18.369 Mathematical Methods in Nanophotonics Spring 2008

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Figure 1: (a) Hexagonal cavity surrounded by perfect-metal walls. (b) Schematic of a function f(x, y) which = 1 in the highlighted region of the cavity and = 0 elsewhere.

18.369 Mid-term Exam

You have two hours. Notice that **all problems have equal weight**, so don't spend too much time on one problem at the expense of the others.

Problem 1: Hexagons (30 points)

Suppose that we have a hexagonal cavity filled with $\varepsilon = 1$ and surrounded by perfectly conducting walls, as shown in fig. 1(i).

- (a) List the symmetry operations and conjugacy classes, and give the character table of this symmetry group ($C_{\rm 6V}$).
- (b) Suppose that we have a function f(x, y) which is 1 in a small region as shown in fig. 1(ii), and zero elsewhere. Using the projection operator, write f(x, y) as a sum of partner functions of the irreducible representations of C_{6V}, by sketching the partner functions [similar to the sketch in fig. 1(ii)].
- (c) Now, suppose that we perturb the cavity by partially filling it with one of various (concentric) dielectric shapes, as shown in fig. 2: (i) a hexagon rotated by 30°; (ii) a hexagon rotated by 15°; (iii) a square (parallel to two sides of the hexagon); and (iv) an equilateral triangle (parallel to three sides of the hexagon). In which of these perturbed cavities would you expect some eigenmodes to have non-accidental degeneracies, and why?



Figure 2: Hexagonal cavity partially filled with dielectric perturbations of various shapes.

Problem 2: Band Diagrams (30 points)

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 quarter-wave stack shown in fig. 3(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. 3(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 out 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



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

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 3: Operators (30 points)

First, recall a few fact derived in class. We know that the time-harmonic electromagnetic field $\mathbf{H}(\mathbf{x})e^{-i\omega t}$ satisfies a Hermitian eigenproblem (for real $\varepsilon > 0$)

$$\nabla \times \frac{1}{\varepsilon(\mathbf{x})} \nabla \times \mathbf{H} = \hat{\Theta} \mathbf{H} = \frac{\omega^2}{c^2} \mathbf{H}, \qquad (1)$$

and this leads to the usual consequences of real ω , orthogonal **H**, etc. You also derived in homework that if $\varepsilon(p, \mathbf{x})$ is also a function of some parameter p, then $d\omega/dp$ is given *exactly* via first-order perturbation theory, in terms of the electric field $\mathbf{E} = \frac{i}{\omega\varepsilon} \nabla \times \mathbf{H}$, by:

$$\frac{d\omega}{dp} = -\frac{\omega}{2} \frac{\int \frac{\partial\varepsilon}{\partial p} |\mathbf{E}|^2}{\int \varepsilon |\mathbf{E}|^2},$$
(2)

where the integrals are over all space (or the unit cell, for a periodic structure).

Now, suppose that $\varepsilon(p, \mathbf{x}, \omega)$ is a function of frequency (the material is *dispersive*) as well as of space and *p*, although for every ω we assume ε is real and positive. Equation (1) *still* holds, but it is no longer an eigenproblem *per se*—the operator $\hat{\Theta}$ now depends upon the "eigenvalue" ω , and the equation must be solved self-consistently for ω and **H**. In this case, answer you these questions two, ere your troubles here are through:

- (a) Which of the following properties of Hermitian eigenproblems is still true of the self-consistent equation $\hat{\Theta}(\omega)\mathbf{H} = \frac{\omega^2}{c^2}\mathbf{H}$, and why? [No need to repeat every detail of proofs given in class; just explain clearly why they do or do not apply here.]
 - (i) ω is real
 - (ii) the solutions H can be chosen to transform as irreducible representations of the space group
 - (iii) for two solutions **H** and **H'** corresponding to frequencies ω and ω' , respectively, then $\omega \neq \omega'$ implies that $\int \mathbf{H}^* \cdot \mathbf{H}' = 0$.
- (b) Derive an expression for $d\omega/dp$ in terms of E, analogous to eq. (2) [but it won't be identical!]. Hint: note that you get a $\Delta \varepsilon$ both from the direct change in Δp and also indirectly from the change $\Delta \omega \approx \frac{d\omega}{dp} \Delta p$.