Matrix elements of the Argonne $v_{18}$ potential

Bogdan Mihaila

Los Alamos National Laboratory, Los Alamos, NM 87545

Abstract

We discuss two approaches to the calculation of matrix elements of the Argonne $v_{18}$ potential. The first approach is applicable in the case of a single-particle basis of harmonic-oscillator wave functions. In this case we use the Talmi transformation, implemented numerically using the Moshinsky transformation brackets, to separate the center-of-mass and relative coordinates degrees of freedom. Integrals involving the radial part of the potential are performed using Gauss-Hermite quadrature formulas, and convergence is achieved for sets of at least 512 points. We validate the calculation of matrix elements of the Argonne $v_{18}$ potential using a second approach suitable for the case of an arbitrary functional form of the single-particle wave functions. When the model space is represented in terms of harmonic-oscillator wave functions, results obtained using these two approaches are shown to be identical within numerical accuracy.

Key words: matrix elements, nucleon-nucleon interaction

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1 Introduction

Direct comparison of experimental data and theory become ambiguous if problems such as the many-body problem are not solved accurately. This is particularly true in nuclear physics, where one uses numerical solutions of the Schrödinger equation to constrain in part the effective interaction between nucleons [[]. Despite tremendous accomplishments in the past decade in carrying out ab initio studies of nuclear structure of light systems [[], numerical solutions of medium and large nuclear systems are yet to be performed in the framework of realistic nuclear interactions [[]].
The matrix elements of the interaction represent the building blocks of any many-body approach which shares features in common with the shell model approach. Here, the model space is represented in terms of a complete set of single-particle wave functions. All possible single-particle configurations with the appropriate properties should in principle be used to diagonalize the Hamiltonian, and obtain the associated spectrum of eigenvalues and eigenfunctions. However, the single-particle model space is in principle infinite. Hence, finite reductions of the model space must be considered and convergence to the continuum limit must be achieved. The efficiency of this procedure is linked to the ability of the functional form of the single-particle wave functions to capture the relevant correlations at both short- and long-range scale.

Traditionally, matrix elements of the interaction are formed in a basis of harmonic-oscillator wave functions. This has the advantage that one can perform an exact separation of the center-of-mass and relative coordinates degrees of freedom using the Talmi transformation approach [19] (via its numerical implementation based on the Moshinsky transformation brackets [20]), and integrals can be accurately performed using Gauss-Hermite quadrature formulas. Therefore, we will by discussing the calculation of the two-body matrix elements in a harmonic-oscillator basis. This is done both for completeness, and for testing purposes, as the more elaborated procedures to be discussed in the second part of this paper will require validation.

Unfortunately, the asymptotic form of the harmonic-oscillator wave functions is Gaussian which leads to densities decaying as $e^{-x^2}$, whereas the natural tail of the nuclear density is exponential, $e^{-x}$. Added flexibility is desirable, and can be achieved by considering linear combinations of harmonic oscillator wave functions [10,11,12], or different functional representations for the hole and particle sides of the spectrum [21]. To this effect, in the second part of this paper, we will discuss the framework of calculating matrix elements of the Argonne $v_{18}$ potential in a basis of single-particle wave functions of arbitrary functional form. Here, the ability of using the Moshinsky transformation brackets approach to perform the separation of the center-of-mass and relative coordinates degrees of freedom is rendered numerically unfeasible, as the required CPU time is of order $N^4$ compared to the calculation involving Moshinsky transformation brackets.

For illustrative and testing purposes, we will apply this approach to the case when the radial part of the single-particle wave functions, $R_{nl}(x)$ can be expanded out into harmonic-oscillator wave functions, $\mathcal{H}\mathcal{O}_{kl}(x)$, i.e.

$$R_{nl}(x) = \sum_{k=1}^{N} A_{nl}^k \mathcal{H}\mathcal{O}_{kl}(x).$$

(1)

This is convenient because we can still use a Gaussian quadrature technique to
perform the numerical computation of the radial integrals. This also allows us
to check of the reliability of our matrix-elements calculation by comparing with
matrix elements calculated in a harmonic-oscillator basis using the procedures
using the Moshinsky transformation brackets.

The paper is organized as follows: In Sec. 2, we review features of the Ar-
gonne \( v_{18} \) potential, together with the definitions of the matrix elements to be
discussed further. Basic aspects of the separation of the center-of-mass and
relative coordinates using the numerical implementation of the Talmi trans-
formation via the Moshinsky transformation-brackets approach, together with
the procedures required for the 7 types of operators part of the Argonne \( v_{18} \)
potential, are discussed in Sec. 3. In Sec. 4 we present the general results
used to calculate the matrix elements of a translationally-invariant two-body
interaction in an arbitrary single-particle basis. The implementation of this
general approach for the particular case of the 7 operators in the Argonne \( v_{18} \)
potential is discussed in Sec. 5. This calculation is carried out in a \( jj \)-coupling
scheme. The part of the calculation involving the isospin part of the interac-
tion is identical in both frameworks. A brief review of this calculation is the
object of Sec. 6. Finally, in Sec. 7 we discuss numerical convergence aspects
of the matrix elements calculation corresponding to a \( ^{16}\text{O} \)-like model space of
harmonic-oscillator single-particle wave functions, and compare with results
obtained using the two frameworks. We also include an appendix on the cal-
culation of large sets of abscissas and weights for the evaluation of integrals
using Gauss-Hermite quadrature formulas, followed by an appendix summa-
rizing results relevant to the calculation of reduced matrix elements used in
Sec. 5.

2 Preliminaries

Consider the two-body approximation of the Hamiltonian describing a system
consisting of protons and neutrons

\[
H = \sum_i T_i + \sum_{i<j} V_{ij} .
\]  

(2)

In the second-quantization representation this becomes

\[
H = \sum_{\alpha\beta} a_\alpha^\dagger \langle \alpha|T|\beta\rangle a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger \langle \alpha\beta|V_{2N}|\gamma\delta\rangle a_\gamma a_\delta ,
\]

(3)

where Greek letters label the single-particle states \( |\alpha\rangle = |nlsjm_j; \frac{1}{2} m_\tau\rangle \), with
\( n \geq 1, s = \frac{1}{2}, j = l \pm \frac{1}{2} \) and \( m_\tau = +\frac{1}{2}(-\frac{1}{2}) \) – for a proton (neutron). The parity
of these states is \((-1)^l\). In this work we will assume that the radial part of the single-particle wave functions, \(R_{nl}(x)\), is simply given by the radial part of the harmonic oscillator wave functions \(HO_{kl}(x)\), subject to the normalization conditions

\[
\int_0^\infty [x^2 \, dx] \, R_{nl}(x) \, R_{n'l'}(x) = \delta_{n \, n'} \delta_{l \, l'} .
\] (4)

Here, \(x = r/b\), with \(b\) the oscillator parameter. We note that the single-particle radial functions \(R_{nl}(r)\) are defined in terms of the radial functions \(R_{nl}(x)\) such that they satisfy the normalization condition

\[
\int_0^\infty [r^2 \, dr] \, R_{nl}(r) \, R_{n'l'}(r) = \delta_{n \, n'} \delta_{l \, l'} .
\] (5)

Thus, we have

\[
R_{nl}(r) = \frac{1}{b^{3/2}} \, R_{nl}(x) .
\] (6)

2.1 Argonne \(v_{18}\) potential

The Argonne \(v_{18}\) potential \[16\] is an updated version of the nonrelativistic Argonne potential \[22\] that fits both \(np\) data and \(pp\) data, as well as low-energy \(nn\) data scattering parameters and deuteron properties. The potential was fit directly to the Nijmegen \(NN\) scattering database, which contains 1787 \(pp\) and 2514 \(np\) data in the range 0-350 MeV, together with the \(nn\) scattering length measured in \(d(\pi^-,\gamma)nn\) experiments and the deuteron binding energy. The fit has a \(\chi^2\) per datum of 1.09.

The strong interaction part of the Argonne \(v_{18}\) potential is projected into an operator format with 18 terms:

i) a charge-independent part that has 14 operator components (as in the older Argonne \(v_{14}\) \[22\]), featuring 7 basic operators,

\[1, \sigma_i \cdot \sigma_j, \, S_{ij}, \, \ell \cdot S, \, \ell^2, \, \ell^2 (\sigma_i \cdot \sigma_j), \, (\ell \cdot S)^2 ,\]

and their charge-independent counterparts

\[\tau_i \cdot \tau_j, \, (\sigma_i \cdot \sigma_j) (\tau_i \cdot \tau_j), \, S_{ij} (\tau_i \cdot \tau_j), \, (\ell \cdot S) (\tau_i \cdot \tau_j), \, \ell^2 (\tau_i \cdot \tau_j), \, \ell^2 (\sigma_i \cdot \sigma_j) (\tau_i \cdot \tau_j), \, (\ell \cdot S)^2 (\tau_i \cdot \tau_j) ;\]

ii) a charge-independence breaking part that has three charge-dependent operators
where $T_{ij} = 3 \tau_i \tau_j - \tau_i \cdot \tau_j$ is the isotensor operator, defined analogous to the $S_{ij}$ operator, and iii) one charge-asymmetric operator

$$
\tau_{zi} + \tau_{zj}.
$$

In principle, there could be more charge-independence breaking terms, such as $(\ell \cdot S) T_{ij}$ or $S_{ij} (\tau_{zi} + \tau_{zj})$, but the scattering data are not sufficiently precise to identify them at present. The potential also includes a complete electromagnetic potential, containing Coulomb, Darwin-Foldy, vacuum polarization, and magnetic moment terms with finite-size effects.

### 2.2 Two-body matrix elements

Matrix elements of the two-body interaction can be specified either in particle-particle (pp) coupling or in particle-hole (ph) coupling. Either set of matrix elements completely specify the two-body interaction. We define ph-coupled matrix elements as

$$
\langle (34)_L | V | (12)_L \rangle = \sum_{m_1 m_2 m_3 m_4} \langle 12 | V | 34 \rangle \times (-)^{j_3 - j_4} \langle j_1 m_1 j_3 - m_3 | \lambda \mu \rangle \langle j_4 m_4 j_2 - m_2 | \lambda \mu \rangle.
$$

Correspondingly, the pp-coupled matrix elements are defined as

$$
\langle (13)_L | V | (42)_L \rangle = \sum_{m_1 m_2 m_3 m_4} \langle 12 | V | 34 \rangle \langle j_1 m_1 j_3 - m_3 | L M \rangle \langle j_3 m_3 j_4 m_4 | L M \rangle.
$$

In practice, the calculation of the two-body matrix elements using a harmonic-oscillator single-particle basis set is carried out in pp coupling. Subsequently, ph-coupled matrix elements are evaluated from their pp counterpart, using the relationship

$$
\langle (13)_L | V | (42)_L \rangle = \sum_{L} (-)^{j_3 + j_4 + L} (2L + 1) \left\{ \begin{array}{ccc} j_1 & j_3 & \lambda \\ j_4 & j_2 & L \end{array} \right\} \langle (12)_L | V | (34)_L \rangle. \tag{13}
$$

Conversely, we have

$$
\langle (12)_L | V | (34)_L \rangle = \sum_{L} (-)^{j_3 + j_4 + L} (2\lambda + 1) \left\{ \begin{array}{ccc} j_1 & j_2 & L \\ j_4 & j_3 & \lambda \end{array} \right\} \langle (13)_L | V | (42)_L \rangle. \tag{14}
$$
It is useful to introduce here some notations we will be using throughout the rest of this paper. First, we note that, by definition, the scalar product of two tensor operators of rank $k$, $U^{(k)}$ and $V^{(k)}$, is introduced as

$$
(U^{(k)} \odot V^{(k)}) = \sum_q (-)^q U_q^{(k)} V_{-q}^{(k)} .
$$

(15)

In turn, the definition of the spherical tensor product of two tensor operators, $A^{(k_1)}$ and $B^{(k_2)}$, is

$$
\left[ A^{(k_1)} \otimes B^{(k_2)} \right]_q^{(k)} = \sum_{q_1 q_2} \langle k_1 q_1 k_2 q_2 | k q \rangle A^{(k_1)}_{q_1} B^{(k_2)}_{q_2} .
$$

(16)

Second, we note that the angular degrees of freedom will be described in terms of the unnormalized spherical harmonics, defined in terms of their normalized counterparts such that (23, Eq. 2.5.31)

$$
C_q^{(k)}(\hat{r}) = \sqrt{\frac{4\pi}{k}} Y_{kq}(\hat{r}) .
$$

(17)

The unnormalized spherical harmonics satisfy the orthogonality conditions

$$
\int d\Omega \: C_{q_1}^{(k_1)}(\hat{r})^* C_{q_2}^{(k_2)}(\hat{r}) = \frac{4\pi}{2k_1 + 1} \delta_{k_1 k_2} \delta_{q_1 q_2} .
$$

(18)

For completeness, we list here useful properties of the unnormalized spherical harmonics:

i) $C^{(0)}(\hat{r}) = 1$.

ii) $C_q^{(k)}(\hat{r})^* = (-)^q C_{-q}^{(k)}(\hat{r})$.

iii) $\left( C^{(k)}(\hat{r}) \otimes C^{(k)}(\hat{p}) \right) = P_k(\cos \omega)$, where $\omega$ is the angle between $\hat{r}$ and $\hat{p}$.

iv) $\left[ C^{(k_1)}(\hat{r}) \otimes C^{(k_2)}(\hat{r}) \right]^{(k)} = \langle k_1 0 k_2 0 | k 0 \rangle C^{(k)}(\hat{r})$.

v) $C_{q_1}^{(k_1)}(\hat{r}) C_{q_2}^{(k_2)}(\hat{r}) = \sum_{kq} C_q^{(k)}(\hat{r}) \langle k_1 0 k_2 0 | k 0 \rangle \langle k_1 q_1 k_2 q_2 | k q \rangle$.

Finally, in the interest of brevity, throughout the remainder of this paper we will follow the conventions, and will be referring directly to the equation numbers, found in Ref. [23].

3 Matrix elements calculation using harmonic-oscillator wave functions

Provided that the single-particle wave functions are harmonic-oscillator wave functions, one can use Talmi transformation [19] via the Moshinsky trans-
formation brackets \[20\] to exactly factorize a product of two single-particle wave functions into a part which depends only on the center-of-mass degrees of freedom, and a part which depends only on the relative-motion degrees of freedom. For completeness, we will review now the technical details of this procedure.

3.1 Moshinsky transformation brackets

Consider a two-particle system in a harmonic oscillator potential. We shall characterize the two particles by their coordinates and quantum numbers. For the purpose of our discussion, we introduce two system of coordinates:

- **laboratory frame**, where the two particles are described by their coordinates with respect to the center of the potential well, \( \vec{r}_1 \) and \( \vec{r}_2 \), and corresponding radial, \( n_1 \) and \( n_2 \), and orbital quantum numbers, \( l_1 \) and \( l_2 \).
- **center-of-mass frame**, where the system is characterized by the relative coordinate \( \vec{r} \) and the coordinate \( \vec{R} \) of the center of mass of the two particles, defined as

\[
\vec{r} = \frac{1}{\sqrt{2}} (\vec{r}_1 - \vec{r}_2), \quad \vec{R} = \frac{1}{\sqrt{2}} (\vec{r}_1 + \vec{r}_2); \quad (19)
\]

the radial and orbital quantum numbers \( n, l \) will correspond to the relative motion, and \( N, L \) to that of the center of mass.

The eigenkets in the two coordinate systems may be written as follows:

- **laboratory frame**

\[
|n_1 n_2 (l_1 l_2) \lambda \mu \rangle = \sum_{m_1 m_2} \langle l_1 m_1 l_2 m_2 | \lambda \mu \rangle |n_1 l_1 m_1 \rangle |n_2 l_2 m_2 \rangle; \quad (20)
\]

- **center-of-mass frame**

\[
|n N (l L) \lambda \mu \rangle = \sum_{m M} \langle l m L M | \lambda \mu \rangle |n l m \rangle |N L M \rangle . \quad (21)
\]

The Moshinsky transformation brackets are defined as the expansion coefficients of the eigenket \[20\] in a series of eigenkets \[21\]. We have \[20\]

\[
|n_1 n_2 (l_1 l_2) \lambda \mu \rangle = \sum_{n l NL} \langle n l N L | \lambda \mu \rangle |n_1 l_1 n_2 l_2 \lambda \rangle |n N (l L) \lambda \mu \rangle. \quad (22)
\]

This transformation is independent of the magnetic quantum number \( \mu \), and the transformation bracket vanishes for all combinations of its parameters which do not satisfy the total angular momentum

\[
\vec{\lambda} = \vec{\ell}_1 + \vec{\ell}_2 = \vec{\ell} + \vec{L}, \quad (23)
\]
E \propto (2n_1 + l_1 + 3/2) + (2n_2 + l_2 + 3/2) \\
= (2n + l + 3/2) + (2\Lambda + L + 3/2).
\tag{24}

conservation laws. Therefore, the transformation bracket vanishes for all combinations of its parameters which do not satisfy the energy condition (24), and any summations over \( \lambda \) will be restricted by the corresponding triangle relations:

\begin{align*}
|l_1 - l_2| &\leq \lambda \leq l_1 + l_2, \\
|l - L| &\leq \lambda \leq l + L.
\tag{25}
\end{align*}

We calculate the two-body matrix element in a harmonic oscillator single-particle basis using the Moshinsky transformation brackets, and obtain

\begin{align*}
\langle n_1n_2 (l_1 \frac{1}{2} j_1, (l_2 \frac{1}{2}) j_2) ; JM_J \mid V \mid n_3n_4 (l_3 \frac{1}{2} j_3, (l_4 \frac{1}{2}) j_4) ; JM_J \rangle \\
= \hat{\lambda} \hat{\lambda}' \sum_{nN\Lambda \lambda' n'N'\Lambda'} \langle n_1 l_1 n_2 l_2 \lambda' \mid n' l' N' L' \lambda' \rangle \langle n_3 l_3 n_4 l_4 \lambda \mid n l N L \lambda \rangle \\
\times \left\{ \begin{array}{c}
\frac{1}{2} j_1 \\
\frac{1}{2} j_2
\end{array} \right\} \left\{ \begin{array}{c}
\frac{1}{2} j_3 \\
\frac{1}{2} j_4
\end{array} \right\} \\
\times \langle n' N' (l' L') \lambda' \left( \frac{1}{2} \frac{1}{2} \right) \lambda' ; JM_J \mid V \mid nN (lL) \lambda \left( \frac{1}{2} \frac{1}{2} \right) \lambda ; JM_J \rangle.
\tag{26}
\end{align*}

For a particular choice of the potential, \( V \), all we have to do is to calculate the matrix element

\begin{align*}
\langle n' N' (l' L') \lambda' \left( \frac{1}{2} \frac{1}{2} \right) \lambda' ; JM_J \mid V \mid nN (lL) \lambda \left( \frac{1}{2} \frac{1}{2} \right) \lambda ; JM_J \rangle.
\tag{27}
\end{align*}

3.2 Central interaction.

For the case of the central interaction, the potential depends only on the magnitude of the vector \( \vec{r} \), and not on its angular degrees of freedom. We apply the Wigner-Eckart theorem for the case of a zero-rank tensor (23, Eq. 5.4.1a)

\begin{align*}
\langle n' N' (l' L') \lambda \left( \frac{1}{2} \frac{1}{2} \right) \lambda ; JM_J \mid V_c \mid nN (lL) \lambda \left( \frac{1}{2} \frac{1}{2} \right) \lambda ; JM_J \rangle \\
= \frac{1}{J} \langle n' N' (l' L') \lambda \left( \frac{1}{2} \frac{1}{2} \right) \lambda ; JM_J \parallel V_c \parallel nN (lL) \lambda \left( \frac{1}{2} \frac{1}{2} \right) \lambda ; JM_J \rangle.
\tag{28}
\end{align*}
where we have introduced the notation $\hat{J} = \sqrt{2J + 1}$. The reduced matrix element in Eq. (28) is evaluated using (23, Eq. 7.1.7). We have

$$\langle n'N' (l' L')_\lambda (\frac{1}{2} \frac{1}{2})_s'; JM_J \parallel V_c \parallel nN (lL)_\lambda (\frac{1}{2} \frac{1}{2})_s; JM_J \rangle$$

(29)

$$= \delta_{SS'} (-)^{\lambda' + S + J + 0} (2J + 1) \left\{ \begin{array}{c} \lambda' J S \\
J \lambda \ 0 \end{array} \right\} \langle n'N' (l' L')_\lambda \parallel V_c \parallel nN (lL)_\lambda \rangle.$$  

We use (23, Eq. 7.1.7) one more time for the reduced matrix element

$$\langle n'N' (l' L')_\lambda \parallel V_c \parallel nN (lL)_\lambda \rangle$$

(30)

$$= \delta_{NN'} \delta_{LL'} (-)^{\lambda' + L + \lambda + 0} \hat{\lambda}' \left\{ \begin{array}{c} l' \lambda' L \\
\lambda \ l \ 0 \end{array} \right\} \langle n' l' \parallel V_c \parallel n l \rangle.$$  

The Wigner 6$j$ symbols in Eqs. (29,30) are calculated using (23, Eq. 6.3.2). From the Wigner-Eckart theorem (23, Eq. 5.4.1a) we have:

$$\langle n' l' m_l | V_c | n \ l m_l \rangle = \delta_{ll'} \frac{1}{l} \langle n' l' \parallel V_c \parallel n l \rangle$$

(31)

$$= \delta_{ll'} \mathcal{R}\mathcal{M}[V_c](n'l' ; nl),$$

where we have introduced the notation

$$\mathcal{R}\mathcal{M}[V](n'l' ; nl) = \int_0^\infty [r^2 \ d r] \mathcal{H}\mathcal{O}_{n'l'}(r) V(r) \mathcal{H}\mathcal{O}_{nl}(r).$$

(32)

Therefore, Eq. (28) becomes

$$\langle n'N' (l' L')_\lambda (\frac{1}{2} \frac{1}{2})_s'; JM_J \parallel V_c \parallel nN (lL)_\lambda (\frac{1}{2} \frac{1}{2})_s; JM_J \rangle$$

(33)

$$= \delta_{SS'} \delta_{NN'} \delta_{LL'} \delta_{ll'} \delta_{\lambda \lambda'} \mathcal{R}\mathcal{M}[V_c](n'l' ; nl).$$

3.3 Spin-spin interaction

It is convenient to carry out the calculation of the spin-spin interaction matrix element by using the $m$-representation approach outlined above. We have:
where we used the fact that \( \langle \frac{1}{2}\frac{1}{2} S \rangle \) (23), Eq. 7.1.6)

\[ 3.4 \text{ Tensor interaction} \]

We begin the calculation of the tensor interaction matrix element by using (23), Eq. 7.1.6)

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The reduced matrix elements in Eq. (38) are evaluated as follows:

(i) We use ([23], Eq. 7.1.5) – for $S(S') = 0, 1$, to obtain

$$\langle (\frac{1}{2} \frac{1}{2}) S' || [\sigma_1 \otimes \sigma_2]^{(2)} || (\frac{1}{2} \frac{1}{2}) S \rangle = \sqrt{5} \hat{S} \hat{S}' \left\{ \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} 1 \right\} \langle \frac{1}{2} || \sigma_1 || \frac{1}{2} \rangle \langle \frac{1}{2} || \sigma_2 || \frac{1}{2} \rangle$$

with $\langle \frac{1}{2} || \sigma_i || \frac{1}{2} \rangle = \sqrt{6}$ (see Ref. [23], Eq. 5.4.4).

(ii) Next, we use ([23], Eq. 7.1.7) to obtain

$$\langle n' N' (l' L')_\lambda || V_t C^{(2)} || n N (lL)_\lambda \rangle = \delta_{NN'} \delta_{LL'} \delta_{SS'} (-)^{l'+L+\lambda+2} \hat{\lambda} \hat{\lambda}' \left\{ l' \lambda' L \right\} \langle n' l' || V_t C^{(2)} || n l \rangle,$$

(iii) We also have

$$\langle n' l' || V_t C^{(2)} || n l \rangle = \langle l' || C^{(2)} || l \rangle \mathcal{R}\mathcal{M}[V_t](n'' ; nl),$$

where $\langle l' || C^{(k)} || l \rangle$ is given by Eq. (B.1).

We obtain

$$\langle n' N' (l' L')_\lambda || J M_J || V_t S_{12} || n N (lL)_\lambda || J M_J \rangle$$

$$= \delta_{NN'} \delta_{LL'} \delta_{SS'} \delta_{S1} 2 \sqrt{30} (-)^{l'+L+J+1} \hat{\lambda} \hat{\lambda}' \langle 0 2 0 || l' 0 \rangle$$

$$\times \left\{ J S \lambda' \right\} \left\{ l' \lambda' L \right\} \mathcal{R}\mathcal{M}[V_t](n'' ; nl).$$
3.5 Spin-orbit interaction

Similarly to the case of the tensor interaction, we first use (23, Eq. 7.1.6)
\[
\langle n'N' (l'L')_{\lambda'} (\frac{1}{2} \frac{1}{2})_{S'}; JM_J | V_{ls} (\ell \cdot S) | nN (lL)_{\lambda} (\frac{1}{2} \frac{1}{2})_{S}; JM_J \rangle
\]
(44)
\[= (-)^{\lambda + S' + J} \left\{ \begin{array}{c} J \ S' \\ 1 \ \lambda \ S \end{array} \right\} \times \sum_{n''N''} \langle n'N' (l'L')_{\lambda'} || V_{ls} \ell || n''N'' (lL)_{\lambda} \rangle \langle n''N'' (\frac{1}{2} \frac{1}{2})_{S''} || S || nN (\frac{1}{2} \frac{1}{2})_{S} \rangle ,
\]
with the reduced matrix elements calculated as:
(i) We use (23, Eq. 5.4.3) – for \( S = 0, 1 \), to obtain
\[
\langle (\frac{1}{2} \frac{1}{2})_{S''} || S || (\frac{1}{2} \frac{1}{2})_{S} \rangle = \delta_{SS'} \sqrt{S(S+1)(2S+1)} = \sqrt{6} \delta_{S1} \delta_{SS'} .
\]
(45)
(ii) Next, we use (23, Eq. 7.1.7) to obtain
\[
\langle n'N' (l'L')_{\lambda'} || V_{ls} \ell || nN (lL)_{\lambda} \rangle
\]
(46)
\[= \delta_{NN'} \delta_{LL'} (-)^{l'+L+\lambda+1} \hat{\lambda} \hat{\lambda}' \left\{ \begin{array}{c} l' \ \lambda' \\ \lambda \ 1 \end{array} \right\} \langle n' \ell' || V_{ls} \ell || n \ell \rangle .
\]
(iii) Finally, we use \( \langle l || \ell || l' \rangle = \delta_{ll'} \hat{l} \sqrt{l(l+1)} \) (23, Eq. 5.4.3) to obtain
\[
\langle n' \ell' || V_{ls} \ell || n \ell \rangle = \delta_{ll'} \hat{l} \sqrt{l(l+1)} \mathcal{R.M}[V_{ls}](n'l ; nl) .
\]
(47)
Collecting terms, we find
\[
\langle n'N' (l'L')_{\lambda'} (\frac{1}{2} \frac{1}{2})_{S'}; JM_J | V_{ls} (\ell \cdot S) | nN (lL)_{\lambda} (\frac{1}{2} \frac{1}{2})_{S}; JM_J \rangle
\]
(48)
\[= \delta_{NN'} \delta_{LL'} \delta_{SS'} \delta_{S1} \sqrt{6} (-)^{l+L+J} \hat{\lambda} \hat{\lambda}' \sqrt{l(l+1)}
\]
\[\times \left\{ \begin{array}{c} J \ S \ X' \\ 1 \ \lambda \ S \end{array} \right\} \left\{ \begin{array}{c} l \ \lambda' \\ \lambda \ 1 \end{array} \right\} \mathcal{R.M}[V_{ls}](n'l ; nl) .
\]

3.6 \( \ell^2 \) Interaction.

The matrix element of the \( \ell^2 \) interaction can be easily calculated when the matrix element is written in the \( m \) representation, i.e.
\[
\langle n'N' l'm' l'M' S'm_s' \mid V_{12} \ell^2 \mid nN l m_l L M S m_s \rangle = \delta_{NN'} \delta_{LL'} \delta_{MM'} \delta_{\ell \ell'} \delta_{m_m m_m'} \delta_{SS'} \delta_{m_s m_s'} \ l(l+1) \ \mathcal{R} \mathcal{M}[V_{12}](n'l; nl).}
\]

We use the transformation

\[
\langle n'N' (l' L')_\lambda (\frac{1}{2} \frac{1}{2})_s' \mid J M_J \mid V_{12} \ell^2 \mid nN (IL)_\lambda (\frac{1}{2} \frac{1}{2})_s \mid J M_J \rangle = \sum_{m_l M m_s \mu' \mu} \langle l' m' l'M' \mid \lambda' \mu' \rangle \langle \lambda' \mu' S' m_s' \mid J M_J \rangle \times \sum_{m_l M m_s \mu' \mu} \langle l m_l L M \mid \lambda \mu \rangle \langle \lambda \mu S m_s \mid J M_J \rangle \times \langle n'N' l'm' l'M' S'm_s' \mid V_{12} \ell^2 \mid nN l m_l L M S m_s \rangle,
\]

substitute Eq. (49), and employ the orthogonality properties of the Clebsch-Gordon coefficients, to obtain

\[
\langle n'N' (l' L')_\lambda (\frac{1}{2} \frac{1}{2})_s' \mid J M_J \mid V_{12} \ell^2 \mid nN (IL)_\lambda (\frac{1}{2} \frac{1}{2})_s \mid J M_J \rangle = \delta_{\lambda\lambda'} \delta_{NN'} \delta_{LL'} \delta_{\ell \ell'} \delta_{SS'} \ l(l+1) \ \mathcal{R} \mathcal{M}[V_{12}](n'l; nl).
\]

3.7 $\ell^2 (\sigma_1 \cdot \sigma_2)$ interaction

The derivation of the matrix element for the $\ell^2 (\sigma_1 \cdot \sigma_2)$ interaction follows closely the calculation of the matrix element corresponding to the $\ell^2$ interaction. We first perform a transformation to the $m$ representation where the calculation of the matrix element is particularly simple, i.e.

\[
\langle n'N' (l' L')_\lambda (\frac{1}{2} \frac{1}{2})_s' \mid J M_J \mid V_{12s} \ell^2 (\sigma_1 \cdot \sigma_2) \mid nN (IL)_\lambda (\frac{1}{2} \frac{1}{2})_s \mid J M_J \rangle = \sum_{m_s \mu' \mu} \langle \lambda' \mu' S' m_s' \mid J M_J \rangle \langle \lambda \mu S m_s \mid J M_J \rangle \times \langle n'N' \lambda' \mu' S'm_s' \mid V_{12s} \ell^2 (\sigma_1 \cdot \sigma_2) \mid nN \lambda \mu S m_s \rangle,
\]

which gives:

\[
\langle n'N' (l' L')_\lambda (\frac{1}{2} \frac{1}{2})_s' \mid J M_J \mid V_{12s} \ell^2 (\sigma_1 \cdot \sigma_2) \mid nN (IL)_\lambda (\frac{1}{2} \frac{1}{2})_s \mid J M_J \rangle = \delta_{\lambda\lambda'} \delta_{SS'} \delta_{NN'} \delta_{LL'} \delta_{\ell \ell'} 2 \left[ S(S+1) - \frac{3}{2} \right] l(l+1) \ \mathcal{R} \mathcal{M}[V_{12s}](n'l; nl).
\]
3.8 Quadrupole spin-orbit interaction

For the purpose of generalizing this matrix-element calculation to the case of an arbitrary set of single-particle wave functions, it is convenient to approach this calculation by first noting that

\[
(\ell \cdot S)^2 = \sum_{j=0}^{2} j \left[ (\ell \otimes \ell)^{(j)} \otimes (S \otimes S)^{(j)} \right]^{(0)}. \tag{54}
\]

A close inspection of the above equation shows that some of the pieces of the quadrupole spin-orbit interaction may be incorporated into the calculation of the other previous interactions involving the relative orbital angular momentum operator, \( \ell \).

(i) Case \( j = 0 \).

\[
\left[ (\ell \otimes \ell)^{(0)} \otimes (S \otimes S)^{(0)} \right]^{(0)} = \frac{1}{6} \ell^2 \left( 3 + \sigma_1 \cdot \sigma_2 \right), \tag{55}
\]

where we have used \( (\sigma_{i,x}^2 = \sigma_{i,y}^2 = \sigma_{i,z}^2 = 1) \)

\[
S^2 = \frac{1}{2} \left( 3 + \sigma_1 \cdot \sigma_2 \right). \tag{56}
\]

Therefore, we can introduce the modified radial amplitudes of the \( \ell^2 \) and \( \ell^2 \left( \sigma_1 \cdot \sigma_2 \right) \) interactions:

\[
\tilde{V}_{l2} = V_{l2} + \frac{1}{2} V_{ls2}, \tag{57}
\]
\[
\tilde{V}_{l2ss} = V_{l2ss} + \frac{1}{6} V_{ls2}. \tag{58}
\]

(ii) Case \( j = 1 \).

\[
\sqrt{3} \left[ (\ell \otimes \ell)^{(1)} \otimes (S \otimes S)^{(1)} \right]^{(0)} = -\frac{1}{2} \ell \cdot S, \tag{59}
\]

where we have used the definition of the angular momentum quantum operator, \( \vec{J} \times \vec{J} = i \vec{J} \). Similarly, we introduce the modified radial amplitude for the
spin-orbital interaction, as:
\[ \hat{V}_{ls} = V_{ls} - \frac{1}{2} V_{ls^2}. \] (60)

(iii) Case \( j = 2 \).
\[ \sqrt{5} \left[ [\ell \otimes \ell]^{(2)} \otimes [S \otimes S]^{(2)} \right]^{(0)} = \frac{\sqrt{5}}{2} \left[ [\ell \otimes \ell]^{(2)} \otimes [\sigma_1 \otimes \sigma_2]^{(2)} \right]^{(0)}. \] (61)

We notice that the only component of the \((\ell \cdot S)^2\) interaction that we have not addressed yet is the one corresponding to \( j = 2 \).

To calculate the corresponding matrix element we first use ([23], Eq. 7.1.6)
\[ \langle n' N' (l' l')_{\lambda'} (\ell \cdot S) \rangle \langle \lambda S \rangle \langle n N (l l)_{\lambda} \rangle = \delta_{N N'} \delta_{L L'} \delta_{S S'} \delta_{j j} \frac{1}{2} \left[ \ell \otimes \ell \right]^{(2)} \langle n' N' (l' l')_{\lambda'} \parallel \ell \otimes \ell \rangle \langle n N (l l)_{\lambda} \parallel n N \rangle. \] (62)

with the reduced matrix elements calculated as:

(i) We use ([23], Eq. 7.1.1), to obtain
\[ \langle n' N' (l' l')_{\lambda'} \parallel \ell \otimes \ell \rangle \langle n N (l l)_{\lambda} \parallel n N \rangle = \delta_{l l'} \delta_{j j} \frac{1}{2} \left[ \ell \otimes \ell \right]^{(2)} \langle n' N' (l' l')_{\lambda'} \parallel \ell \otimes \ell \rangle \langle n N (l l)_{\lambda} \parallel n N \rangle. \] (63)

(ii) Next, we use ([23], Eq. 7.1.7) to obtain
\[ \langle n' N' (l' l')_{\lambda'} \parallel \ell \otimes \ell \rangle \langle n N (l l)_{\lambda} \parallel n N \rangle = \delta_{N N'} \delta_{L L'} \delta_{S S'} \delta_{j j} \frac{1}{2} \left[ \ell \otimes \ell \right]^{(2)} \langle n' N' (l' l')_{\lambda'} \parallel \ell \otimes \ell \rangle \langle n N (l l)_{\lambda} \parallel n N \rangle. \] (64)

with ([23], Eq. 7.1.1)
\[ \langle n N' \mid \ell \otimes \ell \rangle \langle n l \rangle = \delta_{N N'} \delta_{L L'} \delta_{S S'} \delta_{j j} \frac{1}{2} \left[ \ell \otimes \ell \right]^{(2)} \langle n N' (l l)_{\lambda} \parallel \ell \otimes \ell \rangle \langle n N (l l)_{\lambda} \parallel n N \rangle. \] (65)
Collecting terms, we find

\[
\langle n'N'(l' L')_N \frac{1}{\sqrt{2}}; JM \rangle |V_{ls2}(\ell \otimes \ell'' \otimes [S \otimes S]^j(0) \rangle |nN(lL)\frac{1}{\sqrt{2}}; JM \rangle = \delta_{NN'} \delta_{\ell L} \delta_{SS'} \delta_{S1} \delta_{S2} \frac{6(-)^{l+L+J+1} \hat{j}\hat{j}'}{l(l+1)(2l+1)}
\]

\[
\times \left\{ \begin{array}{c} 1 \ 1 \ j \\ 1 \ 1 \ 1 \ \end{array} \right\} \left\{ \begin{array}{c} 1 \ 1 \ j \\ l \ l \ l \ \end{array} \right\} \left\{ \begin{array}{c} J \ S' \ \lambda' \\ j \ \lambda \ S \ \end{array} \right\} \left\{ \begin{array}{c} l \ \lambda' \ L \\ \lambda \ l \ j \ \end{array} \right\} \mathcal{R} \mathcal{M}[V_{ls2}](n'l; nl).
\]

4 Two-body matrix elements calculation

Unlike the case of harmonic-oscillator single-particle basis set, the calculation (and storage) of the two-body matrix elements using single-particle wave functions that can be represented as linear combinations of harmonic-oscillator wave functions is performed more efficiently in \( ph \) coupling. The \( ph \)-coupled matrix-element calculation is based on the following two lemmas:

**Lemma 1:** Provided that the two-body potential can be factorized into parts depending only on the \( \vec{r}_1 \) or \( \vec{r}_2 \) coordinates, respectively,

\[
V(\vec{r}_1, \vec{r}_2) = \left( U^{(k)}(\vec{r}_1) \otimes V^{(k)}(\vec{r}_2) \right),
\]

then \( ph \)-coupled matrix elements of the two-body interaction are given by

\[
\langle (13) \lambda | U^{(k)}(\vec{r}_1) \otimes V^{(k)}(\vec{r}_2) \rangle |(42) \lambda \rangle = (-)^{j_2+j_4+1} \frac{2l+1}{2\lambda+1} \langle 1 \parallel U^{(\lambda)} \parallel 3 \rangle \langle 2 \parallel V^{(\lambda)} \parallel 4 \rangle \delta_{k \lambda}.
\]

Using the definition of the scalar product of two tensor operators of rank \( k \), Eq. (65), we calculate the matrix elements of the \( U_q^{(k)}(\vec{r}_1)V_{-q}^{(k)}(\vec{r}_2) \) operator in the \( m \)-representation, using the Wigner-Eckart theorem

\[
\langle 12 | U^{(k)}(\vec{r}_1) | V^{(k)}(\vec{r}_2) | 34 \rangle = \frac{(-)^{j_2-m_3}}{k} \langle j_1 m_1 j_3 - m_3 | k q \rangle \langle 1 \parallel U^{(k)} \parallel 3 \rangle \times \frac{(-)^{j_4-m_4}}{k} \langle j_2 m_2 j_4 - m_4 | k - q \rangle \langle 2 \parallel V^{(k)} \parallel 4 \rangle,
\]

where we have also introduced the notation \( \hat{k} = \sqrt{2k+1} \). Then, Eq. (69) is obtained using the orthonormality of the Clebsch-Gordon coefficients, together with the definition of \( ph \)-coupled matrix elements, Eq. (66).
We note the identity:

\[
\left[ U^{(k)}(\vec{r}_1) \otimes V^{(k)}(\vec{r}_2) \right]^{(0)} = \frac{(-)^k}{k} \left( U^{(k)}(\vec{r}_1) \otimes V^{(k)}(\vec{r}_2) \right),
\]

where the spherical tensor product of two tensor operators, \( A^{(k_1)} \) and \( B^{(k_2)} \), was defined in Eq. (16).

**Lemma 2:** Provided that the spatial part of the two-body interaction has the form \( V(r) C^{(k)}(\hat{r}) \), with \( k \) a positive integer or zero, then the variables \( \vec{r}_1 \) and \( \vec{r}_2 \) can be separated in the sense that

\[
r^\alpha V(r) C^{(k)}(\hat{r}) = \sum_{k_1,k_2} i^{k_2-k_1} \frac{(2k_1+1)(2k_2+1)}{2k+1} \langle k_0 k_2 0 | k 0 \rangle \times u^{(k_1 k_2;k)}(r_1,r_2) \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(k)},
\]

where \( \alpha \) is a positive integer exponent, and \( \vec{r} = \vec{r}_1 - \vec{r}_2 \) indicates the relative-motion coordinate. We have also introduced the notations

\[
u^{(k_1 k_2;k)}(r_1,r_2) = \frac{2}{\pi \sqrt{2}} \int_0^{\infty} dp \; p^2 \; v_{\alpha k}(p) j_{k_1}(pr_1) j_{k_2}(pr_2),
\]

and

\[
v_{\alpha k}(p) = \int_0^{\infty} dr \; r^{\alpha} V(r) j_{k}(pr).
\]

To prove lemma 2, we first introduce the asymmetric Fourier transform of the operator \( V(r) C^{(k)}(\hat{r}) \)

\[
\tilde{v}^{(\alpha k)}(\vec{p}) = \frac{1}{(2\pi)^3} \int d^3r \; r^{\alpha} V(r) C^{(k)}(\hat{r}) e^{i\vec{p} \cdot \vec{r}}
\]

and, conversely,

\[
r^{\alpha} V(r) C^{(k)}(\hat{r}) = \int d^3p \; \tilde{v}^{(\alpha k)}(\vec{p}) e^{-i\vec{p} \cdot \vec{r}}.
\]

We use the plane wave expansion in terms of unnormalized spherical harmonics,

\[
e^{i\vec{p} \cdot \vec{r}} = \sum_{l} i^l (2l + 1) j_l(pr) \left( C^{(l)}(\hat{r}) \otimes C^{(l)}(\hat{p}) \right),
\]

together with the orthogonality conditions of spherical harmonics, and carry out the angular
part of the integral (74). Then, \( \tilde{v}(p) \) becomes
\[
\tilde{v}^{(\alpha k)}(p) = \left( -\frac{i}{2\pi^2} \right)^k C^{(k)}(p) v_{\alpha \kappa}(p).
\] (77)

From Eq. (75), we can write
\[
r^{\alpha} V(r) C^{(k)}(\hat{r}) = \left( -\frac{i}{2\pi^2} \right)^k \int d^3p v_{\alpha \kappa}(p) C^{(k)}(\hat{p}) e^{ip \cdot \hat{r}}.
\] (78)

The angular part of the last integral can be carried out explicitly using the definition of the relative coordinate, \( \vec{r} = \vec{r}_1 - \vec{r}_2 \), and by applying Eq. (76) twice for \( \exp(i \vec{p} \cdot \vec{r}_1) \) and \( \exp(-i \vec{p} \cdot \vec{r}_2) \), respectively. The following integral is evaluated using the above properties of the unnormalized spherical harmonics:
\[
\int d\Omega_p \left[ C^{(k_1)}(\hat{p}) \right]^* \left[ C^{(k_2)}(\hat{p}) \right]^* C^{(k)}(\hat{p}) = \frac{4\pi}{2k+1} \langle k_1 0 k_2 0 | k 0 \rangle \langle k_1 q_1 k_2 q_2 | k q \rangle.
\] (79)

To finalize our proof, we use the definition of the spherical tensor product of rank \( k \) obtained from the tensor operators \( C^{(k_1)}(\hat{r}_1) \) and \( C^{(k_2)}(\hat{r}_2) \).

5 Matrix elements calculation using arbitrary single-particle wave functions

It is convenient to evaluate two-body matrix elements in \( ph \) angular momentum coupling using lemma 1. Then, according to lemma 2, \( ph \) matrix elements factorize in two parts, which depend on the coordinates of the first and the second particle, respectively. Hence, the appropriate angular-momentum coupling for each single-particle wave function \( |\alpha\rangle \) is provided in the \((lsj)\)-coupling, with the individual orbital angular momentum \( l_\alpha \) and spin \( s_\alpha \) are coupled to a total angular momentum \( j_\alpha \). For an operator \( O^{(k)} \) which depends only on the orbital angular momentum components, in the \((lsj)\)-coupling scheme we have:

i) (see [23], 7.1.7)
\[
\langle (l_1 \frac{1}{2})_{j_1} \parallel O^{(k)} \parallel (l_2 \frac{1}{2})_{j_2} \rangle = F(l_1 j_1; l_2 j_2; k) \langle l_1 \parallel O^{(k)} \parallel l_2 \rangle,
\] (80)

with
\[
F(l_1 j_1; l_2 j_2; k) = (-)^{l_1 + j_2 + \frac{1}{2} + k} \sum_{j_1 j_2} \begin{pmatrix} l_1 & j_1 & \frac{1}{2} \\ j_2 & l_2 & k \end{pmatrix}.
\] (81)
ii) (see [23], 7.1.5 and 5.4.4)
\[
(\langle l_{\frac{1}{2}} j_1, l_{\frac{1}{2}} j_2 \parallel \mathcal{O}^{(k_1)} \otimes \sigma \rangle^{(k_2)} \parallel l_{\frac{1}{2}} j_2 \rangle = G(l_1 j_1; l_2 j_2; k_1 k_2) \langle l_1 \parallel \mathcal{O}^{(k_1)} \parallel l_2 \rangle ,
\]
(82)
with
\[
G(l_1 j_1; l_2 j_2; k_1 k_2) = \sqrt{6} \hat{j}_1 \hat{j}_2 \hat{k}_2
\]
\[
\begin{pmatrix}
  l_1 & l_2 & k_1 \\
  \frac{1}{2} & \frac{1}{2} & 1 \\
  j_1 & j_2 & k_2
\end{pmatrix}.
\]
(83)

We can now proceed to discussing the calculation of the two-body matrix elements of the Argonne $v_{18}$ potential: We will first evaluate the radial part of the matrix element, which can be performed independently of the way we handle the angular and spin/isospin degrees of freedom of the interaction. Next, we will discuss the angular and spin part of the 7 basic operators corresponding to the Argonne $v_{18}$ potential.

5.1 Radial part of the two-body matrix element

The radial part of the two-body matrix elements is defined as
\[
R_{\alpha \kappa; k_1 k_2}^{n_1 l_1 n_2 l_2; n_3 l_3 n_4 l_4} = \frac{2}{\pi} \int_0^\infty \left[ p^2 dp \right] v_{\alpha \kappa}(p)
\times \int_0^\infty \left[ r_1^2 dr_1 \right] \mathcal{R}_{n_1 l_1}(r_1) \left[ \mathcal{O}^{(1)} \mathcal{R}_{n_3 l_3}(r_1) \right] j_{k_1}(pr_1)
\times \int_0^\infty \left[ r_2^2 dr_2 \right] \mathcal{R}_{n_2 l_2}(r_2) \left[ \mathcal{O}^{(2)} \mathcal{R}_{n_4 l_4}(r_2) \right] j_{k_2}(pr_2) ,
\]
(84)
where $v_{\alpha \kappa}(p)$ was defined in Eq. [73] and the operators $\mathcal{O}^{(1,2)}$ are operators acting only on the radial part of the single-particle wave functions. The functional form of the radial wave functions in Eq. (84) is not restricted to that of a harmonic-oscillator wave function. Therefore, at this point we need to carefully consider what is the most efficient numerical strategy to computing (84) for the particular radial form of the wave functions under consideration. For illustrative (and testing) purposes, in the following we will confine our discussion to the case of a basesis of single-particle wave functions defined as linear combinations of harmonic-oscillator wave functions [see Eq. (1)], in which case some of the integrals in (84) can be efficiently performed using Gauss-Hermite quadrature formulas.
Treating separately the integral
\[
\int_0^\infty [r_1^2 \, dr_1] \mathcal{R}_{n_1l_1} (r_1) \left[ \mathcal{O}^{(1)} \mathcal{R}_{n_3l_3} (r_1) \right] j_{k_1} (p r_1) ,
\]
we first change variables such that \(x_i' = r_i \left( \sqrt{2}/b \right)\) with \(q' = p \left( b/\sqrt{2} \right)\), and we recall that (see discussion surrounding Eq. (6))
\[
R_{nl} (\sqrt{2} x') = b^{3/2} R_{nl} (r) .
\]
Next, we perform the harmonic-oscillator expansion
\[
R_{n_1l_1} (\sqrt{2} x_1') \left[ \mathcal{O}^{(1)} R_{n_3l_3} (\sqrt{2} x_1') \right] = \sum_n A_{n_1l_1 n_3l_3}^{n_{k_1}} \mathcal{HO}_{n_{k_1}} (x_1') .
\]
Therefore, the integral (85) becomes
\[
\frac{1}{(\sqrt{2})^3} \sum_n A_{n_1l_1 n_3l_3}^{n_{k_1}} \left[ \sqrt{\frac{\pi}{2}} \tilde{\mathcal{HO}}_{nk_1} (q') \right] ,
\]
where we have introduced the notation, \(\tilde{\mathcal{HO}}_{n\ell} (q) = (-)^n \mathcal{HO}_{n\ell} (q)\), which denotes the Fourier transform of the harmonic-oscillator wave function, \(\mathcal{HO}_{n\ell}\), and the coefficients \(A_{n_1l_1 n_3l_3}^{n_{k_1}}\) are calculated as
\[
A_{n_1l_1 n_3l_3}^{n_{k_1}} = \int_0^\infty \left[ x_1'^2 \, dx_1' \right] R_{n_1l_1} (\sqrt{2} x_1') \left[ \mathcal{O}^{(1)} R_{n_3l_3} (\sqrt{2} x_1') \right] \mathcal{HO}_{nk_1} (x_1') .
\]
This integral is conveniently performed using Gaussian quadratures. Similarly, we have:
\[
\int_0^\infty [r_2^2 \, dr_2] \mathcal{R}_{n_2l_2} (r_2) \left[ \mathcal{O}^{(2)} \mathcal{R}_{n_4l_4} (r_2) \right] j_{k_2} (p r_2) = \frac{1}{(\sqrt{2})^3} \sum_m A_{n_2l_2 n_4l_4}^{m_{k_2}} \left[ \sqrt{\frac{\pi}{2}} \tilde{\mathcal{HO}}_{mk_2} (q') \right] ,
\]
where the coefficients \(A_{n_2l_2 n_4l_4}^{m_{k_2}}\) are given as
\[
A_{n_2l_2 n_4l_4}^{m_{k_2}} = \int_0^\infty \left[ x_2'^2 \, dx_2' \right] R_{n_2l_2} (\sqrt{2} x_2') \left[ \mathcal{O}^{(2)} R_{n_4l_4} (\sqrt{2} x_2') \right] \mathcal{HO}_{mk_2} (x_2') .
\]
Using Equations (88) and (90), the radial part of the two-body matrix elements becomes
\[
R_{n_1l_1 n_2l_2; n_3l_3 n_4l_4}^{\alpha \kappa; k_1k_2} = \frac{1}{(b \sqrt{2})^3} \sum_n A_{n_1l_1 n_3l_3}^{nk_1} \sum_m A_{n_2l_2 n_4l_4}^{mk_2} \times \int_0^\infty [q^2 dq] v_{\alpha \kappa}(\mathbf{r} \cdot q') \mathcal{H}\mathcal{O}_{n_1l_1}(q') \mathcal{H}\mathcal{O}_{mk_2}(q') .
\] (92)

5.2 Central interaction

The central interaction depends only on the magnitude of the relative distance \( r \) between the two particles, i.e.

\[
V_C = V_c(r) C^{(0)}(\mathbf{r}) .
\] (93)

The strategy to calculating the \( ph \) matrix element

\[
\langle (l_1 \frac{1}{2})_{j_1} | (l_2 \frac{1}{2})_{j_2} ; \lambda \mu | V_C | (l_4 \frac{1}{2})_{j_4} (l_2 \frac{1}{2})_{j_2} ; \lambda \mu \rangle,
\]

is emblematic for the rest of this section: (For simplicity, we will not concern ourselves here with the radial degrees of freedom. The radial part of the matrix elements is calculated using the approach discussed in the previous section.) First, we use lemma 2 and separate \( V_C \) into tensor-operator components which depend on either \( \mathbf{r}_1 \) or \( \mathbf{r}_2 \). We have

\[
V_C = \sum_k (2k + 1) u^{(kk;00)}(r_1, r_2) \left( C^{(k)}(\mathbf{r}_1) \otimes C^{(k)}(\mathbf{r}_2) \right) .
\] (94)

Second, we use lemma 1 to calculate the \( ph \) matrix element of the corresponding interaction. For the central interaction, this procedure leads to

\[
\langle (l_1 \frac{1}{2})_{j_1} (l_3 \frac{1}{2})_{j_3} ; \lambda \mu | V_C | (l_4 \frac{1}{2})_{j_4} (l_2 \frac{1}{2})_{j_2} ; \lambda \mu \rangle = (-1)^{j_2+j_4+1} u^{(\lambda\lambda;00)}(r_1, r_2)
\]

\[
\times \langle (l_1 \frac{1}{2})_{j_1} || C^{(\lambda)}(\mathbf{r}_1) || (l_3 \frac{1}{2})_{j_3} \rangle \langle (l_2 \frac{1}{2})_{j_2} || C^{(\lambda)}(\mathbf{r}_2) || (l_4 \frac{1}{2})_{j_4} \rangle,
\] (95)

which gives

\[
\langle (l_1 \frac{1}{2})_{j_1} (l_3 \frac{1}{2})_{j_3} ; \lambda \mu | V_C | (l_4 \frac{1}{2})_{j_4} (l_2 \frac{1}{2})_{j_2} ; \lambda \mu \rangle = (-1)^{j_2+j_4+1} u^{(\lambda\lambda;00)}(r_1, r_2)
\]

\[
\times F(l_1j_1; l_3j_3; \lambda) \langle l_1 || C^{(\lambda)} || l_3 \rangle F(l_2j_2; l_4j_4; \lambda) \langle l_2 || C^{(\lambda)} || l_4 \rangle .
\] (96)

5.3 Spin-spin interaction

By definition, the spin-spin interaction is introduced as

\[
V_S = V_s(r) \sigma_1 \cdot \sigma_2 ,
\] (97)
where we can write
\[ \sigma_1 \cdot \sigma_2 = -\sqrt{3} \left[ \sigma_1 \otimes \sigma_2 \right]^{(0)} . \] (98)

We perform the recoupling
\[ \left[ \left[ C^{(k)}(r_1) \otimes C^{(k)}(r_2) \right]^{(0)} \otimes \left[ \sigma_1 \otimes \sigma_2 \right]^{(0)} \right]^{(0)} \]
\[ = \frac{1}{k \sqrt{3}} \sum_l (-)^l \left[ \left[ C^{(k)}(r_1) \otimes \sigma_1 \right]^{(l)} \otimes \left[ C^{(k)}(r_2) \otimes \sigma_2 \right]^{(l)} \right] , \] (99)

and obtain
\[ \langle (l_1 \frac{1}{2})_{j_1} (l_3 \frac{1}{2})_{j_3} : \lambda \mu \mid V_S \mid (l_4 \frac{1}{2})_{j_4} (l_2 \frac{1}{2})_{j_2} : \lambda \mu \rangle \]
\[ = \frac{(-)^{\lambda + j_2 + j_4}}{2\lambda + 1} \sum_k (-)^k (2k + 1) u^{(kk;00)}(r_1, r_2) \]
\[ \times G(l_1, j_1; l_3, j_3; k \lambda) \langle l_1 \parallel C^{(k)} \parallel l_3 \rangle G(l_2, j_2; l_4, j_4; k \lambda) \langle l_2 \parallel C^{(k)} \parallel l_4 \rangle , \] (100)

with \(|\lambda - 1| \leq k \leq \lambda + 1 .

5.4 Tensor interaction

The tensor interaction is defined as:
\[ V_T = V_t(r) S_{12} , \] (101)

where the operator \( S_{12} \) defined in Eq. (39) is written now as

\[ S_{12} = \sqrt{30} \left[ C^{(2)}(\vec{r}) \otimes [\sigma_1 \otimes \sigma_2]^{(2)} \right]^{(0)} . \] (102)

Using a recoupling scheme similar to Eq. (99),
\[ \left[ \left[ C^{(k_1)}(r_1) \otimes C^{(k_2)}(r_2) \right]^{(2)} \otimes \left[ \sigma_1 \otimes \sigma_2 \right]^{(2)} \right]^{(0)} \]
\[ = -(-)^{k_2} \sqrt{3} \sum_k \left\{ \begin{array}{ccc} k_1 & k_2 & 2 \\ 1 & 1 & k \end{array} \right\} \left[ \left[ C^{(k_1)}(r_1) \otimes \sigma_1 \right]^{(k)} \otimes \left[ C^{(k_2)}(r_2) \otimes \sigma_2 \right]^{(k)} \right] , \] (103)
we obtain
\[\langle (l_1^{\frac{1}{2}})_{j_1} (l_3^{\frac{1}{2}})_{j_3} ; \lambda \mu | V_T | (l_2^{\frac{1}{2}})_{j_4} (l_4^{\frac{1}{2}})_{j_2} ; \lambda \mu \rangle = \frac{(-)^{j_2+j_4+1}}{2\lambda + 1} \]
\[\times \sqrt{6} \sum_{k_1} (2k_1 + 1) G(l_1; j_1; l_3; j_3; k_1 \lambda) \langle l_1 || C^{(k_1)} || l_3 \rangle \sum_{k_2} i^{k_1+k_2} (2k_2 + 1) \]
\[\times u^{(k_1, k_2; 20)}(r_1, r_2)(k_1 0 k_2 0 | 2 0) \left\{ \begin{array}{c} k_1 \ k_2 \ 2 \\ 1 \ 1 \ \lambda \end{array} \right\} G(l_2; j_2; l_4; j_4; k_2 \lambda) \langle l_2 || C^{(k_2)} || l_4 \rangle . \] (104)

5.5 Spin-orbit interaction

The spin-orbit interaction is given by:
\[V_{LS} = V_{ls}(r) \ell \cdot S , \] (105)

where the orbital angular momentum operator and the total spin operator are defined as
\[\vec{\ell} = \frac{1}{2} \vec{r} \times (\vec{p}_1 - \vec{p}_2) , \quad \text{and} \quad \vec{S} = \frac{1}{2} (\vec{\sigma}_1 + \vec{\sigma}_2) , \] (106)

respectively. Using the tensor operator properties:
\[\vec{r}_m = r C_m^{(1)}(\hat{r}) , \quad \text{and} \quad (\vec{x} \times \vec{y})_m = -i \sqrt{2} [x \otimes y]_m^{(1)} , \] (107)

we can write
\[\ell = \frac{\hbar}{\sqrt{2}} r \left[ C^{(1)}(\hat{r}) \otimes (\nabla_2 - \nabla_1) \right]^{(1)} . \] (108)

Then, we use lemma 2, and obtain:
\[rV_{ls}(r) C^{(1)}(\vec{r}) = \sum_{k_1, k_2} i^{k_2 - k_1 - 1} \]
\[\times \frac{(2k_1 + 1)(2k_2 + 1)}{3 \sqrt{2}} \langle k_1 0 k_2 0 | 1 0 \rangle u^{(k_1 k_2; 11)}(r_1, r_2) \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} . \] (109)
Recoupling the \( C^{(k_1)}(\hat{r}_1) \) and \( C^{(k_2)}(\hat{r}_2) \) operators with the appropriate gradient operators, we obtain:

\[
V_{ls}(r) = \sum_{k_1 k_2} \frac{1}{\sqrt{2}} \sum_{k} \frac{k}{\sqrt{6}} \left\{ k_1 k_2 1 \right\} u^{(k_1 k_2, 1)}(r_1, r_2) \left\{ - \left[ C^{(k_1)}(\hat{r}_1) \otimes \left[ C^{(k_2)}(\hat{r}_2) \otimes \nabla_2 \right]^{(k)} \right]^{(1)} + (-)^{k_1 + k_2 + 1} \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(k)} \right\} .
\]

Next, using the triangle conditions for the angular momentum arguments of the Wigner 6j symbol, we derive the conditions: \( |k_1 - k_2| \leq 1 \leq k_1 + k_2 \), \( |k_2 - 1| \leq k \leq k_2 + 1 \) and \( |k_1 - 1| \leq k \leq k_1 + 1 \). These conditions together with the condition that \( k_1 + k_2 \) is odd, derived from the Clebsch-Gordan coefficient in \( \{110\} \), can be satisfied only if \( k \) equals either \( k_1 \) or \( k_2 \). Therefore, we can write Eq. \( \{110\} \) as

\[
V_{ls}(r) = \frac{1}{\sqrt{2}} \sum_{k_1 k_2} \frac{1}{\sqrt{6}} \sum_{k} \left\{ k_1 k_2 1 \right\} u^{(k_1 k_2, 1)}(r_1, r_2) \left\{ - \left[ C^{(k_1)}(\hat{r}_1) \otimes \left[ C^{(k_2)}(\hat{r}_2) \otimes \nabla_2 \right]^{(k_1)} \right]^{(1)} + \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(k)} \right\} ,
\]

with \( k_1 + k_2 + 1 \) even.

Taking the inner products of Eq. \( \{111\} \) with \( S \), and using the following identities valid for operators \( A^{(k)} \) and \( B^{(\ell)} \) that commute with all components \( \sigma_i \)

\[
\left( \left[ A^{(k)}(1) \otimes B^{(\ell)}(2) \right]^{(1)} \otimes \sigma_1 \right) = (-)^k \frac{\sqrt{3}}{\ell} \left( \left[ A^{(k)}(1) \otimes \sigma_1 \right]^{(\ell)} \otimes B^{(\ell)}(2) \right) ,
\]

\[
\left( \left[ A^{(k)}(1) \otimes B^{(\ell)}(2) \right]^{(1)} \otimes \sigma_2 \right) = (-)^{k+1} \frac{\sqrt{3}}{k} \left( A^{(k)}(1) \otimes \left[ B^{(\ell)}(2) \otimes \sigma_2 \right]^{(k)} \right) ,
\]

the operators in Eq. \( \{111\} \) give the following contributions to the \( ph \)-coupled matrix element \( \langle (l_{3/2})_{j_3} (l_{3/2})_{j_3} ; \lambda \mu | V_{LS} | (l_{4/2})_{j_4} (l_{2/2})_{j_2} ; \lambda \mu \rangle \):
\[
\left( C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \otimes \nabla_2 \right)^{(k_1)} \left( 1 \right) \otimes S \right)
\]
\[
\Rightarrow \delta_{(k_1)} \left( - \right)^{\lambda + j_2 + j_3 + 1} \frac{\sqrt{3}}{\lambda (2\lambda + 1)} \times \left[ G(l_1; j_1; l_3; j_3; \lambda \lambda) \langle l_1 \parallel C^{(\lambda)} \parallel l_3 \rangle F(l_2; j_2; l_4; j_4; \lambda) CG_2(\lambda k_2, k_2 \lambda)
\]
\[
- F(l_1; j_1; l_3; j_3; \lambda) \langle l_1 \parallel C^{(\lambda)} \parallel l_3 \rangle G(l_2; j_2; l_4; j_4; \lambda) CG_2(\lambda k_2, k_2 \lambda) \right],
\]
and
\[
\left( \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \otimes \nabla_2 \right]^{(k_1)} \left( 1 \right) \otimes S \right)
\]
\[
\Rightarrow \left( - \right)^{k_1 + j_2 + j_3 + 1} \frac{\sqrt{3}}{\lambda (2\lambda + 1)} \times \left[ \delta_{k_2 \lambda} G(l_1; j_1; l_3; j_3; k_1 \lambda) CG_1(k_1, k_1) F(l_2; j_2; l_4; j_4; \lambda) \langle l_2 \parallel C^{(\lambda)} \parallel l_4 \rangle
\]
\[
- \delta_{k_1 \lambda} F(l_1; j_1; l_3; j_3; \lambda) CG_1(\lambda k_2, \lambda \lambda) G(l_2; j_2; l_4; j_4; k_2 \lambda) \langle l_2 \parallel C^{(k_2)} \parallel l_4 \rangle \right],
\]
and
\[
\left( \left[ C^{(k_2)}(\hat{r}_1) \otimes C^{(k_1)}(\hat{r}_2) \otimes \nabla_1 \right]^{(k_1)} \left( 1 \right) \otimes S \right)
\]
\[
\Rightarrow \left( - \right)^{k_2 + j_2 + j_3 + 1} \frac{\sqrt{3}}{\lambda (2\lambda + 1)} \times \left[ \delta_{k_1 \lambda} G(l_1; j_1; l_3; j_3; k_1 \lambda) \langle l_1 \parallel C^{(k_2)} \parallel l_3 \rangle F(l_2; j_2; l_4; j_4; \lambda) CG_2(k_2 \lambda, \lambda \lambda)
\]
\[
- \delta_{k_2 \lambda} F(l_1; j_1; l_3; j_3; \lambda) \langle l_1 \parallel C^{(\lambda)} \parallel l_3 \rangle G(l_2; j_2; l_4; j_4; k_1 \lambda) CG_2(\lambda k_1, k_1 k_1) \right],
\]
and
\[
\left( \left[ C^{(k_2)}(\hat{r}_1) \otimes \nabla_1 \right]^{(k_1)} \left( 1 \right) \otimes S \right)
\]
\[
\Rightarrow \delta_{k_1 \lambda} \left( - \right)^{\lambda + j_2 + j_3 + 1} \frac{\sqrt{3}}{\lambda (2\lambda + 1)} \times \left[ G(l_1; j_1; l_3; j_3; \lambda \lambda) CG_1(k_2 \lambda, k_2 \lambda) F(l_2; j_2; l_4; j_4; \lambda) \langle l_2 \parallel C^{(\lambda)} \parallel l_4 \rangle
\]
\[
- F(l_1; j_1; l_3; j_3; \lambda) CG_1(k_2 \lambda, k_2 \lambda) G(l_2; j_2; l_4; j_4; \lambda \lambda) \langle l_2 \parallel C^{(\lambda)} \parallel l_4 \rangle \right],
\]
where we have introduced the notations

\[
CG_1(k_1k_2, l_1l_2) = \langle l_1 \parallel u^{(k_1k_2,11)}(r_1, r_2) \left[ C^{(l_1)}(\hat{r}_1) \otimes \nabla(1) \right]^{(l_2)} \parallel l_3 \rangle ,
\]

\[
CG_2(k_1k_2, l_1l_2) = \langle l_2 \parallel u^{(k_1k_2,11)}(r_1, r_2) \left[ C^{(l_1)}(\hat{r}_2) \otimes \nabla(2) \right]^{(l_2)} \parallel l_4 \rangle .
\]

\[\text{(118)}\]

\[\text{(119)}\]

5.6 $\ell^2$ interaction

The $\ell^2$ interaction is defined as

\[
V_{L2} = V_{l2}(r) \ell^2 ,
\]

where we can write

\[
\ell^2 = -\sqrt{3} \left[ \ell \otimes \ell \right]^{(0)} .
\]

\[\text{(120)}\]

\[\text{(121)}\]

It is useful to discuss this as a particular case of the more general operator

\[
\left[ \ell \otimes \ell \right]^{(j)} = -\frac{1}{2} \left[ \left[ r \otimes (p_1 - p_2) \right]^{(1)} \otimes \left[ r \otimes (p_1 - p_2) \right]^{(1)} \right]^{(j)} .
\]

\[\text{(122)}\]

We begin by using the definition of the spherical components of an arbitrary vector, $a$, i.e. $^{(23)}$, 5.9.4

\[
a_{\pm1} = \mp \frac{1}{\sqrt{2}} (a_x \pm ia_y) ; \quad a_0 = a_z .
\]

\[\text{(123)}\]

Then, we can show that

\[
\left[ r_m, p_n \right] = i\hbar (-)^m \delta_{n,-m} ,
\]

\[\text{(124)}\]

and

\[
\left[ (r_1 - r_2)_m, (p_1 - p_2)_n \right] = 2i\hbar (-)^m \delta_{n,-m} .
\]

\[\text{(125)}\]
We can change the coupling scheme and combine the two $\vec{r}$s, in Eq. (122), into a single tensor operator dependent on the relative-coordinate unit vector:

$$\left[ r \otimes (p_1 - p_2) \right]^{(1)} \otimes \left[ r \otimes (p_1 - p_2) \right]^{(1)}_m$$

$$= 3 \vec{r}^2 \sum_{\kappa \kappa'} \hat{\kappa} \hat{\kappa}' \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ \kappa & \kappa' & j \end{pmatrix} \left\langle 1 0 1 0 \mid \kappa 0 \right\rangle \left[ C^{(\kappa)}(\vec{r}) \otimes [(p_1 - p_2) \otimes (p_1 - p_2)]^{(\kappa')} \right]^{(j)}_m$$

$$+ 6 i \vec{r} (-)^j \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & j \end{pmatrix} \left[ C^{(1)}(\vec{r}) \otimes (p_1 - p_2) \right]^{(j)}_m.$$

Because of the cross product property, $\vec{p}_m \times \vec{p}_n = 0$, $\kappa$ and $\kappa'$ cannot be equal to 1. (The parameter $\kappa$ is also restricted to even values only because of the Clebsch-Gordan coefficient in (126).) Then, we can write

$$\left[ \ell \otimes \ell \right]^{(j)} = \frac{3}{2} \vec{r}^2 \sum_{\kappa \kappa' = 0, 2} \hat{\kappa} \hat{\kappa}' \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ \kappa & \kappa' & j \end{pmatrix} \left\langle 1 0 1 0 \mid \kappa 0 \right\rangle$$

$$\times \left[ C^{(\kappa)}(\vec{r}) \otimes \left( (\nabla_1 - \nabla_2) \otimes (\nabla_1 - \nabla_2) \right)^{(\kappa')} \right]^{(j)}$$

$$- 3 \vec{r} (-)^j \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & j \end{pmatrix} \left[ C^{(1)}(\vec{r}) \otimes (\nabla_1 - \nabla_2) \right]^{(j)}.$$

In the particular case of the $\ell^2$ interaction, the rank $j$ is equal to 0, and we can use the symmetry properties of the Wigner 6$j$ and 9$j$ symbols ([23], 6.4.14 and 6.3.2) to obtain the tensor-product form of $\ell^2$ as

$$\ell^2 = \frac{3}{2} \vec{r}^2 \sum_{\kappa = 0, 2} \hat{\kappa} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & \kappa \end{pmatrix} \left\langle 1 0 1 0 \mid \kappa 0 \right\rangle \left[ C^{(\kappa)}(\vec{r}) \otimes \left( (\nabla_1 - \nabla_2) \otimes (\nabla_1 - \nabla_2) \right)^{(\kappa)} \right]^{(0)}$$

$$- \sqrt{3} \vec{r} \left[ C^{(1)}(\vec{r}) \otimes (\nabla_1 - \nabla_2) \right]^{(0)}.$$

(128)
We expand the unnormalized spherical harmonics $C^{(\kappa)}(\hat{r})$ and $C^{(1)}(\hat{r})$ using lemma 2, to obtain

$$V_2(r) \ell^2 = \frac{3}{2} \sum_{\kappa=0,2} \frac{1}{\hat{k}} \left\{ \begin{array}{ccc} 1 & 1 & 1 \\ 1 & \kappa & 1 \end{array} \right\} (129)$$

$$\times \langle 1 0 1 0 | \kappa 0 \rangle \sum_{k_1k_2} \delta^{k_2-k_1-\kappa}(2k_1+1)(2k_2+1) \langle k_1 0 k_2 0 | \kappa 0 \rangle$$

$$\times u^{(k_1k_2,\kappa)}(r_1, r_2) \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ (\nabla_1 - \nabla_2) \otimes (\nabla_1 - \nabla_2) \right]^{(\kappa)} \langle 0 \rangle$$

$$- \frac{1}{\sqrt{3}} \sum_{k_1k_2} \delta^{k_2-k_1-1}(2k_1+1)(2k_2+1) \langle k_1 0 k_2 0 | 1 0 \rangle u^{(k_1k_2,11)}(r_1, r_2)$$

$$\times \left\{ \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes \nabla_2 \right\}^{(0)} - \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes \nabla_1 \right\}^{(0)}.$$ 

The operators in Eq. (129) give rise to contributions to the matrix element $\langle (l_{1_2}^{1/2})_{j_1} (l_{2_2}^{1/2})_{j_2} ; \lambda \mu | V_{L2} | (l_{1_2}^{1/2})_{j_4} (l_{2_2}^{1/2})_{j_3} ; \lambda \mu \rangle$ similar to the contributions of the $\ell^2 (\sigma_1 \cdot \sigma_2)$ and quadrupole spin-orbit operators discussed in the subsequent sections. Therefore, it is useful to base the calculation of the $\ell^2$ matrix element on several general results.

First, let us discuss the case of the matrix elements involving only one gradient operator in Eq. (129), which are very similar to those discussed in the case of the spin-orbit interaction. We have the general identities:

$$\left[ \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes \nabla_2 \right]^{(j)}$$

$$= (-)^{j} \sqrt{3} \sum_{k} \hat{k} \left\{ \begin{array}{ccc} k_1 & k_2 \ 1 & j \end{array} \right\} \left[ C^{(k_1)}(\hat{r}_1) \otimes \left[ C^{(k_2)}(\hat{r}_2) \otimes \nabla_2 \right]^{(k)} \right]^{(j)},$$

and

$$\left[ \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes \nabla_1 \right]^{(j)}$$

$$= (-)^{k_2} \sqrt{3} \sum_{k} (-)^{k} \hat{k} \left\{ \begin{array}{ccc} k_2 & k_1 \ 1 & j \end{array} \right\} \left[ \left[ C^{(k_1)}(\hat{r}_1) \otimes \nabla_1 \right]^{(k)} \otimes C^{(k_2)}(\hat{r}_2) \right]^{(j)}.$$

For the $\ell^2$ interaction we are only interested in $j = 0$. We obtain:

$$\left[ \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes \nabla_2 \right]^{(0)}$$

$$\Rightarrow \delta_{k_1 \lambda} \frac{(-)^{\lambda+j_2+j_4+1}}{\lambda (2\lambda + 1)} F(l_1j_1; l_3j_3; \lambda) \langle l_1 \parallel C^{(k_1)} \parallel l_3 \rangle F(l_2j_2; l_4j_4; \lambda) CG_2(\lambda k_2, k_2 \lambda),$$

28
and
\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes \nabla_1 \right]^{(0)}
\]
\[
\Rightarrow \delta_{k_2\lambda} \frac{(-)^{\lambda+j_2+j_2+1}}{\lambda (2\lambda + 1)} F(l_1; l_3; \lambda) CG_1(k_1 \lambda, k_1 \lambda) F(l_2; l_4; \lambda) \langle l_2 \parallel C^{(\lambda)} \parallel l_4 \rangle.
\]

Next, we multiply the operator expressions in the first sum in Eq. (129) to obtain
\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ (\nabla_1 - \nabla_2) \otimes (\nabla_1 - \nabla_2) \right]^{(\kappa)} \right]^{(0)}
\]
\[
= \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_2 \otimes \nabla_2 \right]^{(\kappa)}
\]
\[
- 2 \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_1 \otimes \nabla_2 \right]^{(\kappa)}
\]
\[
+ \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_1 \otimes \nabla_1 \right]^{(\kappa)}
\right]^{(0)}.
\]

Now, we have to change the coupling and separate the operators depending on the coordinates of the first particle, from the operators depending on the coordinates of the second particle. Hence, the matrix elements involving two gradient operators in Eq. (129), are calculated using the following identities:
\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_2 \otimes \nabla_2 \right]^{(\kappa')} \right]^{(j)}
\]
\[
= \sum_k (-)^{k_1+k_2+k'+j} \hat{k} \hat{k}' \begin{cases} k_1 & k_2 & k \\ k' & j & k \end{cases} \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \otimes \left[ \nabla_2 \otimes \nabla_2 \right]^{(\kappa')} \right]^{(k)}
\]
and
\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_1 \otimes \nabla_2 \right]^{(\kappa')} \right]^{(j)}
\]
\[
= \sum_k \hat{k} \hat{k}' \hat{k}' \hat{k} \begin{cases} k_1 & k_2 & k \\ k' & j & k \end{cases} \left[ C^{(k_1)}(\hat{r}_1) \otimes \nabla_1 \right]^{(k)} \otimes \left[ C^{(k_2)}(\hat{r}_2) \otimes \nabla_2 \right]^{(k')}^{(j)},
\]
and
\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_1 \otimes \nabla_1 \right]^{(\kappa')} \right]^{(j)}
\]
\[
= \sum_k (-)^{k_2+k'-\kappa+k} \hat{k} \hat{k}' \begin{cases} k_2 & k_1 & k \\ k' & j & k \end{cases} \left[ C^{(k_2)}(\hat{r}_2) \otimes \left[ \nabla_1 \otimes \nabla_1 \right]^{(\kappa')} \right]^{(k)} \otimes \left[ C^{(k_1)}(\hat{r}_1) \right]^{(j)}.
\]
Again, for the $\ell^2$ interaction, we are only interested in the case $j = 0$. We obtain:

$$
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_2 \otimes \nabla_2 \right]^{(\kappa)}(0) \\
\Rightarrow \delta_{k_1 \lambda} \left( - \right)^{\lambda+j_2+j_4+1} \frac{\lambda}{2(2\lambda+1)} F(l_1j_1; l_3j_3; \lambda) \langle l_1 \parallel C^{(\lambda)} \parallel l_3 \rangle \\
\times F(l_2j_2; l_4j_4; \lambda) CGG_2(\lambda k_2 \kappa, k_2 \kappa \lambda),
$$

and

$$
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_1 \otimes \nabla_2 \right]^{(\kappa)}(0) \\
\Rightarrow \frac{(-)^{k_2+j_2+j_4}}{2\lambda+1} \hat{\kappa} \left\{ \begin{array}{c} k_1 \\ k_2 \\ \kappa \\ 1 \\ 1 \\ \lambda \\
\end{array} \right\} \\
\times F(l_1j_1; l_3j_3; \lambda) F(l_2j_2; l_4j_4; \lambda) CGCG(k_1 k_2 \kappa, k_1 \lambda k_2 \lambda),
$$

and

$$
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_1 \otimes \nabla_1 \right]^{(\kappa)}(0) \\
\Rightarrow \delta_{k_2 \lambda} \left( - \right)^{\lambda+j_2+j_4+1} \frac{\lambda}{2(2\lambda+1)} F(l_1j_1; l_3j_3; \lambda) CGG_1(k_1 \lambda \kappa, k_1 \kappa \lambda) \\
\times F(l_2j_2; l_4j_4; \lambda) \langle l_2 \parallel C^{(\lambda)} \parallel l_4 \rangle.
$$

Here we have introduced the notations

$$
CGG_1(k_1 k_2 \kappa, k \lambda) = \langle l_1 \parallel u^{(k_1 k_2, 2\kappa)}(r_1, r_2) \left[ C^{(k)}(\hat{r}_1) \otimes \left[ \nabla_1 \otimes \nabla_1 \right]^{(1)} \right]^{(\lambda)} \parallel l_3 \rangle
$$

(141)

$$
CGG_2(k_1 k_2 \kappa, k \lambda) = \langle l_2 \parallel u^{(k_1 k_2, 2\kappa)}(r_1, r_2) \left[ C^{(k)}(\hat{r}_2) \otimes \left[ \nabla_2 \otimes \nabla_2 \right]^{(2)} \right]^{(\lambda)} \parallel l_4 \rangle
$$

(142)

and

$$
CGCG(k_1 k_2 \kappa, l_1 l_2 \lambda_1 \lambda_2) = \langle l_1 \parallel u^{(k_1, 2\kappa)}(r_1) \left[ C^{(l_1)}(\hat{r}_1) \otimes \nabla_1 \right]^{(l_2)} \parallel l_3 \rangle \\
\times \langle l_2 \parallel u^{(k_2, 2\kappa)}(r_2) \left[ C^{(l_1)}(\hat{r}_2) \otimes \nabla_2 \right]^{(l_2)} \parallel l_4 \rangle.
$$

(143)

5.7 $\ell^2 (\sigma_1 \cdot \sigma_2)$ interaction

The $\ell^2 (\sigma_1 \cdot \sigma_2)$ interaction is given by:
Accordingly, using Eqs. (138–140) and Eqs. (132,133) we obtain the interaction. We have:

\[
V_{LS} = V_{LS}(r) \ell^2 (\sigma_1 \cdot \sigma_2) = (-\sqrt{3}) \ell^2 [\sigma_1 \otimes \sigma_2]^{(0)}.
\] (144)

Since the \(\ell^2 (\sigma_1 \cdot \sigma_2)\) interaction differs from the \(\ell^2\) interaction only through the spin part, \((\sigma_1 \cdot \sigma_2)\), we can use Eq. (129) and add the corresponding spin interaction. We have:

\[
V_{LS}(r) \ell^2 (\sigma_1 \cdot \sigma_2) = \frac{3}{2} \sum_{\kappa=0,2} \frac{1}{k} \left\{ \begin{array}{ccc} 1 & 1 & 1 \\ 1 & \kappa & 1 \end{array} \right\} (145)
\]

\[
\times \langle 1 0 1 0 | \kappa 0 \rangle \sum_{k_1k_2} \delta_{k_2-k_1-\kappa} (2k_1+1)(2k_2+1) \langle k_1 0 k_2 0 | \kappa 0 \rangle (k_1k_2,\kappa)(r_1, r_2)
\]

\[
\times \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ (\nabla_1 - \nabla_2) \otimes (\nabla_1 - \nabla_2) \right]^{(\kappa)} (\sigma_1 \cdot \sigma_2)
\]

\[
- \frac{1}{\sqrt{3}} \sum_{k_1k_2} \delta_{k_2-k_1-1} (2k_1+1)(2k_2+1) \langle k_1 0 k_2 0 | 1 0 \rangle (k_1k_2,11)(r_1, r_2)
\]

\[
\times \left\{ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right\}^{(1)} (\sigma_1 \cdot \sigma_2)
\]

\[
- \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes \nabla_1 (\sigma_1 \cdot \sigma_2) \right\}.
\]

Accordingly, using Eqs. (138,140) and Eqs. (132,133) we obtain the contributions to the \(ph\) matrix element \((l_{\frac{1}{2}}j_{1}; l_{\frac{1}{2}}j_{3} ; \lambda \mu \mid V_{LS} \mid l_{\frac{1}{2}}j_{4}; l_{\frac{1}{2}}j_{2} ; \lambda \mu )\):

\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_2 \otimes \nabla_2 \right]^{(\kappa)} (\sigma_1 \cdot \sigma_2) \right\}^{(0)}
\]

\[
\Rightarrow (-)^{\lambda+j_2+j_4} \frac{1}{k_1(2\lambda+1)} G(l_{1}j_{1}; l_{3}j_{3} ; k_1\lambda \lambda \parallel l_{3}) \langle l_{1} \parallel C^{(k_1)} \parallel l_{3} \rangle
\]

\[
\times G(l_{2}j_{2}; l_{4}j_{4} ; k_1\lambda \lambda) CGG_{2}(k_1k_2\kappa, k_2k_1),
\]

and

\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_1 \otimes \nabla_2 \right]^{(\kappa)} (\sigma_1 \cdot \sigma_2) \right\}^{(0)}
\]

\[
\Rightarrow (-)^{\lambda+k_2+j_2+j_4+1} \frac{1}{2\lambda+1} \hat{\kappa} \sum_{k} (-)^{k} \left\{ \begin{array}{ccc} k_1 & k_2 & \kappa \\ 1 & 1 & k \end{array} \right\}
\]

\[
\times G(l_{1}j_{1}; l_{3}j_{3} ; k_\lambda \lambda) G(l_{2}j_{2}; l_{4}j_{4} ; k_\lambda \lambda) CGG_{2}(k_1k_2\kappa, k_1k_2k),
\]

31
and

\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \otimes \left[ \nabla_1 \otimes \nabla_1 \right]^{(\kappa)} \left( \sigma_1 \cdot \sigma_2 \right) \] (148)
\]

\[
\Rightarrow \frac{(-)^{\lambda+j_2+j_4}}{k_2 (2\lambda + 1)} G(l_1 j_1; l_3 j_3; k_2\lambda) \ CGG_1(k_1 k_2 \kappa, k_1 \kappa k_2)
\times G(l_2 j_2; l_4 j_4; k_2\lambda) \ \langle l_2 \parallel C^{(k_2)} \parallel l_4 \rangle,
\]

and

\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes \nabla_2 \] (0) \ (\sigma_1 \cdot \sigma_2) \] (149)
\]

\[
\Rightarrow \frac{(-)^{\lambda+j_2+j_4}}{k_1 (2\lambda + 1)} G(l_1 j_1; l_3 j_3; k_1\lambda) \ \langle l_1 \parallel C^{(k_1)} \parallel l_3 \rangle
\times G(l_2 j_2; l_4 j_4; k_1\lambda) \ CGG_2(k_1 k_2, k_2 k_1),
\]

and

\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes \nabla_1 \] (0) \ (\sigma_1 \cdot \sigma_2) \] (150)
\]

\[
\Rightarrow \frac{(-)^{\lambda+j_2+j_4}}{k_2 (2\lambda + 1)} G(l_1 j_1; l_3 j_3; k_2\lambda) \ CGG_1(k_1 k_2, k_1 k_2)
\times G(l_2 j_2; l_4 j_4; k_2\lambda) \ \langle l_2 \parallel C^{(k_2)} \parallel l_4 \rangle.
\]

5.8 Quadrupole spin-orbit interaction

The quadrupole spin-orbit interaction, \( V_{LS2} \), is given as the radial factor, \( V_{ls}(r) \), multiplying the operator \( (\ell \cdot \mathbf{S})^2 \) defined in Eq. (54). As discussed in Sec. 3, the \( j = 0, 1 \) components in Eq. (54) can be incorporated by introducing modified radial amplitudes of the spin-orbit, \( \ell \cdot \mathbf{S} \) and \( \ell^2 \) \( (\sigma_1 \cdot \sigma_2) \) interactions, see Eqs. (57, 58, 60). The only component of the interaction that we have not addressed yet is the one in Eq. (61), corresponding to \( j = 2 \).
In general, we can use Eq. (127) and write

\[
V_{ls2}(r) \left[ \ell \otimes \ell \right]^{(j)} = \frac{3}{2} r^2 \sum_{\kappa \kappa'=0,2} \frac{\tilde{F}'}{\tilde{K}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}^{(j)} (\kappa \kappa' j) \tag{151}
\]

\[
\times \langle 1010 \mid \kappa \rangle \sum_{k_1 k_2} i^{k_2-k_1-\kappa}(2k_1+1)(2k_2+1)\langle k_1 0 k_2 0 \mid \kappa \rangle u^{(k_1 k_2,2\kappa)}(r_1, r_2)
\times \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \left[ (\nabla_1 - \nabla_2) \otimes (\nabla_1 - \nabla_2) \right]^{(\kappa')}^{(j)}
- r \left( - \right)^j \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & j \end{pmatrix} \sum_{k_1 k_2} i^{k_2-k_1-1}(2k_1+1)(2k_2+1) \langle k_1 0 k_2 0 \mid 10 \rangle
\times u^{(k_1 k_2,1)}(r_1, r_2) \left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \otimes (\nabla_1 - \nabla_2)^{j}.\]

Using Eqs. (135, 137) and Eqs. (130, 131), with \( j = 2 \), we couple \( C^{(k)}(\hat{r}_1) \) with \( \nabla_1 \), and \( C^{(l)}(\hat{r}_2) \) with \( \nabla_2 \) dependent operators, respectively. The contributions to the \( ph \)-coupled matrix element \( \langle (l_{1\frac{1}{2}}; j_1, l_{3\frac{1}{2}}; j_3 ; \lambda \mu) \mid V_{ls2} \mid (l_{1\frac{1}{2}}; j_4, l_{3\frac{1}{2}}; j_2) ; \lambda \mu \rangle \) are:

\[
\left[ C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \otimes \nabla_2 \otimes \nabla_2 \right]^{(\kappa)} \left[ (\kappa')^{(2)} \otimes [\sigma_1 \otimes \sigma_2]^{(2)} \right]^{(0)} \tag{152}
\]

\[
\Rightarrow \frac{(-)^{k+j_2+j_4}}{2\lambda + 1} \sqrt{5} \begin{pmatrix} k_1 & k & 2 \\ 1 & 1 & \lambda \end{pmatrix} \times G(1, j_1; l_{3j_3}; k_1 \lambda) G(1 \parallel C^{(k_1)} \parallel l_3) G(l_{2j_2}; l_{4j_4}; k \lambda) CGG_2(k_1 k_2 \kappa, k_2 k' k),
\]

and

\[
\left[ \left[ C^{(k_1)}(\hat{r}_1) \otimes \nabla_1 \right]^{(k)} \otimes \left[ C^{(k_2)}(\hat{r}_2) \otimes \nabla_2 \right]^{(k')} \left[ (\kappa')^{(2)} \otimes [\sigma_1 \otimes \sigma_2]^{(2)} \right]^{(0)} \tag{153}
\]

\[
\Rightarrow \frac{(-)^{k'+j_2+j_4+1}}{2\lambda + 1} \sqrt{5} \begin{pmatrix} k & k' & 2 \\ 1 & 1 & \lambda \end{pmatrix} \times G(1, j_1; l_{3j_3}; k \lambda) G(l_{2j_2}; l_{4j_4}; k' \lambda) CGCG(k_1 k_2 \kappa, k_1 k k' k'),
\]
and

\[
\left[ \left[ C^{(k_1)}(\hat{r}_1) \otimes \left[ \nabla_1 \otimes \nabla_1 \right]^{(k')}^{(k)} \otimes C^{(k_2)}(\hat{r}_2) \right]^{(2)} \otimes \left[ \sigma_1 \otimes \sigma_2 \right]^{(2)} \right]^{(0)}
\]

\[
\Rightarrow \frac{(-)^{k_2+j_2+j_4+1}}{2\lambda+1} \sqrt{5} \begin{pmatrix} k & k_2 & 2 \\ 1 & 1 & \lambda \end{pmatrix}
\]

\[
\times G(l_1j_1; l_3j_3; k\lambda) CGG_1(k_1k_2k, k_1k'k) G(l_2j_2; l_4j_4; k\lambda) \langle l_2 \parallel C^{(k_2)} \parallel l_4 \rangle ,
\]

and

\[
\left[ \left[ C^{(k_1)}(\hat{r}_1) \otimes \left[ C^{(k_2)}(\hat{r}_2) \otimes \nabla_2 \right]^{(k')}^{(k)} \otimes \left[ \sigma_1 \otimes \sigma_2 \right]^{(2)} \right]^{(0)}
\]

\[
\Rightarrow \frac{(-)^{k+j_2+j_4}}{2\lambda+1} \sqrt{5} \begin{pmatrix} k_1 & k & 2 \\ 1 & 1 & \lambda \end{pmatrix}
\]

\[
\times G(l_1j_1; l_3j_3; k_1\lambda) \langle l_1 \parallel C^{(k_1)} \parallel l_3 \rangle G(l_2j_2; l_4j_4; k\lambda) CG_2(k_1k_2, k_2k) ,
\]

and

\[
\left[ \left[ \left[ C^{(k_1)}(\hat{r}_1) \otimes \nabla_1 \right]^{(k')}^{(k)} \otimes C^{(k_2)}(\hat{r}_2) \right]^{(2)} \otimes \left[ \sigma_1 \otimes \sigma_2 \right]^{(2)} \right]^{(0)}
\]

\[
\Rightarrow \frac{(-)^{k_2+j_2+j_4}}{2\lambda+1} \sqrt{5} \begin{pmatrix} k & k_2 & 2 \\ 1 & 1 & \lambda \end{pmatrix}
\]

\[
\times G(l_1j_1; l_3j_3; k\lambda) CG_1(k_1k_2, k_1k) G(l_2j_2; l_4j_4; k_2\lambda) \langle l_2 \parallel C^{(k_2)} \parallel l_4 \rangle .
\]

### 6 Isospin matrix-elements calculation

Independent of the functional form of the single-particle wave functions, the isospin dependence of the matrix elements is worked out in a proton-neutron basis representation. We find it convenient to introduce the proton/neutron creation/destruction operators, $\tau_{\pm}$, in terms of its Cartesian components, as

\[
\tau_{\pm} = \frac{1}{2}(\tau_x \pm i\tau_y) , \quad \tau_0 = \tau_z ,
\]

such that

\[
\tau_+ |p\rangle = 0 \quad \tau_+ |n\rangle = |p\rangle \quad \tau_- |n\rangle = 0 \quad \tau_- |p\rangle = |n\rangle .
\]
Reciprocally, we have

\[
\tau_x = \tau_+ + \tau_- , \quad (158)
\]
\[
\tau_y = \frac{1}{i} (\tau_+ - \tau_-) , \quad (159)
\]

where the Cartesian components of the isospin operator are the usual Pauli matrices

\[
\tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \tau_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \quad (160)
\]

With these definitions, the expectation values of the various isospin-dependent operators are computed, in terms of the matrices

\[
\langle \tau' | \tau_+ | \tau \rangle = \begin{cases} 1 & \text{if } |\tau\rangle = |n\rangle \text{ and } |\tau'\rangle = |p\rangle , \\ 0 & \text{otherwise} , \end{cases} \quad (161)
\]
\[
\langle \tau' | \tau_- | \tau \rangle = \begin{cases} 1 & \text{if } |\tau\rangle = |p\rangle \text{ and } |\tau'\rangle = |n\rangle , \\ 0 & \text{otherwise} , \end{cases} \quad (162)
\]
\[
\langle \tau' | \tau_0 | \tau \rangle = \begin{cases} 1 & \text{if } |\tau\rangle = |\tau'\rangle = |p\rangle , \\ -1 & \text{if } |\tau\rangle = |\tau'\rangle = |n\rangle , \\ 0 & \text{otherwise} . \end{cases} \quad (163)
\]

In particular, we note the identity:

\[
\tau_1 \cdot \tau_2 = 2 (\tau_+ \tau_- + \tau_+ \tau_2) + \tau_0 \tau_2 . \quad (164)
\]

7 Results and Discussions

To study the numerical accuracy of the approach described in the previous sections, we will consider all possible \(ph\)-coupled matrix elements, NME, of the Argonne \(v_{18}\) potential that can be formed in a \(^{16}\)O-like model space of single-particle harmonic-oscillator wave functions, \(\mathcal{HO}_{nl}\), with \(l \leq 6\) and \(n \leq 6\): the states involving \(\mathcal{HO}_{10}\) and \(\mathcal{HO}_{11}\), i.e. \((nlj) = \{(10\frac{1}{2}), (11\frac{1}{2}), (11\frac{3}{2})\}\), are taken to be hole (occupied) states, and all others are particle (unoccupied) states.
We will begin by studying the convergence of the matrix elements calculated using the Moshinsky transformation-brackets approach outlined in Sec. 3. Up to intrinsic round-off errors, the numerical accuracy of the matrix element calculation is tied to the calculation of the radial part of the matrix element, given in Eq. (32). While this is not the only possible way to calculate this integral, we find it instructive to perform this integral using the Gauss-Hermite quadrature formula. This approach is applicable because the asymptotic form of the product of two harmonic-oscillator wave functions is Gaussian, and the potential itself falls to zero, as \( r \) goes to infinity. To study the convergence of the matrix elements with NGAUS, the number of abscissas and weights in the Gauss-Hermite quadrature set, it is convenient to introduce the parameter \( \varepsilon \leq y > x \), which represents the number of matrix elements characterized by a percentage change in the numerical value of the matrix element between \( x\% \) and \( y\% \) when doubling the number of grid points, NGAUS.

Results for the 7 types of operators discussed in the Argonne \( v_{18} \) potential are presented in Tables 1-7. We find that the calculation of the matrix-elements converges relatively fast with the number of points in the Gauss-Hermite
Table 3
Convergence of matrix elements of the tensor interaction of the Argonne $v_{18}$ potential calculated using the Moshinsky transformation-brackets approach outlined in Sec. 3. Similar to table 1.

| NGAUS | NME | $\varepsilon > 1$ | $\varepsilon \leq 1$ | $\varepsilon \leq 0.1$ | $\varepsilon \leq 0.01$ | $\varepsilon \leq 0.001$ |
|-------|-----|-----------------|------------------|---------------------|---------------------|---------------------|
| 64    | 45853 | 16337          | 20967           | 7729                | 751                 |
| 128   | 45853 | 1907           | 12680           | 6663                | 3845                |
| 256   | 45853 | 121            | 1851            | 12795               | 6667                |
| 512   | 45853 | 6              | 147             | 2111                | 13314               |

Table 4
Convergence of matrix elements of the spin-orbit interaction of the Argonne $v_{18}$ potential calculated using the Moshinsky transformation-brackets approach outlined in Sec. 3. Similar to table 1.

| NGAUS | NME | $\varepsilon > 1$ | $\varepsilon \leq 1$ | $\varepsilon \leq 0.1$ | $\varepsilon \leq 0.01$ | $\varepsilon \leq 0.001$ |
|-------|-----|-----------------|------------------|---------------------|---------------------|---------------------|
| 64    | 41255 | 7931           | 20655           | 10778               | 1724                |
| 128   | 41255 | 10             | 108             | 556                 | 5059                |
| 256   | 41255 | 0              | 8               | 78                  | 428                 |
| 512   | 41255 | 0              | 0               | 6                   | 66                  |

Table 5
Convergence of matrix elements of the $\ell^2$ interaction of the Argonne $v_{18}$ potential calculated using the Moshinsky transformation-brackets approach outlined in Sec. 3. Similar to table 1.

| NGAUS | NME | $\varepsilon > 1$ | $\varepsilon \leq 1$ | $\varepsilon \leq 0.1$ | $\varepsilon \leq 0.01$ | $\varepsilon \leq 0.001$ |
|-------|-----|-----------------|------------------|---------------------|---------------------|---------------------|
| 64    | 30650 | 5560           | 15907           | 7636                | 1421                |
| 128   | 30650 | 0              | 130             | 254                 | 7045                |
| 256   | 30650 | 0              | 0               | 82                  | 158                 |
| 512   | 30650 | 0              | 0               | 0                   | 82                  |

quadrature set, NGAUS, with the one notable exception of the matrix element of the tensor interaction. In order to converge the tensor matrix element we require a large set of Gauss-Hermite abscissas. Obtaining such a set is in fact a nontrivial endeavor, and we have described in Appendix A a practical approach to achieve this. The difficulty in converging numerically the tensor matrix element is related to the fact that the radial shape of the tensor interaction has a longer range than the other components of the Argonne $v_{18}$ potential. Hence the deviations from the $e^{-x^2}$ tail of the integrand in Eq. (32) are more pronounced in the case of the tensor interaction. A larger cutoff and a finer Gauss-Hermite grid is needed for an accurate numerical evaluation, which in turn leads to a larger NGAUS number of points.
Table 6
Convergence of matrix elements of the $\ell^2(\sigma_1 \cdot \sigma_2)$ interaction of the Argonne $v_{18}$ potential calculated using the Moshinsky transformation-brackets approach outlined in Sec. 3. Similar to table 1.

| NGAUS | NME  | $\varepsilon > 1$ | $\varepsilon \leq 1$ | $\varepsilon \leq 0.1$ | $\varepsilon \leq 0.01$ | $\varepsilon \leq 0.001$ |
|-------|------|------------------|---------------------|----------------------|----------------------|----------------------|
| 64    | 44261 | 8280             | 22408               | 11709                | 1715                 |
| 128   | 44261 | 2                | 89                  | 765                  | 8686                 |
| 256   | 44261 | 0                | 0                   | 2                    | 163                  |
| 512   | 44261 | 0                | 0                   | 0                    | 0                    |

Table 7
Convergence of matrix elements of the quadrupole spin-orbit interaction in the Argonne $v_{18}$ potential calculated using Moshinsky transformation-brackets approach outlined in Sec. 3. Similar to table 1.

| NGAUS | NME  | $\varepsilon > 1$ | $\varepsilon \leq 1$ | $\varepsilon \leq 0.1$ | $\varepsilon \leq 0.01$ | $\varepsilon \leq 0.001$ |
|-------|------|------------------|---------------------|----------------------|----------------------|----------------------|
| 64    | 46726 | 17572            | 22013               | 6245                 | 787                  |
| 128   | 46726 | 31               | 408                 | 5549                 | 21721                |
| 256   | 46726 | 0                | 10                  | 106                  | 1412                 |
| 512   | 46726 | 0                | 0                   | 0                    | 6                    | 49                   |

We conclude that a parameter value, NGAUS=512, is large enough to assure a good accuracy of all components of the Argonne $v_{18}$ matrix elements, including the tensor part of the interaction, as indicated by the sharp decrease in the parameter $\varepsilon_{>0.1}$ for NGAUS=512. This statement is supported by results of an independent calculation, to be discussed next.

Next, we will compare the calculation of the Argonne $v_{18}$ matrix elements using the Moshinsky transformation-brackets approach described in Sec. 3 with the more general calculation of the same matrix elements in the framework outlined in Sec. 5. With the exception of unavoidable round-off errors, the source of possible numerical loss of accuracy in the calculation of the matrix elements presented here is linked to the calculation of the integrals discussed in Sec. 5.1. First, we are concerned with the integrals in Eqs. (73) and (92): Given that the integrand vanishes for large values of the integration variables, and in order to maintain the approach general, we will evaluate these integrals by choosing a large cutoff and discretizing the integrand on a fine grid. Because these integrals only have to be performed once in the beginning of the calculation, and that the results can be stored on disk for future reference, we have chosen a radial cutoff of 25 fm and a momentum cutoff of 30 fm$^{-1}$ in Eqs. (73) and (92), respectively, together with uniform grids of 8000 points, and have performed these integrals using the Simpson rule.

Second, we have to perform the integrals involving the radial parts of the
Table 8
Convergence of matrix elements of the various components of the Argonne $v_{18}$ potential calculated using the approach outlined in Sec. 5. Calculations were performed for values of the number of abscissas and weights in the Gauss-Hermite quadrature set, NGAUS, equal to 32, 64, 96 and 128. Here we study the evolution of the parameter $\varepsilon_{\leq y}^{\geq x}$, which indicates how many matrix elements out of the total number of matrix elements, NME, that can be formed in a $^{16}$O-like model space of harmonic-oscillator single-particle wave functions, $R_{nl}$, with $l \leq 6$ and $n \leq 6$, are characterized by a relative error between $x\%$ and $y\%$ when the number of grid points, NGAUS, changes. Calculations for larger values of NGAUS, (NGAUS=96 or 128 where appropriate) have resulted in zero values of the parameter $\varepsilon_{\leq y}^{\geq x}$.

| Operator | NGAUS | NME  | $\varepsilon_{\geq 1}$ | $\varepsilon_{\leq 1}$ | $\varepsilon_{\leq 0.1}$ | $\varepsilon_{\leq 0.01}$ | $\varepsilon_{\leq 0.001}$ |
|----------|-------|------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| 1        | 64    | 23950| 0                       | 20                      | 411                     | 17243                   |
| $\sigma_i \cdot \sigma_j$ | 64    | 43796| 0                       | 137                     | 1425                    | 22048                   |
| $S_{ij}$ | 64    | 45853| 17844                   | 4704                    | 3795                    | 17892                   |
| $S_{ij}$ | 96    | 45853| 0                       | 4                       | 23                      | 378                     |
| $\ell \cdot S$ | 64    | 41255| 10                      | 109                     | 636                     | 5191                    |
| $\ell^2$ | 64    | 30650| 0                       | 115                     | 257                     | 3011                    |
| $\ell^2 (\sigma_i \cdot \sigma_j)$ | 64    | 44261| 0                       | 9                       | 294                     | 3659                    |
| $(\ell \cdot S)^2$ | 64    | 46726| 22                      | 230                     | 2971                    | 16467                   |

Table 9
Comparison of the matrix elements of the 7 operators in the Argonne $v_{18}$ potential calculated using the center-of-mass separation of variables for harmonic-oscillator wave functions such as described in Sec. 3 and the general procedure outlined in Sec 5. Here, the parameter $\varepsilon_{\leq y}^{\geq x}$ reflects the changes between the Moshinsky-transformation based result (NGAUS=512) and the matrix elements calculated using the approach presented in Sec. 5 for NGAUS=96.

| Operator | NME  | $\varepsilon_{\geq 1}$ | $\varepsilon_{\leq 1}$ | $\varepsilon_{\leq 0.1}$ | $\varepsilon_{\leq 0.01}$ | $\varepsilon_{\leq 0.001}$ |
|----------|------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| 1        | 23950| 0                       | 0                       | 0                       | 0                       | 0                       |
| $\sigma_i \cdot \sigma_j$ | 43796| 0                       | 0                       | 0                       | 188                    |
| $S_{ij}$ | 45853| 0                       | 8                       | 187                     | 3365                   |
| $\ell \cdot S$ | 41255| 0                       | 0                       | 0                       | 2                      |
| $\ell^2$ | 30650| 0                       | 0                       | 0                       | 0                      |
| $\ell^2 (\sigma_i \cdot \sigma_j)$ | 44261| 0                       | 0                       | 0                       | 0                      |
| $(\ell \cdot S)^2$ | 46726| 0                       | 0                       | 0                       | 4                      |

single-particle wave functions, as seen in Eqs. (89) and (91). For an arbitrary functional form of the single-particle wave functions, these calculations can become computationally expensive, as they may have to be repeated for
the calculation of each and every matrix element. For the case of a linear combination of harmonic-oscillator single-particle basis, these integrals can be performed using Gauss-Hermite quadrature formulas.

We study the convergence of the matrix elements with the number of abscissas and weights in the Gauss-Hermite quadrature set, NGAUS, by computing the value of the parameter \( \varepsilon \leq y_{\geq x} \), which represents the number of matrix elements characterized by a percentage change in the numerical value of the matrix element between \( x\% \) and \( y\% \) as the number of grid points, NGAUS, changes. We have performed calculations using 4 sets of Gauss-Hermite quadrature points, corresponding to values of the NGAUS parameter of 32, 64, 96, and 128. Results for the 7 types of operators part of the Argonne \( v_{18} \) potential are presented in Table 8. We find that the calculation of the matrix-elements is fully converged for a value of the NGAUS parameter, NGAUS=96, for all components of the Argonne \( v_{18} \) potential, with the exception of the tensor interaction, which requires a larger set of NGAUS=128 Gauss-Hermite quadrature points. The slower convergence of the tensor-interaction matrix element follows the trend observed in the case of the calculation based on the Moshinsky transformation brackets, and is due to the fact that the tensor interaction in the Argonne \( v_{18} \) potential has a longer range and more structure than the other components of the interaction.

In order to ascertain the numerical accuracy and correctness of the approach presented in Sec. 5, we have also compared with results of the calculation of the matrix elements using the Moshinsky transformation brackets discussed earlier. Results are displayed in Table 9. Here, the parameter \( \varepsilon \leq y_{\geq x} \) reflects the changes between the Moshinsky transformation-brackets result (NGAUS=512) and the matrix elements calculated using the approach discussed in Sec. 4 for NGAUS=96. The two calculations lead to numerically identical matrix elements, which is quite remarkable since the two approaches are very different. This validates both theoretical approaches.

In summary, in this paper we discussed two approaches for the calculation of two-body matrix elements of the Argonne \( v_{18} \) potential. The first approach is only applicable to the specific case of a harmonic-oscillator single-particle wave function representation. In this case, the matrix elements are calculated using the Talmi transformation (implemented numerically using the Moshinsky transformation brackets) which allows for the separation of the center-of-mass and relative coordinates degrees of freedom. Integrals involving the radial part of the potential were performed using Gauss-Hermite quadrature formulas, and convergence was achieved for sets of at least 512 Gauss points. This procedure was designed to validate the calculation of matrix elements of the Argonne \( v_{18} \) potential using an approach suitable for an arbitrary functional form of the single-particle wave functions. The latter approach represents the main thrust of this paper. This general framework is suitable for the calculation of ma-
trix elements involving a representation of the single-particle wave functions given by linear combinations of harmonic-oscillator wave functions such as in Refs. [10][11][12], and/or the two-scale functional representation for the hole and particle sides of the spectrum such as outlined in Ref. [21]. For a model space represented in terms of harmonic-oscillator wave functions, results obtained using the approaches discussed in Sec. 3 and Sec. 5 are shown to be identical within numerical accuracy.

A Generator of large-$N$ Gauss-Hermite quadrature sets

The algorithm used to generate the Gauss-Hermite quadrature abscissas and weights represents an adaption of the algorithm described in Ref. [25].

The Gauss-Hermite quadrature formula allows for the efficient numerical computation of the integral
\[ \int_{-\infty}^{\infty} dx \ f(x) \ e^{-x^2} \approx \sum_{j=1}^{N} w_j \ f(x_j), \]  (A.1)
where $x_j$ are the roots of the $H_N(x)$ Hermite polynomial. The $N$-points Gauss-Hermite becomes exact provided that $f(x)$ is a polynomial. In order to avoid the overflow problems related to the standard recurrence relation of the Hermite polynomials, i.e.
\[ H_{j+1}(x) = 2x \ H_{j}(x) - 2j \ H_{j-1}(x), \]  (A.2)
one uses instead the the orthonormal set of polynomials, $\tilde{H}_j(x)$, which are generated using the recurrence relation
\[ \tilde{H}_{-1} = 0, \quad \tilde{H}_0 = \pi^{-1/4}, \]
\[ \tilde{H}_{j+1}(x) = x \sqrt{\frac{2}{j+1}} \ \tilde{H}_j(x) - \sqrt{\frac{j}{j+1}} \ \tilde{H}_{j-1}(x). \]

Then, the formula for the Gauss-Hermite weights is
\[ w_j = \frac{2}{|\tilde{H}_j'(x_j)|^2}, \]  (A.4)
where $\tilde{H}_j'(x)$ denotes the derivative of the polynomial $\tilde{H}_j(x)$, which is calculated as
\[ \tilde{H}_j'(x) = \sqrt{2j} \ \tilde{H}_{j-1}(x). \]  (A.5)
The roots of the Hermite polynomial $\tilde{H}_N(x)$ are symmetric about the origin, so we only have to calculate half of them, e.g. the positive ones. The roots are
estimated using the formulas put forward by Szegő for the largest root of the Hermite polynomial $H_N(x)$ [26], i.e.

$$x_N^{[0]} \simeq \sqrt{2N + 1} - 1.85575 (2N + 1)^{-1/6}, \quad (A.6)$$

and by Stroud and Secrest [27] for the second-largest root,

$$x_{N-1}^{[0]} \simeq x_N - 1.14 N^{-426} / x_N, \quad (A.7)$$

the third-largest root

$$x_{N-2}^{[0]} \simeq 1.86 x_{N-1} - 0.86 x_N, \quad (A.8)$$

the fourth-largest root

$$x_{N-3}^{[0]} \simeq 1.91 x_{N-2} - 0.91 x_{N-1}, \quad (A.9)$$

and all other positive roots

$$x_j^{[0]} \simeq 2x_{j-1} - x_{j-2}. \quad (A.10)$$

Subsequently, a root-finding algorithm is employed to improve these solutions. For added accuracy, all calculations are performed in quadruple precision, even though the Gauss-Hermite quadrature sets are ultimately used in double precision.

Press et al. [25] propose the commonly-used Newton’s method to achieve this task. In this approach, the $i^{th}$ approximation of the root $x_j$ is obtained as

$$x_j^{[i]} = x_j^{[i-1]} - \frac{H_N(x_j^{[i-1]})}{H'_N(x_j^{[i-1]})}. \quad (A.11)$$

In our experience, this procedure is able to successfully produce all $N$-points Gauss-Hermite quadrature sets of abscissas and weights for $N \lesssim 200$. For larger sets, one must replace the root finder and use Muller’s method instead (see page 364 in Ref. [25].) This method uses a quadratic interpolation among the 3 most recent estimates of the solution. To begin the search, we have chosen the first 3 guesses of the solution as $x_j^{[0]}$, given by the Szegő’s or Stroud’s approximations described above, together with the coordinates $x_j^{[0]} \pm 0.1$. It is important for this root-finding algorithm to be allowed to carry out the search in the complex plane, even though the roots of the Hermite polynomial are real. Muller’s method allows for the calculation of Gauss-Hermite quadrature sets with $N \lesssim 600$.

To further improve the algorithm and reach higher values of $N$, it has been noticed that the coordinate dropped after the first estimate performed using
Muller's method, must be the one which is the farthest away from this estimate. This allows for the calculation of Gauss-Hermite quadrature sets with \( N \lesssim 1050 \), at which point we are very close to the natural numerical barrier encountered in numerical computations performed using 32-bit CPUs, even when using quadruple precision. Because, these sets where large enough to provide convergence for the purpose of our matrix-elements calculations, and because our calculations are carried out entirely on 32-bit platforms, we have not investigated this matter further.

Because of the symmetry of the Gauss-Hermite quadrature set and the fact that our integrals involve only the radial coordinate in a spherical coordinates, we define the parameter \( N_{\text{GAUS}} \) as half the value of the integer \( N \) in Eq. (A.1).

## B Reduced matrix elements

In this appendix we list commonly used reduced matrix elements, relevant to the calculations described in this paper.

### B.1 \( C^{(k)}(r) \)

The reduced matrix element of the unnormalized spherical harmonic is ([23], Eq. 5.4.6)

\[
\langle l_1 \parallel C^{(k)}(r) \parallel l_2 \rangle = \hat{l}_2 \langle l_2 0 k 0 \mid l_1 0 \rangle ,
\]

with the selection rules \( \ell_1 + \ell_2 + k = \text{even} \), and \( |l_1 - l_2| \leq k \leq l_1 + l_2 \).

### B.2 \( [C^{(k_1)}(r) \otimes \nabla]^{(k_2)} \)

Using ([23], 7.1.1) we obtain

\[
\langle n_1 l_1 \parallel [C^{(k_1)}(r) \otimes \nabla]^{(k_2)} \parallel n_2 l_2 \rangle = (-)^{l_1 + l_2 + k_2} \hat{k}_2 \sum_{l} \begin{pmatrix} k_1 & 1 & k_2 \\ l_2 & l_1 & l \end{pmatrix} \langle l_1 \parallel C^{(k_1)}(r) \parallel l \rangle \langle n_1 l \parallel \nabla \parallel n_2 l_2 \rangle ,
\]

subject to the selection rules: \( |k_1 - 1| \leq k_2 \leq k_1 + 1 \). The reduced matrix elements of the gradient operator are obtained from the gradient formula (see ...
The only nonzero components are

\[
\langle n_1(l_1 = l_2 - 1) \| \nabla \| n_2 l_2 \rangle = -\sqrt{l_2} \int_0^\infty [r^2 \, dr] R_{n_1 l_1}(r) \left[ \left( \frac{d}{dr} + \frac{l_2 + 1}{r} \right) R_{n_2 l_2}(r) \right],
\]

(B.3)

and

\[
\langle n_1(l_1 = l_2 + 1) \| \nabla \| n_2 l_2 \rangle = \sqrt{l_2 + 1} \int_0^\infty [r^2 \, dr] R_{n_1 l_1}(r) \left[ \left( \frac{d}{dr} - \frac{l_2}{r} \right) R_{n_2 l_2}(r) \right].
\]

(B.4)

### B.3 \[ C^{(k_1)}(\hat{r}) \otimes [\nabla \otimes \nabla]^{(j)} \]^{(k_2)}

Using (23, 7.1.1) we obtain

\[
\langle n_1 l_1 \| [C^{(k_1)}(\hat{r}) \otimes [\nabla \otimes \nabla]^{(j)}]^{(k_2)} \| n_2 l_2 \rangle
\]

(B.5)

\[
= (-)^{l_1 + l_2 + k_2} \frac{\hbar^2}{k_2} \sum_{l} \left\{ \begin{array}{ccc} k_1 & j & k_2 \\ l_2 & l_1 & l \end{array} \right\} \langle l_1 \| [C^{(k_1)}(\hat{r})] \| l \rangle \langle n_1 l_1 \| [\nabla \otimes \nabla]^{(j)} \| n_2 l_2 \rangle,
\]

with the selection rules: \(|\ell - 1| \leq \kappa \leq \ell + 1\). The allowed reduced matrix elements are

\[
\langle n_1(l_1 = l_2 - 2) \| [\nabla \otimes \nabla]^{(j)} \| n_2 l_2 \rangle = \sqrt{l_2(l_2 - 1)} \left\{ \begin{array}{ccc} 1 & 1 & j \\ l_2 & l_2 - 2 & l_2 - 1 \end{array} \right\}
\]

(B.6)

\[
\times (-)^j \int_0^\infty [r^2 \, dr] R_{n_1 l_1}(r) \left\{ \left[ \frac{d^2}{dr^2} + \frac{2l_2 + 1}{r} \frac{d}{dr} + \frac{(l_2 - 1)(l_2 + 1)}{r^2} \right] R_{n_2 l_2}(r) \right\},
\]

and

\[
\langle n_1(l_1 = l_2) \| [\nabla \otimes \nabla]^{(j)} \| n_2 l_2 \rangle
\]

(B.7)

\[
= - \left\{ \begin{array}{ccc} 1 & 1 & j \\ l_2 & l_2 & l_2 - 1 \end{array} + (l_2 + 1) \left\{ \begin{array}{ccc} 1 & 1 & j \\ l_2 & l_2 & l_2 + 1 \end{array} \right\} \right\} \times (-)^j \int_0^\infty [r^2 \, dr] R_{n_1 l_1}(r) \phi(r) \left\{ \left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l_2(l_2 + 1)}{r^2} \right] R_{n_2 l_2}(r) \right\},
\]
and
\[ \langle n_1(l_1 = l_2 + 2) \parallel \nabla \otimes \nabla \parallel n_2 l_2 \rangle = \sqrt{(l_2 + 1)(l_2 + 2)} \left\{ \begin{array}{l} 1 \\ l_2 \end{array} , \begin{array}{l} l_2 \\ l_2 + 2 \end{array} + j \right\} \]
\[ \times (-1)^j \int_0^\infty [r^2 dr] R_n n_1 (r) \left\{ \left[ \frac{d^2}{dr^2} - \frac{2l_2 + 1}{r} \frac{d}{dr} + \frac{l_2(l_2 + 2)}{r^2} \right] R_n n_2 (r) \right\}. \]
(B.8)

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