18.369 Mathematical Methods in Nanophotonics Spring 2008

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18.325 Problem Set 1

Problem 1: Adjoints and operators

- (a) We defined the adjoint \dagger of states and operators by: $\langle H_1 | H_2 \rangle = |H_1\rangle^{\dagger} |H_2\rangle$ and $\langle H_1 | \hat{O} | H_2 \rangle = (\hat{O}^{\dagger} | H_1 \rangle)^{\dagger} |H_2\rangle$. Show that for a *finite-dimensional* Hilbert space, where $|H\rangle$ is a column vector h_n $(n = 1, \dots, d)$, \hat{O} is a square $d \times d$ matrix, and $\langle H^{(1)} | H^{(2)} \rangle$ is the ordinary conjugated dot product $\sum_n h_n^{(1)*} h_n^{(2)}$, the above adjoint definition corresponds to the conjugate-transpose for both matrices and vectors.
- (b) Show that if Ô is simply a number o, then Ô[†] = o^{*}. (This is not the same as the previous question, since Ô here can act on infinitedimensional (continuous) spaces.)
- (c) If a linear operator \hat{O} satisfies $\hat{O}^{\dagger} = \hat{O}^{-1}$, then the operator is called **unitary**. Show that a unitary operator preserves inner products (that is, if we apply \hat{O} to every element of a Hilbert space, then their inner products with one another are unchanged). Show that the eigenvalues u of a unitary operator have unit magnitude (|u| = 1) and that its eigenvectors can be chosen to be orthogonal to one another.
- (d) For a non-singular operator \hat{O} (i.e. \hat{O}^{-1} exists), show that $(\hat{O}^{-1})^{\dagger} = (\hat{O}^{\dagger})^{-1}$. (Thus, if \hat{O} is Hermitian then \hat{O}^{-1} is also Hermitian.)

Problem 2: Completeness

- (a) Prove that the eigenvectors |n⟩ of a finitedimensional Hermitian operator Ô (a d × d matrix) are complete: that is, that any ddimensional vector can be expanded as a sum ∑_n c_n |n⟩ in the eigenvectors with some coefficients c_n. It is sufficient to show that there are d linearly independent eigenvectors |n⟩:
 - (i) Show that every $d \times d$ Hermitian matrix O has at least one nonzero eigenvector $|1\rangle$

(... use the fact that every polynomial with nonzero degree has at least one (possibly complex) root).

- (ii) Show that the space of V₁ = {|v⟩ | ⟨v|1⟩ = 0} orthogonal to |1⟩ is preserved (transformed into itself or a subset of itself) by Ô. From this, show that we can form a (d 1) × (d 1) Hermitian matrix whose eigenvectors (if any) give (via a similarity transformation) the remaining (if any) eigenvectors of O.
- (iii) By induction, form an orthonormal basis of d eigenvectors for the d-dimensional space.
- (b) Suppose that we have an *infinite*-dimensional Hermitian operator Ô that can be simulated on a computer (with arbitrary, but finite, memory and time): its solutions can be approximated to arbitrary accuracy by a finite-dimensional Hermitian operator (e.g. Ô discretized on a finite grid). Argue that the infinite-dimensional eigenvectors form a complete basis for anything that we care about; can you give an example of a sense in which they do *not* form a complete basis?¹
- (c) Completeness is not automatic for eigenvectors in general. Give an example of a non-singular non-Hermitian operator whose eigenvectors are not complete. (A 2 × 2 matrix is fine. This case is also called "defective.")

Problem 3: Maxwell eigenproblems

(a) In class, we eliminated E from Maxwell's equations to get an eigenproblem in H alone, of the form Ô |H⟩ = ω²/c² |H⟩. Show that if you instead eliminate H, you cannot get a Hermitian eigenproblem in E except for the trivial case ε = constant. Instead, show that you get a generalized Hermitian eigenproblem of the form |E⟩ = ω²/c² B̂ |E⟩, where both and B̂ are Hermitian operators.

 $^{^{1}}$ For a more precise discussion of the completeness of continous Hermitian operators, see e.g. Courant & Hilbert, *Methods of Mathematical Physics* vol. 1.

- (b) For any generalized Hermitian eigenproblem where \hat{B} is positive definite (i.e. $\langle E|\hat{B}|E\rangle > 0$ for all $|E\rangle \neq 0^2$), show that the eigenvalues are real and that different eigenvectors $|E_1\rangle$ and $|E_2\rangle$ satisfy a modified kind of orthogonality. Show that \hat{B} for the **E** eigenproblem above was indeed positive definite.
- (c) Show that both the $|E\rangle$ and $|H\rangle$ formulations lead to generalized Hermitian eigenproblems with real ω if we allow magnetic materials $\mu(\mathbf{x}) \neq 1$ (but require μ real, positive, and independent of \mathbf{H} or ω).
- (d) μ and ϵ are only ordinary numbers for *isotropic* media. More generally, they are 3×3 matrices (technically, rank 2 tensors)—thus, in an *anisotropic medium*, by putting an applied field in one direction, you can get dipole moment in different direction in the material. Show what conditions these matrices must satisfy for us to still obtain a generalized Hermitian eigenproblem in **E** (or **H**) with real eigen-frequency ω .

Problem 4: Projection operators

The representation-theory handout gives a formula for the projection operator from a state onto its component that transforms as a particular representation. Prove the correctness of this formula (using the Great Orthogonality Theorem).

Problem 5: Symmetries of a field in a metal box

In class, we considered a two-dimensional (xy) problem of light in an $L \times L$ square of air $(\varepsilon = 1)$ surrounded by perfectly conducting walls (in which $\mathbf{E} = 0$). We solved the case of $\mathbf{H} = H_z(x, y)\hat{\mathbf{z}}$ and saw solutions corresponding to three different representations of the symmetry group $(C_{4\mathbf{V}})$.

- (a) Solve for the eigenmodes of the other polarization: $\mathbf{E} = E_z(x, y)\hat{\mathbf{z}}$ (you will need the \mathbf{E} eigenproblem from above), with the boundary condition that $E_z = 0$ at the metal walls.
 - (i) Sketch and classify the solutions according to the representations of C_{4V} enumerated in class.
- (b) Consider the solutions in a triangular box with side L. Don't try to solve this analytically; instead, use symmetry to sketch out what the possible solutions will look like for both E_z and H_z polarizations.
 - (i) List the symmetry operations in the space group (choose the origin at the center of the triangle so that the space group is symmorphic), and break them into conjugacy classes. (This group is traditionally called C_{3V}). Verify that the group is closed under composition (i.e. that the composition of two operations always gives another operation in the group) by giving the "multiplication table" of the group (whose rows and columns are group members and whose entries give their composition).
 - (ii) Find the character table of C_{3V} , using the rules from the representation-theory hand-out.
 - (iii) Give unitary representation matrices D for each irreducible representation of C_{3V} .
 - (iv) Sketch possible $\omega \neq 0$ E_z and H_z solutions that would transform as these representations. What representation should the lowest- ω mode (excluding $\omega = 0$) of each polarization correspond to? If there are any (non-accidental) degenerate modes, show how given one of the modes we can get the other orthogonal eigenfunction(s) (e.g. in the square case we could get one from the 90° rotation of the other for a degenerate pair).

²Here, when we say $|E\rangle \neq 0$ we mean it in the sense of generalized functions; loosely, we ignore isolated points where **E** is nonzero, as long as such points have zero integral, since such isolated values are not physically observable. See e.g. Gelfand and Shilov, *Generalized Functions*.