Physics 715. HW 4 Solutions

1. Consider a two-dimensional square lattice with the lattice constant $a$. Nearest neighbor atoms of mass $m$ are coupled by harmonic forces with the spring constants $\kappa_\parallel$ and $\kappa_\perp$:

$$U = U_\parallel + U_\perp$$

$$U_\parallel = \left( \frac{\kappa_\parallel}{2} \right) \sum_{<ij>} \left[ \mathbf{b}_{<ij>} \cdot (\mathbf{u}_j - \mathbf{u}_i) \right]^2$$

$$U_\perp = \left( \frac{\kappa_\perp}{2} \right) \sum_{<ij>} \left[ \mathbf{b}_{<ij>} \times (\mathbf{u}_j - \mathbf{u}_i) \right]^2$$

where $\mathbf{b}_{<ij>}$ is a unit vector in the direction of the bond connecting nearest neighbor points $i$ and $j$, i.e. it is either $\pm \mathbf{a}_1/a$ or $\pm \mathbf{a}_2/a$. (see Figure).

(a) Derive phonon dispersion laws for this lattice and verify that $\omega_j(k) \to 0$ when $k \to 0$.

(b) Draw the first Brillouin zone (BZ) for this lattice, and verify that the derivative $\partial \omega_j(k)/\partial k$ is zero in the direction perpendicular to the BZ boundary (by symmetry, it is sufficient to consider only one segment of the boundary).
(c) In which directions the classification of waves in terms of trans-
verse and longitudinal is exact (Hint: do not miss directions along
which the two phonon branches have the same energy—one is free to
rotate the eigenvector basis at points of degeneracy).
(d) What relation between $\kappa_{\parallel}$ and $\kappa_{\bot}$ has to be satisfied for all
modes to be transverse or longitudinal?

Solution

General analysis. The problem is two-dimensiona and there is one
atom in the basis. Hence, there are two phonon modes correspon-
ding to two different directions of the eigenvectors. The structure of the
interaction is such that the $x$ and $y$ components of the displacements
are not coupled to each other. Hence, the problem decouples into two
independent parts: for $x$ and $y$ components of the displacements. Each
of the problems yields one mode with the eigenvector along the $x$- and
$y$-direction, correspondingly. Moreover, since the whole problem is ob-
viously symmetric with respect to re-labelling directions, $x \leftrightarrow y$, we
actually need to solve for only one mode, say, the $x$-mode.

(a) With the given interaction, we readily see that the spring matrix
$A^{xx}(n)$ has only five non-zero elements corresponding to one on-site
(i.e. $n = 0$) and four nearest-neighbor couplings:

$$A^{xx}(0) = 2(\kappa_{\parallel} + \kappa_{\bot}), \quad A^{xx}(\pm \hat{e}_1) = -\kappa_{\parallel}, \quad A^{xx}(\pm \hat{e}_2) = -\kappa_{\bot},$$

where $\hat{e}_1 = (1, 0)$ and $\hat{e}_2 = (0, 1)$ are unit displacements in the space
of integer vectors $n$. In terms of the dimensionless wavevector $g$ we
thus get (since there is only one type of atoms, we set mass equal to
unity and do not distinguish between $C$ and $\tilde{C}$):

$$C^{xx}(g) = \sum_n A^{xx}(n) e^{-ig.n} = A^{xx}(0) +$$

$$+ A^{xx}(-\hat{e}_1) e^{ig.\hat{e}_1} + A^{xx}(\hat{e}_1) e^{-ig.\hat{e}_1} + A^{xx}(-\hat{e}_2) e^{ig.\hat{e}_2} + A^{xx}(\hat{e}_2) e^{-ig.\hat{e}_2} =$$

$$= 2(\kappa_{\parallel} + \kappa_{\bot}) - \kappa_{\parallel} \left(e^{ig_1} + e^{-ig_1}\right) - \kappa_{\bot} \left(e^{ig_2} + e^{-ig_2}\right) =$$

$$2$$
\[ \begin{align*}
&= 2\kappa_\parallel (1 - \cos g_1) + 2\kappa_\perp (1 - \cos g_2) \\
&\equiv 4\kappa_\parallel \sin^2 \frac{g_1}{2} + 4\kappa_\perp \sin^2 \frac{g_2}{2}.
\end{align*} \]

[Do not forget about the trigonometric relation \( 1 - \cos x = 2\sin^2(x/2) \).]

Our matrix \( C^{xx}(g) \) is a trivial \( 1 \times 1 \) matrix, and we immediately write

\[ \omega_x^2(g) = 4\kappa_\parallel \sin^2 \frac{g_1}{2} + 4\kappa_\perp \sin^2 \frac{g_2}{2} \quad (m = 1). \]

The answer for \( \omega_y^2(g) \) is obtained by symmetry \( x \leftrightarrow y, \, 1 \leftrightarrow 2 \):

\[ \omega_y^2(g) = 4\kappa_\perp \sin^2 \frac{g_1}{2} + 4\kappa_\parallel \sin^2 \frac{g_2}{2} \quad (m = 1). \]

Restoring the mass and introducing the dimensional wavevector \( \mathbf{k} \) \( (k_x = g_1/a, \, k_y = g_2/a) \), we write

\[ \begin{align*}
\omega_x^2(\mathbf{k}) &= \frac{4\kappa_\parallel}{m} \sin^2 \frac{k_x a}{2} + \frac{4\kappa_\perp}{m} \sin^2 \frac{k_y a}{2}, \\
\omega_y^2(\mathbf{k}) &= \frac{4\kappa_\perp}{m} \sin^2 \frac{k_x a}{2} + \frac{4\kappa_\parallel}{m} \sin^2 \frac{k_y a}{2}.
\end{align*} \quad (1, 2) \]

In the limit of \( ka \ll 1 \) we get the acoustic behavior:

\[ \begin{align*}
\omega_x^2(\mathbf{k}) &\approx \frac{\kappa_\parallel}{m} (k_x a)^2 + \frac{\kappa_\perp}{m} (k_y a)^2 \quad (ka \ll 1), \\
\omega_y^2(\mathbf{k}) &\approx \frac{\kappa_\perp}{m} (k_x a)^2 + \frac{\kappa_\parallel}{m} (k_y a)^2 \quad (ka \ll 1).
\end{align*} \]

(b) The Brillouin zone is the square \( k_x, k_y \in [\pm \frac{\pi}{a}, \pm \frac{\pi}{a}] \); the directions perpendicular to the BZ boundaries are, respectively, the \( x \) and \( y \) directions. Differentiating both sides of Eq. (1) with respect to \( k_x \) and \( k_y \) we find

\[ \omega_x \frac{\partial \omega_x}{\partial k_x} \propto \sin k_x a, \quad \omega_x \frac{\partial \omega_x}{\partial k_y} \propto \sin k_y a. \]

Since \( \omega_x \neq 0 \) at the BZ boundary, we conclude that

\[ \left. \frac{\partial \omega_x}{\partial k_x} \right|_{k_y = \pm \frac{\pi}{a}} = 0, \quad \left. \frac{\partial \omega_x}{\partial k_y} \right|_{k_x = \pm \frac{\pi}{a}} = 0. \]
Similar result for $\omega_y$ follows by symmetry. [Clearly, it can be obtained explicitly by differentiating (2).]

(c) There are three cases:
1.) $k = (k_x, 0)$. In this case, the $y$-mode is transverse and the $x$-mode is longitudinal.
2.) $k = (0, k_y)$. In this case, the $x$-mode is transverse and the $y$-mode is longitudinal.
3.) $k_y = \pm k_x$. In this case both modes have the same frequency, and without loss of generality one can use any two orthogonal vectors as the displacement eigenvectors; for example, the transverse and longitudinal with respect to $k$.

(d) That would require a complete degeneracy between the two modes, $\omega_x(k) = \omega_y(k)$ for any $k$. In accordance with Eqs. (1)-(2), this takes place if and only if $\kappa_\parallel = \kappa_\perp$.

2. **Diatomic chain.** Consider a one-dimensional diatomic chain: $ABABAB....$
The masses of the atoms $A$ and $B$ are $m_1$ and $m_2$. The distance between two adjacent atoms $A$ and $B$ is $a/2$. The interaction is only between the adjacent atoms $A$ and $B$; the interaction is harmonic with the spring constant $\kappa$.
(a) Solve for the phonons. (b) Study the limit $m_1 \rightarrow m_2$: Interpret the result at $m_1 = m_2$ in terms of the single-atomic chain; explain a subtle difference between the cases $m_1 = m_2$ and $|m_1 - m_2| \ll m_1$.

**Solution**

(a) We select the origin of the primitive cell in such a way that the mass $m_1$ is at the coordinate $x_1^{(0)} = -a/4$ and that the mass $m_2$ is at the coordinate $x_2^{(0)} = a/4$. Since there is only one spring constant $\kappa$, we set it equal to unity and then restore at the very end by $\omega \rightarrow \omega\sqrt{\kappa}$. Since we are in 1D, there are no axes superscripts, and we are dealing with the matrix $A_{j_1j_2}(n)$, where $j_1, j_2 = 1, 2$ and $n = 0, \pm 1, \pm 2, \ldots$. 4
The only non-zero elements are (below $\hat{e}$ is the unit):

$$A_{11}(0) = 2, \quad A_{22}(0) = 2, \quad A_{12}(0) = A_{21}(0) = -1.$$ 

Introducing dimensionless wavevector $g$, for the matrix

$$\tilde{C}_{j_1j_2}(g) = \sum_{n=-\infty}^{\infty} \frac{A_{j_1j_2}(n)}{\sqrt{m_1m_2}} e^{-ign},$$

we get

$$\tilde{C}_{11}(g) = \frac{2}{m_1}, \quad \tilde{C}_{22}(g) = \frac{2}{m_2},$$

$$\tilde{C}_{12}(g) = -\frac{1 + e^{ig}}{\sqrt{m_1m_2}}, \quad \tilde{C}_{21}(g) = -\frac{1 + e^{-ig}}{\sqrt{m_1m_2}},$$

which brings us to the characteristic equation (below $\lambda = \omega^2$)

$$\left| \begin{array}{cc}
\frac{2}{m_1} - \lambda & -\frac{1 + e^{ig}}{\sqrt{m_1m_2}} \\
-\frac{1 + e^{-ig}}{\sqrt{m_1m_2}} & \frac{2}{m_2} - \lambda
\end{array} \right| = 0.$$

$$\lambda^2 - 2 \frac{m_1 + m_2}{m_1m_2} \lambda + \frac{4 \sin^2(g/2)}{m_1m_2} = 0. \quad (3)$$

$$\lambda_{\pm} = \frac{2}{m} \left[ 1 \pm \sqrt{1 - \eta \sin^2(g/2)} \right], \quad (4)$$

where

$$m = \frac{m_1 + m_2}{2}, \quad \eta = \frac{4m_1m_2}{(m_1 + m_2)^2}. \quad (5)$$

Restoring $\kappa$ and replacing $g \rightarrow ka$ (note that the period of the lattice is $a$ because there are two atoms in the basis), we write the final answer

$$\omega^2_{\pm}(k) = \left( \frac{2}{\eta} \right) \frac{\kappa}{m} \left[ 1 \pm \sqrt{1 - \eta \sin^2(ka/2)} \right], \quad (ka \in [-\pi, \pi]). \quad (6)$$

The sign minus corresponds to the acoustic branch.

(b) To explore the case $m_1 \rightarrow m_2$, introduce the relevant parameter

$$\xi = \frac{|m_1 - m_2|}{m_1 + m_2} \ll 1.$$
Observing that $\eta = 1 - \xi^2$, we have

$$\omega^2_\pm(k) = \frac{2\kappa}{m(1 - \xi^2)} \left[ 1 \pm \sqrt{1 - (1 - \xi^2) \sin^2(ka/2)} \right], \quad (ka \in [-\pi, \pi]).$$

At $\xi = 0$ (i.e. $m_1 = m_2$), we have

$$\omega^2_-(k) = \frac{2\kappa}{m} \left[ 1 - \cos \frac{ka}{2} \right] = \frac{4\kappa}{m} \sin^2 \frac{ka}{4}, \quad (ka \in [-\pi, \pi]),$$

$$\omega^2_+(k) = \frac{2\kappa}{m} \left[ 1 + \cos \frac{ka}{2} \right] = \frac{4\kappa}{m} \cos^2 \frac{ka}{4}, \quad (ka \in [-\pi, \pi]),$$

or

$$\omega_-(k) = 2\sqrt{\kappa/m} \left| \sin \frac{ka}{4} \right|, \quad (ka \in [-\pi, \pi]),$$

$$\omega_+(k) = 2\sqrt{\kappa/m} \cos \frac{ka}{4}, \quad (ka \in [-\pi, \pi]).$$

Now we observe that

$$\omega_+(k) = 2\sqrt{\kappa/m} \cos \frac{ka}{4} \equiv 2\sqrt{\kappa/m} \left| \sin \frac{ka \pm 2\pi}{4} \right| \quad (ka \in [-\pi, \pi]),$$

meaning that the mode $\omega_+(k)$ coincides with the mode $\omega_-(k)$ extended to the second BZ, and then translated by the primitive reciprocal lattice vector. This is not a coincidence. At $m_1 = m_2$, the system becomes identical to a single-atomic chain with the lattice period $a_0 = a/2$ and correspondingly the first BZ being $ka_0 \in [-\pi, \pi]$, twice as large as the diatomic one. What we get is just a re-parametrization of the single-atomic dispersion in terms of diatomic nomenclature. At any finite $\xi$, however, there appears a qualitative difference at $k$’s close to the boundaries of BZ. To explore the behavior at the BZ boundaries, we expand the dispersion in the vicinity of the BZ boundary $k_{BZ} = \pm \pi/a$ up to the leading correction in $\Delta k = k - k_{BZ}$:

$$\sin^2 \frac{ka}{2} \approx 1 - \frac{(\Delta k a)^2}{8}.$$

Preserving only the leading corrections (which are $\sim \xi$), we obtain

$$\omega_\pm(k \to k_{BZ}) \approx \sqrt{\frac{2\kappa}{m}} \left[ 1 \pm \frac{1}{2} \sqrt{\xi^2 + \frac{(\Delta k a)^2}{8}} \right], \quad (|\Delta k a| \ll 1).$$

We see that there opens a gap between the two branches. The value of the gap scales as $\xi$. 

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3. **Chain with alternating interaction.** Consider a one-dimentional chain of atoms of the same mass \( m \), with the harmonic interaction between the nearest-neighbor atoms characterized by alternating spring constants: \( \kappa_1, \kappa_2, \kappa_1, \kappa_2, \ldots \). The distance between the nearest-neighbor atoms is \( a/2 \).

(a) Solve for the phonons. (b) Study the limit \( \kappa_1 \to \kappa_2 \): Interpret the result at \( \kappa_1 = \kappa_2 \) in terms of the chain with non-alternating interaction; explain a subtle difference between the cases \( \kappa_1 = \kappa_2 \) and \( |\kappa_1 - \kappa_2| \ll \kappa_1 \).

**Solution**

(a) The idea of this problem is very close to that of the previous problem of diatomic chain: there are two atoms per basis. In a very close analogy to the previous problem, for the non-zero elements \( A_{j_1j_2}(n) \) we have

\[
A_{11}(0) = A_{22}(0) = \kappa_1 + \kappa_2, \quad A_{12}(0) = A_{21}(0) = -\kappa_1.
\]

\[
A_{12}(-1) = A_{21}(1) = -\kappa_2.
\]

Note that now the spring constants are different and we must keep them explicitly. The masses are equal, and we set \( m = 1 \) (we restore \( m \) in the final answer by \( \omega \to \omega/\sqrt{m} \)). With the dimensionless wavevector \( g \), for the matrix \( C_{j_1j_2}(g) \) we find

\[
C_{11} = C_{22} = \kappa_1 + \kappa_2,
\]

\[
C_{12}(g) = -\kappa_1 - \kappa_2 e^{ig}, \quad C_{21}(g) = -\kappa_1 - \kappa_2 e^{-ig}.
\]

The characteristic equation for \( \lambda = \omega^2 \) thus reads

\[
\begin{vmatrix}
\kappa_1 + \kappa_2 - \lambda & -\kappa_1 - \kappa_2 e^{ig} \\
-\kappa_1 - \kappa_2 e^{-ig} & \kappa_1 + \kappa_2 - \lambda
\end{vmatrix} = 0.
\]

\[
(\kappa_1 + \kappa_2 - \lambda)^2 - (\kappa_1 + \kappa_2)^2 + 4\kappa_1\kappa_2 \sin^2(g/2) = 0.
\]
\[ \lambda_{\pm} = 2\kappa \left[ 1 \pm \sqrt{1 - \eta \sin^2(g/2)} \right], \quad (7) \]

where
\[ \kappa = \frac{\kappa_1 + \kappa_2}{2}, \quad \eta = \frac{4\kappa_1\kappa_2}{(\kappa_1 + \kappa_2)^2}. \quad (8) \]

Restoring \( m \) and replacing \( g \to ka \), we write the final answer
\[ \omega_{\pm}^2(k) = \frac{2\kappa}{m} \left[ 1 \pm \sqrt{1 - \eta \sin^2(ka/2)} \right], \quad (ka \in [-\pi, \pi]). \quad (9) \]

Note a very close similarity between (7)-(9) and (3)-(6).

(b) The above-mentioned similarity between (7)-(9) and (3)-(6) allows one to immediately reduce this part of the problem to corresponding part of the previous one. Introducing the relevant parameter
\[ \xi = \frac{|\kappa_1 - \kappa_2|}{\kappa_1 + \kappa_2} \ll 1 \]

and observing that \( \eta = 1 - \xi^2 \) we realize that we are dealing with exactly the same mathematical relations (up to a negligibly different global pre-factor of \( 1/(1 - \xi^2) \approx 1 \)) that in the previous problem, so that the previous analysis applies literally, and there is no need to repeat it!