18.325 Problem Set 3

Due Tuesday, 18 October 2005.

Problem 1: Perturbation theory

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

(i) That is, assume we have the solution $\hat{A}^{(0)}|u^{(0)}\rangle = u^{(0)}\hat{B}^{(0)}|u^{(0)}\rangle$ to an unperturbed system and find the first-order correction $u^{(1)}$ when we change *both* $\hat{A}$ and $\hat{B}$ by small amounts $\Delta\hat{A}$ and $\Delta\hat{B}$. You may assume that $u^{(0)}$ 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 1 for the E_z (TM) polarization. Originally, this box was filled with air ($\varepsilon = 1$). Now, suppose that we increase ε by some small constant $\Delta\varepsilon$ in the lower-left $\frac{L}{2}\times\frac{L}{2}$ corner of the box. What is the first-order $\Delta\omega$ for the first four (lowest ω) modes of the TM polarization? What happens to the degenerate modes?

(c) In class, we calculated the band gap $\Delta\omega$ that appeared in a uniform (1d) material $\varepsilon(x) = \varepsilon_1$ when *half* of the unit cell a was changed to $\varepsilon_1 - \Delta\varepsilon$ for some small $\Delta\varepsilon$, by using perturbation theory. In particular, we derived the gap between the first two bands that appears at $k = \pi/a$, the edge of the Brillouin zone.

(i) Now, you should compute the gap that appears between band 2 and band 3 at $k = 0$, the *center* of the Brillouin zone, to first order. However, do it more generally: assume that the ε_1 region has thickness d_1 and that the $\varepsilon_1 - \Delta\varepsilon$ region has thickness $a - d_1$, repeated with period a, and compute $\Delta\omega$ as a function of d_1.

(ii) At what d_1 values does this gap at $k = 0$ disappear ($\Delta\omega = 0$)? What is $\Delta\omega$ for the quarter-wave stack thicknesses?

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.

(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?

Problem 3: Space group of k

Consider the structure of problem 2. What are the symmetry operations of its space group? How are these reduced (if at all) if we consider $\hat{\Theta}_k$—that is, what is the space group as a function of k? In class, when we derived the band gap, we took the modes at $k = \pi/a$ to be of even/odd (cos/sin) form; why was this justified?

Give an example of a 1d periodic structure in which the modes at $k = \pi/a$ are *not* even or odd. Is the band diagram of this structure still symmetric (i.e. $\omega(-k) = \omega(k)$)?

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) Via first-order perturbation theory, derive an *exact* expression for the rate of change $\frac{d\omega}{d(\Delta\varepsilon)}$ of the defect-mode frequency ω of a single defect layer $\varepsilon_2 + \Delta\varepsilon$ layer, as $\Delta\varepsilon$ is changed. Your expression should be in terms of the eigenfield $\mathbf{E}$ of the localized defect state at the current $\Delta\varepsilon$. Verify your formula numerically by showing, at a couple of different values of $\Delta\varepsilon$, that it correctly predicts the slope of your ω vs. $\Delta\varepsilon$ curve above. (Note that you can export $\mathbf{E}$ to Matlab and compute the necessary integrals there or, for the Scheme lovers among you, you can compute the integral directly in MPB using the compute-energy-in-objects or compute-field-integral function.)

(e) Is there a minimum $\Delta\varepsilon$ (of an ε_2 layer) to create a defect mode, or is a defect mode localized even for infinitesimal $\Delta\varepsilon$? Support your conjecture[1] with numerical evidence. (Don't forget that, like in problem set 2, as the mode becomes less localized you must increase the computational cell size. Another thing to be careful about is how accurately you know the location of the gap edge—compute the gap edge using the same resolution as you are using to compute the defect, and you may need to increase both resolutions.)

(f) 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).

[1] In mathematics, we never merely "guess." We conjecture, or perhaps we postulate an ansatz.