Physics 285a Problem Set 10

posted November 16, 2023, due November 29, 2023

Problem 1. He wave function

a) Assume that both electrons in the helium atom or in a helium-like ion occupy the same orbital wave function

$$\psi(\vec{r}) \;=\; \frac{1}{\sqrt{\pi}}\beta^{-\frac{3}{2}}\, e^{-\frac{r}{\beta}}\,.$$

For which value of β is the expectation value of the two-body Hamiltonian

$$\hat{H} \;=\; \sum_{i=1,2}\left(\frac{\vec{p}^2}{2\mu} - \frac{KZ}{r_i}\right) + \frac{K}{|\vec{r}_1 - \vec{r}_2|}$$

a minimum? How do β and the minimal energy depend on the charge number Z? (Hint: Use the Legendre polynomial expansion of $|\vec{r}_1 - \vec{r}_2|^{-1}$.) Why do we use this form for ψ?

b) Calculate the expectation values of $\hat{H}$in the ^1P and ^3P states of the helium atom, constructed by appropriate angular momentum coupling from the 1s2p configuration. Use hydrogenic single-particle wave functions with the parameter β as obtained in (a).

Problem 2. Basic Group theory This and the following problems will serve as a review for group theory for further discussions in class. Although more materials will be posted for reference, you are more than welcome to use any textbooks.

Take the symmetry of a pyramid over a square (see Fig. 1).

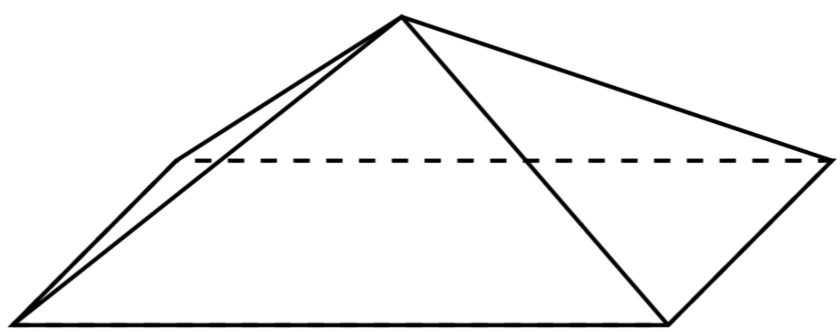

Figure 1: Pyramid with a square base

(a) List all group elements and create a multiplication table.

(b) List all possible subgroups (there are 10 of them, among them two trivial) and give examples of objects/spaces/molecules/etc. with that symmetry (and not higher).

(c) List all classes and give the dimensions of all the irreducible representations. Construct a character table. This can be done if one assumes that there is always the trivial 1D representation and one 1D representation where all proper rotations are 1 and all improper rotations are -1. There is one obvious two dimensional representation. The other representations can be found by using the character orthogonality relation. Proof (a posteriori) that the 2D representation is in fact irreducible.

Problem 3.

SU(2):

(a) Show that the matrices

$$U = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}$$

are the most general 2D unitary matrices with det $U = 1$. Show that they constitute a group (which is called "$SU(2)$").

(b) Take the functions

$$f_m^{(j)}(\rho) = \frac{u^{j+m}\, v^{j-m}}{\sqrt{(j+m)!(j-m)!}},$$

where $\rho = (u, v)$, $j = 0, \pm\frac{1}{2}, \pm, \ldots$, and $m = -j, \ldots j-1, j$. How does $P_U f_m^{(j)}(\rho)$ look in general? Use the $f_m^{(j)}$ as basis functions to create a 1D, 2D, and 3D irreducible representation for $SU(2)$. (Irreducibility can be proved using the special form for all Us of all dimensions and using Schurs lemma. You do not need to do that.)

(c) Take the two matrices

$$A = \begin{pmatrix} -z & x+iy \\ x-iy & z \end{pmatrix} \quad \text{and} \quad A' = \begin{pmatrix} -z' & x'+iy' \\ x'-iy' & z' \end{pmatrix},$$

where x, y, z and x', y', z' are real numbers and $A' = UAU^{-1}$. Write the form of x', y', z' explicitly as functions of x, y, z, depending on the parameters a and b. Show that the matrix R with $\mathbf{r}' = R\mathbf{r}$ is a regular rotation in 3 dimensions and therefore a member (and a representation) of $O^+(3)$.

(d) Show this in particular for the example of $U(\alpha)$ with $a = e^{-i\alpha/2}$ and $b = 0$ and $a = -e^{-i\alpha/2}$ and $b = 0$, leading to $-U(\alpha)$. What is the difference is the two resulting matrices R? If we generalize this example (which can be done but you dont have to), what can we therefore conclude for the relationship between $SU(2)$ and $O^+(3)$? (This is what allowed us to find the half-integer representations in class.)

Problem 4.

Time reversal:

Define the time reversal (or Kramers') operator

$$Kf(\mathbf{r}, t) = f^*(\mathbf{r}, -t)$$

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(a) Show that any real Hamiltonian $H(\mathbf{r})$ is invariant under time reversal.

(b) Assume $K\left|m_s\right\rangle = (-1)^{m_s}\left|-m_s\right\rangle$ for spin functions and $K\left|l, m_l\right\rangle = (-1)^{m_l}\left|l, -m_l\right\rangle$. Do the proof for (l, m_l) only. Show first (using the spin functions) that we can assume $K^2 = -1$ if there is spin present. So we know for a regular single electron function ψ that $K^2\psi = -\psi$. Are ψ and $K\psi$ linearly independent? What do we find therefore for the degeneracy of these wavefunctions if the Hamiltonian is real? What happens if there are two electrons?

(c) Why does this (single electron) symmetry get lost if we add an external magnetic field (but not if the magnetic field is internal, e.g., generated by the electron spin)?

This can be generalized into Kramers Theorem, which states that, without an external magnetic field, the Hamiltonian is invariant under time reversal and no combination of external electric fields can ever remove the resulting degeneracy completely. (E.g., if one has an F=2 manifold in Hydrogen it is 5-fold degenerate, and while we can apply a magnetic field to Zeeman split all five levels, complete splitting of this level can never be accomplished with any combination of electric fields alone.)