Teach Yourself Group Representation Theory

This problem set applies techniques of group theory to quantum mechanical perturbation theory. Prior knowledge of group theory is not needed, and you can teach yourself more about these concepts by reading in Landau and Lifshitz *Quantum Mechanics: non-relativistic theory.* Feel free to stop by my office for help if you need it.

Although this problem looks long and complicated, in fact very little calculation is required.

1. Consider the $l = 0$ and $l = 1$ spherical harmonics $Y_{00}(\theta, \phi)$ and $Y_{1m}(\theta, \phi)$ $(m = 0, \pm 1)$ as a set of four functions $\{f_1, f_2, f_3, f_4\}$. These functions form a basis for a four-dimensional representation of the improper rotation group $O(3)$. That is, they transform into linear combinations of each other under rotations so that

$$\hat{R} f_i(\theta, \phi) = \sum_j M_{ij}(\hat{R}) f_j(\theta, \phi).$$

Find the matrix $\mathbf{M}(\psi, \hat{z})$ representing a rotation by angle ψ around the $\hat{z}$ axis, find the matrix $\mathbf{M}(90°, \hat{x})$ representing a rotation by angle 90° around the $\hat{x}$ axis, and find the matrix $\mathbf{M}(\sigma_v)$ representing reflection through the xz plane. By inspecting these matrices verify that the four dimensional representation is *reducible*, consisting of two *irreducible* representations that always transform only within themselves. One of the irreducible representations is the *unit* representation, so-called because the associated block of $\mathbf{M}$ is a 1×1 matrix consisting of the number 1 independently of the rotation $\hat{R}$. Discuss the relationship between the basis functions f_i, the irreducible representations, and the $n = 2$ states $\{|2, l, m >\}$ of the hydrogen atom.

2. Consider the linear Stark effect on the $n = 2$ level of hydrogen (see Cohen-Tannoudji, p. 1279). Show that the electrostatic potential function $W_S = -q\mathcal{E}\mathbf{Z}$ lowers the symmetry group from $O(3)$ to $C_{\infty v}$, the group of rotations by angle ψ around $\hat{z}$ and/or reflections through vertical planes. Use the functions f_1, f_2, f_3, f_4 defined previously as the basis of a representation of the group $C_{\infty v}$. By studying the transformations of this set, identify the irreducible representations of $C_{\infty v}$ contained in this basis. How many times is the *unit* representation contained?

3. Group theory proves that if a function $f(\mathbf{r})$ belongs to the basis of an irreducible representation (other than the *unit* representation) of any spatial symmetry group, then its integral vanishes,

$$\int d\mathbf{r} f(\mathbf{r}) = 0. \tag{1}$$

Similarly, if two functions $f_i(\mathbf{r})$ and $f_j(\mathbf{r})$ are basis functions of *different* irreducible representations, then their inner product vanishes,

$$\langle i|j\rangle = \int d\mathbf{r} f_i^*(\mathbf{r}) f_j(\mathbf{r}) = 0. \tag{2}$$

See Landau and Lifshitz §97 "Selection rules for matrix elements" for explanation. We will use these rules to identify vanishing matrix elements $\langle i|W_S|j\rangle$.

(i) First consider the group $C_{\infty v}$ and note that the perturbation W_S itself transforms as the unit representation of this group. Prove that the product $W_S f_i$ transforms identically to f_i under $C_{\infty v}$. Use this observation together with rule (2) to show that the matrix $\langle i|W_S|j\rangle$ has a block diagonal structure. Write down a 4×4 matrix showing the values 0 you have just obtained and indicating the dimensionalities of the remaining blocks.

(ii) Now consider the group $O(3)$. Note that W_S is proportional to $f_2 = Y_{10}$, and use your knowledge of the addition of angular momenta (see Cohen-Tannoudji, p. 1046) to express the products $W_S f_i$ as sums of functions in the basis set f_1, f_2, f_3, f_4 and other functions you may wish to define. Finally, use rule (1) find additional zeros of the matrix $\langle i|W_S|j\rangle$ not previously recognized in part *(i)*.

4. Sketch the energy level diagram as a function of applied field predicted by first order degenerate perturbation theory. Label every state according to the irreducible representation of $C_{\infty v}$ under which it transforms and indicate the degeneracy of each level. Note the massive crossing of levels at zero applied field. Discuss which degeneracy at zero field can be explained by the $O(3)$ symmetry group and which degeneracy can not be explained by the $O(3)$ symmetry. *Is* there a symmetry-based explanation for this unexpected higher degeneracy?