Two-body matrix elements of Pauli-projected excentric single-particle orbits

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Abstract

We present explicit analytical formulae for two-body matrix elements between Pauli-projected single-particle orbits generated by gaussians shifted from the centre of a nuclear core, which is populated by nucleons occupying harmonic-oscillator orbits. Such shifted gaussian orbits appear in the generator-coordinate model of two-cluster systems and, as ingredients of generating functions, in the resonating group model as well. A Pauli projection is to be understood as a projection onto the subspace not occupied by the core nucleons. This is an exact procedure to take into account the Pauli principle in the limit in which the core is infinitely heavy, thus the procedure to be presented is very useful in the microscopic description of large-core plus small-cluster systems, such as involved in $\alpha$-decay problems.

§1. Introduction

The more complex the nuclear system, the more complicated it is to allow for the Pauli principle. In single-configuration models, like the extreme shell model, the Pauli principle is exactly allowed for by choosing the single-particle (s.p.) orbits orthogonal to each other and prescribing single population; hence the interpretation of the Pauli principle as an exclusion principle. For multiconfiguration one-centre models with a passive and massive core, like the multiconfiguration shell model, the Pauli principle between the core and valence particles is exactly observed by choosing the valence orbits orthogonal to those occupied by the core particles. However, for a multicentre system, such as a two-cluster system, the antisymmetrization between the clusters has to be carried through explicitly, and that implies tremendous technical complications [1].

In this paper we consider the case when one of the clusters, the “core”, is substantially heavier than the other, “the cluster”. In the limit, in which the core is completely passive and infinitely heavy, the Pauli principle can again be taken into account by an orthogonality requirement, but it is not so easy to fulfil this requirement. The subject of this paper is just to show a technique for the treatment of the most critical aspect of such a model, that of the calculation of the two-body potential matrix elements.

The wave function of the core $A$ is taken to be an harmonic-oscillator (h.o.) shell model Slater determinant, and that of the cluster $a$, which is assumed to contain at most four nucleons, is restricted
to be 0s h.o. orbits around a centre displaced from the centre of the core. The two-centre shell model underlying this picture forms a basis of the generator-coordinate model (GCM) of the two-cluster system. The orthogonality condition is imposed on the s.p. functions of cluster $a$ by an operator that projects out the states filled in the core.

Though this model may look rather restrictive, it can serve as a starting point for more sophisticated models. In particular, the condition of the infinite mass of the core can be lifted by applying a transformation that shifts the centre of mass (c.m.) of the system from the centre of the core to the joint c.m. [1]. By further transformations the GCM can be replaced by a resonating-group model [1] or by one in which the relative motion is represented by an h.o. basis [2] or by a single-centre basis spanned by gaussians of different widths [3]. Any of these transformations only involves the generator coordinates (and not the physical ones), so they do not interfere with antisymmetrization and can be performed on the matrix elements. All of these transformations can be performed analytically, but they should be performed before the angular-momentum projection.

The model with Pauli-projected s.p. orbits is useful especially for the description of core+$\alpha$ systems. Since the relation of the Pauli-projected orbits to the core orbits is the same as that of the valence shell-model orbits, the Pauli-projected orbits can be treated, to some extent, as shell-model orbits. In particular, the configurations they can form are just like ordinary shell-model configurations. The only difference is that they are not orthogonal to the ordinary valence orbits, thus a diagonalization over a non-orthogonal basis is required. Such cluster configurations have been used in the description of $\alpha$ decay [3, 4, 5].

To calculate the overlaps and s.p. matrix elements between such Pauli-projected s.p. orbits is straightforward with the well-known techniques [1]. The calculation of the two-body matrix elements is, however, not so simple. The two-body matrix elements reduce to integrals of products of h.o. and shifted gaussian functions. It seems to be natural to expand the gaussians in terms of h.o. functions [3] and then use the conventional technique, but this recipe leads to infinite summations, and the numerical expenditure is enormous. The procedure we show avoids this, by evaluating these integrals directly.

The plan of the paper is as follows. In §2 we briefly summarize the essentials of the method of the Pauli-projected s.p. orbits. In §3 we express the matrix element of an interaction term as a sum of sixteen terms and derive a general formula for these terms. In §4 we specialize this formula for some terms, and in §5 we give a brief summary. The paper is concluded with an Appendix containing a glossary of the formulae we used in the derivation.

§2. Pauli-projected single-particle orbits

A general state of the $a + A$ two-cluster system can be written in the form $\Psi = A\{\phi_{LM}(r) \Phi_a(\xi_a)\Phi_A(\xi_A)\}$, where $\Phi$ are antisymmetrized cluster internal states, the function $\phi$ describes the relative motion of angular momentum $LM$ and $A$ is an intercluster antisymmetrizer normalized in the pattern of $A = N^{-1/2} \sum_{i=1}^{N} (-1)^{P_i} P_i$. A GCM representation can be obtained by expanding $\phi_{LM}(r)$ in terms of angular-momentum projected gaussians displaced with respect to the centre:

$$\phi_{LM}(r) = \sum_k f_k \int d\mathbf{z}_k Y_{LM} (\mathbf{z}_k) \varphi^b_{\mathbf{z}_k}(r),$$  

(1)
where the gaussians are 0s h.o. functions of parameter $b$,

$$\varphi^b_s(r) = \left(\frac{b}{\pi}\right)^{3/4} \exp \left\{ -\frac{b}{2}(r-s)^2 \right\}. \tag{2}$$

Accordingly, $\Psi$ will take the form $\Psi = \sum_k f_k \Psi_k$, with $\Psi_k$ to be discussed below.

Let us assume that the two intrinsic states are single configurations of h.o. states $\varphi_{\alpha,000}^\beta$ and $\varphi_{n_i,l_i,m_i}^\beta$ $(n_1,l_1,m_1,...,n_A,l_A,m_A)$, of parameters $\alpha$ and $\beta$, respectively. If, in addition, the core is taken infinitely heavy, $\Phi_A$ reduces to a Slater determinant of $\{\varphi_{n_i,l_i,m_i}^\beta\}$, and, by choosing $b = 4\alpha$, so does $\varphi_{s_k}^b(r) \Phi_a(\xi_a)$. The corresponding $a + A$-particle state thus reads

$$\Psi_k = A\{\varphi_{s_k}^b(r - s_k) \Phi_a(\xi_a) \Phi_c(\xi_c)\}$$

$$= \left[(a + A)!\right]^{-1/2} \det\{\varphi_{s_k}^\alpha(r_1)(1)\ldots \varphi_{s_k}^\alpha(r_a)\chi_a(a)$$

$$\times \varphi_{n_i,l_i,m_i}^\beta(r_{a+1})(a+1)\ldots \varphi_{n_A,l_A,m_A}^\beta(r_{a+A})(a+A+1)\chi_{a+A}(a+A)\}. \tag{3}$$

The coordinates $\mathbf{r}_i$ are those with respect to the total c.m., but, the mass being infinity, the c.m. can be fixed at the origin, so $\mathbf{r}_i$ may be interpreted as the usual s.p. coordinates. The symbol $\chi_i(i)$ stands for a spin-isospin state. The function $\Psi_k$ may be cast into an even more useful form,

$$\Psi_k = [(a + A)!]^{-1/2} \det\{\psi_{s_k}(r_1)(1)\ldots \psi_{s_k}(r_a)\chi_a(a)$$

$$\times \varphi_{n_i,l_i,m_i}^\beta(r_{a+1})(a+1)\ldots \varphi_{n_A,l_A,m_A}^\beta(r_{a+A})(a+A)\}, \tag{4}$$

where

$$\psi_{s_k}(r_j) = (1 - P_j) \varphi_{s_k}^\alpha(r_j) = \varphi_{s_k}^\alpha(r_j) - \sum_{i=1}^A \varphi_{n_i,l_i,m_i}^\beta(r_j) \langle \varphi_{n_i,l_i,m_i}^\beta | \varphi_{s_k}^\alpha \rangle,$$  \tag{5}

with $P_j = \sum_i^A \varphi_{n_i,l_i,m_i}^\beta(r_j) \langle \varphi_{n_i,l_i,m_i}^\beta |$. We call the s.p. states $\psi_{s_k}(r)$ Pauli-projected s.p. orbits. The function $\Psi_k$ of eq. (4) is equal to that of eq. (3) because (3) is obtained from (4) by adding linear combinations of columns $a+1,...,a+A$ to columns $1,...,a$.

The advantage of using (5) rather than (4) is that the s.p. states involved in eq. (5) are all orthogonal to each other. The matrix elements between two states of the type of eq. (5) can be expressed in terms of the s.p. states more easily, which helps to separate the problem of the valence nucleons from that of the core (4). In particular, the two-body matrix elements of Slater determinants built up of orthogonal s.p. states can be expressed simply by the two-body matrix elements of the s.p. states.

### §3. Matrix elements

We shall consider the two-body matrix elements of the form factor, $e^{-\frac{1}{2}(r_2-r_1)}$, of a gaussian two-body potential between the Pauli-projected s.p. functions $\psi_{s_k}(r)$:

$$\langle \psi_{s_k}(r_1) | \psi_{s_k}(r_2) \big| e^{-\frac{1}{2}(r_2-r_1)} | \psi_{s_k}(r_1) \psi_{s_k}(r_2) \rangle$$

$$= \langle (1 - P_1) \varphi_{s_k}^\alpha(r_1) | (1 - P_2) \varphi_{s_k}^\alpha(r_2) \big| e^{-\frac{1}{2}(r_2-r_1)} | (1 - P_1) \varphi_{s_k}^\alpha(r_1) | (1 - P_2) \varphi_{s_k}^\alpha(r_2) \rangle. \tag{7}$$

It should be noted that the s.p. states in the bra and ket have no definite angular momenta, but a state of good angular momentum can be easily constructed from any of $\psi_{s_k}$ by taking $\int d\mathbf{s} Y_{lm}(\hat{\mathbf{s}}) \psi_{s_k}$.
Since, however, the projection of the total angular momentum in eq. (1) also involves the s.p. states other than those in the two-particle matrix element (7), it is more natural to include this projection at a later stage, which is out of the scope of this paper. Moreover, as is obvious from eq. (1), the projection of the full orbital angular momentum only requires a single operation by \( \int d\textbf{s}Y_{LM}(\hat{\textbf{s}}) \). The only thing we shall do in this paper to facilitate angular-momentum projecting is that we shall express the matrix element (7) in terms of \( s, \hat{s}, s' \) and \( \hat{s}' \).

By letting \( 1 - \mathcal{P}_i \) act term by term, this matrix element is written as a sum of 16 terms. Each of these terms contains two-body matrix elements of different combinations of h.o. and gaussian wave functions. To write the two-body matrix elements of the orbits \( \varphi_s^\alpha \) and \( \mathcal{P}_r \varphi_s^\alpha \) as special cases of a general formula, we introduce the notation

\[
M(q_1q_2|q'_1q'_2) = \langle \mathcal{P}_1^q \varphi_s^\alpha(r_1) \mathcal{P}_2^q \varphi_s^\alpha(r_2) \left| e^{-\frac{i}{\hbar}(\mathbf{r}_2 - \mathbf{r}_1)^2} \right| \mathcal{P}_1^q \varphi_s^\alpha(r_1) \mathcal{P}_2^q \varphi_s^\alpha(r_2) \rangle,
\]

which runs over all terms when each quotient \( q_i \) runs over 0 and 1. With these, (7) can be expressed as

\[
\langle \psi_s(r_1) | \psi_s(r_2) \rangle \left| e^{-\frac{i}{\hbar}(\mathbf{r}_2 - \mathbf{r}_1)^2} \right| \psi_{s'}(r_1) \psi_{s'}(r_2) \rangle = M(00|00) - M(10|00) - M(01|00) - M(00|10) - M(11|00) + M(01|10) + M(10|01) + M(11|10) + M(01|11) - M(10|11) - M(11|01) - M(11|10).
\]

It is obvious that any two-body matrix elements that involve shell-model orbits \( \varphi_{n_l,m_l}^\beta \) instead of some of the Pauli-projected eccentric states \( \psi_s \) are built up from the same building blocks, but are simpler, and can be derived analogously.

The calculations are simplified by the following symmetry relations:

\[
M(10|11) = M(01|11), \quad M(11|10) = M(01|01) = M(01|11)', \quad (10)
\]

\[
M(00|10) = M(00|01), \quad M(10|00) = M(00|00) = M(00|01)', \quad (11)
\]

\[
M(10|10) = M(01|01)', \quad M(11|00) = M(00|11)', \quad M(10|01) = M(01|10)', \quad (12)
\]

where \( M(q_1q_2|q'_1q'_2) \) differs from \( M(q_1q_2|q'_1q'_2)' \) in that the parameters \( s \) and \( s' \) are exchanged.

It is convenient to factorize the h.o. function as

\[
\varphi_{nlm}^\beta(r) = e^{-\frac{\alpha}{2}r^2} \overline{\varphi}_{nlm}^\beta(r).
\]

With the introduction of \( A_{nl}(s) \) through

\[
\langle \varphi_s^\alpha | \varphi_{nlm}^\beta \rangle = A_{nl}(s) Y_{lm}(\hat{s}),
\]

the matrix elements of eq. (8) take the form

\[
M(q_1q_2|q'_1q'_2) = \mathcal{N}_{q_1}(s) \mathcal{N}_{q_2}(s) \mathcal{N}_{q'_1}(s') \mathcal{N}_{q'_2}(s') \times \sum_{\{n_{l1}m_{l1}\}q_{l1}} A_{n_{l1}}(s) Y_{l_{1}m_{1}}(\hat{s}) A_{n_{l2}}(s) Y_{l_{2}m_{2}}(\hat{s}) A_{n'_{l1}}(s') Y_{l'_{1}m'_{1}}(\hat{s'}) A_{n'_{l2}}(s') Y_{l'_{2}m'_{2}}(\hat{s'}) \times \int d\mathbf{r}_1 \int d\mathbf{r}_2 \overline{\varphi}_{n_{l1}m_{l1}}^\beta(\mathbf{r}_1) \varphi_{n_{l2}m_{l2}}^\beta(\mathbf{r}_2) e^{-\frac{i}{\hbar}(\mathbf{r}_1 - \mathbf{r}_2)^2} e^{-\frac{i}{\hbar}(\mathbf{r}_1 - \mathbf{r}_2)^2} \times e^{-\frac{\alpha}{2}(r_1^2 + r_2^2)} \overline{e^{-\frac{\alpha}{2}(r_1^2 + r_2^2)}} e^{-\frac{\alpha}{2}(r_1^2 + r_2^2)},
\]

(15)
with the notations \( \alpha_i = (1 - q_i) \alpha \), \( \beta_i = q_i \beta \) and

\[
N_q(s) = \left[ \left( \frac{\alpha}{\beta} \right)^{3/4} \frac{1}{\langle \varphi_\alpha^\beta | \varphi_000 \rangle} \right]^{1-q}.
\]

As to the summation limits, if \( q_i = 1 \) then \( \{n_i,l_i,m_i\} \) runs over the filled orbits, but, if \( q_i = 0 \), then there is just one term, \( \{n_i = 0, l_i = 0, m_i = 0\} \). For \( A_{nl} \), an explicit formula is given in eq. (33) of the Appendix.

It is useful to couple the angular momenta of the h.o. wave functions of the same arguments and make use of the formula [6]

\[
[\hat{\varphi}_{n1l1}^\beta(r) \hat{\varphi}_{n2l2}^\beta(r)]_{lm} = \left( \frac{\beta}{\pi} \right)^{3/4} \sum_n T_{n1l1n2l2}^{nl} \hat{\varphi}_{nlm}^\beta(r)
\]

(17)

(the coefficient \( T_{n1l1n2l2}^{nl} \) is given in eq. (54) of the Appendix), to obtain

\[
M(q_1q_2|q_1'q_2') = \left( \frac{\beta}{\pi} \right)^{3/2} N_{q_1}(s) N_{q_2}(s) \sum_{(n_1l_1)_{q_1}} \sum_{(n_1l_1)'_{q_1}} A_{n_1l_1}(s) A_{n_2l_2}(s) A_{n_1l_1'}(s') A_{n_1l_2'}(s')
\]

\[
\times \sum_{\lambda' \lambda'LM} \left[ Y_{l_1}(\hat{s}) Y_{l_1'}(\hat{s}') \right]_{\lambda} \left[ Y_{l_2}(\hat{s}) Y_{l_2'}(\hat{s}') \right]_{\lambda'} \sum_{N' \lambda'LM} T_{n1l1n2l2}^{NN' \lambda'} T_{n1l1n2l2}^{NN' \lambda} I_{\lambda'LM}^{NN'}
\]

(18)

with

\[
I_{\lambda'LM}^{NN'} = \int dr_1 \int dr_2 \left[ \hat{\varphi}_{N\lambda}^\beta \hat{\varphi}_{N'\lambda'}^\beta \right]_{LM} \times e^{-\frac{1}{2} \sum_{i=1}^2 (a_i(r_i - s)^2 + \beta_i r_i^2)} e^{-\frac{1}{2} \beta_i(r_2 - r_1)^2} e^{-\frac{1}{2} \sum_{i=1}^2 (a_i(r_i - s)^2 + \beta_i r_i^2)}
\]

(19)

The summations over the angular momenta are restricted by the well-known rules, i.e. \( |l_1 - l_1'| \leq \lambda \leq l_1 + l_1' \), and \( M = -L, ..., L \). The coefficient \( T_{n1l1n2l2}^{nl} \) is non-zero if a triangle inequality (see \( (53) \) in the Appendix) of the quantum numbers is satisfied. In eq. (18) the spherical harmonics can be recoupled so that those belonging to the same argument can be combined:

\[
\left[ Y_{l_1}(\hat{s}) Y_{l_1'}(\hat{s}') \right]_{\lambda} \left[ Y_{l_2}(\hat{s}) Y_{l_2'}(\hat{s}') \right]_{\lambda'} = \lambda \lambda' \sum_{w} \hat{\ell}^{\lambda \lambda'} \left( \begin{array}{c} l_1 \ l_2 \ l_1' \ l_2' \\ \lambda \ \lambda' \ \lambda \end{array} \right) S_{l_1l_2}^{w} S_{l_1'l_2'}^{w} \left[ Y_{l}(\hat{s}) Y_{l'}(\hat{s}') \right]_{LM}^w
\]

(20)

where \( \hat{J} = \sqrt{2J + 1} \) and

\[
S_{l_1l_2}^{w} = \frac{i \hat{l}_1 \hat{l}_2}{\sqrt{4 \pi}} |l_10l_20|00).
\]

(21)

In §4 we shall see that at least one of the angular momenta in the 9j-symbol is zero in all practical cases, therefore (20) reduces to a simpler form.

The integral \( I_{\lambda'LM}^{NN'} \) can be determined using the that generating function of \( \varphi_{nlm}^\beta \) [9],

\[
g(p) = e^{2 \sqrt{\beta} p - p^2}.
\]

(22)

With this, \( \hat{\varphi}_{nlm}^\beta \) can be expressed as

\[
\hat{\varphi}_{nlm}^\beta = \left( \frac{\beta}{\pi} \right)^{3/4} \sum_{n} \frac{c_{nl} \ d_n^2 \ d_{n+l}}{(2n + l)! \ d^{2n+l}} \left( \int dp Y_{lm}(p)g(p) \right) \bigg|_{p=0},
\]

\[
c_{nl} = (-1)^n \sqrt{\frac{n!(2n + 2l + 1)!}{4\pi^{2n+l}}},
\]

(23)
Thus the integral $I^{NN'}_{(\lambda')LM}$ can be determined from the matrix element of the generator function

$$G(p, p') = \int dr_1 \int dr_2 g(p) e^{-\frac{i}{2} \sum_{i=1}^{2} (\alpha_i (r_i - s)^2 + \beta_i r_i^2)} e^{-\frac{i}{2} \sum_{i=1}^{2} (\alpha'_i (r_i - s)^2 + \beta'_i r_i^2)} g(p'),$$

as

$$I^{NN'}_{(\lambda')LM} = \left( \frac{\beta}{\pi} \right)^{3/2} \frac{c_{N\lambda'} c_{N'}^{\lambda}}{(2N + \lambda)! (2N' + \lambda')!}$$

$$\times \frac{\partial^{2N + \lambda + 2N' + \lambda'}}{\partial p^{2N + \lambda} \partial \bar{p}^{2N' + \lambda'}} \left( \int d\bar{p} \int d\bar{p}' [Y_{\lambda\mu}(\bar{p}) Y_{\lambda'\mu'}(\bar{p}')]_{LM} G(p, p') \right) \bigg|_{p = 0, p' = 0}.$$  

With the abbreviations

$$a_1 = \frac{1}{2} (\alpha_1 + \alpha'_1 + \beta_1 + \beta'_1 + \vartheta), \quad a_2 = \frac{1}{2} (\alpha_2 + \alpha'_2 + \beta_2 + \beta'_2 + \vartheta),$$

$$d = 4a_1 a_2 - \vartheta^2, \quad A_1 = \frac{\vartheta^2}{d}, \quad A_2 = \frac{\alpha_1^2 + \alpha'_1^2 + \beta_1^2 + \beta'_1^2}{d},$$

$$B_1 = \frac{\vartheta^2}{d} - A_1, \quad B_2 = \frac{\vartheta^2}{d} - A_2, \quad B = \frac{\vartheta}{d}, \quad v = 2A_1 \alpha_1 + 2A_2 \alpha_2 + B(\alpha_1 \alpha'_1 + \alpha'_2),$$

$$u = \frac{1}{2} (\alpha_1 + \alpha'_2) - A_1 \alpha_1 - A_2 \alpha_2 - B \alpha_1 \alpha_2, \quad u' = \frac{1}{2} (\alpha'_1 + \alpha'_2) - A_1 \alpha'_1 - A_2 \alpha'_2 - B \alpha'_1 \alpha'_2,$$

$$t = (2A_1 \alpha_1 + 2A_2), \quad r = (2A_1 \alpha'_1 + 2A_2), \quad t' = (2A_2 \alpha_2 + 2A_1), \quad r' = (2A_2 \alpha'_2 + 2A_1),$$

$$Q = ts + rs',$$

the double integral $G(p, p')$ is expressible as

$$G(p, p') = \left( \frac{4\pi^2}{d} \right)^{3/2} \exp\{-us^2 - u's'^2 + vss' - B_1 P^2 - B_2 P'^2 + BPp' + PQ + PP'Q'\}.  \tag{27}$$

The explicit forms of these coefficients in the exponent for different values of $q_i$ and $q'_i$ are collected in table 1. To be able to carry out the operations prescribed by (25), we expand the exponentials containing $P$ and $P'$ into the power series

$$G(p, p') = \left( \frac{4\pi^2}{d} \right)^{3/2} \exp\{-us^2 - u's'^2 + vss'\} \sum_{\nu_1 \nu_2 \mu_1 \mu_2} \frac{(-1)^{\nu_1 + \nu_2}}{\nu_1! \nu_2! \mu_1! \mu_2!} p^{2\nu_1 + \mu_1 + \kappa} p^{2\nu_2 + \mu_2 + \kappa}$$

$$\times B_1^{\nu_1} B_2^{\nu_2} \left( \frac{2\sqrt{\beta}}{d} \right)^{2(\nu_1 + \nu_2 + \kappa) + \mu_1 + \mu_2} B^{\nu_1} B^{\nu_2} \sum_{\lambda l \mu \nu} C_{\mu_1 \lambda_1} C_{\mu_2 \lambda_2} C_{\nu l}$$

$$\times \sum_{m_1 m_2 m} Y_{\lambda_1 m_1}(\hat{p}) Y_{\lambda_1 m_1}(\hat{Q}) Y_{\lambda_2 m_2}(\hat{p}') Y_{\lambda_2 m_2}(\hat{Q}') Y_{l m}(\hat{p}) Y_{l m}(\hat{p}'), \tag{28}$$

where we used the expression

$$(ab)^n = a^n b^n \sum_{l(n)} C_{nl} \sum_{m=-l}^{l} Y_{lm}(\hat{a}) Y_{lm}(\hat{b})^*, \quad C_{nl} = \frac{4\pi n!}{(n-l)!(n+l+1)!}. \tag{29}$$

In this formula $\sum_{l(n)}$ stands for a summation over $l = 0, 2, ..., n-2, n$ if $n$ is even, and $l = 1, 3, ..., n-2, n$ if $n$ is odd.

It is straightforward to recouple the spherical harmonics in (28):

$$\sum_{m_1 m_2 m} Y_{\lambda_1 m_1}(\hat{p})^* Y_{\lambda_1 m_1}(\hat{Q}) Y_{\lambda_2 m_2}(\hat{p}')^* Y_{\lambda_2 m_2}(\hat{Q}') Y_{l m}(\hat{p}) Y_{l m}(\hat{p}')^*$$

$$= \sum_{\lambda \lambda' LM} (-1)^l \lambda \lambda' W(\lambda_1 L \lambda'; \lambda_2 \lambda) S_{\lambda l}^\lambda S_{\lambda' l}^{\lambda'} [Y_{\lambda}(\hat{p}) Y_{\lambda}(\hat{p}')]^* [Y_{\lambda}(\hat{Q}) Y_{\lambda}(\hat{Q}')]_{LM}. \tag{30}$$
After substituting (30) into (28) and inserting (28) in (25) the derivations and the integrations in (25) can be carried out, with the result

$$I_{(\lambda\chi)^{\prime}LM}^{NN'\prime} = \exp\{ -u s^2 - u' s'^2 + v s s' \} \sum_{\mu_1 = 0}^{2N + \lambda + 2N' + \lambda'} \sum_{\mu_2 = 0}^{2N + \lambda + 2N' + \lambda'} \sum_{\lambda_1(\mu_1) \lambda_2(\mu_2)} G_{\mu_1 \lambda_1 \mu_2 \lambda_2}^{(NN'\chi'\lambda')} Q^{\mu_1} Q'^{\mu_2} \left[ Y_{\lambda_1}(\hat{Q}) Y_{\lambda_2}(\hat{Q'}) \right]_{LM},$$

where

$$G_{\mu_1 \lambda_1 \mu_2 \lambda_2}^{(NN'\chi'\lambda')} = \left( \frac{4\pi\beta}{d} \right)^{3/2} \Lambda_{\chi'} (2\sqrt{\beta})^{2N + \lambda + 2N' + \lambda'} c_{NN'\chi'\lambda'} C_{\mu_1 \lambda_1} C_{\mu_2 \lambda_2} \times \sum_{\nu_1 \mu_2 \kappa} \left( \frac{-1}{\nu_1 + \nu_2} \right) B_{1}^{\nu_1} B_{2}^{\nu_2} B^\kappa \sum_{l} (-1)^{l} W(\lambda_1 L l \lambda'; \lambda_2 \lambda) C_{\nu l} S_{\lambda_1 l}^\lambda S_{\lambda_2 l}^\lambda',$$

and the summation indices should fulfill the constraints

$$2\nu_1 + \mu_1 + \kappa = 2N + \lambda, \quad 2\nu_2 + \mu_2 + \kappa = 2N' + \lambda'.$$

The vectors $\hat{Q}$ and $\hat{Q'}$ are linear combinations of $s$ and $s'$. To facilitate the angular-momentum projection, it is useful to expand the $Q$- and $Q'$-dependent factor of eq. (31) in terms of $s$ and $s'$:

$$Q^{\mu_1} Q'^{\mu_2} \left[ Y_{\lambda_1}(\hat{Q}) Y_{\lambda_2}(\hat{Q'}) \right]_{LM} = \sum_{k_1 = 0}^{n} a_{k_1}^{n-k} \sum_{\lambda_1(k)} \sum_{\lambda_2(n-k)} H_{\lambda_1 \lambda_2 L}^{nk} \left[ Y_{\lambda_1}(\hat{a}) Y_{\lambda_2}(\hat{b}) \right]_{LM},$$

where the coefficients $F_{\lambda_1 \lambda_2 \lambda_1' \lambda_2' L}^{nk}$ are given in eq. (37) of the Appendix. One can verify this expansion immediately by using the well-known expression (2)

$$(a + b)^n Y_{lm}(\mathbf{a} + \mathbf{b}) = \sum_{k = 0}^{n} a_{k} b_{n-k} \sum_{\lambda_1(k)} \sum_{\lambda_2(n-k)} H_{\lambda_1 \lambda_2 L}^{nk} \left[ Y_{\lambda_1}(\hat{a}) Y_{\lambda_2}(\hat{b}) \right]_{LM},$$

where $H_{\lambda_1 \lambda_2 L}^{nk}$ is given in eq. (36) of the Appendix.

With (31) and (34) substituted into eq. (18), our final expression for $M(q_1 q_2 | q'_1 q'_2)$ becomes

$$M(q_1 q_2 | q'_1 q'_2) = \left( \frac{\beta}{\pi} \right)^{3/2} N_{q_1}(s) N_{q_2}(s) N_{q'_1}(s') N_{q'_2}(s') \exp\{ -u s^2 - u' s'^2 + v s s' \} \times \sum_{(\nu_{l_1} \lambda_{l_1})_{q_1}} A_{n_1 n_1'} \left( s \right) A_{n_2 n_2'} \left( s' \right) \sum_{\lambda \lambda'} \sum_{l l'} \sum_{l' L} (-1)^{l} L^2 l l' \Lambda_{\lambda' \lambda} \left( l_1 \ell_1' \ell_1 \ell_1' \lambda \lambda' \lambda' \lambda \right) S_{l_1 l_2} S_{l_1' l_2'}.$$
§4. Special cases

In this section we substitute the values of \(q_i\) and \(q'_i\) into eq. (36) and determine the concrete forms of \(M(q_1q'_2 | q'_1q'_2)\).

(1) \(M(11|11)\). This case reduces to combinations of two-body matrix elements of h.o. functions. These matrix elements are extensively used in shell-model calculations [7]. From table 1 we see that \(t = t' = r = r' = 0\), i.e. \(Q = Q' = 0\), \(u = u' = v = 0\), and then only the terms with \(\mu_i = k_i = \lambda_i = 0, (i = 1, 2)\) survive in equation (36). Moreover, as

\[
F_{\lambda_1\lambda_2\lambda'_1\lambda'_2}^{0000} = \delta_{\lambda_10}\delta_{\lambda_20}\delta_{\lambda'_10}\delta_{\lambda'_20}\delta_{L0}
\]  

the the Racah, the 9j-symbol and the \(S_{II'}^L\) coefficients in equation (36) are reduced as:

\[
W(ll00;0L') = \frac{(-1)^{l-l'}}{l},
\]

\[
\begin{pmatrix}
 l_1 & l'_1 & \lambda \\
 l_2 & l'_2 & \lambda'
\end{pmatrix} = \delta_{\lambda\lambda'}\delta_{l'0}\delta_{l'l} \frac{(-1)^{\lambda+l+l'}l'}{\lambda l}W(l_1l_2l'_1l'_2;\lambda l)
\]

and

\[
S_{II'}^L = \frac{1}{\sqrt{4\pi}}\delta_{II'}, \quad S_{I0I'}^L = \frac{1}{\sqrt{4\pi}}\delta_{I'I'}.
\]

By using these results, eq. (36) reads as

\[
M(11|11) = \left( \frac{\beta}{\pi} \right)^{3/2} \sum_{\lambda} \sum_{l_1l_2} A_{n_1l_1}(s)A_{n_2l_2}(s)A_{n'_1l'_1}(s')A_{n'_2l'_2}(s') \sum_{l_0} \hat{\lambda}(-1)^l \frac{1}{4\pi}W(l_1l_2l'_1l'_2;\lambda l)
\]

\[
\times S_{l_1l_2}^{l_0} S_{l_1l_2}^{l'_0} \sum_m Y_{lm}(s)Y_{lm}(s') \sum_{NN'} T_{n_1l_1n'_1l'_1}^{N\lambda} T_{n_2l_2n'_2l'_2}^{N\lambda} G_{0000}^{(N\lambda N'\lambda)0}.
\]

In this case the coefficient \(G_{0000}^{(N\lambda N'\lambda)0}\) can be expressed in a simpler form. From eq. (33) it follows that \(\kappa = 2N + \lambda - 2\nu_1\) and \(\nu_2 = N' - N + \nu_1\), and then by substituting \(B_1, B_2\) and \(B\) (see table 1) into eq. (32), reducing the Racah and the \(S_{II'}^L\) coefficients, \(G_{0000}^{(N\lambda N'\lambda)0}\) is given by

\[
G_{0000}^{(N\lambda N'\lambda)0} = (4\pi)^2 \left( \frac{4\pi\beta}{d} \right)^{3/2} e^{\lambda+\lambda'} \left( \frac{2\sqrt{\beta}}{\beta} \right)^{2N+\lambda+2N'+\lambda} (-1)^{N+N'+\lambda} \hat{\lambda} \left( \frac{\theta/2}{\theta + \beta} \right)^{N+N'+\lambda} \sum_{\nu_1} \nu_1!(N' - N + \nu_1)!\nu_1!(N - \nu_1)!\nu_1!(2N + 2\lambda - 2\nu_1 + 1)!!
\]

The summation over \(\nu_1\) can be carried out [3] and our final expression is

\[
G_{0000}^{(N\lambda N'\lambda)0} = (4\pi)^2 \left( \frac{4\pi\beta}{d} \right)^{3/2} e^{\lambda+\lambda'} \left( \frac{-\theta/2}{\theta + \beta} \right)^{N+N'+\lambda} \left( -1 \right)^{\lambda} 2^\lambda (4\pi)^2 \hat{\lambda} \left( \frac{\theta/2}{\theta + \beta} \right)^{N+N'+\lambda} \sum_{\nu_1} \nu_1!(N' - N + \nu_1)!\nu_1!(N - \nu_1)!\nu_1!(2N + 2\lambda - 2\nu_1 + 1)!!
\]

\[
\times \frac{(2N + 2N' + 2\lambda + 1)!!}{N!N'(2N + 2\lambda + 1)!!(2N' + 2\lambda + 1)!!}.
\]
(2) $M(01|11)$. Now we do not have so simple expressions as in the previous case. The first simplification is that $r = r' = 0$, i.e. $\mathbf{Q} = ts$, $\mathbf{Q}' = t's$ and $u' = v = 0$ (see table 1). The summation over $k_i (i = 1, 2)$ is then restricted to $k_i = \mu_i (i = 1, 2)$. The coefficient $F^{\mu_1 \mu_2 \mu_2}_{\lambda_1 \lambda_2 \lambda_1 \lambda_2 L}$ can easily be evaluated:

$$F^{\mu_1 \mu_2 \mu_2}_{\lambda_1 \lambda_2 \lambda_1 \lambda_2 L} = \sqrt{4\pi} \delta_{\lambda_1} \delta_{\lambda_2} \delta_{\lambda_1} \delta_{\lambda_2} S^L_{\lambda_1 \lambda_2}.$$  \hspace{1cm} (43)

From this it follows that $\lambda_2 = 0$, thus the Racah coefficient and $S^L_{\lambda_1 \lambda_2}$ in equation (43) can be written as:

$$W(ll'00; LL') = \frac{\delta_{\mu L}}{L'} \delta_{LL'}, \quad S^L_{\lambda_1 \lambda_2} = \frac{1}{\sqrt{4\pi}} \delta_{LL'}$$  \hspace{1cm} (44)

An other simplification to be used is that when $q_1 = 0$, then $n_1 = l_1 = 0$. From this it follows that the coefficient $T^{N\lambda}_{n_1 l_1 n_1 l_1}$ is

$$T^{N\lambda}_{00 n_1 l_1} = \delta_{n_1 N} \delta_{l_1 \lambda}$$  \hspace{1cm} (45)

and the 9j-symbol, similarly as in the first case, can be expressed by a Racah coefficient.

Let us put all these together to find

$$M(01|11) = \left( \frac{\alpha \beta}{\pi^2} \right)^{3/4} \exp\{-us^2\} \sum (n_1 l_1) \sum (n_1 l_1) \sum A_{n_2 l_2}(s)A_{n_1 l_1}(s')A_{n_1 l_1}(s) \sum_{\lambda L} \lambda' L \frac{(-1)^{l_1 + l_2 - L}}{2l_1 + 2l_2} \delta_{l_1 l_2} \delta_{l_1 l_2} \delta_{\lambda \lambda'} \sum_{n' m'} T^{N\lambda}_{n_2 l_2 n_2 l_2} \sum_{\mu_1 \mu_2 \lambda_1 \lambda_2} G^\mu_{\mu_1 \mu_2 \lambda_1 \lambda_2} T^{\mu_1 \mu_2 \mu_2}_{\lambda_1 \lambda_2 \lambda_1 \lambda_2} S^L_{\lambda_1 \lambda_2}.$$  \hspace{1cm} (46)

(3) $M(01|10)$. As we can see in Table 1, all coefficients differ from zero. There is one gaussian in the bra and one in the ket, that is $q_1 = q_2 = 0$ and $n_1 = n_2 = l_1 = l_2 = 0$. It follows that

$$T^{N\lambda}_{00 n_1 l_1} = \delta_{n_1 N} \delta_{l_1 \lambda}, \quad T^{N\lambda}_{n_2 l_2 00} = \delta_{n_2 N} \delta_{l_2 \lambda},$$  \hspace{1cm} (47)

and the 9j-symbol, as it contains two zero elements, can be substituted by

$$\left( \begin{array}{ccc} 0 & l_1' & \lambda \\ l_2 & 0 & \lambda' \\ l & l' & L \end{array} \right) = \left( \begin{array}{c} (-1)^{l_1' + l_2 - L} \\ 2l_1 + 2l_2 \end{array} \right) \delta_{l_1' \lambda} \delta_{l_2 \lambda} \delta_{l_1 l_2}$$  \hspace{1cm} (48)

That is all one can do in this case and thus equation (36) becomes

$$M(01|10) = \left( \frac{\alpha}{\pi} \right)^{3/2} \exp\{-us^2 - u's^2 + vss'\} \sum A_{n_2 l_2}(s)A_{n_1 l_1}(s') \sum_{\lambda L} \sum_{\mu_1 = 0} \sum_{\mu_2 = 0} \frac{2n_1 + l_1' 2n_2 + l_2}{2l_1 + 2l_2} \sum_{\mu_1 \mu_2 \lambda_1 \lambda_2} G^\mu_{\mu_1 \mu_2 \lambda_1 \lambda_2} T^{\mu_1 \mu_2 \mu_2}_{\lambda_1 \lambda_2 \lambda_1 \lambda_2} S^L_{\lambda_1 \lambda_2}.$$  \hspace{1cm} (49)

(4) $M(01|01)$. Now $q_1 = q_2 = 0$ and $n_1 = n_2 = l_1 = l_2 = 0$, consequently $T^{N\lambda}_{0000} = \delta_{N\lambda}$ and therefore $\mu_1 = k_1 = 0$. Then the coefficients will reduce to

$$F^{001}_{002} = \frac{1}{\sqrt{4\pi}} \delta_{LL_2} H^{12}_{12},$$  \hspace{1cm} (50)
and after repeating the steps used in the previous cases, i.e. reducing the 9j-, Racah and S-symbols, the expression \({\text{eq. 36}}\) yields

\[
M(01|01) = \left(\frac{\alpha^2}{\pi^2}\right)^{3/4} \exp\{-us^2 - u's'^2 + vss'\} \sum_{n_2l_2} A_{n_2l_2}(s) A_{n_2l_2}(s') \sum_{L} T_{n_2l_2n_2l_2}^{N'\ell} \sum_{\mu_2=0}^{2N'+L} \\
\times G(00\mu_2L) \sum_{k_2} t^{k_2} N\mu_2 \sum_{\lambda_2} H_{\lambda_2}^{k_2} \sum_{L'} (-1)^{L+L'} W(l_2l_2\lambda_1\lambda_2; LL') \\
\times S_{l_2\lambda_2'} \sum_{M'} Y_{L'M'}(\bar{s}) Y_{L'M'}(\bar{s}').
\]

where the coefficient \(G\) can be written as

\[
G(00\mu_2\lambda_2) = \left(\frac{4\beta}{d}\right)^{3/2} c_{N'\lambda'} (2\sqrt{\beta})^{2N'+\lambda'} \sum_{\nu_2+\mu_2=2N'+\lambda'} \frac{(-1)^\nu_2}{\nu_2! \mu_2!} B_{\nu_2}^{\mu_2} C_{\mu_2\lambda'}, \quad (49)
\]

(5) \(M(00|11)\). In this case both gaussians are in the bra, and \(u' = v = 0, r = r' = 0\), therefore \(Q = ts, Q = t's\) just as in case (2). In addition, now \(n_1 = l_1 = n_2 = l_2 = 0\), so the result of case (2) can be simplified further:

\[
M(00|11) = \left(\frac{\alpha}{\pi}\right)^{3/2} \exp\{-us^2\} \sum_{n_1l_1} A_{n_1l_1}(s) A_{n_1l_1}(s') \sum_{L} T_{n_1l_1n_1l_1}^{N'\ell} \sum_{\mu_1=0}^{2N'+\lambda'} \sum_{\mu_2=0}^{\ell} \sum_{\lambda_1} \sum_{\lambda_2} G_{\mu_1\lambda_1\mu_2\lambda_2}^{n_1l_1n_1l_1} \\
\times t^{\mu_1} t^{\mu_2} s^{\mu_1+\mu_2} \sum_{M} Y_{LM}(\bar{s}) Y_{LM}(\bar{s}').
\]

(6) \(M(00|01)\). Using the results of case (4), one finds

\[
M(00|01) = \left(\frac{\alpha^3}{\beta \pi^2}\right)^{3/4} \exp\{-us^2 - u's'^2 + vss'\} \sum_{n_1l_1} \sum_{\mu_2} G(00\mu_2l_2) \sum_{k_2} t^{k_2} N\mu_2 \sum_{\lambda_2} H_{\lambda_2}^{k_2} \sum_{m_2} Y_{\lambda_2m_2}(\bar{s}) Y_{\lambda_2m_2}(\bar{s}').
\]

(7) \(M(00|00)\) This is the simplest case, overlap of four gaussians is just

\[
M(00|00) = \left(\frac{\alpha}{\alpha + \theta}\right)^{3/2} \exp\{-us^2 - u's'^2 + vss'\} \quad (50)
\]

§5. Conclusions

All summation in formula (36) are finite, so after angular momentum projection it is straightforward to apply it, or its special cases given in §4, in numerical calculations [10]. If, in any of the states involved there are other nucleons in Pauli-projected orbits, their overlaps may bring in factors of the form of \(\exp\{vss'\}\). Grouping these factors together with \(\exp\{vss'\}\) of eq. [6], the product has to be
expanded into its multipoles. The functions $Y_{LM}(\hat{s})Y_{LM}(\hat{s}')^*$ appearing in this way should be coupled with $Y_{L'M'}(\hat{s})Y_{L'M'}(\hat{s}')^*$, respectively. The infinite summation involved in the multipole expansion is then eliminated by the angular momentum projection, which can be achieved by the operations $\int d\hat{s}Y^*_{LM}(\hat{s})$ and $\int d\hat{s}'Y_{L'M'}(\hat{s}')$.

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§6. Appendix

In this paper we used the standard definition of the harmonic oscillator function (see e.g. [6])

$$\varphi_{nlm}(r) = \left(\frac{\beta}{\pi}\right)^{3/4} e^{-\frac{\beta r^2}{2}} \frac{n!4\pi^{n+l}}{(2n+2l+1)!!} \left(\sqrt{\beta r}\right)^l L_n^{l+1/2}(\beta r^2) Y_{lm}(\hat{r})$$

(51)

with $L_n^{l+1/2}(x)$ being associated the Laguerre polynomial

$$L_n^{l+1/2}(x) = \frac{(2n+2l+1)!!}{2^n} \sum_{s=0}^n \frac{(-1)^s 2^s}{(2s+2l+1)!!(n-s)!} x^s.$$  

(52)

The radial part (see eq. (14)) of the overlap of a harmonic oscillator function of width parameter $\beta$ and a gaussian of width parameter $\alpha$ and of displacement vector $s$ is

$$A_{nl} = \sqrt{4\pi} \left(\frac{n!(2n+2l+1)!!}{2^n l!}\right)^{1/2} \frac{4\alpha\beta}{(\alpha+\beta)^2} e^{-\frac{\alpha\beta}{2(\alpha+\beta)^2} s^2} \sum_{k=0}^n (-1)^k \frac{2^{k+l}}{k!(n-k)!(2k+2l+1)!!} \left(\frac{\alpha-\beta}{\alpha+\beta}\right)^{n-k} \left(\frac{\alpha\sqrt{\beta}s}{\alpha+\beta}\right)^{2k+l}$$

(53)

The combination coefficients of product of two h. o. functions of the same argument $\alpha$ and $\beta$ is given by

$$T^{NL}_{nln'l'} = \left(\frac{n!n'!2^{N+L}(2n+2l+1)!!(2n'+2l'+1)!!}{(2N+2L+1)!!2^{n+l+2n'+l'}N'!}\right)^{1/2} \langle l0'0|L0L \hat{P}\rangle L \sum_{ss'} (-1)^{s+s'}$$

$$\times \frac{(2s+2s'+l+l'+L+1)!!(s+s'+\frac{1}{2}(l+l'-L))!}{(2s+2l+1)!!(2s'+2l'+1)!!(n-s)!(n'-s')!(s+s'-N+\frac{1}{2}(l+l'-L))!},$$

(54)

where the quantum numbers must satisfy the triangular condition

$$|2n+l-2n'-l| \leq 2N+L \leq 2n+l+2n'+l'.$$

(55)

The expansion coefficients in equation (35) are

$$H^{nk}_{\lambda_1\lambda_2} = \left(\frac{n}{k}\right) C_{k\lambda_1} C_{n-k\lambda_2} S^{\lambda_1}_{\lambda_2},$$

(56)
The detailed form of the coefficients of equation (34) is
\[
F_{\lambda_1\lambda_2\lambda_1'\lambda_2'}^{\mu_1\mu_2k_1k_2} = \sum_{l_1l_2l_1'l_2'} H_{l_1l_1'}^{\mu_1k_1} H_{l_2l_2'}^{\mu_2k_2} S_{l_1l_2}^{\lambda_1'} S_{l_1'l_2'}^{\lambda_2'} \begin{pmatrix} l_1 & l_1' & \lambda_1 & \lambda_1' \\ l_2 & l_2' & \lambda_2 & \lambda_2' \end{pmatrix} (L).
\]

The range of the summation variables are determined by those of the coefficient \(H_{\lambda_1\lambda_2l}^{nk}\) and those of the 9\(j\) symbol.

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