Physics 362 : Assignment 10

Max Gould
Reed College, Portland, OR 97202
(Dated: April 5, 2012)

PROBLEM 10.1

(a)

The harmonic potential energy for a one-dimensional monatomic Bravais lattice may be described by the following equation including interactions between each particle in the lattice structure:

$$U = \sum_i \sum_{j>0} \frac{1}{2}\ \kappa_j\ \Big[u_i - u_{i+j}\Big]^2$$

κ_j representing the associated spring constant of the j^{th} atom. The equation of motion for the m^{th} atom in this structure may be defined as:

$$M\ \ddot{u}_m = -\frac{\partial U}{\partial u_m}$$

In taking this derivative, there are two main components that result. The first is the case in the sum over i when $i = m$. This results in a sum over j as follows:

$$\sum_{j>0} \frac{1}{2}\ \kappa_j\ \frac{\partial}{\partial u_m}\ \Big[u_m - u_{m+j}\Big]^2$$

$$\sum_{j>0} \kappa_j\ \Big[u_m - u_{m+j}\Big]$$

The other component is a series of terms when $i \neq m$. In each of these cases, the only term that survives in the sum over j after the derivative is taken is the one with u_m in it which corresponds to $i = m - j$. After the derivative is taken, each of these terms have the following form:

$$\kappa_j\ \Big[u_m - u_{m-j}\Big]$$

These must be summed over all m however to account for each surviving term. The resulting equation when both components are considered is as follows:

$$M\ \ddot{u}_m = -\sum_{j>0} \kappa_j\ \Big[2\ u_m - u_{m-j} - u_{m+j}\Big]$$

The normal modes corresponding to a single unified frequency, ω, must have a solution of the following form:

$$u_m = A_m e^{-i\omega t}$$

Plugging this into our equation of motion and canceling out all of the exponents, we get:

$$A_m\ M\ \omega^2 = \sum_{j>0} \kappa_j\ \Big[2\ A_m - A_{m-j} - A_{m+j}\Big]$$

In order to make this true for all m, we'll define the constant, A_m, as follows:

$$A_m = A_0\ e^{ikma}$$

Introducing this back into our equation and canceling out all of the A_0s, we get:

$$M\ \omega^2\ e^{ikma} = \sum_{j>0} \kappa_j\ \Big[2\ e^{ikma} - e^{-ijka}\ e^{ikma} - e^{ijka}\ e^{ikma}\Big]$$

We can further cancel out all of the exponents from the definition of A_m, leaving us with:

$$M\ \omega^2 = \sum_{j>0} \kappa_j\ \Big[2 - e^{-ijka} - e^{ijka}\Big]$$

$$\omega^2 = \sum_{j>0} \frac{\kappa_j}{M}\ \Big[2 - 2\cos(j\ k\ a)\Big]$$

$$\omega^2 = \sum_{j>0} \frac{\kappa_j}{M}\ 4\ \sin^2\left(\frac{j\ k\ a}{2}\right)$$

$$\omega = 2\sqrt{\sum_{j>0} \frac{\kappa_j}{M}\ \sin^2\left(\frac{j\ k\ a}{2}\right)}$$

(b)

In the long-wavelength limit ($ka \ll 1$), we can expand the sine-squared term as a Maclaurin Series:

$$\omega = 2 \sqrt{\sum_{j>0} \frac{\kappa_j}{M} \sin^2\left(\frac{j\ k\ a}{2}\right)}$$

$$= 2 \sqrt{\sum_{j>0} \frac{\kappa_j}{M} \left[\left(\frac{j\ k\ a}{2}\right)^2 + \mathcal{O}(j^4)\right]}$$

$$\approx \sqrt{\sum_{j>0} \frac{\kappa_j}{M} (j\ k\ a)^2}$$

$$\approx a\ |k| \sqrt{\sum_{j>0} \frac{\kappa_j}{M} j^2}$$

(c)

The above approximation only holds however if the sum converges. When $\kappa_j = j^{-p}$ for $1 < p < 3$, the sum does not converge and a different method of approximation must be used. In this case, we'll just determine the k-dependence of ω, and we'll do this by replacing the sum over j by an integral.

In order to do this, we'll define a new variable, $x = j\ k\ a$, where $dx = k\ a$ represents the spacing between adjacent j values. For small k, dx is very small, allowing us to take the integral over x-space:

$$\omega = 2 \sqrt{\sum_{j>0} \frac{\kappa_j}{M} \sin^2\left(\frac{j\ k\ a}{2}\right)}$$

$$= 2 \sqrt{\sum_{j>0} \frac{1}{M\ j^p} \sin^2\left(\frac{x}{2}\right)}$$

$$= 2 \sqrt{(k\ a)^{p-1} \sum_{j>0} \frac{1}{M\ (j\ k\ a)^p} \sin^2\left(\frac{x}{2}\right)\ k\ a}$$

$$= 2\ (k\ a)^{(p-1)/2} \sqrt{\sum_{j>0} \frac{1}{M} \frac{\sin^2(x/2)}{x^p}\ dx}$$

Now because we were summing over all positive values of j, and since k and a are both positive, we can replace the sum with an integral over x from zero to infinity:

$$\omega \approx 2\ (k\ a)^{(p-1)/2} \sqrt{\int_{x=0}^{\infty} \frac{1}{M} \frac{\sin^2(x/2)}{x^p}\ dx}$$

$$\approx 2\ (k\ a)^{(p-1)/2} \sqrt{-\frac{1}{2\ M} \sin\left(\frac{\pi\ p}{2}\right)\ \Gamma(p-1)}$$

The integral here was computed with the aid of Mathematica for values of $p < 3$. Since the remaining terms from the integral are not k-dependent however, the k-dependence becomes simply:

$$\omega \propto k^{(p-1)/2}$$

PROBLEM 10.2

(a)

We're asked to determine the frequencies of the normal modes of a one-dimensional monatomic Bravais lattice with two distinct atom types functioning as an ion pair. To this end, we may write our equations of motion as follows:

$$M_1\ \ddot{u}_j = -\kappa\ (2\ u_j - v_j - v_{j-1})$$

$$M_2\ \ddot{v}_j = -\kappa\ (2\ v_j - u_j - u_{j+1})$$

It stands to reason that our solutions will take the following form:

$$u_j = A\ e^{i(kR_j - \omega t)}$$

$$v_j = B\ e^{i(kR_j - \omega t)}$$

Substituting these back into our equations of motion and canceling out the exponents, we get:

$$A\ M_1\ \omega^2 = \kappa\ (2\ A - B - B\ e^{-ika})$$

$$B\ M_2\ \omega^2 = \kappa\ (2\ B - A - A\ e^{ika})$$

This can be re-written as a matrix equation as follows:

$$\omega^2 \begin{pmatrix} A \\ B \end{pmatrix} = \kappa \begin{pmatrix} \frac{2}{M_1} & -\frac{1+e^{-ika}}{M_1} \\ -\frac{1+e^{ika}}{M_2} & \frac{2}{M_2} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

This corresponds to an eigenvalue problem which we can solve by taking the determinant as follows:

$$\begin{vmatrix} \frac{2\ \kappa}{M_1} - \omega^2 & -\frac{\kappa}{M_1}\ (1+e^{-ika}) \\ -\frac{\kappa}{M_2}\ (1+e^{ika}) & \frac{2\ \kappa}{M_2} - \omega^2 \end{vmatrix} = 0$$

$$\frac{4\ \kappa^2}{M_1\ M_2} - \frac{2\ \kappa\ (M_1+M_2)\ \omega^2}{M_1\ M_2} + \omega^4 = \frac{\kappa^2}{M_1\ M_2}\ (2 + e^{-ika} + e^{ika})$$

$$\frac{2\ \kappa^2}{M_1\ M_2}(1-\cos(k\ a)) - \frac{2\ \kappa\ (M_1+M_2)\ \omega^2}{M_1\ M_2} + \omega^4 = 0$$

The foregoing equation takes the form of a quadratic with respect to ω. We can solve it therefore simply by employing the quadratic formula:

$$\omega^2 = \frac{\kappa\ (M_1+M_2)}{M_1\ M_2} \pm \frac{1}{2}\ \sqrt{\frac{4\ \kappa^2\ (M_1+M_2)^2}{(M_1\ M_2)^2} - \frac{8\ \kappa^2}{M_1\ M_2}(1-\cos(k\ a))}$$

$$= \frac{\kappa\ (M_1+M_2)}{M_1\ M_2} \pm \frac{\kappa}{M_1\ M_2}\ \sqrt{(M_1+M_2)^2 - 2\ M_1\ M_2\ (1-\cos(k\ a))}$$

$$= \frac{\kappa}{M_1\ M_2}\ \left[M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2\ M_1\ M_2\ \cos(k\ a)} \right]$$

(b)

In the special case in which $M_1 \gg M_2$, we can simplify the dispersion relation as follows:

$$\omega^2 = \frac{\kappa}{M_1\ M_2}\ \left[M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2\ M_1\ M_2\ \cos(k\ a)} \right]$$

$$= \frac{\kappa}{M_2}\ \left[1 + \frac{M_2}{M_1} \pm \sqrt{1 + \frac{M_2^2}{M_1^2} + 2\ \frac{M_2}{M_1}\ \cos(k\ a)} \right]$$

$$\approx \frac{\kappa}{M_2}\ \left[1 \pm 1 \right]$$

This leads to the following two resultant frequencies of the normal modes:

$$\Rightarrow \quad \omega = 0\ ,\ \sqrt{\frac{2\ \kappa}{M_2}}$$

The none-zero frequency here is of the form of a damped harmonic oscillator of mass M_2. The $\sqrt{2}$ term here represents the damping term where the damping ratio, ζ, of the traditional damped harmonic oscillator is related to it by the equation, $\sqrt{2} = \sqrt{1-\zeta^2}\ \Rightarrow\ \zeta = \sqrt{-1}$.

(c)

In the case in which $M_1 \approx M_2$, we can relate our ionic dispersion relation to the dispersion relation of the simple monatomic linear chain. The relation simplifies as follows given our assumption:

$$\omega^2 = \frac{\kappa}{M_1\ M_2}\ \left[M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2\ M_1\ M_2\ \cos(k\ a)} \right]$$

$$\approx \frac{\kappa}{M^2}\ \left[2\ M \pm \sqrt{2\ M^2 + 2\ M^2\ \cos(k\ a)} \right]$$

$$\approx \frac{\kappa}{M}\ \left[2 \pm \sqrt{2 + 2\ \cos(k\ a)} \right]$$

$$\approx \frac{\kappa}{M}\left[2 \pm \sqrt{4\ \sin^2\left(\frac{k\ a}{2}\right)}\right]$$

$$\approx \frac{2\ \kappa}{M}\left[1 \pm \left|\sin\left(\frac{k\ a}{2}\right)\right|\right]$$

If we define the dispersion relation of the monatomic linear chain as ω_1, the dispersion relation of the ionic chain in terms of ω_1 becomes:

$$\Rightarrow \quad \omega^2 \approx \frac{2\ \kappa}{M} \pm \frac{1}{2}\ \omega_1^2$$

PROBLEM 10.3

(a)

Given a two-dimensional square lattice, we're asked to calculate the dynamical matrix, $\mathbf{D}(\mathbf{k})$, of the system. While the lattice is two-dimensional however, the atoms are free to move in three dimensions, allowing for fully three dimensions of polarizability. For this reason, we may simply derive our result by simplifying down from the three-dimensional case. The harmonic matrix, $\mathbb{H}$, for our system may therefore be defined as the three-dimensional harmonic matrix for which z (the vertical component of $\mathbf{R}_i - \mathbf{R}_j$) is set to zero:

$$\mathbb{H}(r) = \frac{1}{2\ r^2}\begin{pmatrix} A\ r^2 + B\ x^2 & B\ x\ y & 0 \\ B\ x\ y & A\ r^2 + B\ y^2 & 0 \\ 0 & 0 & A\ r^2 \end{pmatrix}$$

Our dynamical matrix may then be defined in terms of $\mathbb{H}$ as follows:

$$\mathbf{D}(\mathbf{k}) = \sum_i\ \mathbb{H}(R)\ \left[1 - e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}\right]$$

$$\mathbf{D}(\mathbf{k}) = \frac{1}{2\ a^2}\left[\begin{pmatrix} A\ a^2 & 0 & 0 \\ 0 & (A+B)\ a^2 & 0 \\ 0 & 0 & A\ a^2 \end{pmatrix}(2 - e^{ik_y a} - e^{-ik_y a})\right.$$

$$\left. + \begin{pmatrix} (A+B)\ a^2 & 0 & 0 \\ 0 & A\ a^2 & 0 \\ 0 & 0 & A\ a^2 \end{pmatrix}(2 - e^{ik_x a} - e^{-ik_x a})\right]$$

$$\mathbf{D}(\mathbf{k}) = \frac{1}{2}\left[\begin{pmatrix} A & 0 & 0 \\ 0 & A+B & 0 \\ 0 & 0 & A \end{pmatrix}(2 - 2\ \cos(k_y\ a))\right.$$

$$\left. + \begin{pmatrix} A+B & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & A \end{pmatrix}(2 - 2\ \cos(k_x\ a))\right]$$

$$\mathbf{D}(\mathbf{k}) = 2\left[\begin{pmatrix} A & 0 & 0 \\ 0 & A+B & 0 \\ 0 & 0 & A \end{pmatrix}\sin^2\left(\frac{k_y\ a}{2}\right)\right.$$

$$\left. + \begin{pmatrix} A+B & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & A \end{pmatrix}\sin^2\left(\frac{k_x\ a}{2}\right)\right]$$

(b)

In order to determine the normal mode frequencies for each of the possible polarization directions, we must refer back to our equation of motion:

$$\omega^2\ \boldsymbol{\epsilon} = \frac{1}{M}\ \mathbf{D}(\mathbf{k})\ \boldsymbol{\epsilon}$$

$\boldsymbol{\epsilon}$ represents the polarization direction, so the eigenvalue problem decomposes into three basic equations:

$$\left|\frac{1}{M}\ \mathbf{D}(\mathbf{k}) - \begin{pmatrix} \omega_1^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right| = 0$$

$$\left|\frac{1}{M}\ \mathbf{D}(\mathbf{k}) - \begin{pmatrix} 0 & 0 & 0 \\ 0 & \omega_2^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right| = 0$$

$$\left|\frac{1}{M}\ \mathbf{D}(\mathbf{k}) - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \omega_3^2 \end{pmatrix}\right| = 0$$

We solve these equations in the attached Mathematica documentation for this problem. Choosing the positive frequencies we get:

$$\omega_1 = \sqrt{\frac{1}{M}\left[(A+B)\ \sin^2\left(\frac{k_x\ a}{2}\right) + A\ \sin^2\left(\frac{k_y\ a}{2}\right)\right]}$$

$$\omega_2 = \sqrt{\frac{1}{M}\left[(A+B)\ \sin^2\left(\frac{k_y\ a}{2}\right) + A\ \sin^2\left(\frac{k_x\ a}{2}\right)\right]}$$

$$\omega_3 = \sqrt{\frac{A}{M}\left[\sin^2\left(\frac{k_x\ a}{2}\right) + \sin^2\left(\frac{k_y\ a}{2}\right)\right]}$$

(c)

In order to get a picture of what these frequencies look like, we'll plot they're behavior over the following walk in k-space shown in red:

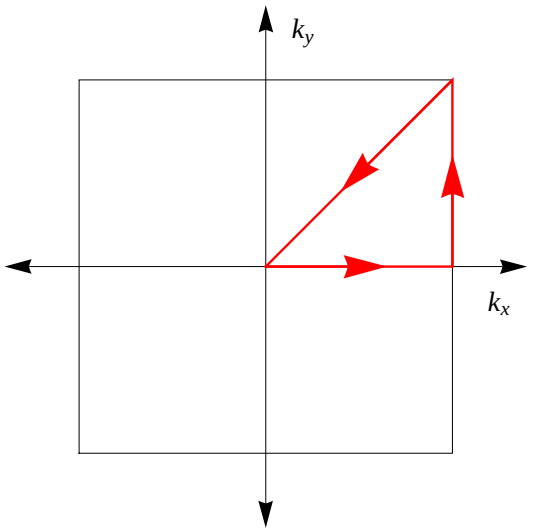

FIG. 1. Walk over one octant of the first Brillouin zone.

The following plot displays the entire walk in sequence for all three frequencies (see Mathematica documentation for reference):

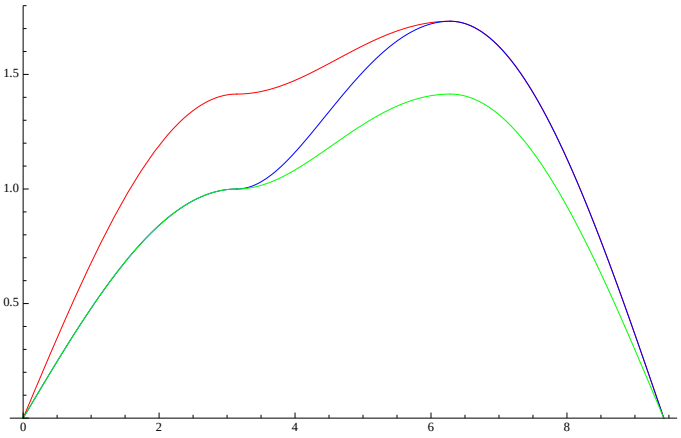

FIG. 2. Red = ω_1, Blue = ω_2, Green = ω_3