

Phys 507B - Solid State Physics II

Assignment 3: Optical properties from charged excitations. Due March 3rd

1. Sum rule for the dielectric function.

The dielectric function is subject to various *sum rules*. For example, show that the Kramers-Kronig relations imply

$$\int_0^\infty \text{Im}[\epsilon(\omega)] \omega d\omega = \frac{\pi e^2 N}{2m^* V}, \quad (1)$$

no matter what the frequency distribution of oscillators in the medium.

2. Semiclassical theory of phonon-polaritons.

Here we consider the following Hamiltonian density as a model for a optical phonon interacting with light:

$$\mathcal{H} = \frac{1}{2n} \mathbf{\Pi}^2 + \frac{1}{2} n \omega_T^2 - \gamma_{12} \mathbf{u} \cdot \mathbf{E} - \frac{1}{2} \gamma_{22} \mathbf{E}^2, \quad (2)$$

where $\mathbf{u} = \mathbf{u}(\mathbf{r}, t)$ is the elastic displacement field modelling the phonons, with n the mass density, ω_T the transverse phonon frequency, and $\mathbf{\Pi} = n\dot{\mathbf{u}}$ the momentum associated to the phonon field. The electric field \mathbf{E} represents light, with the coupling constants γ_{12} and γ_{22} to be determined below. Note how this Hamiltonian is isotropic. Physically, γ_{12} represents the coupling of phonons to electric field, while γ_{22} represents all the terms that contribute to χ_e but don't depend on phonons (e.g. the polarizability of the electronic cloud).

The modes of vibration have to satisfy the Hamiltonian equations of motion together with Maxwell's equations. Considering that $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$ these are:

$$\begin{aligned} \dot{\mathbf{u}} &= \frac{\partial \mathcal{H}}{\partial \mathbf{\Pi}}, \\ \dot{\mathbf{\Pi}} &= -\frac{\partial \mathcal{H}}{\partial \mathbf{u}}, \\ \nabla \cdot (\epsilon_0 \mathbf{E} + \mathbf{P}) &= 0, \\ \nabla \cdot \mathbf{B} &= 0, \\ \nabla \times \mathbf{B} &= \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}}{\partial t}, \\ \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t}. \end{aligned} \quad (3)$$

- (a) Find the equation of motion for the phonon field (the first two equations above). Also, find the electric polarization using the definition

$$\mathbf{P} = -\frac{\partial \mathcal{H}}{\partial \mathbf{E}}. \quad (4)$$

Considering the $\omega = 0$ (zero frequency or static case), use the equation of motion and the polarization to show that

$$\left(\frac{\gamma_{12}^2}{n\omega_T^2} + \gamma_{22} \right) = (\epsilon(0) - \epsilon_0). \quad (5)$$

Now consider $\omega = \infty$; in this case, argue that $\mathbf{u} = 0$ and relate γ_{22} to $\epsilon(\infty)$.

- (b) Search for a *longitudinal* solution of the equations with the form $E_z, P_z, u_z \propto e^{i(kz-\omega t)}$, and all other fields equal to zero. Are the phonons coupled to photons in this case? For which frequency is this an allowed solution? Call it ω_L and relate to $\epsilon(0)$, $\epsilon(\infty)$, and ω_T .
- (c) Now look for transverse solutions of the form

$$\begin{aligned} E_x &= E_0 e^{i(kz-\omega t)}; & P_x &= P_0 e^{i(kz-\omega t)}; \\ u_x &= u_0 e^{i(kz-\omega t)}; & H_y &= H_0 e^{i(kz-\omega t)}. \end{aligned} \quad (6)$$

Assume all other fields are zero, and write the resulting equations as a homogeneous system. Determine the polariton dispersion analytically and make a sketch labelling the phonon like and photon like branches.

3. Plasmons: Semiclassical model.

Consider a *jellium* model for a thin sheet of metal: Think of the atomic ions as forming a fixed positive background with charge density $\rho_+ = -n e$ (here n is the number of electrons per unit volume and $e < 0$ is the electron's charge); the conduction electrons form a uniform jellium with charge density $\rho_- = n e$. The vibrational modes of the conduction electron gas with respect to this positive matrix is called a plasmon.

- (a) Assume that the electron gas is displaced by an amount z with respect to its positive background along the direction perpendicular to the plane (the $\hat{\mathbf{z}}$ direction). From Newton's law, find the equation of motion for z , and show that the frequency of oscillation of the plasma will be

$$\omega_p^2 = \frac{ne^2}{\epsilon_0 m^*}. \quad (7)$$

Hint: Use Gauss' law to find the internal electric field (the "depolarizing field") created by displacing the electron gas by z .

- (b) Assume an external electric field of the form $E_{\text{ext}}e^{-i\omega t}$ is applied perpendicular to the plasma. Find the response of the system (its polarization as a function of ω) and show that the dielectric constant is given by

$$\epsilon_{\perp}(\omega) = \epsilon_0 \left(1 - \frac{\omega_p^2}{\omega^2} \right). \quad (8)$$

*Hint: There is a tricky issue here: The dielectric constant is defined from $P = \epsilon_0 \chi_e E_{\text{int}}$, **not from** $P = \epsilon_0 \chi_e E_{\text{ext}}$. Note that for external field perpendicular to the metal sheet we will get $E_{\text{int}} = E_{\text{ext}} - \frac{ne}{\epsilon_0} z = E_{\text{ext}} - P/\epsilon_0$.*

- (c) Now assume the external field $E_{\text{ext}}e^{-i\omega t}$ is applied *parallel* to the metal's plane. If the displacement of the plasma is x , argue that there will be no depolarizing field (i.e. $E_{\text{int}} = E_{\text{ext}}$) and find the polarization induced along the \hat{x} direction. Compute the dielectric constant $\epsilon_{\parallel}(\omega)$, and show that the result is identical to Eq. (8). Hence $\epsilon(\omega)$ is isotropic despite the fact that the system is quite anisotropic! Sketch $\epsilon(\omega)$ as a function of ω and label the frequency regions where the metal will be transparent, as well as the frequency region where the metal will absorb light (where does the photon energy go to?).

4. Surface plasmons.

Consider a semi-infinite plasma on the positive side of the plane $z = 0$. A solution of Laplace's equation $\nabla^2 \phi = 0$ in the plasma is $\phi_i(x, z) = A \cos(kx)e^{-kz}$, whence $E_{zi} = kA \cos(kx)e^{-kz}$, and $E_{xi} = kA \sin(kx)e^{-kz}$. Here i means inside ($z > 0$) and o means outside ($z < 0$).

- (a) Show that in the vacuum $\phi_o(x, z) = A \cos(kx)e^{kz}$ for $z < 0$ satisfies the boundary condition that the tangential component of \mathbf{E} be continuous at the boundary; that is, find E_{xo} .
- (b) Note that $\mathbf{D}_i = \epsilon(\omega)\mathbf{E}_i$; $\mathbf{D}_o = \mathbf{E}_o$. Show that the boundary condition that the normal component of \mathbf{D} be continuous at the boundary requires that $\epsilon(\omega) = -1$. Use the dielectric function of the free electron gas [Eq. (8) derived above] to find the Stern-Ferrell result:

$$\omega_s^2 = \frac{1}{2}\omega_p^2 \quad (9)$$

for the frequency ω_s of a surface plasma oscillation.