

Figure 1: Electric fields  $(E_z)$  of eigenmodes inside a 2d metal box. Blue/white/red indicate positive/zero/negative fields.

# 18.369 Problem Set 2 Solutions

### **Problem 1: Projection operators**

Consider the action of  $\hat{P}_i^{(\alpha)}$  on a partner function  $\phi_j^{(\alpha')}$ , as defined in the handout. We obtain  $\hat{P}_i^{(\alpha)}\phi_j^{(\alpha')} = \frac{d_{\alpha}}{|G|}\sum_{g\in G} D_{ii}^{(\alpha)}(g)^* \hat{O}_g \phi_j^{(\alpha')} = \frac{d_{\alpha}}{|G|}\sum_{g\in G} D_{ii}^{(\alpha)}(g)^* [\sum_{i'} \phi_{i'}^{(\alpha')} D_{i'j}^{(\alpha')}(g)]$ . If we perform the  $\sum_g$  first, then from the Great Orthogonality Theorem we get  $\sum_{i'} \delta_{ii'} \delta_{ij} \delta_{\alpha\alpha'} \phi_{i'}^{(\alpha')} = \delta_{ij} \delta_{\alpha\alpha'} \phi_i^{(\alpha)}$ . Thus, for a state  $\psi = \sum_{\alpha} \sum_i c_i^{(\alpha)} \phi_i^{(\alpha)}$  decomposed into partner functions (as proved in class),  $\hat{P}_i^{(\alpha)} \psi = c_i^{(\alpha)} \phi_i^{(\alpha)}$ . Q.E.D.

### Problem 2: Symmetries of a field in a square metal box

(a) For  $\mathbf{E} = E_z(x, y)\hat{\mathbf{z}}$  in air ( $\varepsilon = 1$ ), we get  $\nabla \times \nabla \times \mathbf{E} = -\nabla^2 E_z \hat{\mathbf{z}} = \frac{\omega^2}{c^2} E_z$ . The solutions of this are sines and cosines, and to satisfy the  $E_z = 0$  boundary conditions at x = 0, L and y = 0, L we must have:

$$E_z = A \sin\left(\frac{n\pi}{L}x\right) \sin\left(\frac{m\pi}{L}y\right)$$

where n and m are positive integers and A is an amplitude. The corresponding frequency is  $\omega = c \frac{\pi}{L} \sqrt{n^2 + m^2}$ . This solutions are plotted in Figure 1 for the first few values of n and m.

- (b) Since E is a vector, we can treat  $E_z$  as an ordinary scalar field here (no funny -1 factors under reflections). Therefore, from the field plots we can see that n = m = 1 (and, in fact, any n = m =odd) transforms as  $\Gamma_1$  (the trivial representation) and n = m = 2 (and any n = m = even) transforms as  $\Gamma_4$  (even with diagonal mirror planes and odd with horizontal/vertical mirrors). Any  $n \neq m$  state is (at least) doubly degenerate (with the (m, n) state), such as the (n, m) = (2, 1) and (1, 2) states shown in Fig. 1. There are three cases:
  - (i) If n is even and m is odd or vice versa, e.g. (n,m) = (2,1), then it transforms as  $\Gamma_5$ .
  - (ii) If both n and m are odd, e.g. (n, m) = (3, 1), then it forms a 2×2 reducible representation with (m, n). To decompose it into irreducible representations, we just take the sum and difference of the two eigenmodes. The (n, m)+(m, n) state transforms as Γ<sub>1</sub>, and (n, m)-(m, n) transforms as Γ<sub>3</sub>. This is shown in the left two panels of Fig. 2.
  - (iii) If both n and m are even, e.g. (n, m) = (4, 2), then it again forms a  $2 \times 2$  reducible representation with (m, n). The (n, m) + (m, n) state transforms as  $\Gamma_4$ , and (n, m) (m, n) transforms as  $\Gamma_2$ . This is shown in the right two panels of Fig. 2.



Figure 2: Electric fields  $(E_z)$  of eigenmodes inside a 2d metal box for accidentally degenerate (n, m) states  $n \neq m$ . By forming linear combinations as shown, we can create eigenmodes which transform as, from left to right:  $\Gamma_1$ ,  $\Gamma_3$ ,  $\Gamma_4$ , and  $\Gamma_2$ . Blue/white/red indicate positive/zero/negative fields.

#### Problem 3: Symmetries of a field in a triangular metal box

Now we consider the solutions in a *triangular* box with side L.

(a) The different symmetry operations in the space group of a triangle are shown in Figure 3 : three mirror planes  $\sigma$ , and counter-clockwise rotation  $C_3$  by 120° (and also  $C_3^{-1}$ , clockwise rotation), and of course the identity *E*. There are three conjugacy classes: {*E*}, { $\sigma_1, \sigma_2, \sigma_3$ }, and { $C_3, C_3^{-1}$ }. This is because  $\sigma_3 = C_3^{-1}\sigma_1C_3$ ,  $\sigma_2 = C_3\sigma_1C_3^{-1}$ , and  $C_3^{-1} = \sigma_1C_3\sigma_1$ . The multiplication table of the group is:

0	E	$C_3$	$C_3^{-1}$	$\sigma_1$	$\sigma_2$	$\sigma_3$
E	E	$C_3$	$C_{3}^{-1}$	$\sigma_1$	$\sigma_2$	$\sigma_3$
$C_3$	$C_3$	$C_{3}^{-1}$	E	$\sigma_3$	$\sigma_1$	$\sigma_2$
$C_{3}^{-1}$	$C_3^{-1}$	E	$C_3$	$\sigma_2$	$\sigma_3$	$\sigma_1$
$\sigma_1$	$\sigma_1$	$\sigma_2$	$\sigma_3$	E	$C_3$	$C_{3}^{-1}$
$\sigma_2$	$\sigma_2$	$\sigma_3$	$\sigma_1$	$C_{3}^{-1}$	E	$C_3$
$\sigma_3$	$\sigma_3$	$\sigma_1$	$\sigma_2$	$C_3$	$C_{3}^{-1}$	E

(b) The character table of  $C_{3v}$  must have only three representations since there are three classes, and the sum of the squares of the dimensions must equal 6 (the number of elements in the group). From this, the only possibility is for the representations to have dimensions 1, 1, and 2 (this gives the first column of the table). The first row must be the trivial representation, and by applying the orthogonality relations we get the other two rows:

	E	$2C_3$	$3\sigma$
$\Gamma_1$	1	1	1
$\Gamma_2$	1	1	-1
$\Gamma_3$	2	-1	0

where  $\Gamma_{1\dots 3}$  are traditional names for these three representations.

we get:					
E	$C_3$	$C_{3}^{-1}$	$\sigma_1$	$\sigma_2$	$\sigma_3$
x	$(-x+y\sqrt{3})/2$	$(-x-y\sqrt{3})/2$	$(-x-y\sqrt{3})/2$	$(-x+y\sqrt{3})/2$	x

and therefore if we operate the  $\Gamma_3$  projection operator  $\hat{P}^{(3)} = \frac{2}{6} \overline{(2\hat{O}_E - \hat{O}_{C_3} - \hat{O}_{C_3^{-1}})}$  on  $f(\mathbf{x}) = x$  we



Figure 3: Symmetries of  $C_{3v}$  (triangle symmetries): three mirror planes  $\sigma$ , and rotation  $C_3$  by 120°.

get simply x—thus, the function x must itself be a partner function for  $\Gamma_3$  and no other representation. Moreover, the operation of the space group on x is clearly spanned by the orthogonal functions x and y, and so we must have a representation given simply by the  $2 \times 2$  rotation matrices that transform the functions  $\{x, y\}$ :

E	$C_3$	$C_{3}^{-1}$	$\sigma_1$	$\sigma_2$	$\sigma_3$
$\left(\begin{array}{cc}1&0\\0&1\end{array}\right)$	$\begin{array}{ccc} \frac{1}{2} \left( \begin{array}{cc} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{array} \right) \end{array}$	$ \begin{array}{c c} \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \end{array} $	$\begin{array}{ccc} \frac{1}{2} \left( \begin{array}{cc} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{array} \right) \end{array}$	$ \begin{array}{c c}                                    $	$\left(\begin{array}{cc}1&0\\0&-1\end{array}\right)$
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where to get  $\sigma_1$  and  $\sigma_2$  we used  $\sigma_1 = \sigma_3 C_3$  and  $\sigma_2 = \sigma_3 C_3^{-1}$  from the multiplication table above. The unitarity of these matrices follows immediately from the fact that they come from the 2 × 2 rotation matrices, and can be easily verified in any case. Their traces clearly match those in the character table.

(d)  $E_z$  field patterns that transform as these representations are very crudely sketched in Figure 4, where + and - denote maxima and minima of the field. Note that because **E** is a vector, the component  $E_z$  transforms as an ordinary scalar in the xy plane, and "even" and "odd" fields are what we expect; note also that the boundary conditions require  $E_z$  to go to zero at the edges of the triangle, so all extrema must lie in the interior. The  $\Gamma_3$  mode must be doubly degenerate, of course, and can be chosen so that one mode is even with respect to a *single* one of the mirror planes and the other mode is odd with respect to that mirror plane, as shown. (For example, in our  $\{x, y\}$  representation matrices above, this even/odd plane was  $\sigma_3$ , although of course the modes could be rotated to be even/odd around any of the three  $\sigma$ 's.) From the representation matrices, we can see that one degenerate partner may be found by operating  $(\hat{O}_{C_3} - \hat{O}_{C_3^{-1}})/\sqrt{3}$  on the other—i.e., by the difference of its 120° and  $-120^\circ$  rotations (this will give an *orthogonal* mode because it will have opposite even-odd symmetry under one of the mirror planes). The lowest-order  $E_z$  mode should be  $\Gamma_1$  (fewest nodes  $\rightarrow$  smallest  $\nabla^2$  term in eigenproblem). A less crude sketch would be to show contours of the field as in class, but in lieu of that I opted to show you an exact numerical calculation of the first few eigenmodes of this



Figure 4: Sketch of possible  $E_z$  field patterns (for the lowest- $\omega$  modes of each symmetry) in the triangular cavity corresponding to the three representations. Note that a  $\Gamma_3$  mode must be doubly degenerate with two field patterns roughly as shown.



Figure 5:  $E_z$  field plots of first few lowest- $\omega$  modes in a triangular air cavity surrounded by metal (black) with side L, from a numerical calculation. The corresponding frequencies  $\omega L/2\pi c$  (and representations) are, from left to right: 1.16 ( $\Gamma_1$ ), 1.78 ( $\Gamma_3$ ), 2.32 ( $\Gamma_1$ ), 2.60 ( $\Gamma_3$ ), 2.93 ( $\Gamma_3$ ), and 3.08 ( $\Gamma_2$ ). Note that the second, fourth, and fifth modes (from left) are doubly degenerate (their degenerate partner is not shown, but can be found by subtracting 120° and  $-120^\circ$  rotations of the field). (Slight asymmetries in the  $\Gamma_2$  state are due to the finite computational grid resolution.)

cavity, in Figure. 5, which illustrates all three representations (note that the lowest  $\omega$  mode of each representation looks much like our "guess"). The lowest frequency mode of  $E_z$  transforms like  $\Gamma_1$  because that has the fewest oscillations (only a single extremum).

The  $H_z$  field sketches, in Figure 6, are somewhat different, for two reasons. First, **H** is a pseudovector, so  $H_z$  transforms as a pseudo-scalar and our normal conceptions of "even" and "odd" are reversed. Second, because of the boundary conditions the extrema of  $H_z$  tend to occur on the boundaries of the triangle, at least for the low- $\omega$  modes. So, for example, now the  $\Gamma_1$  mode looks *odd* with respect to all of the mirror planes, and will only appear for higher- $\omega$  modes. The  $\Gamma_2$  mode is the one that looks most symmetric, but because the extrema lie on the boundaries there will tend to be a minima in the center of the triangle for the lowest- $\omega$  mode. The lowest-order  $H_z$  mode should be  $\Gamma_3$ , since it has the fewest nodal planes. The corresponding numerical calculations are shown in Figure 7. Here, the least-oscillatory (lowest- $\omega$ ) mode corresponds to  $\Gamma_3$ , with only two extrema. Note that the numerical  $\Gamma_1$  mode is higher-order (each of our sketched extrema is split into two) than our cartoon (I couldn't find any lower-order  $\Gamma_1$  modes, and I'm not quite sure why...).

(e) We want an operation on one partner function that gives us the other (with some sign/coefficient), i.e. which corresponds to a matrix of the form  $\begin{pmatrix} 0 & \pm 1 \\ \pm 1 & 0 \end{pmatrix}$ . By inspection of the  $\Gamma_3$  representation matrices from (c), there are several ways to get a matrix of this form. For example,  $(E + 2C_3)/\sqrt{3}$  or (more symmetrically)  $(C_3 - C_3^{-1})/\sqrt{3}$ , or  $(\sigma_1 - \sigma_2)/\sqrt{3} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ . That means, if we have a solution  $\psi$  corresponding to one of the degenerate partner functions of  $\Gamma_3$ , then, for example,  $(\hat{O}_{\sigma_1} - \hat{O}_{\sigma_2})\psi/\sqrt{3}$  gives us the other orthogonal partner function.

### **Problem 3: Cylindrical symmetry**

(a) If D is a representation where D(φ) is the matrix corresponding to rotation by an angle φ around the z axis, then we must have D(φ + Δφ) = D(φ)D(Δφ) by definition of representations (rotating by Δφ followed by φ is exactly the same as rotating by φ + Δφ). Therefore, as we derived in class for the translation group (which had the same property), the representations must all be of the form D<sup>(m)</sup>(φ) = e<sup>-imφ</sup> where m is some number characterizing the representation (k in class). For the translation group, this number was a completely arbitrary real number (it could even be complex, if we allowed divergent representations). Here, however, we have a further constraint: rotation by 2π must be the same as doing nothing, and therefore we must have D(2π) = 1 for D to represent the group. This implies that m is an integer (so that e<sup>-i2πm</sup> = 1).



Figure 6: Sketch of possible  $H_z$  field patterns (for low- $\omega$  modes) in the triangular cavity corresponding to the three representations. Note that a  $\Gamma_3$  mode must be doubly degenerate with two field patterns roughly as shown.



Figure 7:  $H_z$  field plots of the lowest- $\omega$  mode for each irreducible representation of  $C_{3v}$  in a triangular air cavity surrounded by metal (black) with side L, from a numerical calculation. The corresponding frequencies  $\omega L/2\pi c$  (and representations) are, from left to right: 0.66 ( $\Gamma_3$ ), 1.14 ( $\Gamma_2$ ), and 3.01 ( $\Gamma_1$ ). Note that the leftmost mode is doubly degenerate (its degenerate partner is not shown, but can be found by subtracting  $120^\circ$  and  $-120^\circ$  rotations of the field). (Slight asymmetries in the  $\Gamma_1$  state are due to the finite computational grid resolution.) There are 8 modes (not shown) with frequencies between 0.66 and 1.74.

Note, by the way, that you might be tempted to form  $2 \times 2$  representation matrices via the ordinary (x, y) rotation  $R = \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix}$ , but this is reducible:  $R = \exp \begin{pmatrix} 0 & i\phi \\ -i\phi & 0 \end{pmatrix}$ , which can be diagonalized into  $1 \times 1$  representations  $e^{\pm i\phi}$ .

(b) If ψ(r, φ, z) transforms like D<sup>(m)</sup>, then rotating by θ (sending ψ(r, φ, z) → ψ(r, φ - θ, z)) must be just multiplication by e<sup>-imθ</sup>. This means that ψ must be of the form ψ<sub>m</sub>(r, z)e<sup>imφ</sup>. Since we further have translational symmetry in z, we must have ψ = ψ<sub>mk</sub>(r)e<sup>imφ+ikz</sup>. That is, we now have a one-dimensional function and should obtain a one-dimensional Hermitian eigenproblem in r.

If we plug this  $\psi$  into  $-\nabla^2 \psi = \frac{\omega^2}{c^2} \psi$ , we can apply the form of  $\nabla^2$  in cylindrical coordinates and obtain:

$$-\psi_{km}'' - \frac{1}{r}\psi_{km}' + (\frac{1}{r^2}m^2 + k^2)\psi_{km} = \frac{\omega^2}{c^2}\psi_{km},$$

where primes denote differentiation by r, which after a slight rearrangement becomes:

$$r^2\psi_{km}'' + r\psi_{km}' + (k_{\perp}^2r^2 - m^2)\psi_{km} = 0,$$

where  $k_{\perp}^2 = \frac{\omega^2}{c^2} - k^2$ . Now, make a change of variables:  $x = k_{\perp}r$ ,  $y(x) = \psi_{km}(x/k_{\perp})$ , and we find:

$$x^{2}y'' + xy' + (x^{2} - m^{2})y = 0,$$

which is precisely Bessel's equation of order m. The solutions of this are  $J_m(x)$  and  $Y_m(x)$ , the Bessel functions of the first and second kinds. However,  $Y_m(x)$  diverges at x = 0, which we can't allow (physical wave solutions can't blow up in empty space). So, the eigensolution must by  $y(x) = J_m(x)$  (choosing an arbitrary amplitude of 1), and thus

$$\psi(r,\phi,z) = J_m(k_\perp r)e^{im\phi + ikz}.$$

We're not done yet, because we haven't found  $k_{\perp}$ . This is determined by the boundary condition  $\psi|_{r=R} = 0$ . That means we must have  $J_m(k_{\perp}R) = 0$ , or  $k_{\perp}^{(n)} = x_{m,n}/R$  where the  $x_{m,n}$  are the



Figure 8: The first few bands of the scalar wave equation in a cylindrical waveguide. Plotted are lowest four bands for m = 0 (blue),  $m = \pm 1$  (thick red), and  $m = \pm 2$  (dashed green). Also, shown, for reference, is the light line  $\omega = ck$  of air (all modes lie above this and are therefore extended in the air core).

zeros of  $J_m$ . Solving for  $\omega$  from  $k_{\perp}$ , we finally get a discrete sequence of bands:

$$\omega_{mk}^{(n)}(k) = c\sqrt{k^2 + \left(\frac{x_{m,n}}{R}\right)^2}.$$

Note, moreover, that  $J_{-m} = J_m$ , and therefore the bands for  $m \neq 0$  are *doubly degenerate* (this actually also follows from mirror symmetry). To sketch the bands, we can choose dimensionless units (c = 1, R = 1), and the result is shown in figure 8.

(c) The  $\psi_{mk}(r)e^{im\phi+kz}$  must be orthogonal  $(\int \psi_1^*\psi_2 r \, dr \, d\phi \, dz = 0$  for eigenfunctions of different eigenvalues) since they are eigenfunctions of a Hermitian operator. For two different m and k values, they are orthogonal since  $\int e^{i(m_1-m_2)\phi} d\phi = 0$  for  $m_1 \neq m_2$  (which follows from group theory since they correspond to different representations). For the same m, we must have that the r integral is zero, and hence, changing variables to u = r/R, we have:

$$\int_0^1 J_m(x_{m,n}u) \cdot J_m(x_{m,n'}u) \, u \, du = 0$$

for different zeros  $n \neq n'$ . (This is a well-known identity that is used in Fourier-Bessel series expansions.)

## **Problem 5: Conservation Laws**

(a) A current J modifies Ampere's law:  $\nabla \times \mathbf{H} = \frac{4\pi}{c} \mathbf{J} - i \frac{\omega}{c} \varepsilon \mathbf{E}$  (where we have cancelled the  $e^{-i\omega t}$  time-dependence in every term). Therefore, when we take Faraday's law  $\nabla \times \mathbf{E} = i \frac{\omega}{c} \mathbf{H}$  and operate  $\nabla \times$  on both sides, we get

$$(\nabla \times \nabla \times -\frac{\omega^2}{c^2}\varepsilon)\mathbf{E} = 4\pi i \frac{\omega}{c^2} \mathbf{J}.$$

This is indeed of the form  $\hat{A}\mathbf{E} = \mathbf{b}$ , where  $\hat{A} = \nabla \times \nabla \times -\frac{\omega^2}{c^2}\varepsilon$  is a linear operator and  $\mathbf{b} = 4\pi i \frac{\omega}{c^2} \mathbf{J}$  is a given right-hand side.

- (b) Suppose that E solves ÂE = b, and that b transforms as some representation α of the space group. Therefore, P̂<sup>(α)</sup>b = b, where P̂<sup>(α)</sup> = d<sub>α</sub>/|C| Σ<sub>g</sub> χ<sup>(α)</sup>(g)\*Ô<sub>g</sub> is the projection operator for that representation. Moreover, by definition of the space group we must have [Â, Ô<sub>g</sub>] = 0 for any g in the space group. Since is linear, and P̂<sup>(α)</sup> is merely a linear combination of the Ô<sub>g</sub>'s, then [Â, Ô<sub>g</sub>] = 0 (∀g) ⇒ [Â, P̂<sup>(α)</sup>] = 0. Therefore ÂE = b = P̂<sup>(α)</sup>b = P̂<sup>(α)</sup>ÂE = ÂP̂<sup>(α)</sup>E, and thus Â(1 P̂<sup>(α)</sup>)E = 0. Therefore, either E transforms as α (P̂<sup>(α)</sup>E = E), or the component of E that doesn't transform as α lies in the null space of —that is, Â is singular and we didn't have a unique solution E in the first place.
- (c) If  $\omega$  is one of the eigenfrequencies, then  $\hat{A}$  is singular— $\hat{A}$  operating on an eigenstate  $\mathbf{E}_0$  will give zero by definition (since it is the generalized eigenequation as you derived in problem set 1). In a finite system (i.e. compact support, not necessarily finite-dimensional), then physically you can get a divergent (non-harmonic) solution, exactly like the case where you drive a harmonic oscillator at the resonant frequency. Alternatively, if J is orthogonal to the eigenstate  $E_0$  (e.g. they are partner functions of different representations), then there will be a solution, but it won't be unique because you can add any multiple of  $\mathbf{E}_0$  while satisfying the equation (although one could easily impose some additional condition to make it unique). In an infinite system, the question is more subtle because the eigenstate in question (if it is an extended mode) can have infinitesimal overlap with  $\mathbf{J}$  (if  $\mathbf{J}$  is localized). In this case, you can get a finite response, but to make it unique you have to impose some additional boundary conditions. The classic example of this is a localized antenna source (e.g. a dipole) in vacuum –vacuum has eigenmodes (planewaves) at every  $\omega$  ( $\omega = c |\mathbf{k}|$ ), but the resulting field is a finite-amplitude spherical wave(s) emanating from the antenna, not a divergence (except at the antenna itself, if J itself diverges as for a point source). To get a unique solution, however, we have to impose a boundary condition that there are no incoming waves from infinity (which would satisfy Maxwell's equations, but wouldn't be very physical). Hopefully, we will get a chance to discuss such Green's functions in greater depth later in the course.