5.73

Quiz 33 ANSWERS

1. Consider the nd^2 electronic configuration. Denote the 10 possible spin-orbitals as $2\alpha, 2\beta, 1\alpha, 1\beta, 0\alpha, 0\beta, -1\alpha, -1\beta, -2\alpha, -2\beta$, and use the above as the standard order.

A. Fill each of the M_L, M_S boxes on the diagram below with all of the appropriate nonzero Slater determinants.

M_S \ M_L	4	3	2	1	0
1		$2\alpha1\alpha$	$2\alpha0\alpha$	$2\alpha{-1}\alpha$ $1\alpha0\alpha$	$2\alpha{-2}\alpha$ $1\alpha{-1}\alpha$
0	$2\alpha2\beta$	$2\alpha1\beta$ $2\beta1\alpha$	$2\alpha0\beta$ $0\beta2\alpha$ $1\alpha1\beta$	$2\alpha{-1}\beta$ $2\beta{-1}\alpha$ $1\alpha0\beta$ $1\beta0\alpha$	$2\alpha{-2}\beta$ $2\beta{-2}\alpha$ $1\alpha{-1}\beta$ $1\beta{-1}\alpha$ $0\alpha0\beta$

B. What are all of the L-S terms that belong to nd^2?

^3F, ^3P, ^1G, ^1D, ^1S

C. The linear combination of the two Slater determinants in the $|M_L = 3, M_S = 0\rangle$ box that corresponds to the $|^1G\ M_L = 3, M_S = 0\rangle$ many-electron basis state is $2^{-1/2}[||2\alpha1\beta|| - ||2\beta1\alpha||]$. Use orthogonality with the $|^1G\ 3\ 0\rangle$ basis state to derive the linear combination of two Slater determinants that corresponds to $|^3F\ 3\ 0\rangle$.

$$\left|{}^1G\ M_L = 3, M_S = 0\right\rangle = 2^{-1/2}\left[\left\|2\alpha1\beta\right\| - \left\|2\beta1\alpha\right\|\right]$$

by orthogonality $\left|{}^3F\ M_L = 3, M_S = 0\right\rangle = 2^{-1/2}\left[\left\|2\alpha1\beta\right\| + \left\|2\beta1\alpha\right\|\right]$

D. Calculate $\left\langle \ {}^1\mathrm{G} \quad 3 \quad 0 \ \left|\mathbf{H}^{SO}\right| \ {}^3\mathrm{F} \quad 3 \quad 0 \ \right\rangle = \hbar^2\zeta_{nd}$ [?].

You need only consider $\mathbf{H}^{SO} = \sum_i \zeta_{nd}\ell_{iz}\mathbf{s}_{iz}$.

$$\left\langle {}^1\mathrm{G}\ \mathrm{M}_L = 3, M_\mathrm{S} = 0 \middle| \mathbf{H}^{\mathrm{SO}} \middle| {}^3\mathrm{F}\ \mathrm{M}_L = 3, M_\mathrm{S} = 0 \right\rangle$$

$$= \zeta_{nd}\left[\left\langle \left|2\alpha 1\beta\right| \middle| \ell_z\mathbf{s}_z \middle| \left|2\alpha 1\beta\right| \right\rangle - \left\langle \left|2\beta 1\alpha\right| \middle| \ell_z\mathbf{s}_z \middle| \left|2\beta 1\alpha\right| \right\rangle\right.$$

$$= \zeta_{nd}\hbar^2\left[2\left(\frac{1}{2}\right) + 1\left(-\frac{1}{2}\right) - 2\left(-\frac{1}{2}\right) - 1\left(\frac{1}{2}\right)\right]$$

$$= \zeta_{nd}\hbar^2\left[1 - \frac{1}{2} + 1 - \frac{1}{2}\right] = \zeta_{nd}\hbar^2 1$$