PH563 Assignment 2

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Question 1.

(a) False.
C_{4v} is an abelian group. So, all its irreps are one-dimensional and its wavefunctions non-degenerate.

(b) False.
The dimension of the tensor product of two representations is the product of their individual dimensions, not their sum.

(c) False.
We need to look at the transition amplitude $\langle 10| e\hat{Y} |00\rangle$ to check if the transition is forbidden. The unit irrep A_1 is present in the decomposition of the tensor product of irreps for this amplitude, so it will evaluate to a non-zero quantity.

Question 2.

(a) iv. χ_{B_2}
The character for a tensor product of representations is the product of individual characters, which in this case, clearly from the character table is χ_{B_2}

(b) iii. 6-dimensional vector space
The dimension of the tensor product of two representations is the product of their individual dimensions.

Question 3.

(a) Consider the character table of C_{3v}

C_{3v}	e	C_3	σ_v
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Using the Great Orthogonality Theorem,

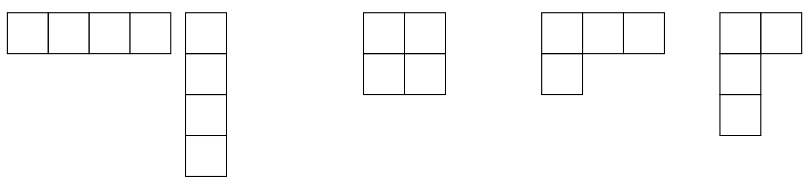
$$a_\alpha = \frac{1}{|G|} \cdot \left(\sum_i n_i \chi(i) \chi_\alpha(i) \right) , \tag{1}$$

and the characters given, we get,

$$a_{A_1} = \frac{1}{6} \cdot (1 \cdot 1 \cdot 7 + 2 \cdot 1 \cdot 1 + 3 \cdot 1 \cdot (-3)) = 0 , \tag{2}$$
$$a_{A_2} = \frac{1}{6} \cdot (1 \cdot 1 \cdot 7 + 2 \cdot 1 \cdot 1 + 3 \cdot (-1) \cdot (-3)) = 3 \text{ , and} \tag{3}$$
$$a_E = \frac{1}{6} \cdot (1 \cdot 2 \cdot 7 + 2 \cdot (-1) \cdot 1 + 3 \cdot 0 \cdot (-3)) = 2 . \tag{4}$$

(b) C_s is abelian, so it has no symmetric degeneracies. All 2-dimensional degeneracies of C_{3v} split into two non-degenerate states.

(g) $\mathfrak{S}(4)$ has irreps with dimensions $\{1, 1, 2, 3, 3\}$. They are represented by the Young's diagrams given below, left to right:



(h) The electric dipole moment and magnetic dipole moment operators are given by:

$$\hat{\mu}_E = (q\hat{X}, q\hat{Y}, q\hat{Z}),\ \hat{\mu}_B = \frac{g}{2m}(\hat{L}_x, \hat{L}_y, \hat{L}_z) \tag{5}$$

with

$$\hat{Z} \in A_1 \tag{6}$$
$$\hat{X}, \hat{Y}, \hat{L}_x, \hat{L}_y \in A_2 \tag{7}$$
$$\hat{L}_z \in E \tag{8}$$

following the product rules

$$A_1 \otimes \Gamma = \Gamma \text{ for any irrep } \Gamma \tag{9}$$
$$A_2 \otimes A_2 = A_1 \tag{10}$$
$$A_2 \otimes E = E \tag{11}$$
$$E \otimes E = A_1 \oplus A_2 \oplus E . \tag{12}$$

So in any of the required integral computations, we will have a term from A_1 and thus, the questioned transitions will be disallowed.