# 18.369 Problem Set 3

Due Monday, 12 March 2007.

#### **Problem 1: Variational Theorem**

Suppose that we have a generalized Hermitian eigenproblem  $\hat{A} |\psi\rangle = \lambda \hat{B} |\{\rangle \psi\}$  on some Hilbert space  $|\psi\rangle$  with  $\hat{A}^{\dagger} = \hat{A}$ ,  $\hat{B}^{\dagger} = \hat{B}$ , and  $\hat{B}$  positive-definite.

- (a) In class, during our "quick and dirty" proof of the variational theorem, we relied on the fact that a weighted average  $\sum w_n x_n / \sum w_n$ for  $w_n \ge 0$  is always between min  $x_n$  and max  $x_n$ . Prove this (hint: use induction on the number of terms in the sum).
- (b) Derive the variational theorem via the "quick and dirty" method as in class: assuming a complete basis of eigenstates  $|n\rangle$  with eigenvalues  $\lambda_n$ , show that  $\lambda_{\min} \leq F\{|\psi\rangle\} \leq \lambda_{\max}$  for some functional  $F\{|\psi\rangle\}$  and the minimum and maximum eigenvalues (if any)  $\lambda_{\min}$  and  $\lambda_{\max}$ . (For example, if  $\hat{B} = 1$  then we have an ordinary eigenproblem, and  $F\{|\psi\rangle\} = \langle \psi | \hat{A} | \psi \rangle / \langle \psi | \psi \rangle$  as in class.)
- (c) Without using completeness, show that extrema of your functional  $F\{|\psi\rangle\}$  only occur when  $|\psi\rangle$  is an eigenstate of the generalized eigenproblem. Do this by the using property that, at an extremum  $|\psi\rangle$ , the functional must be *stationary*: that is, if we add any small  $|\delta\psi\rangle$  to  $|\psi\rangle$  at an extremum, the change  $F\{|\psi\rangle + |\delta\psi\rangle\} - F\{|\psi\rangle\}$  is zero to first order in  $|\delta\psi\rangle$ . You should be able to show that this stationary condition implies that  $|\psi\rangle$  satisfies the eigen-equation.
- (d) Assume that we have a periodic structure  $\varepsilon$  and therefore the electric field **E** can be chosen in the form of a Bloch mode  $\mathbf{E} = e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\mathbf{E}_{\mathbf{k}}(\mathbf{x})$  for some Bloch wavevector  $\mathbf{k}$ , where  $\mathbf{E}_{\mathbf{k}}(\mathbf{x})$  is periodic. Use the variational theorem for the generalized eigenproblem, which you derived above, to write an expression the minimum eigenvalue  $\omega_{\min}(\mathbf{k})$  as the minimum of some space of possible periodic field patterns  $\mathbf{E}_{\mathbf{k}}$ .

### Problem 2: Guided modes in periodic waveguides

In class, we showed by a variational proof that any  $\varepsilon(y)$ , in two dimensions, gives rise to at least one guided mode whenever  $\varepsilon(y)^{-1} = \varepsilon_{lo}^{-1} - \Delta(y)$ for  $\int \Delta > 0$  and  $\lim_{y \to \pm \infty} \Delta(y) = 0$ . At least, we showed it for the TE polarization (**H** in the  $\hat{\mathbf{z}}$  direction). Now, you will show the same thing much more generally, but using the same basic technique.

- (a) Let  $\varepsilon(x, y)^{-1} = 1 \Delta(x, y)$  be a periodic function  $\Delta(x, y) = \Delta(x + a, y)$ , with  $\Delta$  going to zero at  $y \to \pm \infty$  and  $\int_0^a \int_{-\infty}^\infty \Delta(x, y) dx dy > 0$ . Prove that at least one TE guided mode exists, by choosing an appropriate (simple!) trial function of the form  $\mathbf{H}(x, y) = u(x, y) e^{ikx} \hat{\mathbf{z}}$ . That is, show by the variational theorem that  $\omega^2 < ck^2$  for the lowest-frequency eigenmode. (It is sufficient to show it for  $|k| < \pi/a$ , by periodicity in k-space.)
- (b) Prove the same thing as in (a), but for the TM polarization (**E** in the  $\hat{\mathbf{z}}$  direction). Hint: you will need to pick a trial function of the form  $\mathbf{H}(x, y) = [u(x, y)\hat{\mathbf{x}} + v(x, y)\hat{\mathbf{y}}]e^{ikx}$ where u and v are some (simple!) functions such that  $\nabla \cdot \mathbf{H} = 0.^1$

### Problem 3: 2d Waveguide Modes

Consider the two-dimensional dielectric waveguide of thickness h that we first introduced in class:

$$\varepsilon(y) = \begin{cases} \varepsilon_{hi} & |y| < h/2 \\ \varepsilon_{lo} & |y| \ge h/2 \end{cases}$$

where  $\varepsilon_{hi} > \varepsilon_{lo}$ . Look for solutions with the "TM" polarization  $\mathbf{E} = E_z(x, y)\hat{\mathbf{z}}e^{-i\omega t}$ . The boundary conditions are that  $E_z$  is continuous and  $\partial E_z/\partial y \ (\sim H_x)$  is continuous, and that we require the fields to be finite at  $x, y \to \pm \infty$ ,

(a) Prove that we can set  $\varepsilon_{lo} = 1$  without loss of generality, by a change of variables in

<sup>&</sup>lt;sup>1</sup>You might be tempted, for the TM polarization, to use the **E** form of the variational theorem that you derived in problem 1, since the proof in that case will be somewhat simpler: you can just choose  $\mathbf{E}(x,y) = u(x,y)e^{ikx}\hat{\mathbf{z}}$  and you will have  $\nabla \cdot \varepsilon \mathbf{E} = 0$  automatically. However, this will lead to a slightly weaker condition  $\int (\varepsilon - 1) > 0$  instead of  $\int \Delta = \int \frac{\varepsilon - 1}{\varepsilon} > 0$ .

Maxwell's equations. In the subsequent sections, therefore, set  $\varepsilon_{lo} = 1$  for simplicity.

- (b) Find the guided-mode solutions  $E_z(x, y) = e^{ikx}E_k(y)$ , where the corresponding eigenvalue  $\omega(k) < ck$  is below the light line.
  - (i) Show for the |y| < h/2 region the solutions are of sine or cosine form, and that for |y| > h/2 they are decaying exponentials.
  - (ii) Match boundary conditions ( $E_z$  and  $H_x$  are continuous) at  $y = \pm h/2$  to obtain an equation relating  $\omega$  and k. You should get a transcendental equation that you cannot solve explicitly. However, you can "solve" it graphically and learn a lot about the solutions in particular, you might try plotting the left and right hand sides of your equation (suitably arranged) as a function of  $k_{\perp} = \sqrt{\frac{\omega^2}{c^2}} \varepsilon_{hi} - k^2$ , so that you have two curves and the solutions are the intersections.
  - (iii) From the graphical picture, derive an exact expression for the number of guided modes as a function of k. Show that there is exactly one guided mode, with even symmetry, as  $k \to 0$ , as we argued in class.

## Problem 4: Numerical computations with MPB

For this problem, you will gain some initial experience with the MPB numerical eigensolver described in class, and which is available on Athena in the meep locker. Refer to the class handouts, and also to the online MPB documentation at jdj.mit.edu/mpb/doc. For this problem, you will study the simple 2d dielectric waveguide (with  $\varepsilon_{hi} = 12$ ) that you analyzed analytically above, along with some variations thereof start with the sample MPB input file (2dwaveguide.ctl) that was introduced in class and is available on the course web page.

(a) Plot the TM  $(E_z)$  even modes as a function of k, from k = 0 to a large enough k that you get at least four modes. Compare where these modes start being guided (go below the light line) to your analytical prediction from problem 1. Show what happens to this "crossover point" when you change the size of the computational cell.

- (b) Plot the fields of some guided modes on a log scale, and verify that they are indeed exponentially decaying away from the waveguide. (What happens at the computational cell boundary?)
- (c) Modify the structure so that the waveguide has  $\varepsilon = 2.25$  instead of air on the y < -h/2side. Show that there is a low- $\omega$  cutoff for the TM guided bands, as we argued in class, and find the cutoff frequency.
- (d) Create the waveguide with the following profile:

$$\varepsilon(y) = \begin{cases} 2 & 0 \le y < h/2 \\ 0.8 & -h/2 < y < 0 \\ 1 & |y| \ge h/2 \end{cases}.$$

Should this waveguide have a guided mode as  $k \to 0$ ? Show numerical evidence to support your conclusion (careful: as the mode becomes less localized you will need to increase the computational cell size).