Problem 1: Discrete Bloch (34 points)

Suppose you have an infinite sequence of identical masses \( m \), which can move without friction in 1d (x), connected by spring constants \( k \), which are repeating with period \( N \): \( k_{n+N} = k_n \). Denote the displacement of the \( n \)-th mass from equilibrium by \( x_n \), where \( k_n \) is the spring between \( x_n \) and \( x_{n+1} \). Newton’s laws give the following equation:

\[
 m \frac{d^2 x_n}{dt^2} = k_n (x_{n+1} - x_n) + k_{n-1} (x_{n-1} - x_n).
\]

We want to find the time-harmonic modes (normal modes, eigenmodes): solutions of the form \( x_n = X_n e^{-i\omega t} \) where \( X_n \) is time-independent.

(a) Bloch’s theorem tells us that we can choose eigenvectors in the form \( X_n = X_0 e^{ikn} \), where \( X_{N+n} = X_n \) (periodic). This corresponds to the irrep \( D_k(m) = e^{-ikNn} \) for translation by \( mN \): \( X_{n-mN} = D_k(m) X_n \). Note that \( k \) and \( k + 2\pi/N \) give the same irrep, so the Brillouin zone is \( k \in [-\pi/N, \pi/N] \).

If we plug this \( X_n e^{-i\omega t} \) into the Newton equation above, and multiply both sides by \( e^{-ikn} \), we obtain

\[
 -m\omega^2 X_n^k = k_n (X_{n+1}^k - X_n^k) + k_{n-1} (X_{n-1}^k - e^{-i\omega t} X_n^k).
\]

Since the \( X_n^k \) are periodic, there are only \( N \) independent equations, which we can write in matrix form (after dividing both sides by \(-m\))

\[
 \frac{1}{m} \begin{pmatrix}
 k_1 + k_N & -k_1 e^{ik} & \cdots & -k_N e^{-i\omega t} \\
 -k_1 e^{-i\omega t} & k_2 + k_1 & \cdots & -k_2 e^{-i\omega t} \\
 \vdots & \vdots & \ddots & \vdots \\
 k_N e^{i\omega t} & k_N - 2 e^{-i\omega t} & \cdots & k_{N-1} e^{-i\omega t}
 \end{pmatrix}
 A_k
 \begin{pmatrix}
 X_1^k \\
 X_2^k \\
 \vdots \\
 X_N^k
 \end{pmatrix}
 = \omega(k)^2 \begin{pmatrix}
 X_1^k \\
 X_2^k \\
 \vdots \\
 X_N^k
 \end{pmatrix},
\]

in which we have an \( N \times N \) (obviously) Hermitian matrix \( A_k \).

Since \( A_k \) is Hermitian and (less obviously) positive-semidefinite, it follows that \( \omega^2 \) is real and \( \geq 0 \), hence \( \omega(k) \) is real.

(b) For \( N = 1 \), we have the \( 1 \times 1 \) problem

\[
 \omega^2 X_1^k = \frac{k_1}{m} \left[ 2 - e^{i\omega t} - e^{-i\omega t} \right] = \frac{k_1}{m} [2 - 2\cos(k)] = \frac{4k_1}{m} \sin^2(k/2),
\]

where we have simplified the result using the half-angle identity, and hence

\[
 \omega(k) = \pm 2 \frac{k_1}{m} \sin(k/2).
\]

In the irreducible Brillouin zone (IBZ) \([0, \pi]\), this just rises in the usual sine fashion from \( \omega(0) = 0 \) (where all the masses move together and there is no oscillation) to a zero-slope “band edge” at \( \omega(\pi) = 2\sqrt{k_1/m} \) (where the masses are moving in exactly alternating fashion: effectively simple harmonic motion with spring constant \( 4k_1 \)).
Problem 3: Min–Max (33 points)

(c) We should expect that increasing a single spring to \( k'_1 > k_1 \) should localize an oscillating mode: since increasing \( k_1 \) causes the \( \omega \) to increase, this \( k'_1 \) will push a mode “up into the gap” above the band edge. As in class, frequencies above the band edge are exponentially decaying in the surrounding periodic regions.

Conversely, decreasing a single spring constant tries to pull frequencies down, but there is no gap at lower frequencies to be pulled down into (the bulk bands extend all the way to \( \omega = 0 \)). So, we wouldn’t expect to create a localized state by a defect \( k'_1 < k_1 \).

(d) The \( k_1 = k_2 = k_3 \) case is just a supercell: we will see the \( \sin(k/2) \) dispersion relation above simply “folded” into the new IBZ \( k \in [0, \pi/3] \). Then, if we make the spring constants slightly different, band gaps should open up around the folding points at the edges of the IBZ.

Problem 2: Degeneracy (33 points)

Suppose you have a 2d-periodic structure \( \epsilon(x,y) \). In class, we said that, in the long-wavelength limit (\( \lambda \gg \) period), the wave solutions “see” only a “homogenized” average medium: the solutions (averaged over a unit cell) are identical to those of the solutions in a homogeneous medium \( \epsilon_{\text{eff}} \). In general, \( \epsilon_{\text{eff}} \) is anisotropic (a 3 \times 3 matrix). Let’s consider only the TE polarization (in-plane \( E \)), for which we only have a 2 \times 2 \( \epsilon_{\text{eff}} \). You can assume that \( \epsilon_{\text{eff}} \) must real-symmetric and positive-definite if \( \epsilon(x,y) \) is real-symmetric and positive-definite (this is easy to prove).

(a) Suppose we have an eigenvector \( \mathbf{E} \) of \( \epsilon_{\text{eff}} \): \( \epsilon_{\text{eff}} \mathbf{E} = \lambda \mathbf{E} \). Because the system has \( C_n \) symmetry, the vector \( C_n \mathbf{E} \) should also be an eigenvector with the same eigenvalue \( \lambda \) (\( C_n \) must commute with \( \epsilon_{\text{eff}} \)). If \( n > 2 \), then \( C_n \mathbf{E} \) is linearly independent from \( \mathbf{E} \) (whereas for \( n = 1 \) and \( n = 2 \) it is parallel or antiparallel, respectively). Since this forms a basis for the 2d plane, and \( \epsilon_{\text{eff}} \) is isotropic is isotropic in that basis, it is isotropic in every basis. If you want an orthonormal basis, then any linear combination of \( \mathbf{E} \) and \( C_n \mathbf{E} \) is also an eigenvector of \( \lambda \), so we can use Gram–Schmidt to make an orthonormal basis of such eigenvectors, and in this basis we again have \( \epsilon_{\text{eff}} = \lambda \mathbf{I} \) where \( \mathbf{I} \) is the 2 \times 2 identity. This basis spans the 2d plane, so \( \epsilon_{\text{eff}} \) is isotropic (for the in-plane TE polarization).

(b) In the limit \( |k| \to 0 \) our lowest band always has \( \omega \to 0 \): it is the long-wavelength limit. In this limit, we have an effectively homogeneous isotropic material \( \epsilon_{\text{eff}} \) and hence the eigensolution is \( \omega_1(k_c) \approx c_{k_c}/\sqrt{\epsilon_{\text{eff}}} \) with two polarizations \( E_x \hat{x} \) and \( E_y \hat{y} \).

However, all the solutions must also be partners of an irrep of \( C_{nv} \). These solutions clearly transform as \( (x,y) \), so they fall into the 2d irrep given by the coordinate-rotation matrices. Hence they are exactly degenerate.

Furthermore, the solutions for \( \omega_1 \) are continuous functions of \( k_c \). So, if they fall into a 2d irrep for long wavelengths (small \( k_c \)) then they must be in the same 2d irrep at all wavelengths (all \( k_c \)): there is no way for a function to continuously go from being a partner of one irrep to another without passing through zero (which is not possible for eigenfunctions). Hence \( \omega_1(k_c) \) is doubly degenerate at all \( k_c \).

Problem 3: Min–Max (33 points)

- The correct statement is

\[
\hat{\lambda}_2 = \inf_{\mathcal{H}_2 \subseteq \mathcal{H}} \left[ \sup_{u \in \mathcal{H}_2} R\{u\} \right].
\]

This follows from the following two observations:

- First, for any \( \mathcal{H}_2 \subseteq \mathcal{H} \), let us choose a basis \( \{b_1, b_2\} \), where (as suggested) without loss of generality we can choose \( b_2 \perp u_1 \). i.e. \( b_2 = \sum_{n>1} c_n u_n \) for some \( c_n \), with \( c_1 = 0 \). Then \( R\{b_2\} \geq \hat{\lambda}_2 \) because it is a weighted average of the \( \lambda_n \geq \hat{\lambda}_2 \) for \( n > 1 \). Hence

\[
\sup_{u \in \mathcal{H}_2} R\{u\} \geq R\{b_2\} \geq \hat{\lambda}_2.
\]
Second, if $\mathcal{H}_2 = \text{span of } \{u_1, u_2\}$, the $R\{u\}$ is a weighted average of $\lambda_1$ and $\lambda_2$, so its supremum is $R\{u_2\} = \lambda_2$ similar to class.