Phys 507A - Solid State Physics I

Assignment 3: Classical waves: Sound and light. *Due Mar. 2nd*

1. *Sound dispersion of a diatomic linear chain: Acoustic and optical branches.* Consider a linear chain in which alternate ions have mass M_1 and M_2, and only nearest neighbors interact.

   (a) Show that the dispersion relation for the normal modes is

   $$\omega^2 = \frac{K}{M_1 M_2}\left(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos ka}\right). \tag{1}$$

   (b) Discuss the form of the dispersion relation and the nature of the normal modes when $M_1 \gg M_2$.

   (c) Compare the dispersion relation with that of the monatomic chain when $M_1 \approx M_2$.

2. *Counting the number of branches.* Consider a d-dimensional crystal with s atoms per unit cell.

   (a) What is the number of acoustic wave branches?

   (b) What is the number of optical wave branches?

3. *Acoustic phonons in a cubic crystal.*

   (a) Write down the Christoffel wave equation for a wave in a cubic crystal propagating along the [111] direction.

   (b) Find the dispersion and the polarization vector of each mode.
   Hint: The roots of $x^3 - 3x + 2 = 0$ are $x = 1$ and $x = -2$. One of these will be longitudinal, and the other will be transverse (doubly degenerate).

4. *Optical behavior of a simple soft mode ferroelectric.* Consider the following model free energy density for a ferroelectric material,

   $$\mathcal{F} = \frac{a}{2}P_z^2 + \frac{b}{4}P_z^4 + \frac{P_x^2 + P_y^2}{2\chi_\perp} - \boldsymbol{P}\cdot\boldsymbol{E}, \tag{2}$$

   where $\boldsymbol{P} = (P_x, P_y, P_z)$ is the electric dipole moment per unit volume of the material, and $\boldsymbol{E}$ is the applied electric field. The parameters b and $\chi_\perp$ are constants independent of temperature; the parameter a is assumed to depend on temperature according to $a = a_0(T - T_c)$, where T is the temperature and T_c is the critical temperature for a phase transition from paraelectric to ferroelectric.

(a) Assume $\boldsymbol{E} = 0$. Sketch the energy as a function of P_z for $T > T_c$ and for $T < T_c$. What is the difference?

Hint: When $T < T_c$, $\mathcal{F}$ is a double well potential.

(b) At thermal equilibrium, the system will choose a state that minimizes $\mathcal{F}$. Show that at $T < T_c$ the system has two stable phases with two possible values of spontaneous polarization $\mathbf{P}_0 \neq \mathbf{0}$ (Assume $\boldsymbol{E} = 0$). Note that a spontaneous polarization or ferroelectric moment exists even when $\boldsymbol{E} = 0$, a remarkable result. What is the magnitude of $\boldsymbol{P}_0$?

Assume light is incident on the material, exciting it with an electric field of the form $\boldsymbol{E} = \boldsymbol{E}_\omega e^{i\omega t}$. The electric polarization of the material will respond according to Newton's second law of motion,

$$\frac{\partial^2 \boldsymbol{P}}{\partial t^2} = -f \frac{\partial \mathcal{F}}{\partial \boldsymbol{P}}, \tag{3}$$

where f is a constant [dimensions of $Q^2/(ML^3)$]. In the following, assume the polarization response is given by $\boldsymbol{P} = \boldsymbol{P}_0 + \delta \boldsymbol{P}_\omega e^{i\omega t}$, with $\delta \boldsymbol{P}_\omega$ small; drop all terms that are quadratic or higher order in $\delta \boldsymbol{P}_\omega$.

(c) Compute the electric susceptibility tensor as a function of frequency in the paraelectric phase ($T > T_c$). The susceptibility tensor is the matrix $\boldsymbol{\chi}(\omega)$ in $\delta \boldsymbol{P}_\omega = \boldsymbol{\chi}(\omega) \cdot \boldsymbol{E}_\omega$.

How many poles in $\boldsymbol{\chi}(\omega)$? Each pole can be interpreted as an optical phonon associated to vibrations of the material's internal electric polarization. Dielectric resonance happens when the frequency of light is equal to one of these poles. Consider the reflectivity,

$$r = \left| \frac{1 - \sqrt{\epsilon}}{1 + \sqrt{\epsilon}} \right|. \tag{4}$$

What happens to the reflectivity when the frequency of light satisfies the dielectric resonance condition?

(d) Compute the electric susceptibility tensor as a function of frequency in the ferroelectric phase ($T < T_c$). Sketch the frequency of the pole in χ_{zz} as a function of temperature as the temperature is changed from above T_c to below T_c. This phenomena is called mode softening; measurements of the reflectivity as a function of temperature can be used to measure T_c and to determine whether the material has a phase transition.