Homework 4 solutions

Problem 1

Displacements between cells are related to one another through a phase $e^{i\mathbf{k}\cdot\mathbf{r}}$, according to the Bloch theorem. We want the displacement pattern on the second atom in the fourth cell and first atom in the fifth cell when $\mathbf{k} = \hat{\mathbf{x}}\pi/a$, given the displacement pattern in the zeroth cell $u_0 = (0.1a,\, -0.05a)$. Using the Bloch theorem, we therefore have

$$u_4 = e^{i\frac{\pi}{a}4a}u_0 = u_0 \tag{9}$$

$$u_5 = e^{i\frac{\pi}{a}5a}u_0 = -u_0. \tag{10}$$

Adding these to the coordinates of the atoms in the fourth and fifth cells and taking the difference yields

$$\boxed{\Delta\,(\text{atom 4b} \leftrightarrow \text{atom 5a}) = 0.617a} \tag{11}$$

Problem 2

The potential energy of this configuration of atoms is

$$U = \frac{1}{2}k\left[(x_1 - x_2)^2 + (x_2 - x_3)^2 + (x_3 - x_4)^2 + \right]. \tag{46}$$

The force constant matrix is given by the second derivative of the energy with respect to displacements. Therefore,

$$K = \begin{pmatrix} k & -k & 0 & 0 \\ -k & 2k & -k & 0 \\ 0 & -k & 2k & -k \\ 0 & 0 & -k & k \end{pmatrix}. \tag{47}$$

The equation of motion can be written in matrix form as

$$M\ddot{\mathbf{x}} = -K\mathbf{x}, \tag{48}$$

where $M = mI_4$. Assuming our solutions are oscillatory–that is, assuming $\mathbf{x} \propto e^{i\omega t}$, this becomes

$$\omega^2 M\mathbf{x} = K\mathbf{x}. \tag{49}$$

This is a *generalized eigenvalue problem*. Rearranging, we can write it as a *regular eigenvalue problem*:

$$\left(M^{-1}K - \omega^2 I_4\right)\mathbf{x} = 0. \tag{50}$$

Since we have 4 atoms, each with one degree of freedom, this system will have 4 eigenvalues and 4 associated normal modes. One eigenvalue will be 0, which will be associated with translations along the x-axis, and the other 3 eigenvalues will be non-zero. Calculating the frequencies explicitly, we have

$$\omega_0 = 0 \tag{51}$$

$$\omega_1 = \sqrt{\left(2 - \sqrt{2}\right)\frac{k}{m}} \tag{52}$$

$$\omega_2 = \sqrt{\frac{2k}{m}} \tag{53}$$

$$\omega_3 = \sqrt{\left(2 + \sqrt{2}\right)\frac{k}{m}} \tag{54}$$

Problem 3

The potential energy for the closed loop configuration is given by

$$U = \frac{1}{2}K\left[(x_1 - x_2)^2 + (x_2 - x_3)^2 + (x_3 - x_4)^2 + (x_4 - x_1)^2\right]. \tag{55}$$

The force constant matrix is then

$$K = \begin{pmatrix} 2K & -K & 0 & -K \\ -K & 2K & -K & 0 \\ 0 & -K & 2K & -K \\ -K & 0 & -K & 2K \end{pmatrix}. \tag{56}$$

Note that this is exactly the same force constant matrix as in **Problem 12**, but with non-zero elements for $K_{14} = K_{41}$. The eigenfrequencies for this system are

$$\omega_0 = 0 \tag{57}$$

$$\omega_1 = \sqrt{\frac{2K}{m}} \tag{58}$$

$$\omega_2 = \sqrt{\frac{2K}{m}} \tag{59}$$

$$\omega_3 = \sqrt{\frac{4K}{m}}. \tag{60}$$

Let us now do this using periodic boundary conditions. We will use the same machinery as in Problem 4. Recall that the dynamical matrix is given by

$$D_{\mu\nu}(\mathbf{k}) = \sum_{n'} \frac{1}{\sqrt{m_\mu m_\nu}} D_{\mu\nu}(\mathbf{r}_n - \mathbf{r}_{n'}) e^{-i\mathbf{k}\cdot(\mathbf{r}_n - \mathbf{r}_{n'})}. \tag{61}$$

We already explicitly calculated the force constant matrix, but it will be useful for calculating the dynamical matrix if we write it in terms of indices. Doing so, we have

$$D_{\mu\nu}(\mathbf{r}_n - \mathbf{r}_{n'}) = K\left(2\delta_{nn'} - \delta_{n(n'-1)} - \delta_{n(n'+1)}\right). \tag{62}$$

Plugging in, we then have

$$\begin{aligned} D_{\mu\nu}(\mathbf{k}) &= \frac{K}{m}\sum_{n'}\left(2\delta_{nn'} - \delta_{n(n'-1)} - \delta_{n(n'+1)}\right) e^{-i\mathbf{k}\cdot(\mathbf{r}_n - \mathbf{r}_{n'})} \\ &= \frac{K}{m}\left[2 - e^{-ika} - e^{ika}\right] \\ &= \frac{2K}{m}\left(1 - \cos ka\right). \end{aligned} \tag{63}$$

As in **Problem 7**, the periodicity restricts the allowed values of k to be

$$k = \frac{2\pi n}{aN} = \frac{2\pi n}{4a}. \tag{64}$$

The allowed values of k are then $k = \pi/a\,\{0, \pm 1/2, 1\}$. Note that we are using $-\pi/2a$ rather than $3\pi/2a$ to stay in the first Brillouin zone. Finally, since $D(\mathbf{k}) = \omega^2(\mathbf{k})$, the eigenfrequencies are

$$\omega_0 = 0 \tag{65}$$

$$\omega_1 = \sqrt{\frac{2K}{m}} \tag{66}$$

$$\omega_2 = \sqrt{\frac{2K}{m}} \tag{67}$$

$$\omega_3 = \sqrt{\frac{4K}{m}}. \tag{68}$$

Problem 4

The energy of this chain is given by the sum of the energy in each spring:

$$\begin{aligned} U &= \frac{1}{2}K\sum_n \left[u(r_n) - u(r_{n+1})\right]^2 \\ &= \frac{1}{2}K\sum_n \left[u^2(r_n) - 2u(r_n)u(r_{n+1}) + u^2(r_{n+1})\right] \\ &= K\sum_n \left[u^2(r_n) - u(r_n)u(r_{n+1})\right], \end{aligned} \tag{12}$$

where we shifted the sum for the last term and combined it with the first. The dynamical matrix is given by

$$D_{\mu\nu}(\mathbf{k}) = \sum_{n'} \frac{1}{\sqrt{m_\mu m_\nu}} D_{\mu\nu}(\mathbf{r}_n - \mathbf{r}_{n'}) e^{-i\mathbf{k}\cdot(\mathbf{r}_n - \mathbf{r}_{n'})}, \tag{13}$$

where $D_{\mu\nu}(\mathbf{r}_n - \mathbf{r}_{n'}) = \frac{\partial^2 U}{\partial u_\mu(\mathbf{r}_n)\partial u_\nu(\mathbf{r}_{n'})}$ is the force constant matrix. The force constant matrix is (see `lecture06.pdf` if you need a reminder on how to calculate it)

$$D_{\mu\nu}(\mathbf{r}_n - \mathbf{r}_{n'}) = K\left(2\delta_{nn'} - \delta_{(n+1)n'} - \delta_{(n-1)n'}\right). \tag{14}$$

Plugging in to the formula for the dynamical matrix yields

$$\begin{aligned} D_{\mu\nu}(\mathbf{k}) &= \frac{K}{m}\sum_{n'} \left(2\delta_{nn'} - \delta_{n'(n-1)} - \delta_{n'(n+1)}\right) e^{-i\mathbf{k}\cdot(\mathbf{r}_n - \mathbf{r}_{n'})} \\ &= \frac{K}{m}\left[2 - e^{-ika} - e^{ika}\right] \\ &= \frac{2K}{m}\left(1 - \cos ka\right) = \omega^2(\mathbf{k}). \end{aligned} \tag{15}$$

Thus, we have our dispersion relation. Note that because of the periodicity, the only allowed k are $k = 2\pi n/Na$, and there are N of them. A plot of the dispersion is shown in Figure 2.

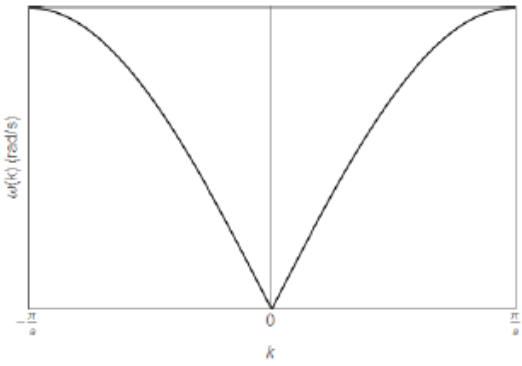

Figure 2: Dispersion relation for the 1D infinite chain.

To calculate the density of states, we will use

$$g(E) = \frac{a}{\pi}\frac{1}{|dE/dk|}. \tag{16}$$

Plugging in the dispersion relation, we find

$$g(E) = \frac{1}{\pi}\sqrt{\frac{2K}{m}}\left|\frac{\sqrt{1-\cos ka}}{\sin ka}\right|. \tag{17}$$

The density of states diverges at the zone boundary. A plot of of the density of states is shown in Figure 3.

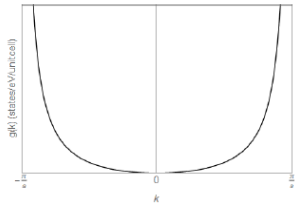

Figure 3: Density of state of the 1D infinite chain.

Problem 5

From the lecture notes, we recall that the dispersion relation for the generalized one-dimensional elastic chain is

$$\omega(k) = \sqrt{\frac{2}{m}\sum_p \kappa_p(1-\cos kap)}. \tag{20}$$

This is similar to **Problem 7**, but here we have an additional sum over spring constants. The sound velocity is the group velocity at small k. Expanding the dispersion relation about small k yields

$$\omega(k) \approx \frac{ak}{\sqrt{m}}\sqrt{\sum_p \kappa_p p^2}. \tag{21}$$

Taking the derivative with respect to k, we find the sound velocity to be

$$\boxed{v_s = \frac{a}{\sqrt{m}}\sqrt{\sum_p \kappa_p p^2}} \tag{22}$$

Problem 6

The potential energy for this system is given by

$$U = \frac{1}{2}\sum_n \left[\kappa\left(u_1(r_n) - u_2(r_n)\right)^2 + \gamma\left(u_2(r_n) - u_1(r_{n+1})\right)^2\right], \tag{23}$$

where, similar to our expression in **Problem 7**, $u_i(r_n)$ is the displacement of atom i relative to its associated Bravais lattice point r_n. Note that atom 1 is located on the Bravais lattice point r_n and atom 2 is located at $r_n + d = r_n + a/2$, in the middle of the primitive cell. Now, recall that the dynamical matrix is given by

$$D_{\mu\nu}(\mathbf{k}) = \sum_{n'} \frac{1}{\sqrt{m_\mu m_\nu}} D_{\mu\nu}(\mathbf{r}_n - \mathbf{r}_{n'}) e^{-i\mathbf{k}\cdot(\mathbf{r}_n - \mathbf{r}_{n'})}, \tag{24}$$

where $D_{\mu\nu}(\mathbf{r}_n - \mathbf{r}_{n'}) = \frac{\partial^2 U}{\partial u_\mu(\mathbf{r}_n)\partial u_\nu(\mathbf{r}_{n'})}$ is the force constant matrix. Note that this expression differs from the one in Ashcroft & Mermin. This definition yields an eigenvalue problem, while A&M's definition yields a generalized eigenvalue problem. To calculate the force constant matrix, we will first need the first derivatives of the potential:

$$\frac{\partial U}{\partial u_1(r_n)} = \kappa(u_1(r_n) - u_2(r_n)) + \gamma(u_1(r_n) - u_2(r_{n-1})) \tag{25}$$

$$\frac{\partial U}{\partial u_2(r_n)} = \kappa(u_2(r_n) - u_1(r_n)) + \gamma(u_2(r_n) - u_1(r_{n+1})). \tag{26}$$

The force constant matrix elements are then

$$\frac{\partial^2 U}{\partial u_1(r_n)\partial u_1(r_{n'})} = (\kappa + \gamma)\delta_{nn'} \tag{27}$$

$$\frac{\partial^2 U}{\partial u_1(r_n)\partial u_2(r_{n'})} = -\kappa\delta_{nn'} - \gamma\delta_{(n-1)n'} \tag{28}$$

$$\frac{\partial^2 U}{\partial u_2(r_n)\partial u_1(r_{n'})} = -\kappa\delta_{nn'} - \gamma\delta_{(n+1)n'} \tag{29}$$

$$\frac{\partial^2 U}{\partial u_2(r_n)\partial u_2(r_{n'})} = (\kappa + \gamma)\delta_{nn'}. \tag{30}$$

Plugging in to our expression for the dynamical matrix, we have

$$\begin{aligned} D_{11}(\mathbf{k}) &= \sum_{n'} \frac{\delta_{nn'}}{m}(\kappa + \gamma)e^{-ik(na - n'a)} \\ &= \frac{\kappa + \gamma}{m} \end{aligned} \tag{31}$$

$$D_{22}(\mathbf{k}) = \frac{\kappa + \gamma}{m} \tag{32}$$

$$\begin{aligned} D_{12}(\mathbf{k}) &= \sum_{n'} \frac{1}{m}\left(-\kappa\delta_{nn'} - \gamma\delta_{(n-1)n'}\right) e^{-ik(na - (n'+1/2)a)} \\ &= -\frac{1}{m}\left[\kappa e^{ika/2} + \gamma e^{-ika/2}\right] \end{aligned} \tag{33}$$

$$\begin{aligned} D_{21}(\mathbf{k}) &= \sum_{n'} \frac{1}{m}\left(-\kappa\delta_{nn'} - \gamma\delta_{(n+1)n'}\right) e^{-ik((n+1/2)a - n'a)} \\ &= -\frac{1}{m}\left[\kappa e^{-ika/2} + \gamma e^{ika/2}\right] = D_{12}^*(\mathbf{k}). \end{aligned} \tag{34}$$

The eigenvalues are

$$\omega_\pm^2(k) = \frac{1}{m}\left(\kappa + \gamma \pm e^{-iak}\sqrt{e^{2iak}\left(2\kappa\gamma\cos(ak) + \kappa^2 + \gamma^2\right)}\right) \tag{35}$$

and the corresponding eigenvectors are

$$\mathbf{u}_\pm(k) = \left(\mp\frac{e^{-\frac{1}{2}iak}\sqrt{e^{2iak}\left(2\gamma\kappa\cos(ak) + \gamma^2 + \kappa^2\right)}}{\kappa + \gamma e^{iak}}, 1\right). \tag{36}$$

Evaluating these eigenvectors at Γ and simplifying, we have

$$\boxed{u_\pm(\Gamma) = (\mp 1, 1)} \tag{37}$$

And at the zone-edge ($k = \pi/a$), we have

$$\boxed{u_\pm\left(\frac{\pi}{a}\right) = (\pm i, 1)} \tag{38}$$

Problem 7

The general form of B is

$$B(G) = \begin{pmatrix} e^{iGx_1} & 0 \\ 0 & e^{iGx_2} \end{pmatrix}, \tag{39}$$

where x_1 and x_2 are the basis vectors for our system. Since we set $x_1 = 0$ and $x_2 = a/2$ in **Problem 10**, we have

$$B(G) = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{iGa}{2}} \end{pmatrix}. \tag{40}$$

Using B to make a similarity transformation of $D(\mathbf{k})$ yields

$$\begin{aligned} D'(\mathbf{k}) &= B^{-1} D(\mathbf{k}) B \\ &= \frac{1}{m} \begin{pmatrix} \kappa + \gamma & -\left(\kappa e^{ia(k+G)/2} + \gamma e^{-ia(k-G)/2}\right) \\ -\left(\kappa e^{-ia(k+G)/2} + \gamma e^{ia(k-G)/2}\right) & (\kappa + \gamma) \end{pmatrix}. \end{aligned} \tag{41}$$

It is not obvious that this equals $D(\mathbf{k} + \mathbf{G})$, but recall that $D(\mathbf{k}) = \omega^2(\mathbf{k})$. Calculating the eigenvalues, we find

$$(\omega')^2_{\pm}(k) = \omega^2_{\pm}(k + G) = \omega^2_{\pm}(k). \tag{42}$$

Therefore, the eigenvalues are periodic in reciprocal space, and $D'(\mathbf{k}) = D(\mathbf{k} + \mathbf{G})$.

The eigenvalue problem with the transformed matrix is

$$\begin{aligned} 0 &= \left[D'(\mathbf{k}) - (\omega')^2 I)\right] \mathbf{v} \\ &= \left[B^{-1} D(\mathbf{k}) B - (\omega')^2 I)\right] \mathbf{v}. \end{aligned} \tag{43}$$

Can we act on this equation to get an eigenvalue problem for $D(\mathbf{k})$ in terms of the eigenvectors $\mathbf{v}$ of $D'(\mathbf{k})$? We can. Left multiplying by B and inserting $I = B^{-1}B$ just left of the eigenvector, we have

$$\begin{aligned} 0 &= B\left[B^{-1} D(\mathbf{k}) B - \omega^2 I)\right] B^{-1} B\mathbf{v} \\ &= \left[D(\mathbf{k}) - \omega^2 I)\right] B\mathbf{v}. \end{aligned} \tag{44}$$

Note that here we have used our previous result from this problem, where we showed that $D'(\mathbf{k})$ and $D(\mathbf{k})$ have the same eigenvalues. Comparing with **Problem 4**, we see that the eigenvectors for the transformed matrix and the original matrix are related by B:

$$\mathbf{u} = B\mathbf{v}. \tag{45}$$

Problem 8

(a) For each value of k, there are $3N$ normal modes and corresponding eigenfrequencies. Since there are 6 distinct bands, this tells us there are 2 atoms.

(b) The lowest three modes are the acoustic modes, and the upper three modes are the optical modes. The branches are labeled in Figure 4.

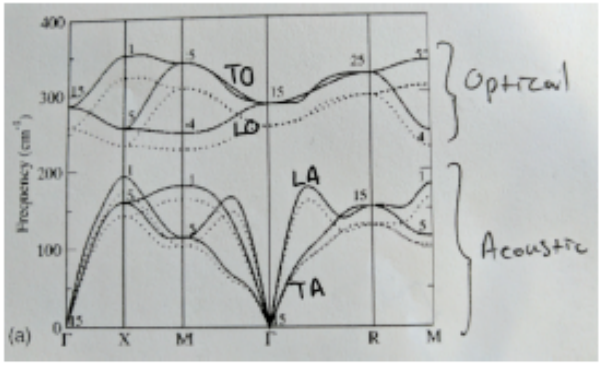

Figure 4: Labeled branches of the phonon band structure.

(c) The speed of sound is the group velocity of the transverse acoustic mode, which is given by

$$v_g = \frac{\partial \omega}{\partial k} \approx \frac{\Delta \omega}{\Delta k}. \tag{18}$$

Note that this is true at small values of k, but we will have to estimate it using larger values of k because we do not have the data used to make the plot. To calculate the derivative numerically, we will use the frequency at Γ and the frequency at $X/4$. NiAl has a $B2$ crystal structure, which is a BCC lattice where the body-centered atom is a different species than the atoms at the corners. Therefore, the high-symmetry k-points Γ and $X/4$ labeled in the phonon dispersion are located at $(0, 0, 0)$ and $\frac{2\pi}{4a}(1, 0, 0)$, respectively, and from the paper cited, the lattice constant is $a_{\mathrm{NiAl}} = 2.906\,\text{Å}$. The frequencies at these points are approximately $\omega(\Gamma) = 0\,\mathrm{cm}^{-1}$ and $\omega_L(X/4) = 50\,\mathrm{cm}^{-1}$ for the lower branch and $\omega_U(X/4) = 90\,\mathrm{cm}^{-1}$ for the upper branch. Plugging in (and taking care with the units!) to calculate the velocities for each branch and then averaging them, we therefore can estimate the group velocity along the Γ to X direction as

$$\boxed{v_g\,(\Gamma \to X) = 388.5\,\mathrm{m\,s}^{-1}} \tag{19}$$