

18.369 Problem Set 3 Solutions

Problem 1: Variational Theorem

- (a) Choose $F\{\psi\} = \langle \psi, \hat{A}\psi \rangle / \langle \psi, \hat{B}\psi \rangle$. Suppose we have eigenstates ψ_n with eigenvalues λ_n , and recall from pset 1 that they can be chosen orthogonal, with $\langle \psi_n, \hat{B}\psi_m \rangle = \delta_{n,m}$ and thus $\langle \psi_n, \hat{A}\psi_m \rangle = \lambda_n \delta_{n,m}$. For this part, we assume the eigenstates are complete, so any ψ can be written $\psi = \sum_n c_n \psi_n$ for some coefficients c_n . Then,

$$F\{\psi\} = \frac{\sum_{n,m} c_n^* c_m \langle \psi_n, \hat{A}\psi_m \rangle}{\sum_{n,m} c_n^* c_m \langle \psi_n, \hat{B}\psi_m \rangle} = \frac{\sum_n |c_n|^2 \lambda_n}{\sum_n |c_n|^2}.$$

Assuming $\psi \neq 0$, then $\langle \psi, \hat{B}\psi \rangle = \sum_n |c_n|^2 > 0$, and this is precisely a weighted average of the λ_n 's. Therefore, by part (a), it lies between the minimum and maximum λ_n 's (if any).

- (b) Let us write $F\{\psi + \delta\psi\} - F\{\psi\}$, dropping any terms of second order or higher in $\delta\psi$:

$$\begin{aligned} F\{\psi + \delta\psi\} - F\{\psi\} &= \frac{\langle \psi, \hat{A}\psi \rangle + \langle \delta\psi, \hat{A}\psi \rangle + \langle \psi, \hat{A}\delta\psi \rangle}{\langle \psi, \hat{B}\psi \rangle + \langle \delta\psi, \hat{B}\psi \rangle + \langle \psi, \hat{B}\delta\psi \rangle} - \frac{\langle \psi, \hat{A}\psi \rangle}{\langle \psi, \hat{B}\psi \rangle} + O(\delta^2) \\ &= \left[\frac{\langle \delta\psi, \hat{A}\psi \rangle}{\langle \psi, \hat{B}\psi \rangle} - \frac{\langle \psi, \hat{A}\psi \rangle \langle \delta\psi, \hat{B}\psi \rangle}{\langle \psi, \hat{B}\psi \rangle^2} \right] + [\text{c.c.}] + O(\delta^2) \\ &= \left[\frac{\langle \delta\psi, \dots \rangle}{\langle \psi, \hat{B}\psi \rangle} (\hat{A}\psi - F\{\psi\} \hat{B}\psi) \right] + [\text{c.c.}] + O(\delta^2) \end{aligned}$$

where ‘‘c.c.’’ denotes the complex conjugate of the bracketed expression.¹ Here, we have used the fact that $\frac{1}{u+\delta} = \frac{1}{u} - \frac{\delta}{u^2} + O(\delta^2)$ in order to move the $\langle \delta\psi, \hat{B}\psi \rangle$ from the denominator to the numerator. Now, in order for this to be true for *all* variations $\delta\psi$, which must be the case at an extremum, the parenthesized expression (\dots) must be zero.² But this parenthesized expression is just the eigenequation $\hat{A}\psi - \lambda \hat{B}\psi = 0$ where $\lambda = F\{\psi\}$ is just a number. This is only satisfied when ψ is an eigenstate and λ is the corresponding generalized eigenvalue. Q.E.D.

- (c) For the the electric field, we saw in pset 1 that we obtain a generalized eigenproblem with $\hat{A} = \nabla \times \nabla \times$ and $\hat{B} = \epsilon$, with the constraint that $\nabla \cdot \epsilon \mathbf{E} = 0$ (the absence of free charge). For the Bloch mode $\mathbf{E} = e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} \mathbf{E}_{\mathbf{k}}(\mathbf{x})$, we simply replace ∇ with $\nabla + i\mathbf{k}$ to get the eigenequation for $\mathbf{E}_{\mathbf{k}}$. Furthermore, since $\nabla \times$ is Hermitian, we write $\langle E, \hat{A}E \rangle$ as $\int |\nabla \times \mathbf{E}|^2$. Thus, our variational theorem becomes:

$$\frac{\omega_{\min}(\mathbf{k})^2}{c^2} = \min_{\substack{\mathbf{E}_{\mathbf{k}} \\ (\nabla + i\mathbf{k}) \cdot \mathbf{E}_{\mathbf{k}} = 0}} \frac{\int |(\nabla + i\mathbf{k}) \times \mathbf{E}_{\mathbf{k}}|^2}{\int \epsilon |\mathbf{E}_{\mathbf{k}}|^2},$$

where the integration is over the unit cell.

Problem 2: Guided modes in periodic waveguides

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

$$\int_0^a \int_{-\infty}^{\infty} (1 - \Delta) |(\nabla + i\mathbf{k}) \times \mathbf{H}_{\mathbf{k}}|^2 dx dy - k^2 \int_0^a \int_{-\infty}^{\infty} |\mathbf{H}_{\mathbf{k}}|^2 dx dy < 0$$

for the trial Bloch envelope $\mathbf{H}_{\mathbf{k}} = \mathbf{H} e^{-i\mathbf{k} \cdot \mathbf{x}}$, $\mathbf{k} = k\hat{\mathbf{x}}$, and $\epsilon^{-1} = 1 - \Delta$.

¹Note that in writing $\langle \delta\psi | \hat{A} | \psi \rangle = \langle \psi | \hat{A} | \delta\psi \rangle^*$, we have used the fact that \hat{A} is Hermitian, and similarly for \hat{B} .

²At first sight, since we are adding the complex conjugate, it might seem that only the real part of the $[\dots]$ quantity must be zero. However, if the imaginary part were nonzero, then we could send $\delta\psi \rightarrow i\delta\psi$ and get a non-zero quantity.

- (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, $\int |u|^2 = 2a \int_0^\infty e^{-2y/L} dy = aL$ over the unit cell. In this case, the variational criterion above becomes, exactly as in class except for the factor of a :

$$\begin{aligned} \int_0^a \int_{-\infty}^{\infty} (1 - \Delta) (k^2 + L^{-2}) e^{-2|y|/L} dx dy - k^2 aL &< 0 \\ &= \frac{a}{L} - \int_0^a \int_{-\infty}^{\infty} \Delta \cdot (k^2 + L^{-2}) e^{-2|y|/L} dx dy, \end{aligned}$$

which becomes negative in the limit $L \rightarrow \infty$ thanks to our assumption that $\int_0^a \int_{-\infty}^{\infty} \Delta(x, y) dx dy > 0$. Note that the fact that $\lim_{y \rightarrow \pm\infty} \Delta = 0$ ensures that we can interchange the limits and integration, because it makes the integrand uniformly convergent in L .

- (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 $(\nabla + i\mathbf{k}) \cdot [u(y)\hat{\mathbf{x}} + v(y)\hat{\mathbf{y}}] = 0 = iku + v'$, 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 $u(y) = -\frac{iy}{kL^2} e^{-y^2/2L^2}$. Recall the Gaussian integrals $\int_{-\infty}^{\infty} e^{-y^2/L^2} dy = L\sqrt{\pi}$ and $\int_{-\infty}^{\infty} y^2 e^{-y^2/L^2} dy = L^3\sqrt{\pi}/2$. So, $\int |\mathbf{H}|^2 = a \int |u|^2 + |v|^2 = aL\sqrt{\pi}[1 + \frac{1}{k^2L^2}]$. Also, $(\nabla + i\mathbf{k}) \times [u(y)\hat{\mathbf{x}} + v(y)\hat{\mathbf{y}}] = -u'\hat{\mathbf{z}} + ik\hat{\mathbf{y}}$. So,

$$|\nabla \times \mathbf{H}|^2 = |(\nabla + i\mathbf{k}) \times \mathbf{H}_{\mathbf{k}}|^2 = |u'|^2 + k^2|v|^2 = k^2 \left[1 + \frac{1}{k^4L^4} \left(1 - \frac{y^2}{L^2} \right) \right] e^{-y^2/L^2}.$$

Then, if we look at our variational criterion, we have two terms: $\int |\nabla \times \mathbf{H}|^2$ and $-\int \Delta \cdot |\nabla \times \mathbf{H}|^2$. The latter is uniformly convergent and goes to $-k^2 \int \Delta$ as $L \rightarrow \infty$, by inspection. Combining the former with the $-k^2 \int |\mathbf{H}|^2$ term in the variational criterion, we get:

$$\begin{aligned} \int |\nabla \times \mathbf{H}|^2 - k^2 \int |\mathbf{H}|^2 &= a \int_{-\infty}^{\infty} k^2 \left[1 + \frac{1}{k^4L^4} \left(1 - \frac{y^2}{L^2} \right) \right] e^{-y^2/L^2} dy - k^2 aL\sqrt{\pi} \left[1 + \frac{1}{k^2L^2} \right] \\ &= a \int_{-\infty}^{\infty} \frac{k^2}{k^4L^4} \left(1 - \frac{y^2}{L^2} \right) e^{-y^2/L^2} dy - \frac{k^2 aL\sqrt{\pi}}{k^2L^2} \\ &= \frac{a}{k^2L^4} L\sqrt{\pi} \left(1 - \frac{L^2}{2L^2} \right) - \frac{a\sqrt{\pi}}{L}, \end{aligned}$$

which goes to zero as $L \rightarrow \infty$. Thus:

$$\int (1 - \Delta) |(\nabla + i\mathbf{k}) \times \mathbf{H}_{\mathbf{k}}|^2 - k^2 \int |\mathbf{H}_{\mathbf{k}}|^2 \rightarrow -k^2 \int_0^a \int_{-\infty}^{\infty} \Delta(x, y) dx dy < 0.$$

as $L \rightarrow \infty$. Q.E.D.

Problem 3: 2d Waveguide Modes

- (a) Maxwell's equations are (in terms of \mathbf{H}) given by the eigen-equation $\nabla \times \frac{1}{\varepsilon} \nabla \times \mathbf{H} = \frac{\omega^2}{c^2} \mathbf{H}$. Suppose that we replace ε by $\alpha\varepsilon$ where α is some constant. By inspection, one obtains the *same* eigensolution \mathbf{H} with ω replaced by $\omega/\sqrt{\alpha}$ (we just divided both sides by α). Thus, scaling epsilon everywhere by a constant just trivially scales the eigenvalues (we could have alternatively rescaled the fields: $\mathbf{H}(\mathbf{x}) \rightarrow \mathbf{H}(\mathbf{x}\sqrt{\alpha})$). Therefore, we can set $\varepsilon_{l_0} = 1$ by simply recalcing ε by $\alpha = 1/\varepsilon_{l_0}$, 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 $-\nabla^2 E_z = \frac{\omega^2}{c^2} \epsilon E_z$, and when we plug in the e^{ikx} form we get:

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

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

- (i) In any region where ϵ is constant, the above equation is solved simply by sines and cosines if $\omega^2 \epsilon - k^2 > 0$ 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 $E_k = A \cos(k_\perp y)$ or $A \sin(k_\perp y)$, where

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

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 ($\omega^2 \epsilon_{lo} < k^2$), we must have exponentials...and requiring the solutions to be finite at infinity we must have $E_k = B e^{-\kappa y}$ for $y > h/2$ and $\pm B e^{\kappa y}$ for $y < -h/2$ (with \pm depending on whether the state is even or odd, where:

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

where we define $f = \epsilon_{lo}/\epsilon_{hi} < 1$ (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 $A \cos(k_\perp h/2) = B e^{-\kappa h/2}$, and continuity of $E'_k \sim H_x$ implies that $-k_\perp A \sin(k_\perp h/2) = -\kappa B e^{-\kappa h/2}$. 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 case. So, there are no imaginary k_\perp solutions, as promised—this means that the guided modes must always be *above* the light line for ϵ_{hi} , which makes physical sense (they must correspond to *propagating* modes in the ϵ_{hi} region and *evanescent* modes in the ϵ_{lo} regions).

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

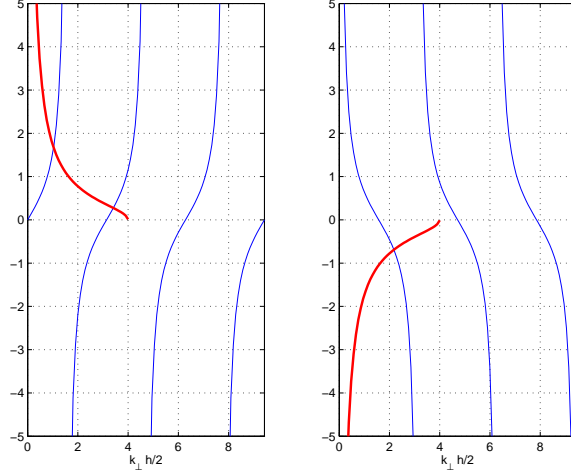


Figure 1: Plot of the two transcendental equations for even modes (left plot) and odd modes (right plot) as a function of $k_{\perp}h/2$. The thick lines show the right hand sides, while the thin lines show the left hand sides (tan or cot) of the equations, and the intersections correspond to guided-mode solutions. This plot is for the particular case of $f = 0.1$ and $kh/2 = 2$.

through zero when $k_{\perp}h/2 + \pi/2$ is an integer multiple of π . Therefore, the number of even modes is simply the number of zero crossings before k_{\perp}^{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 greatest³ 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 $k \rightarrow 0$ 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/ϵ is continuous (since $H'_k \sim D_x = D_{\parallel}$). Thus, for example for the $\cos(k_{\perp}y)$ mode (the *odd* mode, since \mathbf{H} is a pseudovector), we have $-k_{\perp}A \sin(k_{\perp}h/2)/\epsilon_{hi} = -\kappa B e^{-\kappa h/2}/\epsilon_{lo}$. Therefore, both the tan and cot in the transcendental equations get multiplied by $f = \epsilon_{lo}/\epsilon_{hi}$. What effect does this have on the solutions? Multiplying by $f < 1$ *decreases* the tangent curves, but does *not* change the locations of their zeros. Therefore, the *number* of modes at a given k is *unaffected*. However, the intersection point is clearly pulled towards *larger* values

³There 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.

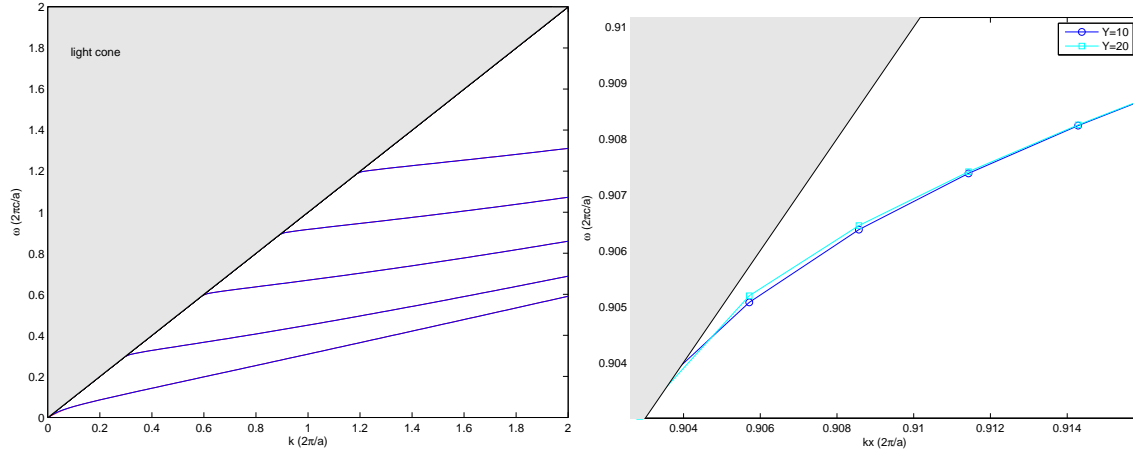


Figure 2: Band diagram (ω vs. k) for five even TM bands of $\epsilon_{hi} = 12$ waveguide structure with thickness $h = a$. *Right*: zoom in on point where band 4 enters the light cone, showing effect of increasing cell size from $Y = 10$ (blue) to $Y = 20$ (red).

of k_{\perp} when the tan/cot is shrunk, which corresponds to *smaller* values of κ , the decay rate. Therefore, the modes are *less* strongly confined for the H_z (TE) polarization. (Later in the class, we will see how this generally follows from the boundary conditions and the variational theorem.)

Problem 4: Numerical computations with MPB

- 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.
- 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`, 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

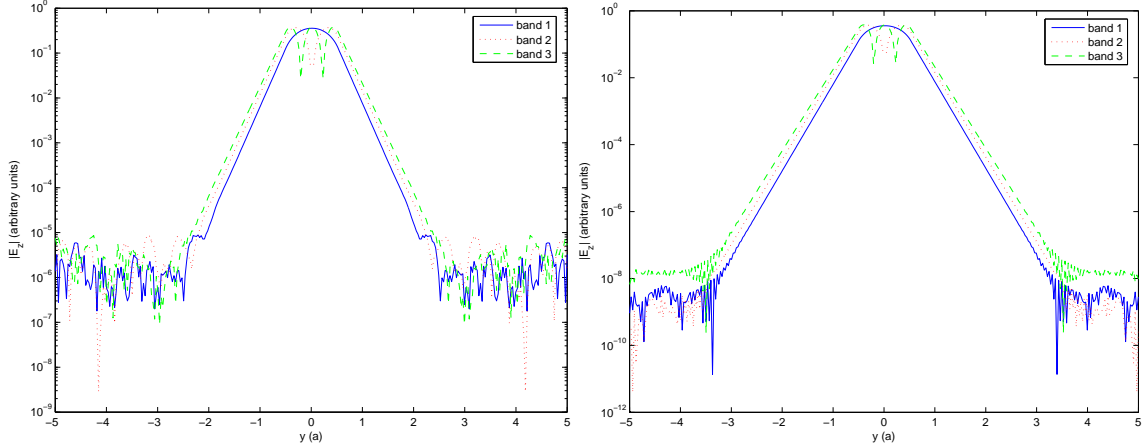


Figure 3: Fields $|E_z|$ for first three even TM modes of $\epsilon_{hi} = 12$ waveguide, for $Y = 10$ cell at $ka/2\pi = 1$, showing exponential decay (straight line on log scale) until “noise floor” caused by finite numerical error in the fields is reached. *Left*: default (10^{-7}) tolerance in MPB. *Right*: decreased (10^{-14}) tolerance in MPB; we can’t decrease the tolerance much further because of floating-point errors.

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 $\epsilon = 2.25$ instead of air on the $y < -h/2$ side, we simply modify the geometry list to:

```
> (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 $\epsilon = 2.25$, 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 $\int \Delta(y) dy = \int (1 - 1/\epsilon) dy = (h/2) \cdot (0.5 - 0.25) > 0$, 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 ω (large λ), we don’t need such

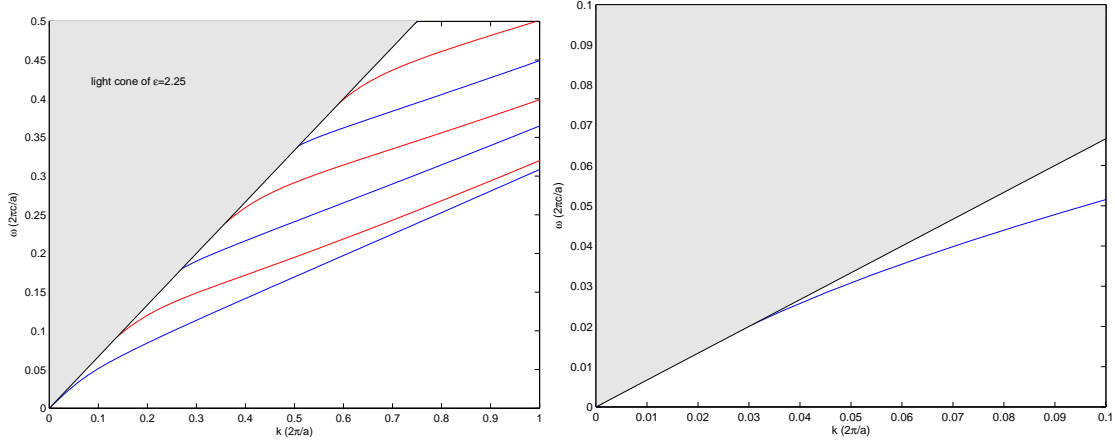


Figure 4: TM (blue) and TE (red) bands of $\epsilon_{hi} = 12$ waveguide with $\epsilon = 2.25$ on one side, which causes a cutoff in the modes. (The light cone here is $\omega \geq ck/\sqrt{2.25}$.) At right is the same band diagram, but zoomed in to show the cutoff for the first TM band, using a larger ($Y = 40$) cell.

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 $k \rightarrow 0$. 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 $k \rightarrow 0$, 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 ω the curve would diverge towards $-\infty$).

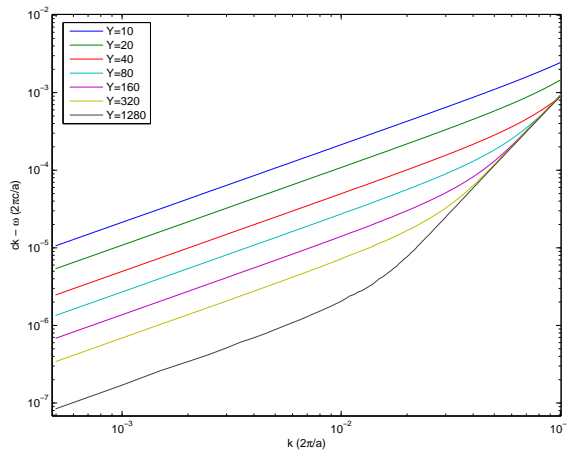


Figure 5: The amount $ck - \omega$ by which the lowest TM mode of the $\epsilon_{hi} = \{2, 0.8\}$ system is below the light line, as a function of k , on a log-log scale (straight line = power law). As we increase the size of the computational cell Y from 10 to 1280, this curve decreases for small k (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.