Homework Assignment #6

1. **Continuum wave equation.** Show that for long wavelengths the equation of motion,

\[ M \frac{d^2u}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s), \]

reduces to the continuum elastic wave equation

\[ \frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \]

where \( v \) is the velocity of sound.

2. **Diatomic chain.** Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternately \( C \) and \( 10C \). Let the masses be equal, and let the nearest-neighbor separation be \( a/2 \). Find \( \omega(K) \) at \( K = 0 \) and \( K = \pi/a \). Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as \( \text{H}_2 \).

3. **Atomic vibrations in a metal.** Consider point ions of mass \( M \) and charge \( e \) immersed in a uniform sea of conduction electrons. The ions are imagined to be in stable equilibrium when at regular lattice points. If one ion is displaced a small distance \( r \) from its equilibrium position, the restoring force is largely due to the electric charge within the sphere of radius \( r \) centered at the equilibrium position. Take the number density of ions (or of conduction electrons) as \( \frac{4}{3\pi R^3} \), which defines \( R \).

   (a) Show that the frequency of a single ion set into oscillation is \( \omega = \sqrt{\frac{e^2}{MR^3}} \).

   (b) Estimate the value of this frequency for sodium, roughly.

   (c) From (a), (b), and some common sense, estimate the order of magnitude of the velocity of sound in metal.

4. **Soft phonon modes.** Consider a line of ions of equal mass but alternating in charge, with \( e_p = e(-1)^p \) as the charge on the \( p \)th ion. The interatomic potential is the sum of two contributions: (1) a short-range interaction of force constant \( C_{iR} = \gamma \) that acts between nearest-neighbors only, and (2) a coulomb interaction between all ions.

   (a) Show that the contribution of the coulomb interaction to the atomic force constants is \( C_{pC} = 2(-1)^p \frac{e^2}{p^3 a^3} \), where \( a \) is the equilibrium nearest-neighbor distance.

   (b) From \( \omega^2 = \frac{2}{M} \sum_{p>0} C_p (1 - \cos pKa) \), here \( C \) includes both nearest neighbor and other neighbors, show that the dispersion relation may be written as

\[ \omega^2 / \omega_0^2 = \sin^2 \left( \frac{1}{2} Ka \right) + \sigma \sum_{p=1}^{\infty} (-1)^p (1 - \cos pKa) p^{-3}, \]

where \( \omega_0^2 \equiv 4\gamma / M \) and \( \sigma = e^2 / \gamma a^3 \).

   (c) Show that \( \omega^2 \) is negative (unstable mode) at the zone boundary \( Ka = \pi \) if \( \sigma > 0.475 \) or \( 4/7\zeta(3) \), where \( \zeta \) is a Riemann zeta function.

   Show further that the speed of sound at small \( Ka \) is imaginary if \( \sigma > 2(\ln 2)^{-1} = 0.721 \). Thus \( \omega^2 \) goes to zero and the lattice is unstable for some value of \( Ka \) in the interval \((0, \pi)\) if \( 0.475 < \sigma < 0.721 \). Notice that the phonon spectrum is not that of a diatomic lattice because the interaction of any ion with its neighbors is the same as that of any other ion.
5. For a 1D lattice, if \( k_1 - k_2 = \frac{2\pi m}{a} \),

(a) Show that \( k_1 \) and \( k_2 \) describe the same elastic wave.

(b) For a special case of \( k_1 = \frac{\pi}{3a} \) and \( k_2 = \frac{7\pi}{3a} \), make a plot of \( \cos(k_1 x) \) and \( \cos(k_2 x) \) versus \( x/a \). Confirm the conclusion of (a) from the plot.