Math 126 Problem set 3.

Using character tables.

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1 The Clebsch Gordon decomposition.

1.1 The group D_4.

From the last problem set we know that D_4 has one two dimensional irreducible representation and four one dimensional irreducible representations. The top line of the table below gives the conjugacy classes (with the number of elements in each class). Here $[r_4]$ denotes the conjugacy class consisting of the rotations of order 4, i.e. through 90^o and 270^o. There are three types of elements of order two: rotation through 180^o which is equal to r_4^2 for either choice of r_4, and so this conjugacy class contains a single element, the reflections through the side bisectors (denoted by r_2+) and the reflections through the diagonals (denoted by $r_2\times$). The trace of a rotation in the plane through angle θ is $2\cos\theta$ while the trace of any reflection in the plane is 0. So the bottom line in the table below gives the character of the representation of D_4 acting on the plane as symmetries of the square, and since 4+4=8, we see that this representation is irreducible. Each of the $\chi_i,\ i = 1, 2, 3, 4$ satisfy $(\chi_i, \chi_i) = 1$. You can check (don't hand this in) that $\chi_i(ab) = \chi_i(a)\chi_i(b)$ for all elements a, b of D_4 for $i = 1, 2, 3, 4$ so each is indeed the character of a one dimensional representation, and that any two distinct rows are orthogonal, so that the table is indeed the character table of D_4.

$8D_4$	$[e]$	$2[r_4]$	$[r_4^2]$	$2[r_2+]$	$2[r_2\times]$
χ_1	1	1	1	1	1
χ_2	1	1	1	-1	-1
χ_3	1	-1	1	-1	1
χ_4	1	-1	1	1	-1
χ_5	2	0	-2	0	0

Let ρ_i denote the irreducible representation chose character is χ_i. So, for example, ρ_5 is the two dimensional representation corresponding to symmetries of the square, and is on a two dimensional vector space, call it V. The space $V \otimes V$ is four dimensional, and we get a representation $\rho_5 \otimes \rho_5$ of D_4 on this four dimensional space.

1. What is the decomposition of this four dimensional representation into irreducibles ?

We know that for any representation ρ of any group on any vector space V, the representation $\rho \otimes \rho$ on $V \otimes V$ has character χ^2 if χ is the character of r. The space $V \otimes V$ is the direct sum of the space $S^2(V)$ - the space of symmetric tensors and $\wedge^2(V)$ - the space of anti-symmetric tensors. For any basis $e_1 \ldots, e_n$ of V, the elements $e_i \otimes e_j + e_j \otimes e_i, \;\; i \leq j$ form a basis of $S^2(V)$ and the elements $e_i \otimes e_j - ej \otimes e_i, \;\; i < j$ form a basis of $\wedge^2(V)$. The decomposition of

$$V \otimes V = S^2(V) \oplus \wedge^2(V)$$

is invariant under the representation $r \otimes r$. In other words, $r \otimes r$ decomposes into $r^{sym} \oplus r^{ant}$, a direct sum of the representation on $S^2(V)$, the space of symmetric tensors, and the representation on $\wedge^2(V)$, the space of anti-symmetric tensors. Here is a formula for the characters of each of these representations:

$$\chi^{sym}(a) = \frac{1}{2}(\chi(a)^2 + \chi(a^2)), \quad \chi^{ant}(a) = \frac{1}{2}(\chi(a)^2 - \chi(a^2)).$$

Proof. Since we may assume that $r(a)$ i unitary, and we can diagonalize any unitary operator, we may assume that the e_i chosen above are eigenvalues of $r(a)$, say with eigenvalue λ_i. Then $e_i \otimes e_j + e_j \otimes e_i$ is an eigenvalue of $r^{sym}(a)$ with eigenvalue $\lambda_i \lambda_j$ so

$$\chi^{sym}(a) = \operatorname{tr} r^{sym}(a) = \sum_{i \leq j} \lambda_i \lambda_j = \sum \lambda_i^2 + \sum_{i<j} \lambda_i \lambda_j = \frac{1}{2}\left(\sum_i \lambda_i\right)^2 + \frac{1}{2}\sum_i \lambda_i^2$$

and

$$\chi^{alt}(a) = \sum_{i<j} \lambda_i \lambda_j = \frac{1}{2}\left(\sum_i \lambda_i\right)^2 - \frac{1}{2}\sum \lambda_i^2. \quad \square$$

2. If V is two dimensional, then $S^2(V)$ is three dimensional and $\wedge^2(V)$ is one dimensional. Which of the irreducibles you found in problem **1** are in the decomposition of $S^2(V)$ and which are in $\wedge^2(V)$?

1.2 The group T.

The group T has twelve elements, and its character table was given in the handout. (The header of the last column should be $3[r_2]$ describing the 180^o rotations about the lines joining the midpoints of opposite edges. The subscript was misprinted as a superscript.)

For any two characters in the table, we have

$$\chi_i \chi_j = \sum_k C_{ijk} \chi_k$$

where the C_{ijk} are non-negative integers. We thus get a "multiplication table". All this is true for any group. For the group T we clearly have

$$\chi_1 \chi_i = \chi_i \;\; \forall\, i, \chi_2^2 = \chi_3,\; \chi_3^2 = \chi_2,\; \chi_2 \chi_3 = \chi_1 \;\text{ and } \chi_i \chi_4 = \chi_4, \quad i = 1, 2, 3.$$

3. What is the expansion of χ_4^2?

χ_4 is the character of the representation ρ_4 of T acting on the three dimensional space V as rotational symmetries of the tetrahedron. So χ_4^2 is the character of the representation $\rho_4 \otimes \rho_4$ acting on the nine dimensional space $V \otimes V$, and the coefficients C_{44k} that you computed in problem **3** gives the decomposition of $\rho_4 \otimes \rho_4$ into irreducibles. Now $S^2(V)$ is six dimensional and $\wedge^2(V)$ is three dimensional.

4. Which of the irreducibles occur in $S^2(V)$ and which in $\wedge^2(V)$?

2 Macroscopic properties of crystals.

In this section we will be examining representations of finite subgroups G of $O(3)$ which occur as the "point groups" of crystals. We will let V denote the (complexified) three dimensional space on which the group $O(3)$ acts, so we get a representation ρ_V of G on V. There is another representation of G on V given by

$$\tilde{\rho}_V(a) := \det(\tilde{\rho}_V(a))\rho_V(a).$$

If G contains only rotations, i.e. is a subgroup of $SO(3)$, these two representations are the same; but if G contains reflections they are different. In the physics literature a vector which transforms according to the representation ρ_V is called a **polar** vector while an element of V under the representation $\tilde{\rho}_V$ us called an **axial** vector. For example, the electric dipole moment $\mathbf{P}$ is a polar vector while the magnetic moment $\mathbf{M}$ is an axial vector. (You do not need to know what these are, only which representation they belong to.)

The electrical conductivity tensor is an element of $S^2(V)$ which transforms according to the restriction of $\rho_V \otimes \rho_V$ to $S^2(V)$. The piezoelectricity tensor is an element of $V \otimes V \otimes V$ which transforms according to $\rho_V \otimes \rho_V \otimes \rho_V$. Again, you do not need to know what these are to do the following problems.

A **permanent** electric dipole moment, magnetic moment, etc. is an element of the corresponding representation which is invariant under the representation; so if it is not zero, it must belong to a subrepresentation which is equivalent to the trivial representation. For example, the three dimensional representation of the group T is irreducible and so any crystal associated to this symmetry group can not have a non-zero permanent electric or magnetic dipole moment.

5. What is the dimension of the space of possible permanent piezoelectricity tensors for the group T? In other words, how many times does $\rho_V \otimes \rho_V \otimes \rho_V$ contain the trivial representation?

There are two subgroups of $O(3)$ which are isomorphic as abstract groups to S_3. One is the group $D_3 \subset SO(3)$ consisting of all three dimensional rotational symmetries of the triangle, so consisting of the identity, rotation through 120^o and 240^o about the z-axis (so our equilateral triangle is in the x, y-plane and centered at the origin), and the 180^o rotations about the angle bisectors.

The other is the group C_{3v} which contains the identity, rotation through 120^o and 240^o about the z-axis, and reflections in the planes which are perpendicular to and bisect the sides. This group is the group of all symmetries of a right pyramid on an equilateral base and is not a subgroup of $SO(3)$. For example, C_{3v} is the symmetry group of the ammonia molecule NH_3.

6. Using the character table for S_3, determine which of the groups D_3 and C_{3v} can possess a non-zero permanent electric dipole moment and which can possess a non-zero permanent magnetic moment.