Physics 220, Spring 2010, Homework 3, fun with $O$, Due April 28

1. Write the 24 elements of $O$ as $S_4$ permutations of the 4 body diagonals (between opposite vertices). Label vertices on the bottom face of the cube as $1, 2, 3, 4$ with 1 and 3 diagonally across from each other and 2 and 4 diagonally across from each other. The vertices on the top face of the cube are $5, 6, 7, 8$. Body diagonal connects vertices 1 and 8, body diagonal 2 connects vertices 2 and 7, body diagonal 3 connects vertices 3 and 6, and body diagonal 4 connects vertices 4 and 5. Write each $O$ group element as particular permutations of the eight vertices (as a subgroup of $S_8$) and show that each corresponds to a particular distinct $S_4$ permutation element of the 4 body diagonals.

2. The representation $F_1$ of $O$ is how a vector, such as $\vec{r}$, transforms under this discrete subgroup of the rotation group $SO(3)$ [1]. In this problem you will do some checks that $(zy, xz, xy)$ transforms as the other 3d representation, $F_2$. Consider the examples of $C_2$ and $C_4$ elements that act on $F_1$ as

$$C_2 : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \qquad C_2 : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

   If we put the center of the cube at the origin, with edges parallel to the $\hat{x}$, $\hat{y}$, $\hat{z}$ axes, the above $C_2$ is a $\pi$ rotation around the line $x = y$ and $C_4$ is a rotation by $2\pi/4$ around the $\hat{z}$ axis. You can easily verify that the traces of the above matrices, and also $C_4^2$ (squaring the above $C_4$ matrix) agree with the characters in the $F_1$ irrep of the $C_2$, $C_4$, and $C_4^2$ conjugacy classes, as given in lecture.

   Write out the $3 \times 3$ matrices for $C_2$, $C_4$, and $C_4^2$ acting on the basis $(yz, xz, xy)$ and verify that the characters of these are as given in lecture for the $F_2$ irrep.

3. A system has Hamiltonian $H = H_0 + H_1$, where $H_0$ has symmetry group $O$ and perturbation $H_1$ preserves the subgroup $T$. As in lecture, call the $T$ irreps $A_0$ (trivial),

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[1] The cross product of two vectors $\vec{v} \times \vec{w}$ also transforms in the representation $F_1$, because it transforms exactly the same as a vector under all ordinary rotations. The cross product is an axial vector, and the difference between that and an ordinary, or "polar", vector shows up under reflections in a plane, or inversions, i.e. elements of $O(3)$ rather than $SO(3)$. Since $O$ only contains proper rotations, both polar and axial vectors transform the same. On the other hand, $O$ is isomorphic to $T_d$, the tetrahedral group augmented by reflections in a plane, and in this description the two 3d irreps *do* correspond to polar and axial vectors.

$E$ (sum of two complex conjugate 1d irreps), and $F$ (corresponding to $\vec{r}$). Call the $O$ irreps $A_0$ (trivial), $A_1$ (another 1d irrep), $E$ (2d irrep), $F_1$ (corresp to $(x,y,z)$), and $F_2$ (corresp to $(yz,xz,xy)$).

(a) Find how each $O$ irrep splits into $T$ irreps.

(b) Suppose that the first five energy levels of $H_0$ correspond to irreps $A_0$, $A_1$, $E$, $F_1$, and $F_2$, in that order. The small perturbation changes the energy of a $O$ level with the $T$ irreps affected as: lowered for $A_0$, raised for $F$, and no change for $E$. Draw a qualitative picture of the first five $H_0$ energy levels, and their splitting due to $H_1$, indicating the degeneracies of the levels before and after the splitting. (Draw the splitting size as small compared with the initial separation of the first five $H_0$ energy levels.)

4. Consider again a system with $H_0$ having symmetry group $O$. Find the selection rule when a photon is emitted (dipole radiation with $H_1$ in the rep corresponding to $\vec{r}$). List all possible leading order transitions, e.g. can one have a $F_2 \leftrightarrow A_0$ transition? Etc. For each of the five possible initial irreps, list which of the 5 final possible irreps it can transition to up emitting a photon.

5. Consider again a system with $H_0$ with symmetry group $O$, and now find the selection rules for leading order radiation due to quadrupole radiation (a pair of photons, in the $\ell = 2$ state). Recall $Q_{ij}$ transforms as the symmetrized product of two vectors $\vec{v}$ and $\vec{w}$, i.e. $v_i w_j + v_j w_i$, omitting the trace part (the dot product $\vec{v}\cdot\vec{w}$). So consider $F_1 \otimes F_1$ and subtract out the $A_0$ irrep (this is $\vec{v}\cdot\vec{w}$), and also subtract out the antisymmetric part corresponding to $\vec{v}\times\vec{w} = -\vec{w}\times\vec{v}$ (as discussed in the footnote, this is in the $F_1$ irrep). What's left is the $O$ representation of the 5 quadrupole states $Q_{ij}$ as a sum of $O$ irreps. Now use this information to find the selection rules for all of the allowed transitions due to quadrupole radiation.

6. Consider the 3d rotation group $SO(3)$. All rotations by some angle $\theta$, around whatever axis, are in the same conjugacy class[2]. The character of all group elements in this conjugacy class is $\chi_j(\theta) = \mathrm{Tr}D(R_{\widehat{z}}(\theta) = \sum_{m=-j}^{+j} e^{im\theta} = \sin[(j+\frac{1}{2})\theta]/\sin(\theta/2)$.

Suppose that an electron in an atom is in a $j = 2$ state ("d-state"), with all five energy levels initially degenerate. Now apply an external field as a perturbation, which

[2] To see this, label a rotation by angle $\theta$ about some axis $\widehat{n}$ as $R_{\widehat{n}}(\theta)$. Conjugating by another group element, $R_{\widehat{n}_1}(\theta_1)R_{\widehat{n}}(\theta)R_{\widehat{n}_1}(\theta_1)^{-1} = R_{\widehat{n}_2}(\theta)$, where $\widehat{n}_2 = R_{\widehat{n}_1}(\theta_1)\widehat{n}$ is what we get by rotating the axis $\widehat{n}$.

breaks the full rotation symmetry to the $O$ octahedral subgroup. To find how the $j = 2$ energy levels split, find how the 5d, $j = 2$ irrep. of the full rotation group decomposes into a sum of irreps of the $O$ subgroup: $D_{j=2} = \oplus(O\ irreps)$. To do this, write again the $O$ character table, and include the character $\chi_{j=2}(\theta)$ for the appropriate rotation angles $\theta$ corresponding to the various discrete rotations of the $O$ conjugacy classes (e.g. $\theta = 2\pi/3$ for the $2\pi/3$ rotations around the body diagonal axes. Using this character table, you can read off how $D_{j=2}$ decomposes into a sum of $O$ irreps. Draw a qualitative picture of the associated splitting of the 5-fold degeneracy. What degeneracies remain?

7. This is similar to the above problem, but now consider two non-equivalent (different energy level) $d$ electrons in an atom. Ignore spin. Initially the atom is free (no applied field, so $H = H_0$), and the energy levels are ordered so that the energy increases with increasing $\ell_{tot}$.

(a) Draw a diagram where the vertical axis is the energy, and draw all the energy levels and indicate their degeneracies. (This part is just addition of angular momentum).

(b) Now, in the same diagram, let the horizontal axis denote the strength of the applied external field, which breaks the rotation symmetry down to $O$. When the field is weak, $H = H_0 + H_1$ and $H_1$ can be treated as a perturbation. Indicate how the $H_0$ energy levels are split by $H_1$ when the field is weak.

(c) Now, in the same diagram, farther along the horizontal axis, show what happens when the applied external field is strong. The point is that, when the field is strong, the energy level of each $d$ electron state is strongly modified, depending on its $O$ representation (as in problem 6). So the two $d$ electrons form energy levels arranged according to definite tensor products of those $O$ representations. The energy levels are rearranged from those in part (b), with some energy level crossings, such that now they are grouped with $O$ irreps nearby if they together sum to terms appearing on the RHS of the tensor product of the $O$ irreps appearing in problem 6.