18.369 Problem Set 4

Due Monday, 30 March 2008.

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 $\nabla\times\nabla\times\mathbf{E} = \frac{\omega^2}{c^2}\varepsilon\mathbf{E}$ for a small change $\Delta\varepsilon$, 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 ($\varepsilon = 1$). Now, suppose that we increase ε by some small constant $\Delta\varepsilon$ 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: $\varepsilon_1 = 12$ and $\varepsilon_2 = 1$, with thicknesses d_1 and $d_2 = a - d_1$, respectively. To help you with this, I've created a sample input file *bandgap1d.ctl* 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 $d_{1,2} = a\sqrt{\varepsilon_{2,1}}/[\sqrt{\varepsilon_1}+\sqrt{\varepsilon_2}]$ (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 $\lambda = 2\pi c/\omega = 1.55\mu$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?

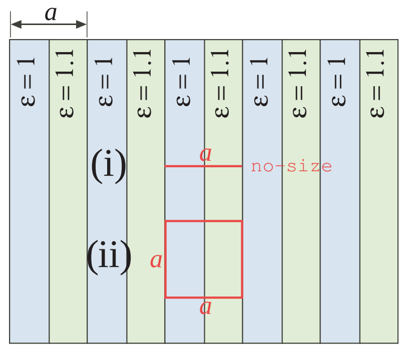

Figure 1: (For problem 3.) Two MPB unit cells for the band structure of a 1d-periodic structure: (i) a 1d $a\times$`no-size` unit cell (ii) a 2d $a\times a$ unit cell.

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 $a\times$`no-size`$\times$`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 $a \times a \times$`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 $\Delta\varepsilon$, 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.ctl* that is posted on the course web page.

(a) When there is *no* defect ($\Delta\varepsilon$), 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.

(b) 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 $\Delta\varepsilon = 1$, 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?

(c) Gradually increase the ε of a single ε_2 layer, and plot the defect ωas a function of $\Delta\varepsilon$ as the frequency sweeps across the gap. At what $\Delta\varepsilon$ 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.)

(d) 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 asympotic 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: Dispersion

Derive the width of a narrow-bandwidth Gaussian pulse propagating in 1d (x) in a dispersive medium, as a function of time, in terms of the dispersion parameter $D = \frac{2\pi c}{v_g^2 \lambda^2} \frac{dv_g}{d\omega} = -\frac{2\pi c}{\lambda^2} \frac{d^2 k}{d\omega^2}$ as defined in class. That is, assume that we have a pulse whose fields can be written in terms of a Fourier transform of a Gaussian distribution:

$$\text{fields} \sim \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-(k-k_0)^2/2\sigma^2} e^{i(kx-\omega t)} dk,$$

with some width σ and central wavevector $k_0 \gg \sigma$. Expand ω to second-order in k around k_0 and compute the inverse Fourier transform to get the spatial distribution of the fields, and define the "width" of the pulse in space as the standard deviation of the $|\text{fields}|^2$. That is, width $= \sqrt{\int (x-x_0)^2 |\text{fields}|^2 dx / \int |\text{fields}|^2 dx}$, where x_0 is the center of the pulse (i.e. $x_0 = \int x |\text{fields}|^2 dx / \int |\text{fields}|^2 dx$).

You should be able to show, as argued in class, that D asymptotically (after a long time, or equivalently for large x_0) gives the pulse spreading in time per unit distance per unit wavelength (bandwidth).

It is helpful to recall some properties of Gaussian functions. Suppose we have the function $F(k) = e^{-k^2/2s^2}$. Its Fourier transform is then $f(x) \sim e^{-x^2 s^2/2}$, with some proportionality constant. Moreover, if we define the width Δx via $\Delta x^2 = \int x^2 |f(x)|^2 dx / \int |f(x)|^2 dx$, then by a standard Gaussian integral this yields $\Delta x = 1/s\sqrt{2}$. If σ is complex, then $|f(x)|^2 \sim e^{-x^2 \Re s^2}$ and we get $\Delta x = 1/\sqrt{2\Re s^2}$ instead.