PHYS455 Homework set VI, Wednesday, March 2, 2005
(Due at 11am, March 9, 2005)

Correlated Lattice Vibrations and Phonons

As discussed in previous lectures, one can introduce the following coordinates for lattice sites in a **cubic** crystal

$$\mathbf{R} = (n_x, n_y, n_z)a, n_\mu = 0, \pm 1, \pm 2, ..., \mu = x, y, z. \tag{1}$$

The position of an atom at site $\mathbf{R}$ then is characterized by the following vector

$$\mathbf{r}(\mathbf{R}) = \mathbf{R} + \mathbf{u}(\mathbf{R}). \tag{2}$$

In the Debye-Einstein model, the energy for atoms in a crystal is

$$E = \sum_{\mathbf{R}} \frac{\mathbf{P}^2(\mathbf{R})}{2M} + \frac{1}{2} M\omega^2 \sum_{<\mathbf{R}\mathbf{R}'>} |\mathbf{U}(\mathbf{R}) - \mathbf{U}(\mathbf{R}')|^2. \tag{3}$$

The second sum is over all neighboring sites.

a) Introduce

$$\mathbf{P}(\mathbf{R}) = \frac{1}{\sqrt{V_L}} \sum_{\mathbf{Q}} \mathbf{P}(\mathbf{Q}) \exp(i\mathbf{Q}\cdot\mathbf{R}), \tag{4}$$

V_L is the number of lattice sites in a crystal.

Show that

$$\sum_{\mathbf{R}} \mathbf{P}^2(\mathbf{R}) = \sum_{\mathbf{Q}} \mathbf{P}^2(\mathbf{Q}). \tag{5}$$

b)

Introduce

$$\mathbf{U}(\mathbf{R}) = \frac{1}{\sqrt{V_L}} \sum_{\mathbf{Q}} \mathbf{U}(\mathbf{Q}) \exp(-i\mathbf{Q}\cdot\mathbf{R}). \tag{6}$$

Show that

$$\frac{1}{2} M\omega^2 \sum_{<\mathbf{R}\mathbf{R}'>} |\mathbf{U}(\mathbf{R}) - \mathbf{U}(\mathbf{R}')|^2 = \sum_{\mathbf{Q}} \frac{1}{2} M\Omega^2(\mathbf{Q})\mathbf{U}^2(\mathbf{Q}). \tag{7}$$

Calculate $\Omega(\mathbf{Q})$ as a function of ω, a and $\mathbf{Q}$.

For the rest of calculations $\Omega(\mathbf{Q})$ should be replaced with its asymptotical form at small $|\mathbf{Q}|$ or the linear dispersion.

c) $\mathbf{P}_\mu(\mathbf{R})$ and $U_\mu(\mathbf{R})$ are a pair of ordinary conjugate variables. Use the definitions for $\mathbf{P}(\mathbf{Q})$ and $\mathbf{U}(\mathbf{Q})$ in a) and b), further show that

$$[\mathbf{P}_\mu(\mathbf{Q}), U_\nu(\mathbf{Q}')] = i\hbar\delta_{Q,Q'}\delta_{\mu\nu}. \tag{8}$$

d) So far you have shown that the Debye-Einstein Hamiltonian is equivalent to

$$H = \sum_{Q} H_Q, H_Q = \frac{\mathbf{P}^2(\mathbf{Q})}{2M} + \frac{1}{2} M\Omega^2(\mathbf{Q})\mathbf{U}^2(\mathbf{Q}) \tag{9}$$

for a set of decoupled harmonic oscillators.

e) Unlike in the case of photons, Q can't be infinity because of periodical structure of a crystal. The total number of modes should be equal to the number of lattice sites ("this is called conservation of phase volume"). Show that under this constraint the upper cut-off of Q, Q_D is

$$\frac{4\pi Q_D^3}{3}\frac{1}{(2\pi)^3} = \frac{1}{a^3}. \tag{10}$$

Again a is the lattice constant of the cubic crystal. Define $\Omega(Q_D)$ as the Debye frequency Ω_D for a crystal. Express ω in the Hamiltonian in terms of Ω_D.

f) Calculate the energy and heat capacity of a crystal described by the above Hamiltonian. Hint: Calculate the energy for the $\mathbf{Q}$th oscillator and sum up energies of all oscillators.

Problem 2 Problem 7.64, page 313, the textbook (part a), b) only).