

5.73

Quiz 33

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.

$M_L \backslash M_S$	4	3	2	1	0
1					
0					

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

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

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

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