Abstract. Euler angles determining rotations of a system as a whole are conveniently separated in three–particle basis functions. Analytic integration of matrix elements over Euler angles is done in a general form. Results for the Euler angle integrated matrix elements of a realistic NN interaction are listed. The partial wave decomposition of correlated three–body states is considered.
Elimination of Rotational Degrees of Freedom in Expansion Methods for Three Nucleons

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1 Introduction

When expansion methods are applied in three-particle problems matrix elements (ME) are to be calculated which are six-dimensional integrals. It is expedient to choose Euler angles, representing rotations of a system as a whole, as three of the six degrees of freedom and to carry out the integration over Euler angles analytically. Then one is left with integrations that are three-dimensional only. Such low-dimension integrations can very efficiently be done with regular quadratures. The elimination of rotational degrees of freedom has been used by several groups [1, 2, 3] at solving both the three-nucleon Schrödinger dynamic equation and that of the method of integral transforms [4]. No restrictions on the form of basis functions arise in such an approach, and in conjunction with use of an appropriate set of basis functions the techniques are probably the fastest and easiest ones to solve most of the nuclear three-body problems of interest. Therefore, it seems useful to list the formalism. In Sec. 2 the separation of Euler angles is performed for general form three-particle functions. In Sec. 3 analytic integration over Euler angles of general type ME is carried out which is applied in Sec. 4 to calculate the ME pertaining to a realistic NN interaction. The partial wave decomposition of correlated basis functions is considered in Sec. 3 as well. Sec. 5 contains comments on symmetry properties of Euler angle integrated ME.

In Ref. [5] most of the ME considered in Sec. 4 were also calculated, however, our techniques are different. Both the results and techniques of the present paper are substantially simpler. Besides, we present the general formula for Euler angle integrated ME, and our choice of the body reference frame leads to simplifications.

Contrary to the correlated basis functions case, ME of one-body and two-body operators can be calculated in a simple way without the Euler angle inte-
gration when e.g. uncorrelated hyperspherical harmonics are used as a basis set. However, the present techniques are helpful also in the latter case when ME of NNN force or those involving two–body subsystems at solving reaction problems are considered.

While the formulae are written down below for the case of the three–nucleon problem they may be applicable also beyond these frames.

2 Separation of Euler Angles

We use the Jacobi vectors

\[ u = \frac{1}{\sqrt{2}} (r_2 - r_1), \quad v = \sqrt{\frac{2}{3}} \left( r_3 - \frac{r_1 + r_2}{2} \right) \]  

where \( r_i \) are nucleon positions, and we consider three–dimensional rotations \( u, v \rightarrow u', v' \). We interpret rotations as rotations of a coordinate system so that a rotation \( a \rightarrow a' \) means that \( \{a_x, a_y, a_z\} \equiv a \) and \( \{a'_x, a'_y, a'_z\} \equiv a' \) are coordinates of a vector in the old and new coordinate systems, respectively. Spatial components \( F_{LM} \), with given total orbital momentum and its projection quantum numbers, of three–particle basis functions transform under rotations as \[ F_{LM}'(u', v') = \sum_{M'=-L}^{L} D_{MM'}^{L}(\omega)F_{LM}(u, v) \]

where \( \omega \) denotes collectively three Euler angles parameterizing a rotation and \( D_{MM'}^{L} \) are the Wigner D–functions.

In order to separate the Euler angle dependence of \( F_{LM}(u, v) \) we consider rotations \( u' = u'(u, v) \), \( v' = v'(u, v) \) which are different for different \( u, v \) vectors, so that \( \omega = \omega(u, v) \). We use the inverse relation

\[ F_{LM}(u, v) = \sum_{M'=-L}^{L} D_{MM'}^{L}(\omega)F_{LM'}(u', v'). \]  

At given \( u \) and \( v \), we choose the new coordinate system in a way that it corresponds to a body reference frame associated with the \( u, v \) plane. The corresponding body–frame coordinates \( u'_x, v'_y \) may be expressed in terms of scalars \( u, v, (u \cdot v) \). Treated in this way, Eq. (2) becomes an expansion of \( F_{LM}(u, v) \) over D–functions depending on Euler angles with coefficients depending on scalar variables. The Euler angles determine positions of the body reference frame with respect to a laboratory reference frame.

In particular, a convenient choice \[ \] is to direct the \( z \)–axis of the body reference frame along the vector \( u \), and to place the \( x \)–axis of the body reference frame in the \( u, v \) plane in a way that the projection of the vector \( v \) onto this axis is positive. Then one has

\[ u'_x = 0, \quad u'_y = 0, \quad u'_z = u, \quad v'_x = v\sqrt{1-t^2}, \quad v'_y = 0, \quad v'_z = vt \]
Elimination of Rotational Degrees of Freedom

where \( t = (\bar{u} \cdot \bar{v}) \), \( \bar{u} \) and \( \bar{v} \) being the unit vectors in the directions of \( u \) and \( v \).

As a result, one comes to the expansion

\[
F_{LM}(u, v) = \sum_{M'=-L}^{L} D_{MM'}^L(\omega)F_{LM'}(u, v, t)
\]

(4)

where the Euler angles \( \omega \) parametrize the above defined rotation into the body reference frame, and the notation \( F_{LM}(u', v') \equiv F_{LM}(u'_x, u'_y, u'_z, v'_x, v'_y, v'_z) \) taken at the space point from (3):

\[
F_{LM}(u, v, t) \equiv F_{LM}(u'_x = 0, u'_y = 0, u'_z = u, v'_x = v\sqrt{1-t^2}, v'_y = 0, v'_z = vt).
\]

(5)

Writing down the formulae we shall consider \( F_{LM} \) to be real which is commented below in connection with Eq. (19).

The coordinates \( \omega \equiv \{\alpha, \beta, \gamma\} \), \( u, v, t \) ranging between their natural boundaries realize a mapping onto the whole phase space \( (u, v) \). The correspondence between the points in the phase space and the \( \alpha, \beta, \gamma, u, v, t \) coordinates is a one–to–one correspondence everywhere except for the exceptional sub–areas where the \( u, v \) plane is undefined and hence the body reference frame cannot be defined. These are sub–areas where vectors \( u \) and \( v \) are collinear, or \( u = 0 \), or \( v = 0 \). Many sets of Euler angles correspond to the same point in the phase space if the point belongs to these sub–areas. For the case of integrands which are non–singular in the exceptional sub–areas the contribution of these sub–areas to ME vanishes (not speaking of the fact that the phase space volume element suppresses the contributions of \( u = 0 \) and \( v = 0 \) sub–areas, see Eq. (7) below).

Therefore, one can transform the integration over \( u, v \) into the integration over \( \alpha, \beta, \gamma, u, v, t \) and apply Eq. (4).

Our basis functions \( F_{LM} \) are regular single–valued functions of the points of the phase space. This is in contrast to D–functions themselves which do not possess such property in the above mentioned exceptional sub–areas. While this does not cause problems when Eq. (4) is used for integration purposes, use of products of D–functions and functions of internal variables as basis functions would be a disadvantage.

Let us also comment on the aspect of symmetry with respect to particle permutations. A well–known way to get totally antisymmetric three–nucleon basis

\footnote{In addition, it is easy to see that Eq. (4) remains valid in the exceptional sub–areas where \( u \) and \( v \) are collinear, and where \( v = 0 \). Both sides of Eq. (4) turn to \( Y_{LM}\beta, \alpha f(u, v) \) in these sub–areas, and integration over them using the coordinates \( \alpha, \beta, \gamma, u, v, t \) leads to correct results.}

\footnote{At given \( L \) and \( M \) values D–functions form a complete set of \( 2L + 1 \) functions of three coordinates determining the position of a system as a whole. Constraining the basis set \( F_{LM} \), for example, can use another set of \( 2L + 1 \) functions instead of D–functions which have the same property but which are basically polynomials of the components of the vectors \( u, v \) and are regular in the whole phase space. These functions are to be multiplied by functions of three internal variables. This basis proved to be very efficient in atomic physics. When such a basis is used to calculate ME of some simple operators there is no need to apply Eq. (4). The integrands in the left–hand side of Eq. (5) below can be decomposed in a closed form into the sum of components with given \( L \) values. Only the \( L = 0 \) component contributes to the right–hand side of (6), and no summation over \( M' \) is then required, see (7).}
functions is to combine spatial basis functions that are components of irreducible representations of the three–particle permutation group with spin–isospin functions of conjugated symmetry. The corresponding spatial basis functions are often constructed via application of symmetrization operators to complete sets of initial ”simple” functions. It is convenient, and sufficient, to use the expansion of symmetrized functions involving one and the same body reference frame described above. In contrast to the basis functions themselves, this reference frame does not possess symmetry properties with respect to permutations of three particles. The arising symmetrized functions $F_{\text{sym}}$ are expressed in terms of initial functions $F$ with the help of relations of the type

$$F_{\text{sym}}(u, v) = \sum_P C_P F(Pu, Pv)$$

where $P$ are particle permutations, and $C_P$ are given coefficients. Hence, the required body–system components of symmetrized functions are obtained with the help of such type relations applied at the points $(u', v')$ given by Eq. (3). One thus needs to form linear combinations of the corresponding vectors

$$Pu' = a_P u' + b_P v', \quad Pv' = c_P u' + d_P v'$$

and to calculate initial functions at the points $(Pu', Pv')$. When, alternatively, the basis functions antisymmetric with respect to nucleon permutations are obtained via a direct antisymmetrization of angular momentum coupled products of space functions and spin–isospin functions the procedure is similar.

ME between functions of the form (4) will be calculated below. The volume element is

$$d\tau = dudv = d\omega d\tau_{\text{int}}, \quad d\tau_{\text{int}} = u^2 v^2 dudvdt.$$ (7)

Here the relationship $d\bar{u}d\bar{v} = d\omega dt$, see Appendix, is used. The overlap–type integrals are

$$\int d\tau G^*_{L'M'}\hat{O}_{u,v,t} F_{LM} = \delta_{LL'} \delta_{M'M'} 8\pi^2 (2L + 1)^{-1}$$

$$\times \int d\tau_{\text{int}} \sum_{M''=\pm L} G_{LM'M''}(u, v, t)\hat{O}_{u,v,t} F_{LM'M''}(u, v, t).$$ (8)

Here $\hat{O}_{u,v,t}$ is an operator acting on $u, v, t$, and the orthogonality properties (A.37) are used.

3 Matrix Elements of Tensor Operators

To calculate ME it is expedient to decompose the operators into sums of tensors irreducible with respect to rotations. Performing integration over Euler angles analytically is then possible in practically important cases. The following relations are useful to this aim.

1. Let $\hat{O}_{k\kappa}$ be the irreducible tensor operator of the rank $k$. We obtain its Euler angle integrated reduced ME $(G_{L'}|\hat{O}_{k\kappa}|F_L)$ defined as usual,

$$(G_{L'M'}|\hat{O}_{k\kappa}|F_{LM}) = C^{L'M'}_{LMkk}(2L' + 1)^{-1/2}(G_{L'}|\hat{O}_{k\kappa}|F_L),$$
where \( C^{L'M'}_{LM\kappa\kappa} \) are the Clebsh–Gordan coefficients. The result is

\[
\left( G_{L'} || \hat{O}_k || F_L \right) = 8\pi^2(2L' + 1)^{-1/2} \int d\tau_{int} \sum_{M'M''} C^{L'M'}_{LM\kappa\kappa} G^{L'M'}_{LM\kappa\kappa} \hat{O}_{k\kappa} F_{LM}.
\]

(9)

Here \( \hat{O}_{k\kappa} F_{LM} \) means the quantity \( \hat{O}_{k\kappa} F_{LM} \) taken at the space point from \( \hat{O}_k \).

The relation (6) is useful when one is able to calculate \( \hat{O}_{k\kappa} F_{LM} \) in a simple way. The cases when the operator \( \hat{O}_{k\kappa} \) includes multiplications by functions and differentiations fall into this category, cf. the next section.

To get Eq. (6) we define the states

\[
(OF)^{kL}_{L_0 M_0} = \sum_{\kappa + M = M_0} C^{L_0 M_0}_{LM\kappa\kappa} \hat{O}_{k\kappa} F_{LM}.
\]

(10)

Since \( \hat{O}_{k\kappa} \) is an irreducible tensor these states possess definite rotational quantum numbers \( L_0, M_0 \). One therefore can expand them, as in Eq. (6), in terms of products of D–functions and the body–system functions \( (OF)^{kL}_{L_0 M_0} (u, v, t) \) defined similar to Eq. (5). Writing down the relation inverse to (10) and utilizing this expansion gives

\[
\hat{O}_{k\kappa} F_{LM} = \sum_{L_0 M_0 M'} C^{L_0 M_0}_{LM\kappa\kappa} D^{L_0 M_0}_{M_0 M'} (\omega)(OF)^{kL}_{L_0 M_0}.
\]

Use of this relation, the D–function expansion of \( G_{L'M'} \), and Eq. (6) gives

\[
\int d\tau G_{L'M'}^{*} \hat{O}_{k\kappa} F_{LM} = 8\pi^2(2L' + 1)^{-1} C^{L'M'}_{LM\kappa\kappa} \int d\tau_{int} \sum_{M''} G_{L'M''}^{*} (OF)^{kL}_{L_0 M_0}.
\]

Substitution of the body–system version of Eq. (11) here,

\[
(OF)^{kL}_{L_0 M_0} = \sum_{M + \kappa = M''} C^{L'M''}_{LM\kappa\kappa} \hat{O}_{k\kappa} F_{LM},
\]

(11)

gives Eq. (6).

More complicated ME can also be integrated over Euler angles. Let us comment on e.g. the ME of the square of a three-nucleon Hamiltonian \( \hat{H}^2 = (\hat{T} + \hat{V})^2 \) entering the well–known Temple lower bound for binding energy. ME of \( \hat{T}^2 \) are calculated like the overlap integrals (6) with \( F_{LM} \to \hat{T} F_{LM}, \ G_{LM} \to \hat{T} G_{LM} \), ME of \( \hat{T} \hat{V} + \hat{V} \hat{T} \) are calculated using the same replacements and Eq. (6), and ME of \( \hat{V}^2 \) are given by the sum of contributions of the form

\[
\left\langle (G_{L_2} \otimes \chi_{S_2})_{JM} \left| \left( \hat{O}_{k_2} \cdot \hat{\Sigma}_{k_2} \right) \left( \hat{O}_{k_1} \cdot \hat{\Sigma}_{k_1} \right) \right| (F_{L_1} \otimes \varphi_{S_1})_{JM} \right\rangle
\]

(12)

where \( \hat{O}_k \) and \( \hat{\Sigma}_k \) are the rank \( k = 0, 1, \) and 2 tensor operators, \( (\hat{O}_k \cdot \hat{\Sigma}_k) \) is their scalar product (6), and \( (F_L \otimes \varphi_{S})_{JM} \) symbolizes the LSJ coupling. The operators \( \hat{O}_k \) and \( \hat{\Sigma}_k \) act in the coordinate subspace and the spin–isospin subspace, respectively, and they are irreducible with respect to rotations.

To calculate ME (12) one performs recouplings, see Appendix, leading to spatial and spin states of the type \((OF)^{L_1}_{LM} \cdot (OG)^{L_2}_{LM} \cdot (\Sigma \varphi)^{S_1}_{SM_1} \cdot (\Sigma \chi)^{S_2}_{SM_2} \).
are real as well. This is seen from the body–system version (12),

$$\sum_{M_1, M_2, \kappa_1, \kappa_2} I(M_1, \kappa_1, M_2, \kappa_2)J(M_1, \kappa_1, M_2, \kappa_2),$$

(13)

$$I(M_1, \kappa_1, M_2, \kappa_2) = \int d\tau \int \hat{O}_{k_1 k_2} G_{L_2 M_2} \hat{O}_{k_1 k_2} F_{L_1 M_1}.$$ 

$$J(M_1, \kappa_1, M_2, \kappa_2) = 8\pi^2 (-1)^{S_1 - S_2} \sum_{L S} (2S + 1) \left\{ \begin{array}{ccc} S & L & J \\ L_1 & S_1 & k_1 \end{array} \right\} \left\{ \begin{array}{ccc} S & L & J \\ L_2 & S_2 & k_2 \end{array} \right\}$$

$$\times C^{L_1, \kappa_1}_{L_1, M_1, \kappa_1} C^{L_2, \kappa_2}_{L_2, M_2, \kappa_2} \left\langle (\Sigma \chi)_{S M_1} (\Sigma \varphi)_{S M_2} \right\rangle.$$ 

Here $M_s$ is arbitrary.

2. The partial wave decomposition

$$F_{L M}(u, v) = \sum_{l_1 l_2} Y^{l_1 l_2}_{L M}(\bar{u}, \bar{v}) f_{l_1 l_2 L}(u, v),$$

(14)

$$Y^{l_1 l_2}_{L M}(\bar{u}, \bar{v}) = \sum_{m_1 + m_2 = M} C^{L M}_{l_1, m_1, l_2, m_2} Y^{l_1}_{l_1}(\bar{u}) Y^{l_2}_{l_2}(\bar{v})$$

(15)

of correlated three–body states could also help to calculate ME between them. This applies e.g. to ME of a non–local NN interaction, or NN interaction with $l$-dependent form factors. To perform the decomposition we need to calculate the overlap integrals

$$f_{l_1 l_2 L}(u, v) = \int d\bar{u} d\bar{v} Y^{l_1 l_2 *}_{L M}(\bar{u}, \bar{v}) F_{L M}(u, v).$$

(16)

If used directly, Eq. (16) implies the four–dimensional integration to get $f$ at each $u, v$ point. But separating Euler angles and performing integration over them analytically one can replace the four–dimensional integration with a single–dimensional one. Indeed, similar to Eq. (8), using the Eq. (4)–type expansion for both factors in the right–hand side of Eq. (16) we obtain that

$$f_{l_1 l_2 L}(u, v) = 8\pi^2 (2L + 1)^{-1} \int_{-1}^{1} dt \sum_{\lambda = -\lambda} Y^{l_1 l_2}_{L M}(t) F_{L M}(u, v, t),$$

(17)

where $Y^{l_1 l_2}_{L M}(t)$ are the body–system values of $Y^{l_1 l_2 *}_{L M}(\bar{u}, \bar{v})$,

$$Y^{l_1 l_2}_{L M}(t) = A^{l_1 l_2}_{L M} Y_{l_1 M}(\cos \theta = t, \varphi = 0), \quad A^{l_1 l_2}_{L M} = [(2l_1 + 1)/(4\pi)]^{1/2} C^{L M}_{1 l_1 0 l_2 M},$$

(18)

and $\lambda = \min(l_2, L)$.

If in the expansion (14) the functions $f_{l_1 l_2 L}(u, v)$ are real then the body–system functions $F_{L M}$ are real as well. This is seen from the body–system version of Eq. (14)

$$F_{L M}(u, v, t) = \sum_{l_1 l_2} Y^{l_1 l_2}_{L M}(t) f_{l_1 l_2 L}(u, v)$$

(19)

In the usual case of T–invariant Hamiltonians the expansion coefficients are real for such a choice of basis functions.
since, with the choice made of the body reference frame, the functions $Y^{l_1l_2}_{LM}$ entering (19) are also real.

4 Matrix Elements of NN Interaction and Kinetic Energy

The basis functions are antisymmetric with respect to particle permutations so it is sufficient to calculate the ME of an interaction between a pair of particles. We consider here such an interaction, e.g. $V(12)$, that includes the operators

$$\hat{k}^2, \hat{l}^2, (\hat{l} \cdot (\hat{s}_1 + \hat{s}_2)), S_{12} = 3(\mathbf{n} \cdot \sigma_1)(\mathbf{n} \cdot \sigma_2) - (\sigma_1 \cdot \sigma_2),$$
$$S_{12}^{ll} = 3(\hat{l} \cdot \sigma_1)(\hat{l} \cdot \sigma_2) - \hat{l}^2(\sigma_1 \cdot \sigma_2), S_{12}^{kk} = 3(\hat{k} \cdot \sigma_1)(\hat{k} \cdot \sigma_2) - \hat{k}^2(\sigma_1 \cdot \sigma_2)$$

(20)
times factors $V(r)$ and isospin and spin projection operators. Here $\mathbf{n} = \mathbf{r}/r$, $r = r_2 - r_1$, $\mathbf{k} = (1/2)(\mathbf{k}_2 - \mathbf{k}_1) = -i\partial/\partial \mathbf{r}$, $\mathbf{l} = \mathbf{r} \times \mathbf{k}$, and $\sigma_i$ are the Pauli matrices. Most frequently used versions of the realistic NN interaction are of this form. We shall use Eq. (4) to obtain ME of the above operators integrated over Euler angles. Initial ME can alternatively be calculated using Eqs. (14), (17) but the first of these procedures is faster.

Within e.g. the approximation of equal proton and neutron mass (denoted with $m$) ME of kinetic energy are expressed in terms of those of the $\hat{k}^2$ operator.

Indeed, kinetic energy $\hat{\mathcal{E}}_1$ of nucleons in the center–of–mass system can be taken into account in (21). For $\mu$ such that the corresponding Euler angle integrated reduced ME

$$\langle G|\hat{\mathcal{E}}_1|F \rangle = (A - 1)(4m)^{-1}\langle G|\hat{\mathcal{E}}_1|F \rangle = (A - 1)(\hbar^2/m)\langle G|\hat{k}^2|F \rangle.$$

Final expressions for the Euler angle integrated ME of the operators (20) are given by Eqs. (21), (23), (24), (27), (28), (29), and (34) below. ME of the $l s$ force and of further operators in (20) are expressed in the usual way [6] in terms of the reduced ME of spatial components of those operators. In the $l s$ force case, the corresponding Euler angle integrated reduced ME

$$\left(G_{L'}||V(r)\hat{l}||F_L \right)$$

of the operator $V(r)\hat{l}_\mu$ are required. Equation (4) gives

$$\left(G_{L'}||V(r)\hat{l}||F_L \right) = 8\pi^2(2L' + 1)^{-1/2} \int d\tau_{int}V(r) \sum_{MM',M+\frac{1}{2}}^{M+\frac{1}{2}} C_{LM1\mu}^{LM'} G_{LM'}^{1\mu} \hat{l}_\mu F_{LM}.$$  

(21)

Here the quantities $\hat{l}_\mu F_{LM}$ are defined as above. One has $\hat{l}_0 F_{LM} = 0$ which is taken into account in (21). For $\mu = \pm 1$ these quantities are of the form

$$\hat{l}_{\pm 1} F_{LM} = -\frac{u}{\sqrt{2}} \left( \frac{\partial}{\partial u'_x} \pm i \frac{\partial}{\partial u'_y} \right) F_{LM}.$$  

(22)

where the derivatives are taken at the space point from (4). The derivatives can be calculated numerically, and high accuracy is attained in this way. To perform this for symmetrized basis functions one needs to apply Eq. (4) at space points $(u, v)$ that are obtained from Eq. (3) by the replacement of $u'_x = 0$, or $u'_y = 0$, with small non–zero values of these quantities.
Only real parts are to be collected in the right–hand side of (22) when the functions \( f_{ll_1l_2} \) are real in Eq. (14). Indeed, the quantities \( \hat{l}_{\pm 1} F_{LM} \) are real in this case which is seen using the expansion of \( \hat{l}_{\pm 1} F_{LM} \) over \( Y_{L \pm l}^{l_1l_2} \).

When calculating ME of the \( \hat{k}^2 \) operator it is convenient to express them in terms of the quantities that already appear in ME (21). (The same is done below also in Eqs. (24) and (28).) For this purpose one writes down the integrand in the form \( V(r) \sum_{\mu} (\hat{l}_\mu G_{LM}^\ast) (\hat{l}_\mu F_{LM}) \), expresses \( \hat{l}_\mu F_{LM} \) and \( \hat{l}_\mu G_{LM} \) in terms of the Eq. (10) type quantities, uses subsequently Eqs. (4) and (8), and uses expressions of Eq. (11) type and the orthogonality property of Clebsch–Gordan coefficients. This gives

\[
\int d\tau G_{LM}^\ast V(r)\hat{k}^2 F_{LM} = \delta_{LL'}\delta_{MM'}8\pi^2(2L + 1)^{-1} \int d\tau_{int} V(r) \sum_{M'', \mu = \pm 1} \hat{l}_\mu G_{LM''} \hat{l}_\mu F_{LM''}. \tag{23}
\]

The Euler angle integrated ME of the \( \hat{k}^2 \) operator are obtained as

\[
\int d\tau G_{LM}^\ast \hat{k}^2 F_{LM} = (1/2) \int d\tau G_{LM}^\ast \Delta_u F_{LM} = \delta_{LL'}\delta_{MM'}4\pi^2 \int d\tau \left( \frac{\partial G_{LM}^\ast}{\partial u} \frac{\partial F_{LM}}{\partial u} + G_{LM}^\ast \frac{l^2}{u^2} F_{LM} \right) = \delta_{LL'}\delta_{MM'}4\pi^2 \int d\tau \left\{ (\partial/\partial u) G_{LM''} (\partial/\partial u) F_{LM''} + u^{-2} \sum_{M'', \mu = \pm 1} l_\mu G_{LM''} l_\mu F_{LM''} \right\}. \tag{24}
\]

When ME of the operator \( 1/2[V(r)\hat{k}^2 + \hat{k}^2 V(r)] \) are considered the integrand in the last line of (24) is obviously to be replaced with

\[
V(r) \left\{ \sum_{M''} (\partial/\partial u) G_{LM''} (\partial/\partial u) F_{LM''} + u^{-2} \sum_{M'', \mu = \pm 1} l_\mu G_{LM''} l_\mu F_{LM''} \right\} + 2^{-1/2} V'(r) \sum_{M''} \left\{ G_{LM''} (\partial/\partial u) F_{LM''} + (\partial/\partial u) G_{LM''} F_{LM''} \right\}. \]

The quantities \( S_{12}, S_{12}^{ll}, \) and \( S_{12}^{kk} \) in (21) can be written as

\[
3 \sum_{i,j=1}^{3} X_{ij}^{(2)} \Sigma_{ij}^{(2)} = (3/2) \sum_{\mu = -2}^{2} X^{(2)}_\mu \Sigma^{(2)}_{-\mu} (-1)^\mu
\]

where \( X_{ij}^{(2)} \) and \( \Sigma_{ij}^{(2)} \) are the Cartesian components of a space tensor and spin tensor, respectively, and \( X^{(2)}_\mu \) and \( \Sigma^{(2)}_\mu \) are the corresponding spherical components. The latter are linear combinations \( \Sigma \) of the Cartesian ones, and in particular \( X^{(2)}_0 = X^{(2)}_{zz}, \Sigma^{(2)}_0 = \Sigma^{(2)}_{zz} \). In our case

\[
\Sigma^{(2)}_{ij} = (1/2)(\sigma_{i1}\sigma_{j2} + \sigma_{1j}\sigma_{2i}) - (1/3)\delta_{ij}(\sigma_{1} \cdot \sigma_{2}).
\]
One thus has

\[
S_{12} = \frac{3}{2} \sum_{\mu=-2}^{2} \mathcal{N}_\mu^{(2)} \Sigma^{(2)}_{-\mu}(-1)^\mu,
\]

\[
S_{12}^{kl} = \frac{3}{2} \sum_{\mu=-2}^{2} \mathcal{L}_\mu^{(2)} \Sigma^{(2)}_{-\mu}(-1)^\mu,
\]

\[
S_{12}^{kk} = \frac{3}{2} \sum_{\mu=-2}^{2} \mathcal{K}_\mu^{(2)} \Sigma^{(2)}_{-\mu}(-1)^\mu.
\]

The tensors \(\mathcal{N}_\mu^{(2)}, \mathcal{L}_\mu^{(2)}, \text{and } \mathcal{K}_\mu^{(2)}\) are

\[
\mathcal{N}_\mu^{(2)} = 4(\pi/5)^{1/2} Y_{2\mu}(n),
\]

\[
\mathcal{L}_\mu^{(2)} = 4(\pi/5)^{1/2} \{Y_{2\mu}(\hat{l})\}_{\text{sym}},
\]

\[
\mathcal{K}_\mu^{(2)} = 4(\pi/5)^{1/2} Y_{2\mu}(\hat{k}),
\]

where \(Y_{2\mu}(x) = x^2 Y_{2\mu}(\hat{x})\) are the solid spherical harmonics. The \(\mu = 0\) components of these tensors are

\[
\mathcal{N}_0^{(2)} = 3n_z^2 - 1, \quad \mathcal{L}_0^{(2)} = 3l_z^2 - l^2, \quad \mathcal{K}_0^{(2)} = 3\hat{k}_z^2 - \hat{k}^2.
\]

To perform integration over Euler angles in the reduced ME of the first of the tensors \([23]\) one uses Eq. \([3]\). One has \(\mathcal{N}_0^{(2)} = 2\delta_{\mu0}\) that gives

\[
\left(F_L||V(r)\mathcal{N}^{(2)}||G_L\right) = 16\pi^2(2L' + 1)^{-1/2} \int d\tau_{int} V(r) \sum_M C_{LM}^{(2)}^{(2)} F_{LM} G_{LM}.
\]

The Euler angle integrated reduced ME of the two other tensors \([23]\) will be obtained via calculating the corresponding ME of the operators \([26]\). Proceeding in the same way as at the derivation of Eq. \([23]\) we come to the following expressions

\[
\left(G_L||V(r)\mathcal{L}^{(2)}||F_L\right) = 8\pi^2 \int V(r) \sum_{\mu_1=\pm 1,M_1,\mu_2=\pm 1,M_2} f(L_1,L_2,M_1,M_2,\mu_1,\mu_2) l_{\mu_2} G_{LM} l_{\mu_1} F_{LM},
\]

\[
\left(G_L||V(r)\delta^{(2)} + \kappa^{(2)} V(r)||F_L\right) = 8\pi^2 \int d\tau_{int} \sum_{\mu_1=M_1\mu_2=M_2} f(L_1,L_2,M_1,M_2,\mu_1,\mu_2) [V(r)\nabla_{\mu_2} G_{LM} F_{LM} \nabla_{\mu_1} F_{LM}]
\]

\[
+ 2^{-1/2} V'(r) \left(\delta_{\mu_10} \nabla_{\mu_2} G_{LM} F_{LM} + \delta_{\mu_20} G_{LM} \nabla_{\mu_1} F_{LM}\right)
\]

which contain the quantity

\[
f(L_1,L_2,M_1,M_2,\mu_1,\mu_2) = \frac{(2L_2 + 1)^{1/2} C_{LM}^{L_2 M_2}}{C_{L_1 M_1}^{L_1 M_1}} S(L_1,L_2,M_1,M_2,\mu_1,\mu_2),
\]

\[
S(L_1,L_2,M_1,M_2,\mu_1,\mu_2) = 3 \sum_{L'} (2L' + 1)^{-1} C_{L_1 M_1}^{L_1 M_1} C_{L_2 M_1}^{L_2 M_1} C_{L_1 M_2}^{L_1 M_2} C_{L_2 M_2}^{L_2 M_2} - \frac{\delta_{\mu_12} \delta_{\mu_22} \delta_{LM} \delta_{L_1 L_2}}{2L + 1}.
\]
It is implied here that $|L_1 - L_2| \leq 2$. The value of $M$ in (30) is arbitrary provided that $C_{L_1,M_2}^{L_2,M_0} \neq 0$. In (31) $M' = \mu_1 + M_1 = \mu_2 + M_2$. In (32) $\nabla = \partial / \partial r$. The quantities $\nabla_{\mu} F_{LM}$ and $\nabla_{\mu} G_{LM}$ are real at the same conditions as above.

The summation in (31) can be done in a closed form. For this purpose, let us perform a transformation of the sum. It follows from the general structure of the ME [3] that the equality $S = C_{L_1,M_2}^{L_2,M_0}S'$ with $S'$ being independent of $M$ holds true. Then multiplying $S$ by $C_{L_1,M_2}^{L_2,M_0}$, summing over $M$ and using the relation $\sum_M \left( C_{L_1,M_2}^{L_2,M_0} \right)^2 = (2L_2 + 1)/5$ one concludes that the quantity (30) may be represented as $5(2L_2 + 1)^{-1/2}$. According to (35) it holds true. Then multiplying (35) by $S_0 = \sum_M C_{L_1,M_2}^{L_2,M_0}S$. And due to the relation $\sum_M C_{L_1,M_2}^{L_2,M_0} = 0$ the last term from (31) is eliminated in the course of the summation. As a result, one obtains

$$f(L_1, L_2, M_1, M_2, \mu_1, \mu_2) = 15(2L_2 + 1)^{-1/2} \sum_{L,M'} g(L_1, L_2, L') C_{L_1,M_1,\mu_1}^{L,M'} C_{L_2,M_2,\mu_2}^{L,M'}, \quad (32)$$

$$g(L_1, L_2, L') = (2L' + 1)^{-1} \sum_M C_{L_1,M_2}^{L_2,M_0}C_{L_1,M_1,\mu_1}^{L,M}C_{L_2,M_2,\mu_2}^{L,M}. \quad (33)$$

(The summation over $M'$ in (32) is a formal one.) Now we perform the summation in (33) with the help of Eq. 8.7.(13) in [3] obtaining

$$g(L_1, L_2, L') = (-1)^{L_1 + L'}(2L_2 + 1)^{1/2} \sqrt{\frac{2}{15}} \left\{ \begin{array}{ccc} 1 & 1 & 2 \\ L_1 & L_2 & L' \end{array} \right\}. \quad (34)$$

We substitute this into (32) and perform the summations with the help of Eq. 8.7.(32) in [3]. Finally, we obtain that in (28), (29)

$$f(L_1, L_2, M_1, M_2, \mu_1, \mu_2) = (6/5)^{1/2}(-1)^{\mu_1 + M_2} C_{L_1,M_1,\mu_1}^{2, M_{1,-2}} C_{L_2,M_2,\mu_2}^{2, \mu_1, -\mu_2}. \quad (34)$$

It is implied here that $\mu_1 + M_1 = \mu_2 + M_2$, otherwise $f = 0$.

The formulae in this section have been verified in three–nucleon computations.

5 Symmetry relations

We write down the formulae for (components of) states possessing definite parity $(-1)^I$. The relation

$$F_{I-M} = (-1)^{I+L+M} F_{LM} \quad (35)$$

holds true. According to (35) $F_{L,M=0}$ vanishes when $I + L$ is odd. To obtain (35) one notes that in Eq. (19) $Y_{L,-M}^{L_{1,2}} = (-1)^{l_1 + l_2 + L + M} Y_{L,M} V_{L_{1,2}}^{L_{1,2}}$.

Let us assume that the quantities $\hat{O}_{kr} F_{LM}$ have definite parity $(-1)^k$ (that is related to the parity of $F_{LM}$ and that of the operator). Then

$$\hat{O}_{k,-k} F_{LM} = (-1)^{i+L+M+k+k} \hat{O}_{kr} F_{LM}. \quad (36)$$

Eq. (36) is obtained expressing its left–hand side in terms of the functions $(OF)_{LM}^{LM}$ from Eq. (4) and applying Eq. (35) to them.
The integrands in Eqs. (8), (17), (27), and (23) may be written, up to the notation of summation, as

\[ \sum_{M} X(M) \quad \text{and} \quad \sum_{M \mu} X(M, \mu). \]

Due to Eqs. (35) and (36) one has

\[ X(-M) = (-1)^I X(M), \quad X(-M, -\mu) = (-1)^{I + I'} X(M, \mu), \]

where \((-1)^I\) and \((-1)^{I'}\) are the parities of the two states entering an ME. Then, when parities are the same, one can apply e.g. the relations

\[ \sum_{M} X(M) = X(0) + 2 \sum_{M > 0} X(M), \quad \sum_{M \mu} X(M, \mu) = \sum_{\mu} X(0, \mu) + 2 \sum_{M > 0, \mu} X(M, \mu) \]

to speed up the summations. When parities are opposite the sums vanish as it should be.

The integrands in Eqs. (13), (21), (28), and (29) may be written as

\[ \sum_{M' \mu = \pm 1} X(M, M', \mu) \quad \text{and} \quad \sum_{M' \mu = \pm 1} X(M_1, \mu_1, M_2, \mu_2). \]

One has, with the same definitions of \((-1)^I\) and \((-1)^{I'}\) as above,

\[ X(-M, -M', -\mu) = (-1)^{I + I'} X(M, M', \mu), \]
\[ X(-M_1, -\mu_1, -M_2, -\mu_2) = (-1)^{I + I'} X(M_1, \mu_1, M_2, \mu_2). \]

When one of the summation variables above is expressed in terms of the others this leads to the sums of the form

\[ \sum_{m_1 m_2} Y(m_1, m_2), \quad \sum_{m_1 m_2 m_3} Y(m_1, m_2, m_3) \]

with the similar property \(Y(-m_1, \ldots, -m_i) = (-1)^{I + I'} Y(m_1, \ldots, m_i)\). Then, when parities are the same, at a particular choice of summation variables one can apply e.g. the relations of the type

\[ \sum_{M \mu} Y(M, \mu) = \sum_{\mu} Y(0, \mu) + 2 \sum_{M > 0, \mu} Y(M, \mu), \]
\[ \sum_{M_1 \mu_1 \mu_2} Y(M_1, \mu_1, \mu_2) = \sum_{\mu_1 \mu_2} Y(0, \mu_1, \mu_2) + 2 \sum_{M_1 > 0, \mu_1 \mu_2} Y(M_1, \mu_1, \mu_2). \]

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Appendix

The known relationship $d\bar{u}d\bar{v} = d\omega dt$ is obtained as follows. Let us recall the definition, see (6), of the Euler angles $\omega \equiv \{\alpha, \beta, \gamma\}$: the angles $\alpha$ and $\beta$ are the azimuthal angle and polar angle determining the direction of the vector $\bar{u}$, and the angle $\gamma$ corresponds to a rotation of an intermediate reference frame around its $z$–axis coinciding with the $\bar{u}$ direction. (This rotation brings the $x$–axis of the intermediate reference frame into the $\bar{u}, \bar{v}$ plane.) Let us perform the integration over $d\bar{v}$ choosing some fixed reference frame with the $z$–axis directed along $\bar{u}$. Then one can write $d\bar{u}d\bar{v} = d\alpha \sin \beta d\beta d\gamma$ where $\alpha$ is the azimuthal angle of the vector $\bar{v}$ in the chosen reference frame. But, by the definition of $\gamma$, $\alpha$ differs from $\gamma$ only by a constant, so that $d\alpha = d\gamma$. This gives the desired expression taking into account that $d\omega = d\alpha \sin \beta d\beta d\gamma$.

The D–function orthogonality relations we use are (6)

$$\int d\omega D^L_{M_2}M_1(\omega)D^{L_2}_{M_1'}M_1'(\omega) = \frac{8\pi^2}{2L_1+1}\delta_{L_1}\delta_{L_2}\delta_{M_1}M_1'\delta_{M_1'}M_2'. \quad (A.37)$$

To obtain (12) we need to expand the states of the form

$$\left(\hat{O}_k \cdot \hat{\Sigma}_k\right)|\left(F_l \otimes \varphi_s\right)_{JM}\rangle$$

over those of the form

$$|\left(\left(OF\right)^{L_k}_{L} \otimes \left(S\varphi\right)^{S_k}_{S}\right)_{JM}\rangle.$$

The expansion coefficients are the same as if $\hat{O}_k$ and $\hat{\Sigma}_k$ were not operators but states of independent subsystems with angular momenta $k$. Hence, these coefficients are the recoupling coefficients for four angular momenta (6), i.e. basically $9j$–symbols. Our initial states include scalar products so that two of the four angular momenta are coupled to zero angular momentum. Therefore, the $9j$–symbols reduce to $6j$–symbols in our case.

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