18.369 Mathematical Methods in Nanophotonics
Spring 2008

18.325 Problem Set 4

Problem 1: Group velocity and material dispersion

Suppose that we have a dispersive medium with some frequency-dependent dielectric constant $\varepsilon(\omega)$. (We still assume $\varepsilon(\omega) > 0$ and real, however.[1]) In this case, our eigen-equation becomes a "self-consistent" equation $\hat{\Theta}|H\rangle = \frac{\omega^2}{c^2}|H\rangle$, since the eigen-operator $\hat{\Theta}$ depends on the eigenvalue ω.

(a) Explain why ω is still real, and why first-order perturbation theory (and thus the Hellman-Feynman theorem) still holds for such a self-consistent Hermitian eigen-like problem. Give a property of Hermitian eigen problems that is *not* true any longer for the self-consistent problem.

(b) Apply the Hellman-Feynman theorem to the self-consistent problem $\hat{\Theta}_{\mathbf{k}}|H_{\mathbf{k}}\rangle = \frac{\omega^2}{c^2}|H_{\mathbf{k}}\rangle$ in order to get an expression for the group velocity $\mathbf{v}_g = \frac{d\omega}{d\mathbf{k}}$. Note that you will have to use the chain rule, because varying $\mathbf{k}$ causes $\hat{\Theta}_{\mathbf{k}}$ to change directly and it also causes ε to change due to the change in ω: $\frac{d\hat{\Theta}_{\mathbf{k}}}{d\mathbf{k}} = \frac{\partial\hat{\Theta}_{\mathbf{k}}}{\partial\mathbf{k}} + \frac{\partial\hat{\Theta}}{\partial\varepsilon} \cdot \frac{d\varepsilon}{d\omega} \cdot \mathbf{v}_g$.

(c) Show that your $\mathbf{v}_g$ is the ratio of mean flux to mean energy density, where the energy density is now the "dispersive" energy density $\frac{1}{8\pi}\left(\frac{d(\omega\varepsilon)}{d\omega}|\mathbf{E}|^2 + |\mathbf{H}|^2\right)$, as derived e.g. in Jackson (*Classical Electrodynamics*).

Problem 2: Dispersion

Derive the width of a narrow-bandwidth Gaussian pulse propagating in 1d (x) in a dispersive medium, as a function of time, in terms of the dispersion parameter $D = \frac{2\pi c}{v_g^2\lambda^2}\frac{dv_g}{d\omega} = -\frac{2\pi c}{\lambda^2}\frac{d^2k}{d\omega}$ as defined in class. That is, assume that we have

a pulse whose fields can be written in terms of a Fourier transform of a Gaussian distribution:

$$\text{fields} \sim \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-(k-k_0)^2/2\sigma^2}e^{i(kx-\omega t)},$$

with some width σ and central wavevector $k_0 \gg \sigma$. Expand ω to second-order in k around k_0 and compute the inverse Fourier transform to get the spatial distribution of the fields, and define the "width" of the pulse in space as the standard deviation of the $|\text{fields}|^2$. That is,

$$\text{width} = \sqrt{\int (x-x_0)^2|\text{fields}|^2 dx / \int |\text{fields}|^2 dx},$$

where x_0 is the center of the pulse (i.e. $x_0 = \int x|\text{fields}|^2 dx / \int |\text{fields}|^2 dx$).

Problem 3: Projected band diagrams and omni-directional reflection

Starting with the bandgap1d.ctl MPB control file from problem set 3, which computes the frequencies as a function of k_x. Modify it to compute the frequencies as a function of k_y for some range of k_y (e.g. 0 to 2, in units of $2\pi/a$ ... recall that the k_y Brillouin zone is infinite!) for some fixed value of k_x, and to use $\varepsilon_2 = 2.25$ instead of 1.[2]

(a) Compute and plot the TM projected band diagram for the quarter-wave stack with ε of 12 and 2.25. That is, plot $\omega(k_y)$ for several bands, first with $k_x = 0$, then $k_x = 0.1$, then 0.2, then ... then 0.5, and interpolate intermediate k_x to shade in the "continuum" regions of the projected bands. Verify that the extrema of these continua lie at either $k_x = 0$ or $k_x = 0.5$ (in units of $2\pi/a$), i.e. at the B.Z. edges.

(b) Compute and plot the TE projected band diagram as well.

(c) Find the size $\Delta\omega/\omega_{\text{mid}}$ of the range of omni-directional reflection (from an interface with air). Vary the layer thicknesses d_1 or d_2 slightly and see how the size of the omni-directional gap changes...do the quarter-wave thicknesses lead to the maximum omni-directional gap?

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[1] Strictly speaking, any dispersive ε must be complex to satisfy causality (see e.g. Jackson, *Classical Electrodynamics*, or Google "Kramers-Kronig relations"), but for weak dispersion we can neglect the absorption loss (imaginary part) to a first approximation.

[2] You might want to add a "kx" parameter via "(define-param kx 0)" so that you can change k_x from the command line with "mpb kx=0.3 ...".

Problem 4: Fabry-Perot Waveguides

Modify the MPB defect1d.ctl file from problem set 3 to compute the defect mode as a function of k_y (for $k_x = 0$).

(a) Changing a single ε_2 layer by $\Delta\varepsilon = 4$, with an $N = 20$ supercell, plot the first 80 bands as a function of k_y for some reasonable range of k_y. Overlay your TM projected band diagram from problem 3, above, to show that the bands fall into two categories: modes that fall within the projected "continuum" regions from problem 3, and discrete guided bands that lie within the empty spaces. (If there are any bands *just* outside the *edge* of the continuum region, increase the supercell size to check whether those bands are an artifact of the finite size.) Plot the fields for the guided bands (a couple of nonzero k_y points will do) to show that they are indeed localized.

(b) Modify the structure and plot the new band diagram(s) (if necessary) to give examples of:

  (i) "index-guided" bands that do not lie within a band gap

  (ii) a band in the gap that intersects a continuum region

  (iii) a band in the gap that asymptotically approaches, but does not intersect, the continuum regions