DEPARTMENT OF PHYSICS & ASTRONOMY

PHAS3226 QUANTUM MECHANICS

Problem Paper 3 - solutions

Solutions to be handed in on Tuesday 16 November 2010

1. (a) *The component of spin S in the direction of the unit vector $\hat{\mathbf{n}}$ is $S_n = \mathbf{S} \cdot \hat{\mathbf{n}}$ and has two normalized eigenfunctions*

$$|\chi_{\hat{\mathbf{n}}}^+\rangle = \cos(\theta/2)\,|\alpha\rangle + \sin(\theta/2)\,\mathrm{e}^{i\phi}|\beta\rangle \qquad \text{and} \qquad |\chi_{\hat{\mathbf{n}}}^-\rangle = -\sin(\theta/2)\,\mathrm{e}^{-i\phi}|\alpha\rangle + \cos(\theta/2)\,|\beta\rangle$$

satisfying $S_n|\chi_{\hat{\mathbf{n}}}^+\rangle = \frac{\hbar}{2}|\chi_{\hat{\mathbf{n}}}^+\rangle$ and $S_n|\chi_{\hat{\mathbf{n}}}^-\rangle = -\frac{\hbar}{2}|\chi_{\hat{\mathbf{n}}}^-\rangle$, *where (θ, ϕ) are the polar angles of the unit vector $\hat{\mathbf{n}}$. If $|\psi\rangle = \psi_1(\mathbf{r})|\alpha\rangle + \psi_2(\mathbf{r})|\beta\rangle$ is a normalized state, show that the probability of obtaining the value $\hbar/2$ in a measurement of S_n is* [10]

$$P(S_n = \hbar/2) = |\psi_1(\mathbf{r})|^2 \cos^2(\theta/2) + |\psi_2(\mathbf{r})|^2 \sin^2(\theta/2) + \sin\theta\,\mathrm{Re}\left(\psi_1^*\psi_2\mathrm{e}^{-i\phi}\right).$$

Expand the state $|\psi\rangle$ in terms of the eigenstates of S_n as

$$|\psi\rangle = a|\chi_{\hat{\mathbf{n}}}^+\rangle + b|\chi_{\hat{\mathbf{n}}}^-\rangle = \psi_1(\mathbf{r})|\alpha\rangle + \psi_2(\mathbf{r})|\beta\rangle. \tag{1}$$

The probability of obtaining state with $S_n = \frac{1}{2}\hbar$ i.e. to be in state $|\chi_{\hat{\mathbf{n}}}^+\rangle$ is given by $|a|^2$. But

$$\begin{aligned} a &= \langle\chi_{\hat{\mathbf{n}}}^+|\psi\rangle = \psi_1(\mathbf{r})\langle\chi_{\hat{\mathbf{n}}}^+|\alpha\rangle + \psi_2(\mathbf{r})\langle\chi_{\hat{\mathbf{n}}}^+|\beta\rangle & (2)\\ &= \psi_1(\mathbf{r})\cos(\theta/2) + \psi_2(\mathbf{r})\sin(\theta/2)\,\mathrm{e}^{-i\phi}. & (3)\end{aligned}$$

Hence

$$\begin{aligned} |a|^2 &= \left(\psi_1^*(\mathbf{r})\cos(\theta/2) + \psi_2^*(\mathbf{r})\sin(\theta/2)\,\mathrm{e}^{i\phi}\right)\left(\psi_1(\mathbf{r})\cos(\theta/2) + \psi_2(\mathbf{r})\sin(\theta/2)\,\mathrm{e}^{-i\phi}\right),\\ &= |\psi_1(\mathbf{r})|^2\cos^2(\theta/2) + |\psi_2(\mathbf{r})|^2\sin^2(\theta/2)\\ &\quad + \psi_2^*(\mathbf{r})\sin(\theta/2)\,\mathrm{e}^{i\phi}\psi_1(\mathbf{r})\cos(\theta/2) + \psi_1^*(\mathbf{r})\cos(\theta/2)\,\psi_2(\mathbf{r})\sin(\theta/2)\,\mathrm{e}^{-i\phi},\\ &= |\psi_1(\mathbf{r})|^2\cos^2(\theta/2) + |\psi_2(\mathbf{r})|^2\sin^2(\theta/2) + 2\,\mathrm{Re}\left(\psi_1^*(\mathbf{r})\,\psi_2(\mathbf{r})\cos(\theta/2)\sin(\theta/2)\,\mathrm{e}^{-i\phi}\right),\\ &= |\psi_1(\mathbf{r})|^2\cos^2(\theta/2) + |\psi_2(\mathbf{r})|^2\sin^2(\theta/2) + \mathrm{Re}\left(\psi_1^*(\mathbf{r})\,\psi_2(\mathbf{r})\sin(\theta)\,\mathrm{e}^{-i\phi}\right),\\ &= |\psi_1(\mathbf{r})|^2\cos^2(\theta/2) + |\psi_2(\mathbf{r})|^2\sin^2(\theta/2) + \sin\theta\,\mathrm{Re}\left(\psi_1^*(\mathbf{r})\,\psi_2(\mathbf{r})\sin(\theta)\,\mathrm{e}^{-i\phi}\right).\end{aligned}$$

(b) *Obtain, using the raising and/or lowering operators, the six wave functions $|j,m\rangle$ for the p-states of an electron in terms of the spherical harmonics Y_1^m ($\equiv |1,m\rangle$, $m = -1, 0, 1$) and the spinors $|\alpha\rangle$ ($\equiv |\frac{1}{2},\frac{1}{2}\rangle$) and $|\beta\rangle$ ($\equiv |\frac{1}{2},-\frac{1}{2}\rangle$).* [10]

For the p-state electron the orbital quantum number $\ell = 1$, has three z-projections $m = 1, 0, -1$, i.e. states $|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$ ($\equiv Y_\ell^m = Y_1^1, Y_1^0, Y_1^{-1}$). The two spin states $|\alpha\rangle$ ($\equiv |\frac{1}{2},\frac{1}{2}\rangle$) and $|\beta\rangle$ ($\equiv |\frac{1}{2},-\frac{1}{2}\rangle$) have $m_s = \frac{1}{2}$ and $-\frac{1}{2}$ respectively. The maximum total angular momentum has $J = \ell + \frac{1}{2}$, the minimum is $J = \ell - \frac{1}{2}$. The highest (top) state has $J = \frac{3}{2}$, $M_J = \frac{3}{2}$ and is clearly given by

$$\psi\left(\frac{3}{2},\frac{3}{2}\right) = Y_1^1\alpha; \qquad |\frac{3}{2},\frac{3}{2}\rangle = |1,1\rangle|\frac{1}{2},\frac{1}{2}\rangle \tag{4}$$

as $M_J = m_\ell + m_s$. The state $J = \frac{3}{2}$, $M_J = -\frac{3}{2}$ is clearly given by

$$\psi\left(\frac{3}{2},-\frac{3}{2}\right) = Y_1^{-1}\beta; \qquad |\frac{3}{2},-\frac{3}{2}\rangle = |1,-1\rangle|\frac{1}{2},-\frac{1}{2}\rangle. \tag{5}$$

The state $J = \frac{3}{2}$, $M_J = \frac{1}{2}$ can be obtained from the $J = \frac{3}{2}$, $M_J = \frac{3}{2}$ one by application of the lowering operator $\hat{J}_-$. Recall that in general $\hat{J}_-|J,M\rangle = \sqrt{J(J+1) - M(M-1)}\hbar|J,M-1\rangle$, thus

$$\hat{J}_-|\frac{3}{2},-\frac{3}{2}\rangle = \sqrt{\frac{3}{2}\left(\frac{3}{2}+1\right) - \frac{3}{2}\left(\frac{3}{2}-1\right)}\hbar|\frac{3}{2},\frac{1}{2}\rangle = \sqrt{3}\hbar|\frac{3}{2},\frac{1}{2}\rangle. \tag{6}$$

In terms of the individual orbital and spin angular momenta, $\hat{J}_- = \hat{L}_- + \hat{S}_-$ so using $\hat{L}_-|\ell,m_\ell\rangle = \sqrt{\ell(\ell+1) - m_\ell(m_\ell-1)}\hbar|\ell,m_\ell-1\rangle$ and $\hat{S}_-|s,m_s\rangle = \sqrt{s(s+1) - m_s(m_s-1)}\hbar|s,m_s-1\rangle$, with

$\ell = 1$, $m_\ell = 1$, $s = \frac{1}{2}$, $m_s = \frac{1}{2}$,

$$\begin{aligned} \hat{J}_-|\frac{3}{2},\frac{3}{2}\rangle &= \left(\hat{L}_- + \hat{S}_-\right)|1,1\rangle|\frac{1}{2},\frac{1}{2}\rangle, \qquad (7)\\ &= \left(\hat{L}_-|1,1\rangle\right)|\frac{1}{2},\frac{1}{2}\rangle + |1,1\rangle\hat{S}_-|\frac{1}{2},\frac{1}{2}\rangle, \\ \sqrt{3}\hbar|\frac{3}{2},\frac{1}{2}\rangle &= \sqrt{2}\hbar|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle + \hbar|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle \equiv \sqrt{2}\hbar Y_1^0\alpha + \hbar Y_1^1\beta, \qquad (8)\\ |\frac{3}{2},\frac{1}{2}\rangle &= \sqrt{\frac{2}{3}}\hbar|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle + \frac{1}{\sqrt{3}}|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle \equiv \sqrt{\frac{2}{3}}\hbar Y_1^0\alpha + \frac{1}{\sqrt{3}}\hbar Y_1^1\beta. \qquad (9) \end{aligned}$$

The state $J = \frac{3}{2}$, $M_J = -\frac{1}{2}$ can be obtained from the $J = \frac{3}{2}$, $M_J = \frac{1}{2}$ state by application of $\hat{J}_-$ or by applying $\hat{J}_+$ to the state $J = \frac{3}{2}$, $M_J = -\frac{3}{2}$,

$$\begin{aligned} \hat{J}_+|\frac{3}{2},-\frac{3}{2}\rangle &= \left(\hat{L}_+ + \hat{S}_+\right)|1,-1\rangle|\frac{1}{2},\frac{-1}{2}\rangle, \qquad (10)\\ &= \left(\hat{L}_+|1,-1\rangle\right)|\frac{1}{2},-\frac{1}{2}\rangle + |1,-1\rangle\hat{S}_+|\frac{1}{2},-\frac{1}{2}\rangle, \\ \sqrt{3}\hbar|\frac{3}{2},-\frac{1}{2}\rangle &= \sqrt{2}\hbar|1,0\rangle|\frac{1}{2},-\frac{1}{2}\rangle + \hbar|1,-1\rangle|\frac{1}{2},\frac{1}{2}\rangle \equiv \sqrt{2}\hbar Y_1^0\beta + \hbar Y_1^{-1}\alpha, \qquad (11)\\ |\frac{3}{2},-\frac{1}{2}\rangle &= \sqrt{\frac{2}{3}}\hbar|1,0\rangle|\frac{1}{2},-\frac{1}{2}\rangle + \frac{1}{\sqrt{3}}|1,-1\rangle|\frac{1}{2},\frac{1}{2}\rangle \equiv \sqrt{\frac{2}{3}}\hbar Y_1^0\beta + \frac{1}{\sqrt{3}}\hbar Y_1^{-1}\alpha. \qquad (12) \end{aligned}$$

The state $J = \frac{1}{2}$, $M_J = \frac{1}{2}$ must be a linear combination of $Y_1^0\alpha = |1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle$ and $Y_1^1\beta = |1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle$ since $M_J = m_\ell + m_s$, thus

$$|\frac{1}{2},\frac{1}{2}\rangle = a|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle + b|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle. \qquad (13)$$

But

$$\begin{aligned} \hat{J}_+|\frac{1}{2},\frac{1}{2}\rangle &= 0 = \left(\hat{L}_+ + \hat{S}_+\right)\left[a|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle + b|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle\right] \qquad (14)\\ &= \left[a\left(\hat{L}_+|1,0\rangle\right)|\frac{1}{2},\frac{1}{2}\rangle + b|1,1\rangle\hat{S}_+|\frac{1}{2},-\frac{1}{2}\rangle\right] \\ 0 &= a\sqrt{2}\hbar|1,1\rangle|\frac{1}{2},\frac{1}{2}\rangle + b\hbar|1,1\rangle|\frac{1}{2},\frac{1}{2}\rangle = \left(a\sqrt{2}+b\right)\hbar|1,1\rangle|\frac{1}{2},\frac{1}{2}\rangle \qquad (15) \end{aligned}$$

giving $a\sqrt{2} + b = 0$. Normalization requires $|a|^2 + |b|^2 = 1$, so $|a|^2 + 2|a|^2 = 1$ and $a = \frac{1}{\sqrt{3}}$. Hence

$$|\frac{1}{2},\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle - \sqrt{\frac{2}{3}}|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle \equiv \frac{1}{\sqrt{3}}Y_1^0\alpha - \sqrt{\frac{2}{3}}Y_1^1\beta. \qquad (16)$$

Applying $\hat{J}_-$ gives

$$\begin{aligned} \hat{J}_-|\frac{1}{2},\frac{1}{2}\rangle &= \left(\hat{L}_- + \hat{S}_-\right)\left(\frac{1}{\sqrt{3}}|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle - \sqrt{\frac{2}{3}}|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle\right), \qquad (17)\\ \hbar|\frac{1}{2},-\frac{1}{2}\rangle &= \sqrt{\frac{2}{3}}\hbar|1,-1\rangle|\frac{1}{2},\frac{1}{2}\rangle + \frac{1}{\sqrt{3}}|1,0\rangle\hbar|\frac{1}{2},-\frac{1}{2}\rangle - \sqrt{\frac{2}{3}}\sqrt{2}\hbar|1,0\rangle|\frac{1}{2},-\frac{1}{2}\rangle, \\ |\frac{1}{2},-\frac{1}{2}\rangle &= \sqrt{\frac{2}{3}}|1,-1\rangle|\frac{1}{2},\frac{1}{2}\rangle - \frac{1}{\sqrt{3}}|1,0\rangle|\frac{1}{2},-\frac{1}{2}\rangle \equiv \sqrt{\frac{2}{3}}Y_1^{-1}\alpha - \sqrt{\frac{1}{3}}Y_1^0\beta. \qquad (18) \end{aligned}$$

Note the state $J = \frac{1}{2}$, $M_J = \frac{1}{2}$ could also be found by requiring it to be orthogonal to the state

$J=\frac{3}{2}$, $M_J=\frac{1}{2}$ i.e.

$$\begin{aligned}
\langle\frac{3}{2},\frac{1}{2}|\frac{1}{2},\frac{1}{2}\rangle &= 0,\\
0 &= \left(\sqrt{\frac{2}{3}}\hbar\langle 1,0|\langle\frac{1}{2},\frac{1}{2}|+\frac{1}{\sqrt{3}}\langle 1,1|\langle\frac{1}{2},-\frac{1}{2}|\right)\left(a|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle+b|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle\right),\\
0 &= \sqrt{\frac{2}{3}}\hbar a+\frac{1}{\sqrt{3}}b,
\end{aligned}$$

as before.

2. (a) *Show that the operator $\hat{L}\cdot\hat{S}$ can be expressed in terms of the raising and lowering operators $\hat{L}_+$, $\hat{L}_-$, $\hat{S}_+$, S_-, and the components $\hat{L}_z$, $\hat{S}_z$ by $\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}=\frac{1}{2}\left(\hat{L}_+\hat{S}_-+\hat{L}_-\hat{S}_+\right)+\hat{L}_z\hat{S}_z$.}* [4]

The operator $\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}=\hat{L}_x\hat{S}_x+\hat{L}_y\hat{S}_y+\hat{L}_z\hat{S}$. But the the raising/lowering operators $\hat{L}_\pm=\hat{L}_x\pm i\hat{L}_y$ give $\hat{L}_x=\frac{1}{2}\left(\hat{L}_++\hat{L}_-\right)$ and $\hat{L}_y=\frac{1}{2i}\left(\hat{L}_+-\hat{L}_-\right)$ and similar relations for $\hat{S}_x$ and $\hat{S}_y$. Thus

$$\begin{aligned}
\hat{\mathbf{L}}\cdot\hat{\mathbf{S}} &= \frac{1}{2}\left(\hat{L}_++\hat{L}_-\right)\frac{1}{2}\left(\hat{S}_++\hat{S}_-\right)+\frac{1}{2i}\left(\hat{L}_+-\hat{L}_-\right)\frac{1}{2i}\left(\hat{S}_+-\hat{S}_-\right)+\hat{L}_z\hat{S} && (19)\\
&= \frac{1}{2}\left(\hat{L}_+\hat{S}_-+\hat{L}_-\hat{S}_+\right)+\hat{L}_z\hat{S}. && (20)
\end{aligned}$$

(b) *If a particle has spin $\frac{1}{2}$ and is in a state with orbital angular momentum ℓ, there are two basis states, $|\ell,s,\ell_z,s_z\rangle$ which can be expressed in terms of the individual states as $|\ell,s,\ell_z,s_z\rangle=|\ell,\ell_z\rangle|s,s_z\rangle$ with total z-component of angular momentum $m\hbar$, namely*

$$|a\rangle\equiv|\ell,m-\tfrac{1}{2},\tfrac{1}{2}\rangle=|\ell,m-\tfrac{1}{2}\rangle|\tfrac{1}{2},\tfrac{1}{2}\rangle$$

and

$$|b\rangle\equiv|\ell,\tfrac{1}{2},m+\tfrac{1}{2},-\tfrac{1}{2}\rangle=|\ell,m+\tfrac{1}{2}\rangle|\tfrac{1}{2},-\tfrac{1}{2}\rangle.$$

With these two states $|a\rangle$, $|b\rangle$ as a basis show that the matrix representation of the operator $\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}$ is (*Hint: express $L\cdot S$ in terms of the raising and lowering operators $\hat{L}_+$, $\hat{L}_-$, $\hat{S}_+$, S_-, and the components $\hat{L}_z$, $\hat{S}_z$.*) [16]

$$\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}=\begin{pmatrix}\frac{1}{2}\left(m-\frac{1}{2}\right) & \frac{1}{2}\left[\left(\ell+\frac{1}{2}\right)^2-m^2\right]^{1/2}\\ \frac{1}{2}\left[\left(\ell+\frac{1}{2}\right)^2-m^2\right]^{1/2} & -\frac{1}{2}\left(m+\frac{1}{2}\right)\end{pmatrix}\hbar^2.$$

The matrix representation of $\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}$ with the basis states, $|a\rangle$, $|b\rangle$ is

$$\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}=\begin{pmatrix}\langle a|\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|a\rangle & \langle a|\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|b\rangle\\ \langle b|\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|a\rangle & \langle b|\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|b\rangle\end{pmatrix}. \qquad (21)$$

In general $\hat{L}_\pm|\ell,m\rangle=\sqrt{\ell\left(\ell+1\right)-m\left(m\pm1\right)}\hbar|\ell,m\pm1\rangle$ with a similar relation for $\hat{S}_\pm$. Thus explicitly

$$\begin{aligned}
\hat{L}_+|\ell,m-\tfrac{1}{2}\rangle &= \sqrt{\ell\left(\ell+1\right)-\left(m-\tfrac{1}{2}\right)\left(m+\tfrac{1}{2}\right)}\hbar|\ell,m+\tfrac{1}{2}\rangle, && (22)\\
&= \sqrt{\ell^2+\ell+\frac{1}{4}-m^2}\hbar|\ell,m+\tfrac{1}{2}\rangle,\\
&= \sqrt{\left(\ell+\tfrac{1}{2}\right)^2-m^2}\hbar|\ell,m+\tfrac{1}{2}\rangle. && (23)
\end{aligned}$$

Similarly for

$$\begin{aligned}
\hat{L}_-|\ell,m+\tfrac{1}{2}\rangle &= \sqrt{\ell\left(\ell+1\right)-\left(m+\tfrac{1}{2}\right)\left(m-\tfrac{1}{2}\right)}\hbar|\ell,m-\tfrac{1}{2}\rangle, && (24)\\
&= \sqrt{\left(\ell+\tfrac{1}{2}\right)^2-m^2}\hbar|\ell,m-\tfrac{1}{2}\rangle. && (25)
\end{aligned}$$

For $\hat{S}_{\pm}$, $\hat{S}_{+}|\frac{1}{2},-\frac{1}{2}\rangle = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)-\left(-\frac{1}{2}\right)\left(\frac{1}{2}\right)}\hbar|\frac{1}{2},\frac{1}{2}\rangle = \hbar|\frac{1}{2},\frac{1}{2}\rangle$, $\hat{S}_{+}|\frac{1}{2},\frac{1}{2}\rangle = \hat{S}_{-}|\frac{1}{2},-\frac{1}{2}\rangle = 0$ and $\hat{S}_{-}|\frac{1}{2},\frac{1}{2}\rangle = \hbar|\frac{1}{2},-\frac{1}{2}\rangle$.

To evaluate the matrix elements, $\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|a\rangle = \left(\frac{1}{2}\left(\hat{L}_{+}\hat{S}_{-}+\hat{L}_{-}\hat{S}_{+}\right)+\hat{L}_z\hat{S}\right)|\ell,m-\frac{1}{2}\rangle|\frac{1}{2},\frac{1}{2}\rangle$ note that $\hat{L}$ operators only operate on the $|\ell,m\pm\frac{1}{2}\rangle$ states and $\hat{S}$ operators only operate on the$|\frac{1}{2},\pm\frac{1}{2}\rangle$ states. Hence using the relations above for the action of $\hat{L}$ and $\hat{S}$ operators on the states gives

$$\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|a\rangle = \left(\frac{1}{2}\left(\hat{L}_{+}\hat{S}_{-}+\hat{L}_{-}\hat{S}_{+}\right)+\hat{L}_z\hat{S}\right)|\ell,m-\tfrac{1}{2}\rangle|\tfrac{1}{2},\tfrac{1}{2}\rangle \tag{26}$$

$$\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|\ell,m-\tfrac{1}{2}\rangle|\tfrac{1}{2},\tfrac{1}{2}\rangle = \frac{1}{2}\sqrt{\left(\ell+\tfrac{1}{2}\right)^2-m^2}\hbar|\ell,m+\tfrac{1}{2}\rangle\hbar|\frac{1}{2},-\frac{1}{2}\rangle+\left(m-\tfrac{1}{2}\right)\hbar\frac{1}{2}\hbar|\ell,m-\tfrac{1}{2}\rangle|\tfrac{1}{2},\tfrac{1}{2}\rangle \tag{27}$$

and

$$\begin{aligned}\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|b\rangle &= \left(\frac{1}{2}\left(\hat{L}_{+}\hat{S}_{-}+\hat{L}_{-}\hat{S}_{+}\right)+\hat{L}_z\hat{S}_z\right)|\ell,m+\tfrac{1}{2}\rangle|\tfrac{1}{2},-\tfrac{1}{2}\rangle && (28)\\ &= \frac{1}{2}\sqrt{\left(\ell+\tfrac{1}{2}\right)^2-m^2}\hbar|\ell,m-\tfrac{1}{2}\rangle\hbar|\frac{1}{2},\frac{1}{2}\rangle+\left(m+\tfrac{1}{2}\right)\hbar\left(-\frac{1}{2}\hbar\right)|\ell,m-\tfrac{1}{2}\rangle|\tfrac{1}{2},\tfrac{1}{2}\rangle && (29)\end{aligned}$$

Hence using the orthogonality of the states $|\ell,m+\frac{1}{2}\rangle$, $|\ell,m-\frac{1}{2}\rangle$, $|\frac{1}{2},\frac{1}{2}\rangle$ and $|\frac{1}{2},-\frac{1}{2}\rangle$ gives

$$\begin{aligned}\langle a|\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|a\rangle &= \frac{1}{2}\left(m-\tfrac{1}{2}\right)\hbar^2,\\ \langle a|\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|b\rangle &= \frac{1}{2}\left(\left(\ell+\tfrac{1}{2}\right)^2-m^2\right)\hbar^2,\\ \langle b|\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|a\rangle &= \frac{1}{2}\left(\left(\ell+\tfrac{1}{2}\right)^2-m^2\right)\hbar^2,\\ \langle b|\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|b\rangle &= -\frac{1}{2}\left(m+\tfrac{1}{2}\right)\hbar^2.\end{aligned}$$

3. (a) *Write down, without proof, the wave functions for two spin-$\frac{1}{2}$ particles which as eigenstates $|S,S_z\rangle$ of definite total angular momentum S and z-component S_z.* [4]

The singlet state, $S=0$, is

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left(\alpha_1\beta_2-\beta_1\alpha_2\right). \tag{30}$$

The triplet states , $S=1$, are

$$\begin{aligned}|1,1\rangle &= \alpha_1\alpha_2, && (31)\\ |1,0\rangle &= \frac{1}{\sqrt{2}}\left(\alpha_1\beta_2+\beta_1\alpha_2\right), && (32)\\ |1,-1\rangle &= \beta_1\beta_2. && (33)\end{aligned}$$

(b) *Suppose that particles a and b interact through a magnetic dipole-dipole potential*

$$V = A\frac{\left(\boldsymbol{\sigma}_a\cdot\boldsymbol{\sigma}_b\right)r^2-3\left(\boldsymbol{\sigma}_a\cdot\mathbf{r}\right)\left(\boldsymbol{\sigma}_b\cdot\mathbf{r}\right)}{r^5},$$

where r is the inter-particle separation and σ_a and σ_b are the Pauli matrices referring to particles a and b respectively. If the two particles are a fixed distance d apart along the z-axis, show that (Hint; express V in terms of the total spin operator $\hat{\mathbf{S}}^2$ and z-component $\hat{S}_z$ and recall, $\boldsymbol{\sigma}^2=\sigma_x^2+\sigma_y^2+\sigma_z^2=3$)

i. *V does not mix the states $|S,S_z\rangle$, i.e. the off-diagonal elements are zero,*

ii. *and that the diagonal elements are*

$$\langle 1,1|V|1,1\rangle = \langle 1,-1|V|1,-1\rangle = -2\frac{A}{d^3}; \qquad \langle 1,0|V|1,0\rangle = 4\frac{A}{d^3}; \qquad \langle 0,0,|V|0,0\rangle = 0.$$

As the two particles are separated by a **fixed** distance d along the z-axis, the dipole-dipole interaction reduces to

$$V = A\frac{(\boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b)\, d^2 - 3\,(\boldsymbol{\sigma}_{az})\,(\boldsymbol{\sigma}_{bz})\, d^2}{d^5} = \frac{A}{d^3}\left[(\boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b) - 3\,(\sigma_{az})\,(\sigma_{bz})\right] \tag{34}$$

since $\mathbf{r} = d\hat{\mathbf{z}}$ so $\boldsymbol{\sigma}_a \cdot \mathbf{r} = \boldsymbol{\sigma}_a \cdot \hat{\mathbf{z}} d = \sigma_{az}$, and similarly for $\boldsymbol{\sigma}_b \cdot \mathbf{r}$.
The total spin

$$\mathbf{S} = \mathbf{S}_a + \mathbf{S}_b = \frac{\hbar}{2}\,(\boldsymbol{\sigma}_a + \boldsymbol{\sigma}_b) \tag{35}$$

and

$$\mathbf{S}^2 = \frac{\hbar^2}{4}\left(\boldsymbol{\sigma}_a^2 + \boldsymbol{\sigma}_b^2 + 2\boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b\right) \tag{36}$$

and so

$$\boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b = \frac{1}{2}\left(\frac{4}{\hbar^2}\mathbf{S}^2 - \boldsymbol{\sigma}_a^2 - \boldsymbol{\sigma}_b^2\right). \tag{37}$$

But $\boldsymbol{\sigma}^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = 3$ so

$$\boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b = \frac{2}{\hbar^2}\mathbf{S}^2 - 3. \tag{38}$$

Similarly since $S_z = \frac{\hbar}{2}\,(\sigma_{az} + \sigma_{bz})$, then

$$\begin{aligned} \sigma_{az}\sigma_{bz} &= \frac{1}{2}\left(\frac{4}{\hbar^2}\hat{S}_z^2 - \sigma_{az}^2 - \sigma_{bz}^2\right), \\ &= \frac{2}{\hbar^2}\hat{S}_z^2 - 1. \end{aligned} \tag{39}$$

Using eq(**??**) and eq(**??**) in eq(34) gives

$$\begin{aligned} V &= \frac{A}{d^3}\left[\left(\frac{2}{\hbar^2}\mathbf{S}^2 - 3\right) - 3\left(\frac{2}{\hbar^2}\hat{S}_z^2 - 1\right)\right], \\ & \frac{2A}{d^3\hbar^2}\left[\mathbf{S}^2 - 3\hat{S}_z^2\right]. \end{aligned} \tag{40}$$

Thus since $\hat{\mathbf{S}}^2|S, S_z\rangle = S\,(S+1)\,\hbar^2|S, S_z\rangle$ and $\hat{S}_z|S, S_z\rangle = S_z\hbar|S, S_z\rangle$ then $\hat{S}_z^2|S, S_z\rangle = S_z^2\hbar^2|S, S_z\rangle$ and

$$V|S, S_z\rangle = \frac{2A}{d^3\hbar^2}\left[\mathbf{S}^2 - 3\hat{S}_z^2\right]|S, S_z\rangle = \frac{2A}{d^3\hbar^2}\left[S\,(S+1)\,\hbar^2 - 3S_z^2\hbar^2\right]|S, S_z\rangle. \tag{41}$$

Hence the matrix elements are

$$\langle S', S_z'|V|S, S_z\rangle = \frac{2A}{d^3\hbar^2}\left[S\,(S+1)\,\hbar^2 - 3S_z^2\hbar^2\right]\langle S', S_z'|S, S_z\rangle. \tag{42}$$

Since the states $|S, S_z\rangle$ are orthonormal, i.e. $\langle S', S_z'|S, S_z\rangle = \delta_{S'S}\delta_{S_z'S_z}$ eq(**??**) shows that the off-diagonal matrix elements are all zero. [2]
The diagonal elements are [8]

$$\begin{aligned} \langle 1, 1|V|1, 1\rangle &= \frac{2A}{d^3\hbar^2}\left[2\hbar^2 - 3\hbar^2\right] = -\frac{2A}{d^3}, & (43) \\ \langle 1, 0|V1, 0\rangle &= \frac{2A}{d^3\hbar^2}\left[2\hbar^2\right] = \frac{4A}{d^3}, & (44) \\ \langle 1, -1|V|1, -1\rangle &= \frac{2A}{d^3\hbar^2}\left[2\hbar^2 - 3\hbar^2\right] = -\frac{2A}{d^3}, & (45) \\ \langle 0, 0|V|0, 0\rangle &= 0. & (46) \end{aligned}$$

(c) *At time $t = 0$ the two spins are pointing towards each other. By expressing this state in terms of a linear combination of the $|S, S_z\rangle$ states show that after a time $t = \frac{\pi \hbar d^3}{4A}$ the spins will be pointing away from each other.* [6]

Recall from the second year course, that the general solution of the time-dependent Schrödinger equation is $|\psi(t)\rangle = \sum_n c_n |\phi_n\rangle e^{-iE_n t/\hbar}$ where $|\phi_n\rangle$ satisfies the time-independent Schrödinger equation $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$ with energy eigenvalue E_n.

At time $t = 0$ if the two spins are pointing towards each other the spin state $|\psi(0)\rangle$ must be either $\alpha_1\beta_2$ or $\beta_1\alpha_2$ depending on which particles are labelled a and b. Taking the first case $\alpha_1\beta_2$, then state can be expressed in terms of the total spin states $|S, S_z\rangle$ as

$$|\psi(0)\rangle = \alpha_1\beta_1 = \frac{1}{\sqrt{2}}\left[|1,0\rangle + |0,0\rangle\right]. \tag{47}$$

Thus the general time-dependent wavefunction is

$$|\psi(t)\rangle = a|1,0\rangle e^{-iE_{10}t/\hbar} + b|0,0\rangle e^{-iE_{00}t/\hbar} \tag{48}$$

where E_{10} and E_{00} are the energies of the $|1,0\rangle$ and $|0,0\rangle$ states respectively. These are found from the time-independent Schrödinger equation $V|S, S_z\rangle = E_{SS_z}|S, S_z\rangle$. Hence $E_{SS_z} = \langle S, S_z|V|S, S_z\rangle$ and so $E_{10} = \langle 1,0|V|1,0\rangle = \frac{4A}{d^3}$ and $E_{00} = \langle 0,0|V|0,0\rangle = 0$, and thus

$$|\psi(t)\rangle = a|1,0\rangle e^{-i4At/\hbar d^3} + b|0,0\rangle. \tag{49}$$

Thus evaluating eq(**??**) at $t = 0$ and comparing with equ(**??**) gives $a = b = \frac{1}{\sqrt{2}}$, and hence

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}|1,0\rangle e^{-i4At/\hbar d^3} + \frac{1}{\sqrt{2}}|0,0\rangle. \tag{50}$$

Express this in terms of the individual particle spin states gives

$$\begin{aligned}
|\psi(t)\rangle &= \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}(\alpha_1\beta_2 + \beta_1\alpha_2)\right] e^{-i4At/\hbar d^3} + \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}(\alpha_1\beta_2 - \beta_1\alpha_2)\right], \\
&= \frac{1}{2}\left(e^{-i4At/\hbar d^3} + 1\right)\alpha_1\beta_2 + \frac{1}{2}\left(e^{-i4At/\hbar d^3} - 1\right)\beta_1\alpha_2 \\
&= e^{-i2At/\hbar d^3}\frac{1}{2}\left[\left(e^{-i2At/\hbar d^3} + e^{i2At/\hbar d^3}\right)\alpha_1\beta_2 + \left(e^{-i2At/\hbar d^3} - e^{i2At/\hbar d^3}\right)\right]\beta_1\alpha_2 \\
&= e^{-i2At/\hbar d^3}\left[\alpha_1\beta_2\cos\left(\frac{2At}{\hbar d^3}\right) - i\beta_1\alpha_2\sin\left(\frac{2At}{\hbar d^3}\right)\right].
\end{aligned} \tag{51}$$

Thus initially at $t = 0$ the system is in a pure $\alpha_1\beta_2$ state. It is in a pure $\beta_1\alpha_2$ state when $\cos\left(\frac{2At}{\hbar d^3}\right) = 0$, i.e. when $\frac{2At}{\hbar d^3} = (2n+1)\pi/2$, with n a positive integer. Thus the spins are first pointing away from each other at a time $t = \pi\hbar d^3/4A$.