

# 5.73

## Quiz 30 ANSWERS

1.

The six np spin orbitals, listed in standard order, are:  $1\alpha, 1\beta, 0\alpha, 0\beta, -1\alpha, -1\beta$ .  
The number 1, 0, -1 refers to  $m_l$ , and  $\alpha, \beta$  refers to  $m_s = 1/2, -1/2$ .

Matrix elements of a one-electron operator,  $\mathbf{F} = \mathbf{f}(i)$ , are

$$\Delta_{so} = 0 \langle \|a, a_i\| \mathbf{F} \|a, a_i\| \rangle = \sum \langle a_i | \mathbf{f} | a_i \rangle$$

$$\Delta_{so} = 0 \langle \|a, b\| \mathbf{F} \|a, a_i\| \rangle = \langle b | \mathbf{f} | a_i \rangle$$

$$\langle p1 | \ell_+ | p0 \rangle = \langle p0 | \ell_+ | p-1 \rangle = 2^e; \langle \alpha | \mathbf{s}_+ | \beta \rangle = 1$$

A.  $\mathbf{F} \equiv \sum_i -\gamma B_z (\ell_{z_i} + 2\mathbf{s}_{z_i})$ . Evaluate  $\langle \mathbf{F} \rangle$  for  $\psi = \|1\alpha 0\beta\|$ .

This operator operates sequentially on electrons #1 and #2.

$$\begin{aligned} & \left\langle \|1\alpha 0\beta\| \sum_{i=1}^2 -\gamma B_z (\ell_{z_i} + 2s_{z_i}) \|1\alpha 0\beta\| \right\rangle \\ &= -\gamma B_z \hbar \left[ \underbrace{1+0}_{\ell_z} + \underbrace{2(1/2) + 2(-1/2)}_{s_z} \right] = -\gamma B_z \hbar \end{aligned}$$

Recall  $\ell_z |n p \lambda\rangle = \hbar \lambda |n p \lambda\rangle$ .

B.  $\mathbf{F} \equiv \mathbf{J}_+ = \sum_i (\ell_{+i} + \mathbf{s}_{+i})$ . Evaluate  $\langle \|1\alpha 0\alpha\| \mathbf{F} \|1\alpha -1\alpha\| \rangle$ .

[HINT:  $\mathbf{F}$  is a sum, not a product, of two one-electron operators.]

There is an orbital mismatch in position #2. This is where we must put our  $1e^-$  operator. This mismatch is "fixed" by  $\ell_+$  and NOT by  $\mathbf{s}_+$ .

$$\begin{aligned} & \left\langle \|1\alpha 0\alpha\| \sum_i (\ell_{+i} + \mathbf{s}_{+i}) \|1\alpha -1\alpha\| \right\rangle = \langle 0\alpha | \ell_+ | -1\alpha \rangle \\ &= \hbar [1 \cdot 2 - (-1) \cdot 0]^{1/2} = \sqrt{2} \hbar \end{aligned}$$

C. 
$$\mathbf{F} = \sum_i \ell_i \cdot \mathbf{s}_i = \sum_i \left[ \ell_{zi} \mathbf{s}_{zi} + \frac{1}{2} (\ell_{+i} \mathbf{s}_{-i} + \ell_{-i} \mathbf{s}_{+i}) \right].$$

Evaluate  $\langle |1\alpha 0\beta\rangle | \mathbf{F} | |1\alpha - 1\alpha\rangle$

The orbital mismatch is in position #2. It is "fixed" by  $1/2 \ell_+ \mathbf{s}_-$ .

$$\begin{aligned} \left\langle |1\alpha 0\beta\rangle \left| \sum_i \left[ \ell_{zi} \mathbf{s}_{zi} + \frac{1}{2} (\ell_{+i} \mathbf{s}_{-i} + \ell_{-i} \mathbf{s}_{+i}) \right] \right| |1\alpha - 1\alpha\rangle \right\rangle &= \left\langle 0\beta \left| \frac{1}{2} \ell_+ \mathbf{s}_- \right| -1\alpha \right\rangle \\ &= \frac{1}{2} \hbar^2 [1 \cdot 2 - (-1) \cdot 0]^{1/2} \\ &= 2^{-1/2} \hbar^2 \end{aligned}$$

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