

5.73

Quiz 30

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 α, β refers to $m_s = 1/2, -1/2$.

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

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

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

$$\langle p1 | \ell_+ | p0 \rangle = \langle p0 | \ell_+ | p-1 \rangle = 2^{1/2}; \langle \alpha | s_+ | \beta \rangle = 1$$

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

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.]

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

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