18.369 Midterm Exam Solutions (Spring 2016)

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_n 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:

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

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 $X_n = X_n^k e^{ikn}$, where $X_{N+n}^k = X_n^k$ (periodic). This corresponds to the irrep $D_k(m) = e^{-ikNm}$ 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

$$-m\omega^2 X_n^k = k_n\left(X_{n+1}^k e^{ik} - X_n^k\right) + k_{n-1}\left(X_{n-1}^k e^{-ik} - X_n^k\right).$$

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 $-m$)

$$\underbrace{\frac{1}{m}\begin{pmatrix} k_1+k_N & -k_1e^{ik} & & & -k_Ne^{-ik} \\ -k_1e^{ik} & k_2+k_1 & -k_2e^{-ik} & & \\ & \ddots & \ddots & \ddots & \\ & & k_{N-2}e^{-ik} & k_{N-1}+k_{N-2} & k_{N-1}e^{ik} \\ k_Ne^{ik} & & & k_{N-1}e^{-ik} & k_N+k_{N-1} \end{pmatrix}}_{A_k}\underbrace{\begin{pmatrix} X_1^k \\ X_2^k \\ \vdots \\ X_{N-1}^k \\ X_N^k \end{pmatrix}}_{\mathbf{X}^k} = \omega(k)^2\mathbf{X}^k,$$

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 ω^2 is real and ≥ 0, hence $\omega(k)$ is **real**.

(b) For $N = 1$, we have the 1×1 problem

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

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

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

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 $4k_1$).

(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 ω^2 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 $\varepsilon(x,y)$. 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 ε_{eff}. In general, ε_{eff} is anisotropic (a 3×3 matrix). Let's consider only the TE polarization (in-plane $\mathbf{E}$), for which we only have a 2×2 ε_{eff}. You can assume that ε_{eff} must real-symmetric and positive-definite if $\varepsilon(x,y)$ is real-symmetric and positive-definite (this is easy to prove).

(a) Suppose we have an eigenvector $\mathbf{E}$ of ε_{eff}: $\varepsilon_{\text{eff}}\mathbf{E} = \lambda\mathbf{E}$. Because the system has C_n symmetry, the vector $C_n\mathbf{E}$ should also be an eigenvector with the same eigenvalue λ (C_n must commute with ε_{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 ε_{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 λ, so we can use Gram–Schmidt to make an orthonormal basis of such eigenvectors, and in this basis we again have $\varepsilon_{\text{eff}} = \lambda I$ where I is the 2×2 identity. This basis spans the 2d plane, so ε_{eff} is isotropic (for the in-plane TE polarization).

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

However, all the solutions must also be partners of an irrep of $C_{n\text{v}}$. 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 ω_1 are continous functions of k_z. So, if they fall into a 2d irrep for long wavelengths (small k_z) then they must be in the same 2d irrep at all wavelengths (all k_z): there is no way for a functio to continously go from being a partner of one irrep to another without passing through zero (which is not possible for eigenfunctions). Hence $\omega_1(k_z)$ is doubly degenerate at all k_z.

Problem 3: Min–Max (33 points)

- The correct statement is

$$\lambda_2 = \inf_{\mathscr{H}_2 \subseteq \mathscr{H}} \left[\sup_{u \in \mathscr{H}_2} R\{u\} \right].$$

  This follows from the following two observations:

  - First, for any $\mathscr{H}_2 \subseteq \mathscr{H}$, 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 $R\{b_2\} \geq \lambda_2$ because it is a weighted average of the $\lambda_n \geq \lambda_2$ for $n > 1$. Hence

$$\sup_{u \in \mathscr{H}_2} R\{u\} \geq R\{b_2\} \geq \lambda_2.$$

- Second, if $\mathscr{H}_2 =$ span of $\{u_1, u_2\}$, the $R\{u\}$ is a weighted average of λ_1 and λ_2, so its supremum is $R\{u_2\} = \lambda_2$ similar to class.