18.369 Problem Set 3 Solutions

Problem 1: (10+15 points)

In both parts of this problem, we need to prove that the variational quotient \( \langle H, \hat{a} H \rangle / \langle H, H \rangle < k^2 \) for some trial function \( H \), or equivalently that

\[
\int_0^a \int_{-\infty}^\infty (1-\Delta) |(\nabla + ik) \times H_k|^2 \, dx \, dy - k^2 \int_0^a \int_{-\infty}^\infty |H_k|^2 \, dx \, dy < 0
\]

for the trial Bloch envelope \( H_k = H e^{-ik x} \), \( k = \mathbf{k} \hat{x} \), and \( \varepsilon^{-1} = 1 - \Delta \).

(a) We will choose \( u(x,y) = e^{-|y|/L} \) for some \( L > 0 \), exactly as in class—that is, it is the simplest conceivable periodic function of \( x \), a constant. Thus, \( \int |u|^2 = 2a \int_0^a e^{-2y/L} \, dy = aL \) over the unit cell. In this case, the variational criterion above becomes, exactly as in class except for the factor of \( a \):

\[
\int_0^a \int_{-\infty}^\infty (1-\Delta) \left(k^2 + L^{-2}\right) e^{-2|y|/L} \, dx \, dy - k^2 aL < 0
\]

which becomes negative in the limit \( L \to \infty \) thanks to our assumption that \( \int_0^a \int_{-\infty}^\infty \Delta(x,y) \, dx \, dy > 0 \). Note that the fact that \( \int |\Delta| < \infty \) ensures that we can interchange the limits and integration, via the dominated convergence theorem.

(b) Let us assume that we can choose \( u(y) \) and \( v(y) \) to be functions of \( y \) only (i.e., again the trivial constant-function periodicity in \( x \)). The fact that \( \nabla \cdot \mathbf{H} = 0 \) implies that \( (\nabla + ik) \cdot [u(y) \hat{x} + v(y) \hat{y}] = 0 = iku + v', \) and therefore \( u = iv' / k \). Therefore, it is convenient to choose \( v(y) \) to be a smooth function so that \( u \) is differentiable. Let us choose

\[
v(y) = e^{-y^2/2L^2}
\]

in which case \( u(y) = \frac{-i}{kL} e^{-y^2/2L^2} \). Recall the Gaussian integrals \( \int_{-\infty}^\infty e^{-x^2/2L^2} \, dx = \sqrt{\pi} L \) and \( \int_{-\infty}^\infty x^2 e^{-x^2/2L^2} \, dx = L^3 \sqrt{\pi} / 2. \) So, \( \int |\mathbf{H}|^2 = a \int |u|^2 + |v|^2 = aL \sqrt{\pi} \left[1 + \frac{1}{2kL^2}\right] \). Also, \( (\nabla + ik) \times [u(y) \hat{x} + v(y) \hat{y}] = (ikv - u') \hat{y}. \)

So,

\[
|\nabla \times \mathbf{H}|^2 = |(\nabla + ik) \times H_k|^2 = |u'|^2 + k^2 |v|^2 = k^2 \left[1 + \frac{1}{k^2L^2} \left(1 - \frac{y^2}{L^2}\right)\right] e^{-y^2/2L^2}.
\]

Then, if we look at our variational criterion, we have two terms: \( \int |\nabla \times \mathbf{H}|^2 \) and \( -\int \Delta |\nabla \times \mathbf{H}|^2 \). Again, we can swap limits with integration in the latter by the dominated convergence theorem. Combining the former with the \( -k^2 \int |\mathbf{H}|^2 \) term in the variational criterion, we get:

\[
\int |\nabla \times \mathbf{H}|^2 - k^2 \int |\mathbf{H}|^2 = \frac{a \int_{-\infty}^\infty k^2 \left[1 + \frac{1}{k^2L^2} \left(1 - \frac{y^2}{L^2}\right)\right] e^{-y^2/2L^2} \, dy - k^2 aL \sqrt{\pi} \left[1 + \frac{1}{k^2L^2}\right]} \]

\[
= \frac{a \int_{-\infty}^\infty k^2 \left[1 + \frac{1}{k^2L^2} \left(1 - \frac{y^2}{L^2}\right)\right] e^{-y^2/2L^2} \, dy - k^2 aL \sqrt{\pi}} \]

\[
= \frac{a k^2 L \sqrt{\pi} \left[1 - \frac{L^2}{2k^2L^2}\right] - \frac{a \sqrt{\pi}}{L}} \]

which goes to zero as \( L \to \infty \). Thus:

\[
\int (1-\Delta) |(\nabla + ik) \times H_k|^2 - k^2 \int |H_k|^2 \to -k^2 \int_{-\infty}^a \int_{-\infty}^\infty \Delta(x,y) \, dx \, dy < 0.
\]

as \( L \to \infty \). Q.E.D.
Problem 2: (5+15 points)

(a) Maxwell’s equations are (in terms of $\mathbf{H}$) given by the eigen-equation $\nabla \times \frac{1}{\sqrt{\varepsilon}} \nabla \times \mathbf{H} = \frac{\omega^2}{c^2} \mathbf{H}$. Suppose that we replace $\varepsilon$ by $\alpha \varepsilon$ where $\alpha$ is some constant. By inspection, one obtains the same eigen-solution $\mathbf{H}$ with $\omega$ replaced by $\omega/\sqrt{\alpha}$ (we just divided both sides by $\alpha$). Thus, scaling epsilon everywhere by a constant just trivially scales the eigenvalues. [We could have alternatively rescaled the geometry and fields: $\varepsilon(x) \rightarrow \varepsilon(x/\sqrt{\alpha})$ and $\mathbf{H}(x) \rightarrow \mathbf{H}(x/\sqrt{\alpha})$.] Therefore, we can set $\varepsilon_{lo} = 1$ (that is, $\alpha = 1/\varepsilon_{lo}$), without loss of generality.

(b) Since we are looking for “TM” solutions $E_z(x,y) = e^{ikx}E_k(y)$, i.e. with $\mathbf{E}$ in the $z$ direction, then we already saw from the last problem set that the eigen-equation simplifies to $-\nabla^2 E_z = \frac{\omega^2}{c^2} \varepsilon E_z$, and when we plug in the $e^{ikx}$ form we get:

$$-\frac{d^2}{dy^2} E_y = (\omega^2 \varepsilon - k^2) E_y$$

(where I have chosen $c = 1$ units for simplicity).

(i) In any region where $\varepsilon$ is constant, the above equation is solved simply by sines and cosines if $\omega^2 \varepsilon - k^2 > 0$ and by exponentials otherwise. Since we have a $y = 0$ mirror plane, the solutions can be chosen either even or odd, and therefore in the $|y| < h/2$ region we have solutions $E_k = A \cos(k \cdot y)$ or $A \sin(k \cdot y)$, where

$$k_\perp = \sqrt{\omega^2 \varepsilon_{hi} - k^2}.$$  

If $k_\perp$ is imaginary, these become cosh and sinh solutions, but we will see below that this won’t happen. In the $|y| > h/2$ region, since we are looking for solutions below the light line ($\omega^2 \varepsilon_{lo} < k^2$), we must have exponentials...and requiring the solutions to be finite at infinity we must have $E_k = Be^{-\kappa y}$ for $y > h/2$ and $\pm Be^{\kappa y}$ for $y < -h/2$ (with $\pm$ depending on whether the state is even or odd, where:

$$\kappa = \sqrt{k^2 - \omega^2 \varepsilon_{lo}} = \sqrt{k^2 (1 - f) - k_\perp^2 f},$$

where we define $f = \varepsilon_{lo}/\varepsilon_{hi} < 1$ (the dielectric contrast), and we have used the definition of $k_\perp$ from above.

(ii) Let’s consider first the even solutions (cosine). Continuity of $E_k$ implies that $A \cos(k \cdot h/2) = Be^{-\kappa h/2}$, and continuity of $E_k' \sim H_k$ implies that $-k_\perp A \sin(k \cdot h/2) = -\kappa Be^{-\kappa h/2}$. Dividing these two equations, we find:

$$\tan(k_\perp h/2) = \frac{\kappa}{k_\perp} = \frac{\sqrt{k^2 (1 - f) - k_\perp^2 f}}{k_\perp}.$$  

Similarly, for the odd solutions (sine), we obtain:

$$\cot(k_\perp h/2) = -\frac{\sqrt{k^2 (1 - f) - k_\perp^2 f}}{k_\perp}.$$

These are transcendental equations for $k_\perp$. We plot the left and right hand sides of these two equations in figure 1, where the intersections of the curves give the guided-mode solutions.

What about imaginary $k_\perp$ solutions? In this case, the left hand side (tan or cot) would be purely imaginary, while the right hand side would also be purely imaginary, so it seems like there might be some such solutions. Consider the even mode (tan) equation. The tangent of an imaginary $k_\perp$ is always imaginary with the same sign as the imaginary part of $k_\perp$, whereas the right hand side will be imaginary with the opposite sign ($1/i = -i$)—because of that, the two curves will never intersect for imaginary $k_\perp$ and there will be no solution. Conversely for the odd-mode
Figure 1: Plot of the two transcendental equations for even modes (left plot) and odd modes (right plot) as a function of $k_{\perp}h/2$. The thick lines show the right hand sides, while the thin lines show the left hand sides (tan or cot) of the equations, and the intersections correspond to guided-mode solutions. This plot is for the particular case of $f = 0.1$ and $kh/2 = 2$.

So, there are no imaginary $k_{\perp}$ solutions, as promised—this means that the guided modes must always be above the light line for $\epsilon_{hi}$, which makes physical sense (they must correspond to propagating modes in the $\epsilon_{hi}$ region and evanescent modes in the $\epsilon_{lo}$ regions).

(iii) We can see immediately that the right-hand side of the transcendental equations is a real number only when $k_{\perp} \leq |k|\sqrt{\frac{1}{f} - 1} = k_{\perp}^{\text{max}}$. Furthermore, we will clearly have an intersection for every branch of the tangent/cotangent curve that passes through zero before $k_{\perp}^{\text{max}}$. The tangent curves pass through zero whenever $k_{\perp}h/2$ is an integer multiple of $\pi$, and the cotangent curves pass through zero when $k_{\perp}h/2 + \pi/2$ is an integer multiple of $\pi$. Therefore, the number of even modes is simply the number of zero crossings before $k_{\perp}^{\text{max}}$, namely:

$$
\# \text{ even modes} = \left\lfloor \frac{|k|h\sqrt{\frac{1}{f} - 1}}{2\pi} \right\rfloor + 1,
$$

where the +1 is for the first branch of the tangent (which has a zero crossing at $k_{\perp} = 0$ and therefore always intersects the right-hand-side at least once). Here, by $\lfloor x \rfloor$ we mean the greatest integer $\leq x$. Similarly, the number of odd modes is also given by the number of zero crossings:

$$
\# \text{ odd modes} = \left\lfloor \frac{|k|h\sqrt{\frac{1}{f} - 1} + \pi}{2\pi} \right\rfloor,
$$

where in this case we see that we will not have any odd guided modes for $|k|h\sqrt{\frac{1}{f} - 1} < \pi$. Therefore, as $k \to 0$ we get exactly one (even) guided mode.

Just for fun, let’s look at the TE polarization ($\mathbf{H}$ in the $\hat{z}$ direction). For the $H_z = H_k e^{ikx}$ polarization, we have very similar equations except that the boundary conditions are that $H_k$ is continuous and $H_k'/\epsilon$ is continuous.

\footnote{There is some ambiguity about whether to define the mode as guided when the argument of $\lfloor x \rfloor$ here is exactly an integer, because that corresponds to the case where the mode is exactly on the light line and hence has $\kappa = 0$. If we don’t call that a guided mode, then we have to modify our formula by one in that case, but since this situation has measure zero in the parameter space, the question has no practical significance.}
Figure 2: Band diagram ($\omega$ vs. $k$) for five even TM bands of $\varepsilon_{hi} = 12$ waveguide structure with thickness $h = a$. Right: zoom in on point where band 4 enters the light cone, showing effect of increasing cell size from $Y = 10$ (blue) to $Y = 20$ (red).

Figure 2: Band diagram ($\omega$ vs. $k$) for five even TM bands of $\varepsilon_{hi} = 12$ waveguide structure with thickness $h = a$. Right: zoom in on point where band 4 enters the light cone, showing effect of increasing cell size from $Y = 10$ (blue) to $Y = 20$ (red).

Problem 3: (5+5+10+10 points)

(a) The 2dwaveguide.ctl file by default is already for a large enough $k$ (0 to $2 \cdot 2\pi / a$) to get five even modes (in fact, there are more, as we would see if we increased num-bands, and the result is shown in figure 2 (left). If we double the size of the computational cell (from $Y = 10$ to $Y = 20$), then the change is insignificant—we can’t even see on the regular graph. If we zoom in on the crossover point for band 4, as in figure 2 (right), then we can see a slight change, but only to the point of the band that is above the light line. To get the crossover points, I increased the number of $k$ points to k-interp=100, and then interpolated the intersection points. The first band, of course, is guided starting at $k = 0$, just as we predicted. The next three bands intersect the light line at $ka / 2\pi$ of 0.2979, 0.5954, and 0.8926, respectively. Our analytical prediction from problem 2 was that we would get a new even mode whenever $kh\sqrt{1/f - 1/2\pi}$ was an integer, i.e. for $kh / 2\pi$ an integer multiple of $1 / \sqrt{1/f - 1}$. In this case, $h = a = 1$, and $f = 1/12$, so we should get modes starting at $ka / 2\pi$ of 0.3015, 0.6030, and 0.9045. This matches our numerical calculation to an accuracy of better than 2%, which is as good as we can expect without increasing the number of $k$ points, etc.

(b) If we plot the fields at $ka / 2\pi = 1$ on a log scale in figure 3(left), we see that the amplitude decays as a straight line (thus, exponentially) at first, but then just becomes noisy. What is going on here? The answer is twofold. First, MPB solves for the modes by an iterative process, optimizing the Rayleigh quotient until some tolerance (by default, $10^{-7}$) in the eigenvalue is achieved. However, because very small values of the field have little effect on the eigenvalue, MPB does not try to converge them, and thus we see random tiny values once the field decays beyond a certain point. We can improve the accuracy of the small field values by reducing this tolerance...if we run MPB with tolerance=1e-14,
Figure 3: Fields $|E_z|$ for first three even TM modes of $\varepsilon_{hi} = 12$ waveguide, for $Y = 10$ cell at $ka/2\pi = 1$, showing exponential decay (straight line on log scale) until "noise floor" caused by finite numerical error in the fields is reached. Left: default ($10^{-7}$) tolerance in MPB. Right: decreased ($10^{-14}$) tolerance in MPB; we can’t decrease the tolerance much further because of floating point errors.

we see the field shown in figure 3(right), which decays linearly (exponentially) for a much larger range of $y$. It still has some noise at the boundaries, however, because the finite precision of floating point arithmetic does not let us get more accurate than this in our computation. If we reduce the cell size, however, so that it did not decay so much before reaching the boundary, however, we would see the field flatten out to a minimum value at the boundary for even modes (or go to a node for odd modes), due to the periodic boundary conditions.

(c) To put $\varepsilon = 2.25$ instead of air on the $y < -h/2$ side, we simply modify the geometry list to:

```lisp
> (set! geometry
>  (list (make block (center 0 (/ Y -4) 0)
>        (size infinity (/ Y 2) infinity)
>        (material (make dielectric (epsilon 2.25))))
>  (make block (center 0 0 0)
>        (size infinity h infinity)
>        (material (make dielectric (epsilon eps-hi))))))
```

That is, we added another block, of $\varepsilon = 2.25$, before the waveguide block. The new block has width $Y/2$, but where it overlaps with the waveguide the waveguide takes precedence (because it comes after in the geometry list). Now: **BE CAREFUL** – the original 2dwaveguide.ctl file computed the $y$-even and $y$-odd modes separately, but now there is no $y = 0$ mirror plane. We must just use (run-te) and (run-tm).

Now, if we plot the TM and TE modes, it looks at first as if there is no cutoff for the fundamental TM mode! This isn’t the case, however. The problem is that, for modes very near the light cone, they become delocalized and our computational cell needs to be larger. If we increase the size to $Y = 40$, and zoom in on the origin, we see that the first TM mode does indeed have a cutoff at around $\omega a/2\pi c = 0.02$ (whereas the TE cutoff is at a frequency around 0.1).

(d) This waveguide **should** have a TM (and a TE) guided mode for all values of $k$, because $\int \Delta y dy = \int (1 - 1/\varepsilon) dy = (h/2) \cdot (0.5 - 0.25) > 0$, applying our variational proof from class and from problem 2.
To show this numerically, we look at the first TM guided mode, for small values of $k$: we change num-bands to 1, kmax to 0.1, and k-interp to 200. (Similar to (c), above, we modify the geometry to contain two blocks of thickness $h/2$.) Since we are looking at small $\omega$ (large $\lambda$), we don’t need such a high resolution and reduce resolution to 10; this will allow us to look at much larger computational cells. Then, in figure 5, we plot $ck - \omega$, how far we are above the light cone—this should be positive for guided modes and should go to zero for $k \to 0$. This is precisely what we see, plotting on a log-log scale to see the power-law dependence.

However, we have to be careful: as $k \to 0$, we must increase the computational cell size so that the guided mode does not “see” the boundary. In particular, as we increase $Y$ from 10 to 20 to ... to 1280, we see that $ck - \omega$ is indeed converging to a positive, decreasing function (at the right side of the plot), whereas small $k$ values (at the left side of the plot) are not yet converged, but the trend is clear: it is going towards a steeper power-law decay (whereas if there were a cutoff $\omega$ the curve would diverge towards $-\infty$).
Figure 5: The amount $ck - \omega$ by which the lowest TM mode of the $\varepsilon_{hi} = \{2, 0.8\}$ system is below the light line, as a function of $k$, on a log-log scale (straight line = power law). As we increase the size of the computational cell $Y$ from 10 to 1280, this curve decreases for small $k$ (where the large wavelength is strongly affected by a finite computational cell), and is clearly converging (at the right side of the plot) to a steeper power-law decay.