1. (a) Just like in class when we solved the chain with two different spring constants, label each lattice point by the pair \((R, i)\). Here \(R = na\) is the 1d Bravais lattice vector labeling the unit cell, and \(i = 1, 2\) is the basis index telling us which atom inside the unit cell we’re looking at. In this notation, the Hamiltonian is

\[
H = \frac{1}{2M_1} \sum_R p_{R1}^2 + \frac{1}{2M_2} \sum_R p_{R2}^2 + \frac{K}{2} \sum_R (u_{R1} - u_{R2})^2 + \frac{K}{2} \sum_R (u_{R2} - u_{R+1})^2. \tag{1}
\]

I am going to solve this by a trick, which is to rescale the momenta (and the coordinates), in order to make this problem look like one we already solved, where both masses are the same. To do this in a symmetric fashion, define \(M = \sqrt{M_1M_2}\), and write for the kinetic part of the Hamiltonian:

\[
H_K = \frac{1}{2M} \sqrt{\frac{M_2}{M_1}} \sum_R p_{R1}^2 + \frac{1}{2M} \sqrt{\frac{M_1}{M_2}} \sum_R p_{R2}^2. \tag{2}
\]

We want to get rid of the square root factors. To do that, define new momenta by

\[
p_{R1}' = (M_2/M_1)^{1/4} p_{R1}, \tag{3}
\]

\[
p_{R2}' = (M_2/M_1)^{-1/4} p_{R2}. \tag{4}
\]

In terms of these, we have \(H_K = (1/2M) \sum_R (p_{R1}')^2\).

It is now convenient to define

\[
\alpha \equiv (M_2/M_1)^{1/4} = \sqrt{\frac{M_2}{M_1}} = \sqrt{\frac{M}{M_1}}. \tag{5}
\]

If we make this transformation without also changing the coordinates \(u_{R1}\), we will spoil the commutation relations. So we should also change to the new coordinates:

\[
u_{R1}' = (1/\alpha) u_{R1}, \tag{6}
\]

\[
u_{R2}' = \alpha u_{R2}, \tag{7}
\]

which can be checked to satisfy the canonical commutation relations \([u_{R1}', p_{R1}'] = i\hbar \delta_{ij} \delta_{RR'}\).

Plugging this into the potential part of the Hamiltonian we have

\[
H_p = \frac{K}{2} \sum_R \left[\alpha u_{R1}' - \frac{1}{\alpha} u_{R2}'\right]^2 + \frac{K}{2} \sum_R \left[\frac{1}{\alpha} u_{R2}' - \alpha u_{R+1}'\right]^2. \tag{8}
\]

Fourier transforming this exactly as we did in class, we get

\[
H_p = \frac{K}{2} \sum_{k \in \text{B.Z.}} \left[\alpha u_{k1}' - \frac{1}{\alpha} u_{k2}'\right]^\dagger \left[\alpha u_{k1}' - \frac{1}{\alpha} u_{k2}'\right] + \frac{K}{2} \sum_{k \in \text{B.Z.}} \left[\frac{1}{\alpha} u_{k2}' - e^{ika} \alpha u_{k1}'\right]^\dagger \left[\frac{1}{\alpha} u_{k2}' - e^{ika} \alpha u_{k1}'\right]. \tag{9}
\]

\[
= \frac{K}{2} \sum_{k \in \text{B.Z.}} [u_{k1}'^\dagger] D_{ij}(k)[u_{kj}']. \tag{10}
\]

Here, \(k \in \text{B.Z.}\) means \(-\pi/a \leq k < \pi/a\), and the matrix \(D(k)\) is

\[
D(k) = \begin{pmatrix}
2\alpha^2 & -1 - e^{-ika} \\
-1 - e^{ika} & 2/\alpha^2
\end{pmatrix}. \tag{11}
\]

If \(\lambda\) is an eigenvalue of \(D(k)\), then the corresponding frequency is given by \(\omega^2 = (K/M)\lambda\). (Note that, here, we didn’t include the factor of \(K\) inside \(D(k)\).)
The eigenvalues of $D(k)$ are

$$\lambda = \frac{2(\alpha^2 + 1/\alpha^2) \pm \sqrt{4(\alpha^2 + 1/\alpha^2)^2 - 4(2 - 2\cos(k\alpha))}}{2}$$

(12)

$$= (\alpha^2 + 1/\alpha^2) \pm \sqrt{\alpha^4 + 1/\alpha^4 + 2\cos(k\alpha)}$$

(13)

$$= \frac{M_2}{M} + \frac{M_1}{M} \pm \sqrt{\frac{M_2}{M} + \frac{M_1}{M} + \frac{1}{M^2}} \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos(k\alpha)}$$

(14)

$$= \frac{M_2}{M} + \frac{M_1}{M} \pm \sqrt{1/M^2} \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos(k\alpha)}$$

(15)

$$= \frac{1}{M^2} \left[ M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos(k\alpha)} \right].$$

(16)

And therefore

$$\omega^2 = \frac{K}{M} \lambda$$

(18)

$$= \frac{K}{M^2} \left[ M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos(k\alpha)} \right]$$

(19)

$$= \frac{K}{M_1M_2} \left[ M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos(k\alpha)} \right].$$

(20)

(b) First, let’s approximate $\omega^2$ in the limit $M_1 \gg M_2$. The square root in $\omega^2$ is

$$\sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos(k\alpha)} = M_1 \sqrt{1 + 2\frac{M_1}{M_2} \cos(k\alpha) + \left(\frac{M_2}{M_1}\right)^2}$$

(21)

$$\approx M_1 \sqrt{1 + 2\frac{M_1}{M_2} \cos(k\alpha)}$$

(22)

$$\approx M_1 + M_2 \cos(k\alpha),$$

(23)

where the last line was obtained by Taylor expansion of the square root (i.e. the function $\sqrt{1+x}$), to leading order.

Putting this in, for the negative root we have

$$\omega^2 \approx \frac{K}{M_1M_2} \left[ M_1 + M_2 - M_1M_2\cos(k\alpha) \right]$$

(24)

$$= \frac{K}{M_1}(1 - \cos(k\alpha)),$$

(25)

This is exactly the frequency for a one-dimensional chain of atoms with mass $M_1$ and spring constant $K/2$. So we can guess that these normal modes involve motion of the heavy atoms. They are connected by two springs joined together by a light (almost massless) atom, so it’s effectively like they’re joined by a new spring that’s twice as long as the original one. This explains the fact that the effective spring constant is $K/2$, since if we take a spring made out of some material, and replace it with a new one of the same material but twice as long, the spring constant should go down by a factor of 2.

On the other hand, for the positive root we have

$$\omega_+ \approx \frac{2K}{M_2}.$$

(26)

This describes motion of the light atoms, but with frequencies that are independent of $k$. Since all the modes in this branch have the same frequency, it suggests we can think of them as independent, identical harmonic oscillators. Indeed we can: each light atom can be viewed as connected to two nearby, very heavy “walls” (the heavy atoms). The light atom is connected to each wall with a spring of spring constant $K$. So, effectively, it feels a spring constant $2K$, since it gets a force from both springs when it moves. Eq. (26) is exactly the frequency for a single harmonic oscillator with spring constant $2K$ and mass $M_2$. Therefore, these modes describe independent oscillations of the light atoms confined between pairs of immobile heavy atoms.
(c) For simplicity, I will just consider the case \( M_1 = M_2 = M \). Then

\[
\omega^2_{\pm} = \frac{K}{M} (2 \pm \sqrt{2 + 2 \cos(ka)})
\]

(27)

\[
= \frac{K}{M} (2 \pm \sqrt{4 \cos^2(ka/2))})
\]

(28)

\[
= \frac{K}{M} (2 \pm 2 |\cos(ka/2)|)
\]

(29)

\[
= \frac{2K}{M} (1 \pm \cos(ka/2)).
\]

(30)

In the last line, we used the fact that \(-\pi/a \leq k < \pi/a\) – the cosine is always positive in this range.

Now, for a monatomic chain with lattice spacing \( a/2 \), there is only one branch of normal modes and the frequency is

\[
\omega^2 = \frac{2K}{M} (1 - \cos(ka/2)).
\]

(31)

Here, \( k \) lives in the range \(-2\pi/a \leq k < 2\pi/a\). So within the smaller range, this is the same frequency as \( \omega_- \) above.

What about the other branch, \( \omega_+ \)? Consider \( \pi/a < k < 2\pi/a \). Then

\[
\omega^2(k) = \frac{2K_0}{M} \left[ 1 + \cos \left( \frac{ka}{2} - \pi \right) \right]
\]

(32)

\[
= \frac{2K_0}{M} \left[ 1 + \cos \left( \frac{k - (2\pi/a)}{2} \right) \right]
\]

(33)

\[
= \omega^2_+(k - 2\pi/a).
\]

(34)

So this says that \( \omega^2 \) for \( \pi/a < k < 2\pi/a \) gives the same frequencies as \( \omega^2_+ \) for \(-\pi/a < k < 0\). Similarly, we can get the \( \omega^2_+ \) frequencies for \( k > 0 \) by considering \( \omega^2(k) \) for \(-2\pi/a < k < -\pi/a\).

The point here is that \( \omega^2_{\pm}(k) \) are the exactly same frequencies as in \( \omega^2(k) \). They’ve just been divided up into two different branches.

2. (a) Our starting point here is A & M Equation 22.37,

\[
\omega^2_{\pm}(k) = \frac{K + G}{M} \pm \frac{1}{M} \sqrt{K^2 + G^2 + 2KG \cos(ka)}.
\]

(35)

Here the crystal momentum \( k \) lies in the range \(-\pi/a \leq k < \pi/a\). Note that \( a \) is the unit cell size, and hence \( a/2 \) is the spacing between nearest-neighbor atoms.

When \( \Delta = 0, K = G = K_0 \) and

\[
\omega^2_{\pm}(k) = \frac{2K_0}{M} \pm \frac{K_0}{M} \sqrt{2 + 2 \cos(ka)}
\]

(36)

\[
= \frac{2K_0}{M} \left( 1 \pm \cos(ka/2) \right),
\]

(37)

where the algebra is exactly the same as in Eq. (27) above.

Actually, we already showed above in problem 3c that this is the same as the dispersion relation for a monatomic chain with spring constant \( K_0 \).

(b) In terms of \( K_0 \) and \( \Delta \), we have

\[
\omega^2_{\pm}(k) = \frac{2K_0}{M} \pm \frac{1}{M} \sqrt{(K_0 + \Delta)^2 + (K_0 - \Delta)^2 + 2(K_0^2 - \Delta^2) \cos(ka)}
\]

(38)

\[
= \frac{2K_0}{M} \pm \frac{K_0}{M} \sqrt{2(1 + \cos(ka)) + (\Delta/K_0)^2(1 - 2 \cos(ka))}
\]

(39)

As long as \( 2(1 + \cos(ka)) \) is not small, then we can expand the square root in powers of \((\Delta/K_0)^2\), and the leading correction to the \( \Delta = 0 \) result will be proportional to \((\Delta/K_0)^2\).

However, if \( ka = \pi \), then \( 2(1 + \cos(ka)) = 0 \), and it’s clear that the leading correction to \( \omega^2_{\pm}(k) \) is proportional to \( \Delta/K_0 \). More generally, if \( ka = \pi + \pi \Delta/K_0 \), then \( 1 + \cos(ka) \) will be of order \((\Delta/K_0)^2\).

So for any \( k \) in this range, the leading correction to \( \omega^2_{\pm} \) will be proportional to \( \Delta/K_0 \).
3. (a) We start from the potential energy of the solid in terms of the pair potential, A & M 22.3:

\[ U = \frac{1}{2} \sum_{R, \mathbf{R}'} \phi[R - R' + \mathbf{u}(R) - \mathbf{u}(R')] \tag{40} \]

We want to expand this to second order in \( \mathbf{u}(\mathbf{R}) \), and, upon Fourier transforming, to put it in the form

\[ H_p = \frac{1}{2} \sum_{k} \left[ u^1(k)'' D^{\mu\nu}(k) [u(k)]'' \right]. \tag{41} \]

To goal of this problem is to show that \( D^{\mu\nu}(k) \) has the form written in A & M 22.97. It’s obvious based on what we’ve done in class and also from the discussion in the book that the frequencies are given by \( \omega = \sqrt{\lambda/M} \), where \( \lambda \) are eigenvalues of \( D \), so we will not show that here.

Let’s return to the potential energy in terms of the pair potential. Since we assume only nearest-neighbor atoms interact, we can write

\[ U = \frac{1}{2} \sum_{\mathbf{R}} \sum_{\mathbf{a}} \phi[\mathbf{u} + \mathbf{u} R + \mathbf{a}) - \mathbf{u}(\mathbf{R})], \tag{42} \]

where the sum over \( \mathbf{a} \) is over the 12 vectors connecting \( \mathbf{R} \) to its nearest neighbors. Defining \( \delta \mathbf{u} = \mathbf{u}(\mathbf{R} + \mathbf{a}) - \mathbf{u}(\mathbf{R}) \), we have

\[ \phi[\delta \mathbf{u}] = \phi[\sqrt{d^2 + \delta \mathbf{u}^2 + 2\mathbf{a} \cdot \delta \mathbf{u}}], \tag{43} \]

where we used the fact that \( \phi(r) = \phi(|r|) \). We need to expand this in \( \delta \mathbf{u} \), keeping all terms up through second order.

First, let’s expand the square root using \( \sqrt{1 + x} = 1 + x/2 - x^2/8 + \mathcal{O}(x^3) \). We drop all terms higher than second order.

\[ \sqrt{d^2 + \delta \mathbf{u}^2 + 2\mathbf{a} \cdot \delta \mathbf{u}} = d \sqrt{1 + \frac{\delta \mathbf{u}^2}{d^2} + \frac{2\mathbf{a} \cdot \delta \mathbf{u}}{d^2}} = d \left[ 1 + \frac{1}{2} \left( \frac{\delta \mathbf{u}^2}{d^2} + \frac{2\mathbf{a} \cdot \delta \mathbf{u}}{d^2} \right) - \frac{1}{8} \left( \frac{2\mathbf{a} \cdot \delta \mathbf{u}}{d^2} \right)^2 \right] \]

\[ = d + \frac{\mathbf{a} \cdot \delta \mathbf{u}}{2d} + \frac{\delta \mathbf{u}^2}{2d} - \frac{(\mathbf{a} \cdot \delta \mathbf{u})^2}{2d^3} \]

\[ = d + \hat{\mathbf{a}} \cdot \delta \mathbf{u} + \frac{\delta \mathbf{u}^2}{2d} - \frac{(\mathbf{a} \cdot \delta \mathbf{u})^2}{2d}, \tag{47} \]

where in the last line we defined \( \hat{\mathbf{a}} = \mathbf{a}/d \).

Next, let’s expand the pair potential itself, again dropping all terms higher than second order.

\[ \phi[\sqrt{d^2 + \delta \mathbf{u}^2 + 2\mathbf{a} \cdot \delta \mathbf{u}}] = \phi[d + \hat{\mathbf{a}} \cdot \delta \mathbf{u} + \frac{\delta \mathbf{u}^2}{2d} - \frac{(\mathbf{a} \cdot \delta \mathbf{u})^2}{2d}] \]

\[ = \phi(d) + \phi'(d) \left[ \hat{\mathbf{a}} \cdot \delta \mathbf{u} + \frac{\delta \mathbf{u}^2}{2d} - \frac{(\mathbf{a} \cdot \delta \mathbf{u})^2}{2d} \right] + \frac{1}{2} \phi''(d)(\hat{\mathbf{a}} \cdot \delta \mathbf{u})^2 \]

\[ = \phi(d) + \phi'(d)(\hat{\mathbf{a}} \cdot \delta \mathbf{u}) + \frac{\phi'(d)}{2d} \delta \mathbf{u}^2 + \frac{1}{2} \phi''(d) - \phi'(d)/d \right)(\hat{\mathbf{a}} \cdot \delta \mathbf{u})^2 \tag{50} \]

Ignoring the unimportant constant term, this gives us three different contributions to \( H_p \). Let’s deal with them in turn. The second, linear, term of Eq. (50) gives us

\[ H_p^1 = \frac{\phi'(d)}{2} \sum_{\mathbf{R}} \sum_{\mathbf{a}} \hat{\mathbf{a}} \cdot [\mathbf{u}(\mathbf{R} + \mathbf{a}) - \mathbf{u}(\mathbf{R})] \tag{51} \]

\[ = \frac{\phi'(d)}{2} \sum_{\mathbf{R}} \sum_{\mathbf{a}} \hat{\mathbf{a}} \cdot [\mathbf{u}(\mathbf{R}) - \mathbf{u}(\mathbf{R})] = 0. \tag{52} \]

To get to the second line, in the first term only we made the change of variables \( \mathbf{R} \rightarrow \mathbf{R} - \mathbf{a} \). So the linear term vanishes – this needs to happen if we’re expending about a stable minimum of the energy.
Next, consider the contribution to $H_p$ coming from the third term of Eq. (50). This is

$$H_{p2} = \frac{\phi'(d)}{4d} \sum_{R} \sum_{a} [u(R + a) - u(R)]^2$$

$$= \frac{1}{N} \frac{\phi'(d)}{4d} \sum_{k} \sum_{k',a} e^{iR(k + k')} [e^{ik \cdot a} - 1] [e^{ik' \cdot a} - 1] u(k) \cdot u(k')$$

$$= \frac{\phi'(d)}{4d} \sum_{k} \sum_{a} \left| e^{ik \cdot a} - 1 \right|^2 u(k) \cdot u(k)$$

$$= \frac{\phi'(d)}{4d} \sum_{k} \sum_{a} 4 \left[ 1 - \cos(k \cdot a) \right] u(k) \cdot u(k)$$

$$= \frac{\phi'(d)}{4d} \sum_{k} \sum_{a} 4 \sin^2(k \cdot a/2) u(k) \cdot u(k)$$

$$= \frac{1}{2} \sum_k [u(k) \cdot] u^\mu D^\mu \nu_{\!_{2}}(k) [u(k)]^\nu,$$

where

$$D^\mu \nu_{\!_{2}}(k) = \frac{2\phi'(d)}{d} \delta^\mu \nu \sum_a \sin^2(k \cdot a/2).$$

Finally, consider the contribution to $H_p$ coming from the last term of Eq. (50). This is

$$H_{p3} = \frac{1}{4} [\phi''(d) - \phi'(d)/d] \sum_{R} \sum_{a} \left( \hat{a} \cdot [u(R + a) - u(R)] \right)^2$$

$$= \frac{1}{4} [\phi''(d) - \phi'(d)/d] \sum_{k} \sum_{a} \hat{a}^\mu \hat{a}^\nu [u(R + a) - u(R)]^\mu [u(R + a) - u(R)]^\nu$$

$$= \frac{1}{4} [\phi''(d) - \phi'(d)/d] \sum_{k} \sum_{a} \hat{a}^\mu \hat{a}^\nu \left| e^{ik \cdot a} - 1 \right|^2 [u(k)]^\mu [u(k)]^\nu$$

$$= \left[ \phi''(d) - \phi'(d)/d \right] \sum_{k} \sum_{a} \hat{a}^\mu \hat{a}^\nu \sin^2(k \cdot a/2) [u(k)]^\mu [u(k)]^\nu$$

$$= \frac{1}{2} \sum_k [u(k) \cdot] u^\mu D^\mu \nu_{\!_{3}}(k) [u(k)]^\nu,$$

where

$$D^\mu \nu_{\!_{3}}(k) = 2[\phi''(d) - \phi'(d)/d] \sum_a \hat{a}^\mu \hat{a}^\nu \sin^2(k \cdot a/2).$$

Putting things together, we have

$$D^{\mu \nu}(k) = D^{\mu \nu}_{\!_{2}}(k) + D^{\mu \nu}_{\!_{3}}(k) = \sum_a \sin^2(k \cdot a/2) [A \delta^{\mu \nu} + B \hat{a}^\mu \hat{a}^\nu],$$

where $A = 2\phi'(d)/d$ and $B = 2[\phi''(d) - \phi'(d)/d]$. This is the desired form.

(b) Since $k = kx$, we have $k \cdot a = 0$ and $\sin^2(k \cdot a/2) = 0$ for $a = (a/2)(\pm y \pm z)$. So only the other eight $a$’s contribute to the sum over $a$ in Eq. (66). For the other eight $a$’s, we have $k \cdot a = \pm ka/2$, so that $\sin^2(k \cdot a/2) = \sin^2(ka/4)$. Therefore, we have

$$D^{\mu \nu}(k) = \sin^2(ka/4) \sum_a [A \delta^{\mu \nu} + B \hat{a}^\mu \hat{a}^\nu],$$

where the prime over the sum means we only sum over those eight $a$’s with a nonzero component in the $x$-direction. The result of doing this sum is

$$D^{\mu \nu}(k) = \sin^2(ka/4) \left[ 8A \delta^{\mu \nu} + B (x+y)^\mu (x+y)^\nu + (x-y)^\mu (x-y)^\nu + (x+z)^\mu (x+z)^\nu + (x-z)^\mu (x-z)^\nu \right].$$
We can find the eigenvalues of $D^{\mu\nu}(k)$ by guessing that the eigenvectors are $x, y, z$. We have

$$D^{\mu\nu}(k)x^\nu = \sin^2(ka/4)(8A + 4B)x^\nu$$  \hspace{1cm} (69)
$$D^{\mu\nu}(k)y^\nu = \sin^2(ka/4)(8A + 2B)y^\nu$$  \hspace{1cm} (70)
$$D^{\mu\nu}(k)z^\nu = \sin^2(ka/4)(8A + 2B)z^\nu.$$  \hspace{1cm} (71)

The eigenvector $x$ corresponds to the longitudinal polarization, and the other two eigenvectors to the transverse polarization. The usual formula

$$\omega = \sqrt{\lambda/M}$$

gives the frequencies written in $A$ & $M$.

(c) Here we have $k(k/\sqrt{3})(x + y + z)$, so we have $k \cdot a = \pm(ka/\sqrt{3})$ for $a = \pm(a/2)(x + y), \pm(a/2)(x + z), \pm(a/2)(y + z)$. For all other $a$'s, $k \cdot a = 0$ and $\sin^2(k \cdot a/2) = 0$. Therefore we have

$$D^{\mu\nu}(k) = \sin^2(ka/2\sqrt{3}) \sum_a \left[ A\delta^{\mu\nu} + B\hat{a}^\mu\hat{a}^\nu \right],$$  \hspace{1cm} (72)

where the sum is only over the six $a$'s for which $k \cdot a \neq 0$. Doing the sum we have

$$D^{\mu\nu}(k) = \sin^2(ka/2\sqrt{3})[6A\delta^{\mu\nu} + (x + y)^\mu(x + y)^\nu + (x + z)^\mu(x + z)^\nu + (y + z)^\mu(y + z)^\nu].$$  \hspace{1cm} (73)

We guess that the (orthogonal but non-normalized) eigenvectors are

$$e_1 = x + y + z$$  \hspace{1cm} (74)
$$e_2 = x - y$$  \hspace{1cm} (75)
$$e_3 = x + y - 2z.$$  \hspace{1cm} (76)

The first one is parallel to $k$ and corresponds to longitudinal polarization. The other two lie in the plane perpendicular to $k$ and are thus transverse. Acting on these with the matrix $D(k)$ we find

$$D^{\mu\nu}(k)e_1^\nu = \sin^2(ka/2\sqrt{3})[6A + 4B]e_1^\mu$$  \hspace{1cm} (77)
$$D^{\mu\nu}(k)e_2^\nu = \sin^2(ka/2\sqrt{3})[6A + B]e_2^\mu$$  \hspace{1cm} (78)
$$D^{\mu\nu}(k)e_3^\nu = \sin^2(ka/2\sqrt{3})[6A + B]e_3^\mu.$$  \hspace{1cm} (79)

Again, the two transverse polarizations are degenerate, and we have

$$\omega_L = \sin(ka/2\sqrt{3})\sqrt{\frac{6A + 4B}{M}}$$  \hspace{1cm} (80)
$$\omega_T = \sin(ka/2\sqrt{3})\sqrt{\frac{6A + B}{M}}.$$  \hspace{1cm} (81)