## 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.

$M_{\rm L}$	4	3	2	1	0
1		2α1α	2α0α	2α-1α 1α0α	2α-2α 1α-1α
0	2α2β	2α1β 2β1α	2α0β 0β2α 1α1β	2α-1β 2β-1α 1α0β 1β0α	2α-2β 2β-2α 1α-1β 1β-1α 0α0β

- B. What are all of the L-S terms that belong to nd<sup>2</sup>?

  <sup>3</sup>F, <sup>3</sup>P, <sup>1</sup>G, <sup>1</sup>D, <sup>1</sup>S
- 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  $2^{-1/2}[\|2\alpha 1\beta\| \|2\beta 1\alpha\|]$ . Use orthogonality with the  $|^1G\ 3\ 0\rangle$  basis state to derive the linear combination of two Slater determinants that corresponds to  $|^3F\ 3\ 0\rangle$ .

$$\begin{vmatrix} ^{1}G \ M_{L} = 3, M_{S} = 0 \end{vmatrix} = 2^{-1/2} \left[ ||2\alpha 1\beta|| - ||2\beta 1\alpha|| \right]$$
by orthogonality  $|^{3}F \ M_{L} = 3, M_{S} = 0 \rangle = 2^{-1/2} \left[ ||2\alpha 1\beta|| + ||2\beta 1\alpha|| \right]$ 

D. Calculate  $\langle {}^{1}G \ 3 \ 0 \ | \mathbf{H}^{SO} | {}^{3}F \ 3 \ 0 \rangle = \hbar^{2}\zeta_{nd}$  [?]. You need only consider  $\mathbf{H}^{SO} = \sum_{i} \zeta_{nd} \ell_{iz} \mathbf{s}_{iz}$ .

$$\langle {}^{1}G M_{L} = 3, M_{S} = 0 | \mathbf{H}^{SO} | {}^{3}F M_{L} = 3, M_{S} = 0 \rangle$$

$$= \zeta_{nd} \left[ \langle || 2\alpha 1\beta || \ell_{z} \mathbf{s}_{z} || 2\alpha 1\beta || \rangle - \langle || 2\beta 1\alpha || \ell_{z} \mathbf{s}_{z} || 2\beta 1\alpha || \rangle$$

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

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

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