

18.369 Problem Set 4

Due Friday, April 4 2014.

Problem 1: Perturbation theory

(a) In class, we derived the 1st-order correction in the eigenvalue for an ordinary Hermitian eigenproblem $\hat{O}\psi = \lambda\psi$ for a small perturbation $\Delta\hat{O}$. Now, do the same thing for a *generalized* Hermitian eigenproblem $\hat{A}\psi = \lambda\hat{B}\psi$.

(i) That is, assume we have the solution $\hat{A}^{(0)}\psi^{(0)} = \lambda^{(0)}\hat{B}^{(0)}\psi^{(0)}$ to an unperturbed system (where $\hat{A}^{(0)}$ and $\hat{B}^{(0)}$ are Hermitian, and $\hat{B}^{(0)}$ is positive-definite) and find the first-order correction $\lambda^{(1)}$ when we change *both* \hat{A} and \hat{B} by small amounts $\Delta\hat{A}$ and $\Delta\hat{B}$. You may assume that $\lambda^{(0)}$ is non-degenerate, for simplicity.

(ii) Now, apply this solution to the generalized eigenproblem $\nabla \times \nabla \times \mathbf{E} = \frac{\omega^2}{c^2} \epsilon \mathbf{E}$ for a small change $\Delta\epsilon$, and show that the first-order correction $\Delta\omega$ is the same as the one derived in class using the \mathbf{H} eigenproblem.

(b) Recall the problem of the modes in an $L \times L$ metal box that we solved in class for the H_z (TE) polarization, and which you solved in problem set 2 for the E_z (TM) polarization as $\sin(n\pi x/L)\sin(m\pi y/L)$ for nonzero integers n and m . Originally, this box was filled with air ($\epsilon = 1$). Now, suppose that we increase ϵ by some small constant $\Delta\epsilon$ in a $\frac{L}{2} \times \frac{L}{2}$ square in the *center* of the box (oriented parallel to the metal box). What is the first-order $\Delta\omega$ for the solutions (n,m) equal to $(1,1)$, $(1,2)$, and $(1,3)$? (Note that you have to use degenerate perturbation theory for degenerate modes.)

Problem 2: Band gaps in MPB

Consider the 1d periodic structure consisting of two alternating layers: $\epsilon_1 = 12$ and $\epsilon_2 = 1$, with thicknesses d_1 and $d_2 = a - d_1$, respectively. To help you with this, I've created a sample input file `bandgap1d.ctf` that is posted on the course web page.

(a) Using MPB, compute and plot the fractional TM gap size (of the *first* gap, i.e. lowest ω) vs. d_1 for d_1 ranging from 0 to a . What d_1 gives the largest gap? Compare to the "quarter-wave" thicknesses $d_{1,2} = a\sqrt{\epsilon_{2,1}}/[\sqrt{\epsilon_1} + \sqrt{\epsilon_2}]$

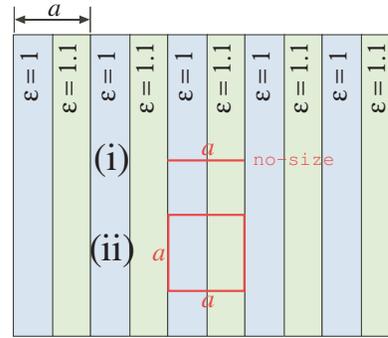


Figure 1: (For problem 3.) Two MPB unit cells for the band structure of a 1d-periodic structure: (i) a 1d $a \times \text{no-size}$ unit cell (ii) a 2d $a \times a$ unit cell.

(see section "size of the band gap" in chapter 4 of the book).

- (b) Given the optimal parameters above, what would be the physical thicknesses in order for the mid-gap vacuum wavelength to be $\lambda = 2\pi c/\omega = 1.55\mu\text{m}$? (This is the wavelength used for most optical telecommunications.)
- (c) Plot the 1d TM band diagram for this structure, with d_1 given by the quarter wave thickness, showing the first five gaps. Also compute it for $d_1 = 0.12345$ (which I just chose randomly), and superimpose the two plots (plot the quarter-wave bands as solid lines and the other bands as dashed). What special features does the quarter-wave band diagram have?

Problem 3: Bands and supercells

Note: this problem does *not* require you to do any numerical calculations in MPB etcetera—it actually appeared on the spring 2007 midterm.

Calvin Q. Luss, a Harvard student, posts to the MPB mailing list that he has discovered a bug in MPB. He writes:

I'm getting ready to do a 2d-crystal calculation, but first I wanted to do a 1d crystal as a test case since I know the band diagram analytically for that (from Yeh's book). I used the structure shown in fig. 1(i), with a 1d computational cell of $a \times \text{no-size} \times \text{no-size}$, and plotted the TM band structure $\omega(k_x)$ (for $\mathbf{k} = (k_x, 0, 0)$ with k_x from 0 to 0.5 in MPB units, i.e. from 0 to π/a)—everything works fine!

Then I do the same calculation but with a computational cell of $a \times a \times \text{no-size}$, as shown in fig. 1(ii), and the result is wrong! I get all sorts of extra bands at bogus frequencies; why doesn't the result match the 1d computation, since the structure hasn't changed? I think it must be a bug; you MIT people obviously don't know what you're doing.

Sketch the plots that Calvin got from his two calculations, and explain why MPB is correctly answering exactly the question that he posed. Sketch at least 4 bands in the 1d calculation, and at least 6 bands in the 2d calculation (not counting degeneracies), and label any bands that are doubly (or more?) degenerate.

(You can use the fact that the ϵ contrast in this case is only 10%—the structure is *nearly* homogeneous—to help you sketch out the bands more quantitatively. But no need to be *too* quantitative, however: you don't need to use perturbation theory or anything like that; a reasonable guess is sufficient.)

Problem 4: Defect modes in MPB

In MPB, you will create a (TM polarized) defect mode by increasing the dielectric constant of a single layer by $\Delta\epsilon$, pulling a state down into the gap. The periodic structure will be the same as the one from problem 2, with the quarter-wave thickness $d_1 = 1/(1 + \sqrt{12})$. To help you with this, I've created a sample input file *defect1d.ctf* that is posted on the course web page.

- When there is *no* defect ($\Delta\epsilon$), plot out the band diagram $\omega(k)$ for the $N = 5$ supercell, and show that it corresponds to the band diagram of problem 2 “folded” as expected.
- Create a defect mode (a mode that lies in the band gap of the periodic structure) by increasing the ϵ of a single ϵ_1 layer by $\Delta\epsilon = 1$, and plot the E_z field pattern. Do the same thing by increasing a single ϵ_2 layer. Which mode is even/odd around the mirror plane of the defect? Why?
- Gradually increase the ϵ of a single ϵ_2 layer, and plot the defect ω as a function of $\Delta\epsilon$ as the frequency sweeps across the gap. At what $\Delta\epsilon$ do you get two defect modes in the gap? Plot the E_z of the second defect mode. (Be careful to increase the size of the supercell for modes near the edge of the gap, which are only weakly localized.)

- The mode must decay exponentially far from the defect (multiplied by an $e^{i\frac{\pi}{a}x}$ sign oscillation and the periodic Bloch envelope, of course). From the E_z field computed by MPB, extract this asymptotic exponential decay rate (i.e. κ if the field decays $\sim e^{-\kappa x}$) and plot this rate as a function of ω , for the first defect mode, as you increase ϵ_2 as above (vary ϵ_2 so that ω goes from the top of the gap to the bottom).

Problem 5: Local Density of States

- In Jackson (*Classical Electrodynamics*), the electric field of a radiating dipole $\mathbf{J}(\mathbf{x}, t) = -i\omega\mathbf{p}\delta(\mathbf{x})e^{-i\omega t}$ at the origin in vacuum is given in spherical coordinates (radius r , radial direction \mathbf{n}), with $k = \omega/c$, as

$$\mathbf{E} = \frac{1}{4\pi\epsilon_0} \left\{ k^2(\mathbf{n} \times \mathbf{p}) \times \mathbf{n} \frac{1}{r} + [3\mathbf{n}(\mathbf{n} \cdot \mathbf{p}) - \mathbf{p}] \left(\frac{1}{r^3} - \frac{ik}{r^2} \right) \right\} e^{i(kr - \omega t)}$$

Note the divergence as $r \rightarrow 0$. The total power radiated by this dipole is computed from the Poynting flux to be $P = \frac{c^2 Z_0 k^4}{12\pi} |\mathbf{p}|^2$, where $Z_0 = \sqrt{\mu_0/\epsilon_0}$. Show that you obtain the *same* P by taking the $r \rightarrow 0$ limit of $-\frac{1}{2}\Re[\mathbf{E}^* \cdot \mathbf{J}]$ (regardless of the direction \mathbf{n} from which you approach the origin). (Taylor expanding e^{ikr} will be helpful.)

- Re-do the derivation, from the notes in class, of relating the LDOS to the power radiated by a dipole source. Now, however, suppose that a small positive imaginary part is added to ϵ somewhere, which shifts all the eigenfrequencies by a small amount $\omega_n \rightarrow \omega_n - i\gamma_n$ ($\gamma_n > 0$).
 - Show that, even for complex ϵ , we still have an orthogonality relationship on the eigenfields \mathbf{E}^n using an *unconjugated inner product* $(\mathbf{E}, \mathbf{E}') = \int \epsilon \mathbf{E} \cdot \mathbf{E}'$. (This is not a true inner product because it may be zero for a nonzero \mathbf{E} , e.g. $\mathbf{E} = (1, i)$. However, this cannot happen if the eigenfunctions \mathbf{E}^n arise from a sufficiently small perturbation of the eigenfunctions of the real-symmetric $\hat{\Theta}$ for which the norm is nonzero.)
 - Assuming that completeness of the eigenfunctions still holds (true for a sufficiently small perturbation), expand the δ function in the LDOS derivation.
 - Show that you obtain a sum of Lorentzians ($\sim 1/[(\omega - \omega_n)^2 + \gamma_n^2]$), one for each

mode, instead of delta functions, if you keep only terms to lowest order in γ_n ($\ll \omega_n$). Show that in the limit $\gamma_n \rightarrow 0$ you recover the delta functions from class (i.e. that the Lorentzians approach functions that are zero except at ω_n , and approach a finite integral with the correct coefficient).