Assignment 8

1. In a diatomic structure in 2D comprising of atoms of mass M and m, spring cnstant α, the dispersion relation is given by

$$\omega^2 = \alpha\left(\frac{M+m}{Mm}\right) \pm \alpha\sqrt{\left(\frac{M+m}{Mm}\right)^2 - \frac{2}{Mm}(1-\cos(ka))}. \quad (1)$$

   (a) Find ω for acoustic phonons in the small k limit, i.e $\cos(ka) \approx 1 - \frac{k^2a^2}{2}$.

   (b) Find ω for optical phonons in the small k limit.

   (c) Insert these $\omega's$ into the characteristic equation

$$\begin{vmatrix} \omega^2 M - 2\alpha & \alpha(1+e^{-ika}) \\ \alpha(1+e^{ika}) & \omega^2 m - 2\alpha \end{vmatrix} = 0 \quad (2)$$

   and find the ratios of the amplitudes for acoustic and optic modes. Attach a physical meaning to these modes.

2. Consider a monoatomic 1D crystal. Suppose each atom of mass m is connected to its neighboring $\pm p$ atoms ($p \geq 1$). Each interaction is represented by a strength $\alpha_{|p|}$. Write down an expression for the potential energy and force on each atom.

3. Show that the dispersion relation for a monoatomic 1D chain's longitudinal motion is periodic in the reciprocal space. How many modes exist in the FBZ?

4. (a) Write an expression for the total energy U for phonon modes in a 2D structure

at temperature T. Consider only longitudinal vibrations. Consider $k_B T >> \hbar\omega$ (i.e. the high temperature limit).

(b) Find the heat capacity $C_V = \partial U/\partial T$ upto second order in T. Use

$$g(\omega) = \frac{L}{\pi a} \frac{1}{\sqrt{\frac{\alpha}{m} - \left(\frac{\omega}{2}\right)^2}} \tag{3}$$

In the process, you will need to specify the maximum value (cut-off) of the frequency, and you need to know the dispersion relation

$$\omega = 2\sqrt{\frac{\alpha}{m}} \left|\sin(\frac{ka}{2})\right| . \tag{4}$$