18.369 Midterm Exam Solutions (Spring 2018)

Problem 1: Irreps

(a) Since $D(n)D(n') = D(n+n')$, it follows as in class that $D(n) = e^{-isn}$ for some s. (In particular, note that $D(n) = D(1)^n$ and $D(1) \neq 0$.) Since $D(N) = 1$ (rotation by C_N^N), it follows that $s = \frac{2\pi}{N}k$ for some integer k, i.e. we have the 1d irreps

$$D^{(k)}(n) = e^{-\frac{2\pi i}{N}kn}.$$

Furthermore, since we have N rotations in the C_N group, all in their own conjugacy class, it must be that we have exactly N irreps. This is true because

$$D^{(k+N)}(n) = e^{-\frac{2\pi i}{N}kn - 2\pi ni} = D^{(k)}(n),$$

i.e. only $k = 0, 1, \ldots, N-1$ are distinct irreps.

(b) Similar to class and in homework, a partner function of $D^{(k)}$ is of the of the form

$$\phi_\ell = \phi_0 e^{\frac{2\pi i}{N}k\ell}$$

for any constant ϕ_0, so that $\phi_{\ell-n} = D^{(k)}(n)\phi_\ell$. (Note that this is periodic: $\phi_{\ell+N} = \phi_\ell$.) Since all of the eigenvectors can be chosen in the form of partner functions, these are our eigenvectors. We an just plug them in to $\hat{\Theta}\phi$ to find the eigenvalues. The ℓ-th of $\hat{\Theta}\phi$ is

$$\frac{\kappa}{m}\left(2\phi_\ell - \phi_{\ell+1} - \phi_{\ell-1}\right) = \frac{\kappa}{m}\left(2 - e^{\frac{2\pi i}{N}k} - e^{-\frac{2\pi i}{N}k}\right)\phi_0 e^{\frac{2\pi i}{N}k\ell} = \frac{2\kappa}{m}\left(1 - \cos(2\pi k/N)\right)\phi_\ell,$$

confirming that ϕ_ℓ is an eigenvector with eigenvalue

$$\omega_k^2 = \frac{2\kappa}{m}\left(1 - \cos(2\pi k/N)\right) = \frac{2\kappa}{m}\sin^2\left(\frac{\pi k}{N}\right) = \omega_{k+N}^2 = \omega_{-k}^2 = \omega_{N-k}^2$$

for $k = 0, 1, \ldots, N-1$. (Note that we have exactly N linearly independent eigenvectors for our $N \times N$ matrix. Note also that the eigenvalues are real and nonnegative, which must be true for a real-symmetric positive-semidefinite matrix.) Hence the eigenfrequencies are:

$$\omega_k = \pm\sqrt{\frac{2\kappa}{m}}\sin\left(\frac{\pi k}{N}\right).$$

(c) For odd N, we also have the mirror symmetries σ:

(i) There are N mirror-symmetry planes, one through each vertex (bisecting the opposite edge). (Note that if N were even, we would have $N/2$ mirror planes through vertices and $N/2$ mirror planes through edges.)

(ii) The rotation C_N^n is conjugate to C_N^{-n} under a mirror flip. Ever mirror plane is conjugate to every other mirror plane under a rotation. Hence there are the following conjugacy classes: $C_N^0 = E$, the $\frac{N-1}{2}$ pairs $C_N^{\pm n}$ for $n = 1, \ldots \frac{N-1}{2}$, and the $N\sigma$ conjugacy class of mirror planes. (Note that if N were even, the mirror planes through vertices and faces would be in different conjugacy classes.)

(iii) There are $1 + \frac{N-1}{2} + 1 = \frac{N+3}{2}$ conjugacy classes, and hence **there are $\frac{N+3}{2}$ irreps**. The sum of their dimensions^2 must equal the number of elements in the group, $2N$. A further hint comes from the 2-fold degeneracies of the eigenvalues $\omega_k^2 = \omega_{N-k}^2$ for $k = 1, 2, \ldots$, which lets us know to expect 2-dimensional irreps. If you count how many 2d irreps you can half, it turns out that you must have **2 1d irreps and $\frac{N-1}{2}$ 2d irreps.** This gives a sum of dimensions^2 equal to $1 + 1 + 2^2\frac{N-1}{2} = 2 + 2N - 2 = 2N$, which is the correct sum. Indeed, the degenerate eigenvalues above for $k \neq 0$ correspond to partners of 2d irreps (while $k = 0$ is the trivial 1d irrep).

In fact, this is precisely the $C_{N\mathrm{v}}$ group . In pset 2 you analyzed $C_{3\mathrm{v}}$ and you found that it had two 1d irreps and $1 = \frac{3-1}{2}$ 2d irreps, exactly consistent with the general result here. (In the fall 2005 midterm there was an example of $C_{5\mathrm{v}}$, which had two 1d irreps and $2 = \frac{5-1}{2}$ 2d irreps, again consistent with our result here.)

One thing that you may find surprising is that there are *two* 1d irreps, but we only have *one* nondegenerate eigenvalue above at $\omega_0 = 0$. Why is this? The key thing is to understand what a mirror plane σ through a vertex ℓ does to ϕ_ℓ. Since ϕ_ℓ represents a displacement going *around* the circle tangentially, a mirror flip through ℓ must send $\phi_\ell \to -\phi_\ell$. That means the zero-frequency eigenfunction $\phi_\ell = \phi_0$ *cannot* transform as the trivial representation $D(g) = 1$. Instead, it must transform as the *other* 1d irrep, in which $D(n) = 1$ and $D(\sigma) = -1$. To get the trivial irrep, we would actually have to consider a *different physical problem* with the same symmetry group, for example oscillations in the *radial* direction from a ring of masses.

Problem 2: Index guiding

In class and in homework, you considered the problem of index-guiding: localization in a higher-index region with translational symmetry. In this problem, you should do the same thing but with a different wave equation, the Schrödinger equation, whose eigenmode equation for time-harmonic modes $\psi(\mathbf{x})e^{-i\omega t}$ is:

$$\hat{H}\psi = \underbrace{\left(-\nabla^2 + V\right)}_{\hat{H}}\psi = \omega\psi$$

where $V(\mathbf{x})$ is a "potential" function. In particular, we consider an x-independent potential $V(y)$ in 2d, as depicted in figure **??**, that $= 0$ for $|y| > h$ and is otherwise negative "on average," i.e. $\int_{-\infty}^{\infty} V(y)\,dy < 0$. You are also given that $\int_{-\infty}^{\infty} |V|\,dy$ is finite.

Note that $\hat{H}$ is Hermitian under the usual inner product $\langle\phi,\psi\rangle = \int \phi^*\psi$ for functions ϕ,ψ that decay sufficiently rapidly, and $\langle\psi,\hat{H}\psi\rangle = \int(|\nabla\psi|^2 + V|\psi|^2)$ via integration by parts.

(a) Solutions $\psi_k(y)e^{ikx}$ satisfy the "reduced" eigenproblem $\hat{H}_k\psi_k = \omega(k)\psi_k$ with $\hat{H} = -\frac{d^2}{dy^2} + k^2 + V(y)$. Note that the k dependence is purely in the form of an additive constant k^2, so it follows that $\omega(k) = \omega(0) + k^2$.

Furthermore, similar to the Maxwell case from class, we expect that the eigenvalues will be divided into the "light cone" — a continuous range of ω corresponding solutions in the infinite $V = 0$ regions — and one or more discrete guided modes pulled down below the light cone by the $V < 0$ region. The light cone, the solution for $V = 0$, is just planewaves $e^{i(kx+k_y y)}$ for all real numbers k_y, with eigenvalues $\omega = k^2 + k_y^2$. This gives the light cone as a continuous region $\omega \geq k^2$.

As we will show explicitly in the next part, there is at least one guided mode below the light cone. There could be more than one if the $V < 0$ region is big/deep enough, but in any case there will be a finite number. Unlike the Maxwell case, however, we will *not* get more more higher-order modes as we increase k, because of the $\omega(k) = \omega(0) + k^2$ property from above: whatever guided modes we have will maintain a fixed separation from the light cone.

A typical band diagram is shown in figure 1.

(b) Similar to class and homework, we will use a trial function $\psi_k(y) = e^{-\alpha|y|}$ in the limit of small $\alpha > 0$. We need to show $\frac{\langle\psi,\hat{H}\psi\rangle}{\langle\psi,\psi\rangle} < k^2$, i.e.

$$\alpha + \frac{k^2}{\alpha} + \int_{-\infty}^{\infty} Ve^{-2\alpha|y|}dy = \int_{-\infty}^{\infty}\left(\alpha^2 + k^2 + V\right)e^{-2\alpha|y|}dy = \boxed{\langle\psi_k,\hat{H}_k\psi_k\rangle < k^2\langle\psi_k,\psi_k\rangle} = k^2\int_{-\infty}^{\infty} e^{-2\alpha|y|}dy = \frac{k^2}{\alpha}.$$

Cancelling the k^2/α terms, we obtain the condition

$$\alpha + \int_{-\infty}^{\infty} Ve^{-2\alpha|y|}dy < 0$$

for some $\alpha > 0$. It suffices, therefore, to show that the left-hand side is negative for $\lim_{\alpha\to 0^+}$. Since $\left|Ve^{-2\alpha|y|}\right| \leq |V|$ and $\int|V| < \infty$ by assumption, we can use the dominated convergence theorem to interchange the limit and the integral. The limit of the left-hand-side is therefore $0 + \int V$, which is < 0 by assumption. It follows that we have at least one

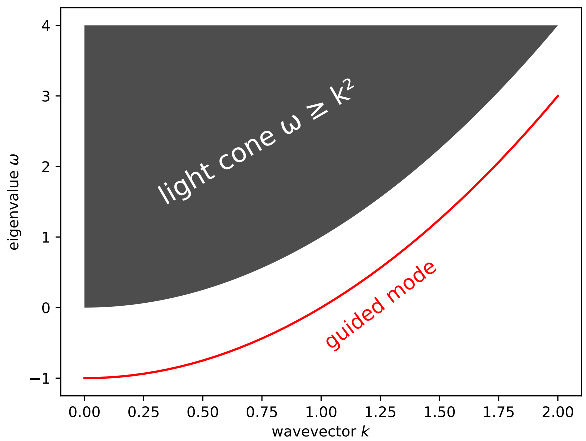

Figure 1: Schematic guided modes of a "channel" in the 2d Schrödinger equation.

eigenvalue below the light cone, i.e. a guided mode for all k.

(The problem only asked you to prove it for $k \neq 0$, since in the Maxwell case you don't have guided modes at $k = 0$, but in the Schrödinger case we have a guided mode at all k as depicted in figure 1.)

Problem 3: Projected band diagram

(a) The projection is done as follows:

(i) The edge of the projected Brillouin zone is at $k_d = \frac{\pi}{a\sqrt{2}}$ (π divided by the period).Since $|M| = \frac{\pi}{a}\sqrt{2}$, this means that the edge of the projected Brillouin zone is at $M/2$.

(ii) The projected bands are shown as a shaded region in figure 2, with the points labeled above and below the gap. Also shown are the folded bands from a supercell calculation (inset)—this is very helpful, because MPB will fold the bands for you without making mistakes.

Note that the original Γ–M/2 curve becomes the bottom of the lower continuum, which then "folds back" so that M (point b) lies back at $k_d = 0$. The X point (c and f) projects onto $k_d = \frac{\pi}{a\sqrt{2}}$.

(b) The (exact) projected band diagrams for $N = 1$, $N = 7$, and $N = 25$ are shown in figure 3.

As $N \to \infty$, we should get a continuum of guided bands filling up the intersectino of the light cone $\omega \geq ck_d$ (above red line) with the gap—if the air defect is infinitely wide, the solutions are exactly the planewaves of air—and indeed we can see a good approximation of that for $N = 25$. As N decreases, we will get fewer and fewer guided bands, eventually just one for $N = 1$.

A more subtle feature is clearly visible in the $N = 25$ diagram: where the light line hits the edge of the Brillouin zone and "folds back," there is a line of avoided crossings. This is essentially because the "folded" light line is an approximate solution (a planewave propagating along the defect) for a wide defect, which for a finite width turns into avoided crossings.

Another surprising feature is the fact that the $N = 1$ guided band is nearly (but not exactly) flat (about 2% bandwidth). I don't have any simple (non-numerical) explanation for this, however, and I don't expect you to have guessed it.

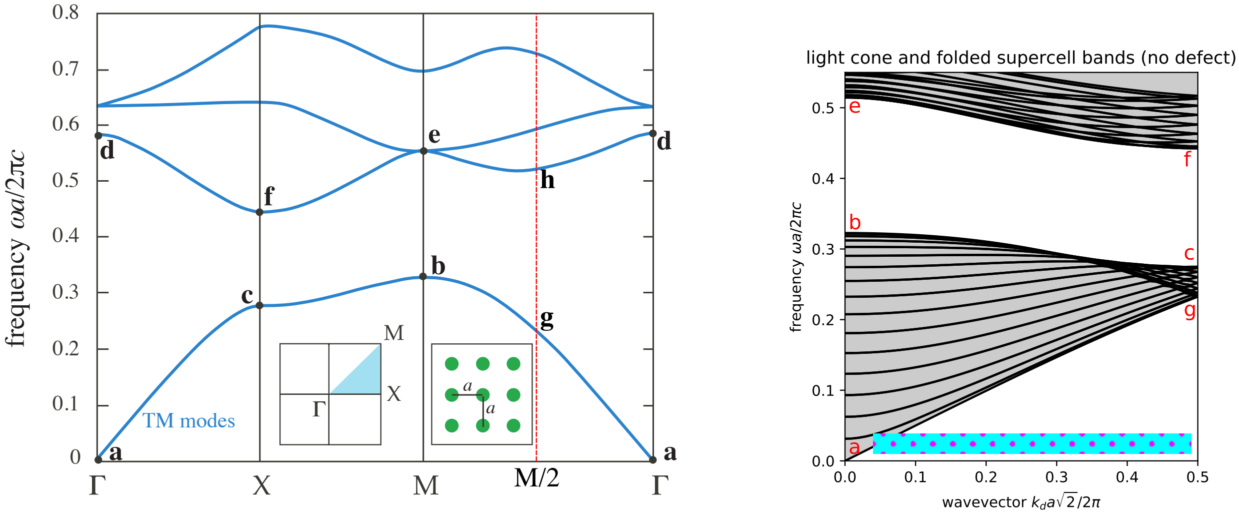

Figure 2: Left: band diagram and Brillouin zone (inset) for a square lattice of dielectric rods (period a, radius $0.2a$, $\varepsilon = 8.9$). Right: projected TM band diagram (shaded) along the diagonal direction. The inset shows a supercell, and black lines are the folded bands for this finite supercell (with periodic boundary conditions in the lateral direction). Red letters label the points indicated at left.

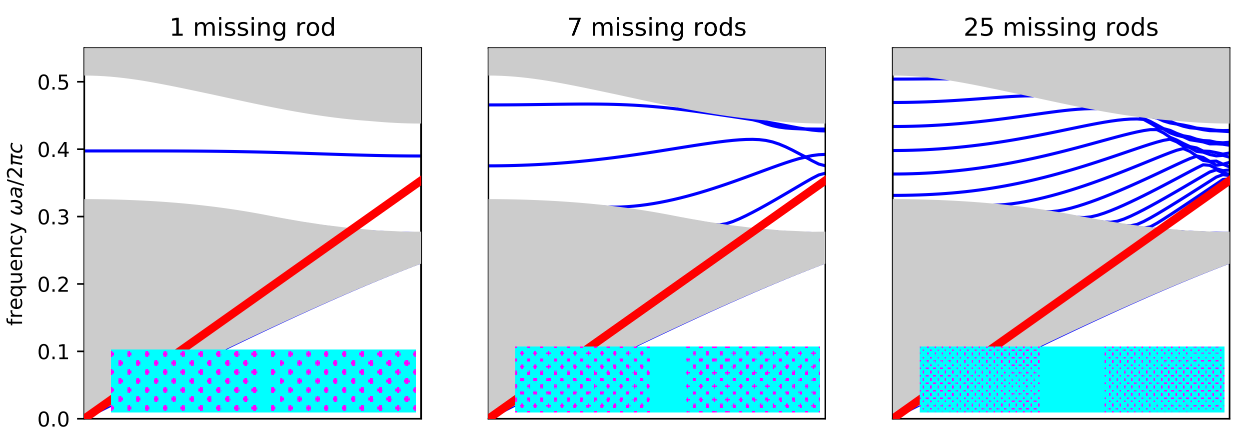

Figure 3: Projected TM band diagram for linear defects of N rows of rods along the diagonal direction of a square lattice of rods, for $N = 1, 7, 25$, with the geometry shown as insets. The gray shaded region is the spectrum of the bulk crystal, the blue curves are guided bands in the gap, and the red line is the light line $\omega = ck_d$.