Physics 472 Homework 5 Solutions

1. $$|\chi\rangle = \begin{pmatrix} -3i/4 \\ \sqrt{6}/4 \\ i/4 \end{pmatrix} \qquad s = 1$$

a) $$P(\hbar) = |\langle 1,1|\chi\rangle|^2 = \underline{\underline{\frac{9}{16}}}$$

$$P(0) = |\langle 1,0|\chi\rangle|^2 = \underline{\underline{\frac{6}{16}}} = \frac{3}{8}$$

$$P(-\hbar) = |\langle 1,-1|\chi\rangle|^2 = \underline{\underline{\frac{1}{16}}}$$

b) $$\hat{S}_x = \begin{pmatrix} 0 & \hbar/\sqrt{2} & 0 \\ \hbar/\sqrt{2} & 0 & \hbar/\sqrt{2} \\ 0 & \hbar/\sqrt{2} & 0 \end{pmatrix}$$

From last semester's final exam, problem 3, we know the eigenvectors:

$$|1,1\rangle_x = \begin{pmatrix} 1/2 \\ \sqrt{2}/2 \\ 1/2 \end{pmatrix} \qquad |1,0\rangle_x = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \qquad |1,-1\rangle_x = \begin{pmatrix} \frac{1}{2} \\ -\sqrt{2}/2 \\ \frac{1}{2} \end{pmatrix}$$

$${}_x\langle 1,1|\chi\rangle = \left(\frac{1}{2}, \frac{\sqrt{2}}{2}, \frac{1}{2}\right)\begin{pmatrix} -3i/4 \\ \sqrt{6}/4 \\ i/4 \end{pmatrix} = \frac{-3i}{8} + \frac{\sqrt{12}}{8} + \frac{i}{8} = \frac{\sqrt{12} - 2i}{8}$$

$$P(\hbar) = \frac{\sqrt{12} - 2i}{8} \cdot \frac{\sqrt{12} + 2i}{8} = \frac{12 + 4}{64} = \underline{\frac{1}{4}}$$

$${}_x\langle 1,0|\chi\rangle = \left(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}}\right)\begin{pmatrix} -3i/4 \\ \sqrt{6}/4 \\ i/4 \end{pmatrix} = \frac{-3i}{4\sqrt{2}} - \frac{i}{4\sqrt{2}} = \frac{-4i}{4\sqrt{2}} = \frac{-i}{\sqrt{2}}$$

$$P(0) = \underline{\frac{1}{2}}$$

$${}_x\langle 1,-1|\chi\rangle = \left(\frac{1}{2}, -\frac{\sqrt{2}}{2}, \frac{1}{2}\right)\begin{pmatrix} -\frac{3i}{4} \\ \sqrt{6}/4 \\ i/4 \end{pmatrix} = -\frac{3i}{8} - \frac{\sqrt{12}}{8} + \frac{i}{8} = \frac{-\sqrt{12}-2i}{8}$$

$$P(-\hbar) = \frac{(-\sqrt{12}-2i)(-\sqrt{12}+2i)}{8\cdot 8} = \frac{12+4}{64} = \underline{\underline{\frac{1}{4}}}$$

c)

$$S_y = \begin{pmatrix} 0 & -i\hbar/\sqrt{2} & 0 \\ i\hbar/\sqrt{2} & 0 & -i\hbar/\sqrt{2} \\ 0 & i\hbar/\sqrt{2} & 0 \end{pmatrix}$$

$$S_y\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \hbar\begin{pmatrix} a \\ b \\ c \end{pmatrix} \qquad \left.\begin{matrix} -\frac{i\hbar}{\sqrt{2}} b = \hbar a \rightarrow b = \sqrt{2}ia \\ \frac{i\hbar}{\sqrt{2}} b = \hbar c \rightarrow b = -\sqrt{2}ic \end{matrix}\right\} c = -a$$

$$|1,1\rangle_y = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2}i \\ -1 \end{pmatrix}$$

$$S_y\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0 \qquad \begin{matrix} -\frac{i\hbar}{2} b = 0 \Rightarrow b = 0 \\ \frac{i\hbar}{\sqrt{2}} a - \frac{i\hbar}{2} c = 0 \Rightarrow a = c \end{matrix} \qquad |1,0\rangle_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

$$S_y\begin{pmatrix} a \\ b \\ c \end{pmatrix} = -\hbar\begin{pmatrix} a \\ b \\ c \end{pmatrix} \qquad \left.\begin{matrix} -\frac{i\hbar}{2} b = -\hbar a \rightarrow b = -\sqrt{2}ia \\ \frac{i\hbar}{\sqrt{2}} b = -\hbar c \rightarrow b = \sqrt{2}ic \end{matrix}\right\} c = -a$$

$$|1,-1\rangle_y = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2}i \\ -1 \end{pmatrix}$$

$${}_y\langle 1,1|\chi\rangle = \frac{1}{2}\left(1, -\sqrt{2}\,i, -1\right)\begin{pmatrix} -3i/4 \\ \sqrt{6}/4 \\ i/4 \end{pmatrix} = \frac{1}{2}\left(\frac{-3i}{4} \quad \frac{\sqrt{12}\,i}{4} - \frac{i}{4}\right)$$

$$= \frac{-\sqrt{12}-4}{8}\,i = \frac{-\sqrt{3}-2}{4}\,i$$

$$P(\hbar) = \left(\frac{-\sqrt{3}-2}{4}\right)^2 = \frac{3+4+4\sqrt{3}}{16} = \underline{\underline{\frac{7+4\sqrt{3}}{16}}}$$

$${}_y\langle 1,0|\chi\rangle = \frac{1}{\sqrt{2}}\left(1, 0, 1\right)\begin{pmatrix} -3i/4 \\ \sqrt{6}/4 \\ i/4 \end{pmatrix} = \frac{1}{\sqrt{2}}\left(\frac{-3i}{4} + \frac{i}{4}\right) = \frac{-2i}{4\sqrt{2}}$$

$$= \frac{-i}{2\sqrt{2}}$$

$$P(0) = \underline{\frac{1}{8}}$$

$${}_y\langle 1,-1|\chi\rangle = \frac{1}{2}\left(1, +\sqrt{2}\,i, -1\right)\begin{pmatrix} -3i/4 \\ \sqrt{6}/4 \\ i/4 \end{pmatrix} = \frac{1}{2}\left(\frac{-3i}{4} + \frac{\sqrt{12}\,i}{4} - \frac{i}{4}\right)$$

$$= \frac{+\sqrt{12}-4}{8}\,i = \frac{+\sqrt{3}-2}{4}\,i$$

$$P(-\hbar) = \frac{3+4-4\sqrt{3}}{16} = \underline{\underline{\frac{7-4\sqrt{3}}{16}}}$$

d) Using the probabilities from parts (a)-(c):

$$\langle S_x\rangle = \frac{1}{4}\hbar + \frac{1}{2}\cdot 0 + \frac{1}{4}(-\hbar) = \underline{0}$$

$$\langle S_y\rangle = \frac{7+4\sqrt{3}}{16}\hbar + \frac{1}{8}\cdot 0 + \frac{7-4\sqrt{3}}{16}(-\hbar) = \frac{8\sqrt{3}}{16}\hbar = \underline{\frac{\sqrt{3}}{2}\hbar}$$

$$\langle S_z\rangle = \frac{9}{16}\hbar + \frac{3}{8}\cdot 0 + \frac{1}{16}(-\hbar) = \frac{8}{16}\hbar = \underline{\frac{1}{2}\hbar}$$

Using matrix multiplication:

$$\langle S_x \rangle = \langle \chi | S_x | \chi \rangle = \left(\frac{+3i}{4}, \frac{\sqrt{6}}{4}, \frac{-i}{4} \right) \begin{pmatrix} 0 & \frac{\hbar}{\sqrt{2}} & 0 \\ \frac{\hbar}{\sqrt{2}} & 0 & \frac{\hbar}{\sqrt{2}} \\ 0 & \frac{\hbar}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} -3i/4 \\ \sqrt{6}/4 \\ i/4 \end{pmatrix}$$

$$= \left(\frac{+3i}{4}, \frac{\sqrt{6}}{4}, \frac{-i}{4} \right) \begin{pmatrix} \frac{\sqrt{3}}{4}\hbar \\ \frac{-2i}{4\sqrt{2}}\hbar \\ \frac{\sqrt{3}}{4}\hbar \end{pmatrix}$$

$$= \left(\frac{3\sqrt{3}\,i}{16} - \frac{2\sqrt{3}\,i}{16} - \frac{\sqrt{3}\,i}{16} \right)\hbar = \underline{0}$$

$$\langle S_y \rangle = \langle \chi | S_y | \chi \rangle = \left(\frac{3i}{4}, \frac{\sqrt{6}}{4}, \frac{-i}{4} \right) \begin{pmatrix} 0 & \frac{-i\hbar}{\sqrt{2}} & 0 \\ i\hbar/\sqrt{2} & 0 & -i\hbar/\sqrt{2} \\ 0 & \frac{i\hbar}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} -3i/4 \\ \sqrt{6}/4 \\ i/4 \end{pmatrix}$$

$$= \left(\frac{3i}{4}, \frac{\sqrt{6}}{4}, \frac{-i}{4} \right) \begin{pmatrix} -i\frac{\sqrt{3}}{4}\hbar \\ \hbar/\sqrt{2} \\ \frac{i\sqrt{3}}{4}\hbar \end{pmatrix} = \left(\frac{3\sqrt{3}}{16} + \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{16} \right)\hbar = \frac{8\sqrt{3}}{16}\hbar$$

$$= \underline{\underline{\frac{\sqrt{3}}{2}\hbar}}$$

$$\langle S_z \rangle = \langle \chi | S_z | \chi \rangle = \left(\frac{3i}{4}, \frac{\sqrt{6}}{4}, \frac{-i}{4} \right) \begin{pmatrix} \frac{-3i}{4}\hbar \\ 0 \\ -\frac{i}{4}\hbar \end{pmatrix}$$

$$= \frac{9}{16}\hbar - \frac{1}{16}\hbar = \underline{\underline{\frac{1}{2}\hbar}}$$

Answers agree with those on previous page.

e) $\langle S_x \rangle = 0 = \hbar \sin\theta \cos\phi$ $\left.\begin{matrix} \\ \end{matrix}\right\}$ $\cos\phi = 0$

$\langle S_y \rangle = \frac{\sqrt{3}}{2}\hbar = \hbar \sin\theta \sin\phi$ $\left.\begin{matrix} \\ \end{matrix}\right\}$ $\sin\phi > 0$ $\left.\begin{matrix} \\ \end{matrix}\right\}$ $\underline{\underline{\phi = \frac{\pi}{2}}}$

$\langle S_z \rangle = \frac{1}{2}\hbar = \hbar \cos\theta$ $\quad \cos\theta = \frac{1}{2}$ $\quad \underline{\underline{\theta = \frac{\pi}{3}}}$

Check $\sin\theta = \sin\frac{\pi}{3} = \frac{\sqrt{3}}{2}$ ✓

$|\chi\rangle$ points along axis in y-z plane, 60° from z-axis.

2. Griffiths 5.12

a)

H	$(1s)$		
He	$(1s)^2$		
Li	$(1s)^2$	$(2s)$	
Be	$(1s)^2$	$(2s)^2$	
B	$(1s)^2$	$(2s)^2$	$(2p)$
C	"	"	$(2p)^2$
N	"	"	$(2p)^3$
O	"	"	$(2p)^4$
F	"	"	$(2p)^5$
Ne	"	"	$(2p)^6$

b) H : $s = \frac{1}{2}$, $l = 0 \Rightarrow j = \frac{1}{2}$ $\qquad {}^2S_{1/2}$

He : $s = 0$ (antisymmetric, due to Pauli exclusion)
$l = 0$
$\Rightarrow j = 0$ $\qquad {}^1S_0$

Li : Ignore the closed 1s shell.
$s = \frac{1}{2}$, $l = 0 \Rightarrow j = \frac{1}{2}$ $\qquad {}^2S_{\frac{1}{2}}$

Be : same argument as He
$s = 0$, $l = 0 \Rightarrow j = 0$ $\qquad {}^1S_0$

B : Ignore the closed 1s and 2s shells
$s = \frac{1}{2}$, $l = 1 \Rightarrow j = \frac{3}{2}$ or $\frac{1}{2}$

${}^2P_{\frac{1}{2}}$ or ${}^2P_{3/2}$

C : 2 electrons in $l=1$ orbitals

$s=0$ or 1 ; $l=0, 1,$ or 2

Antisymmetry of overall state requires either

A. $s=0$ with $l=0$ or 2 $\Rightarrow$ $j=0$ or 2

B. or $s=1$ with $l=1$ $\Rightarrow$ $j=0, 1,$ or 2

A. possibilities : ${}^1S_0$, ${}^1D_2$

B. possibilities : ${}^3P_0$, ${}^3P_1$, ${}^3P_2$

N : 3 electrons in $l=1$ orbitals

$s=\frac{3}{2}$ or $\frac{1}{2}$; $l=0, 1, 2,$ or 3

This is complicated. It turns out that the only ladders with definite exchange symmetry are

$s=\frac{3}{2}$ symmetric

$l=3$ symmetric

$l=0$ antisymmetric

So the only possibility is $s=\frac{3}{2}$, $l=0$

I'll discuss this more in the next problem.

${}^4S_{3/2}$

3. Griffiths 5.13

a) $S=1$ states have lower energy than $S=0$.

b) Carbon has $S=1$ from Hund's first rule. $S=1$ is symmetric under exchange.

For 2 electrons each with $l=1$, the $L=2$ ladder is symmetric under exchange, so this violates the Spin-Statistics Thm.

c) Boron has $s=\frac{1}{2}$, $l=1 \Rightarrow j=\frac{3}{2}$ or $\frac{1}{2}$

$\underline{j=\frac{1}{2}}$ has lower energy ${}^2P_{1/2}$

d) C : Hund's 1^{st} rule $\rightarrow$ $s=1$ is lower

From previous problem, $s=1$ goes with $L=1$ to have total antisymmetry

$J=0, 1,$ or $2 \Rightarrow J=0$ has lowest energy by Hund's 3^{rd} rule

$\underline{{}^3P_0}$

N: Hund's 1^{st} rule $\rightarrow$ $s=\frac{3}{2}$ is lowest (symmetric)

The only spatial state that is antisymmetric under exchange is $L=0$

N: continued. One way to see this is to take the $|s=\tfrac{3}{2}, m_s=\tfrac{3}{2}\rangle = |\uparrow\uparrow\uparrow\rangle$ state.

Since all electrons have spin up, they must occupy different spatial orbitals: $m_l = 1, 0,$ and -1.

So the z-component of the total orbital angular momentum is zero. The only way to assure that is to have $L=0$.

If your interested, here is what the $L=0$ state looks like in the $|m_{l1}\ m_{l2}\ m_{l3}\rangle$ basis, where this is shorthand for $|l_1\ m_{l1}\rangle \otimes |l_2\ m_{l2}\rangle \otimes |l_3\ m_{l3}\rangle$

$$
\begin{aligned}
|L=0, m_L=0\rangle = \frac{1}{\sqrt{6}}\Big\{ & |1\ 0\ -1\rangle - |0\ 1\ -1\rangle \\
& - |1\ -1\ 0\rangle + |-1\ 1\ 0\rangle \\
& + |0\ -1\ 1\rangle - |-1\ 0\ 1\rangle \Big\}
\end{aligned}
$$

If you check this, you'll see that it is antisymmetric under exchange of any 2 particles.

4. a) $s = 0 \Rightarrow l$ even $\quad l = 0, 2, 4, \ldots$

$s = 1 \Rightarrow l$ odd $\quad l = 1, 3, \ldots$

b)

s	l	j	
0	0	0	${}^1S_0$
0	2	2	${}^1D_2$
0	4	4	${}^1G_4$
1	1	2	${}^3P_2$
1	1	1	${}^3P_1$
1	1	0	${}^3P_0$
1	3	4	${}^3F_4$
1	3	3	${}^3F_3$
1	3	2	${}^3F_2$