18.369 Problem Set 4

Problem 1: Perturbation theory

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 $\hat{A}\psi = \lambda\hat{B}\psi$.

(a) 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.

(b) 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 (and given in chapter 2 of the book) using the $\mathbf{H}$ eigenproblem.

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 Jupyter notebook *pset4.ipynb* that is posted on the course web page. You should modify this notebook, and **turn in a PDF** (via *print to PDF* from your browser) of the modified notebook (showing all plots and calculations) **along with your solutions**.

(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 $\lambda = 2\pi c/\omega = 1.55\mu\text{m}$? (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: Defect modes in MPB

In MPB, you will create a (TM polarized) defect mode by increasing the dielectric constant of a single ε_1 layer by $\Delta\varepsilon$, pulling a state down into the gap. The periodic structure will be the same as the one from problem 4 from pset 3, with the quarter-wave thickness $d_1 = 1/(1+\sqrt{12})$. To help you with this, I've created a sample input file *pset4.ipynb* that is posted on the course web page. You should modify this notebook, and **turn in a PDF** (via *print to PDF* from your browser) of the modified notebook (showing all plots and calculations) **along with your solutions**.

(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 ω as 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).