} = -\frac{\mathbf{p}}{\tau} + \mathbf{f(t)}$$

where $\mathbf{p}$ is the electron momentum, $1/\tau$ a damping coefficient representing the collisions of the electron with the atoms of the lattice, and $\mathbf{f(t)}$ is the force exerted by the fields on the electron.

a) Show that for a conduction electron in the field of an electromagnetic wave, one can neglect the magnetic force and write $\mathbf{f(t)} = -e\mathbf{E}$.

b) If ω is the electromagnetic wave angular frequency, upon what condition on the product $\omega\tau$ can we reasonably set $\frac{d\mathbf{p}}{dt} = 0$ in the equation of motion? For $\tau \sim 1 - 10$ fs, for what wave numbers is this condition satisfied?

For the rest of the problem, suppose that we work in the spectral range of far infrared wavelengths.

c) Find the expression of the electric conductivity σ, defined by,

$$\mathbf{J} = \sigma\mathbf{E}$$

d) Using Maxwell's equations, derive the propagation equation for $\mathbf{E}$ in the metal.

e) Looking for a solution of the form $e^{i(\omega t - kx)}$, where k is *a priori* a complex number, find an equation for k. Express the complex refractive index n as a function of σ, ω and the electric permittivity of free space ϵ_0.

f) Prove that the relation you just found can be simplified into,

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

g) Conclude that the intensity of the light beam propagating in the metal follows the law,

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

where I_0 is the intensity of the beam at the surface of the metal, x measures the distance from the surface, and $\delta(\omega)$ is a typical penetration length called *skin depth*. Show that,

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

4 Interband absorption.

Let us consider a direct gap semiconductor. Around the origin, the highest valence band is approximated by the parabola $E_v(k) = -\frac{\hbar^2 k^2}{2m_h}$, where m_h is the

effective mass of a hole at the top of the valence band, and the lowest conduction band is represented by the parabola $E_c(k) = \dfrac{\hbar^2 k^2}{2m_e}$, where m_e is the effective mass of an electron at the bottom of the conduction band. Let E_g be the energy gap.

a) Draw a schematic including all useful data. Give an example of a direct gap semiconductor. Does Si have a direct gap?

b) By absorbing a photon, an electron can jump from the valence to the conduction band. Does k change? Why?

Fermi's golden rule gives the transition rate W for exciting an electron in an initial state i to a final state f by absorption of a photon of angular frequency ω,

$$W = \frac{2\pi}{\hbar}|M|^2 g(\hbar\omega)$$

M is the element of matrix $\langle f|H'|i\rangle$, where H' is the hamiltonian of the perturbation (here the interaction with light). $g(\hbar\omega)$ is the joint density of states. By definition, $g(\hbar\omega)d(\hbar\omega)$ is the number of allowed transitions involving the exchange of an energy between $\hbar\omega$ and $\hbar\omega + d(\hbar\omega)$. In the electric dipole approximation, the perturbing hamiltonian can be simply written,

$$H' = -\mathbf{p} \cdot \mathbf{E}$$

where $\mathbf{p}$ is the dipole moment of the electron, $\mathbf{p} = -e\mathbf{r}$.

c) If a transition occurs, what can be concluded about the states i and f with respect to the total hamiltonian?

d) Explain why in general it is not strictly rigorous to speak of 's-bands', 'p-bands', etc, when describing the band structure of a solid.

However, around the origin, this simplification is legitimate. The angular dependence of the Bloch wave $\psi(\mathbf{r})$ can then be described in terms of the orbital moment quantum number l. If l is even, the wave function will be of positive parity, meaning that $\forall \mathbf{r}, \psi(-\mathbf{r}) = \psi(\mathbf{r})$. If l is odd, we will have a negative parity, meaning that $\forall \mathbf{r}, \psi(-\mathbf{r}) = -\psi(\mathbf{r})$.

e) Selection rules say which transitions are allowed and which are forbidden. For example, in the electric dipole approximation, you cannot have a transition between two states that have the same quantum number l. Can you explain why?

f) Calculate the joint density $g(\hbar\omega)$ for the simplified band structure introduced earlier. You will define the reduced electron-hole mass μ,

$$\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_h}$$

g) We suppose that the quantity $\langle f|r|i\rangle$ is known and is equal to B. Express the

absorption coefficient α in terms of the atomic density, the matrix element B, and all other relevant quantities.