Appendix D

Calculation of the matrix element $\langle \alpha | (\rho_p \rho_n)_0 | \beta \rangle$

We shall give here the expression for the matrix element $\langle \alpha | (\rho_p \rho_n)_0 | \beta \rangle$ where $(\rho_p \rho_n)_0$ is the zeroth multipole of the product $\rho_p \rho_n$ encountered in the chapter IV. One can write the full product $\rho_p \rho_n$ as,

$$\rho_p \rho_n \equiv \rho_p(\vec{r})\, \rho_n(\vec{r})$$
$$= \sum_i^P \sum_j^N \phi_i^*(\vec{r})\, \phi_i(\vec{r})\, \phi_j^*(\vec{r})\, \phi_j(\vec{r}) \qquad D(1)$$

Expanding the single particle orbitals in terms of the basis states, one has,

$$\rho_p \rho_n = \sum_i^P \sum_j^N \sum_{\gamma\gamma'\delta\delta'} C^{i*}_{n_\gamma l_\gamma j_\gamma} C^{i}_{n_{\gamma'} l_{\gamma'} j_{\gamma'}}$$
$$\cdot C^{j*}_{n_\delta l_\delta j_\delta} C^{j}_{n_{\delta'} l_{\delta'} j_{\delta'}}$$
$$\cdot \langle \vec{r} | n_{\gamma'} l_{\gamma'} j_{\gamma'}, m_i \rangle \langle n_\gamma l_\gamma j_\gamma, m_i | \vec{r} \rangle$$
$$\cdot \langle \vec{r} | n_{\delta'} l_{\delta'} j_{\delta'}, m_j \rangle \langle n_\delta l_\delta j_\delta, m_j | \vec{r} \rangle \qquad D(2)$$

The zeroth multipole is obtained in the following way. We have

$$\langle \vec{r} \,|\, n_{\gamma'} l_{\gamma'} j_{\gamma'}, m_i \rangle$$
$$= \sum_{m_{l_{\gamma'}}} C\begin{pmatrix} l_{\gamma'} & 1/2 & j_{\gamma'} \\ m_{l_{\gamma'}} & m_i - m_{l_{\gamma'}} & m_i \end{pmatrix}$$
$$\cdot R_{n_{\gamma'} l_{\gamma'}}(r)\, Y^{l_{\gamma'}}_{m_{l_{\gamma'}}}(\theta, \phi)\, \chi^{1/2}_{m_i - m_{l_{\gamma'}}} \qquad D(3)$$

etc.

After expressing eqn.D(2) in terms of basis states as shown in D(3), the spherical harmonics are coupled in the following way using Clebsch-Gordon series

$$\begin{aligned} \vec{l}_{\gamma} + \vec{l}_{\gamma'} &= \vec{l} \\ \vec{l}_{\delta} + \vec{l}_{\delta'} &= \vec{l}' \\ \vec{l} + \vec{l}' &= \vec{L} \end{aligned} \qquad D(4)$$

Putting L=0 then gives the zeroth multipole of the product ($\rho_p \rho_n$). We shall now give the final expression for the m.e. $\langle \alpha \,|\, (\rho_p \rho_n)_0 \,|\, \beta \rangle$ for the sake of completeness. We have $|\alpha\rangle \equiv |n_\alpha l_\alpha j_\alpha m_\alpha\rangle$. From D(2), D(3) and D(4), after some angular momentum algebra and integration over spin-coordinates, finally,

$\langle \alpha | (\rho_p \rho_n)_0 | \beta \rangle$

$$= \delta_{l_\alpha l_\beta} \delta_{j_\alpha j_\beta} \delta_{m_\alpha m_\beta}$$

$$\cdot \sum_i^P \sum_j^N \sum_{\gamma\gamma'\delta\delta'} C^{i*}_{n_\gamma l_\gamma j_\gamma} C^{i}_{n_{\gamma'} l_{\gamma'} j_{\gamma'}} C^{j*}_{n_\delta l_\delta j_\delta} C^{j}_{n_{\delta'} l_{\delta'} j_{\delta'}}$$

$$\cdot \left[(2l_\gamma+1)(2l_{\gamma'}+1)(2l_\delta+1)(2l_{\delta'}+1) \cdot (2j_\gamma+1)(2j_{\gamma'}+1)(2j_\delta+1)(2j_{\delta'}+1) \right]^{1/2}$$

$$\cdot \sum_l \frac{1}{(4\pi)^2} \cdot \frac{1}{(2l+1)} (-1)^{m_i + l_{\gamma'} - j_{\gamma'} + 1} \cdot (-1)^{m_j + l_{\delta'} - j_{\delta'} + 1}$$

$$\cdot W(j_\gamma \tfrac{1}{2} l\, l_{\gamma'}, l_\gamma j_{\gamma'}) \, C\begin{pmatrix} j_\gamma & j_{\gamma'} & l \\ -m_i & m_i & 0 \end{pmatrix} C\begin{pmatrix} l_\gamma & l_{\gamma'} & l \\ 0 & 0 & 0 \end{pmatrix}$$

$$\cdot W(j_\delta \tfrac{1}{2} l\, l_{\delta'}, l_\delta j_{\delta'}) \, C\begin{pmatrix} j_\delta & j_{\delta'} & l \\ -m_j & m_j & 0 \end{pmatrix} C\begin{pmatrix} l_\delta & l_{\delta'} & l \\ 0 & 0 & 0 \end{pmatrix}$$

$$\cdot \int R_{n_\alpha l_\alpha}(r) R_{n_\beta l_\alpha}(r) R_{n_\gamma l_\gamma}(r) R_{n_{\gamma'} l_{\gamma'}}(r) R_{n_\delta l_\delta}(r) R_{n_{\delta'} l_{\delta'}}(r) \, r^2 \, dr$$

where $W(j_\gamma \tfrac{1}{2} l\, l_{\gamma'}\ ,\ l_\gamma\, j_{\gamma'})$ etc. are Racah coefficients and $C\begin{pmatrix} j_\gamma & j_{\gamma'} & l \\ -m_i & m_i & 0 \end{pmatrix}$ etc. are Clebsch-Gordon coefficients. The integrations over space coordinate r can be carried out easily making use of the Talmi integrals. The expression D(5) is used for calculations in chapter IV.