Homework #6

1. **Continuum wave equation.** Show that for long wavelengths the equation of motion,
\[ M \frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s), \]
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.

**Solution:**
For \( \lambda \gg a \), \( u_{s+1} - u_s \) is small. Replacing \( u_s \) with \( u(x) \), we have \( u_s = u(sa) \),
\[ u_{s\pm 1} = u((s \pm 1)a), \text{ and } \frac{d^2 u_s}{dt^2} = \frac{\partial^2 u(x,t)}{\partial t^2}. \]
Thus
\[ u_{s\pm 1} = u((s \pm 1)a) \approx u(a) \pm \frac{\partial u}{\partial x} a + \frac{1}{2} \frac{\partial^2 u}{\partial x^2} a^2 \]
or
\[ u((s + 1)a) + u((s - 1)a) - 2u(sa) \approx \frac{\partial^2 u}{\partial x^2} a^2 \]
Then \( M \frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s) \) becomes
\[ M \frac{\partial^2 u(x,t)}{\partial t^2} = C \frac{\partial^2 u}{\partial x^2} a^2 \quad \text{or} \quad \frac{\partial^2 u(x,t)}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \]
with \( v = \sqrt{\frac{C a^2}{M}} \).

Note the mass density is \( \rho = M/a^3 \) and the Yong’s modulus is \( Y = \sqrt{C/a} \). Then
\[ v = \sqrt{\frac{C a^2}{M}} = \sqrt{\frac{Y}{\rho}}. \]

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 \( \text{H}_2 \).

**Solution:**

The atoms can be separated into two groups:
The first group has spring \( C \) at the left and spring \( 10C \) at right, and its motion can be described by \( u = A \exp(ikx - i\omega t) \).
The second group has spring 10C at the left and spring C at right, and its motion can be described by

\[
v = B \exp(i k x - i \omega t).
\]

Then the equations of motion for these two groups are:

\[
\begin{align*}
\frac{d^2 u_s}{dt^2} &= 10C(v_{s-1} - u_s) + C(v_{s+1} - u_s) \\
\frac{d^2 v_s}{dt^2} &= C(u_{s-1} - v_s) + 10C(u_{s+1} - v_s)
\end{align*}
\]

Substitute \( u = A \exp(i k x - i \omega t) \) and \( v = B \exp(i k x - i \omega t) \) into these two equations,

\[
\begin{align*}
-m \omega^2 A &= 10C(B e^{-i k a/2} - A) + C(B e^{i k a/2} - A) \\
-m \omega^2 B &= C(A e^{-i k a/2} - B) + 10C(A e^{i k a/2} - B)
\end{align*}
\]

or

\[
\begin{align*}
(11C - m \omega^2) A - C(10e^{-i k a/2} + e^{i k a/2}) B &= 0 \\
-C(10e^{i k a/2} + e^{-i k a/2}) A + (11C - m \omega^2) B &= 0
\end{align*}
\]

To have non-zero solution, we have

\[
\det\left(\begin{array}{cc}
(11C - m \omega^2) & C(10e^{-i k a/2} + e^{i k a/2}) \\
-C(10e^{i k a/2} + e^{-i k a/2}) & (11C - m \omega^2)
\end{array}\right) = 0.
\]

\[
\omega^2 = \frac{C(11 \pm \sqrt{101 + 20 \cos ka})}{m}
\]

At \( k = 0 \), \( \omega_1^2 = \frac{22C}{m} \), \( A = -B \); and \( \omega_2^2 = 0 \), \( A = B \).

At \( k = \pi/a \), \( \omega_1^2 = \frac{20C}{m} \), \( A = iB \); and \( \omega_2^2 = \frac{2C}{m} \), \( A = -iB \).
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 $\frac{4}{(4\pi R^3)^{1/3}}$, which defines $R$. (a) Show that the frequency of a single ion set into oscillation is $\omega = (e^2 / MR^3)^{1/2}$. (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.

Solution:
(a) For a uniformly charged sphere of charge density $\rho$, the electrical field at $r$ within the sphere is $E(r) = \frac{1}{r^2} \rho \frac{4\pi}{3} r^3 = \frac{4\pi \rho r}{3}$. Now $\rho = -\frac{e}{4\pi R^3 / 3} = -\frac{3e}{4\pi R^3}$, so $E(r) = -\frac{er}{R^3}$.

The force acting on the ion is $F = eE = -\frac{e^2 r}{R^3} \equiv -Kr$ with $K = \frac{e^2}{R^3}$.

Then $\omega = \sqrt{\frac{K}{M}} = \sqrt{\frac{e^2}{MR^3}}$.

(b) For Sodium, $M = 23 \times 1.67 \times 10^{-24} \text{ g} = 3.8 \times 10^{-23} \text{ g}$. Taking $R=1\text{ Å}$, we have

$$\omega = \frac{\sqrt{e^2}}{MR^3} = \sqrt{\frac{(4.8 \times 10^{-10})^2}{3.8 \times 10^{-23} \times 10^{-24}}} \approx 10^{14} (1/\text{s})$$

(c) $v \sim \frac{\omega a}{10^4} \times 10^4 = 10^6 \text{ cm/s}.$

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 $C_{pc} = 2(-1)^p e^2 / p^3 a^3$, where $a$ is the equilibrium nearest-neighbor distance. (b) From $\omega^2 = (2/M) \sum_{p > 0} C_p (1 - \cos pKa)$, 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.

Solution:
(a) The force between two ions is \( \pm e^2 / r^2 \).

For two ions at \( s \)th and \((s+p)\)th sites, their separation distance is \( pa \) without ion displacement, and is \( pa + u_{s+p} - u_s \) after the \( s \)th and \((s+p)\)th ions are displaced by \( u_s \) and \( u_{s+p} \), respectively. Then the force between the two ions will change by an amount of

\[
\frac{(-1)^p e^2}{(pa + u_{s+p} - u_s)^2} - \frac{(-1)^p e^2}{(pa)^2} \approx \frac{(-1)^p 2 e^2}{(pa)^3} (u_{s+p} - u_s).
\]

Here \((-1)^p\) accounts for the sign change of the two charges.

(b) The equation of motion for the \( s \)th ion is

\[
m \frac{d^2 u_s}{dt^2} = \gamma (u_{s+1} - u_s) + \gamma (u_{s-1} - u_s) + \sum_{p=1}^{\infty} \frac{(-1)^p 2 e^2}{(pa)^3} (u_{s+p} - u_s + u_{s-p} - u_s).
\]

Let \( u_s = A \exp(ikx_s - i\omega t) \), and substitute it into the above equation.

\[
-m \omega^2 = \gamma (e^{ika} - 1) + \gamma (e^{-ika} - 1) + \sum_{p=1}^{\infty} \frac{(-1)^p 2 e^2}{(pa)^3} (e^{ika} - 1 + e^{-ika} - 1)
\]

\[
= 2 \gamma (\cos ka - 1) + \sum_{p=1}^{\infty} \frac{(-1)^p 4 e^2}{(pa)^3} (\cos pka - 1)
\]

\[
\omega^2 = \frac{2\gamma}{m} (1 - \cos ka) + \frac{4 e^2}{ma^3} \sum_{p=1}^{\infty} \frac{(-1)^p}{p^3} (1 - \cos pka)
\]

\[
= \frac{4\gamma}{m} \sin^2 \left( \frac{ka}{2} \right) + \frac{4 e^2}{ma^3} \sum_{p=1}^{\infty} \frac{(-1)^p}{p^3} (1 - \cos pka)
\]

Define \( \omega_0 \equiv \sqrt{\frac{4\gamma}{m}} \) and \( \sigma \equiv \frac{e^2}{ga^3} \), then

\[
\frac{\omega^2}{\omega_0^2} = \sin^2 \left( \frac{ka}{2} \right) + \sigma \sum_{p=1}^{\infty} \frac{(-1)^p}{p^3} (1 - \cos pka)
\]
(c) At $ka = \pi$, $\cos(pk a) = (-1)^p$ and $\sin \left( \frac{ka}{2} \right) = 1$. Then

$$\frac{\omega^2}{\omega_0^2} = 1 + \sigma \sum_{p=1}^{\infty} \frac{(-1)^p}{p^3} \left( 1 - (-1)^p \right)$$

$$= 1 + \sigma \left[ -\frac{2}{1^3} - \frac{2}{3^3} - \frac{2}{5^3} - \ldots \right] = 1 - 2\sigma \left[ 1 + \frac{1}{3^3} + \frac{1}{5^3} + \ldots \right]$$

$$= 1 - 2.106\sigma$$

If $\sigma > 1/2.106 = 0.475$, $\omega^2 < 0$.

For $ka << 1$,

$$\frac{\omega^2}{\omega_0^2} \approx \left( \frac{ka}{2} \right)^2 + 2\sigma \sum_{p=1}^{\infty} \frac{(-1)^p}{p^3} \left( \frac{kpa}{2} \right)^2$$

$$= \left( \frac{ka}{2} \right)^2 \left[ 1 + 2\sigma \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \right] = \left( \frac{ka}{2} \right)^2 (1 - 2\sigma \ln 2)$$

If $\sigma > 1/2 \ln 2 = 0.721$, $\omega^2 < 0$.

Strong Coulomb interaction makes the lattice unstable.

5. For a 1D lattice, if $k_1 - k_2 = 2\pi n/a$,

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

(b) For a special case of $k_1 = \pi/3a$ and $k_2 = 7\pi/3a$, make a plot of $\cos(k_1x)$ and $\cos(k_2x)$ versus $x/a$. Confirm the conclusion of (a) from the plot.

Solution:

(a) For $u_1 = A \exp(ik_1x - i\omega t)$, $u_2 = A \exp(ik_2x - i\omega t)$, $u_2/u_1 = \exp[(ik_2 - k_1)x]$. For $k_1 - k_2 = 2\pi n/a$ and $x = pa$, $u_2/u_1 = \exp(i2\pi mp) = 1$.

(b) Note the two curves cross at $x/a=$integer.