18.369 Midterm Exam (Spring 2016)

You have two hours. The problems have equal weight, so divide your time accordingly.

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) Apply Bloch's theorem to this problem: write the eigenvectors X_n as $X_n = (\text{something}) \times e^{ikn}$ for a real wavevector k (in what Brillouin zone?), and write down an eigenproblem for eigenvalues $\omega(k)^2$. (You should get an $N \times N$ Hermitian eigenproblem!)

If you do this correctly, your eigenproblem matrix should be both Hermitian and positive-semidefinite. You *don't need to prove this*. But in consequence, it follows from Hermitian + positive-semidefinite that the frequencies $\omega(k)$ are ________________.

(b) For the case of $N = 1$ (identical springs $k_n = k_1$), solve for the dispersion relation $\omega(k)$ and sketch it. Label the irreducible Brillouin zone (IBZ).

(c) If we start with identical springs from (b), and then change *one* spring constant to $k_1' \neq k_1$, explain whether $k_1' > k_1$ or $k_1' < k_1$ (or both, or neither) should be expected to create a localized vibrational state (one in which x_n near k' is oscillating, but these oscillations die off for large $|n|$). No proof required, just a clear argument [based on your dispersion relation from (b) and how ω^2 changes when you increase/decrease k_1].

(d) Sketch the dispersion relation for $N = 3$ (in the IBZ) for both the case of identical springs $k_1 = k_2 = k_3$ (i.e., a supercell) and *slightly* different spring constants.

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) In class, I claimed without proof that, for any $\varepsilon(x,y)$ with C_n symmetry (n-fold rotational symmetry) and $n > 2$, this 2×2 ε_{eff} must be isotropic (a multiple of the identity matrix). Prove this.

Hint: Start with one eigenvector of ε_{eff}, and find another linearly independent one with the same eigenvalue. Use these to construct an orthonormal basis in which it is obvious that ε_{eff} is isotropic.

(b) Consider the 3d time-harmonic Bloch solutions $\mathbf{H}(\mathbf{x},t) = \mathbf{H}_\mathbf{k}(x,y)e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$ for $\mathbf{k} = (0,0,k_z)$, i.e. **out-of-plane propagation**. Suppose that ε has $C_{n\text{V}}$ symmetry for some $n > 2$ (i.e. n-fold rotations + n mirror planes, the symmetry group of the regular n-gon). You are given that this symmetry group as at least one 2d irrep which transforms like the partner functions (x,y), i.e. the 2×2 coordinate-rotation matrices are an irrep. Show that the lowest band $\omega_1(k_z)$ is doubly degenerate.

Hint: use the fact that the long-wavelength limit "sees" an isotropic effective medium, from the previous part, and that the eigenfunction $\mathbf{H}_{\mathbf{k},1}$ for ω_1 is a continuous function of k_z.

Problem 3: Min–Max (33 points)

Suppose that we have a Hermitian operator $\hat{O}$ on some Hilbert space $\mathscr{H}$ (or technically a Sobolev space) with inner product $\langle u, v\rangle$. Recall that the eigenfunctions $\hat{O}u_n = \lambda_n u_n$ can be chosen orthonormal $\langle u_m, u_n\rangle = \delta_{m,n}$. Assume that we have a complete basis of eigenfunctions u_n for $n = 1,2,\ldots$, i.e. any $u \in \mathscr{H}$ can be written $u = \sum_n c_n u_n$ for $c_n = \langle u_n, u\rangle$. Assume that we have an ascending sequence of eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots$. In class, we proved the min–max theorem:

$$\lambda_1 = \min_{u\neq 0\in\mathscr{H}} R\{u\}$$

where $R\{u\} = \langle u, \hat{O}u\rangle / \langle u, u\rangle$ is the Rayleigh quotient. (Technically, I should probably use inf and sup instead of min and max, but let's not worry about that formality.) Recall that if $u = \sum_n c_n u_n$ then, from class,

$$R\{u\} = \frac{\sum_n |c_n|^2 \lambda_n}{\sum_m |c_m|^2},$$

a weighted average of the eigenvalues. We proved the min–max theorem simply by bounding $\lambda_n \geq \lambda_1$ in the numerator, in which case the sums cancel and we obtain $R\{u\} \geq \lambda_1$. Equality is achieved when $u = u_1$.

Now, we want to generalize this to a min–max theorem for λ_2 . One way, as given in class, is to minimize over $u \perp u_1$ for $m < n$ (a technique called "deflation"). Here, you will derive a *different* approach.

- Show that

$$\lambda_2 = \underbrace{\boxed{\text{min or max}}}_{\square}\underbrace{\boxed{\text{min or max}}}_{\lozenge} R\{u\}$$

where you indicate (i) the appropriate "min" or "max" in each box and (ii) the $\square$ and $\lozenge$ are each one of: $\mathscr{H}_2 \subseteq \mathscr{H}$ and $u \neq 0 \in \mathscr{H}_2$, where $\mathscr{H}_2$ indicates any 2-dimensional subspace of $\mathscr{H}$ (i.e. the span of any two linearly independent functions). That is, you are maximizing or minimizing the Rayleigh quotient over all possible 2-dimensional subspaces.

Hint: any two-dimensional subspace $\mathscr{H}_2$ must be spanned by a basis $\{b_1, b_2\}$ where b_1 and b_2 are *not* orthogonal to at *least* two eigenvectors u_n. Without loss of generality, you can choose $b_2 \perp u_1$ (rotate your basis so that b_1 contains any nonzero u_1 component).