

Calculate the spin-orbit splitting of the L-shell hole. With a reference state  $|0\rangle$  the 2p-hole states span a six-dimensional subspace corresponding to the removal of a 2p-electron ( $2p_x, 2p_y, 2p_z$ ) of spin  $\alpha$  or  $\beta$

$$|p_{i\sigma}^{-1}\rangle = a_{i\sigma}|0\rangle \quad i = x, y, z \quad \sigma = \alpha, \beta \quad (1)$$

and the diagonalization of the spin-orbit operator in this basis leads for the atomic case to two degenerate sets of  $J = 1/2$  and  $J = 3/2$

$$V_{ij}^{\sigma\tau} = \langle p_{i\sigma}^{-1} | V | p_{j\tau}^{-1} \rangle = \langle 0 | a_{i\sigma}^\dagger V a_{j\tau} | 0 \rangle \quad (2)$$

Explicit blocking of the spin part yields the matrix

$$\mathbf{V} = \begin{pmatrix} V_{ij}^{\alpha\alpha} & V_{ij}^{\alpha\beta} \\ V_{ij}^{\beta\alpha} & V_{ij}^{\beta\beta} \end{pmatrix} \quad (3)$$

where each subblock is a 3x3 matrix labeled by the  $p$  orbitals. Spin-orbit selection rules give

$$V_{ij}^{\alpha\alpha} = \langle p_{i\alpha}^{-1} | l_z s_z | p_{j\alpha}^{-1} \rangle \quad (4)$$

$$V_{ij}^{\beta\beta} = \langle p_{i\beta}^{-1} | l_z s_z | p_{j\beta}^{-1} \rangle \quad (5)$$

$$V_{ij}^{\alpha\beta} = \langle p_{i\alpha}^{-1} | -l_1 s_{-1} | p_{j\beta}^{-1} \rangle \quad (6)$$

$$V_{ij}^{\beta\alpha} = \langle p_{i\beta}^{-1} | -l_{-1} s_1 | p_{j\alpha}^{-1} \rangle \quad (7)$$

$$(8)$$

and the off-diagonal blocks can be transformed to a common spin component with the Wigner-Eckart theorem (notation  $C_{m_1, m_2, m}^{j_1, j_2, j}$ )

$$V_{ij}^{\alpha\beta} = \langle p_{i\beta}^{-1} | -l_1 s_0 | p_{j\beta}^{-1} \rangle C_{\frac{1}{2}, -1, -\frac{1}{2}}^{\frac{1}{2}, 1, \frac{1}{2}} / C_{\frac{1}{2}, 0, \frac{1}{2}}^{\frac{1}{2}, 1, \frac{1}{2}} = \langle p_{i\beta}^{-1} | -l_1 s_0 | p_{j\beta}^{-1} \rangle \sqrt{2/3} / \sqrt{1/3} = \langle p_{i\beta}^{-1} | (l_x + il_y) s_z | p_{j\beta}^{-1} \rangle \quad (9)$$

$$V_{ij}^{\beta\alpha} = \langle p_{i\beta}^{-1} | -l_{-1} s_0 | p_{j\beta}^{-1} \rangle C_{-\frac{1}{2}, 1, \frac{1}{2}}^{\frac{1}{2}, 1, \frac{1}{2}} / C_{\frac{1}{2}, 0, \frac{1}{2}}^{\frac{1}{2}, 1, \frac{1}{2}} = \langle p_{i\beta}^{-1} | -l_{-1} s_0 | p_{j\beta}^{-1} \rangle (-\sqrt{2/3}) / \sqrt{1/3} = \langle p_{i\beta}^{-1} | (l_x - il_y) s_z | p_{j\beta}^{-1} \rangle \quad (10)$$

and finally

$$V_{ij}^{\alpha\alpha} = \langle p_{i\beta}^{-1} | l_z s_z | p_{j\beta}^{-1} \rangle C_{-\frac{1}{2}, 0, -\frac{1}{2}}^{\frac{1}{2}, 1, \frac{1}{2}} / C_{\frac{1}{2}, 0, \frac{1}{2}}^{\frac{1}{2}, 1, \frac{1}{2}} = -\langle p_{i\beta}^{-1} | l_z s_z | p_{j\beta}^{-1} \rangle \quad (11)$$

i.e.

$$\mathbf{V} = \langle p_{i\beta}^{-1} | \begin{pmatrix} -l_z s_z & (l_x + il_y) s_z \\ (l_x - il_y) s_z & l_z s_z \end{pmatrix} | p_{j\beta}^{-1} \rangle \quad (12)$$