Homework Solution Set # 3
Thursday, September 22, 2016

Exercise 1, page 1086

Consider a deuterium atom (composed of a nucleus of spin $I = 1$ and an electron). The electronic angular momentum is $\vec{J} = \vec{L} + \vec{S}$, where $\vec{L}$ is the orbital angular momentum of the electron and $\vec{S}$ is its spin. The total angular momentum of the atom is $\vec{F} = \vec{J} + \vec{I}$, where $I$ is the nuclear spin. The eigenvalues of $J^2$ and $F^2$ are $J(J + 1)\hbar^2$ and $F(F + 1)\hbar^2$ respectively.

a. What are the possible values of the quantum number $J$ and $F$ for a deuterium atom in the 1s ground state?

In the 1s ground state of the deuterium atom the values of $n$ and $l$ are $n = 1$, $l = 0$ and $s = 1/2$. Therefore the possible values of $J$ are such that $|L - 1/2| \leq J \leq L + 1/2 \Rightarrow |1/2 - 0| \leq J \leq 1 + 1/2 \Rightarrow 1/2 \leq J \leq 1 + 1/2$ leaving the only value possible for $J$ to be $J = 1/2$. With this value of $J$ we can find the possible values of $F$ assuming that $I = 1$, $|J - I| \leq F \leq J + I \Rightarrow |1/2 - 1/2| \leq F \leq 1/2 + 1$. Thus $F = 1/2$ or $F = 3/2$.

b. Same question for the deuterium in the 2p excited state.

In the case of the 2p state of deuterium we have

$$n = 2, \quad l = 1$$

This implies $J$ values such that

$$|L - 1/2| \leq J \leq L + 1/2 \Rightarrow |1 - 1/2| \leq J \leq 1 + 1/2$$

resulting in possible values of $J = 3/2$ and $J = 1/2$.

Now for the case of $J = 1/2$ we have

$$\Rightarrow |I - 1/2| \leq F \leq I + 1/2 \Rightarrow |1/2 - 1/2| \leq F \leq 1 + 1/2$$

leading to $F = 1/2$ and $F = 3/2$.

For the case where $J = 3/2$ we find

$$\Rightarrow |I - 3/2| \leq F \leq I + 3/2 \Rightarrow |1 - 3/2| \leq F \leq 1 + 3/2$$

leading to $F = 1/2$, $F = 3/2$ and $F = 5/2$.

Exercise 2, page 1086

The hydrogen atom nucleus is a proton of spin $I = 1/2$.

a) In the notation of the preceding exercise, what are the possible values of the quantum numbers $J$ and $F$ for a hydrogen atom in the 2p level?

In the case of the 2p state for hydrogen we have $n = 2$ and $l = 1$ and the electron spin $s = 1/2$. This implies that

$$|L - s| \leq J \leq L + s \Rightarrow |L - 1/2| \leq J \leq L + 1/2 \Rightarrow |1 - 1/2| \leq J \leq 1 + 1/2$$
Thus the two possible values of $J$ are $J = 3/2$ and $J = 1/2$.

Now for the case of $J = 1/2$ we have

$$|I - 1/2| \leq F \leq I + 1/2 \Rightarrow |1/2 - 1/2| \leq F \leq 1/2 + 1/2$$

leading to $F = 0$ and $F = 1$

For the case where $J = 3/2$ we find

$$|I - 3/2| \leq F \leq I + 3/2 \Rightarrow |1/2 - 3/2| \leq F \leq 1/2 + 3/2$$

leading to $F = 1$ and $F = 2$

b) Let $\{|n,l,s,J,M_J\rangle\}$ be the basis obtained by adding $\vec{L}$ and $\vec{S}$ to form $\vec{J}$ ($M_J \hbar$ is the eigenvalue of $J_z$); and let $\{|n,l,s,J,I,F,M_F\rangle\}$ be the basis obtained by adding $\vec{J}$ and $\vec{I}$ to form $\vec{F}$ ($M_F \hbar$ is the eigenvalue of $F_z$).

The magnetic operator of the electron is:

$$\vec{M} = \mu_B (\vec{L} + 2\vec{S})/\hbar$$

In each of the subspaces $\mathcal{E}(n = 2, l = 1, s = 1/2, J, I = 1/2, F)$ arising from the $2p$ level and subtended by the $2F + 1$ vectors

$$|n = 2, l = 1, s = 1/2, J, I = 1/2, F, M_F\rangle$$

(8)

corresponding to the fixed values of $J$ and $F$, the projection theorem enables us to write

$$\vec{M} = g_{JF} \mu_B \vec{F}/\hbar$$

(9)

Calculate the various possible Landé factors $g_{JF}$ corresponding to the $2p$ level.

Using the projection theorem Complement $D_X$ we can write

$$\vec{L} = \frac{\langle \vec{L} \cdot \vec{J} \rangle}{J(J+1)\hbar^2} \vec{J}$$

$$\vec{S} = \frac{\langle \vec{S} \cdot \vec{J} \rangle}{J(J+1)\hbar^2} \vec{J}$$

Using the results of Complement $D_X$ of equations 41-a and 41-b after adding the two terms we can write:

$$\langle \vec{L} \cdot \vec{J} \rangle_{E_0, l, s, J} = \frac{\hbar^2}{2} [J(J+1) + L(L+1) - S(S+1)]$$

$$\langle \vec{S} \cdot \vec{J} \rangle_{E_0, l, s, J} = \frac{\hbar^2}{2} [J(J+1) - L(L+1) + S(S+1)]$$

Therefore we obtain that

$$\vec{M} = \frac{\mu_B}{J(J+1)\hbar^3} \left\{ \frac{\hbar^2}{2} [J(J+1) + L(L+1) - S(S+1)] + 2 \times \frac{\hbar^2}{2} [J(J+1) - L(L+1) + S(S+1)] \right\} \vec{J}$$

$$= \frac{\mu_B}{J(J+1)\hbar} \left[ \frac{3}{2} J(J+1) - \frac{1}{2} L(L+1) + \frac{1}{2} S(S+1) \right] \vec{J}$$

Now armed with the relation between $\vec{M}$ and $\vec{J}$ we use the projection theorem again to find the relation between $\vec{M}$ and $\vec{F}$ and deduce the Landé factor.
First let's remember that \( \vec{F} = \vec{I} + \vec{J} \), therefore

\[
\vec{J} = \frac{\langle \vec{J} \cdot \vec{F} \rangle}{F(F+1)\hbar^2} \vec{F}
\]

\[
\langle \vec{J} \cdot \vec{F} \rangle_{E_0, l, s, J, I, F} = \frac{\hbar^2}{2} [F(F+1) + J(J+1) - I(I+1)]
\]

Thus

\[
\vec{J} = \frac{[F(F+1) + J(J+1) - I(I+1)]}{2F(F+1)} \vec{F}
\]

We now replace the expression of \( \vec{J} \) in that of \( \vec{M} \) to obtain:

\[
\vec{M} = \mu_B \frac{\hbar}{2J(J+1)} [3J(J+1) - 2L(L+1) + S(S+1)] \times \frac{[F(F+1) + J(J+1) - I(I+1)]}{2F(F+1)} \vec{F}
\]

\[
\vec{M} = \mu_B \frac{\hbar}{4J(J+1)F(F+1)} [3J(J+1) - 2L(L+1) + S(S+1)] \{F(F+1) + J(J+1) - 3/4 \} \vec{F}
\]

Since \( s = 1/2 \) and \( I = 1/2 \), the above expression becomes

\[
\vec{M} = \mu_B \frac{\hbar}{4J(J+1)F(F+1)} \{3J(J+1) - 3 \} \{F(F+1) + J(J+1) - 3/4 \} \vec{F}
\]

We can write the Landé factor as:

\[
g_{JF} = \frac{\hbar}{4J(J+1)F(F+1)} \{3J(J+1) - 3 \} \{F(F+1) + J(J+1) - 3/4 \}
\]

We can summarize the result for all values of \( J \) and \( F \):

\[
\begin{align*}
    l &= 1, s = 1/2, J = 1/2, \text{ and } F = 0, g_{1/20} = \text{ not defined} \\
    l &= 1, s = 1/2, J = 3/2, \text{ and } F = 1, g_{1/21} = -\frac{1}{6} \\
    l &= 1, s = 1/2, J = 3/2, \text{ and } F = 1, g_{3/21} = \frac{4}{3} \\
    l &= 1, s = 1/2, J = 3/2, \text{ and } F = 2, g_{3/22} = \frac{4}{5}
\end{align*}
\]

Exercise 3, page 1086-1087

Consider a system composed of two spins 1/2 particles whose orbital variables are ignored. The Hamiltonian of the system is:

\[
\hat{H} = \omega_1 \hat{S}_{1z} + \omega_2 \hat{S}_{2z}
\]

where \( S_{1z} \) and \( S_{2z} \) are the projections of the spin \( \hat{S}_1 \) and \( \hat{S}_2 \) of the two particles onto \( O_z \), and \( \omega_1 \) and \( \omega_2 \) are real constants.

a. The initial state of the system, at time \( t = 0 \) is:

\[
|\psi(0)\rangle = \frac{1}{\sqrt{2}} [|+\rangle + |\rangle - +\rangle]
\]

where \( |+\rangle = |\frac{1}{2}, \frac{1}{2}, +\rangle \) and \( |\rangle - +\rangle = |\frac{1}{2}, \frac{1}{2}, -\rangle + |\frac{1}{2}, -\frac{1}{2}, +\rangle \) are two of the common eigenvectors of \( \hat{S}_{1z}^2, \hat{S}_{2z}^2, \hat{S}_{1z} \) and \( \hat{S}_{2z} \). At time \( t, \hat{S}^2 = (\hat{S}_1 + \hat{S}_2)^2 \) is measured, what results can be found and with what probabilities?
First, when a measurement is performed on $\hat{S}^2$ the only possible results of the measurement are eigenvalues of $\hat{S}^2$. In this case, the possible eigenvalues are $S(S+1)\hbar^2$ with $S = 1$ and $S = 0$. Therefore the possible results are $2\hbar^2$ or $0\hbar^2$.

Written in the basis of common vectors of $\hat{S}_1^2$, $\hat{S}_2^2$, $\hat{S}_{1z}$ and $\hat{S}_{2z}$ thus also a common basis of $\hat{H} = \omega_1\hat{S}_{1z} + \omega_2\hat{S}_{2z}$

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} [(|+\rangle + |-\rangle)] = |10\rangle$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} [e^{i\frac{\omega_1}{\hbar}t}|+\rangle + e^{i\frac{\omega_2}{\hbar}t}|-\rangle]$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} [e^{i(\omega_1-\omega_2)t}|+\rangle + e^{-i(\omega_1-\omega_2)t}|-\rangle]$$

where $E_{+} = \frac{\hbar}{2}(\omega_1 - \omega_2)$ and $E_{-} = \frac{\hbar}{2}(\omega_1 + \omega_2)$. The probability to find $2\hbar^2$ when measuring $\hat{S}^2$ at time $t$ is given by

$$P(2\hbar^2) = \langle 1 + 1|\psi(t)\rangle + \langle 10|\psi(t)\rangle + \langle 1-1|\psi(t)\rangle$$

In the next expression we switch from the basis $|SM_S\rangle$ to the basis $|m_S, m_{S_z}\rangle$ to find

$$P(2\hbar^2) = |\langle + | + |\psi(t)\rangle + \frac{1}{\sqrt{2}}(\langle + | - | + \rangle |\psi(t)\rangle + \langle - | \psi(t)\rangle)|^2$$

$$= |0 + \frac{1}{2} \left[ e^{i(\omega_1 - \omega_2)/2t} \right] + \frac{1}{2} \left[ e^{-i(\omega_1 - \omega_2)/2t} \right]|^2$$

$$= |\cos \left( \frac{\omega_1 - \omega_2}{2} \right) t |^2 = \cos^2 \left( \frac{\omega_1 - \omega_2}{2} \right) t$$

while the probability to find $0\hbar^2$ is given by

$$P(0\hbar^2) = |\langle 00 |\psi(t)\rangle|^2$$

switching basis like before we have

$$P(0\hbar^2) = \frac{1}{\sqrt{2}}(|\langle + | - | - \rangle |\psi(t)\rangle)$$

$$= \left| \frac{1}{2} \left[ e^{i(\omega_1 - \omega_2)/2t} \right] - \frac{1}{2} \left[ e^{-i(\omega_1 - \omega_2)/2t} \right] \right|^2$$

$$= \left| i \sin \left( \frac{\omega_1 - \omega_2}{2} \right) t \right|^2 = \sin^2 \left( \frac{\omega_1 - \omega_2}{2} \right) t$$

If the initial state of the system is arbitrary, what Bohr frequencies can appear in the time evolution of $< \hat{S}^2 >$?

Using the Ehrenfest Theorem we can write in general that

$$\frac{d\langle \hat{S}^2 \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{H}, \hat{S}^2] \rangle$$

Since $\hat{H}$ and $\hat{S}^2$ commute then

$$[\hat{H}, \hat{S}^2] = 0 \Rightarrow \frac{d\langle \hat{S}^2 \rangle}{dt} = \text{constant}$$

Thus $< \hat{S}^2 >$ does not evolve in time and thus no frequencies will be needed.

c Same question for $< \hat{S}_z > = < \hat{S}_{1z} + \hat{S}_{2z} >$

If the initial state is arbitrary we can write it in the basis of eigenstates of $\hat{H}$, $\hat{S}_1^2$, $\hat{S}_2^2$, $\hat{S}_{1z}$ and $\hat{S}_{2z}$ as

$$|\psi(0)\rangle = \alpha(0)|+\rangle + \beta(0)|-\rangle + \gamma(0)|-\rangle + \delta(0)|-\rangle$$
since this state is an eigenstate of $\hat{H}$ the time evolution is written as

$$|\psi(t)\rangle = \alpha(0)e^{iE_{+}t/\hbar}|++\rangle + \beta(0)e^{iE_{-}t/\hbar}|+-\rangle + \gamma(0)e^{iE_{-}t/\hbar}|-+\rangle + \delta(0)e^{iE_{+}t/\hbar}|--\rangle$$

where we have

$$E_{+}/\hbar = \frac{\omega_1 + \omega_2}{2} \quad E_{-}/\hbar = -\frac{\omega_1 - \omega_2}{2}$$

the corresponding bra is:

$$\langle \psi(t)| = \alpha(t)^*(|++\rangle + \beta(t)^*(|--\rangle + \gamma(t)^*(-+\rangle + \delta(t)^*(|+\rangle$$

for convenience we leave out in the notation of the coefficients the time dependence in what follows.

$$\langle \hat{S}_x \rangle = \langle \hat{S}_{1x} + \hat{S}_{2x} \rangle$$

$$= (\alpha^*(|+\rangle + \beta^*(|--\rangle + \gamma^*(-+\rangle + \delta^*(-|\rangle \frac{1}{2}(S_{1+} + S_{1-})(\alpha|+\rangle + \beta|+-\rangle + \gamma|-+\rangle + \delta|--\rangle)$$

$$+ (\alpha^*(|+\rangle + \beta^*(|--\rangle + \gamma^*(-+\rangle + \delta^*(-|\rangle \frac{1}{2}(S_{2+} + S_{2-})(\alpha|+\rangle + \beta|+-\rangle + \gamma|-+\rangle + \delta|--\rangle)$$

$$= \frac{1}{2}(\alpha^*\gamma + \beta^*\delta) + \frac{1}{2}(\delta^*\beta + \gamma^*\alpha) + \frac{1}{2}(\alpha^*\beta + \gamma^*\delta) + \frac{1}{2}(\delta^*\gamma + \beta^*\alpha)$$

Both frequencies will appear in the time dependence of $\langle \hat{S}_x \rangle$. 

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