18.369 Problem Set 4 Solutions

Problem 1: Perturbation theory

(a) Generalized perturbations:

(i) Let us write $(\hat{A}^{(0)} + \Delta\hat{A})\psi = \lambda(\hat{B}^{(0)} + \Delta\hat{B})\psi$, where $\psi = \psi^{(0)} + \psi^{(1)} + \cdots$ and $\lambda = \lambda^{(0)} + \lambda^{(1)} + \cdots$ are expansions of the new eigensolutions in powers of the perturbation Δ (since we don't have to worry about breaking degeneracies, by assumption). If we keep only the zero-th order terms, we get the unperturbed problem $\hat{A}^{(0)}\psi^{(0)} = \lambda^{(0)}\hat{B}^{(0)}\psi^{(0)}$. If we only keep terms only up to the 1st order, we get:

$$\hat{A}^{(0)}\psi^{(1)} + \Delta\hat{A}\psi^{(0)} = \lambda^{(1)}\hat{B}^{(0)}\psi^{(0)} + \lambda^{(0)}\hat{B}^{(0)}\psi^{(1)} + \lambda^{(0)}\Delta\hat{B}\psi^{(0)} + O(\Delta^2).$$

Taking the inner product with$\psi^{(0)}$ on both sides, and using the Hermitian property to operate $\hat{A}^{(0)}$ to the left and the fact that $\lambda^{(0)}$ is real, the $\lambda^{(0)}\left\langle \psi^{(0)}, \hat{B}^{(0)}\psi^{(1)} \right\rangle$ terms cancel on both sides, and we obtain:

$$\lambda^{(1)} = \frac{\left\langle \psi^{(0)}, \Delta\hat{A}\psi^{(0)} \right\rangle - \lambda^{(0)}\left\langle \psi^{(0)}, \Delta\hat{B}\psi^{(0)} \right\rangle}{\left\langle \psi^{(0)}, \hat{B}^{(0)}\psi^{(0)} \right\rangle},$$

which is the generalized version of first-order perturbation theory.

(ii) For $\nabla \times \nabla \times \mathbf{E} = \frac{\omega^2}{c^2}\varepsilon\mathbf{E}$ with a small change $\Delta\varepsilon$, we have $\Delta\hat{A} = 0$ and $\Delta\hat{B} = \Delta\varepsilon$. Also, to first order, $\Delta(\frac{\omega^2}{c^2}) = 2\frac{\omega\Delta\omega}{c^2} = \lambda^{(1)}$. Plugging this in above and dividing through by $2\omega/c^2$, we have:

$$\Delta\omega = -\frac{\omega}{2}\frac{\left\langle \mathbf{E}^{(0)}, \Delta\varepsilon\mathbf{E}^{(0)} \right\rangle}{\left\langle \mathbf{E}^{(0)}, \varepsilon\mathbf{E}^{(0)} \right\rangle},$$

which is the same as the expression we derived from the $\mathbf{H}$ eigenproblem in class.

(b) In problem set 2, we found that the TM modes of the $L \times L$ air-filled metal box were of the form $E_z = \sin(\frac{n\pi x}{L})\sin(\frac{m\pi y}{L})$, with $\omega_{nm} = \frac{\pi c}{L}\sqrt{n^2+m^2}$. Therefore, the lowest four nonzero modes are (n,m) of $(1,1)$, $(1,2)$/$(2,1)$, and $(2,2)$, where the middle two are degenerate. If we change the lower-left corner by $\Delta\varepsilon$ (without loss of generality, we can take the lower-left corner to be the $x = 0 \cdots \frac{L}{2}$ and $y = 0 \cdots \frac{L}{2}$ corner), then the first-order frequency shifts are (plugging into the $\Delta\omega$ formula above):

$$\Delta\omega_{11} = -\frac{\pi c\Delta\varepsilon}{L\sqrt{2}}\frac{\left(\int_0^{L/2}\sin^2(\frac{\pi x}{L})dx\right)^2}{\left(\int_0^{L}\sin^2(\frac{\pi x}{L})dx\right)^2} = -\frac{\pi c\Delta\varepsilon}{4L\sqrt{2}}$$

$$\Delta\omega_{22} = -\frac{\pi c\Delta\varepsilon\sqrt{2}}{L}\frac{\left(\int_0^{L/2}\sin^2(\frac{2\pi x}{L})dx\right)^2}{\left(\int_0^{L}\sin^2(\frac{2\pi x}{L})dx\right)^2} = -\frac{\pi c\Delta\varepsilon\sqrt{2}}{4L}.$$

(In fact, $\Delta\omega_{nn} = -\omega_{nn}\Delta\varepsilon/8$ for all n.) The degenerate bands, however, require some care, because the perturbation breaks the C_{4v} symmetry and thus will break the degeneracy. In particular, we need to choose them to diagonalize the perturbation. This can easily be done, however, because the perturbation still has a diagonal mirror plane—thus, we make linear combinations $\psi_\pm$ of the two states that are even and odd with respect to this mirror plane (which swaps x and y), namely:

$$\psi_\pm = \sin(\frac{\pi x}{L})\sin(\frac{2\pi y}{L}) \pm \sin(\frac{2\pi x}{L})\sin(\frac{\pi y}{L})$$

and therefore[1]

$$\Delta\omega_\pm = -\frac{\pi c\sqrt{5}}{2L}\frac{\langle\psi_\pm, \Delta\varepsilon\psi_\pm\rangle}{\langle\psi_\pm,\psi_\pm\rangle} = -\frac{\pi c\sqrt{5}}{2L}\Delta\varepsilon\left(\frac{9\pi^2 \pm 64}{36\pi^2}\right).$$

Note that *both* modes are shifted down in frequency (for $\Delta\varepsilon > 0$), but that the even mode is shifted down more, splitting the degeneracy—this is to be expected, since the even mode is more concentrated in the $\Delta\varepsilon$ region.

Many people get confused by degenerate perturbation theory, so let's be more explicit. Suppose that we didn't have a mirror symmetry, or didn't notice it? Then we would proceed as follows. We have two degenerate states in this case:

$$\psi_1 = \frac{2}{L}\sin(\frac{\pi x}{L})\sin(\frac{2\pi y}{L})$$

$$\psi_2 = \frac{2}{L}\sin(\frac{2\pi x}{L})\sin(\frac{\pi y}{L}),$$

where (with help from the $2/L$ factor) we have *orthonormalized* the states so that $\langle\psi_i, \varepsilon\psi_j\rangle = \delta_{ij}$ for $i, j \in \{1, 2\}$. (This is critically important because orthonormality was assumed in the derivation of degenerate perturbation theory.) Then we must compute the matrix $A_{ij} = \left\langle\psi_i, \Delta\hat{O}\psi_j\right\rangle = -\frac{\omega^2}{c^2}\langle\psi_i, \Delta\varepsilon\psi_j\rangle$ formed by the perturbation $\Delta\varepsilon$ (or more generally $\Delta\hat{O}$ for a Hermitian operator $\hat{O}$); the eigenvalues of A give the shifts $\Delta(\frac{\omega^2}{c^2})$ in the eigenvalues of the states given by the eigenvectors of A. (We'll divide by the usual $2\omega/c^2$ factor to get $\Delta\omega$ from $\Delta(\frac{\omega^2}{c^2})$.) Here, these integrals give the 2×2 matrix:

$$\frac{c^2}{2\omega}A = -\frac{\omega}{2}\begin{pmatrix} \frac{\Delta\varepsilon}{4} & \frac{16\Delta\varepsilon}{9\pi^2} \\ \frac{16\Delta\varepsilon}{9\pi^2} & \frac{\Delta\varepsilon}{4}\end{pmatrix} = -\frac{\omega\Delta\varepsilon}{8}\begin{pmatrix} 1 & \frac{64}{9\pi^2} \\ \frac{64}{9\pi^2} & 1\end{pmatrix}.$$

That is, in this special case all of the diagonal matrix elements happen to be the same—if you forgot to use degenerate perturbation theory, you might have erroneously concluded that the shifts of the eigenvalues were the same for ψ_1 and ψ_2 and there was no splitting. This is not true, however, because A has non-zero off-diagonal elements $\langle\psi_1, \Delta\varepsilon\psi_2\rangle$ and $\langle\psi_2, \Delta\varepsilon\psi_1\rangle$. In particular, the eigenvectors of this 2×2 matrix are simply $(1; \pm 1)$, corresponding to superpositions $\psi_\pm = \psi_1 \pm \psi_2$ of the original eigenstates, with the corresponding eigenvalues of $Ac^2/2\omega$ giving the eigenvalue shifts:

$$\Delta\omega_\pm = -\frac{\omega\Delta\varepsilon}{8}(1 \pm \frac{64}{9\pi^2}),$$

which is the same as our answer above. Thus, diagonalizing A automatically gives us the $\pm$ combinations corresponding to the even/odd states of the only remaining mirror symmetry plane. Above, we used a shortcut—because we know *a priori* that the *perturbed* system still has this mirror symmetry plane, we knew that the degenerate states had to divide into even/odd superpositions, and that these superpositions would automatically diagonalize A (in the diagonalized basis, we can just use ordinary perturbation theory).

(c) Band gaps at $k = 0$:

(i) In the unperturbed system with an "artificial" periodicity, the "folded" modes at $k = 0$ are $e^{\pm ix\cdot 2\pi/a}$ with a frequency of $\omega = c(2\pi/a)/\sqrt{\varepsilon_1}$. To apply degenerate perturbation theory, we need to diagonalize the perturbation $\Delta\varepsilon$. Let us take the $x = 0$ origin to lie at the *center* of a $\Delta\varepsilon$ layer (with thickness d_1, i.e. from $x = -d_1/2$ to $x = d_1/2$).[2] Because $x = 0$ is a mirror plane,

[1] I just did the integrals with Maple. Who has time for this 18.01 nonsense?

[2] In class, we took the $\Delta\varepsilon$ region to be centered at $x = \pm a/2$. The present choice will be a bit more computationally convenient, but it swaps the odd/even modes.

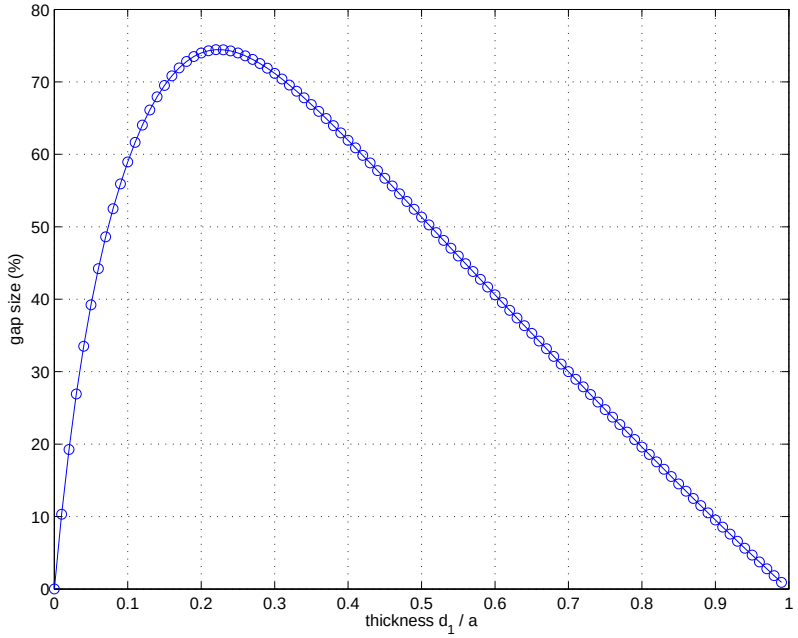

Figure 1: Gap size (% of mid-gap) for ε of 1 and 12 layers (period a) vs. thickness d_1/a of $\varepsilon = 12$ layer. The maximum gap occurs at $d_1 \approx 0.22a$.

it is sufficient to choose our unperturbed modes as $\sin(2\pi x/a)$ and $\cos(2\pi x/a)$, i.e. with odd and even symmetry. The first-order frequency shifts are then, respectively:

$$\Delta\omega_{\text{odd}} = \frac{c\pi\Delta\varepsilon}{a\varepsilon_1\sqrt{\varepsilon_1}} \frac{\int_{-d_1/2}^{d_1/2} \sin^2(2\pi x/a)dx}{\int_{-a/2}^{a/2} \sin^2(2\pi x/a)dx} = \frac{c\pi\Delta\varepsilon}{a\varepsilon_1\sqrt{\varepsilon_1}} \frac{d_1 - \frac{a}{2\pi}\sin(2\pi d_1/a)}{a}$$

$$\Delta\omega_{\text{even}} = \frac{c\pi\Delta\varepsilon}{a\varepsilon_1\sqrt{\varepsilon_1}} \frac{\int_{-d_1/2}^{d_1/2} \cos^2(2\pi x/a)dx}{\int_{-a/2}^{a/2} \cos^2(2\pi x/a)dx} = \frac{c\pi\Delta\varepsilon}{a\varepsilon_1\sqrt{\varepsilon_1}} \frac{d_1 + \frac{a}{2\pi}\sin(2\pi d_1/a)}{a},$$

where as expected, the odd mode is shifted up less than the even mode because the latter is more concentrated in the $\varepsilon - \Delta\varepsilon$ low dielectric, but both modes are shifted up. The gap $\Delta\omega$, expressed as a fractional gap $\Delta\omega/\omega$ to first order, is therefore:

$$\frac{\Delta\omega}{\omega} = \frac{\Delta\omega_{\text{even}} - \Delta\omega_{\text{odd}}}{c(2\pi/a)/\sqrt{\varepsilon_1}} = \frac{\Delta\varepsilon}{\varepsilon_1} \cdot \frac{\sin(2\pi d_1/a)}{2\pi}.$$

(ii) This $k = 0$ gap disappears for $d_1 = 0$ or $d_1 = a$, where the system is uniform ε_1 or $\varepsilon_1 - \Delta\varepsilon$, of course. The (first-order) gap also disappears for $d_1 = a/2$—this exactly corresponds to the quarter-wave thicknesses in the limit of infinitesimal index contrast. Thus, we have confirmed, at least to first order for the infinitesimal $\Delta\varepsilon$ case, the statement from class (and/or course notes) that the quarter-wave stack has an accidental degeneracy (no gap) at the $k = 0$ band crossings.

Problem 2: Band gaps in MPB

(a) To vary d_1 from 0 to a, the easiest thing is to write a loop. One can write a loop in Scheme, modifying the bandgap1d.ctl file, but instead I sometimes find it easier to vary the parameters directly at the Unix

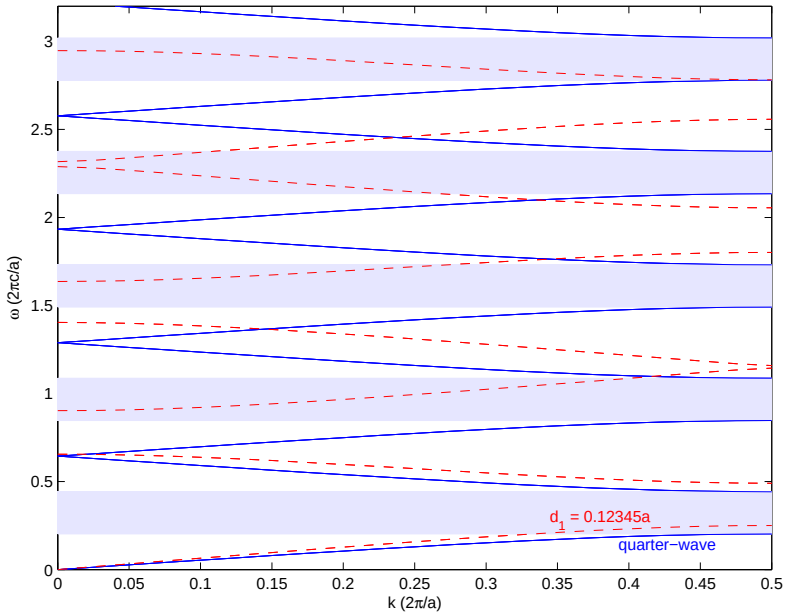

Figure 2: TM band diagram of $\varepsilon = 12/1$ multilayer film, with quarter-wave thickness $d_1 \approx 0.22401a$ (blue, solid) or thickness $d_1 = 0.12345a$ (red, dashed) of the $\varepsilon = 12$ layer. Quarter-wave gaps are shaded blue.

shell that modifies the parameters, using the mpb `d1=0.3` command to modify the `d1` parameter. Using the bash shell (note that the default Athena shell is tcsh, however), one can do a sequence of parameters and extract the results via:

```
(for d in `seq 0 0.01 1`; do echo -n "$d, "; mpbi d1=$d bandgap1d.ctl
|grep Gap |grep "band 1" |cut -d, -f2 |tr -d '%'; done) > p2a.dat
```

This results in the data shown in Figure 1, with the maximum gap at about $0.22a$, which is equal (within our d_1 resolution) to the quarter-wave thickness $d_1/a = 1/(\sqrt{12}+1) \approx 0.22401$, as expected.

(b) At the quarter-wave thickness d_1, the mid-gap is at $\omega a/2\pi c = a/\lambda \approx 0.32217$ (as can be found either from the MPB simulation or from the analytical formula discussed in class). Thus, $a = 0.32217\lambda = 0.32217 \cdot 1.55\mu\text{m} = 0.49936\mu\text{m}$, and $d_1 = 0.22401a = 0.11186\mu\text{m}$ ($d_2 = a - d_1$).

(c) In figure 2 are shown the TM band diagrams for the quarter-wave $d_1 \approx 0.22401a$ and the "random" $d_1 = 0.12345a$. (I increased num-bands to 10 to get this many bands, and increased k-interp to 19 to get smoother plots.) The quarter-wave bands have the following special features (besides having the largest fundamental gap as already noted above). First, all of their gaps $\Delta\omega$ are exactly the same size (in absolute units, not as a percentage of mid-gap). Second, their mid-gap frequencies are spaced exactly at the *odd integer multiples* of the first mid-gap! Third, the quarter-wave structure has no gaps edges at $k = 0$, where the bands are *accidentally degenerate*. (The $d_1 = 0.12345a$ structure *almost* has an accidental degeneracy at $ka/2\pi = 0.5$ between its third and fourth bands, but there is actually a very small gap there.)

Problem 3: Bands and supercells

What Calvin has forgotten is that, with Bloch's theorem, the periodicity in $\mathbf{k}$ is determined by the choice of unit cell—if you employ a supercell, a periodicity larger than the minimum, then this leads to a labelling $\mathbf{k}$ that is "folded" onto the smaller Brillouin zone of the new unit cell.

In particular, the point $(k_x, 0, 0)$ in the *second* calculation (where the y direction has a non-zero periodicity a and thus a finite Brillouin zone $2\pi/a$ in the y direction) corresponds to the points $(k_x, \frac{2\pi n}{a}, 0)$, for all integers n, in the *first* calculation (where the y direction has zero periodicity and thus an infinite Brillouin zone where all k_y are distinct). The results are shown in Fig. 3.

For the 1d unit cell, shown in Fig. 3(top), we see the usual 1d quarter-wave band diagram of non-degenerate bands (considering the TM polarization only). Because the index contrast is so low, the bands are *nearly* the folded bands from $\varepsilon \approx 1.05$ (the mean ε). A small gap opens up at $k_x = \pi/a$, centered on $\omega a/2\pi c = 0.4884$. There is no gap at $k_x = 0$, due to the peculiar accidental degeneracy of the quarter-wave stack at this point.

For the $a \times a$ unit cell, we see two kinds of bands in Fig. 3(bottom). First, the (non-degenerate) bands of the 1d unit cell ($n = 0$) are still solutions, of course, shown in red. The first folded band is for $n = 1$, corresponding to the lowest band at $k_y = \pm\frac{2\pi}{a}$. Since this is *nearly* a homogeneous system, we expect this band to be *nearly* $\omega \approx c\sqrt{k_x^2 + (\pm 2\pi/a)^2}$, which is doubly-degenerate, curved, and is almost degenerate with the 1d bands at $k_x = 0$ (a little below $\omega a/2\pi c = 1$) and at $k_x = 0.5\frac{\pi}{a}$ should be a little below $\sqrt{0.5^2 + 1} = 1.12$. In fact, the first 3 folded bands correspond to the first 3 bands at $n = \pm 1$, with frequencies $\omega \approx c\sqrt{(k_x + \ell\frac{2\pi}{a})^2 + (\pm 2\pi/a)^2}$ for $\ell = 0, -1, 1$. Thus, the 2nd and 3rd folded bands at $k_x = 0$ should be at $\omega \approx \sqrt{2}$. It's hard to tell on this plot because the index contrast is so low, but there *is* a gap in the folded bands at $k_x = 0$, since we are no longer satisfying the quarter-wave condition when $k_y \neq 0$. For the 4th folded band, there is a crossing between two bands: first, the 4th band(s) at $n = \pm 1$, with $\omega \approx c\sqrt{(k_x - 2\frac{2\pi}{a})^2 + (\pm 2\pi/a)^2}$; and second, the 1st band at $n = \pm 2$, with $\omega \approx c\sqrt{k_x^2 + (\pm 4\pi/a)^2}$. The latter is lower ($\omega \approx 2$ vs. $\omega \approx \sqrt{5}$) at $k_x = 0$, and the former is lower ($\omega \approx \frac{\sqrt{13}}{2}$ vs. $\omega \approx \frac{\sqrt{17}}{2}$) at $k_x = \pi/a$. No bands are more than 2-fold degenerate (except at points where they cross, of course).

Problem 4: Defect modes in MPB

For the solution of this problem, I made various modifications to the defect1d.ctl file that was supplied to you. The modified defect1dsol.ctl is given at the end.

(a) The supplied defect1d.ctl just computed the bands at a single $k = 0$ point, which is what we want normally for defect modes but is not what is asked for here. So, I modified the file to paste in the k interpolation code from bandgap1d.ctl, except that it is only invoked when k-interp is nonzero. Also, to show more than one gap we need more bands, so I added an "extra-bands" parameter that controls how many bands beyond the Nth we compute (instead of just 1). Then, running "mpb N=5 k-interp=19 extra-bands=20 defect1dsol.ctl" gives the plot shown in figure xxx (blue lines)—note that, since MPB gives k in units of $2\pi/$(cell size), it is here in units of $2\pi/5a$ and the edge of the folded Brillouin zone is still $k = 0.5$. On top of this, I superimposed the "folded" bands from figure 2,[3] shown as red circles, and we can see that they exactly coincide as expected.

(b) When we increase the ε of a layer, it pulls down a band from the upper edge of the gap, and thus we look at band $N+1$ in the supercell to get the defect mode. The supplied input file is set up to increase the ε of an ε_2 layer by the parameter "deps2". To change an ε_1 layer, the easiest thing is just to swap ε_1 and ε_2: "mpb eps1=1 eps2=12 deps2=1 defect1d.ctl". Unfortunately, it turns out that the ε_1 defect is rather weakly confined, so we also set our supercell size to $N = 120$ (I increased it until I saw clearly

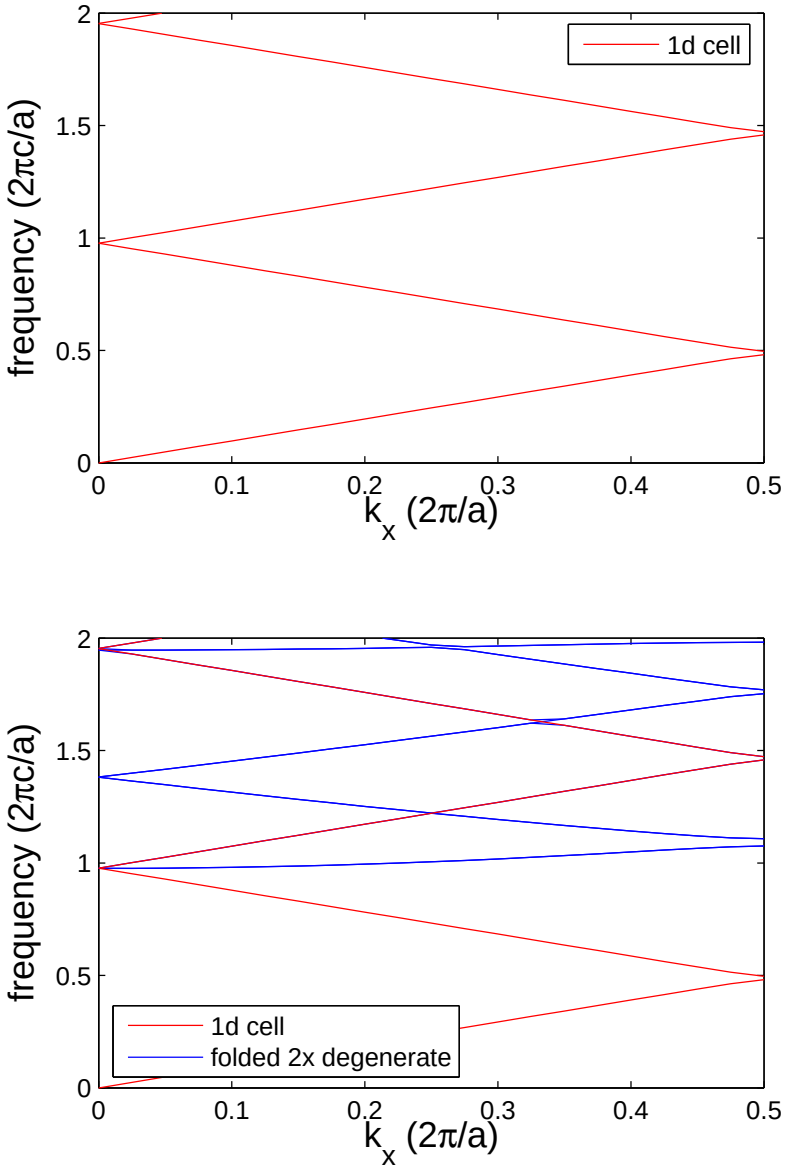

Figure 3: Band diagrams of quarter-wave stack ($\varepsilon = 1.1/1$). *Top*: 1d unit cell. *Bottom:* 2d unit cell (supercell), showing 1d bands (red) and double-degenerate folded bands from $k_y = \frac{2\pi n}{a}$ for $n \neq 0$ (blue).

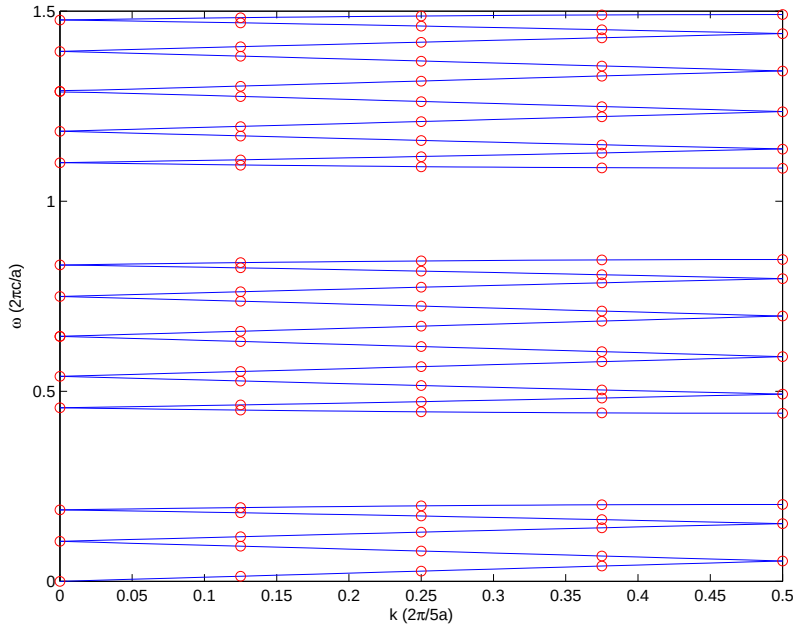

Figure 4: "Folded" band diagram of an $\varepsilon = 12/1$ quarter-wave stack with a supercell of $N = 5$ primitive cells. The supercell computation (blue lines) exactly corresponds with the data of figure 2 (red circles) folded onto this smaller Brillouin zone (note that k is now in units of $2\pi/5a$).

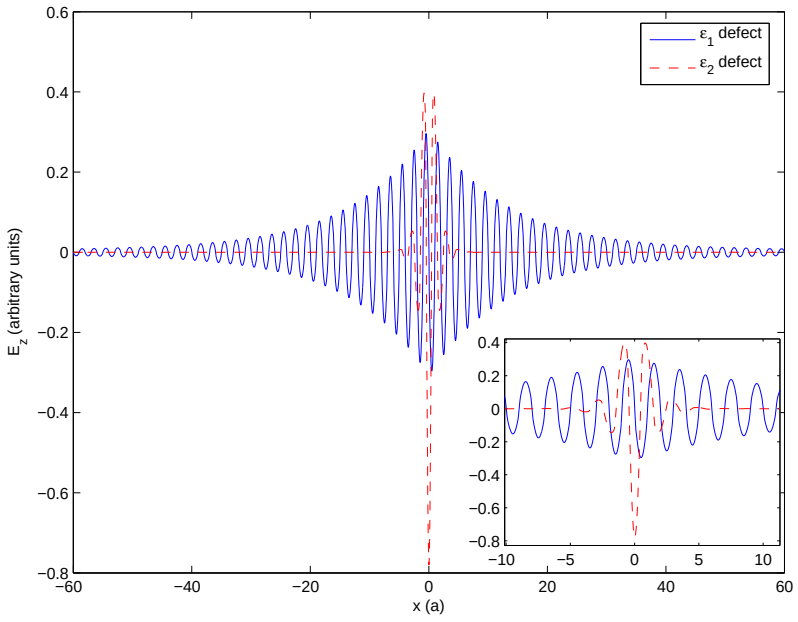

Figure 5: E_z pattern of localized modes formed by adding $\Delta\varepsilon = 1$ to either an $\varepsilon_1 = 12$ layer (blue, solid lines) or to an $\varepsilon_2 = 1$ layer (red, dashed lines). In both cases, the x axis is centered so that $x = 0$ bisects the defect layer. An enlarged view of the region near $x = 0$ is shown in the inset.

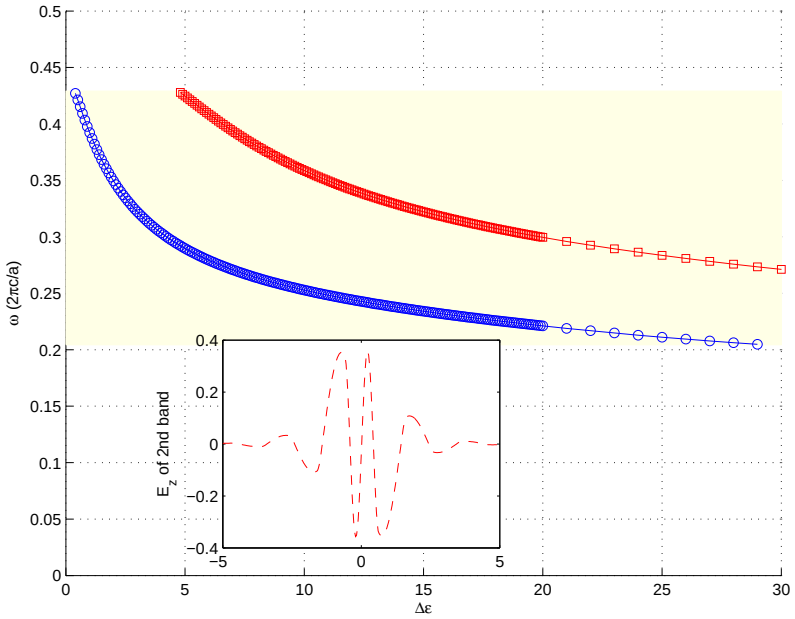

Figure 6: Frequency ω vs. $\Delta\varepsilon$ of point-defect modes formed by increasing a single ε_2 layer by $\Delta\varepsilon$, localizing states in the gap (gap frequencies are shaded yellow). At $\Delta\varepsilon \approx 4.8$, a second defect mode (red squares) enters into the gap; its E_z field at $\Delta\varepsilon = 10$ is inset. (At larger $\Delta\varepsilon$, even higher-order modes are localized, but are not shown here.)

localized modes). The resulting E_z field patterns, increasing ε_1 or ε_2 by $\Delta\varepsilon = 1$, are shown in figure 5.

From the inset of figure 5, we can see that the ε_1 defect mode is *odd* and the ε_2 defect mode is *even* through the center of the defect. The reason for this is that *both* bands are formed by pulling down the *upper* band-edge mode at $k = \pi/a$ (by analytic continuation), and this band edge mode was *odd* in the ε_1 (high-ε) layer and *even* in the ε_2 (low-ε) layer (as we proved when we found the origin of the band gap). From this, we can also see why the ε_2 mode is so much more strongly localized than the ε_1 mode: the latter is odd in the defect layer, and therefore has less field intensity there, and therefore "feels" the perturbation less strongly, and is therefore less localized.

(c) To make this part a little easier, I modified the .ctl file to only output fields when they are inside the gap (as computed from the unit cell) and to also output the frequencies just in that case. Then I did a little loop of deps2 values from the bash shell:

(for dep in 'seq 0 0.1 12'; do mpbi N=30 deps2=$dep extra-bands=2 defect1dsol.ctl |grep gapfreq; done) > p4c.dat

The resulting figure 6 shows the ω as a function of $\Delta\varepsilon$ of the first two defect modes, where the second defect mode (whose E_z is inset for $\Delta\varepsilon = 10$) appears in the gap at $\Delta\varepsilon \approx 4.8$. As it turned out, I need to go to larger values of $\Delta\varepsilon$, all the way to $\Delta\varepsilon = 30$, in order for the first defect mode to reach the lower edge of the gap. Here, we used a supercell $N = 30$, which should be large enough except for modes at very small $\Delta\varepsilon$.

[3] In Matlab, if "k" is the array of k coordinates, then we fold it by first setting "k=5*k" (since the folded bands are in units of $2\pi/5a$), and then repeatedly set "k(k > 0.5) = abs(k(k > 0.5) - 1)".

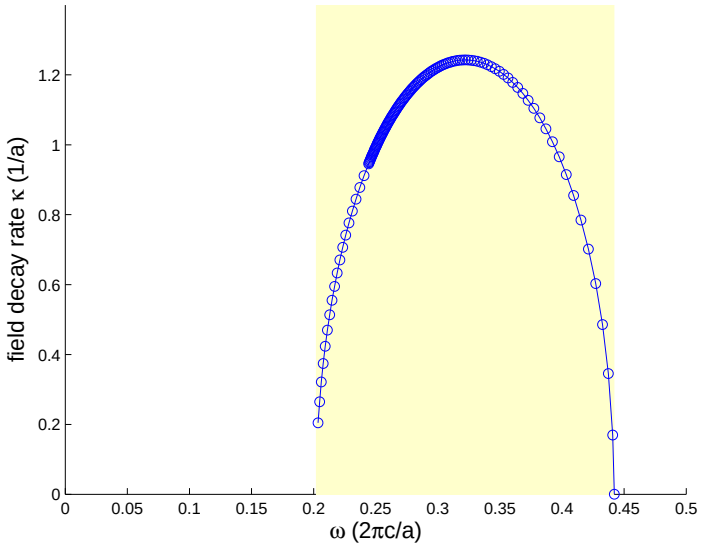

Figure 7: The field decay rate κ ($E_z \sim e^{-\kappa x + i\pi x/a}$) as a function of frequency ω as $\Delta\varepsilon$ ranges from 0 to 30, causing the defect mode to sweep across the gap (see figure 6). The gap frequencies are highlighted in yellow.

(d) To extract the decay rate, it is sufficient to consider two points, at $x = Na/4$ and $x = Na/4+a$, which should have a relative phase of -1 and a relative amplitude of $e^{-\kappa a}$. Or really, any two points separated by a will do, as long as they are far from *both* the defect and the boundaries. Just to make sure we don't accidentally hit a node of the field, I used $Na/4 + 0.182341a$ instead (where the 0.182341 is just a random number). Although we could extract the E_z field amplitudes from the HDF5 file in Matlab or whatever, it is easier to print them directly from MPB using the get-field-point function (which returns the field at a point). See the defect1dsol.ctl file to find out how I did it.

The resulting $\kappa(\omega)$ is plotted in figure 7. Just as we predicted in class, it increases as $\sqrt{\Delta\omega}$ (i.e. in a sideways parabola) away from the gap edges, and peaks in the center of the gap! (The fact that it peaks *exactly* at the center of the gap is a property of the quarter-wave stack, and is not true in general for photonic crystals.)

defect1dsol.ctl

The following is the modified .ctl input file that I used to solve problem 4.

```
(define-param eps1 12)
(define-param eps2 1)
(define-param deps2 0) ; the change in one eps2 layer (default is 0)

; use quarter-wave thickness by default
(define-param d1 (/ (sqrt eps2) (+ (sqrt eps1) (sqrt eps2))))
(define d2 (- 1 d1))

(set! default-material (make dielectric (epsilon eps1)))
```

```
; this is just one block of eps2 at the center... we duplicate it below
(set! geometry (list (make block
                       (center 0)
                       (size d2 infinity infinity)
                       (material (make dielectric (epsilon eps2))))))

; Before we compute the defect modes, let's compute the gap by using
; a size-1 unit cell.
(set! geometry-lattice (make lattice (size 1 no-size no-size)))
(set! k-points (list (vector3 0.5))) ; edge of B.Z. is where gap edges are
(set! num-bands 2) ; only need 2 bands
(run-tm)
(define gap-min (car freqs)) ; the first band's frequency
(define gap-max (cadr freqs)) ; the second band's frequency
(print "gap is from " gap-min " to " gap-max "\n")

(define-param N 15) ; the size of the supercell
(set! geometry-lattice (make lattice (size N no-size no-size)))

; to create the geometry, we have to repeat the epsilon 1 block N times,
(set! geometry (geometric-objects-lattice-duplicates geometry))

; Finally, we have to create the defect.
(set! geometry (append
                geometry
                (list (make block
                       (center 0)
                       (size d2 infinity infinity)
                       (material (make dielectric
                                   (epsilon (+ eps2 deps2))))))))

(set-param! resolution 32) ; 32 pixels/a

; for the defect mode, k does matter (if the supercell is big enough),
; so we just set it to zero.  If k-interp is not zero, however, we will
; indeed compute the (folded) band structure as in problem 4(a).
(define-param k-interp 0)
(if (zero? k-interp)
    (set! k-points (list (vector3 0)))
    (set! k-points (interpolate k-interp (list (vector3 0) (vector3 0.5)))))

; because of the folding, the first band (before the gap) will be folded
; N times.  So, we need to compute N bands plus some extra bands to
; get whatever defect states lie in the gap.   The number of extra bands
; is set by the parameter extra-bands.
(define-param extra-bands 1)
(set! num-bands (+ N extra-bands))

; Now, instead of outputting all of the modes, we'll define a little band
; function to just output the modes in the gap.   A band function is
```

```
; a function of band index, b; when passed to run, this function is
; called for every band computed.  We'll also print the corresponding
; frequency so that we can easily grep for it.  (See also the MPB manual).
(define (output-in-gap b)
  (let ((f (list-ref freqs (- b 1)))) ; the frequency of band b
    (if (and (> f gap-min) (< f gap-max))
        (begin
          (print "gapfreq" b ":, " deps2 ", " f "\n")
          (output-efield-z b)))))

(run-tm output-in-gap) ; run, outputting Ez

; Now that we're done, let's compute the fraction of the field energy
; in the defect layer for the last band, for use in getting the slope
; domega/d(deps2) for problem 4(d).
(get-dfield num-bands) ; get the last band's D
(compute-field-energy) ; compute its epsilon |E|^2 energy density
; compute the fraction of the energy in the defect object (center block).
(define energy-in-defect (compute-energy-in-objects
                          (make block
                            (center 0) (size d2 infinity infinity)
                            (material air))))
(print "predicted slope:, " deps2 ", "
       (* -0.5
          (list-ref freqs (- num-bands 1)) ; omega of last band
          (/ (+ eps2 deps2))
          energy-in-defect) "\n")

; Finally, for problem 4(f), let's compute the decay rate by taking the
; relative amplitude of the field at a random point and the random point
; + a.  (Note that the phase should be -1, or a phase angle of 180 degrees).
(get-efield num-bands)
(define-param fx (+ (/ N 4) 0.182341)) ; a "random" pt. far from the defect
(define field-ratio (/ (vector3-z (get-field-point (vector3 fx)))
                       (vector3-z (get-field-point (vector3 (- fx 1))))))
(print "decay:, "
       deps2 ", "
       (list-ref freqs (- num-bands 1)) ", " ; omega of last band
       (- (log (magnitude field-ratio))) ", " ; decay coefficient kappa
       (magnitude field-ratio) ", "
       (rad->deg (angle field-ratio))
       "\n")
```