

Consider a spin coupled to a magnetic field via the Hamiltonian

$H = \gamma \mathbf{S} \cdot \mathbf{B}$  where the three dimensional magnetic field is  $\mathbf{B} = (B_x, B_y, B_z) = B_0 (1, 1, 0)$ ,  $B_0$  is a constant, and  $\gamma$  is another constant. The three dimensional spin vector is  $\mathbf{S} = (S_x, S_y, S_z)$ , and each  $S_x, S_y, S_z$  are the usual 2x2 spin matrices.

(a) Find the two eigenvalues of the resulting 2x2 Hamiltonian  $H$ .

(b) Find the two normalized-to-one eigenvectors of the 2x2 Hamiltonian  $H$ .

---

$$H = \gamma \vec{S} \cdot \vec{B} = \gamma B_0 (S_x + S_y) = \gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 0 & 1-i \\ 1+i & 0 \end{pmatrix}$$

---

$$\begin{vmatrix} -\lambda & 1-i \\ 1+i & -\lambda \end{vmatrix} = 0; \quad \lambda^2 - \underbrace{(1-i)(1+i)}_2 = 0, \quad \lambda = \pm \sqrt{2}$$

Eigenvalues of  $H$  are then

$$\lambda_H = \pm \gamma B_0 \frac{\hbar}{2} \sqrt{2}$$

$$\text{For } \lambda = +\sqrt{2} \rightarrow \begin{pmatrix} 0 & 1-i \\ 1+i & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \sqrt{2} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}; \begin{pmatrix} (1-i)\beta \\ (1+i)\alpha \end{pmatrix} = \begin{pmatrix} \sqrt{2}\alpha \\ \sqrt{2}\beta \end{pmatrix}$$

$$\text{I.e. } \beta = \frac{(1+i)}{\sqrt{2}} \alpha; \quad \chi_+ = \alpha \begin{pmatrix} 1 \\ \frac{1+i}{\sqrt{2}} \end{pmatrix}$$

$$\chi_+^\dagger \chi_+ = |\alpha|^2 (1, \frac{1-i}{\sqrt{2}}) \begin{pmatrix} 1 \\ \frac{1+i}{\sqrt{2}} \end{pmatrix} = |\alpha|^2 (1 + \frac{1}{2} \cdot 2) = 2|\alpha|^2 = 1$$

$$\alpha = \frac{1}{\sqrt{2}}$$

$$\boxed{\chi_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \frac{1+i}{\sqrt{2}} \end{pmatrix}}$$

$$\text{For } \lambda = -\sqrt{2} \rightarrow \begin{pmatrix} 0 & 1-i \\ 1+i & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -\sqrt{2} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}; \begin{pmatrix} (1-i)\beta \\ (1+i)\alpha \end{pmatrix} = \begin{pmatrix} -\sqrt{2}\alpha \\ -\sqrt{2}\beta \end{pmatrix}$$

$$\text{I.e. } \beta = -\frac{(1+i)\alpha}{\sqrt{2}}; \quad \chi_- = \alpha \begin{pmatrix} 1 \\ -\frac{1+i}{\sqrt{2}} \end{pmatrix}$$

$$\chi_-^\dagger \chi_- = |\alpha|^2 (1, -\frac{1-i}{\sqrt{2}}) \begin{pmatrix} 1 \\ -\frac{1+i}{\sqrt{2}} \end{pmatrix} = |\alpha|^2 [1 + \frac{1}{2} \frac{(1+i-i+1)}{2}]$$

$$= 2|\alpha|^2 = 1 \rightarrow \alpha = \frac{1}{\sqrt{2}}$$

$$\boxed{\chi_- = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\frac{1+i}{\sqrt{2}} \end{pmatrix}}$$

$$\chi_+^\dagger \chi_- = 0$$

$$\chi_+^\dagger \chi_+ = 1$$

$$\chi_-^\dagger \chi_- = 1$$

Consider the spinor  $\chi = A \begin{pmatrix} 2 \\ 1+i \end{pmatrix}$

- Find the normalization A.
- Find the expectation value of the 2x2 spin operator  $S_z$ .
- Find the expectation value of the 2x2 spin operator  $S_x$ .
- Find the expectation value of the 2x2 spin operator  $(S_y)^2$ .
- What is the probability of finding  $+\hbar/2$  if  $S_z$  is measured?

---

$$\begin{aligned} \text{(a)} \quad \chi^\dagger \chi &= |A|^2 (2, 1-i) \begin{pmatrix} 2 \\ 1+i \end{pmatrix} = |A|^2 [4 + (1-i)(1+i)] = \\ &= |A|^2 [4 + 2] = 1 \rightarrow \boxed{A = \frac{1}{\sqrt{6}}} \end{aligned}$$

---

$$\begin{aligned} \text{(b)} \quad \langle S_z \rangle &= \chi^\dagger \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \chi = \frac{\hbar}{2} |A|^2 (2, 1-i) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \\ &= \frac{\hbar}{2} \cdot \frac{1}{6} \cdot (2, 1-i) \begin{pmatrix} 2 \\ -1-i \end{pmatrix} = \frac{\hbar}{12} [4 - (1-i)(1+i)] = \\ &= \frac{\hbar}{12} (4-2) = \boxed{\frac{\hbar}{6}} \end{aligned}$$

$$\begin{aligned}
 (c) \quad \langle S_x \rangle &= \chi^\dagger \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \chi = \frac{\hbar}{2} |A|^2 (2, 1-i) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \\
 &= \frac{\hbar}{2} \cdot \frac{1}{6} (2, 1-i) \begin{pmatrix} 1+i \\ 2 \end{pmatrix} = \frac{\hbar}{12} [2(1+i) + (1-i)2] = \\
 &= \frac{\hbar}{12} [2 + 2i + 2 - 2i] = \boxed{\frac{\hbar}{3}}
 \end{aligned}$$


---

$$(d) \quad (S_y)^2 = \frac{\hbar^2}{4} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

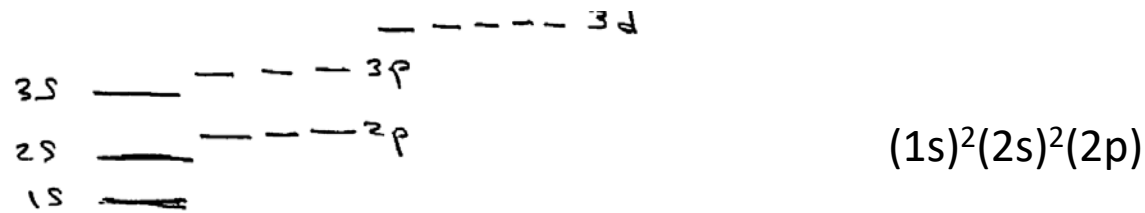
$$\text{Thus, } (S_y)^2 \chi = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \chi = \frac{\hbar^2}{4} \chi$$

$$\langle (S_y)^2 \rangle = \chi^\dagger (S_y)^2 \chi = \frac{\hbar^2}{4} \underbrace{\chi^\dagger \chi}_1 = \boxed{\frac{\hbar^2}{4}} \text{ as expected.}$$


---

$$(e) \quad \chi = \begin{pmatrix} 2/\sqrt{6} \\ (1+i)/\sqrt{6} \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}; \quad \text{Prob. of } +\hbar/2 = |a|^2 = \left(\frac{2}{\sqrt{6}}\right)^2 = \frac{4}{6} = \boxed{\frac{2}{3}}$$

Consider the boron B atom with  $Z=5$ . (a) Write the ground state electronic configuration using the notation  $(1s)^2 \dots$  (b) What is the net spin of boron in the ground state? (c) Using the notation  $^{2S+1}L_J$ , write all the possible values.



Five electrons can be placed as for the ground state.

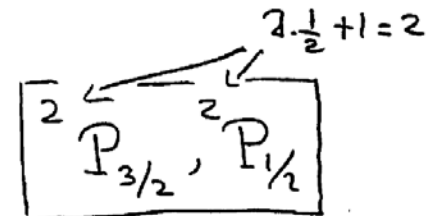
The total spin  $S$  is thus  $1/2$ .

The total orbital angular momentum  $L$  is 1, so well because the 4 lowest energy states have  $l=0$ .

$S=1/2$  and  $L=1$  can be combined as  $3/2$  and as  $1/2$  (i.e.  $J$ )

In the notation  $^{2S+1}L_J$

that means the possibilities are



Consider 4 electrons, each with spin  $\frac{1}{2}$ . Find the possible values of the total spin, including for each value how many times it appears. This is a problem similar to that of the 3 quarks in one of the HWs where the answer was  $3/2, 1/2, 1/2$ .

$\frac{1}{2} \quad \frac{1}{2} \quad \frac{1}{2} \quad \frac{1}{2}$   
 $\underbrace{\hspace{1.5cm}} \quad \underbrace{\hspace{1.5cm}}$   
 can be combined as 1 and 0      can be combined as 1 and 0

1 combined with 1 gives 2, 1, 0  
 1 combined with 0 gives 1  
 0 combined with 1 gives 1  
 0 combined with 0 gives 0

Thus, the answer is

|         |
|---------|
| 2       |
| 1, 1, 1 |
| 0, 0    |

Consider three electrons in a Li atom, one in the lowest energy state  $\psi_{100}(r_1)$  of the H atom, another in  $\psi_{200}(r_2)$ , and a third in  $\psi_{300}(r_3)$ : (a) Write the fully *antisymmetric* wave function of this problem (using the notation  $\psi_{100}(r_1)$  etc of course, not the explicit wave functions). No need to normalize to one. (b) To complete this excited state, as spin portion of the wave function choose the state with the maximum total spin and maximum projection  $m$ .

We start with  $\psi_{100}(r_1) \psi_{200}(r_2) \psi_{300}(r_3)$

$$\left\{ \begin{array}{ll} r_1 \leftrightarrow r_2 & \psi_{100}(r_2) \psi_{200}(r_1) \psi_{300}(r_3) \quad (-) \\ r_2 \leftrightarrow r_3 & \psi_{100}(r_1) \psi_{200}(r_3) \psi_{300}(r_2) \quad (-) \\ r_1 \leftrightarrow r_3 & \psi_{100}(r_3) \psi_{200}(r_2) \psi_{300}(r_1) \quad (-) \end{array} \right.$$

$$\begin{array}{ll} r_1 \leftrightarrow r_2 & \psi_{100}(r_3) \psi_{200}(r_1) \psi_{300}(r_2) \quad (+) \\ r_2 \leftrightarrow r_3 & \end{array}$$

$$\begin{array}{ll} r_1 \leftrightarrow r_3 & \psi_{100}(r_2) \psi_{200}(r_3) \psi_{300}(r_1) \quad (+) \\ r_3 \leftrightarrow r_2 & \end{array}$$

$$\begin{array}{ll} r_2 \leftrightarrow r_1 & \psi_{100}(r_2) \psi_{200}(r_3) \psi_{300}(r_1) \quad (+) \\ r_1 \leftrightarrow r_3 & \end{array}$$

Normalization  
if needed

$$\Psi = \frac{1}{\sqrt{6}} \left[ \begin{aligned} &\psi_{100}(r_1) \psi_{200}(r_2) \psi_{300}(r_3) + \\ &\psi_{100}(r_3) \psi_{200}(r_1) \psi_{300}(r_2) + \\ &\psi_{100}(r_2) \psi_{200}(r_3) \psi_{300}(r_1) - \\ &- \psi_{100}(r_2) \psi_{200}(r_1) \psi_{300}(r_3) - \\ &- \psi_{100}(r_1) \psi_{200}(r_3) \psi_{300}(r_2) - \\ &- \psi_{100}(r_3) \psi_{200}(r_2) \psi_{300}(r_1) \end{aligned} \right]$$

Spinor?  
Simply use

$$|\uparrow\uparrow\uparrow\rangle$$

$$S=3/2, m=3/2$$