Exercises for Physics 560

Problem Set 3; Due Friday, September 16

1) Linear ionic crystal

Consider a line of $2N$ ions of alternating charge $\pm q$ with a repulsive potential energy A/R^n between nearest neighbors.

(a) Show that at the equilibrium separation

$$U(R_0) = -\frac{2Nq^2 \ln 2}{R_0}\left(1 - \frac{1}{n}\right).$$

(b) Let the crystal be compressed so that $R_0 \to R_0(1-\delta)$. Show that the work done in compressing a unit length of the crystal has the leading term $\frac{1}{2}C\delta^2$, where

$$C = \frac{(n-1)q^2 \ln 2}{R_0}.$$

Note: We should not expect to obtain this result from the expression for $U(R_0)$, but must use the complete expression for $U(R)$.

2) Harmonic chain with next-nearest neighbor coupling

Consider a linear lattice of atoms of mass m and lattice spacing a, but introduce an elastic interaction between next-nearest neighbors such that $C(2) = \frac{1}{2}C(1)$. Calculate the frequency of longitudinal acoustic waves as a function of their wavevector. Sketch $\omega(k)$ in the first Brillouin zone.

3) Zero-point fluctuations in 1D

Consider a one-dimensional monatomic crystal with lattice spacing a. The Hamiltonian is

$$H = \sum_{n=1}^{L}\left[\frac{p_n^2}{2m} + \frac{C}{2}(x_n - x_{n-1})^2\right].$$

a) Calculate the zero-point fluctuations of the nearest-neighbor bond length, $\langle 0|(x_n - x_{n-1})^2|0\rangle$. Hint: the displacement operator for the nth atom may be expressed as

$$x_n = L^{-1/2}\sum_k \sqrt{\frac{\hbar}{2m\omega_k}}(a_k e^{ikna} + a_k^\dagger e^{-ikna}).$$

Also, in the limit $L \to \infty$ (which you may utilize) the sum over k may be replaced by an integral, $L^{-1}\sum_k \to (a/2\pi)\int dk$.

b) Calculate the mean squared deviation of the nth atom from its equilibrium position, $\langle 0|x_n^2|0\rangle$. (In evaluating the sum over normal modes, the mode with $k = 0$ should be omitted. This corresponds to displacements of the center of mass, and we are only interested in the displacement of the atom relative to a frame in which the center of mass of the crystal is fixed.)

What does this result suggest about the possible existence of crystalline order in one dimension?