

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 $\nabla \times \nabla \times \mathbf{E} = \frac{\omega^2}{c^2}\epsilon\mathbf{E}$ for a small change $\Delta\epsilon$, and show that the first-order correction $\Delta\omega$ is the same as the one derived in class (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: $\epsilon_1 = 12$ 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 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 $d_{1,2} = a\sqrt{\epsilon_{2,1}}/[\sqrt{\epsilon_1} + \sqrt{\epsilon_2}]$ (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 $\Delta\epsilon$, pulling a state down into the gap. The periodic structure will be the same as the one from problem 2 above 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 ($\Delta\epsilon$), 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.
- (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 $\Delta\epsilon = 1$, 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?
- (c) 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.)
- (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 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).