PHYS852 Quantum Mechanics II, Spring 2010
HOMEWORK ASSIGNMENT 5: Solutions

Topics covered: rotation with spin, exchange symmmetry

1. The Hamiltonian for the deuteron, a bound-state of a proton and neutron, may be written in the form

$$H = \frac{P_p^2}{2M_p} + \frac{P_n^2}{2M_n} + V_1(R) + V_2(R)\vec{S}_p \cdot \vec{S}_n, \tag{1}$$

where R is the relative radial coordinate. Both are spin-1/2 particles, but they are not identical.

(a) The total angular momentum operator is $\vec{S} = \vec{S}_p + \vec{S}_n$. The state $|s_p s_n s\, m\rangle$ is the simultaneous eigenstate of $\vec{S}_p$, $\vec{S}_n$, S^2, and S_z. What are the allowed values of the total spin quantum number s? For each s-value, what are the allowed m quantum numbers.
With $s_p = 1/2$ and $s_n = 1/2$, we find $s_{min} = |s_p - s_n| = 0$, and $s_{max} = s_p + s_n = 1$, so the allowed values of s are $0, 1$. For $s = 0$, only $m = 0$ is allowed, while for $s = 1$, we can have $m = -1, 0, 1$.

(b) Show that $|s_p s_n s\, m\rangle$ is an eigenstate of $\vec{S}_p \cdot \vec{S}_n$, and give the corresponding eigenvalue. Hint, use the fact that $S^2 = (\vec{S}_p + \vec{S}_n) \cdot (\vec{S}_p + \vec{S}_n)$.
We have

$$S^2 = S_p^2 + 2\vec{S}_p \cdot \vec{S}_n + S_n^2 \tag{2}$$

solving for $\vec{S}_p \cdot \vec{S}_n$ gives

$$\vec{S}_p \cdot \vec{S}_n = \frac{1}{2}\left(S^2 - S_p^2 - S_n^2\right) \tag{3}$$

As $|s_p s_n s m\rangle$ an eigenstate of S^2, S_p^2 andS_n^2, then it must also be an eigenstate of $\vec{S}_p \cdot \vec{S}_n$ with eigenvalue $\frac{\hbar^2}{2}\left(s(s+1) - 3\right)$.

(c) Give ten distinct quantum numbers that can be assigned to an eigenstates of this H. Note that this includes s_p and s_n, even though they can never change.
The ten quantum numbers are the three components of the center-of-mass momentum: p_x, p_y, and p_z; the orbital quantum numbers of the relative motion:n, ℓ, and m_ℓ; and the four spin quantum numbers: s_p, s_n, s, and m.

(d) What one-dimensional wave equation would you have to solve to find the energy eigenvalue associated with one of these states?
The radial wave equation would be:

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V_1(r) + \frac{\hbar^2}{2}\left[s(s+1) - 3\right] V_2(r) - E_{n\ell s}\right] R_{n\ell s}(r) = 0 \tag{4}$$

2. Consider a particle of spin $s = 1$, constrained to move on the surface of a sphere. Assume that the Hamiltonian of the particle is

$$H = \frac{L^2}{2I} + \frac{\vec{L} \cdot \vec{S}}{I}, \tag{5}$$

where $\vec{L}$ is the orbital angular momentum operator, I is the moment of inertia, and $\vec{S}$ is the spin operator. find the quantized energy levels and the degeneracy of each level.
With $\vec{J} = \vec{L} + \vec{S}$, simultaneous eigenstates of H, L^2, S^2, J^2, and J_z exist. We can label the $|\ell s j m_j\rangle$, as $s = 1$ never changes, we can drop s. We have then

$$\begin{aligned} H|\ell j m_j\rangle &= \left[\frac{\hbar^2 \ell(\ell+1)}{2I} + \frac{\hbar^2}{2I}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right]\right]|\ell j m_j\rangle \\ &= \frac{\hbar^2}{2I}\left[j(j+1) - 2\right]|\ell j m_j\rangle \end{aligned} \tag{6}$$

so we see that energy depends on j only. This means that states with the same j but different ℓ are degenerate. The degeneracy factor $2j + 1$ counts only those states with the same j for fixed ℓ. We therefore need to multiply by the number of ℓ-values that can give a specific j value to get the total degeneracy of the j^{th} energy level. The easiest way to do this is to make a table:

ℓ	j_{min}	j_{max}
0	1	1
1	0	2
2	1	3
3	2	4
$\vdots$	$\vdots$	$\vdots$

It is easy to see that $j = 0$ can only occur when $\ell = 1$, $j = 1$ can occur for $\ell = 0, 1, 2$, $j = 3$ for $\ell = 2, 3, 4$, etc... So the number of ℓ-values for a given j is 3, except for $j = 0$ which has only 1. This can be formulated as $d_j = (2j + 1)(3 - 2\delta_{j,0}) = 6j + 3 - 2\delta_{j,0}$

3. For Silicon, the ground-state configuration is $(3p)^2$, i.e. there are two valence electrons, each in the $3p$ state.

   (a) What are the possible values for the total spin quantum number, s, where $\vec{S} = \vec{S}_1 + \vec{S}_2$?
   $s = 0, 1$

   (b) What are the possible values for the total angular momentum quantum number, ℓ, where $\vec{L} = \vec{L}_1 + \vec{L}_2$?
   $\ell_1 = 1$, $\ell_2 = 1$, so $\ell = 0, 1, 2$.

   (c) The exchange symmetry of the two-electron spatial wavefunction matches the parity of the quantum number ℓ. Based on this, determine which combinations of s and ℓ are allowed states for the two-electron system.
   $s = 0$ is odd under exchange, while $s = 1$ is even. For ℓ, we have the opposite, $\ell = 0$ is even, $\ell = 1$ is odd, and $\ell = 2$ is even.
   The totally anti-symmetric combinations are therefore $(s, \ell) = (0, 0), (1, 1), (0, 2)$

   (d) For each allowed combination, what are the possible values of the quantum number j, where $\vec{J} = \vec{L} + \vec{S}$?
   For $(s, \ell) = (0, 0)$ we can only have $j = 0$. For $(s, \ell) = (1, 1)$, we can have $j = 0, 1, 2$, and for $(s, \ell) = (0, 2)$ we can only have $j = 2$.

   (e) Assuming that the spin-orbit interaction lifts the degeneracy of the states with different j, how many distinct energy levels make up the fine-structure of the $(3p)^2$ state?
   The allowed j values are $j = 0, 1, 2$, so there would be 3 fine-structure levels.

   (f) Which j levels would shift if a contact interaction between the two valence electrons were added to the Hamiltonian?
   Only states with even orbital exchange symmetry would be affected by a zero-range potential, i.e. $\ell = 0$ or $\ell = 2$. This means only the $j = 0$ an $j = 2$ levels would shift.

4. Let $\vec{J} = \vec{L} + \vec{S}$. Using the method described in the lecture, identify and calculate all non-zero Clebsch-Gordan coefficients for the $\ell = 2$, $s = 1/2$ case.
For starters, we need $j_{max} = \ell + s = 2 + \frac{1}{2} = \frac{5}{2}$ and $j_{min} = |2 - \frac{1}{2}| = \frac{3}{2}$
Starting from $|5/2, 5/2\rangle = |2, 1/2\rangle$, we apply $J_- = L_- + S_-$ to get

$$\begin{aligned} J_-|5/2,5/2\rangle &= L_-|2,1/2\rangle + S_-|2,1/2\rangle \\ \sqrt{\frac{5}{2}\cdot\frac{7}{2} - \frac{5}{2}\cdot\frac{3}{2}}|5/2,3/2\rangle &= \sqrt{2\cdot 3 - 2\cdot 1}|1,1/2\rangle + |2,-1/2\rangle \\ \sqrt{5}|5/2,3/2\rangle &= 2|1,1/2\rangle + |2,-1/2\rangle \\ |5/2,3/2\rangle &= \frac{2}{\sqrt{5}}|1,1/2\rangle + \frac{1}{\sqrt{5}}|2,-1/2\rangle \end{aligned}$$

Applying J_- again gives

$$\begin{aligned} \sqrt{\frac{5}{2}\cdot\frac{7}{2} - \frac{3}{2}\cdot\frac{1}{2}}|5/2,1/2\rangle &= \frac{2}{\sqrt{5}}\left(\sqrt{2\cdot 3 - 1\cdot 0}|0,1/2\rangle + |1,-1/2\rangle\right) + \frac{1}{\sqrt{5}}\sqrt{2\cdot 3 - 2\cdot 1}|1,-1/2\rangle \\ \sqrt{8}|5/2,1/2\rangle &= \frac{2\sqrt{6}}{\sqrt{5}}|0,1/2\rangle + \frac{4}{\sqrt{5}}|1,-1/2\rangle \\ |5/2,1/2\rangle &= \frac{\sqrt{3}}{\sqrt{5}}|0,1/2\rangle + \frac{\sqrt{2}}{\sqrt{5}}|1,-1/2\rangle \end{aligned}$$

After this point, the remaining terms can be found by symmetry, giving:

Table 1: Clebesh Gordan coefficients: $\langle 2, 1/2, m_\ell, m_s | j, m_j \rangle$

j, m_j \ m_ℓ, m_s	2,1/2	2,-1/2	1,1/2	1,-1/2	0,1/2	0,-1/2	-1,1/2	-1,-1/2	-2,1/2	-2,-1/2
5/2,5/2	1	0	0	0	0	0	0	0	0	0
5/2,3/2	0	$1/\sqrt{5}$	$2/\sqrt{5}$	0	0	0	0	0	0	0
5/2,1/2	0	0	0	$\sqrt{2}/\sqrt{5}$	$\sqrt{3}/\sqrt{5}$	0	0	0	0	0
5/2,-1/2	0	0	0	0	0	$\sqrt{3}/\sqrt{5}$	$\sqrt{2}/\sqrt{5}$	0	0	0
5/2,-3/2	0	0	0	0	0	0	0	$2/\sqrt{5}$	$1/\sqrt{5}$	0
5/2,-5/2	0	0	0	0	0	0	0	0	0	1
3/2,3/2	0	$2/\sqrt{5}$	$-1\sqrt{5}$	0	0	0	0	0	0	0
3/2,1/2	0	0	0	$\sqrt{3}\sqrt{5}$	$-\sqrt{2}/\sqrt{5}$	0	0	0	0	0
3/2,-1/2	0	0	0	0	0	$\sqrt{2}/\sqrt{5}$	$-\sqrt{3}/\sqrt{5}$	0	0	0
3/2,-3/2	0	0	0	0	0	0	0	$1/\sqrt{5}$	$-2/\sqrt{5}$	0