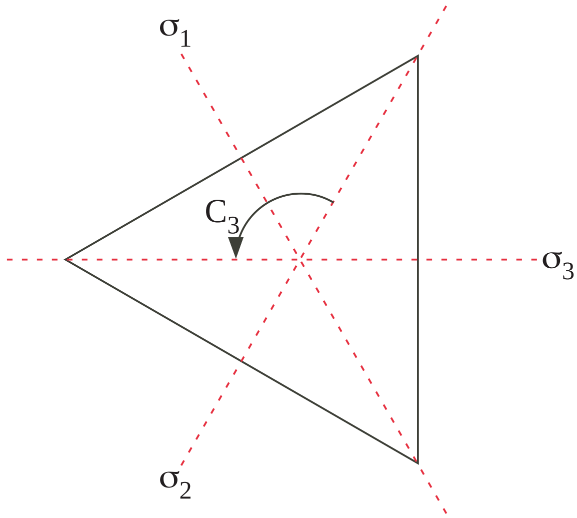

Figure 1: Symmetries of C_{3v} (triangle symmetries): three mirror planes σ, and rotation C_3 by 120°.

18.369 Problem Set 5 Solutions

Problem 3: A triangular metal box (5+5+5+5+5pts)

Consider the two-dimensional solutions in a *triangular* perfect-metal box with side L.

(a) The different symmetry operations in the space group of a triangle are shown in Figure 1 : three mirror planes σ, 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 $\sigma_3 = C_3^{-1}\sigma_1 C_3$, $\sigma_2 = C_3\sigma_1 C_3^{-1}$, and $C_3^{-1} = \sigma_1 C_3 \sigma_1$. The multiplication table of the group is:

$\circ$	E	C_3	C_3^{-1}	σ_1	σ_2	σ_3
E	E	C_3	C_3^{-1}	σ_1	σ_2	σ_3
C_3	C_3	C_3^{-1}	E	σ_3	σ_1	σ_2
C_3^{-1}	C_3^{-1}	E	C_3	σ_2	σ_3	σ_1
σ_1	σ_1	σ_2	σ_3	E	C_3	C_3^{-1}
σ_2	σ_2	σ_3	σ_1	C_3^{-1}	E	C_3
σ_3	σ_3	σ_1	σ_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	$2C_3$	3σ
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	-1	0

where $\Gamma_{1\ldots3}$ are traditional names for these three representations.

(c) For Γ_1 and Γ_2, the representations are one-dimensional and are therefor simply numbers equal to the characters in the character table (± 1, from above). For Γ_3, we must first construct partner functions. Let's guess $f(\mathbf{x}) = x$. If we then operate the different group elements on this, recalling the coordinates rotated counter-clockwise by an angle θ are multiplied by the 2×2 matrix $\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$, we

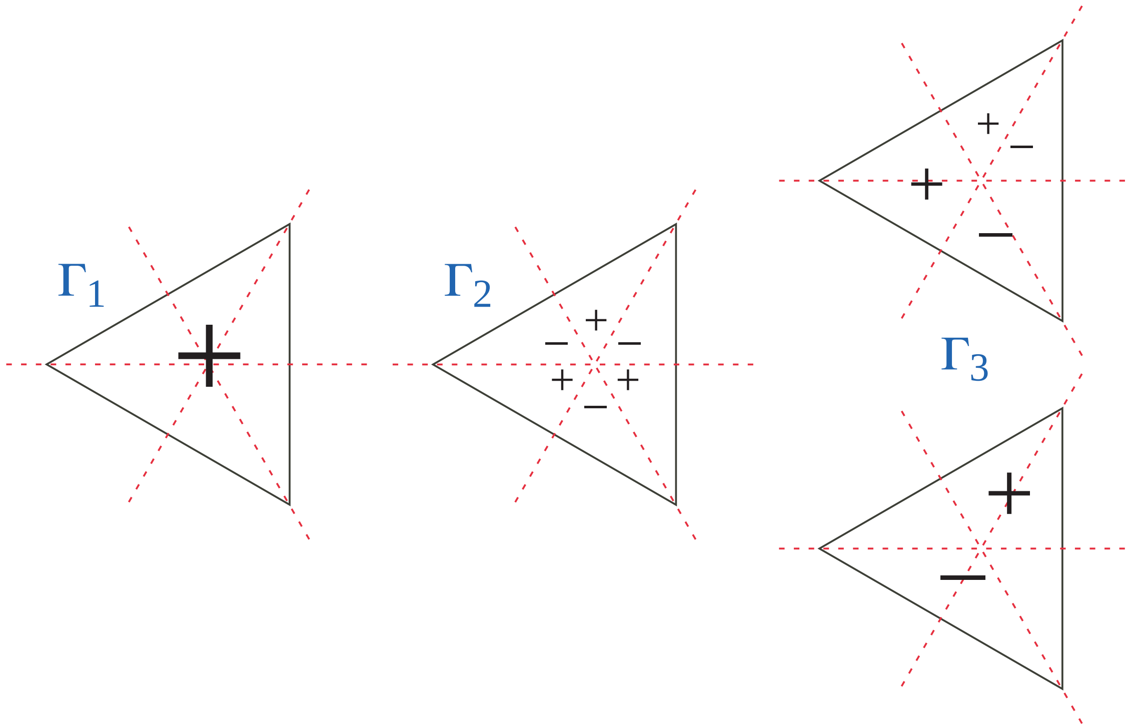

Figure 2: Sketch of possible E_z field patterns (for the lowest-ω modes of each symmetry) in the triangular cavity corresponding to the three representations. Note that a Γ_3 mode must be doubly degenerate with two field patterns roughly as shown.

get:

E	C_3	C_3^{-1}	σ_1	σ_2	σ_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 Γ_3 projection operator $\hat{P}^{(3)} = \frac{2}{6}(2\hat{O}_E - \hat{O}_{C_3} - \hat{O}_{C_3^{-1}})$ on $f(\mathbf{x}) = x$ we get simply x—thus, the function x must itself be a partner function for Γ_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 unitary representation given simply by the 2×2 rotation matrices that transform the functions $\{x,y\}$:

E	C_3	C_3^{-1}	σ_1	σ_2	σ_3
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

where to get σ_1 and σ_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.

Note that the 2×2 (in 2d) or 3×3 (in 3d) rotation matrices always form a representation, but in some groups these matrices are reducible, and in other groups there are multiple 2d irreps and the rotation matrices only give you one of these.

(d) E_z field patterns that transform as these representations are very crudely sketched in Figure 2, where $+$ and $-$ denote maxima and minima of the field. Note that because $\mathbf{E}$ 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 Γ_3 mode must be doubly degenerate, of course, and can be chosen so

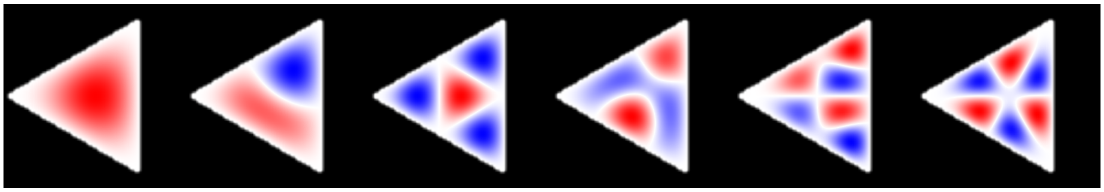

Figure 3: E_z field plots of first few lowest-ω modes in a triangular air cavity surrounded by metal (black) with side L, from a numerical calculation. The corresponding frequencies $\omega L/2\pi c$ (and representations) are, from left to right: 1.16 (Γ_1), 1.78 (Γ_3), 2.32 (Γ_1), 2.60 (Γ_3), 2.93 (Γ_3), and 3.08 (Γ_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 $-120°$ rotations of the field). (Slight asymmetries in the Γ_2 state are due to the finite computational grid resolution.)

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 σ_3, although of course the modes could be rotated to be even/odd around any of the three σ'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 $-120°$ 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 Γ_1 (fewest nodes $\rightarrow$ smallest ∇^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 cavity, in Figure. 3, which illustrates all three representations (note that the lowest ω mode of each representation looks much like our "guess"). The lowest frequency mode of E_z transforms like Γ_1 because that has the fewest oscillations (only a single extremum).

The H_z field sketches, in Figure 4, are somewhat different, for two reasons. First, $\mathbf{H}$ 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-ω modes. So, for example, now the Γ_1 mode looks *odd* with respect to all of the mirror planes, and will only appear for higher-ω modes. The Γ_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-ω mode. The lowest-order H_z mode should be Γ_3, since it has the fewest nodal planes. The corresponding numerical calculations are shown in Figure 5. Here, the least-oscillatory (lowest-ω) mode corresponds to Γ_3, with only two extrema. Note that the numerical Γ_1 mode is higher-order (each of our sketched extrema is split into two) than our cartoon (I couldn't find any lower-order Γ_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 Γ_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 ψ corresponding to one of the degenerate partner functions of Γ_3, then, for example, $(\widehat{\sigma_1} - \widehat{\sigma_2})\psi/\sqrt{3}$ gives us the other orthogonal partner function.

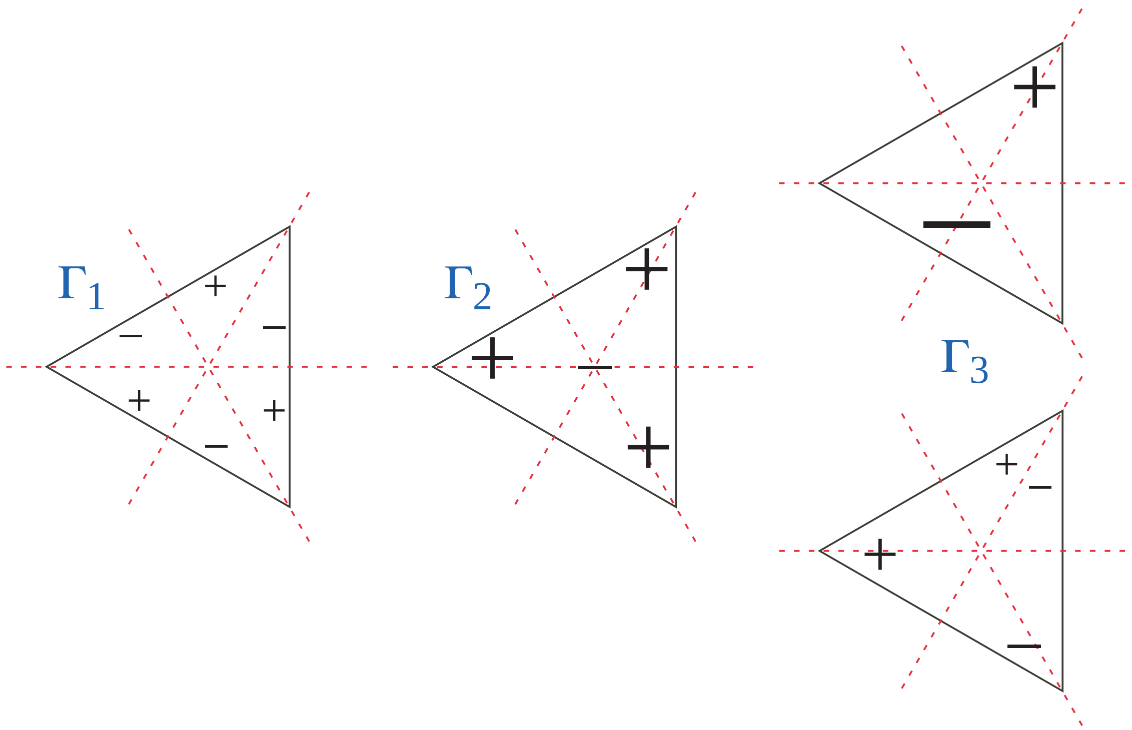

Figure 4: Sketch of possible H_z field patterns (for low-ω modes) in the triangular cavity corresponding to the three representations. Note that a Γ_3 mode must be doubly degenerate with two field patterns roughly as shown.

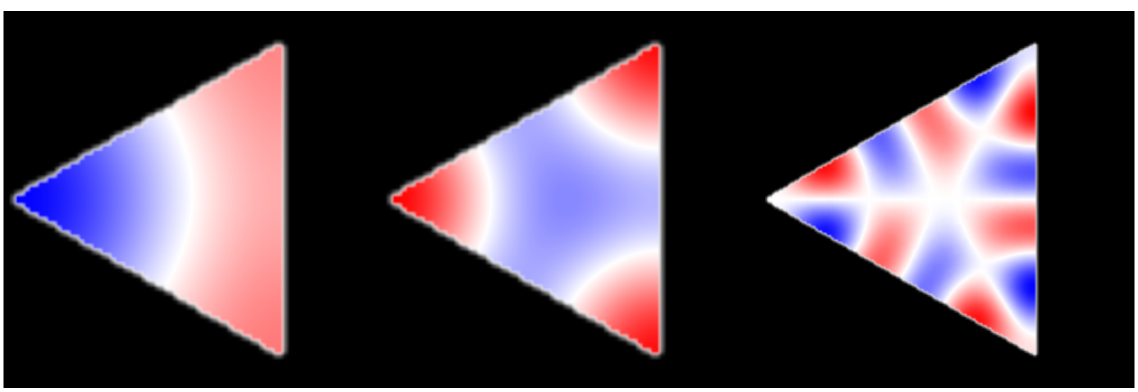

Figure 5: H_z field plots of the lowest-ω mode for each irreducible representation of $C_{3\text{v}}$ in a triangular air cavity surrounded by metal (black) with side L, from a numerical calculation. The corresponding frequencies $\omega L/2\pi c$ (and representations) are, from left to right: 0.66 (Γ_3), 1.14 (Γ_2), and 3.01 (Γ_1). Note that the leftmost mode is doubly degenerate (its degenerate partner is not shown, but can be found by subtracting 120° and $-120°$ rotations of the field). (Slight asymmetries in the Γ_1 state are due to the finite computational grid resolution.) There are 8 modes (not shown) with frequencies between 0.66 and 1.74.