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18.369 Mathematical Methods in Nanophotonics
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18.325 Problem Set 2

Problem 1: Variational Theorem

Suppose that we have a (possibly infinite dimensional) Hermitian operator \hat{O} operating on some Hilbert space $\{|\psi\rangle\}$, and consider the Rayleigh quotient $\langle\psi|\hat{O}|\psi\rangle/\langle\psi|\psi\rangle$. Show that the minimum of this quotient (or, indeed, any extremum) occurs if and only if $|\psi\rangle$ is an eigenstate of \hat{O} . Do this by the using property that, at an extremum $|\psi\rangle$, the quotient must be *stationary*: that is, if we add any small $|\delta\psi\rangle$ to $|\psi\rangle$ at an extremum, the change in the Rayleigh quotient 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.

Problem 2: 2d Waveguide Modes

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

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

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 $x, y \rightarrow \pm\infty$,

- (a) Prove that we can set $\varepsilon_{lo} = 1$ without loss of generality, by a change of variables in 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 at $y = \pm h/2$ to obtain an equation relating ω 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 $k_\perp = \sqrt{\frac{\omega}{c^2}^2 \varepsilon_{hi} - k^2}$, 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 $k \rightarrow 0$, as we argued in class.
- (iv) If you look at the H_z polarization, how do your equations change? (Hint: the boundary conditions from Maxwell’s equations are that \mathbf{H} is continuous, the components \mathbf{E}_\parallel parallel to a dielectric interface is continuous, and the components $\mathbf{D}_\perp = \varepsilon\mathbf{E}_\perp$ perpendicular to a dielectric interface are continuous.) How is the number of guided modes affected at each k ? How about the strength of the confinement (i.e. the exponential decay rate)?

Problem 3: Conservation Laws

- (a) Suppose that introduce a nonzero current $\mathbf{J}(\mathbf{x})e^{-i\omega t}$ into Maxwell’s equations at a given frequency ω , and we want to find the resulting time-harmonic electric field $\mathbf{E}(\mathbf{x})e^{-i\omega t}$ (i.e. we are only looking for fields that arise from the current, with $\mathbf{E} \rightarrow 0$ as $|\mathbf{x}| \rightarrow \infty$ if \mathbf{J} is localized). Show that this results in a linear equation of the form $\hat{A}|E\rangle = |b\rangle$, where \hat{A} is some linear operator and $|b\rangle$ is some known right-hand side in terms of the current density \mathbf{J} .
 - (i) Prove that, if \mathbf{J} transforms as some irreducible representation of the space group then $|E\rangle$ ($= \mathbf{E}$, which you can assume is a unique solution) does also. (This is the analogue of the conservation in *time* that we showed in class, except that now we are proving it in the frequency domain. You could prove it by Fourier-transforming the theorem from class, but do *not* do so—instead, prove it directly from the linear equation here.)

- (ii) Formally, $|E\rangle = \hat{A}^{-1}|b\rangle$, where \hat{A}^{-1} is related to the *Green's function* of the system. What happens if ω is one of the eigenfrequencies?
- (b) Let \hat{U}_t be our time-evolution operator, and we have some space group G of symmetry operators \hat{O}_g ($g \in G$) such that $[\hat{U}_t, \hat{O}_g] = 0$. Now, suppose that we have some state $|\psi(t)\rangle$ that at one time transforms as purely one representation and at a later time transforms as some *other* representation (or some superposition of representation), violating the conservation theorem we proved in class. Show that this implies that \hat{U}_t is a *nonlinear* operator (i.e. it depends on the amplitude of the state). (In class, we implicitly assumed that our operators were linear).¹

Problem 4: Cylindrical symmetry

Suppose that we have a *cylindrical* metallic waveguide—that is, a perfect metallic tube with radius R , which is uniform in the z direction. The interior of the tube is simply air ($\epsilon = 1$).

- (a) This structure has continuous rotational symmetry around the z axis, called the C_∞ group.² Find the irreducible representations of this group (there are infinitely many because it is an infinite group).
- (b) For simplicity, consider the (Hermitian) *scalar* wave equation $-\nabla^2\psi = \frac{\omega^2}{c^2}\psi$ with $\psi|_{r=R} = 0$. Show that, when we look for solutions ψ that transform like one of the representations of the C_∞ group from above, and have z dependence e^{ikz} (from the translational symmetry), then we obtain a Bessel equation (Google it if you've forgotten Mr. Bessel). Write the solutions in terms of Bessel functions, assuming that you are given their zeros $x_{m,n}$ (i.e. $J_m(x_{m,n}) = 0$ for $n = 1, 2, \dots$, where J_m is the Bessel function of the first kind...if you Google for “Bessel function zeros” you can

¹A famous example of this in optics is *third-harmonic generation*. If we have a nonlinear $\epsilon \sim |\mathbf{E}|^2$, we can start with a planewave at (ω, \mathbf{k}) and generate another wave at $(3\omega, 3\mathbf{k})$.

²It also has an infinite set of mirror planes containing the z axis, but let's ignore these for now. If they are included, the group is called $C_{\infty v}$.

find them tabulated). Sketch the dispersion relation $\omega(k)$ for a few bands.

- (c) From the general orthogonality of Hermitian eigenfunctions, derive an orthogonality integral for the Bessel functions.

Problem 5: 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 MIT Server in the mpb locker. Refer to the class handouts, and also to the online MPB documentation at jdl.mit.edu/mpb/doc. For this problem, you will study the simple 2d dielectric waveguide (with $\epsilon_{hi} = 12$) 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 $\epsilon = 2.25$ instead of air on the $y < -h/2$ side. Show that there is a low- ω cutoff for both TM and TE guided bands, as we argued in class, and find the cutoff frequency.
- (d) Create the waveguide with the following profile:

$$\epsilon(y) = \begin{cases} 2 & 0 \leq y < h/2 \\ 0.8 & -h/2 < y < 0 \\ 1 & |y| \geq h/2 \end{cases} .$$

Should this waveguide have a guided mode as $k \rightarrow 0$? Show numerical evidence to support your conclusion (careful: as the mode

becomes less localized you will need to increase the computational cell size).