PHYSICS 232

Homework 1

Due in class, Friday, January 27.

Office Hours, Wednesdays 10:00–11:00 p.m. and at other times if I'm free.

1. The wave function of the hydrogen atom in its ground state is $\psi = \ (\pi a_0^3)^{-1/2} \exp(-r/a_0)$, where $a_0 = \hbar^2/me^2 = 0.529 \times 10^{-8}$ cm. Show that for this state $< r^2 >= 3a_0^2$, and calculate the molar diamagnetic susceptibility of atomic hydrogen.
   Note: The susceptibility per mole is just the volume per mole (a number of order unity) times the susceptibility per unit volume. Since the latter is dimensionless, the units of molar susceptibility are $cm^3/mole$.

2. Consider an electron moving in a potential $V(r)$ in a magnetic field characterized by a vector potential $\mathbf{A}(\mathbf{r})$. For a particular gauge there is an energy eigenstate $\psi(\mathbf{r})$ with energy E.

   Now do a gauge transformation
   $$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \vec{\nabla}\chi(\mathbf{r}).$$
   Show that
   $$\psi'(\mathbf{r}) = \exp\left(-\frac{ie}{\hbar c}\chi(\mathbf{r})\right)\psi(\mathbf{r})$$
   is an eigenstate of the Hamiltonian in the new gauge with the *same* energy E.

   Note: Spin does not enter this problem so neglect it.

3. Apply Hund's rules to obtain the ground state configuration of (a) Eu^{2+}, which has configuration $4f^7 5s^2 5p^6$, (b) Eu^{3+}, (c) Nd^{3+}, and (d) Ho^{3+}.
   Note: you must explain your reasoning to get credit.

4. In this question you will verify the Wigner-Eckart theorem for the special cases of $J = 0$ and $J = 1/2$.

   (a) The components of orbital and spin angular momenta satisfy the following commutation relations
   $$[L_\alpha, L_\beta] = i\epsilon_{\alpha\beta\gamma} L_\gamma, \qquad [S_\alpha, S_\beta] = i\epsilon_{\alpha\beta\gamma} S_\gamma, \qquad [L_\alpha, S_\beta] = 0$$
   where $\epsilon_{\alpha\beta\gamma} = 1$ if $\alpha = x, \beta = y, \gamma = z$ or a cyclic (even) permutation of this, -1 for an an odd permutation, and 0 otherwise. Deduce from these results that
   $$[\mathbf{L} + g_0\,\mathbf{S}, \hat{\mathbf{n}} \cdot \mathbf{J}] = i\hat{\mathbf{n}} \times (\mathbf{L} + g_0\,\mathbf{S})\,, \qquad (1)$$
   where $\hat{\mathbf{n}}$ is a unit (classical) vector and g_0 is a constant, which we will take to be the Landé g-factor of the electron.

   (b) Now consider a state $|0\langle$ with zero total angular momentum J. This has the property that
   $$J_x|0\rangle = J_y|0\rangle = J_z|0\rangle = 0\,.$$
   Deduce from Eq. (1) that
   $$\langle 0|\mathbf{L} + g_0\mathbf{S}|0\rangle = 0\,,$$
   even though the operators $\mathbf{L}^2$ and $\mathbf{S}^2$ need not vanish in the state $|0\rangle$ and, in fact, $(\mathbf{L}+g_0\mathbf{S})|0\rangle$ need not be zero (just orthogonal to $|0\rangle$).

Note: This is a (trivial) example of the Wigner-Eckart theorem. Within states of a given J, the matrix elements of one vector operator, $\mathbf{L} + g_0\mathbf{S}$ here, are proportional those of another vector operator, $\mathbf{J}$ here. In this simple example, $|0\rangle$ is non-degenerate and $\langle 0|\mathbf{J}|0\rangle = 0$ so we must have $\langle 0|\mathbf{L} + g_0\mathbf{S}|0\rangle = 0$ too.

Note too: The Wigner-Eckart theorem also states that $\langle 0|\mathbf{L}|0\rangle$ and $\langle 0|\mathbf{S}|0\rangle$ both vanish separately. This follows from the proof you will obtain for $\mathbf{L} + g_0\mathbf{S}$.

(c) Finally consider the next most complicated case, $J = 1/2$. From Eq. (1) obtain the Wigner-Eckart theorem

$$\langle J\, m_{J'}|\mathbf{L} + g_0\mathbf{S}|J\, m_J\rangle = g(J)\langle J\, m_{J'}|\mathbf{J}|J\, m_J\rangle\,,$$

where $g(J)$ depends on J (and also L and S) but, *and this is the crucial point*, not on m_J or $m_{J'}$.

5. Some organic molecules have a triplet ($S = 1$) excited state at an energy Δ above a singlet ($S = 0$) ground state. Neglecting any orbital contribution to the magnetic moment, find the magnetic moment $\langle\mu\rangle$ in a field H at temperature T

6. Consider a rare earth ion with angular momentum J in a crystal field. Show, from the general formula for the susceptibility discussed in class, that, for temperatures much larger than the crystal field splittings, the paramagnetic susceptibility is just that of the free ion with *no* crystal field splitting. (Hence crystal field slittings can be neglected at sufficiently high temperatures).