Homework 4 Solutions (first four problems only, for Quiz#1)

(1) Energy of lattice wave

a) Monotomic linear lattice, mass \( m \), spacing \( a \), nearest neighbor interaction (spring constant) \( C \). Consider longitudinal wave: \( \Delta r_s = u_s = u \cos(\omega t - ska) \). The total energy of the wave is the sum over all atoms of the energy of each atom. From mechanics, we know that the instantaneous energy of a harmonic oscillator has a kinetic energy term and a potential energy term. The potential term depends only on the force constant and the displacement of the oscillator from equilibrium. Thus the linear lattice can be repeated as a series of springs with masses (atoms) attached.

The potential energy associated with the \( sth \) spring is

\[
PE_s \rightarrow \frac{1}{2} C (u_{s+1} - u_s)^2 = \frac{1}{2} C (u_s - u_{s+1})^2
\]

The kinetic energy associated with the \( sth \) mass is

\[
KE_s \rightarrow \frac{1}{2} M u_s^2 = \frac{1}{2} M \left( \frac{d u_s}{dt} \right)^2
\]

By summing over all atoms we get the total energy:

\[
U(t) = \frac{1}{2} M \sum_s \left( \frac{d u_s}{dt} \right)^2 + \frac{1}{2} C \sum_s (u_s - u_{s+1})^2 \quad \text{(instantaneous)}
\]

b) For longitudinal wave \( u_s = u \cos(\omega t - ska) \), we have \( \frac{d u_s}{dt} = -\omega u \sin(\omega t - ska) \) and

\[
U(t) = \sum_s \left\{ \frac{1}{2} M \omega^2 u^2 \sin^2(\omega t - ska) + \frac{1}{2} Cu^2 \left[ \cos(\omega t - ska) - \cos(\omega t - ska - ka) \right]^2 \right\}
\]

The last term has the form \( \left[ \cos(\alpha - \beta) - \cos \alpha \right]^2 \) with \( \alpha = \omega t - ska, \ \beta = ka \). So we can use the trigonometric identity \( \cos(\alpha - \beta) = \cos \alpha \cos \beta + \sin \alpha \sin \beta \) to write

\[
U(t) = \sum_s \left\{ \frac{1}{2} M \omega^2 u^2 \sin^2 \alpha + \frac{1}{2} Cu^2 \left[ \cos \alpha (\cos \beta - 1) + \sin \alpha \sin \beta \right]^2 \right\}
\]
To get the average, we integrate over the period of wave, $\tau$

$$U = \int_0^\tau U(t) dt \quad \tau = \frac{2\pi}{\omega} = \frac{1}{f}$$

$$\int_0^\tau \sin^2 \alpha dt = \frac{\tau}{2} \; ; \; \int_0^\tau \cos^2 \alpha dt = \frac{\tau}{2} \; ; \; \int_0^\tau 2 \sin \alpha \cos \alpha dt = \int_0^\tau 2 \alpha dt = 0$$

So,

$$U = \frac{1}{2} M \omega^2 u^2 \frac{\tau^2}{\tau} + \frac{1}{2} C u^2 \left[ \frac{\tau}{\tau} (\cos \beta - 1)^2 + \frac{\tau}{\tau} \sin^2 \beta \right]$$

$$U = \frac{1}{4} M \omega^2 u^2 + \frac{1}{4} C u^2 \left[ \cos^2 \beta - 2 \cos \beta + 1 + \sin^2 \beta \right] = \frac{1}{4} M \omega^2 u^2 + \frac{1}{2} C u^2 \left[ 1 - \cos \beta \right]$$

For linear monatomic lattice we have $\omega^2 = \frac{2C}{M} (1-\cos \beta)$. So finally

$$U = \frac{1}{4} M \omega^2 u^2 + \frac{1}{4} M \omega^2 u^2 = \frac{1}{2} M \omega^2 u^2$$

(2) Continuum wave equation

For nearest neighbor-interaction, the force on a given atom (labeled by s) is given by

$$F = C \left( \Delta r_{s+1} - \Delta r_s \right) - C \left( \Delta r_s - \Delta r_{s-1} \right)$$

where we also assume spring constants are equal to $C$. For long wavelength lattice waves, we know $\Delta r_{s+1}$ will nearly in phase and nearly equal amplitude to $\Delta r_s$. Also, $\Delta r_{s-1}$ will be nearly in phase and equal amplitude to $\Delta r_s$. So we can Taylor expand $\Delta r_{s+1}$ and $\Delta r_{s-1}$, thinking of each as a function of the atom average position r. Thus we can write

$$\Delta r_{s+1} \equiv \Delta r \left( r_{s+1} \right) \; ; \; \Delta r_s \equiv \Delta r \left( r_s \right) \; ; \; \Delta r_{s-1} \equiv \Delta r \left( r_{s-1} \right).$$

And by Taylor expansion (to 2nd order)

$$\Delta r_{s+1} \equiv \Delta r \left( r_{s+1} \right) = \Delta r \left( r_s \right) + \frac{d \Delta r}{dr} \bigg|_{r=r_s} \left( r_{s+1} - r_s \right) + \frac{1}{2} \frac{d^2 \Delta r}{dr^2} \bigg|_{r=r_s} \left( r_{s+1} - r_s \right)^2$$
But for uniform lattice constant $d$, $r_{S+1} - r_S = a$. And for lattice oriented along x axis, $r \rightarrow x$ (without loss of generality). Thus,

$$\Delta r_{s+1} = \Delta r_s + \left. \frac{d\Delta r}{dx} \right|_{x=r_S} (a) + \frac{1}{2} \left. \frac{d^2\Delta r}{dx^2} \right|_{x=r_S} (a)^2 + \ldots$$  

* Similarly, we can deduce

$$\Delta r_{s-1} \equiv \Delta r\left(r_{s-1}\right) = \Delta r_s + \left. \frac{d\Delta r}{dx} \right|_{x=r_S} (-a) + \frac{1}{2} \left. \frac{d^2\Delta r}{dx^2} \right|_{x=r_S} (-a)^2 + \ldots$$  

** So,

$$F = C \left( \Delta r_{s+1} - \Delta r_s \right) + C \left( \Delta r_{s-1} - \Delta r_s \right)$$

and we substitute in * and **

$$= C \left( \left. \frac{d\Delta r}{dx} \right|_{x=r_S} (a) + \frac{1}{2} \left. \frac{d^2\Delta r}{dx^2} \right|_{x=r_S} (a)^2 + \frac{d\Delta r}{dx} \right|_{x=r_S} (-a) + \frac{1}{2} \left. \frac{d^2\Delta r}{dx^2} \right|_{x=r_S} (-a)^2 \right)$$

$$= C \left( \frac{1}{2} \left. \frac{d^2\Delta r}{dx^2} \right|_{x=r_S} (a)^2 + \frac{1}{2} \left. \frac{d^2\Delta r}{dx^2} \right|_{x=r_S} (-a)^2 \right) = Ca^2 \left. \frac{d^2\Delta r}{dx^2} \right|_{x=r_S}$$

So using Newton’s law $F = \frac{md^2\Delta r_s}{dt^2}$, we get the wave equation

$$\frac{d^2\Delta r_s}{dt^2} = \frac{ca^2}{m} \left. \frac{d^2\Delta r}{dx^2} \right|_{x=r_S} \equiv \nu^2 \left. \frac{d^2\Delta r_s}{dx^2} \right|_{x=r_S}$$

where

$$\left. \frac{d^2\Delta r}{dx^2} \right|_{x=r_S} \equiv \frac{d^2\Delta r_s}{dx^2}$$

(3) Lattice waves for crystal having basis of two different atoms

At $k = \pi/a$ the solutions for the two branches are $\omega^2 = 2C/M_1$ (acoustical) and $\omega^2 = 2C/M_2$ (optical) where it is assumed $M_1 > M_2$. We substitute these back into the connection equations:
\[
\left(2C-M_1\omega^2\right)u - C\left[1+\exp(-jka)\right]v = 0 \quad (a)
\]
\[
-C\left[1+\exp(jka)\right]u + \left[2C-M_2\omega^2\right]v = 0 \quad (b)
\]
\( (a) \text{ leads to } \frac{u}{v} = \frac{C\left[1+\exp(-jka)\right]}{2C-M_1\omega^2} \quad (c) \)
\( (b) \text{ leads to } \frac{u}{v} = \frac{2C-M_2\omega^2}{C\left[1+\exp(jka)\right]} \quad (d) \)

At \(ka = \pi\), \(\exp(-jka) = \exp(jka) = -1\). So for acoustical branch, \(\omega^2 = 2C/M_1\),

\[
(c) \Rightarrow \frac{u}{v} = \frac{0}{0} \quad (d) \Rightarrow \frac{u}{v} = \frac{2C\left(1-M_2/M_1\right)}{0} \rightarrow \infty
\]

\(u/v \rightarrow \infty\) means that \(u\) is arbitrarily non-zero for \(v = 0\). This means that all the motion is in \(u\) (main atom). For optical branch, \(\omega^2 = 2C/M_2\),

\[
(c) \Rightarrow \frac{u}{v} = \frac{0}{2C\left(1-M_1/M_2\right)} = 0 \quad (d) \Rightarrow \frac{u}{v} = \frac{0}{0} \text{ (undefined)}
\]

\(u/v \rightarrow 0\) means that \(v\) is arbitrary non-zero for \(u = 0\), so that all the motion in \(v\) (satellite atom).

(4) Diatomic Chain

From assumptions of nearest neighbor-interaction, equal masses but unequal spring constants, \(C_1\) and \(C_2\) derived in lecture, the force equations on the atoms in the \(s^{th}\) unit cell

\[
m\frac{d^2\Delta r_1}{dt^2} = C_1 \left(\Delta r_{2,s} - \Delta r_{1,s}\right) - C_2 \left(\Delta r_{1,s} - \Delta r_{2,s-1}\right)
\]
\[
m\frac{d^2\Delta r_{2,s}}{dt^2} = C_2 \left(\Delta r_{1,s+1} - \Delta r_{2,s}\right) - C_1 \left(\Delta r_{2,s} - \Delta r_{1,s}\right)
\]

Assuming the discrete wave solutions

\[
\Delta r_{1,s} = \Delta r_1 e^{j(ksa-\omega t)} \quad , \quad \Delta r_{2,s} = \Delta r_2 e^{j(ksa-\omega t)}
\]

We found the coupled algebraic equations for the amplitudes \(\Delta r_1\) and \(\Delta r_2\).
\[
\begin{pmatrix}
mo^2 - C_1 - C_2 & C_1 + C_2 e^{-jka} \\
C_1 + C_2 e^{jka} & mo^2 - C_1 - C_2
\end{pmatrix}
\begin{pmatrix}
\Delta r_1 \\
\Delta r_2
\end{pmatrix} = 0
\]

A non-trivial solution for \(\Delta r_1\) and \(\Delta r_2\) requires that the 2x2 matrix be non-invertible \(\Rightarrow \det\{\} = 0\)

\[
\Rightarrow m^2 \omega^4 + (C_1 + C_2)^2 - 2m(C_1 + C_2)\omega^2 - \left(C_1^2 + C_2^2 + 2C_1C_2 \cos ka\right) = 0
\]

\[
\omega^2 = \frac{C_1 + C_2}{m} \pm \frac{1}{m} \sqrt{(C_1 + C_2)^2 - 2C_1C_2(1 - \cos ka)} \quad \left\{ \begin{array}{l}
+ \text{ optical branch} \\
- \text{ acoustical branch}
\end{array} \right.
\]

(a) At \(ka = 0\)

\[
\omega^2 = \frac{C_1 + C_2}{m} \pm \frac{C_1 + C_2}{m} = 0 \quad (- \text{ sign, acoustical branch})
\]

\[
\omega^2 = \frac{2(C_1 + C_2)}{m} = \frac{22C}{m} \quad \text{for } C_2 = 10 \cdot C_1 \equiv 10C
\]

or \(\omega = \sqrt{\frac{22C}{m}} \quad (+ \text{ sign, optical branch})\)

(b) At \(ka = \pi, \cos ka = -1\)

\[
\omega^2 = \frac{C_1 + C_2}{m} \pm \frac{1}{m} \sqrt{(C_1 + C_2)^2 - 4C_1C_2}
\]

or \(\omega = \sqrt{\frac{C_1 + C_2}{m} \pm \frac{1}{m} \sqrt{(C_2 - C_1)^2}} = \sqrt{\frac{2C_1}{m}} = \sqrt{\frac{2C}{m}} \quad (-\text{sign, acoustical branch})\)

\[
\omega = \sqrt{\frac{2C_2}{m}} = \sqrt{\frac{20C}{m}} \quad (+\text{sign, optical branch})\)