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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

$\Delta so = 0\ \langle||a_i a_2||\mathbf{F}||a_i a_2||\rangle = \sum\langle a_i|\mathbf{f}|a_i\rangle$

$\Delta so = 0\ \langle||a_i b||\mathbf{F}||a_i a_2||\rangle = \langle b_i|\mathbf{f}|a_2\rangle$

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

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

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

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

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