18.369 Problem Set 5 Solutions

Problem 1: Group Velocity and Material Dispersion (20 points)

First, little bit of background info (you were not required to show this):

- We now technically have a “nonlinear eigenproblem” $\hat{\Theta}_k(\omega)\mathbf{H}_k = \omega^2\mathbf{H}_k$, in which the eigen-operator $\hat{\Theta}_k$ depends on the eigenvalue $\omega^2$. But if $\epsilon(\omega)$ is still real, $\hat{\Theta}_k$ is still Hermitian. Our proof of real eigenvalues and positive-definiteness still work, so $\omega$ is still real. (But our proof of orthogonality of eigenfunctions no longer works, since eigenfunctions at distinct eigenvalues now have different operators $\hat{\Theta}_k$.)

- The derivation of first-order perturbation theory (from which we got $d\omega/dk$) carries through exactly as before, except that you now need to include an additional perturbation $\frac{\partial \hat{\Theta}_k}{\partial \omega} \Delta \omega$ in the operator due to the change in the eigenvalue. This is what gives us the “chain rule” term you were asked to include in $d\omega/dk$.

With that in mind, let’s go ahead and solve the problem. As in class, we’ll just set $c = \epsilon_0 = \mu_0 = 1$ so that we don’t have to deal with all of those annoying SI constant factors. (The book does it in SI units if you are curious.)

The derivation of group velocity is the same as in class, except that there is now an extra term in the numerator of the Hellman-Feynman theorem. In class, we dealt with the partial derivatives like when we first derived perturbation theory (we get $\frac{\partial}{\partial \omega} \hat{\Theta}_k \mathbf{H}_k$). Now we have an additional term $\frac{\partial \hat{\Theta}_k}{\partial \omega} \mathbf{v}_g$. The $\frac{\partial \hat{\Theta}_k}{\partial \omega}$, however is precisely what we would get for a $\Delta \epsilon = \frac{d\epsilon}{d\omega} \mathbf{v}_g$ perturbation like when we first derived perturbation theory (we get $-\frac{\partial \epsilon}{\partial \omega} \nabla \times \mathbf{H}^2 = -\omega^2 \Delta \epsilon |\mathbf{E}|^2$). Therefore, this term of the numerator becomes $-\frac{\partial \epsilon}{\partial \omega} \int (\mathbf{E}, \frac{d\epsilon}{d\omega} \mathbf{v}_g) \mathbf{E}$. In short, we have exactly the expression from class with the addition of this new term:

$$\mathbf{v}_g = \frac{1}{2\omega} \frac{4\omega}{\frac{1}{2} \int (|\mathbf{H}|^2 + \epsilon |\mathbf{E}|^2)} \frac{\int S - \omega \mathbf{v}_g \int |\mathbf{E}|^2 \frac{d\epsilon}{d\omega}}{\frac{1}{2} \int (|\mathbf{H}|^2 + \epsilon |\mathbf{E}|^2)}.$$ 

(Note that, in the denominator, we have used (as in class) the fact that $\int |\mathbf{H}|^2 = \int \epsilon |\mathbf{E}|^2$, which is still true for dispersive media—our derivation from class only relied on $\nabla \times \mathbf{E} = \frac{i}{c} \mathbf{H}$ and $\nabla \times \mathbf{H} = -\frac{i}{c} \mathbf{E}$.) Now, however, we have $\mathbf{v}_g$ on both sides of the equation, so we must solve for it, and obtain:

$$\mathbf{v}_g = \frac{1}{4} \frac{\int S}{\int (|\mathbf{H}|^2 + \epsilon |\mathbf{E}|^2 + \omega \frac{d\epsilon}{d\omega} |\mathbf{E}|^2)} \frac{\int S}{\frac{1}{4} \int \left[|\mathbf{H}|^2 + d\omega(\epsilon) \right] |\mathbf{E}|^2}.$$ 

as desired: the Poynting flux divided by the Brillouin energy density of a lossless dispersive medium, both time-averaged and averaged over the unit cell.


Problem 2: Fabry-Perot waveguides (10+10 points)

(a) Here, we modified bandgap1d.ctl to vary $k_y$ by setting the k-points variable as:

```plaintext
(define-param k-interp 30)
(define-param ky 0)
(define-param k-y-max 2)
(set! k-points (interpolate k-interp (list (vector3 ky 0) (vector3 ky ky-max))))
```

In figure 1 we show the TM projected band diagram for $k_y$ from 0.0 to 0.5 in steps of 0.1 (in units of
Figure 1: TM projected band diagram, vs. $k_y$ for $\varepsilon = 12/2.25$ quarter-wave stack along the $x$ direction. $k_x$ varies from 0 (red) to $\pi/a$ (blue), and the region corresponding to intermediate $k_x$ values is shaded gray. The light line of air ($\omega = c k_y$) is shown as a thick black line.

2$\pi/a$). We also shade (in gray) the region from $k_x = 0.0$ to $k_x = 0.5$ (the red and blue lines), and it is clear that all of the intermediate $k_x$ values do indeed lie between these two curves.

(b) Here, the defect1d.ctl file is modified similarly to the bandgap1d.ctl file to use $\varepsilon_2 = 2.25$ and to compute the bands as a function of $k_y$. (Since it is a supercell, we just use a fixed $k_x = 0$, as $k_x$ should become irrelevant as the supercell size grows.)

Changing a single $\varepsilon_2$ layer by $\Delta \varepsilon = 4$, the resulting TM band diagram is shown in figure 2, overlaid on top of the shaded regions from the previous problem. Most of the bands fall into the shaded regions, corresponding to extended modes. A few discrete guided bands lie within the open regions, however, corresponding to waveguided modes. There are both gap-guided modes, within the band gaps, and a couple of index-guided modes, which lie below the lowest continuum regions. The latter may come as something of a surprise, since our defect still has lower $\varepsilon$ than the $\varepsilon = 12$ layers, but you can think of them in the same sense as “surface states” associated with the $\varepsilon = 12$ layers next to the defect—it is the combination of the defect and the adjacent $\varepsilon = 12$ layers that supports the index-guided modes, which are asymptotically localized just in the $\varepsilon = 12$ layers.

(Note that there are some bands just slightly at the edge of the shaded region. This is due simply to numerical error—finite resolution and supercell size—which causes the extended modes to have slightly different frequencies in defect1d.ctl compared to bandgap1d.ctl.)
Figure 2: TM projected band diagram for $\Delta \varepsilon_2 = 4$ Fabry-Perot defect mode as a function of the $k_y$ (parallel to the quarter-wave stack, which has period $a$).