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Ground state of (16)O

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GROUND STATE OF ^{16}O

BY

Bogdan Mihaila

Diploma (M.Sc.), University of Bucharest (1989)

DISSERTATION

Submitted to the University of New Hampshire
in partial fulfillment of
the requirements for the degree of

Doctor of Philosophy

in

Physics

May 1998

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This dissertation has been examined and approved.

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Date

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Dedication

To my dear parents

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First and foremost, I thank my advisor Professor Jochen Heisenberg. His enthusiasm and creativity have been an inspiration. Without his knowledge and patience, without his friendship and experience, this dissertation would not have been possible. Thank you for believing this research was possible and putting up with my many questions and doubts. I look forward to a continuing relationship for many years to come.

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ABSTRACT

GROUND STATE OF ^{16}O

by

Bogdan Mihaila
University of New Hampshire, May, 1998

We use the coupled cluster expansion ($\exp(S)$ method) to solve the many-body Schrödinger equation in configuration space in a configuration space of 35 $\hbar\omega$. The Hamiltonian includes a nonrelativistic one-body kinetic energy, a realistic two-nucleon potential and a phenomenological three-nucleon potential. Using this formalism we generate the complete ground state correlations due the underlying interactions between nucleons. The resulting ground state wave function is used to calculate the binding energy, the one- and two-body densities for the ground state of ^{16}O. The problem of center-of-mass corrections in calculating observables has been worked out by expanding the center-of-mass correction as many-body operators. For convergence testing purposes, we apply our formalism to the case of the harmonic oscillator shell model, where an exact solution exists. We also work out the details of the calculation involving realistic nuclear wave functions.

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Chapter 1

Introduction.

Motivation. In the last thirty years electron scattering from nuclei has provided a wealth of information mapping out nuclear ground state charge densities [Cv-80], providing precise transition charge and current densities for the excitation of single particle states [Sw-83] and for collective states [Go-80]. The measurement of ground state magnetization densities and the excitation of high multipolarity magnetic excitations, or the single particle knockout reaction to discrete states all have in some way supported the mean-field approach as the lowest order in the description of nuclear structure.

The confirmation of the mean-field approach, however, were more qualitative in nature than quantitative. The form factors for the excitation of the high spin single particle states in ^{208}Pb [Li-79], were described extremely well in shape by the mean-field wave functions, however, the predicted strength was too big by a factor of two. The knockout reactions again were in good agreement with the shapes predicted by the mean-field wave functions but the strength was off by again roughly a factor of two [Le-94].

The general conclusion was that the nuclear correlations are the ones that account for the discrepancies and not the quark degrees of freedom of nucleons. They do not change the shape of the wave functions but they modify the strength due to deoccupation of orbits below the Fermi surface and partial occupation of the orbits above the Fermi surface [Pa-84]. This was confirmed by $(e, e'p)$ experiments in which particles from orbits above the Fermi level were knocked out [Le-94]. Thus, to do justice to the accuracy of the electromagnetic probe,

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we can no longer be satisfied with the mean-field approach, but have to take into account the correlations largely due to the hard repulsive core of the nucleon-nucleon interaction.

Nuclear many-body problem. A major problem in nuclear physics is to understand how nuclear structure comes about from the underlying interactions between nucleons. This requires modeling nuclei as collections of strongly interacting nucleons. The starting point is the solution of the many-body Schrödinger equation for a realistic nuclear Hamiltonians.

Solutions have been proven to be rather difficult to obtain! For the three-nucleon system, this was done only in 1980's via the Fadeev method, first in coordinate [Ch-85], and then in momentum space [Wt-91]. Since then, a variety of methods have been used successfully for studying light nuclear spectra: First, the Correlated Hyperspherical Harmonics (CHH) method [Ki-93, Ki-94] was used to describe the bound states of the A=3 and A=4 nuclei as well as $d+n$ and $d+p$ scattering states at energies below the three-body breakup threshold. Then came the first microscopic calculations that directly produce nuclear shell structure from realistic interactions that fit NN scattering data: in 1996, Pudliner *et al* have reported calculations of ground and low-excited states for nuclei with $A \leq 6$ [Pu-95], and the next year results for nuclei with $A \leq 7$ [Pu-97], using the Green's function Monte Carlo (GMC) method.

However, all these methods are limited in the number of nucleons they can treat, because the dimensions of the necessary grids grow too large. So far, only the Variational Monte Carlo method based calculations with realistic two- and three-nucleon interactions (Argonne $v14$ and Urbana-VII potentials), has enjoyed success in solving the many-body problem for medium nuclei. In this formalism, an optimal trial function is obtained by

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minimizing the energy through the four-body cluster level. The trial wave function is based on products of pair- and triplet-correlation operators acting on a product of single-particle determinants. The pair-correlations operators include central, spin, isospin, tensor, and spin-orbit components, while the triplet-correlation operators include components induced by three-nucleon potentials. Expectation values are evaluated with a cluster expansion for the noncentral correlations. Terms in the expansion are evaluated exactly using the Monte Carlo integration.

Present work. The goal of our effort is to build realistic models of nuclear structure that explicitly account for realistic correlations. There are different ways to account for correlations. As mentioned above, one way is to introduce correlation functions in the many body wave function in real space. This has been quite successful for small nuclei [Wi-91, Pu-95, Pu-97] and has resulted in reasonable descriptions of ^{16}O [Pi-92]. A different approach is to add in configuration space to the uncorrelated ground state multi-particle multi-hole configurations [Ku-78]. Both approaches can be related to each other.

Our aim is twofold: On one hand we want to verify in a more quantitative way the claim that the quenching observed in the transverse electron scattering amplitude is indeed due to correlations. On the other hand, we want to apply this description to single nucleon knockout and double nucleon knockout reactions. In double nucleon knockout the scattering amplitude vanishes without correlations and without two-body (meson exchange) currents. Thus such experiments are a sensitive tool to investigate these two effects.

In a first stage we focus our attention on obtaining a realistic description for the ground state of a double-magic nucleus. We are using the $exp(S)$ coupled-cluster expansion to

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calculate the ground state of ^{16}O. In our treatment we follow closely the formulation of the Bochum group [Ku-78]. However, we solve the equations entirely in configuration space. Furthermore, we truncate in different ways where the significance of terms becomes more transparent

The coupled-cluster method was invented forty years ago by Coester and Kümmel [Co-58, Co-60]. It was not until nearly twenty years later [Ku-78] that the coupled-cluster method was used to carry out the first detailed calculations of larger nuclei with realistic interactions. The idea behind this formalism relies on our ability of expanding the model nuclear wave function in the many-body Hilbert space in terms of two Abelian subalgebras of multi-configurational creation and their Hermitian-adjoint destruction operators. The expansion coefficients carry then the interpretation of nuclear correlations. The fact that we make no artificial separation between "short range" and "long range" correlations is one particular strength of this many-body method.

The derivation of the explicit equations is tedious, but requires only standard techniques. The computation breaks down into two steps: In the first step the G-matrix interaction is calculated inside the nucleus including all the corrections. This results in amplitudes for the $2p2h$ correlations, which are implicitly corrected for the presence of $3p3h$ and $4p4h$ correlations. In the second step the mean field is calculated from these correlations and the single-particle Hamiltonian is solved to give mean-field eigenfunctions and single particle energies. These two steps are iterated until a stable solution is obtained. Calculations are carried out entirely in configuration space where a $35\hbar\omega$ space is used.

The Hamiltonian includes a nonrelativistic one-body kinetic energy, a two-nucleon potential and a supplemental three-nucleon potential. We have chosen the Argonne v-18

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potential as the most realistic nucleon-nucleon interaction available today. The Argonne $v18$ model is one of a new class of NN potentials that accurately fit both pp and nn scattering data up to 350 MeV with a χ^2/datum near one. This necessarily involves the introduction of charge-independence breaking in the strong force. However, the two-body part of that interaction results in over binding and a too large saturation density in nuclear matter Therefore, the NN potential is supplemented by a three-nucleon interaction including a long-range two-pion exchange and a short-range phenomenological component. The Urbana-IX NNN potential is adjusted to reproduce the binding energy of ^{3}H and give reasonable saturation density in nuclear matter when used with Argonne $v18$.

Future plans. Once the calculation of the ^{16}O ground state is completed we intend to extend our formulation to address the calculation of discrete excited states as well as neighboring odd-even nuclei. With the programs working for odd-even nuclei we can then model the (e,e'N) reaction, where the final state has the asymptotic form of a distorted wave times a discrete state of the (A-1) nucleus. However, this is not a solution to the Hamiltonian close to the origin, and thus the wave function needs to be modified in the region of the origin. Finally, we intend to apply this treatment to the two-nucleon knockout reaction. There we have three topics needing to be solved: (a) the inclusion of continuum states, for which we hope to gain experience by modelling the (e,e'N) reaction, (b) the treatment of correlations between the two emerging nucleons, and (c) the description of the (A-2) nucleus for the asymptotic form of the final state and its modification around the origin.

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Chapter 2

Fundamentals.

2.1 Nuclear Many Body Problem.

For a spherically symmetric nuclear system, consisting of both protons and neutrons, the total Hamiltonian is given as

$$\mathbf{H} = \sum_i T_i + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}^{tni} \equiv T + V . \tag{2.1.1}$$

In the *second-quantization* representation this becomes

$$\begin{aligned}\mathbf{H} = & \sum_{\alpha\beta} \mathbf{a}_\alpha^\dagger \langle\alpha|T|\beta\rangle \mathbf{a}_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \mathbf{a}_\alpha^\dagger \mathbf{a}_\beta^\dagger \langle\alpha\beta \,|\, V_{2N} \,|\, \delta\gamma\rangle \mathbf{a}_\gamma \mathbf{a}_\delta \\ & + \frac{1}{6}\sum_{\alpha\beta\gamma\delta\theta\zeta} \mathbf{a}_\alpha^\dagger \mathbf{a}_\beta^\dagger \mathbf{a}_\gamma^\dagger \langle\alpha\beta\gamma \,|\, V_{3N} \,|\, \delta\theta\zeta\rangle \mathbf{a}_\zeta \mathbf{a}_\theta \mathbf{a}_\delta .\end{aligned} \tag{2.1.2}$$

where Greek letters label the single-particle states $|\alpha\rangle = |nlsjm_j; \frac{1}{2}m_\tau\rangle$, with $s = \frac{1}{2}$, $|j = l \pm \frac{1}{2}|$ and $m_\tau = +\frac{1}{2}(-\frac{1}{2})$ - for a proton (neutron). The parity of these states is $(-1)^l$.

We are searching for the N particle eigenfunctions and eigenvalue E of H:

$$H|\Psi\rangle = E|\Psi\rangle . \tag{2.1.3}$$

2.1.1 Single-Particle Radial Wave Functions.

We introduce the functions R_{nl} of the variable $x = r/b$, by their expansion into harmonic oscillator wave functions $\mathcal{HO}_{kl}(x)$, as

$$R_{nl}(x) = \sum_k A_{nl}^k \mathcal{HO}_{kl}(x) , \tag{2.1.4}$$

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and subject to the normalization condition

$$\int_0^\infty x^2\,dx\; R_{nl}(x)\,R_{n'l'}(x) \;=\; \delta_{n\,n'}\delta_{l\,l'}\,. \tag{2.1.5}$$

Then, the single-particle radial functions $\mathcal{R}_{nl}(r)$ are defined in terms of the the radial functions $R_{nl}(x)$ such that they satisfy the normalization condition

$$\int_0^\infty r^2\,dr\; \mathcal{R}_{nl}(r)\,\mathcal{R}_{n'l'}(r) \;=\; \delta_{n\,n'}\delta_{l\,l'}\,. \tag{2.1.6}$$

Thus, we have

$$\mathcal{R}_{nl}(r) \;=\; \frac{1}{b^{3/2}}\,R_{nl}(x)\,. \tag{2.1.7}$$

Note that the tail of the single-particle radial functions $\mathcal{R}_{nl}(r)$ goes like $\exp^{-\frac{r^2}{2}}$ for large x or r.

2.2 Nucleon-Nucleon Potentials.

Traditionally, nucleon-nucleon (NN) potentials are constructed by fitting *np* data for $T = 0$ states and either *np* data for $T = 1$ (Argonne v_{14}, Urbana v_{14}, Bonn potentials) or *pp* data (Reid, Nijmegen 78, Paris potentials), respectively.

Unfortunately, potential models which have been fit only to the *np* data often give a poor description of the *pp* data, even after applying the necessary corrections for the Coulomb interaction. By the same token, potentials fit to *pp* data in $T = 1$ states give only a mediocre description of *np* data. Fundamentally this problem is due to charge-independence breaking in the strong interaction. The Nijmegen *NN* potentials represent one possible way out. However, these models are based on a partial wave analysis. Consequently, they differ in each partial wave and thus introduce nonlocalities from one partial wave to the next that

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are difficult to treat in many-body calculations. Thus, the goal to construct a nonrelativistic potential that can be used easily in many-body calculations and that accurately fits both *np* data and *pp* data.

The Argonne v_{18} potential [1] is an updated version of the nonrelativistic Argonne potential 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, and has an excellent χ^2 per datum of 1.09 . It was also fit to *nn* scattering length measured in $d(\pi^-, \gamma)nn$ experiments and the deuteron binding energy.

The strong interaction part of the potential is projected into an operator format with 18 terms: A charge-independent part that has 14 operator components (as in the older Argonne v_{14})

$$1,\ \sigma_i \cdot \sigma_j,\ S_{ij},\ L \cdot S,\ L^2,\ L^2\ \sigma_i \cdot \sigma_j,\ (L \cdot S)^2 \tag{2.2.1}$$

$$\tau_i \cdot \tau_j,\ (\sigma_i \cdot \sigma_j)\ (\tau_i \cdot \tau_j),\ S_{ij}\ (\tau_i \cdot \tau_j),\ L \cdot S\ (\tau_i \cdot \tau_j),$$

$$L^2(\tau_i \cdot \tau_j),\ L^2\ (\sigma_i \cdot \sigma_j)\ (\tau_i \cdot \tau_j),\ (L \cdot S)^2\ (\tau_i \cdot \tau_j) \tag{2.2.2}$$

And a charge-independence breaking part that has three charge-dependent operators

$$T_{ij},\ (\sigma_i \cdot \sigma_j)\ T_{ij},\ S_{ij}\ T_{ij} \tag{2.2.3}$$

where $T_{ij} = 3\tau_{zi}\tau_{zj} - \tau_i \cdot \tau_j$ is the isotensor operator, defined analogous to the S_{ij} operator; and one charge-asymmetric operator

$$\tau_{zi} + \tau_{zj}\ . \tag{2.2.4}$$

In principle, there could be more charge-independence breaking terms, such as $L \cdot ST_{ij}$ or

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$S_{ij}(\tau_{zi}+\tau_{zj})$, but the scattering data are not sufficiently precise to identify them at present.

The potential includes also a complete electromagnetic potential, containing Coulomb, Darwin-Foldy, vacuum polarization, and magnetic moment terms with finite-size effects.

2.3 Three-Nucleon Interaction Model (Urbana).

The model of the three-nucleon interaction presented below follows closely the formalism described in [Ca-83]. The three-body force is introduced as the sum of two components: a two-pion-exchange ($V_{2\pi 3N}$) interaction, given by the two-pion-exchange model ($V_{2\pi 3N}$) of the three-nucleon interaction; and a repulsive V^I_{3NR} three-nucleon interaction, which was argued ([La-81]) to be necessary in order to help saturate nuclear matter at reasonable density.

2.3.1 Two-Pion-Exchange Interaction.

We shall address first the case of the two-pion-exchange model ($V_{2\pi 3N}$) of the three-nucleon interaction. The two-pion-exchange ($V_{2\pi 3N}$) can be written in the form

$$\begin{aligned} V_{2\pi 3N} \;=\; & \sum_{cycl.} A_{2\pi}\,\{\tau_1\cdot\tau_2\,,\,\tau_1\cdot\tau_3\} \\ & \qquad \times\,\{(S_{12}T(r_{12})+\sigma_1\cdot\sigma_2 Y(r_{12}))\,.\,(S_{13}T(r_{13})+\sigma_1\cdot\sigma_3 Y(r_{13}))\} \\ & +C_{2\pi}\,[\tau_1\cdot\tau_2\,,\,\tau_1\cdot\tau_3]\,[(S_{12}T(r_{12})+\sigma_1\cdot\sigma_2 Y(r_{12}))\,.\,(S_{13}T(r_{13})+\sigma_1\cdot\sigma_3 Y(r_{13}))] \\ & +B(r_{12},r_{13})\,\{\tau_1\cdot\tau_2\,,\,\tau_1\cdot\tau_3\}\,\{(S_{12}+\sigma_1\cdot\sigma_2))\,.\,(S_{13}+\sigma_1\cdot\sigma_3))\}\,. \end{aligned} \tag{2.3.1}$$

Here $\sum_{cycl.}$ represents a cyclic sum over indices 1, 2 and 3; τ, σ and S_{ij} are the isospin, spin and tensor operators, and $\{\,,\,\}$ and $[\,,\,]$ denote anticommutators and commutators. The $T(r)$ and $Y(r)$ are radial functions associated with the tensor and Yukawa parts of the

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one-pion-exchange interaction. The $B(r_{12}, r_{13})$ term comes from the πN S-wave scattering.

Assuming the simple Δ (33 resonance) intermediate-state model, for the Argonne v_{18} potential one gets

$$\begin{aligned} A_{2\pi} &= -\left(\frac{f f^* m_\pi}{12\pi}\right)^2 \frac{2}{9E_{av}} \sim -0.0293\ MeV \\ C_{2\pi} &= \frac{1}{4} A_{2\pi} \\ B(r_{12}, r_{13}) &= 0\,. \end{aligned} \tag{2.3.2}$$

where f and f^* are the πNN and $\pi N\Delta$ coupling constants, and E_{av} is the mean energy denominator.

2.3.2 Repulsive Three-Nucleon Interaction.

Following [Ca-83], we introduce the short range repulsive three-nucleon interaction ($V^I_{3N\,R}$), as

$$V^I_{3N\,R} = U_0 \sum_{cycl.} T^2(r_{12})\, T^2(r_{13})\,. \tag{2.3.3}$$

where the strength U_0 is estimated to be 0.0048 MeV for the Urbana IX potential. This term is meant to simulate the dispersive effects which are required when integrating out Δ degrees of freedom. These contributions are repulsive, and are taken to be independent of spin and isospin in the Urbana representation.

2.4 Matrix Elements Calculation.

Matrix elements of the NN interaction can be specified either in particle-particle (pp) coupling or in particle-hole (ph) coupling. Both of these matrix elements completely specify the interaction, and either set can be calculated from the other set.

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We define *ph*-coupled matrix elements as

$$\begin{aligned}&\langle (1\bar{3})_\lambda \mid V(r) \mid (4\bar{2})_\lambda \rangle \\ &= \sum_{m_1 m_2 m_3 m_4} (-)^{j_3 - m_3} \langle j_1\, m_1\, j_3 - m_3 \mid \lambda\, \mu \rangle \\ &\qquad (-)^{j_2 - m_2} \langle j_4\, m_4\, j_2 - m_2 \mid \lambda\, \mu \rangle \langle 12 \mid V(r) \mid 34 \rangle . \end{aligned} \tag{2.4.1}$$

Correspondingly, the *pp*-coupled matrix elements are defined as

$$\begin{aligned}&\langle (12)_\lambda \mid V(r) \mid (34)_\lambda \rangle \\ &= \sum_{m_1 m_2 m_3 m_4} \langle j_1\, m_1\, j_2\, m_2 \mid \lambda\, \mu \rangle \langle j_3\, m_3\, j_4\, m_4 \mid \lambda\, \mu \rangle \langle 12 \mid V(r) \mid 34 \rangle , \end{aligned} \tag{2.4.2}$$

where the relative coordinate is given as $\vec{r} = \vec{r}_2 - \vec{r}_1$.

The matrix elements calculation is carried out using the *ph*-coupling: *pp*-coupled matrix elements are then evaluated from their *ph* counterpart. using the relationship

$$\langle (12)_L \mid V(r) \mid (34)_L \rangle = \sum_L (-)^{j_3 + j_4 + L} (2\lambda + 1) \begin{Bmatrix} j_1 & j_3 & \lambda \\ j_4 & j_2 & L \end{Bmatrix} \langle (1\bar{3})_\lambda \mid V(r) \mid (4\bar{2})_\lambda \rangle . \tag{2.4.3}$$

Conversely, we have

$$\langle (1\bar{3})_\lambda \mid V(r) \mid (4\bar{2})_\lambda \rangle = \sum_\lambda (-)^{j_3 + j_4 + L} (2L + 1) \begin{Bmatrix} j_1 & j_3 & \lambda \\ j_4 & j_2 & L \end{Bmatrix} \langle (12)_L \mid V(r) \mid (34)_L \rangle . \tag{2.4.4}$$

The foundation of the actual calculation is based on the following two lemmas.

Lemma 1 *[Ho-61] For the particular case when the potential is factorized into parts depending only on the $\vec{r}_1$ or $\vec{r}_2$ coordinates, respectively.*

$$V(r) = \left(U^{(k)}(1) \odot V^{(k)}(2) \right) , \tag{2.4.5}$$

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ph-coupled matrix elements of the N-N interaction are given by

$$\langle (1\bar{3})_\lambda \mid \left(U^{(k)}(1) \odot V^{(k)}(2) \right) \mid (4\bar{2})_\lambda \rangle \;=\; \frac{(-)^{j_2+j_4+1}}{2\lambda+1} \langle 1 \parallel U^{(\lambda)} \parallel 3 \rangle \langle 2 \parallel V^{(\lambda)} \parallel 4 \rangle \, \delta_{k\lambda} \,. \tag{2.4.6}$$

PROOF. According to the definition of the scalar product of two tensor operators of rank k, we have

$$\left(U^{(k)}(1) \odot V^{(k)}(2) \right) \;=\; \sum_q (-)^q \, U_q^{(k)}(1) V_{-q}^{(k)}(2) \,. \tag{2.4.7}$$

We can calculate the matrix elements of the $U_q^{(k)}(1)V_{-q}^{(k)}(2)$ operator in the m-representation, using the Wigner-Eckart theorem

$$\langle 12 \mid U_q^{(k)}(1) V_{-q}^{(k)}(2) \mid 34 \rangle \;=\; \langle 1 \mid U_q^{(k)}(1) \mid 3 \rangle \, \langle 2 \mid V_{-q}^{(k)}(2) \mid 4 \rangle \tag{2.4.8}$$

$$= (-)^{j_3-m_3} \frac{\langle j_1 \, m_1 \, j_3 \, - m_3 \mid k \, q \rangle}{\sqrt{2k+1}} \langle 1 \parallel U^{(k)} \parallel 3 \rangle$$

$$(-)^{j_4-m_4} \frac{\langle j_2 \, m_2 \, j_4 \, - m_4 \mid k \, -q \rangle}{\sqrt{2k+1}} \langle 2 \parallel V^{(k)} \parallel 4 \rangle \,, \tag{2.4.9}$$

Finally, using the orthonormality of the Clebsch-Gordon coefficients, together with the definition of *ph*-coupled matrix elements, Eq. (2.4.1), we obtain the desired result, Eq. (2.4.6).

Lemma 2 *[Da-95] Consider the case when the spatial part of the interaction has the form $V(r)\, C^{(k)}(\hat{r})$, with k some positive integer or zero. Then, we can separate the variables $\vec{r}_1$ and $\vec{r}_2$ as*

$$V(r) C^{(k)}(\hat{r})$$

$$= \sum_{k_1,k_2} i^{k_2-k_1-k} \frac{(2k_1+1)(2k_2+1)}{2k+1} \langle k_1 \, 0 \, k_2 \, 0 \mid k \, 0 \rangle \; u^{(k_1 k_2 ; k)}(r_1, r_2)$$

$$\left[C^{(k_1)}(\hat{r}_1) \odot C^{(k_2)}(\hat{r}_2) \right]^{(k)} \tag{2.4.10}$$

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where

$$u^{(k_1 k_2;k)}(r_1, r_2) \;=\; \frac{2}{\pi}\int_0^\infty \mathrm{d}p\; p^2\; \tilde{V}_k(p)\; j_{k_1}(pr_1)\; j_{k_2}(pr_2) \tag{2.4.11}$$

and

$$\tilde{V}_k(p) \;=\; \int_0^\infty \mathrm{d}r\; r^2\; V(r)\; j_k(pr)\,. \tag{2.4.12}$$

PROOF. Before detailing the actual proof, let us take a moment and introduce the *unnormalized* spherical harmonics by their definition in terms of the *normalized* spherical harmonics, as

$$C_q^{(k)}(\hat{r}) \;=\; \sqrt{\frac{4\pi}{2k+1}}\; Y_{kq}(\hat{r})\,. \tag{2.4.13}$$

The *unnormalized* spherical harmonics satisfy the normalization condition

$$\int d\Omega\; C_{q_1}^{(k_1)}(\hat{r}) C_{q_2}^{(k_2)}(\hat{r}) \;=\; \frac{4\pi}{2k_1+1}\;\delta_{k_1 k_2}\;\delta_{q_1 q_2}\,. \tag{2.4.14}$$

We list here some of their properties, which mirror the properties of the *normalized* spherical harmonics:

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

2. $r_m \;=\; r\, C_m^{(1)}(\hat{r})\,.$

3. $\left[C_q^{(k)}(\hat{r})\right]^* \;=\; (-)^q\, C_{-q}^{(k)}(\hat{r})\,.$

4. $\langle l' \,\|\, C^{(k)}(\hat{r}) \,\|\, l\rangle \;=\; \sqrt{2l+1}\,\langle l\,0\,k\,0 \mid l'\,0\rangle$, with $k+l+l'$ even.

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

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6. $\left[C^{(k_1)}(\hat{r}) \otimes C^{(k_2)}(\hat{r})\right]^{(k)} = \langle k_1\, 0\, k_2\, 0 \mid k\, 0\rangle\, C^{(k)}(\hat{r})$, with $k_1 + k_2 + k$ even.

7. $C^{(k_1)}_{q_1}(\hat{r}) C^{(k_2)}_{q_2}(\hat{r}) = \sum_{kq} \langle k_1\, 0\, k_2\, 0 \mid k\, 0\rangle\, \langle k_1\, q_1\, k_2\, q_2 \mid k\, q\rangle\, C^{(k)}_{q}(\hat{r})$, with $k_1 + k_2 + k$ even.

Going back now to our lemma, we first introduce the asymmetric Fourier transform of the operator $V(r)C^{(k)}(\hat{r})$

$$\tilde{v}^{(k)}(\vec{p}) = \frac{1}{(2\pi)^3} \int \mathrm{d}^3 r\; V(r)\; C^{(k)}(\hat{r})\; \exp(-i\vec{p}\cdot\vec{r}) \tag{2.4.15}$$

and, conversely,

$$V(r)C^{(k)}(\hat{r}) = \int \mathrm{d}^3 p\; \tilde{v}^{(k)}(\vec{p})\; \exp(i\vec{p}\cdot\vec{r})\,. \tag{2.4.16}$$

Using the expansion of a plane wave in spherical waves

$$\exp(i\vec{p}\cdot\vec{r}) = 4\pi \sum_l i^l\, j_l(pr)\, Y_{lm}(\hat{r})\, Y^*_{lm}(\hat{p}) \tag{2.4.17}$$

$$= 4\pi \sum_l i^l\, j_l(pr)\, (2l+1)\, P_l(\cos\omega) \tag{2.4.18}$$

$$= 4\pi \sum_l i^l\, (2l+1)\, j_l(pr)\, \left(C^{(l)}(\hat{r}) \cdot C^{(l)}(\hat{p})\right) \tag{2.4.19}$$

and the orthonormality of the *unnormalized* spherical harmonics in carrying out the angular part of the integral (2.4.15), $\tilde{v}^{(k)}(\vec{p})$ becomes

$$\tilde{v}^{(k)}(\vec{p}) = \frac{(-i)^k}{2\pi^2} C^{(k)}(\hat{p}) \tilde{V}_k(p)\,. \tag{2.4.20}$$

where

$$\tilde{V}_k(p) = \int_0^\infty \mathrm{d}r\; r^2 V(r)\, j_k(pr)\,. \tag{2.4.21}$$

We use Eq. (2.4.20) to calculate the operator $V(r)C^{(k)}(\hat{r})$ from its Fourier Transform. From Eq. (2.4.16), we have

$$V(r)C^{(k)}(\hat{r}) = \frac{(-i)^k}{2\pi^2} \int \mathrm{d}^3 p\; \tilde{V}_k(p)\; C^{(k)}(\hat{p})\; \exp(\vec{p}\cdot\vec{r})\,. \tag{2.4.22}$$

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The angular part of the last integral can be carried out explicitly using the definition $\vec{r} = \vec{r}_2 - \vec{r}_1$, and applying Eq. (2.4.19) twice for $\exp(i\vec{p}\cdot\vec{r}_2)$ and $\exp(-i\vec{p}\cdot\vec{r}_1)$, respectively. Then, we combine some of the above properties of the *unnormalized* spherical harmonics, in order to evaluate the angular integral

$$\int d\Omega_p \, C_{q_1}^{(k_1)}(\hat{p}) C_{q_2}^{(k_2)}(\hat{p}) C_q^{(k)}(\hat{p}) \;=\; (-)^{-q} \, \frac{(2k+1)}{4\pi} \, \langle k_1\, 0\, k_2\, 0 \mid k_3\, 0\rangle \, \langle k_1\, q_1\, k_2\, q_2 \mid k_3\, q_3\rangle \, . \tag{2.4.23}$$

To conclude our proof, we recover the definition of a spherical tensor of rank k:

$$\left[C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2)\right]_q^{(k)} = \sum_{q_1 q_2} \langle k_1\, q_1\, k_2\, q_2 \mid k\, q\rangle \, C_{q_1}^{(k_1)}(\hat{r}_1) \, C_{q_2}^{(k_2)}(\hat{r}_2) \, . \tag{2.4.24}$$

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Chapter 3

Coupled Cluster Method.

3.1 The Uncorrelated Ground State Wave Function.

We introduce the uncorrelated ground state, $|0\rangle$, as the "vacuum" or reference state of the many-body system. The vacuum must play [Bi-91] the basic role of a cyclic vector, with respect to which we can define two Abelian (i.e. mutually commuting) subalgebras of multiconfigurational creation operators $\{C_n^\dagger\}$ and their Hermitian-adjoint destruction operators $\{C_n\}$. Thus, the prime requirement is that arbitrary *ket* and *bra* states within the many-body Hilbert space may then be decomposed as the respective linear combinations:

$$|\Psi\rangle = \sum \psi_n \, C_n^\dagger \, |0\rangle ; \qquad \langle\tilde{\Psi}| = \sum \tilde{\psi}_n \, \langle 0| \, C_n \, . \tag{3.1.1}$$

Here, the set-index n labels a general multiparticle cluster configuration, which in itself is defined with respect to the vacuum. For a number-conserving Fermi system, the standard choice for $|0\rangle$ is the single-particle shell-model (Slater determinant) state formed from an antisymmetrized product of single-particle wave functions. The creation operators $\{C_n^\dagger\}$ then describe configurations formed with respect to this non-interacting, closed-shell state by the formation of multiple pairs of single fermions in (particle) orbits unoccupied in $|0\rangle$ and single vacancies in the corresponding (hole) orbits occupied in $|0\rangle$. In this sense, we shall refer to the multiconfigurational creation and destruction operators, simply as *ph* creation and destruction operators.

We assume such an orthonormal set of single particle wave functions exists. These wave

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functions are solutions to the single particle Hamiltonian given by the Schrödinger equation in the mean field. Then, the uncorrelated ground state is constructed as the single Slater determinant which includes all the occupied orbits. In second quantisation language [Sh-74], this translates into

$$\mathbf{a}_h^\dagger \, |0\rangle \; = \; 0 \, ; \qquad \mathbf{a}_p \, |0\rangle \; = \; 0 \, . \tag{3.1.2}$$

3.2 The Correlated Ground State Wave Function.

The model nuclear wave function $\Phi_0^{(M)} = |\tilde{0}\rangle$ is written in terms of the vacuum state $|0\rangle$ as

$$|\tilde{0}\rangle = e^{\mathbf{S}^\dagger} |0\rangle \, . \tag{3.2.1}$$

Here, $\mathbf{S}^\dagger$ is the cluster correlation operator, which is decomposed in terms of *ph*-creation operators discussed in the previous section ($\mathbf{C}_0^\dagger = \hat{1}$, $\mathbf{C}_1^\dagger = \mathbf{a}_{p_1}^\dagger \mathbf{a}_{h_1}$, $\mathbf{C}_2^\dagger = \mathbf{a}_{p_1}^\dagger \mathbf{a}_{p_2}^\dagger \mathbf{a}_{h_2} \mathbf{a}_{h_1}$, ...), as:

$$\mathbf{S}^\dagger \; = \; \sum_{n=1}^{\infty} \, \frac{1}{n!} \, S_n \, \mathbf{C}_n^\dagger \, . \tag{3.2.2}$$

We shall use a variational approach in order to determine the coefficients S_n.

A variation $\delta|\tilde{0}\rangle$ orthogonal to the correlated ground state can be constructed from any operator $\mathbf{C}_n^\dagger$ as

$$\delta \, |\tilde{0}\rangle \; = \; e^{-\mathbf{S}} \, \mathbf{C}_n^\dagger \, e^{-\mathbf{S}^\dagger} \, |\tilde{0}\rangle \; = \; e^{-\mathbf{S}} \, \mathbf{C}_n^\dagger \, |0\rangle \, . \tag{3.2.3}$$

We have

$$\langle\tilde{0}| \, \delta \, |\tilde{0}\rangle \; = \; \langle 0| \, \mathbf{C}_n^\dagger \, |0\rangle \; = \; 0 \, . \tag{3.2.4}$$

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The variational principle requires that the Hamiltonian between the ground state and such a variation vanishes. Thus, we have

$$\langle\tilde{0}|\,\mathbf{H}\,\delta\,|\tilde{0}\rangle \;=\; \langle 0|\,e^{\mathbf{S}}\,\mathbf{H}\,e^{-\mathbf{S}}\,\mathbf{C}_n^{\dagger}\,|0\rangle \;=\; 0\,. \tag{3.2.5}$$

We are thus led respectively to an equation for the ground state energy eigenvalue E in terms of the cluster correlation coefficients $\{S_n\}$, and a set of formally exact, microscopic, coupled nonlinear equations for these coefficients in which there appear no macroscopic terms like the energy E. These latter equations are all of linked-cluster type, due to the nested commutator expansion (Baker-Hausdorff identity):

$$e^{\mathbf{S}}\,\mathbf{H}\,e^{-\mathbf{S}} \;=\; \mathbf{H} \;+\; [\mathbf{S},\,\mathbf{H}] \;+\; \frac{1}{2!}\,[\mathbf{S},\,[\mathbf{S},\,\mathbf{H}]] \;+\; \cdots\,. \tag{3.2.6}$$

and the fact that all of the individual components of $\mathbf{S}$ commute with each other, so that each element of $\mathbf{S}$ in Eq. (3.2.2) is linked directly to the Hamiltonian. Furthermore, the otherwise infinite series of Eq. (3.2.6) also always terminates in this case after a finite number of terms, since each term in the second-quantized form of the Hamiltonian contains a finite number of destruction operators. Each commutator removes one $\mathbf{a}^{\dagger}$ or a $\mathbf{a}$ from $\mathbf{H}$, since all $\mathbf{a}$ operators occurring in $\mathbf{S}$ commute with each other. We might say that $e^{\mathbf{S}}\,\mathbf{H}\,e^{-\mathbf{S}}$ represents the effective Hamiltonian as Eq. (3.2.5) represents the Hartree-Fock condition for the uncorrelated ground state with this effective Hamiltonian.

For the sake of the argument let us show that the system of equations (3.2.5) is equivalent with the previous CCM equations in the literature [Ku-78, Bi-91]. We start with the exact ground state Schrödinger equation

$$\mathbf{H}\,|\tilde{0}\rangle \;=\; E\,|\tilde{0}\rangle\,. \tag{3.2.7}$$

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which we rewrite in the similarity-transformed form

$$e^{-\mathbf{S}^\dagger}\,\mathbf{H}\,e^{\mathbf{S}^\dagger}\,|0\rangle \;=\; E\,|0\rangle\,. \tag{3.2.8}$$

By taking the inner products of Eq. (3.2.8) with $|0\rangle$ and the complete set of states $\{\mathbf{C}_n^\dagger\,|0\rangle;\; n \neq 0\}$, and recalling that the many-body Hamiltonian is a hermitian operator, $\mathbf{H} = \mathbf{H}^\dagger$, we get what appears to be the Hermitian correspondent of Eq. (3.2.5). Since all quantities here are real, we obtain the desired equivalence:

$$\langle 0|\,\mathbf{C}_n\,e^{-\mathbf{S}^\dagger}\,\mathbf{H}\,e^{\mathbf{S}^\dagger}\,|0\rangle \;=\; \langle 0|\,e^{\mathbf{S}}\,\mathbf{H}\,e^{-\mathbf{S}}\,\mathbf{C}_n^\dagger\,|0\rangle \;=\; 0\,. \tag{3.2.9}$$

3.2.1 The Effective One-Body Hamiltonian.

To simplify the accounting of number of *ph*-excitations we use indices for the two-body Hamiltonian. Corrections due to the three-body part of the Hamiltonian will be discussed in the last section of this chapter. Explicitly we define

$$\begin{aligned}
\mathbf{V}_{20} &= \frac{1}{4}V_{p_1p_2h_1h_2}\mathbf{a}^\dagger_{p_1}\mathbf{a}^\dagger_{p_2}\mathbf{a}_{h_2}\mathbf{a}_{h_1} \;=\; \mathbf{V}^\dagger_{02}\,.\\
\mathbf{V}_{10} &= \frac{1}{2}V_{p_1p_2h_1p_3}\mathbf{a}^\dagger_{p_1}\mathbf{a}^\dagger_{p_2}\mathbf{a}_{p_3}\mathbf{a}_{h_1} \;+\; \frac{1}{2}V_{p_1h_2h_1h_3}\mathbf{a}^\dagger_{p_1}\mathbf{a}^\dagger_{h_2}\mathbf{a}_{h_3}\mathbf{a}_{h_1} \;=\; \mathbf{V}^\dagger_{01}\,.\\
\mathbf{V}_{00} &= V_{p_1h_2h_1p_2}\mathbf{a}^\dagger_{p_1}\mathbf{a}^\dagger_{h_2}\mathbf{a}_{p_2}\mathbf{a}_{h_1}\\
&\quad + \frac{1}{4}V_{p_1p_2p_3p_4}\mathbf{a}^\dagger_{p_1}\mathbf{a}^\dagger_{p_2}\mathbf{a}_{p_4}\mathbf{a}_{p_3} \;+\; \frac{1}{4}V_{h_1h_2h_3h_4}\mathbf{a}^\dagger_{h_1}\mathbf{a}^\dagger_{h_2}\mathbf{a}_{h_4}\mathbf{a}_{h_3}\,.\\
\mathbf{T}_0 &= T_{k_1k_2}\mathbf{a}^\dagger_{k_1}\mathbf{a}_{k_2}\,,\\
\mathbf{H}_0 &= \mathbf{T}_0 + \mathbf{U}_0\,.
\end{aligned} \tag{3.2.10}$$

Here $\mathbf{T}_0$ is the kinetic energy operator. The mean field $\mathbf{U}_0$ will be specified below. We will assume that the orbits are eigenfunctions of this mean field Hamiltonian $\mathbf{H}_0$ with

$$\left[\mathbf{H}_0,\,\mathbf{a}^\dagger_p\right] \;=\; \epsilon_p\mathbf{a}^\dagger_p\,, \qquad [\mathbf{H}_0,\,\mathbf{a}_h] \;=\; -\,\epsilon_h\mathbf{a}_h\,. \tag{3.2.11}$$

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Note here that the mean-field $\mathbf{U}_0$ is not unique and special assumptions can be made in order to optimize the calculation.

We use Eq. (3.2.5) with $n = 1$, $\mathbf{C}_1^\dagger = \mathbf{a}_p^\dagger \mathbf{a}_h$, where we write $\mathbf{a}_p^\dagger \mathbf{a}_h \, |0\rangle = |1p1h\rangle$ to obtain the equation establishing $\mathbf{S}_1$

$$\begin{aligned} 0 \;=\; & \langle 0| \Big\{ \mathbf{T}_0 + \mathbf{V}_{01} + [\mathbf{S}_1, \mathbf{T}_0] + [\mathbf{S}_1, \mathbf{V}_{00}] + [\mathbf{S}_2, \mathbf{V}_{10}] + [\mathbf{S}_3, \mathbf{V}_{20}] \\ & + \frac{1}{2}\Big[\mathbf{S}_1, [\mathbf{S}_1, \mathbf{V}_{10}]\Big] + \Big[\mathbf{S}_1, [\mathbf{S}_2, \mathbf{V}_{20}]\Big] + \frac{1}{6}\Big[\mathbf{S}_1, \Big[\mathbf{S}_1, [\mathbf{S}_1, \mathbf{V}_{20}]\Big]\Big] \Big\} |1p1h\rangle \,. \end{aligned} \tag{3.2.12}$$

There are similar equations that determine $\mathbf{S}_2$, $\mathbf{S}_3$, ... While these equations hold in any basis, there is one basis of particular convenience. This is the *maximum overlap basis* in which $\mathbf{S}_1$ vanishes. Equation (3.2.12) results in the solution $\mathbf{S}_1 = 0$ if the terms that do not contain $\mathbf{S}_1$ vanish. The mean field basis is determined by the condition of the vanishing of $\mathbf{S}_1$ and in the mean field basis we must have

$$0 \;=\; \langle 0| \Big\{ (\mathbf{H}_0 - \mathbf{U}_0) + \mathbf{V}_{01} + [\mathbf{S}_2, \mathbf{V}_{10}] + [\mathbf{S}_3, \mathbf{V}_{20}] \Big\} |1p1h\rangle \,. \tag{3.2.13}$$

Using Eq. (3.2.11), we can show that the expectation value $\langle 0|\mathbf{H}_0|1p1h\rangle$ vanishes. Therefore, Eq. (3.2.13) becomes

$$\langle 0|\mathbf{U}_0|1p1h\rangle \;=\; \langle 0| \Big\{ \mathbf{V}_{01} + [\mathbf{S}_2, \mathbf{V}_{10}] + [\mathbf{S}_3, \mathbf{V}_{20}] \Big\} |1p1h\rangle \,. \tag{3.2.14}$$

Thus those terms establish the elements in the one-body Hamiltonian matrix that connect p and h orbits. The equations establishing the higher order correlations in the mean

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field basis are

$$0 = \langle 0|\Big\{ V_{02} + [S_2, V_{00}] + [S_2, H_0] - [S_2, U_0] + [S_3, V_{10}] + [S_4, V_{20}] + \frac{1}{2}\big[S_2, [S_2, V_{20}]\big] \Big\} |2p2h\rangle , \tag{3.2.15}$$

$$0 = \langle 0|\Big\{ [S_2, V_{01}] + [S_3, V_{00}] + [S_3, H_0] - [S_3, U_0] + [S_4, V_{10}] + [S_5, V_{20}] + \frac{1}{2}\big[S_2, [S_2, V_{10}]\big] + \big[S_3, [S_2, V_{20}]\big] \Big\} |3p3h\rangle . \tag{3.2.16}$$

$$0 = \langle 0|\Big\{ [S_3, V_{01}] + [S_4, V_{00}] + [S_4, H_0] + [S_4, U_0] + [S_5, V_{10}] + [S_6, V_{20}] + \frac{1}{2}\big[S_2, [S_2, V_{00}]\big] + \big[S_3, [S_2, V_{10}]\big] + \big[S_4, [S_2, V_{20}]\big] + \frac{1}{2}\big[S_3, [S_3, V_{20}]\big] + \frac{1}{6}\Big[S_2, \big[S_2, [S_2, V_{20}]\big]\Big] \Big\} |4p4h\rangle . \tag{3.2.17}$$

At this point we will assume that the orbits are eigenfunctions to the single particle Hamiltonian H_0. This allows us to solve these equations as

$$\langle 0|S_2|2p2h\rangle = -\langle 0|\Big\{ V_{02} + [S_2, V_{00}] - [S_2, U_0] + [S_3, V_{10}] + [S_4, V_{20}] + \frac{1}{2}\big[S_2, [S_2, V_{20}]\big] \Big\} \frac{1}{H_0} |2p2h\rangle , \tag{3.2.18}$$

$$\langle 0|S_3|3p3h\rangle = -\langle 0|\Big\{ [S_2, V_{01}] + [S_3, V_{00}] - [S_3, U_0] + [S_4, V_{10}] + [S_5, V_{20}] + \frac{1}{2}\big[S_2, [S_2, V_{10}]\big] + \big[S_3, [S_2, V_{20}]\big] \Big\} \frac{1}{H_0} |3p3h\rangle . \tag{3.2.19}$$

A similar equation allows us to isolate S_4 using Eq. (3.2.17).

We estimate that in our basis there are about 5×10^5 $2p2h$ configurations and about 8×10^9 $3p3h$ configurations. While the number of $2p2h$ configurations is quite accessible, the number of $3p3h$ configurations is prohibitively large, and we cannot store all these numbers. Thus we have to implicitly correct for the presence of these correlations. We do this by inserting the solutions for S_n with $n \geq 3$ back into the equations and thereby obtaining a

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perturbation expansion in $1/E_{ph}$. We write this equation out up to second order for the Eq. (3.2.14) establishing the mean field

$$\begin{aligned}\langle 0|\mathbf{U}_0|1p1h\rangle &= \langle 0|\mathbf{V}_{01}|1p1h\rangle + \langle 0|\left[\mathbf{S}_2, \mathbf{V}_{10}\right]|1p1h\rangle \\ &-\langle 0|\left[\left[\mathbf{S}_2, \mathbf{V}_{01}\right], \frac{1}{\mathbf{H}_0}\mathbf{V}_{20}\right]|1p1h\rangle - \frac{1}{2}\langle 0|\left[\left[\mathbf{S}_2, \left[\mathbf{S}_2, \mathbf{V}_{10}\right]\right], \frac{1}{\mathbf{H}_0}\mathbf{V}_{20}\right]|1p1h\rangle \\ &+\langle 0|\left[\left[\left[\mathbf{S}_2, \mathbf{V}_{01}\right], \frac{1}{\mathbf{H}_0}\mathbf{V}_{00}\right], \frac{1}{\mathbf{H}_0}\mathbf{V}_{20}\right]|1p1h\rangle . \qquad (3.2.20)\end{aligned}$$

This equation establishes the matrix elements of the single particle Hamiltonian $\mathbf{H}_0$ between particle and hole orbits. The matrix elements between hole and hole orbits or between particle and particle orbits are not defined, and any definition may be chosen. As long as $\mathbf{U}_0$ is explicitly kept on the right hand side of Eq. (3.2.18) the explicit choice is merely a question of how fast the resulting series will converge. However, a reasonable choice appears to be that form that we obtain if we replace in the matrix elements obtained in (3.2.20) the hole orbit with a particle orbit in order to get the matrix elements between particle and particle orbits and we change the particle orbit into a hole orbit in order to get the matrix elements between hole and hole orbits. Reference [He-98b] gives a detailed account of the contributions included in our mean field as given by Eq. (3.2.20). Our choice for the other matrix elements corresponds simply in turning the hole line into a particle line or vice versa.

The mean field orbits are the eigenvectors of this matrix, and the eigenvalues are the single particle energies. This procedure now fully defines the mean field used here even though it's definition is not unique.

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3.3 The Internal Hamiltonian.

The Hamiltonian is given in the center of mass as

$$H_{int} = \sum_{i}^{A} \frac{1}{2m} \vec{p}_i^{\,2} + \sum_{i<j}^{A} V(\vec{r}_i - \vec{r}_j) - T_{CM} . \tag{3.3.1}$$

where $T_{CM} \equiv \vec{P}^2/2M$ is the kinetic energy operator of the center of mass (CM), and M is the total mass. This represents the energy in the center of mass frame. The internal Hamiltonian can be rewritten as

$$H_{int} = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{1}{2m} p_i^2 + \sum_{i<j=1}^{A} \left[V(\vec{r}_i - \vec{r}_j) - \frac{\vec{p}_i \cdot \vec{p}_j}{M} \right] . \tag{3.3.2}$$

The $\mathbf{p}_i \cdot \vec{\mathbf{p}}_j/M$ term will be treated as part of the two-body internal potential

$$V_{int}(\vec{r}_i - \vec{r}_j) = V(\vec{r}_i - \vec{r}_j) - \frac{\vec{p}_i \cdot \vec{p}_j}{M} . \tag{3.3.3}$$

Since everywhere in our equations, the Hamiltonian **H** and the potential **V** will be replaced by their *internal* counterparts, we shall drop, from now on, the *int* subscripts.

3.4 Observables.

Ground state expectation values can be evaluated by introducing the operator $\tilde{\mathbf{S}}^\dagger$ as in the normal coupled cluster method as presented in [Bi-91]. The normalized expectation value $\bar{a}$ of any operator **A** can be worked out as

$$\bar{a} = \frac{\langle 0|\, e^{\mathbf{S}}\, \mathbf{A}\, e^{\mathbf{S}^\dagger}\, |0\rangle}{\langle \tilde{0} \,|\, 0\rangle} = \frac{\langle 0|\, e^{\mathbf{S}}\, \mathbf{A}\, e^{-\mathbf{S}}\, e^{\mathbf{S}}\, e^{\mathbf{S}^\dagger}\, |0\rangle}{\langle \tilde{0} \,|\, 0\rangle} . \tag{3.4.1}$$

By inserting the unity operator in the $\{\mathbf{C}_n^\dagger\, |0\rangle\}$ basis, we obtain

$$\bar{a} = \langle 0|\, e^{\mathbf{S}}\, \mathbf{A}\, e^{-\mathbf{S}}\, |0\rangle + \sum_{n} \langle 0|\, e^{\mathbf{S}}\, \mathbf{A}\, e^{-\mathbf{S}}\, \mathbf{C}_n^\dagger\, |0\rangle \frac{\langle 0|\, e^{\mathbf{S}}\, \mathbf{C}_n\, e^{\mathbf{S}^\dagger}\, |0\rangle}{\langle \tilde{0} \,|\, 0\rangle} . \tag{3.4.2}$$

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The expectation value on the right is by definition $\bar{c}_n$, the expectation value of $\mathbf{C}_n$. Thus we can define the new operator

$$\tilde{\mathbf{S}}^\dagger = \sum_{n=1}^{\infty} \bar{c}_n \, \mathbf{C}_n^\dagger \, . \tag{3.4.3}$$

With this, the expectation value for any operator can be expressed as

$$\bar{a} = \langle 0 | \, e^{\mathbf{S}} \, \mathbf{A} \, e^{-\mathbf{S}} \left(1 + \tilde{\mathbf{S}}^\dagger \right) | 0 \rangle \, . \tag{3.4.4}$$

Using the Baker-Hausdorff identity

$$e^{\mathbf{S}} \, \mathbf{A} \, e^{-\mathbf{S}} = \mathbf{A} + [\mathbf{S}, \mathbf{A}] + \frac{1}{2!} [\mathbf{S}, [\mathbf{S}, \mathbf{A}]] + \cdots \tag{3.4.5}$$

we obtain for the expectation value an arbitrary operator $\mathbf{A}$

$$\bar{a} = \langle 0 \, | \, \mathbf{A} \, \tilde{\mathbf{S}}^\dagger \, | \, 0 \rangle + \langle 0 \, | \, [\mathbf{S}, \mathbf{A}] \, \tilde{\mathbf{S}}^\dagger \, | \, 0 \rangle + \cdots \, . \tag{3.4.6}$$

The operators $\tilde{\mathbf{S}}^\dagger$ can be obtained by solving Eq. (3.4.3) in an iterative fashion. Explicitly we write $\tilde{\mathbf{S}}^\dagger$ in the same form as Eq. (3.2.2), with $\tilde{\mathbf{S}}^\dagger$ defined by its decomposition in terms of *ph*-creation operators:

$$\tilde{\mathbf{S}}^\dagger = \sum_{n=1}^{\infty} \frac{1}{n!} \, \tilde{S}_n \, \mathbf{C}_n^\dagger \, . \tag{3.4.7}$$

Finally, in order to make connection with reference [Bi-91], let us mention that the previous procedure is equivalent to parametrizing the *bra* ground state wave function $\langle \tilde{0} |$ as

$$\langle \tilde{0} | \; = \langle 0 | \, \tilde{\mathbf{S}} \, e^{-\mathbf{S}^\dagger} \, . \tag{3.4.8}$$

The *bra* ground state wave function $\langle \tilde{0} |$ is the counterpart to the *ket* correlated ground state $| \tilde{0} \rangle$ given by Eq. (3.2.1).

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3.4.1 Ground State Binding Energy.

We first apply this procedure to the ground state binding energy. The expectation value of the Hamiltonian can be written as

$$\langle E \rangle = \langle 0 | e^{\mathbf{S}} \mathbf{H} e^{-\mathbf{S}} \left(1 + \tilde{\mathbf{S}}^{\dagger}\right) | 0 \rangle \tag{3.4.9}$$

Because of the Hartree-Fock condition expressed in Eq. (3.2.5) the terms involving $\tilde{\mathbf{S}}^{\dagger}$ vanish and we get

$$\langle E \rangle = \langle 0 | e^{\mathbf{S}} \mathbf{H} e^{-\mathbf{S}} | 0 \rangle . \tag{3.4.10}$$

Assuming that $\mathbf{H}$ is at most a two-body operator and taking into account that $\mathbf{S}_1$ vanishes, the last equation becomes

$$\langle E \rangle = \langle 0 | \mathbf{H} | 0 \rangle + \langle 0 | \mathbf{S}_2 \mathbf{V}_{20} | 0 \rangle . \tag{3.4.11}$$

This expression needs to be modified if three-nucleon interactions are present. Also, this expression does not give an upper limit of the ground state energy unless we are exactly at the minimum. In terms of matrix elements the energy can be written as

$$\langle E \rangle = \sum_{h_1 h_2} T_{h_1,h_2} + \frac{1}{2} \sum_{h_1 h_2} V_{h_1 h_2, h_1 h_2} + \frac{1}{4} \sum_{p_1 p_2 h_1 h_2} Z_{p_1 p_2, h_1 h_2} V_{p_1 p_2, h_1 h_2} \tag{3.4.12}$$

3.4.2 Ground State One-Body Density.

By definition, the ground state one-body density is introduced as

$$\rho(\vec{r}) = \sum_{k=1}^{A} \langle \tilde{0} | \delta(\vec{r} - \vec{r}_k) | \tilde{0} \rangle \tag{3.4.13}$$

Since we are dealing with a spherically symmetric nucleus, we shall integrate out the angular degrees of freedom of the system. Then, we write the one-body density operator for a doubly

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magic nucleus, in second quantisation, as

$$\rho^{op}(r) = \sum_{\alpha\beta} \rho_{\alpha\beta}(r)\, \mathbf{a}^{\dagger}_{\alpha}\, \mathbf{a}_{\beta}\,. \tag{3.4.14}$$

Here we use $\rho_{\alpha\beta}(r) = R_{\alpha}(r)\, R_{\beta}(r)$ to denote the radial part of the expectation value $\langle\alpha|\, \delta(\vec{r}-\vec{r}')\, |\beta\rangle$. Thus, we have

$$\rho(r) = \sum_{\alpha\beta} d_{\alpha\beta}\; R_{\alpha}(r)\; R_{\beta}(r)\,, \tag{3.4.15}$$

where the one-body density matrix is obtained using Eq. (3.4.4), as

$$\begin{aligned} d_{\alpha\beta} &= \langle\tilde{0}|\, \mathbf{a}^{\dagger}_{\alpha}\, \mathbf{a}_{\beta}\, |\tilde{0}\rangle \\ &= \langle 0|\, \mathbf{a}^{\dagger}_{\alpha}\mathbf{a}_{\beta}\, |0\rangle + \langle 0|\, \left[\mathbf{S}_2,\, \mathbf{a}^{\dagger}_{\alpha}\mathbf{a}_{\beta}\right]\, \tilde{\mathbf{S}}^{\dagger}_2\, |0\rangle \\ &\quad + \langle 0|\, \mathbf{a}^{\dagger}_{\alpha}\mathbf{a}_{\beta}\, \tilde{\mathbf{S}}^{\dagger}_1\, |0\rangle + \langle 0|\, \left[\mathbf{S}_2,\, \mathbf{a}^{\dagger}_{\alpha}\mathbf{a}_{\beta}\right]\, \tilde{\mathbf{S}}^{\dagger}_1\, |0\rangle \\ &\quad + \langle 0|\, \left[\mathbf{S}_3,\, \mathbf{a}^{\dagger}_{\alpha}\mathbf{a}_{\beta}\right]\, \tilde{\mathbf{S}}^{\dagger}_2\, |0\rangle + \langle 0|\, \left[\mathbf{S}_3,\, \mathbf{a}^{\dagger}_{\alpha}\mathbf{a}_{\beta}\right]\, \tilde{\mathbf{S}}^{\dagger}_3\, |0\rangle \\ &\quad + \frac{1}{2}\, \langle 0|\, \left[\mathbf{S}_2,\, \left[\mathbf{S}_2,\, \mathbf{a}^{\dagger}_{\alpha}\mathbf{a}_{\beta}\right]\right]\, \tilde{\mathbf{S}}^{\dagger}_3\, |0\rangle + \cdots\,. \end{aligned} \tag{3.4.16}$$

The density matrix is a real symmetric matrix with positive definite eigenvalues. We can make a basis transformation such that the density matrix becomes diagonal. This basis represents the "natural" orbits. In this basis the density becomes

$$\rho(r) = \sum_{a} v^{nat}_{a}\; \left[R^{nat}_{a}(r)\right]^2\,. \tag{3.4.17}$$

Here v^{nat}_{a} represents the occupation probability of these natural orbits. This is the only basis in which occupation probabilities have a meaning.

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3.4.3 Ground State Two-Body Density.

We start with the ground state two-body density definition

$$\rho(\vec{r}_1,\vec{r}_2) \;=\; \sum_{mn} \langle\tilde{0}\,|\,\delta(\vec{r}_1-\vec{r}_m)\;\delta(\vec{r}_2-\vec{r}_n)\,|\,\tilde{0}\rangle\,. \tag{3.4.18}$$

In the second quantization representation the two-body density operator can be written as

$$\rho^{op}(\vec{r}_1,\vec{r}_2) \;=\; \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta\,|\,\rho(\vec{r}_1,\vec{r}_2)\,|\,\gamma\delta\rangle\;\mathbf{a}^\dagger_\alpha\;\mathbf{a}^\dagger_\beta\;\mathbf{a}_\delta\;\mathbf{a}_\gamma \tag{3.4.19}$$

Using the completeness relationship of the spherical harmonics

$$\delta(\phi-\phi')\;\delta\left(\cos(\theta)-\cos(\theta')\right) \;=\; \sum_{lm} Y^*_{lm}(\hat{r})\;Y_{lm}(\hat{r}') \tag{3.4.20}$$

we can evaluate the matrix element

$$\begin{aligned}\langle\alpha\beta\,|\,\rho(\vec{r}_1,\vec{r}_2)\,|\,\gamma\delta\rangle \;=\; &\sum_{l_1m_1} R_\alpha(r_1)\;R_\gamma(r_1)\;Y^*_{l_1m_1}(\hat{r}_1)\;\langle j_\alpha m_\alpha\,|\,Y_{l_1m_1}\,|\,j_\gamma m_\gamma\rangle \\ &\sum_{l_2m_2} R_\beta(r_2)\;R_\delta(r_2)\;Y_{l_2m_2}(\hat{r}_2)\;\langle j_\beta m_\beta\,|\,Y^*_{l_2m_2}\,|\,j_\delta m_\delta\rangle\,.\end{aligned} \tag{3.4.21}$$

In order to be consistent with the phase convention of the two-body potential matrix elements, we couple the two-body density matrix elements using the ph angular momentum coupling conventions. Using lemma 1, the angular momentum coupled density is

$$\langle(\alpha\bar{\gamma})_\lambda\,|\,\rho^{\lambda\mu}(\vec{r}_1,\vec{r}_2)\,|\,(\delta\bar{\beta})_\lambda\rangle \;=\; \rho^\lambda_{\alpha\gamma}(r_1)\;\rho^\lambda_{\delta\beta}(r_2)\;\frac{1}{2\lambda+1}\;Y^*_{\lambda\mu}(\hat{r}_1)\;Y_{\lambda\mu}(\hat{r}_2)\,. \tag{3.4.22}$$

Here we have introduced the one-body multipole density $\rho^\lambda_{\alpha\beta}(r)$ which is

$$\begin{aligned}&= (-)^{j_\alpha+1/2}\;R_\alpha(r)\;R_\beta(r)\;\langle j_\alpha\,\|\,Y_{\lambda\mu}\,\|\,j_\beta\rangle \\ &= (-)^{\lambda+1}\sqrt{\frac{(2j_\alpha+1)\,(2j_\beta+1)}{4\pi}}\;\langle j_\alpha 1/2\; j_\beta-1/2\;|\;\lambda 0\rangle\;R_\alpha(r)\;R_\beta(r)\end{aligned} \tag{3.4.23}$$

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if $\ell_\alpha + \ell_\beta + \lambda$ is even, and zero otherwise.

For a spherically symmetric (spin=0) nucleus it is more relevant to calculate $\rho(r_1, r_2, \theta_{12})$ as due to the spherical symmetry the two-body density is dependent on the direction of $\vec{r}_1$ alone. Thus, we can perform an average over the directions of $\vec{r}_2$. This translates into carrying out the sum over the μ component of the angular momentum λ. We obtain the result

$$\rho^{\lambda}_{\alpha\beta\gamma\delta}(r_1, r_2, \theta_{12}) \;=\; \rho^{\lambda}_{\alpha\gamma}(r_1)\; \rho^{\lambda}_{\delta\beta}(r_2)\; P_\lambda(cos\theta_{12}) \tag{3.4.24}$$

Finally, in order to complete the ground state two-body density calculation, we apply again Eq. (3.4.4) to evaluate the two-body density matrix, $\langle\tilde{0}|\, a^\dagger_\alpha\, a^\dagger_\beta\, a_\delta\, a_\gamma\, |\tilde{0}\rangle$. With this, we get the ground state two-body density as

$$\begin{aligned}
\rho(r_1, r_2, \theta_{12}) \;&=\; \langle\tilde{0}|\, \rho_2^{op}\, |\tilde{0}\rangle \\
&=\; \langle 0\,|\,\rho_2^{op}\,|\,0\rangle \;+\; \langle 0\,|\,\rho_2^{op}\tilde{S}_2^\dagger\,|\,0\rangle \;+\; \langle 0\,|\,S_2\rho_2^{op}\,|\,0\rangle \\
&\quad +\, \langle 0\,|\,[S_2,\, \rho_2^{op}]\;\tilde{S}_2^\dagger\,|\,0\rangle \;+\; \langle 0\,|\,\rho_2^{op}\tilde{S}_1^\dagger\,|\,0\rangle \\
&\quad +\, \frac{1}{2}\,\langle 0\,|\,[S_2,\,[S_2,\,\rho_2^{op}]]\,\tilde{S}_2^\dagger\,|\,0\rangle + \cdots .
\end{aligned} \tag{3.4.25}$$

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3.5 Three-Nucleon Interaction Contributions

In this section we will review the corrections necessary to take into account the three-nucleon interaction as part of the general nuclear interaction. As discussed before we consider the three-nucleon interaction as the sum of two components: a long-range two-pion exchange and a short-range phenomenological component.

Given the form (2.1.1) of the Hamiltonian, we write the operator V_{3N} in second quantization as

$$\mathbf{V}_{3N} = \sum_{a_1 b_1 c_1 a_2 b_2 c_2} V_{a_1 b_1 c_1, a_2 b_2 c_2} \mathbf{a}^\dagger_{a_1} \mathbf{a}^\dagger_{b_1} \mathbf{a}^\dagger_{c_1} \mathbf{a}_{c_2} \mathbf{a}_{b_2} \mathbf{a}_{a_2} . \tag{3.5.1}$$

Here, the matrix elements are given as integrals involving the single particle states (including spins)

$$V_{a_1 b_1 c_1, a_2 b_2 c_2} = \langle \phi_{a_1}(1) \phi_{b_1}(2) \phi_{c_1}(3) \mid V_{3N} \mid \phi_{a_2}(1) \phi_{b_2}(2) \phi_{c_2}(3) \rangle . \tag{3.5.2}$$

In addition to being symmetric with respect to the interchange of the particles labelled 2 and 3

$$V_{a_1 b_1 c_1, a_2 b_2 c_2} = V_{a_1 c_1 b_1, a_2 c_2 b_2} . \tag{3.5.3}$$

the integrals (3.5.2) also satisfy the symmetry

$$V_{a_1 b_1 c_1, a_2 b_2 c_2} = V_{c_1 a_1 b_1, c_2 a_2 b_2} . \tag{3.5.4}$$

The last property is a consequence of the cyclic sums involved in the definition of the interaction, which make the interaction invariant with respect to the labelling of the particles.

In previous applications the approximation has been made that such an interaction can be represented by a density dependent two-body interaction. While such a substitution is

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the easiest modification, it has been stated that this is insufficient [Ca-83]. However, the rigorous inclusion of the three-nucleon interaction in configuration space using the coupled-cluster method is seriously hampered by our present computing capabilities and the necessary size of the configuration space. Ideally, we would like to calculate all integrals of the form (3.5.2) without any artificial restrictions. In practice though, we must limit ourselves to calculating matrix elements of the form

$$V_{\alpha a_1 b_1, \beta a_2 b_2} \quad \text{and} \quad V_{\alpha a_1 b_1, a_2 \beta b_2} \quad . \tag{3.5.5}$$

where α and β cannot both denote *particle* orbits for arbitrary $a_1 b_1, a_2, b_2$. We are then faced with a compromise: Since matrix elements of the form (3.5.5) are all we need in order to calculate exactly the first- and second-order (S_2) contributions to the mean-field and binding energy, the leading orders in our expansion are treated rigorously correct. Then we make a reduction of the three-nucleon interaction to an effective two-body interaction, and use this effective interaction when dealing with higher-order corrections (S_n, $n \geq 3$). This is achieved by defining the effective two-body interaction as

$$\mathbf{V}_{3N,den} = \frac{1}{4} \sum_{a_1 b_1 a_2 b_2} V^{3N,den}_{a_1 b_1, a_2 b_2} \, \mathbf{a}^\dagger_{a_1} \mathbf{a}^\dagger_{b_1} \mathbf{a}_{b_2} \mathbf{a}_{a_2} \, . \tag{3.5.6}$$

where we define the matrix element $V^{3N,den}_{a_1 b_1, a_2 b_2}$ to be equal to

$$\begin{aligned} &\langle 0 \,|\, \mathbf{V}^{tni} \mathbf{a}^\dagger_{a_1} \mathbf{a}^\dagger_{a_2} \mathbf{a}_{b_2} \mathbf{a}_{b_1} \,|\, 0 \rangle \\ &\quad = \sum_h \Big\{ V_{h a_1 a_2, h b_1 b_2} - V_{h a_1 a_2, h b_2 b_1} \Big\} \\ &\quad + \sum_h \Big\{ - V_{h a_1 a_2, b_1 h b_2} - V_{h a_2 a_1, b_2 h b_1} + V_{h a_2 a_1, b_1 h b_2} + V_{h a_1 a_2, b_2 h b_1} \Big\} \, . \end{aligned} \tag{3.5.7}$$

The definition (3.5.7) has been inspired by the form of second order (S_2) contributions to

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the binding-energy and has the additional advantage of being fully anti-symmetric, so that all procedures developed when dealing with the nucleon-nucleon interaction [Mi-98a], can be naturally extended to handle the three-nucleon interaction. Note that the first two terms in Eq. (3.5.7) are equivalent to the standard density-dependent reduction of the three-body force.

We shall now detail the changes necessary to take into account the effects of the three-nucleon interaction in the calculation of the binding-energy and mean field using the coupled-cluster formalism.

3.5.1 Binding Energy Corrections.

We are only interested in the total binding energy when the wave function satisfies the Hartree-Fock conditions. Thus, it suffices to compute

$$\langle E \rangle = \langle 0 \,|\, \mathbf{T} \,|\, 0 \rangle + \langle 0 \,|\, \mathbf{V} \,|\, 0 \rangle + \langle 0 \,|\, \mathbf{S}_2\mathbf{V} \,|\, 0 \rangle + \langle 0 \,|\, \mathbf{S}_3\mathbf{V}_{3N} \,|\, 0 \rangle . \tag{3.5.8}$$

The first order corrections to the binding energy are due to the expectation value of the three-nucleon interaction in the uncorrelated ground state. We have

$$\begin{aligned} \langle 0 \,|\, \mathbf{V}_{3N} \,|\, 0 \rangle = \frac{1}{6} \sum_{h_1 h_2 h_3} \Big\{ & V_{h_1 h_2 h_3, h_1 h_2 h_3} - V_{h_1 h_2 h_3, h_1 h_3 h_2} + V_{h_1 h_2 h_3, h_3 h_1 h_2} \\ & - V_{h_1 h_2 h_3, h_3 h_2 h_1} + V_{h_1 h_2 h_3, h_2 h_3 h_1} - V_{h_1 h_2 h_3, h_2 h_1 h_3} \Big\} . \end{aligned} \tag{3.5.9}$$

Using the symmetries (3.5.3, 3.5.4), the last equation becomes

$$\begin{aligned} & \langle 0 \,|\, \mathbf{V}_{3N} \,|\, 0 \rangle \\ & = \sum_{h_1 h_2 h_3} \left\{ \frac{1}{6} V_{h_1 h_2 h_3, h_1 h_2 h_3} - \frac{1}{2} V_{h_1 h_2 h_3, h_1 h_3 h_2} + \frac{1}{3} V_{h_1 h_2 h_3, h_3 h_1 h_2} \right\} . \end{aligned} \tag{3.5.10}$$

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We notice that only the first two terms in Eq. (3.5.10) have the form (3.5.5). However, in this particular case, it is a simple endeavor to calculate the missing third matrix element. We find that the magnitude of this term is small compared to the sum of the terms (3.5.5).

Second order contributions are calculated *exactly* as

$$\langle 0 \,|\, \mathbf{S_2 V} \,|\, 0 \rangle \;=\; \frac{1}{(2!)^4} \sum_{p_1 h_1 p_2 h_2} S_{p_1 h_1 . p_2 h_2} \; V^{3N,den}_{p_2 h_2 . p_1 h_1} \,. \tag{3.5.11}$$

At the present time, the third order corrections have not been evaluated. We intend to closely investigate their size, however, access to a supercomputer is necessary. We will report on our findings as soon as results will be available.

3.5.2 Mean Field Corrections.

In our approach to the coupled cluster formalism, the single particle orbits are eigenfunctions of an mean-field Hamiltonian, defined as the sum of a one-body kinetic energy term and a one-body mean-field potential. The later is not unique, and in the maximum overlap hypothesis $\mathbf{S}_1 = 0$, the mean-field is defined as

$$\langle 0 | \mathbf{U}_0 | 1p1h \rangle \;=\; \langle 0 | \Big\{ \mathbf{V} + [\mathbf{S}_2, \mathbf{V}] + [\mathbf{S}_3, \mathbf{V}] \Big\} | 1p1h \rangle \,. \tag{3.5.12}$$

Correspondingly, the contributions due to the three-nucleon interaction can be written as the sum of three terms

$$\langle 0 \,|\, \mathbf{V}_{3N} \mathbf{a}_p^\dagger \mathbf{a}_h \,|\, 0 \rangle \;+\; \langle 0 \,|\, [\mathbf{S}_2, \mathbf{V}_{3N}] \, \mathbf{a}_p^\dagger \mathbf{a}_h \,|\, 0 \rangle \;+\; \langle 0 \,|\, [\mathbf{S}_3, \mathbf{V}_{3N}] \, \mathbf{a}_p^\dagger \mathbf{a}_h \,|\, 0 \rangle \,. \tag{3.5.13}$$

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In leading order, the three-nucleon interaction correction of the mean-field is given as

$$\langle 0 \,|\, \mathbf{V}_{3N} \mathbf{a}_p^\dagger \mathbf{a}_h \,|\, 0 \rangle = \frac{1}{2} \sum_{h_1 h_2} \Big\{ V_{h_1 h_2 \, h; h_1 h_2 \, p} - V_{h_2 \, h \, h_1, h_2 h_1 \, p} + V_{h_1 h_2, h; h_2, p, h_1} - V_{h_1 h_2 \, h, h_1 \, p \, h_2} + V_{h_2 \, h \, h_1, h_1 h_2 \, p} - V_{h_1 h_2 \, h, h_2 h_1 \, p} \Big\} . \tag{3.5.14}$$

Again, using the symmetries (3.5.3, 3.5.4), Eq. (3.5.14) becomes

$$\langle 0 \,|\, \mathbf{V}_{3N} \mathbf{a}_p^\dagger \mathbf{a}_h \,|\, 0 \rangle = \sum_{h_1 h_2} \Big\{ \frac{1}{2} V_{h_1 h_2 \, h, h_1 h_2 \, p} - V_{h_1 h \, h_2, h_1 h_2 \, p} + V_{h_1 h_2 \, h, h_2 \, p \, h_1} - \frac{1}{2} V_{h_1 h_2 \, h, h_2 h_1 \, p} \Big\} . \tag{3.5.15}$$

The second- and third-order contributions in Eq. (3.5.13) look very similar when one uses the proposed reduction of the three-body force. Eq. (3.5.7), for the account of the $3p3h$ correlations. Then, by making use of the full anti-symmetry of $\mathbf{S}_2$ and $\mathbf{V}_{3N\,den}$ we can show that the required corrections can be written as

$$\sum_{p_1 p_2 h_1 h_2} \Big\{ \Big(V_{h \, p_1 p_2, p \, h_1 h_2} - 2 V_{h \, p_1 p_2, h_1 \, p \, h_2} \Big) Z_{p_1 p_2, h_1 h_2} - \Big(V_{h \, h_1 h_2, p \, p_1 p_2} - 2 V_{h \, h_1 h_2, p_1 \, p \, p_2} \Big) \frac{\langle p_1 \bar{h}_1 \,|\, V_{2N} \,|\, h_2 \bar{p}_2 \rangle}{\epsilon_{ph} + \epsilon_{p_1 h_1} + \epsilon_{p_2 h_2}} \Big\} . \tag{3.5.16}$$

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Chapter 4

Center-of-Mass Corrections.

For the proper description of a scattering process one assumes a nuclear wave function that factorizes into a nuclear center-of-mass wave function, which is taken to be a plane wave, and an intrinsic wave function of coordinates relative to the center-of-mass. The difficulty lies in the ansatz of the wave function as a Slater determinant. Such a wave function generally does not factorize into a center-of mass wave function and a wave function for the nucleus relative to its center-of-mass. Furthermore, for the cases where it factorizes, the center-of-mass wave function is not a plane wave. While this is negligible for heavy nuclei, it is a significant correction for nuclei like ^{16}O.

The calculation usually gives the form factor of the one-body density labeled $F_{sd}(q)$ whereas the experiment requires the form factor with respect to the center-of-mass, labeled $F_{int}(q)$. In the special case of a single Slater determinant of harmonic oscillator single-particle wave functions, it has been shown that the wave function factorizes with a center-of-mass wave function being a Gaussian. This allows us to calculate the form factor in the form

$$F_{sd}(q) = e^{-\frac{1}{4}b^2q^2/A} F_{int}(q) \qquad (4.0.1)$$

where b is the harmonic oscillator length parameter. Because of this exact result it has been customary to apply such a correction also in cases where the single particle wave functions are not harmonic oscillator wave functions and where the presence of correlations has been

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substituted by an effective interaction.

An alternate way [Mi-98b] to deal with this is to calculate directly the form factor in the center-of-mass system. This way the operator can be written as a series of one-body, two-body, ..., to A-body terms. In this chapter we first compare such an expansion with the exact result, for the case where such a result is available. We then apply the same expansion to a realistic wave function of ^{16}O and compare it to the corrections implied by equation (4.0.1).

4.1 The Form Factor of the density

The charge form factor at momentum transfer $\vec{q}$ is given in Born approximation [Ta-59] by

$$F_{int}(\vec{q}) \;=\; \langle \phi_0 \,|\, \sum_k f_k(q^2)\; e^{i\vec{q}\cdot\vec{r'}_k} \,|\, \phi_0 \rangle \,. \tag{4.1.1}$$

where ϕ_0 is the translationally invariant ground state, $\vec{r'}_k$ the distance from the center-of-mass to the kth "point" nucleon and $f_k(q^2)$ the nucleon form factor, which takes into account the finite size of the nucleon k.

The center-of-mass correction has to do with the fact that the origin of the shell-model is not the same as the center-of-mass of the nucleus. Since the many-body Hamiltonian is not translationally invariant, then the model ground state $\Phi_0^{(M)}$ is not translationally invariant either, and thus can lead to incorrect description of observables, especially in small A nuclei.

What we need to establish is the relationship between the model quantities expressed in terms of the coordinates of the laboratory system ($\vec{r}_k$, $k = 1 \ldots A$), and the intrinsic ones ($\vec{r'}_k = \vec{r}_k - \vec{R}_{cm}$, $k = 1 \ldots A-1$), measured from the center-of-mass of the nucleus

$$\vec{R}_{cm} \;=\; \frac{1}{A} \sum_{k=1}^{A} \vec{r}_k \,. \tag{4.1.2}$$

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Formally, this may be viewed as a change of coordinates, from the coordinates of the laboratory system $\vec{r}_k$ to the coordinates of the center-of-mass system $\{\vec{R}_{cm},\ \vec{r'}_k\}$, followed by the removal of the dependence upon $\vec{R}_{cm}$ from the model wave function $\Phi_0^{(M)}$, i.e. we have to construct the intrinsic wave function [Lp-58]

$$\phi_0^{(M)}(\vec{r'}_k) \;=\; \int G(\vec{R}_{cm})\,\Phi_0^{(M)}(\vec{R}_{cm},\vec{r'}_k)\,d\vec{R}_{cm} \tag{4.1.3}$$

independent of $\vec{R}_{cm}$, for an arbitrary function $G(\vec{R}_{cm})$. Note here that, in this formalism, the well-known Gartenhaus-Schwartz transformation [Ga-57, Gi-68] corresponds to taking $G(\vec{R}_{cm}) = \delta(\vec{R}_{cm})$. It is clear now that the arbitrariness of the $G(\vec{R}_{cm})$ function causes some troubles: Since there is no reason to choose a particular $G(\vec{R}_{cm})$, it has been pointed out that the center-of-mass correction for a given model wave function is not uniquely defined [Lp-58]. Nevertheless, the various recipes yield the same result in the limit of the exact wave function of a free nucleus [Fe-71].

The exact nuclear wave function Φ_0 consists of two factors, one of which is a plane wave in the center-of-mass coordinate, $e^{i\vec{P}\cdot\vec{R}_{cm}}$, the other being the intrinsic wave function ϕ_0 of the relative coordinates [Ub-71] $\vec{r'}_k$,

$$\Phi_0(\vec{r}_1\cdots\vec{r}_A) \;=\; e^{i\vec{P}\cdot\vec{R}_{cm}}\;\phi_0(\vec{r'}_1\cdots\vec{r'}_{A-1})\,. \tag{4.1.4}$$

For an approximate model wave function $\Phi_0^{(M)}$ however, all we can hope for is to be able to obtain the decomposition

$$\Phi_0^{(M)} \;=\; \phi_{cm}(\vec{R}_{cm})\;\phi_0^{(M)}(\vec{r'}_1\cdots\vec{r'}_A)\,. \tag{4.1.5}$$

which is approximately correct to the extent that the motion of the intrinsic coordinates

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and the center-of-mass are not correlated. Only then, the factorization

$$F_{sd}(\vec{q}) \;=\; F_{cm}(\vec{q})\; F_{int}(\vec{q}) \tag{4.1.6}$$

is possible. To that approximation, and assuming that the model provides indeed a good description of the internal structure of the nucleus ($\Phi_0 = \Phi_0^{(M)}$ [Ba-61]), equation (4.1.6) is valid with [Fe-71]

$$F_{int}(\vec{q}) \;=\; \langle \Phi_0^{(M)} \mid \sum_k f_k(q^2)\; \hat{e}_k\; e^{i\vec{q}\cdot(\vec{r}_k - \vec{R}_{cm})} \mid \Phi_0^{(M)} \rangle \tag{4.1.7}$$

and

$$F_{cm}(\vec{q}) \;=\; \langle \Phi_0^{(M)} \mid e^{i\vec{q}\cdot\vec{R}_{cm}} \mid \Phi_0^{(M)} \rangle \,. \tag{4.1.8}$$

The form factor (4.1.7) can now be calculated directly by carrying out an expansion in terms of many-body operators:

$$F_{int}(\vec{q}) = \sum_k f_k(q^2) \left\langle e^{i\vec{q}\cdot\vec{r}_k(A-1)/A} \prod_{m\neq k} e^{-i\vec{q}\cdot\vec{r}_m/A} \right\rangle . \tag{4.1.9}$$

Each exponential in equation (4.1.9) can be expressed in terms of the one-body operator which we define by

$$f(\vec{q}\cdot\vec{r}_m) = e^{-i\vec{q}\cdot\vec{r}_m} - 1 \,. \tag{4.1.10}$$

With this we write the form factor as

$$F_{int}(\vec{q}) \;=\; \sum_k f_k(q^2) \left\langle e^{i\vec{q}\cdot\vec{r}_k(A-1)/A} \prod_{m\neq k} (1 + f^*(\vec{q}\cdot\vec{r}_m/A)) \right\rangle \tag{4.1.11}$$

$$\begin{aligned} &= \sum_k f_k(q^2) \left\langle e^{i\vec{q}\cdot\vec{r}_k(A-1)/A} \right\rangle \\ &\quad + \sum_k f_k(q^2) \sum_{m\neq k} \left\langle e^{i\vec{q}\cdot\vec{r}_k(A-1)/A}\; f^*(\vec{q}\cdot\vec{r}_m/A) \right\rangle \\ &\quad + \frac{1}{2} \sum_k f_k(q^2) \sum_{m,n\neq k} \left\langle e^{i\vec{q}\cdot\vec{r}_k(A-1)/A}\; f^*(\vec{q}\cdot\vec{r}_m/A)\; f^*(\vec{q}\cdot\vec{r}_n/A) \right\rangle + \cdots . \end{aligned} \tag{4.1.12}$$

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We intend to apply our formalism to the particular case of doubly magic nuclei (^{16}O). Thus, we can use the spherical symmetry of the nucleus to simplify calculations, in the sense that the form factor $F_{int}(\vec{q})$ should be spherically symmetric too, and we can in turn average the form factor over the directions of $\vec{q}$. We introduce then

$$F_{int}^{(av)}(q) = \frac{1}{4\pi} \int F_{int}(\vec{q})\ d\Omega_q\ . \tag{4.1.13}$$

This allows us to write the different terms in equation (4.1.12) using the second quantization formalism, as follows:

one-body term

$$\sum_{\alpha\beta} f_\alpha(q^2)\ \langle \alpha \mid j_0(qr_1(A-1)/A) \mid \beta \rangle\ \mathbf{a}_\alpha^\dagger \mathbf{a}_\beta \tag{4.1.14}$$

two-body term

$$\sum_{L} (2L+1)$$
$$\sum_{\alpha\beta\gamma\delta} f_\alpha(q^2)\ \left\langle \alpha\beta \left| j_L(qr_1(A-1)/A)\, f_L(qr_2/A)\, \left(\hat{C}_1^{(L)} \cdot \hat{C}_2^{(L)}\right) \right| \gamma\delta \right\rangle\ \mathbf{a}_\alpha^\dagger \mathbf{a}_\beta^\dagger \mathbf{a}_\delta \mathbf{a}_\gamma \tag{4.1.15}$$

three-body term

$$\sum_{L_1 L_2 L_3} i^{L_1-L_2-L_3}\ (2L_2+1)\,(2L_3+1)\,\langle L_3 0\ L_2 0 \mid L_1 0\rangle \sum_{\alpha\beta\gamma\delta\theta\zeta} f_\alpha(q^2)$$
$$\times \left\langle \alpha\beta\gamma \left| j_{L_1}(qr_1(A-1)/A)\, f_{L_2}(qr_2/A)\, f_{L_3}(qr_3/A)\, \left(\hat{C}_1^{(L_1)} \cdot \left[\hat{C}_2^{(L_2)} \cdot \hat{C}_3^{(L_3)}\right]^{(L_1)}\right) \right| \delta\theta\zeta \right\rangle$$
$$\mathbf{a}_\alpha^\dagger \mathbf{a}_\beta^\dagger \mathbf{a}_\gamma^\dagger \mathbf{a}_\zeta \mathbf{a}_\theta \mathbf{a}_\delta \tag{4.1.16}$$

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where we have introduced $f_l(qr) = j_l(qr) - \delta_{l0}$, and $j_l(qr)$ are the spherical Bessel functions of order l. Note that the conversion to second quantization allows for all restrictions in the sums (4.1.12) to be dropped.

4.2 Harmonic Oscillator Shell-Model Calculation

We would like a test of convergence for the proposed many-body expansion. We recall that Eq. (4.1.6) is always exact if $\Phi_0^{(M)}$ is expressed in terms of harmonic oscillator wave functions, provided that the center-of-mass wave function ϕ_{cm} is in one given harmonic oscillator state. Then, the extraction of the center-of-mass coordinate can be done analytically. Elliott and Skyrme [El-54] have shown long time ago, that if the shell-model states are nonspurious, then the center-of-mass moves in its ground state and is described by the $1s$ harmonic oscillator wave function

$$\phi_{cm}(\vec{R}_{cm}) = \left(\frac{A^3}{\pi^3 b^6}\right)^{\frac{1}{4}} \exp\left[-\frac{A R_{cm}^2}{2 b^2}\right] . \tag{4.2.1}$$

where b is the harmonic oscillator length parameter. The center-of-mass form factor can also be evaluated explicitly

$$F_{cm}^{HO}(\vec{q}) = e^{-\frac{1}{4}b^2 q^2/A} . \tag{4.2.2}$$

The correct translation-invariant form factor is thus given in terms of the shell-model form factor by

$$F_{int}(\vec{q}) = e^{\frac{1}{4}b^2 q^2/A} F_{sd}(\vec{q}) . \tag{4.2.3}$$

i.e. F_{sd} must be corrected by dividing through $F_{cm}(q)$. Note that, since the uniqueness of the procedure of carrying out the center-of-mass corrections has been questioned, the use of

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the equation (4.2.3) has been suggested even in the case of a more general nuclear structure model [Ub-71].

We will exploit the analytical nature of these results by testing how fast does the many-body expansion (4.1.12) converge. The shell-model wave function $\Phi_0^{(M)}$ for the harmonic oscillator potential is an independent particle wave function, represented by a simple Slater determinant of single-particle orbits. This state is what we shall call the uncorrelated ground state $|0\rangle$. By taking the expectation value in the model ground state $\Phi_0^{(M)} = |0\rangle$, of the one-, two- and three-body operators in equations (4.1.14), (4.1.15) and (4.1.16), the following relevant expectation values are obtained:

$$\langle 0 \,|\, a_\alpha^\dagger a_\beta \,|\, 0 \rangle = \delta_{\alpha\beta} \tag{4.2.4}$$

$$\langle 0 \,|\, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \,|\, 0 \rangle = \delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma} \tag{4.2.5}$$

$$\begin{aligned}\langle 0 \,|\, a_a^\dagger a_b^\dagger a_c^\dagger a_\zeta a_\theta a_\delta \,|\, 0 \rangle = {} & \delta_{\alpha\delta}\,(\delta_{\beta\theta}\delta_{\gamma\zeta} - \delta_{\beta\zeta}\delta_{\gamma\theta}) - \delta_{\alpha\theta}\,(\delta_{\beta\delta}\delta_{\gamma\zeta} - \delta_{\beta\zeta}\delta_{\gamma\delta}) \\ & + \delta_{\alpha\zeta}\,(\delta_{\beta\delta}\delta_{\gamma\theta} - \delta_{\beta\theta}\delta_{\gamma\delta})\ .\end{aligned} \tag{4.2.6}$$

Using these results and following a straight forward but laborious calculation, the translation-invariant form factor for the harmonic oscillator shell-model can be computed completely up to the third-order in the many-body expansion (4.1.12). The various components involved are presented here, by their corresponding term of origin in the many-body expansion.

One-body term. There is only one contribution to the one-body term of $F_{int}^{(av)}(q)$

$$\mathrm{HO1} = \sum_{nlj} f_{nlj}(q^2)\,(2j+1) \int_0^\infty \mathcal{HO}_{nl}^2(r)\, j_0(\tfrac{A-1}{A} qr)\, r^2\, dr\ . \tag{4.2.7}$$

where $\mathcal{HO}_{nl}(r)$ are the usual radial harmonic oscillator wave functions. Note that, in the previous equation, HO1 is actually the Fourier transform of the one-body density folded

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with the appropriate nucleon form factor, i.e.

$$\mathrm{HO1} \;=\; f_p \int_0^\infty \rho_0^{(p)}(r)\; j_0(\tfrac{A-1}{A}qr)\; r^2\, dr \;+\; f_n \int_0^\infty \rho_0^{(n)}(r)\; j_0(\tfrac{A-1}{A}qr)\; r^2\, dr\,, \tag{4.2.8}$$

where $\rho_0^{(p)}(r)$ and $\rho_0^{(n)}(r)$ are the proton and neutron one-body densities, respectively, corresponding to the uncorrelated ground state $|0\rangle$.

Two-body term. Two different components contribute to the two-body term of $F_{int}^{(av)}(q)$:

1. one component corresponding to the direct contraction $\delta_{\alpha\gamma}\delta_{\beta\delta}$:

$$\begin{aligned}\mathrm{HO2_{dr}} \;=\; & \sum_{n_1 l_1 j_1} f_{n_1 l_1 j_1}(q^2)\; (2j_1+1) \int_0^\infty \mathcal{HO}^2_{n_1 l_1}(r_1)\; j_0(qr_1(A-1)/A)\; r_1^2\, dr_1 \\ & \times \sum_{n_2 l_2 j_2} (2j_2+1) \int_0^\infty \mathcal{HO}^2_{n_2 l_2}(r_2)\; f_0(qr_2/A)\; r_2^2\, dr_2\,: \end{aligned} \tag{4.2.9}$$

2. one component associated with the exchange contraction $\delta_{\alpha\gamma}\delta_{\beta\delta}$:

$$\begin{aligned}\mathrm{HO2_{ex}} \;=\; & \sum_{n_1 l_1 j_1,\, n_2 l_2 j_2} f_{n_1 l_1 j_1,\, n_2 l_2 j_2}(q^2) \sum_L (2L+1)\; \left(\langle (l_1 \tfrac{1}{2}) j_1 \,||\, \hat{C}^{(L)} \,||\, (l_2 \tfrac{1}{2}) j_2 \rangle\right)^2 \\ & \times \int_0^\infty \mathcal{HO}_{n_1 l_1}(r_1) \mathcal{HO}_{n_2 l_2}(r_1)\; j_L(qr_1(A-1)/A)\; r_1^2\, dr_1 \\ & \times \int_0^\infty \mathcal{HO}_{n_1 l_1}(r_2) \mathcal{HO}_{n_2 l_2}(r_2)\; f_L(qr_2/A)\; r_2^2\, dr_2\,. \end{aligned} \tag{4.2.10}$$

where the pair of indices of the nucleon form factor $f(q^2)$ indicate that the two orbits denoted as $(n_1 l_1 j_1)$ and $(n_2 l_2 j_2)$ have the same isospin.

Three-body term. The three-body term contains six contributions to $F_{int}^{(av)}$, out of which two are identical due to the fact that, in equation (4.1.16), the radial and angular parts of the operator dependent upon the coordinates of the 2nd nucleon are the same as the radial

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and angular parts of the operator dependent upon the coordinates of the 3rd nucleon. The different components of the three-body term (4.1.16) are listed below:

1. *term 3.1* ($\delta_{\alpha\delta}\delta_{\beta\theta}\delta_{\gamma\zeta}$):

$$\begin{aligned} \mathrm{HO3_1} \;=\; & \sum_{n_1 l_1 j_1} f_{n_1 l_1 j_1}(q^2)\,(2j_1+1)\int_0^\infty \mathcal{HO}^2_{n_1 l_1}(r_1)\, j_0(qr_1(A-1)/A)\, r_1^2\, dr_1 \\ & \sum_{n_2 l_2 j_2} (2j_2+1)\int_0^\infty \mathcal{HO}^2_{n_2 l_2}(r_2)\, f_0(qr_2/A)\, r_2^2\, dr_2 \\ & \sum_{n_3 l_3 j_3} (2j_3+1)\int_0^\infty \mathcal{HO}^2_{n_3 l_3}(r_3)\, f_0(qr_3/A)\, r_3^2\, dr_3 : \end{aligned} \tag{4.2.11}$$

2. *term 3.2* ($\delta_{\alpha\delta}\delta_{\beta\zeta}\delta_{\gamma\theta}$):

$$\begin{aligned} \mathrm{HO3_2} \;=\; & -\sum_{n_1 l_1 j_1} f_{n_1 l_1 j_1}(q^2)\,(2j_1+1) \\ & \sum_L (-1)^L(2L+1)\int_0^\infty \mathcal{HO}^2_{n_1 l_1}(r_1)\, j_0(qr_1(A-1)/A)\, r_1^2\, dr_1 \\ & \sum_{n_2 l_2 j_2,\, n_3 l_3 j_3} \left(\langle (l_2 \tfrac{1}{2}) j_2 \,||\, \hat{C}^{(L)} \,||\, (l_3 \tfrac{1}{2}) j_3 \rangle \int_0^\infty \mathcal{HO}_{n_1 l_1}(r)\mathcal{HO}_{n_3 l_3}(r)\, f_L(\tfrac{1}{A}qr)\, r^2\, dr \right)^2 : \end{aligned} \tag{4.2.12}$$

3. *term 3.3* ($\delta_{\alpha\theta}\delta_{\beta\delta}\delta_{\gamma\zeta}$): is equal to *term 3.6* ($\delta_{\alpha\zeta}\delta_{\beta\theta}\delta_{\gamma\delta}$):

$$\begin{aligned} \mathrm{HO3_3} \;=\; & \mathrm{HO3_6} \;= \\ = \; & -\sum_{n_1 l_1 j_1,\, n_2 l_2 j_2} f_{n_1 l_1 j_1,\, n_2 l_2 j_2}(q^2) \sum_L (2L+1) \left(\langle (l_1 \tfrac{1}{2}) j_1 \,||\, \hat{C}^{(L)} \,||\, (l_2 \tfrac{1}{2}) j_2 \rangle \right)^2 \\ & \int_0^\infty \mathcal{HO}_{n_1 l_1}(r_1)\mathcal{HO}_{n_2 l_2}(r_1)\, j_L(qr_1(A-1)/A)\, r_1^2\, dr_1 \\ & \int_0^\infty \mathcal{HO}_{n_1 l_1}(r_2)\mathcal{HO}_{n_2 l_2}(r_2)\, f_L(qr_2/A)\, r_2^2\, dr_2 \\ & \sum_{n_3 l_3 j_3} (2j_3+1)\int_0^\infty \mathcal{HO}^2_{n_3 l_3}(r_3)\, f_0(qr_3/A)\, r_3^2\, dr_3 : \end{aligned} \tag{4.2.13}$$

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4. *term 3.4* ($\delta_{\alpha\theta}\delta_{\beta\zeta}\delta_{\gamma\delta}$) is equal to *term 3.5* ($\delta_{\alpha\zeta}\delta_{\beta\delta}\delta_{\gamma\theta}$):

$$HO3_4 = HO3_5 =$$

$$= - \sum_{n_1 l_1 j_1, n_3 l_3 j_3} f_{n_1 l_1 j_1, n_3 l_3 j_3}(q^2) \sum_{n_2 l_2 j_2} \sum_{L_2=|j_1-j_2|}^{j_1+j_2} (2L_2+1) \sum_{L_3=|j_2-j_3|}^{j_2+j_3} (2L_3+1)$$

$$\sum_L (-1)^{\frac{L+L_2+L_3}{2}} \sqrt{2L+1} \langle L_2 0\, L_3 0 \mid L0 \rangle \begin{Bmatrix} L_3 & L & L_2 \\ j_1 & j_2 & j_3 \end{Bmatrix}$$

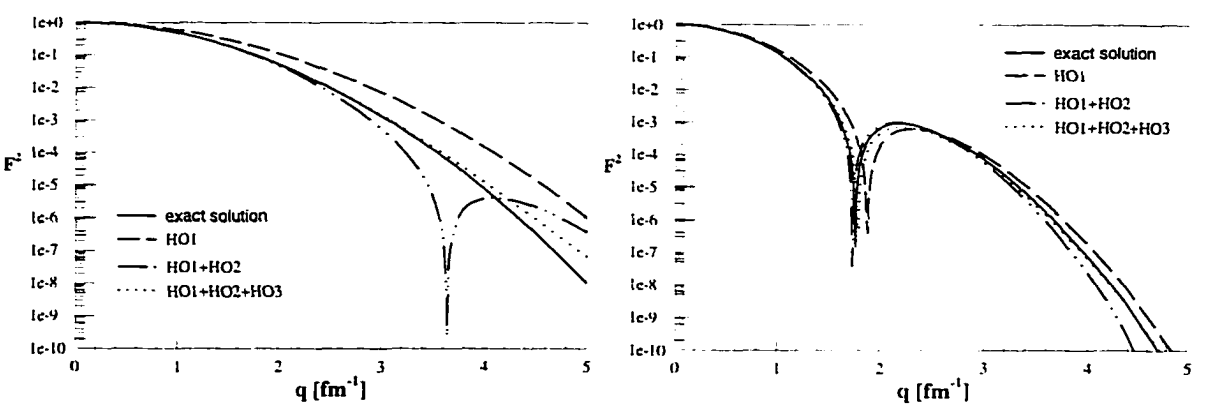
$$\langle (l_1 \tfrac{1}{2}) j_1 \| \hat{C}^{(L)} \| (l_3 \tfrac{1}{2}) j_3 \rangle \int_0^\infty \mathcal{HO}_{n_1 l_1}(r_1) \mathcal{HO}_{n_3 l_3}(r_1)\, j_L(qr_1(A-1)/A)\, r_1^2\, dr_1$$

$$\langle (l_2 \tfrac{1}{2}) j_2 \| \hat{C}^{(L_2)} \| (l_1 \tfrac{1}{2}) j_1 \rangle \int_0^\infty \mathcal{HO}_{n_2 l_2}(r_2) \mathcal{HO}_{n_1 l_1}(r_2)\, f_{L_2}(qr_2/A)\, r_2^2\, dr_2$$

$$\langle (l_3 \tfrac{1}{2}) j_3 \| \hat{C}^{(L_3)} \| (l_2 \tfrac{1}{2}) j_2 \rangle \int_0^\infty \mathcal{HO}_{n_3 l_3}(r_3) \mathcal{HO}_{n_2 l_2}(r_3)\, f_{L_3}(qr_3/A)\, r_3^2\, dr_3 :$$

(4.2.14)

In Fig. 4-1 we illustrate the convergence of the many-body expansion (4.1.12), for the case of the ^{4}He and ^{16}O nuclei, respectively. The solid line represents the *exact* form factor



(a) ^{4}He (b) ^{16}O

Figure 4-1 Convergence of the many-body expansion (4.1.12) of the charge form factor, for the harmonic oscillator shell model case.

in the center-of-mass system, as given by the formula (4.2.3). The agreement is excellent

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for a momentum transfer $q < 3$ fm^{-1}, and remains reasonable good for q up to 4 fm^{-1}. It is expected that the size of the contributions due to correlations (as presented in the next section), is more important than the error made by ignoring higher order terms in the many-body expansion (4.1.12). Also, it is worthwhile mentioning that a correction expected to become increasingly important for high values of the momentum transfer, is the contribution due to the meson-exchange charge density [Sc-90]. However, the inclusion of this correction is beyond the purpose of the present discussion. We conclude that truncating the calculation at the third-order gives us a good approximation of the center-of-mass correction for the independent-particle model wave function case.

Note that leaving out the three-body term in the case of the ^{4}He nucleus, would result in an unacceptable description of the form factor distribution – *false* minima are located at a momentum transfer q as low as 3.6 fm^{-1} –, whereas in the case of the ^{16}O nucleus, the charge form factor changes very little by including the three-body term. This is an indication that expression (4.2.3) can be viewed effectively, as a $1/A$ power expansion of the charge form factor. Therefore, as we consider the applicability of the expansion (4.2.3) for higher values of A, it appears that we can safely drop higher-order terms in the many-body expansion and still hope for a good description charge form factor..

To conclude our study of the convergence of the many-body expansion (4.1.12), let us investigate the influence the given order of approximation has on the inferred mean square charge (rms) radius. It is well known that in the limit of low q the form factor can be approximated as

$$F_{int}(q) = 1 - \frac{1}{6} q^2 \langle r^2 \rangle \qquad (4.2.15)$$

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Table 4.1 Convergence of the mean square charge radius for the case of the ^{4}He and ^{16}O nuclei, and the harmonic oscillator shell model.

Order of approximation	^{4}He	^{16}O
HO1	1.285979	2.250000
HO1 + HO2	1.484927	2.371708
HO1 + HO2 + HO3	1.484922	2.349467
exact value	1.484924	2.349468

and thus is a measure of the rms radius. Table (4.1) shows the convergence of the mean square charge radius for the case of the ^{4}He and ^{16}O nuclei. These results show that the rms radius is little affected by any corrections beyond the two-body term of the expansion (4.1.12). By including the three-body term in Eq. (4.1.12), the rms radius remains virtually the same in the ^{4}He case, and changes by less than 1 % in the ^{16}O case.

4.3 Realistic Nuclear Wave Function Using the exp(S) Method

We shall apply now our formalism to the case of a more complicated model wave function $\Phi_0^{(M)}$ and the particular case of the ^{16}O nucleus. As advertised, the nuclear wave function $\Phi_0^{(M)} = |\tilde{0}\rangle$, has been obtained using the coupled cluster method (or the exp(S) method) together with a *realistic* interaction [He-98a].

The formulas obtained in the previous section are not enough anymore. By replacing the radial harmonic oscillator wave functions, $\mathcal{HO}_{nl}$ by the radial part of new the single-particle wave functions, $\mathcal{R}_{nl}$, we obtain the expectation value of the operator F_{int} in the uncorrelated ground state $|0\rangle$. In this sense, the terms $SM1$, $SM2$ and $SM3$ replace now

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the $HO1$, $HO2$ and $HO3$ contributions derived before. They represent only part of the new picture, since no explicit correction due to the $npnh$ correlations are included.

The correct translation-invariant form factor is given by the expectation value of the operator F_{int} in the correlated ground state $|\tilde{0}\rangle$. As we have previously worked out the one-body and two-body densities for the ground state, we can apply these results to evaluate the first two terms in this expansion.

Using the definition of the one-body density

$$\rho(\vec{r}) = \sum_m \langle \tilde{0} \,|\, \delta(\vec{r} - \vec{r}_m) \,|\, \tilde{0} \rangle \,. \tag{4.3.1}$$

together with the identity

$$\langle \tilde{0} \,|\, e^{i\vec{q}\cdot\vec{r}_k(A-1)/A} \,|\, \tilde{0} \rangle = \langle \tilde{0} | \int d\vec{r}\, e^{i\vec{q}\cdot\vec{r}(A-1)/A}\, \delta(\vec{r} - \vec{r}_k) \,|\, \tilde{0} \rangle \,. \tag{4.3.2}$$

we can write the first term of Eq. (4.1.12) as

$$\begin{aligned} A_1 &= \sum_m f_m(q^2) \, \langle \tilde{0} \,|\, e^{i\vec{q}\cdot\vec{r}_m(A-1)/A} \,|\, \tilde{0} \rangle \\ &= f_p(q^2) \int d\vec{r}\, e^{i\vec{q}\cdot\vec{r}(A-1)/A}\, \rho^{(p)}(\vec{r}) + f_n(q^2) \int d\vec{r}\, e^{i\vec{q}\cdot\vec{r}(A-1)/A}\, \rho^{(n)}(\vec{r}) \,. \end{aligned} \tag{4.3.3}$$

Here, $\rho^{(p)}(\vec{r})$ and $\rho^{(n)}(\vec{r})$ are the proton and neutron ground state one-body densities, which include corrections due to $2p2h$, $3p3h$, and $4p4h$ correlations.

Similarly, we can write the second term as double integral over the ground state two-body density, using

$$\rho(\vec{r}_1, \vec{r}_2) = \sum_{mn} \langle \tilde{0} \,|\, \delta(\vec{r}_1 - \vec{r}_m)\, \delta(\vec{r}_2 - \vec{r}_n) \,|\, \tilde{0} \rangle \,. \tag{4.3.4}$$

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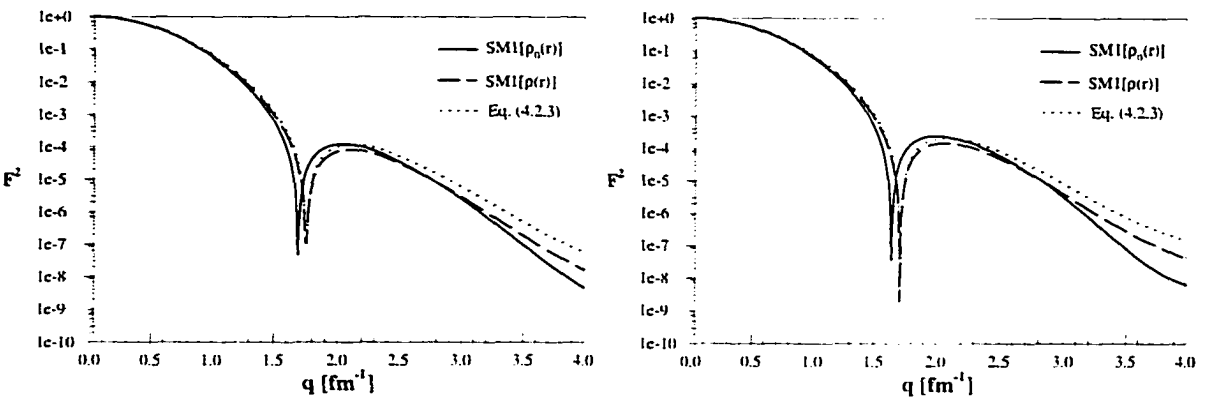
Then, the second term of Eq. (4.1.12) becomes

$$\begin{aligned} A_2 &= \sum_{mn} f_m(q^2)\ \langle \tilde{0} \,|\, e^{i\vec{q}\cdot\vec{r}_m(A-1)/A} f^*(\vec{q}\cdot\vec{r}_n/A) \,|\, \tilde{0}\rangle \\ &= f_p(q^2) \int d\vec{r} \int d\vec{r}'\ e^{i\vec{q}\cdot\vec{r}(A-1)/A}\ f^*(\vec{q}\cdot\vec{r}'/A)\ \left[\rho^{(p,p)}(\vec{r},\vec{r}') + \rho^{(p,n)}(\vec{r},\vec{r}')\right] \\ &\quad + f_n(q^2) \int d\vec{r} \int d\vec{r}'\ e^{i\vec{q}\cdot\vec{r}(A-1)/A}\ f^*(\vec{q}\cdot\vec{r}'/A)\ \left[\rho^{(n,p)}(\vec{r},\vec{r}') + \rho^{(n,n)}(\vec{r},\vec{r}')\right] . \end{aligned} \tag{4.3.5}$$

With these evaluations we include all the terms that were included in evaluating the one- and two-body densities.



(a) Argonne $v18$ (b) Argonne $v18$ plus Urbana IX

Figure 4-2 $SM1[\rho_0(r)]$ and $SM1[\rho(r)]$ form factors compared with the internal form factor calculated according to Eq. (4.2.3).

Figures 4-2 and 4-3 show the various effects of the correlations on the internal charge form factor. We also compare the various approximations of the form factor with the internal form factor suggested by Eq. (4.2.3), which in both cases is plotted as a dotted line.

In the calculation of the translational invariant charge form factor correlations enter at two places. First, the calculation of the one-body operator (A1) includes effects of

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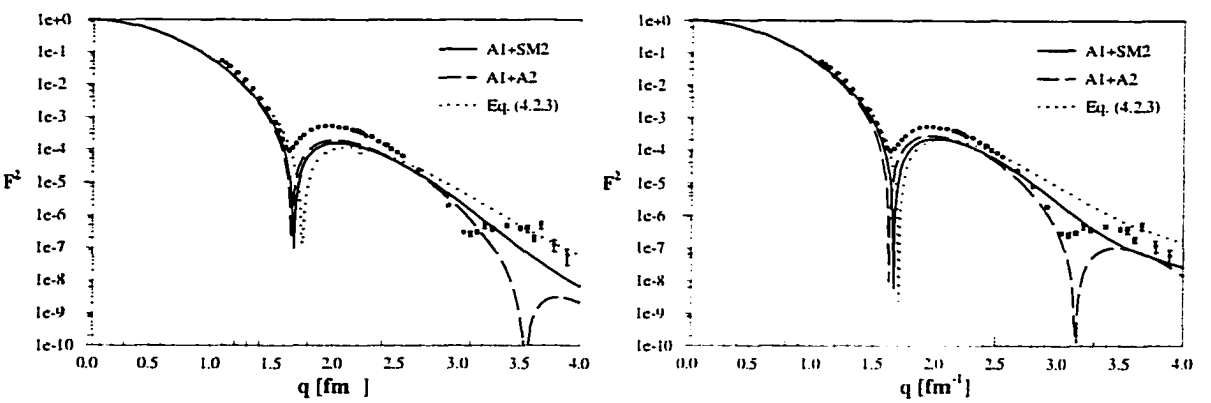
all the correlations, because this term is simply the Fourier transform of the one-body density. In Fig. 4-2, the solid and dashed lines represent the Fourier transform of the one-body density corresponding to the uncorrelated ($|0\rangle$) and correlated ($|\tilde{0}\rangle$) ground state, respectively. These form factors are denoted $SM1[\rho_0(r)]$ and $SM1[\rho(r)]$. Here, the main effect of the correlations is the shifting of the diffraction minimum by 5 % to the right. The new minimum is also predicted by Eq. (4.2.3), which also has a higher tail compared to $SM1[\rho_0(r)]$ and $SM1[\rho(r)]$.



(a) Argonne $v18$ (b) Argonne $v18$ plus Urbana IX

Figure 4-3 Two-body approximations of the translational invariant form factor compared with the internal form factor calculated according to Eq. (4.2.3).

Secondly, as any expectation value taken in the correlated ground state, the center-of mass corrections are modified due to the correlations. In Fig. 4-3, the solid and dashed lines represent the two-body approximations of the translational invariant form factor. Going beyond the leading order ($SM2$) in evaluating the two-body term (.42), leaves the first diffraction minimum virtually unchanged. However, the high q behaviour of the form factor, ($q > 2.5$ fm^{-1}), is dramatically affected. We can see that the $A_1 + A_2$ approximation of the internal charge form factor exhibits a second diffraction minimum, which has been observed

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experimentally by Sick and McCarthy [Si-70], and its presence makes our theory credible. Physically speaking, the hole in the two-body density affects the center of mass motion and thus the center of mass correction to be applied.

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Chapter 5

Results and Conclusions.

5.1 Numerical Modelling

We have chosen the Argonne $v18$ potential [Wi-95] as the underlying NN interaction. This potential gives an excellent fit to the nucleon-nucleon scattering data and the deuteron properties with a χ^2 per datum of 1.09 and thus must be considered to be one of the most realistic interactions available today. For historical reasons, results for the Argonne $v8$ and $v14$ potentials are also reported. However, the two-body part of that interaction results in over binding and a too large saturation density in nuclear matter. For that motive an empirical three-body interaction is added. In Table 5.1 list the values of the strength parameters of the two-pion exchange ($A_{2\pi}$) and the short-range phenomenological (U_0) parts of the three-nucleon interaction, for some of the potentials of the Urbana series.

The calculation in configuration space relies on our ability to calculate two-body matrix

Table 5.1 Strength parameters of the various three-nucleon interactions of the Urbana series.

Potential	$A_{2\pi}$	U_0
Urbana-V	- 0.0333	0.0030
Urbana-VII	- 0.0333	0.0038
Urbana-VIII	- 0.0280	0.0050
Urbana-IX	- 0.0293	0.0048

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elements for the basic interaction with high speed and high precision. We have developed a fast code to compute two-body matrix elements of the N-N interaction. The codes are written in FORTRAN and run on UNIX workstations. They allow us to compute ca. 10^6 matrix elements/minute on a HP-9000/735 workstation and do not depend on the shape of the wave functions. This code has been checked against a calculation using harmonic oscillator wave functions and Moshinsky transformations. The results agreed to at least 10^{-6} in accuracy.

We are using the coupled cluster ($exp(S)$) method to calculate the ground state of ^{16}O. We have solved the main Eq. (3.2.20) that determines the $2p2h$-amplitudes and thus essentially the ground state G-matrix for ^{16}O in a space of 35 $\hbar\omega$ with a harmonic oscillator length parameter b=0.8 fm, excluding those orbits with $\ell \geq 9$. Corrections for $3p3h$ correlations were included in a reduced space of $30\hbar\omega$ and $\ell \leq 6$.

The computation breaks into two steps: In the first step the G-matrix interaction is calculated inside the nucleus including all the corrections as specified by the coupled equations. This results in amplitudes for the $2p2h$-correlations. These amplitudes are implicitly corrected for the presence of $3p3h$-correlations and $4p4h$-correlations. In the second step the mean field is calculated from these correlations and the single-particle Hamiltonian is solved to give mean-field eigenfunctions and single particle energies. These two steps are iterated until a stable solution is obtained. The resulting binding energies for the considered Argonne and Urbana potentials are shown in Table 5.2.

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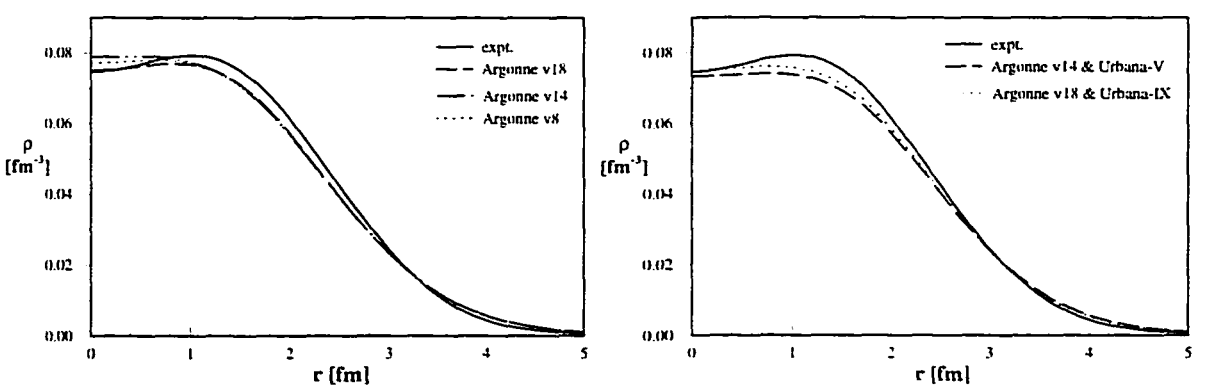
Table 5.2 Energy expectation, charge radii, and proton orbits occupation probabilities.

Potential	E [MeV/nucleon]	rms [fm]	$1d_{5/2}$ [%]	$2s_{1/2}$ [%]
$v8$	- 6.44	2.843	2.08	4.26
$v14$	- 5.66	2.839	1.86	4.98
$v18$	- 4.79	2.840	1.77	3.83
$v14$ plus Urbana-V	- 7.00 (+ 0.27)	2.832	2.40	7.33
$v18$ plus Urbana-IX	- 5.90 (+ 0.27)	2.805	2.65	6.57
expt.	- 8.0	2.73 ± 0.025	2.17 ± 0.12	1.78 ± 0.36

5.2 Densities.

Fig. 5-1 shows the calculated charge density after folding the proton point density with the charge density of the proton and folding the neutron point density with the charge density of the neutron. Also ploted is the *experimental* charge density from Reference [Si-70]. As this



(a) NN interaction.

(b) NN and NNN interaction.

Figure 5-1 Comparison of the *experimental* with the calculated charge density.

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expansion is accurate up to terms of order q^4, it encompasses the result of the rms-radius. The resulting charge radii, shown in Table 5.2, are reasonably close to the experimental one.

In the calculation of the natural orbits we also generate the occupation probabilities for the orbits above the Fermi level. For the Argonne $v8$, $v14$ and $v18$ potentials the occupation probabilities of the $1d_{5/2}$ and the $2s_{1/2}$ proton orbits are summarized in Table 5.2. The occupation probabilities appear to be consistent with the experiment [Li-79], which establishes only the lower limit of these values.

The two-body density represents the probability of finding one nucleon at $\vec{r}_1$ and one nucleon at $\vec{r}_2$. We can divide this by the probability of finding the first nucleon at $\vec{r}_1$. The remaining density represents the probability of finding a second nucleon at $\vec{r}_2$ if the first nucleon is at $\vec{r}_1$. If both nucleons are protons, this density is normalised to a total integral of (Z-1). Figs. 5-2 and 5-3 show these densities for the Argonne $v18$ potential, as a function of $\vec{r}_2$ for various positions of $\vec{r}_1$. We have made no attempt to correct these for the residual CM motion of the nucleus. The densities show the effects of the short range repulsion: they exhibit a deep hole where the first nucleon is located. The fact that the bottom of this hole is not exactly at zero is the result of the approximations associated with our truncation scheme. The two-body densities also show that for large distances the long-range aspect of the ground state nuclear correlations, usually thought to be related with the surface deformation modes, has a significant contribution: when the first nucleon is located closer to the nuclear surface, we observe an enhancement of the density at the symmetrically-opposite position. The picture of a two-body density obtained as the revolution of the spherically symmetric one-body density, with a Gaussian-like distribution centered at the

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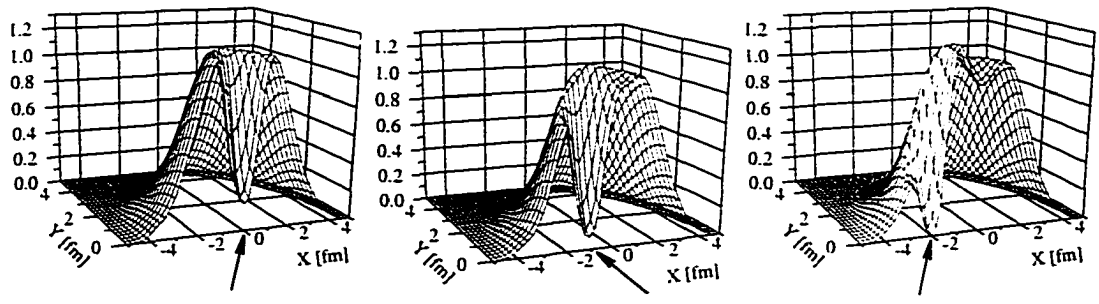
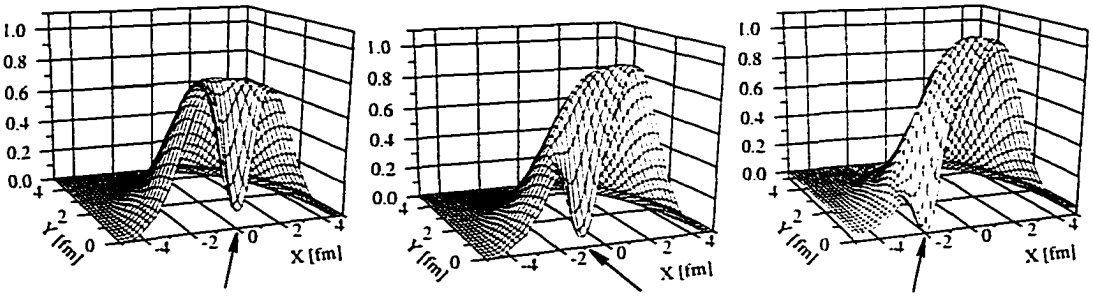


(a) $x_1 = 0.0fm$ (b) $x_1 = 1.0fm$ (c) $x_1 = 2.0fm$

Figure 5-2 The p-p two-body density for three different locations (x_1) of the first proton and the Argonne $v18$ potential.



(a) $x_1 = 0.0fm$ (b) $x_1 = 1.0fm$ (c) $x_1 = 2.0fm$

Figure 5-3 The p-n two-body density for three different proton locations (x_1) and the Argonne $v18$ potential.

location of the first nucleon scooped out of it, is definitely insufficient. For comparison, Figs. 5-4 and 5-5 show the p-p and p-n two-body densities for the Argonne $v18$ plus Urbana IX potential.

5.3 Conclusions.

The aim of this effort was to obtain a reasonable description of the ground state of ^{16}O that explicitly accounts for realistic correlations. We have chosen to describe correlations in configuration space and used the coupled cluster ($exp(\mathbf{S})$) method to calculate the ground

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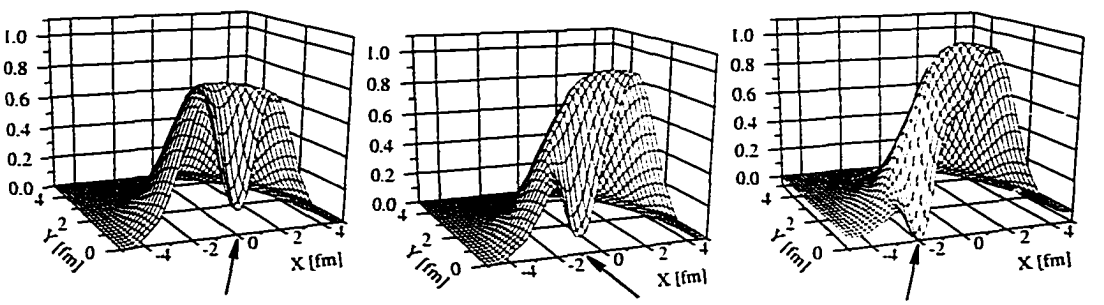
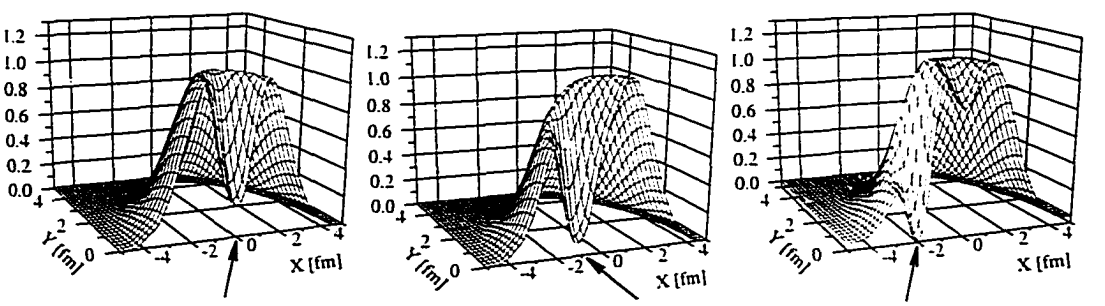


(a) $x_1 = 0.0fm$ (b) $x_1 = 1.0fm$ (c) $x_1 = 2.0fm$

Figure 5-4 The p-p two-body density for three different locations (x_1) of the first proton and the Argonne $v18$ plus Urbana IX potential.



(a) $x_1 = 0.0fm$ (b) $x_1 = 1.0fm$ (c) $x_1 = 2.0fm$

Figure 5-5 The p-n two-body density for three different proton locations (x_1) and the Argonne $v18$ plus Urbana IX potential.

state of ^{16}O.

We have shown that it is possible to choose large enough configuration spaces for the complete and self-consistent calculation of the ground state correlations inside a finite nucleus. This calculation makes no artificial separation between "short range" and "long range" correlations. In fact, the two-body density shows that the correlation function in the surface region of the nucleus has strong contributions from the surface deformation modes. It is largely these modes that cause the strong deoccupation of orbits close to the Fermi surface.

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As any approximation the results presented here are subject to possible improvement in the future. The influence of the size of the configuration space on the actual binding energies and form factors has not been completely explored due to the actual computational limitations. Even though great care has been taken to include all the important terms in our calculation, there is always a chance that a term felt to be small may prove itself to be of importance in a later calculation. With this in mind, the general techniques and conclusions presented here are believed at this time to remain unchanged. Investigations designed to limit the nature of these uncertainties are currently under way.

Calculations were carried out on a HP-9000/735 workstation at the Research Computing Center, and a dual-processor 200 MHz Pentium Pro PC at the Nuclear Physics Group of the University of New Hampshire.

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Bibliography

[Ba-61] F.C. Barker and L.J. Tassie, Il Nuovo Cimento **XIX**. 1211 (1961).

[Bi-91] R. F. Bishop, Theor. Chim. Acta **80**, 95 (1991).

[Ca-83] J. Carlson, V.R. Pandharipande, and R.B. Wiringa, Nucl. Phys. A **401**, 59 (1983).

[Cv-80] J. M. Cavedon, *Thesis de Doctoral d'Etat*, Paris (1980)

[Ch-85] C. R. Chen, G. L. Payne, J. L. Friar, and B. F. Gibson, Phys. Rev. C **31**, 2266 (1985).

[Co-58] F. Coester, Nucl. Phys. **7**, 421 (1958).

[Co-60] F. Coester and H. Kümmel, Nucl. Phys. **17**. 477 (1960).

[Da-95] J. F. Dawson, personal communication (1995).

[Ed-65] A.R. Edmonds, *Angular Momentum in Quantum Mechanics* Princeton University Press, Princeton, 3rd ed., (1965).

[El-54] J.P. Elliott and T.H.R. Skyrme, Proc. Phys. Soc. A **66**. 977 (1954).

[Fe-71] H. Feshbach, A. Gal, and J. Hüfner, Ann. Phys. **66**. 20 (1971).

[Fi-74] M. Fink, Nucl. Phys. A **221**, 163 (1974).

[Ga-57] S. Gartenhaus and C. Schwartz, Phys. Rev. **108**, 482 (1957).

[Gi-68] B.F. Gibson, A. Goldberg, and M.S. Weiss, Nucl. Phys. A **111**. 321 (1968).

[Go-80] D. Goutte, J. B. Bellicard, J. M. Cavedon, B. Frois, M. Huet, P. LeConte, Phan Xuan Ho, S. Platchkov, J. Heisenberg, J. Lichtenstadt, C. N. Papanicolas, and I. Sick, Phys. Rev. Lett. **45**, 1618 (1980).

[He-98a] J.H. Heisenberg and B. Mihaila, nucl-th/9802029 (1998).

[He-98b] J. H. Heisenberg and B. Mihaila, nucl-th/9802031 (1998).

[Ho-61] H. Horie and K. Sasaki, Prog. Theor. Phys. **25**, 475 (1961).

[Ki-93] A. Kievsky, M. Viviani, and S. Rosati, Nucl. Phys. A **551**, 241 (1993).

[Ki-94] A. Kievsky, M. Viviani, and S. Rosati, Nucl. Phys. A **577**, 511 (1994).

[Ku-78] H. Kümmel, K. H. Lührmann, and J. G. Zabolitzky, Phys. Reports **36**, 1 (1978).

[La-81] I. E. Lagaris and V.R. Pandharipande, Nucl. Phys. A **359**. 331 (1981).

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[Le-94] M. Leuschner, J. R. Calarco, F. W. Hersman, H. P. Blok, G. J. Kramer, L. Lapikás, G. van der Steenhoven, P. K. A. de Witt Huberts, and J. Friedrich, Phys. Rev. C **49**, 955 (1994).

[Li-79] J. Lichtenstadt, J. Heisenberg, C. N. Papanicolas, C. P. Sargent, A. N. Courtemanche, and J. S. McCarthy, Phys. Rev. C **20**, 497 (1979).

[Lp-58] H.J Lipkin, Phys. Rev. **110**, 1395 (1958).

[Mi-98a] B. Mihaila and J. H. Heisenberg, nucl-th/9802012 (1998).

[Mi-98b] B. Mihaila and J. H. Heisenberg, nucl-th/9802032 (1998).

[Pa-84] V. R. Pandharipande, C. N. Papanicolas, and J. Wambach, Phys. Rev. Lett. **53**, 1133 (1984).

[Pi-92] S. C. Pieper, R. B. Wiringa, and V. R. Pandharipande, Phys. Rev. C **46**, 1747 (1992).

[Pu-95] B. S. Pudliner, V. R. Pandharipande, J. Carlson, and R. B. Wiringa, Phys. Rev. Lett. **74**, 4396 (1995).

[Pu-97] B. S. Pudliner, V. R. Pandharipande, J. Carlson, S. C. Pieper, and R. B. Wiringa, nucl-th/9705009 (1997).

[Sc-90] R. Schiavilla, V. R. Pandharipande, and D. O. Riska, Phys. Rev. C **41**, 309 (1990).

[Sw-83] O. Schwentker, J. Dawson, J. Robb, J. Heisenberg, J. Lichtenstadt, C. N. Papanicolas, J. Wise, J. S. McCarthy, L. T. van der Bijl, and H. P. Blok, Phys. Rev. Lett. **50**, 15 (1983).

[Sh-74] A. deShalit and H. Feshbach, *Theoretical Nuclear Physics* John Wiley and Sons, New York, Vol. 1 (1979).

[Si-70] I. Sick and J.S. McCarthy, Nucl. Phys. A **150**, 631 (1970).

[Ta-59] L.J. Tassie and F.C. Barker, Phys. Rev. **111**, 940 (1959).

[Ub-71] H. Uberall, *Electron Scattering from Complex Nuclei* (Academic Press, New York, 1971), Vol. 1, p. 183.

[Wi-91] R. B. Wiringa, Phys. Rev. C **43**, 1585 (1991).

[Wi-95] R. B. Wiringa, V. G. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).

[Wt-91] H. Witala, W. Glöckle, and H. Kamada, Phys. Rev. C **43**, 1619 (1991).

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Appendices

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Appendix A

Two-Body Matrix Elements Calculation in the JJ Coupling.

As we have already shown in Chapter 2, it is most convenient to evaluate two-body matrix elements using the *ph* angular momentum coupling. According to our lemma 2, *ph* matrix elements factorize than in two parts, which only depend on the coordinates of the first or second particle, respectively. It is apparent then, that the appropriate angular momentum coupling for each single particle wave function $|\alpha\rangle$ is that when the individual orbital angular momentum l_α and spin s_α are coupled to a total angular momentum j_α. This is what we call the (lsj) coupling scheme.

In this chapter, we present the basics of the two-body matrix elements calculation. We first show how the radial part of the matrix element calculation is carried out, which is independent of what the actual angular part of the interaction is. The specifics related to the angular and/or spin part of the interaction are discussed in the next sections for the seven different operators corresponding to the Argonne $v18$ potential. As a preview, we take now the opportunity to review the fundamental theorems of the angular momentum calculus as presented in Ref. [Ed-65].

Theorem 1 *When the tensor operators $T^{(k_1)}$ and $U^{(k_2)}$ are built up from the same set of coordinates, the reduced matrix element of the tensor product $X^{(K)} = \left[T^{(k_1)} \otimes T^{(k_2)}\right]^{(K)}$ is given by:*

$$\langle \gamma'\ j' \parallel X^{(K)} \parallel \gamma\ j \rangle = (-)^{K+j+j'}\ \hat{K} \sum_{\gamma'' j''} \left\{ \begin{array}{ccc} k_1 & k_2 & K \\ j & j' & j'' \end{array} \right\} \langle \gamma'\ j' \parallel T^{(k_1)} \parallel \gamma''\ j'' \rangle \langle \gamma''\ j'' \parallel T^{(k_2)} \parallel \gamma\ j \rangle . \quad \text{(A.0.1)}$$

Theorem 2 *When the tensor operators $T^{(k_1)}$ and $U^{(k_2)}$ are supposed to work on parts 1 and 2 respectively of a system, the reduced matrix element of the tensor product $X^{(K)} = \left[T^{(k_1)} \otimes T^{(k_2)}\right]^{(K)}$ is given by:*

$$\langle \gamma'\ j'_1 j'_2\ J' \parallel X^{(K)} \parallel \gamma\ j_1 j_2\ J \rangle = \hat{K}\hat{J}\hat{J}' \left\{ \begin{array}{ccc} j'_1 & j_1 & k_1 \\ j'_2 & j_2 & k_2 \\ J & J' & K \end{array} \right\} \sum_{\gamma''} \langle \gamma'\ j'_1 \parallel T^{(k_1)} \parallel \gamma''\ j_1 \rangle \langle \gamma''\ j'_2 \parallel U^{(k_2)} \parallel \gamma''\ j_2 \rangle . \quad \text{(A.0.2)}$$

Here we use the notation $\hat{j} = \sqrt{2j+1}$.

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The following special cases prove themselves to be of a special interest.

Corollary 1 *Scalar product of two commuting tensor operators.*

$$\langle \gamma'\, j'_1 j'_2\, J' M' \mid \left(T^{(k)} \odot U^{(k)}\right) \mid \gamma\, j_1 j_2\, J M \rangle \;=\; \delta_{J J'}\, \delta_{M M'}\, (-)^{j_1+j'_2+J} \left\{ \begin{array}{ccc} J & j'_2 & j'_1 \\ k & j_1 & j_2 \end{array} \right\} \sum_{\gamma''} \langle \gamma'\, j'_1 \parallel T^{(k)} \parallel \gamma''\, j_1 \rangle\, \langle \gamma''\, j'_2 \parallel U^{(k)} \parallel \gamma''\, j_2 \rangle \;. \quad \text{(A.0.3)}$$

Corollary 2 *The reduced matrix element of a tensor operator $T^{(k)}$ working only on part 1 of a system, in the coupled scheme $(\gamma\, j_1 j_2\, J M)$, is*

$$\langle \gamma'\, j'_1 j_2\, J' \parallel T^{(k)} \parallel \gamma\, j_1 j_2\, J \rangle = (-)^{j'_1+j_2+J+k}\, \hat{J}\hat{J}' \left\{ \begin{array}{ccc} j'_1 & J' & j_2 \\ J & j_1 & k \end{array} \right\} \langle \gamma'\, j'_1 \parallel T^{(k)} \parallel \gamma\, j_1 \rangle \,. \quad \text{(A.0.4)}$$

Corollary 3 *Similarly, the reduced matrix element of a tensor operator $U^{(k)}$ working only on part 2 of a system, is*

$$\langle \gamma'\, j_1 j'_2\, J' \parallel U^{(k)} \parallel \gamma\, j_1 j_2\, J \rangle = (-)^{j_1+j_2+J'+k}\, \hat{J}\hat{J}' \left\{ \begin{array}{ccc} j'_2 & J' & j_1 \\ J & j_2 & k \end{array} \right\} \langle \gamma'\, j'_2 \parallel U^{(k)} \parallel \gamma\, j_2 \rangle \,. \quad \text{(A.0.5)}$$

Let us consider now, a couple of examples, which will allow us to introduce notations we will frequently be using in the next sections. Below, the operator $\mathcal{O}^k$ depends only on the angular momentum components, in a (lsj) scheme.

- $$\langle (l_1 \tfrac{1}{2})_{j_1} \parallel \mathcal{O}^{(k)} \parallel (l_2 \tfrac{1}{2})_{j_2} \rangle \;=\; F(l_1 j_1; l_2 j_2; k)\, \langle l_1 \parallel \mathcal{O}^{(k)} \parallel l_2 \rangle \,. \quad \text{(A.0.6)}$$

  with

  $$F(l_1 j_1; l_2 j_2; k) \;=\; (-)^{l_1+\kappa_2+k}\, \hat{j}_1 \hat{j}_2 \left\{ \begin{array}{ccc} l_1 & j_1 & \frac{1}{2} \\ j_2 & l_2 & k \end{array} \right\} . \quad \text{(A.0.7)}$$

- $$\langle (l_1 \tfrac{1}{2})_{j_1} \parallel \left[\mathcal{O}^{(k_1)} \otimes \sigma\right]^{(k_2)} \parallel (l_2 \tfrac{1}{2})_{j_2} \rangle \;=\; G(l_1 j_1; l_2 j_2; k_1 k_2)\, \langle l_1 \parallel \mathcal{O}^{(k_1)} \parallel l_2 \rangle \,, \quad \text{(A.0.8)}$$

  with

  $$G(l_1 j_1; l_2 j_2; k_1 k_2) \;=\; \sqrt{6}\, \hat{j}_1 \hat{j}_2 \hat{k}_2 \left\{ \begin{array}{ccc} l_1 & l_2 & k_1 \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_1 & j_2 & k_2 \end{array} \right\} . \quad \text{(A.0.9)}$$

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A.1 Radial Part of the Two-Body Matrix Elements.

The radial part of the two-body matrix elements is defined as

$$\begin{aligned} R^{\alpha\,\kappa}_{n_1 l_1\, n_2 l_2\,;\, n_3 l_3\, n_4 l_4} \;=\; & \frac{2}{\pi}\int_0^\infty p^2\,dp\; v_{\alpha\,\kappa}(p) \\ & \int_0^\infty r_1^2\,dr_1\; \mathcal{R}_{n_1 l_1}(r_1)\;\left(\mathcal{O}^{(1)}\mathcal{R}_{n_3 l_3}(r_1)\right)\; j_{k_1}(pr_1) \\ & \int_0^\infty r_2^2\,dr_2\; \mathcal{R}_{n_2 l_2}(r_2)\;\left(\mathcal{O}^{(2)}\mathcal{R}_{n_4 l_4}(r_2)\right)\; j_{k_2}(pr_2)\,. \end{aligned} \tag{A.1.1}$$

where

$$v_{\alpha\,\kappa}(p) \;=\; \int_0^\infty r^2\,dr\; r^\alpha\, V(r)\; j_\kappa(pr)\,. \tag{A.1.2}$$

Treating separately the integral

$$\int_0^\infty r_1^2\,dr_1\; \mathcal{R}_{n_1 l_1}(r_1)\;\left(\mathcal{O}^{(1)}\mathcal{R}_{n_3 l_3}(r_1)\right)\; j_{k_1}(pr_1)\,. \tag{A.1.3}$$

we shall first change variable from r_1 to $x_1 = \frac{1}{b}\,r_1$

$$\int_0^\infty x_1^2\,dx_1\; R_{n_1 l_1}(x_1)\;\left(\mathcal{O}^{(1)}R_{n_3 l_3}(x_1)\right)\; j_{k_1}(qx_1)\,. \tag{A.1.4}$$

and then one more time, from x_1 to $x'_1 = \sqrt{2}x_1$, to obtain

$$\frac{1}{(\sqrt{2})^3}\int_0^\infty x'^2_1\,dx'_1\; R_{n_1 l_1}(\tfrac{1}{\sqrt{2}}x'_1)\;\left(\mathcal{O}^{(1)}R_{n_3 l_3}(\tfrac{1}{\sqrt{2}}x'_1)\right)\; j_{k_1}(q'\,x'_1)\,. \tag{A.1.5}$$

with $pr_1 = qx_1 = q'\,x'_1$. In order to carry out the integral explicitly, we use the expansion

$$R_{n_1 l_1}(\tfrac{1}{\sqrt{2}}x'_1)\; R_{n_3 l_3}(\tfrac{1}{\sqrt{2}}x'_1) \;=\; \sum_n A^{nk_1}_{n_1 l_1\, n_3 l_3}\; \mathcal{HO}_{nk_1}(x'_1)\,. \tag{A.1.6}$$

and obtain

$$\frac{1}{(\sqrt{2})^3}\sum_n A^{nk_1}_{n_1 l_1\, n_3 l_3}\int_0^\infty x'^2_1\,dx'_1\; \mathcal{HO}_{nk_1}(x'_1)\; j_{k_1}(q'\,x'_1)\,. \tag{A.1.7}$$

Therefore, the integral (A.1.3) becomes

$$\begin{aligned} & \int_0^\infty r_1^2\,dr_1\; \mathcal{R}_{n_1 l_1}(r_1)\;\left(\mathcal{O}^{(1)}\mathcal{R}_{n_2 l_2}(r_1)\right)\; j_{k_1}(pr_1) \\ & = \frac{1}{(\sqrt{2})^3}\sum_n A^{nk_1}_{n_1 l_1\, n_3 l_3}\left[\sqrt{\frac{\pi}{2}}\,\widetilde{\mathcal{HO}}_{nk_1}(q')\right]\,. \end{aligned} \tag{A.1.8}$$

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where the coefficients $A^{nk_1}_{n_1 l_1\, n_3 l_3}$ are calculated as

$$A^{nk_1}_{n_1 l_1\, n_3 l_3} = \int_0^\infty x'^2_1\, dx'_1\; R_{n_1 l_1}(\tfrac{1}{\sqrt{2}}x'_1)\; \left(\mathcal{O}^{(1)} R_{n_3 l_3}(\tfrac{1}{\sqrt{2}}x'_1)\right)\; \mathcal{HO}_{nk_1}(x'_1)\,. \qquad \text{(A.1.9)}$$

Similarly, we have:

$$\int_0^\infty r_2^2\, dr_2\; \mathcal{R}_{n_2 l_2}(r_2)\; \left(\mathcal{O}^{(2)} \mathcal{R}_{n_4 l_4}(r_2)\right)\; j_{k_2}(pr_2)$$
$$= \frac{1}{(\sqrt{2})^3} \sum_m A^{mk_2}_{n_2 l_2\, n_4 l_4}\; \left[\sqrt{\frac{\pi}{2}}\; \widetilde{\mathcal{HO}}_{mk_2}(q')\right]\,. \qquad \text{(A.1.10)}$$

where the coefficients $A^{mk_2}_{n_2 l_2\, n_4 l_4}$ are given as

$$A^{mk_2}_{n_2 l_2\, n_4 l_4} = \int_0^\infty x'^2_2\, dx'_2\; R_{n_2 l_2}(\tfrac{1}{\sqrt{2}}x'_2)\; \left(\mathcal{O}^{(2)} R_{n_4 l_4}(\tfrac{1}{\sqrt{2}}x'_2)\right)\; \mathcal{HO}_{mk_2}(x'_2)\,. \qquad \text{(A.1.11)}$$

Using Equations (A.1.8) and (A.1.10), the radial part of the two-body matrix elements becomes

$$R^{\alpha\kappa}_{n_1 l_1\, n_2 l_2\, :\, n_3 l_3\, n_4 l_4}$$
$$= \frac{1}{2^3} \int_0^\infty p^2\, dp\; v_{\alpha\kappa}(p) \sum_n A^{nk_1}_{n_1 l_1\, n_3 l_3}\; \widetilde{\mathcal{HO}}_{nk_1}(q') \sum_m A^{mk_2}_{n_2 l_2\, n_4 l_4}\; \widetilde{\mathcal{HO}}_{mk_2}(q')$$
$$= \frac{1}{(\sqrt{2}\,b)^3} \sum_n A^{nk_1}_{n_1 l_1\, n_3 l_3} \sum_m A^{mk_2}_{n_2 l_2\, n_4 l_4}$$
$$\int_0^\infty q'^2\, dq'\; v_{\alpha\kappa}(\tfrac{\sqrt{2}}{b}q')\; \widetilde{\mathcal{HO}}_{nk_1}(q')\; \widetilde{\mathcal{HO}}_{mk_2}(q')\,. \qquad \text{(A.1.12)}$$

Here we have $q' = \frac{b}{\sqrt{2}}p$.

A.2 Central Interaction.

The simplest possible interaction is the so-called central interaction. where the unity operator comes multiplied by a function which depends only on the magnitude of the relative distance r between the two particles.

$$V_C = V_c(r)C^{(0)}(\hat{r}) = \sum_k (2k+1)\; u^{(kk;0)}(r_1, r_2)\; \left(C^{(k)}(\hat{r}_1) \cdot C^{(k)}(\hat{r}_2)\right)\,. \qquad \text{(A.2.1)}$$

The following procedure will be used over and over again in the remainder of this chapter: we use lemma 1 and convert $V_c(r)C^{(0)}(\hat{r})$ into an expression where $\vec{r}_1$ and $\vec{r}_2$ appear separately in different operators. Then we use lemma 2 to calculate the *ph* matrix element of the corresponding interaction.

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Note. All matrix elements presented in this chapter must be multiplied by the constant factor $(-)^{j_2+j_4+1}/(2\lambda+1)$. This factor appears in the expression of the *ph* matrix elements as shown in lemma 2 and has been intentionally left out.

In the case of the central interaction this procedure leads to

$$\begin{aligned}
&\langle n_1 n_3 \,;\, (l_1\tfrac{1}{2})_{j_1}(l_3\tfrac{1}{2})_{j_3}^{-} \,;\, \lambda\mu \mid V_C \mid n_4 n_2 \,;\, (l_4\tfrac{1}{2})_{j_4}(l_2\tfrac{1}{2})_{j_2}^{-} \,:\, \lambda\mu\rangle \\
&\quad = \sum_k (2k+1)\; u^{(kk;00)}(r_1, r_2)\; \delta_{k\lambda} \\
&\qquad \langle (l_1\tfrac{1}{2})_{j_1} \mid C^{(k)}(\hat{r_1}) \mid (l_3\tfrac{1}{2})_{j_3}\rangle\; \langle (l_2\tfrac{1}{2})_{j_2} \mid C^{(k)}(\hat{r_2}) \mid (l_4\tfrac{1}{2})_{j_4}\rangle\,. \qquad \text{(A.2.2)}
\end{aligned}$$

which results into

$$\begin{aligned}
&\langle n_1 n_3 \,;\, (l_1\tfrac{1}{2})_{j_1}(l_3\tfrac{1}{2})_{j_3}^{-} \,;\, \lambda\mu \mid V_C \mid n_4 n_2 \,;\, (l_4\tfrac{1}{2})_{j_4}(l_2\tfrac{1}{2})_{j_2}^{-} \,:\, \lambda\mu\rangle \\
&\quad = (2\lambda+1)\; u^{(\lambda\lambda;00)}(r_1, r_2) \\
&\qquad F(l_1 j_1; l_3 j_3; \lambda)\; \langle l_1 \parallel C^{(\lambda)} \parallel l_3\rangle\; F(l_2 j_2; l_4 j_4; \lambda)\; \langle l_2 \parallel C^{(\lambda)} \parallel l_4\rangle\,. \qquad \text{(A.2.3)}
\end{aligned}$$

A.3 Spin-Spin Interaction.

By definition, the spin-spin interaction is introduced as

$$V_S \;=\; V_s(r)\; \sigma_1 \cdot \sigma_2\,. \qquad \text{(A.3.1)}$$

where

$$\sigma_1 \cdot \sigma_2 \;=\; -\sqrt{3}\; [\sigma_1 \otimes \sigma_2]^{(0)} \qquad \text{(A.3.2)}$$

Then, we get

$$\begin{aligned}
\sigma_1 \cdot \sigma_2 \;\Rightarrow\; & -\sqrt{3}\; \left[\left[C^{(k)}(\hat{r_1}) \otimes C^{(k)}(\hat{r_2}) \right]^{(0)} \otimes [\sigma_1 \otimes \sigma_2]^{(0)} \right]^{(0)} \\
&= \sum_l \frac{(-)^{l+1}}{\sqrt{2k+1}} \left(\left[C^{(k)}(\hat{r_1}) \otimes \sigma_1 \right]^{(l)} \otimes \left[C^{(k)}(\hat{r_2}) \otimes \sigma_2 \right]^{(l')} \right)\,, \qquad \text{(A.3.3)}
\end{aligned}$$

and obtain

$$\begin{aligned}
&\langle n_1 n_3 \,;\, (l_1\tfrac{1}{2})_{j_1}(l_3\tfrac{1}{2})_{j_3}^{-} \,;\, \lambda\mu \mid V_S \mid n_4 n_2 \,;\, (l_4\tfrac{1}{2})_{j_4}(l_2\tfrac{1}{2})_{j_2}^{-} \,:\, \lambda\mu\rangle \\
&\quad = (-)^{\lambda+1} \sum_k (-)^k\; (2k+1)\; u^{(kk;00)}(r_1, r_2) \\
&\qquad G(l_1 j_1; l_3 j_3; k\lambda)\; \langle l_1 \parallel C^{(k)} \parallel l_3\rangle\; G(l_2 j_2; l_4 j_4; k\lambda)\; \langle l_2 \parallel C^{(k)} \parallel l_4\rangle\,, \qquad \text{(A.3.4)}
\end{aligned}$$

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

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A.4 Tensor Interaction.

The tensor interaction is introduced as:

$$V_T = V_t(r)\, S_{12}\,. \tag{A.4.1}$$

where

$$\begin{aligned} S_{12} \;=\; 3(\sigma_1\cdot\hat{r})(\sigma_2\cdot\hat{r}) - \sigma_1\cdot\sigma_2 \;&=\; \sqrt{6}\,\Big(\, C^{(2)}(\hat{r}) \odot [\sigma_1 \odot \sigma_2]^{(2)} \,\Big) \\ &=\; \sqrt{30}\,\Big[\, C^{(2)}(\hat{r}) \odot [\sigma_1 \odot \sigma_2]^{(2)} \,\Big]^{(0)}\,. \end{aligned} \tag{A.4.2}$$

Similar to the previous interactions, we use lemma 1, in order to decouple the $\vec{r}_1$ and $\vec{r}_2$ degrees of freedom. Then we use lemma 2 to calculate the *ph* matrix element of the tensor interaction. We obtain

$$\begin{aligned} &\langle n_1 n_3\,;\, (l_1\tfrac{1}{2})_{j_1}(l_3\tfrac{1}{2})_{j_3}^{-}\,;\, \lambda\mu \mid V_T \mid n_4 n_2\,;\, (l_4\tfrac{1}{2})_{j_4}(l_2\tfrac{1}{2})_{j_2}^{-}\,;\, \lambda\mu\rangle \\ &= \sqrt{6}\sum_{k_1}(2k_1+1)\,G(l_1 j_1; l_3 j_3; k_1\lambda)\,\langle l_1 \parallel C^{(k_1)} \parallel l_3\rangle \\ &\quad \sum_{k_2} i^{k_1+k_2}\, u^{(k_1 k_2;20)}(r_1,r_2)\,(2k_2+1)\,\langle k_1\,0\,k_2\,0 \mid 2\,0\rangle \begin{Bmatrix} k_1 & k_2 & 2 \\ 1 & 1 & \lambda \end{Bmatrix} \\ &\quad G(l_2 j_2; l_4 j_4; k_2\lambda)\,\langle l_2 \parallel C^{(k_2)} \parallel l_4\rangle\,. \end{aligned} \tag{A.4.3}$$

A.5 Spin-Orbit Interaction.

The spin-orbit interaction is given by:

$$V_{LS} \;=\; V_{ls}(r)\,\vec{L}\cdot\vec{S}\,. \tag{A.5.1}$$

where

$$\begin{aligned} \vec{L} \;&=\; \frac{1}{2}\,\vec{r}\times(\vec{p}_2-\vec{p}_1) = \frac{(-i)}{2}\vec{r}\times(\vec{\nabla}_{(2)}-\vec{\nabla}_{(1)})\,. \\ \vec{S} \;&=\; \frac{1}{2}(\vec{\sigma}_1+\vec{\sigma}_2)\,. \end{aligned} \tag{A.5.2}$$

are the orbital angular momentum operator in relative motion and the total spin operator. Using:

- $r_m \;=\; r\,C^{(1)}_m(\hat{r})\,,$
- $[x \odot y]^{(1)}_m \;=\; \dfrac{-i}{\sqrt{2}}\,(\vec{x}\times\vec{y})_m\,,$

we can write

$$\begin{aligned} V_{ls}(r)\vec{L} \;&=\; \frac{1}{2}\,V_{ls}(r)\,\vec{r}\times(\vec{p}_2-\vec{p}_1) \\ &=\; (i\sqrt{2})\,r\,V_{ls}(r)\,\Big[C^{(1)}(\hat{r})\odot(p_2-p_1)\Big]^{(1)} \\ &=\; \sqrt{2}\,r\,V_{ls}(r)\,\Big[\,C^{(1)}(\hat{r})\odot(\nabla_{(2)}-\nabla_{(1)})\,\Big]^{(1)}\,. \end{aligned} \tag{A.5.3}$$

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Then, for $k = 1$ we obtain:

$$rV_{ls}(r)\, C^{(1)}(\hat{r}) = \sum_{k_1 k_2} i^{k_2-k_1-1} \frac{(2k_1+1)(2k_2+1)}{3\sqrt{2}} \langle k_1\, 0\, k_2\, 0 \mid 1\, 0\rangle \; u^{(k_1 k_2, 11)}(r_1, r_2) \left[C^{(k_1)}(\hat{r}_1) \odot C^{(k_2)}(\hat{r}_2)\right]^{(1)} . \quad \text{(A.5.4)}$$

Recoupling the $C^{(k_1)}(\hat{r}_1)$ and $C^{(k_2)}(\hat{r}_2)$ operators with the appropriate gradient operator, we get:

$$\begin{aligned} V_{ls}(r)\vec{L} = & \sum_{k_1 k_2} i^{k_2-k_1-1} (2k_1+1)(2k_2+1) \langle k_1\, 0\, k_2\, 0 \mid 1\, 0\rangle \\ & \sum_k \sqrt{\frac{2k+1}{6}} \begin{Bmatrix} k_1 & k_2 & 1 \\ 1 & 1 & k \end{Bmatrix} u^{(k_1 k_2, 11)}(r_1, r_2) \\ & \Big\{ - \left[C^{(k_1)}(\hat{r}_1) \odot \left[C^{(k_2)}(\hat{r}_2) \odot \nabla_{(2)}\right]^{(k)}\right]^{(1)} \\ & + (-)^{k+k_2+1} \left[\left[C^{(k_1)}(\hat{r}_1) \odot \nabla_{(1)}\right]^{(k)} \odot C^{(k_2)}(\hat{r}_2)\right]^{(1)} \Big\} . \end{aligned} \quad \text{(A.5.5)}$$

From the triangle conditions characterizing the angular momentum arguments of the $6j$ symbol, we get the conditions: $|k_1 - k_2| \leq 1 \leq k_1 + k2$, $|k_2 - 1| \leq k \leq k_2 + 1$ and $|k_1 - 1| \leq k \leq k_1 + 1$. We conclude that k equals either k_1 or k_2. Therefore, Eq. (A.5.5) can be rewritten as:

$$\begin{aligned} V_{ls}(r)\vec{L} = & \frac{1}{\sqrt{2}} \sum_{k_1 k_2} i^{k_1+k_2+1} (2k_1+1)(2k_2+1) \langle k_2\, 0\, 1\, 0 \mid k_1\, 0\rangle \begin{Bmatrix} k_1 & k_2 & 1 \\ 1 & 1 & k_1 \end{Bmatrix} \\ & \Big\{ - u^{(k_1 k_2, 11)}(r_1, r_2) \left[C^{(k_1)}(\hat{r}_1) \odot \left[C^{(k_2)}(\hat{r}_2) \odot \nabla_{(2)}\right]^{(k_1)}\right]^{(1)} \\ & + u^{(k_1 k_2, 11)}(r_1, r_2) \left[\left[C^{(k_1)}(\hat{r}_1) \odot \nabla_{(1)}\right]^{(k_1)} \odot C^{(k_2)}(\hat{r}_2)\right]^{(1)} \\ & + u^{(k_2 k_1, 11)}(r_1, r_2) \left[C^{(k_2)}(\hat{r}_1) \odot \left[C^{(k_1)}(\hat{r}_2) \odot \nabla_{(2)}\right]^{(k_1)}\right]^{(1)} \\ & + u^{(k_2 k_1, 11)}(r_1, r_2) \left[\left[C^{(k_2)}(\hat{r}_1) \odot \nabla_{(1)}\right]^{(k_1)} \odot C^{(k_1)}(\hat{r}_2)\right]^{(1)} \Big\} . \end{aligned} \quad \text{(A.5.6)}$$

with $k_1 + k_2 + 1$ even.

Taking the inner products of Eq. (A.5.6) with $\vec{S}$ and using the identities

$$\left(\left[A^{(k)}_{(1)} \odot B^{(l)}_{(2)}\right]^{(1)} \odot \sigma_{(1)}\right) = (-)^k \sqrt{\frac{3}{2l+1}} \left(\left[A^{(k)}_{(1)} \odot \sigma_1\right]^{(l)} \odot B^{(l)}_{(2)}\right) \quad \text{(A.5.7)}$$

$$\left(\left[A^{(k)}_{(1)} \odot B^{(l)}_{(2)}\right]^{(1)} \odot \sigma_2\right) = -(-)^k \sqrt{\frac{3}{2k+1}} \left(A^{(k)}_{(1)} \odot \left[B^{(l)}_{(2)} \odot \sigma_2\right]^{(k)}\right) \quad \text{(A.5.8)}$$

the operators in Eq. (A.5.6) result into the following four contributions to the *ph*-coupled matrix element $\langle n_1 n_3 \,;\, (l_1 \tfrac{1}{2})_{j_1} (l_3 \tfrac{1}{2})_{j_3} \,;\, \lambda\mu \mid V_{LS} \mid n_4 n_2 \,;\, (l_4 \tfrac{1}{2})_{j_4} (l_2 \tfrac{1}{2})_{j_2} \,;\, \lambda\mu\rangle$

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A.

$$\left(\left[C^{(k_1)}(\hat{r}_1)\otimes\left[C^{(k_2)}(\hat{r}_2)\otimes\nabla_{(2)}\right]^{(k_1)}\right]^{(1)}\odot S\right)$$
$$=\frac{(-)^{k_1}}{2}\sqrt{\frac{3}{2k_1+1}}\left\{\left(\left[C^{(k_1)}(\hat{r}_1)\otimes\sigma_1\right]^{(k_1)}\odot\left[C^{(k_2)}(\hat{r}_2)\odot\nabla_{(2)}\right]^{(k_1)}\right)\right.$$
$$\left.-\left(C^{(k_1)}(\hat{r}_1)\odot\left[\left[C^{(k_2)}(\hat{r}_2)\otimes\nabla_{(2)}\right]^{(k_1)}\odot\sigma_2\right]^{(k_1)}\right)\right\} \tag{A.5.9}$$

$$\Rightarrow\frac{(-)^{\lambda}}{2}\sqrt{\frac{3}{2\lambda+1}}\,\delta_{k_1\lambda}$$
$$\left\{G(l_1j_1;l_3j_3;\lambda\lambda)\,\langle l_1\parallel C^{(\lambda)}\parallel l_3\rangle\,F(l_2j_2;l_4j_4;\lambda)\,CG_2(\lambda k_2.\,k_2\lambda)\right.$$
$$\left.-F(l_1j_1;l_3j_3;\lambda)\,\langle l_1\parallel C^{(\lambda)}\parallel l_3\rangle\,G(l_2j_2;l_4j_4;\lambda\lambda)\,CG_2(\lambda k_2.\,k_2\lambda)\right\} \tag{A.5.10}$$

B.

$$\left(\left[\left[C^{(k_1)}(\hat{r}_1)\otimes\nabla_{(1)}\right]^{(k_1)}\otimes C^{(k_2)}(\hat{r}_2)\right]^{(1)}\odot S\right)$$
$$=(-)^{k_1}\,\frac{\sqrt{3}}{2}\left\{\frac{1}{\sqrt{2k_2+1}}\left(\left[\left[C^{(k_1)}(\hat{r}_1)\odot\nabla_{(1)}\right]^{(k_1)}\odot\sigma_1\right]^{(k_2)}\odot C^{(k_2)}(\hat{r}_2)\right)\right.$$
$$\left.-\frac{1}{\sqrt{2k_1+1}}\left(\left[C^{(k_1)}(\hat{r}_1)\odot\nabla_{(1)}\right]^{(k_1)}\odot\left[C^{(k_2)}(\hat{r}_2)\odot\sigma_2\right]^{(k_1)}\right)\right\} \tag{A.5.11}$$

$$\Rightarrow\frac{(-)^{k_1}}{2}\sqrt{\frac{3}{2\lambda+1}}$$
$$\left\{\delta_{k_2\lambda}\,G(l_1j_1;l_3j_3;k_1\lambda)\,CG_1(k_1\lambda,k_1k_1)\,F(l_2j_2;l_4j_4;\lambda)\,\langle l_2\parallel C^{(\lambda)}\parallel l_4\rangle\right.$$
$$\left.-\delta_{k_1\lambda}\,F(l_1j_1;l_3j_3;\lambda)\,CG_1(\lambda k_2,\lambda\lambda)\,G(l_2j_2;l_4j_4;k_2\lambda)\,\langle l_2\parallel C^{(k_2)}\parallel l_4\rangle\right\} \tag{A.5.12}$$

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C.

$$\left(\left[C^{(k_2)}(\hat{r}_1)\otimes\left[C^{(k_1)}(\hat{r}_2)\otimes\nabla_{(2)}\right]^{(k_1)}\right]^{(1)}\odot S\right)$$
$$=\frac{(-)^{k_2}}{2}\sqrt{3}\left\{\frac{1}{\sqrt{2k_1+1}}\left(\left[C^{(k_2)}(\hat{r}_1)\otimes\sigma_1\right]^{(k_1)}\odot\left[C^{(k_1)}(\hat{r}_2)\odot\nabla_{(2)}\right]^{(k_1)}\right)\right.$$
$$\left.-\frac{1}{\sqrt{2k_2+1}}\left(C^{(k_2)}(\hat{r}_1)\odot\left[\left[C^{(k_1)}(\hat{r}_2)\odot\nabla_{(2)}\right]^{(k_1)}\odot\sigma_2\right]^{(k_2)}\right)\right\} \tag{A.5.13}$$

$$\Rightarrow\frac{(-)^{k_2}}{2}\sqrt{\frac{3}{2\lambda+1}}$$
$$\left\{\delta_{k_1\lambda}\,G(l_1j_1;l_3j_3;k_2\lambda)\,\langle l_1\parallel C^{(k_2)}\parallel l_3\rangle\,F(l_2j_2;l_4j_4;\lambda)\,CG_2(k_2\lambda,\lambda\lambda)\right.$$
$$\left.-\delta_{k_2\lambda}\,F(l_1j_1;l_3j_3;\lambda)\,\langle l_1\parallel C^{(\lambda)}\parallel l_3\rangle\,G(l_2j_2;l_4j_4;k_1\lambda)\,CG_2(\lambda k_1,k_1k_1)\right\} \tag{A.5.14}$$

D.

$$\left(\left[\left[C^{(k_2)}(\hat{r}_1)\otimes\nabla_{(1)}\right]^{(k_1)}\otimes C^{(k_1)}(\hat{r}_2)\right]^{(1)}\odot S\right)$$
$$=\frac{(-)^{k_1}}{2}\sqrt{\frac{3}{2k_1+1}}\left\{\left(\left[\left[C^{(k_2)}(\hat{r}_1)\otimes\nabla_{(1)}\right]^{(k_1)}\odot\sigma_1\right]^{(k_1)}\odot C^{(k_1)}(\hat{r}_2)\right)\right.$$
$$\left.-\left(\left[C^{(k_2)}(\hat{r}_1)\otimes\nabla_{(1)}\right]^{(k_1)}\odot\left[C^{(k_1)}(\hat{r}_2)\odot\sigma_2\right]^{(k_1)}\right)\right\} \tag{A.5.15}$$

$$\Rightarrow\frac{(-)^{\lambda}}{2}\sqrt{\frac{3}{2\lambda+1}}\,\delta_{k_1\lambda}$$
$$\left\{G(l_1j_1;l_3j_3;\lambda\lambda)\,CG_1(k_2\lambda,k_2\lambda)\,F(l_2j_2;l_4j_4;\lambda)\,\langle l_2\parallel C^{(\lambda)}\parallel l_4\rangle\right.$$
$$\left.-F(l_1j_1;l_3j_3;\lambda)\,CG_1(k_2\lambda,k_2\lambda)\,G(l_2j_2;l_4j_4;\lambda\lambda)\,\langle l_2\parallel C^{(\lambda)}\parallel l_4\rangle\right\} \tag{A.5.16}$$

where

$$CG_1(k_1k_2,l_1l_2) = \langle n_1n_2\,;\,l_1\parallel u^{(k_1k_2,11)}(r_1,r_2)\,\left[C^{(l_1)}(\hat{r}_1)\odot\nabla_{(1)}\right]^{(l_2)}\parallel n_3n_4\,;\,l_3\rangle\,, \tag{A.5.17}$$

$$CG_2(k_1k_2,l_1l_2) = \langle n_1n_2\,;\,l_2\parallel u^{(k_1k_2,11)}(r_1,r_2)\,\left[C^{(l_1)}(\hat{r}_2)\odot\nabla_{(2)}\right]^{(l_2)}\parallel n_3n_4\,;\,l_4\rangle\,. \tag{A.5.18}$$

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A.6 L^2 Interaction.

The L^2 interaction is given by:

$$V_{L2} = V_{l2}(r)\, L^2 \tag{A.6.1}$$

where

$$\begin{aligned} L^2 = \vec{L}\cdot\vec{L} &= (-)\sqrt{3}\,[L \circledcirc L]^{(0)} \\ &= (-\sqrt{3})\,\frac{(i\sqrt{2})^2}{4}\,[[r \circledcirc (p_2 - p_1)]^{(1)} \circledcirc [r \circledcirc (p_2 - p_1)]^{(1)}]^{(0)} . \end{aligned} \tag{A.6.2}$$

Since by definition, the spherical components of a vector are

$$a_\pm = \mp\frac{1}{\sqrt{2}}(a_x \pm i\, a_y): \quad a_0 = a_z . \tag{A.6.3}$$

we can show that

$$[r_m, p_n] = (-)^m i\delta_{n-m} \tag{A.6.4}$$

and

$$\begin{aligned} [(r_2 - r_1)_m, (p_2 - p_1)_n] &= r_m(p_2 - p_1)_n - (p_2 - p_1)_n r_m \\ &= [(r_2)_m, (p_2)_n] + [(r_1)_m, (p_1)_n] = (-)^m\, 2i\, \delta_{n-m} . \end{aligned} \tag{A.6.5}$$

Based on this result, we can change the coupling scheme and combine the two $\vec{r}$ s together into a single tensor operator dependent on the relative coordinate unit vector:

$$\begin{aligned} &[[r \circledcirc (p_2 - p_1)]^{(1)} \circledcirc [r \circledcirc (p_2 - p_1)]^{(1)}]^{(J)}_m \\ &= \sum_{m_1 n_1 m_2 n_2 Q_1 Q_2} \langle 1\, m_1\, 1\, n_1 \mid 1\, Q_1\rangle\langle 1\, m_2\, 1\, n_2 \mid 1\, Q_2\rangle \\ &\qquad \langle 1\, Q_1\, 1\, Q_2 \mid j\, m\rangle r_{m_1}(p_2 - p_1)_{m_1} r_{m_2}(p_2 - p_1)_{n_2} \\ &= 3\, r^2 \sum_{\kappa\kappa'} \sqrt{(2\kappa+1)\,(2\kappa'+1)} \begin{Bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ \kappa & \kappa' & j \end{Bmatrix} \langle 1\,0\,1\,0 \mid \kappa\,0\rangle \\ &\qquad \left[C^{(\kappa)}(\hat{r}) \circledcirc [(p_2 - p_1) \circledcirc (p_2 - p_1)]^{(\kappa')}\right]^{(J)}_m \\ &\quad + 6i\, r\, (-)^{-j} \begin{Bmatrix} 1 & 1 & 1 \\ 1 & 1 & j \end{Bmatrix} \left[C^{(1)}(\hat{r}) \circledcirc (p_2 - p_1)\right]^{(J)}_m . \end{aligned} \tag{A.6.6}$$

- *Note 1.* Neither κ or κ' may be equal to one, because of the cross product $\vec{a}\times\vec{a} = 0$. Therefore, the admissible values for κ and κ' are 0 and 2.

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- *Note 2.* In the particular case of the L^2 interaction, the rank j is equal to zero, and by the symmetry properties of the Wigner $9-j$ symbol we have:

$$\left\{ \begin{array}{ccc} 1 & 1 & 1 \\ 1 & 1 & 1 \\ \kappa & \kappa' & 0 \end{array} \right\} = \delta_{\kappa'\kappa} \left\{ \begin{array}{ccc} 1 & 1 & 1 \\ 1 & 1 & 1 \\ \kappa & \kappa & 0 \end{array} \right\} . \tag{A.6.7}$$

Thus, the tensor product form of the L^2 interaction is

$$\begin{aligned} L^2 &= \frac{\sqrt{3}}{2} \left[[r \otimes (p_2 - p_1)]^{(1)} \odot [r \otimes (p_2 - p_1)]^{(1)} \right]^{(0)} \\ &= i \frac{3}{2} r^2 \sum_{\kappa=0,2} \sqrt{2\kappa+1} \left\{ \begin{array}{ccc} 1 & 1 & 1 \\ 1 & 1 & \kappa \end{array} \right\} \langle 1\,0\,1\,0 \mid \kappa 0 \rangle \\ &\qquad \left[C^{(\kappa)}(\hat{r}) \odot [(p_2 - p_1) \odot (p_2 - p_1)]^{(\kappa)} \right]^{(0)} \\ &\quad - i\sqrt{3}\, r \left[C^{(1)}(\hat{r}) \odot (p_2 - p_1) \right]^{(0)} . \end{aligned} \tag{A.6.8}$$

or, equivalently,

$$\begin{aligned} L^2 &= \frac{3}{2} r^2 \sum_{\kappa=0,2} \sqrt{2\kappa+1} \left\{ \begin{array}{ccc} 1 & 1 & 1 \\ 1 & 1 & \kappa \end{array} \right\} \langle 1\,0\,1\,0 \mid \kappa 0 \rangle \\ &\qquad \left[C^{(\kappa)}(\hat{r}) \odot [(\nabla_{(2)} - \nabla_{(1)}) \odot (\nabla_{(2)} - \nabla_{(1)})]^{(\kappa)} \right]^{(0)} \\ &\quad - \sqrt{3}\, r \left[C^{(1)}(\hat{r}) \odot (\nabla_{(2)} - \nabla_{(1)}) \right]^{(0)} . \end{aligned} \tag{A.6.9}$$

We expand the unnormalized spherical harmonics $C^{(\kappa)}(\hat{r})$ and $C^{(1)}(\hat{r})$ lemma 1

$$\begin{aligned} V_{l2}(r) L^2 &= \frac{3}{2} \sum_{\kappa=0,2} \frac{1}{\sqrt{2\kappa+1}} \left\{ \begin{array}{ccc} 1 & 1 & 1 \\ 1 & \kappa & 1 \end{array} \right\} \langle 1\,0\,1\,0 \mid \kappa 0 \rangle \\ &\qquad \sum_{k_1 k_2} i^{k_2 - k_1 - \kappa} (2k_1+1)(2k_2+1) \langle k_1\,0\,k_2\,0 \mid \kappa 0 \rangle\, u^{(k_1 k_2 \kappa 2)}(r_1, r_2) \\ &\qquad \left[\left[C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(\kappa)} \odot [(\nabla_{(2)} - \nabla_{(1)}) \odot (\nabla_{(2)} - \nabla_{(1)})]^{(\kappa)} \right]^{(0)} \\ &\quad - \frac{1}{\sqrt{3}} \sum_{k_1 k_2} i^{k_2 - k_1 - 1} (2k_1+1)(2k_2+1) \langle k_1\,0\,k_2\,0 \mid 1\,0 \rangle\, u^{(k_1 k_2 11)}(r_1, r_2) \\ &\qquad \left\{ \left[\left[C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \odot \nabla_{(2)} \right]^{(0)} \right. \\ &\qquad\quad \left. - \left[\left[C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2) \right]^{(1)} \odot \nabla_{(1)} \right]^{(0)} \right\} . \end{aligned} \tag{A.6.10}$$

We shall find now what the contributions of the operators in Eq. (A.6.10) to the matrix element $\langle n_1 n_3 ; (l_1 \tfrac{1}{2})_{j_1} (l_3 \tfrac{1}{2})_{j_3} ; \lambda\mu \mid V_{L2} \mid n_4 n_2 ; (l_4 \tfrac{1}{2})_{j_4} (l_2 \tfrac{1}{2})_{j_2} ; \lambda\mu \rangle$ are.

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We shall encounter similar operators to those shown in Eq. (A.6.17) a little later in this chapter, when we will be dealing with the quadrupole spin-orbit interaction, with the only difference being that the overall rank of the tensor product will be equal to 2. Therefore, it is useful to derive here results valid for an arbitrary even rank j.

First, we notice the matrix elements of the operators in the second sum are very similar to those discussed in the previous section. We have:

$$\left[\left[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\right]^{(1)}\otimes\nabla_{(2)}\right]^{(j)}$$
$$=(-)^j\sqrt{3}\sum_k\sqrt{2k+1}\begin{Bmatrix}k_1 & k_2 & 1\\ 1 & j & k\end{Bmatrix}\left[C^{(k_1)}(\hat{r}_1)\otimes\left[C^{(k_2)}(\hat{r}_2)\otimes\nabla_{(2)}\right]^{(k)}\right]^{(j)} \tag{A.6.11}$$

$$\left[\left[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\right]^{(1)}\otimes\nabla_{(1)}\right]^{(0)}$$
$$=(-)^{k_2}\sqrt{3}\sum_k(-)^k\sqrt{2k+1}\begin{Bmatrix}k_2 & k_1 & 1\\ 1 & j & k\end{Bmatrix}\left[\left[C^{(k_1)}(\hat{r}_1)\otimes\nabla_{(1)}\right]^{(k)}\otimes C^{(k_2)}(\hat{r}_2)\right]^{(j)} \tag{A.6.12}$$

For the L^2 interactions, we are of course interested only in the case of $j=0$. We get:

D.

$$\left[\left[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\right]^{(1)}\otimes\nabla_{(2)}\right]^{(0)}$$
$$=\left[C^{(k_1)}(\hat{r}_1)\otimes\left[C^{(k_2)}(\hat{r}_2)\otimes\nabla_{(2)}\right]^{(k_1)}\right]^{(0)} \tag{A.6.13}$$

$$\Rightarrow\ \delta_{k_1\lambda}\frac{(-)^{k_1}}{\sqrt{2k_1+1}}F(l_1j_1;l_3j_3;\lambda)\,\langle l_1\parallel C^{(k_1)}\parallel l_3\rangle\,F(l_2j_2;l_4j_4;\lambda)\,CG_2(\lambda k_2,k_2\lambda) \tag{A.6.14}$$

E.

$$\left[\left[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\right]^{(1)}\otimes\nabla_{(1)}\right]^{(0)}$$
$$=\left[\left[C^{(k_1)}(\hat{r}_1)\otimes\nabla_{(1)}\right]^{(k_2)}\otimes C^{(k_2)}(\hat{r}_2)\right]^{(0)} \tag{A.6.15}$$

$$\Rightarrow\ \delta_{k_2\lambda}\frac{(-)^{k_2}}{\sqrt{2k_2+1}}F(l_1j_1;l_3j_3;\lambda)\,CG_1(k_1\lambda,k_1\lambda)\,F(l_2j_2;l_4j_4;\lambda)\,\langle l_2\parallel C^{(\lambda)}\parallel l_4\rangle \tag{A.6.16}$$

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Secondly, in the first sum, we multiply through the operator expressions to obtain

$$\begin{aligned}
&\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\otimes\big[(\nabla_{(2)}-\nabla_{(1)})\otimes(\nabla_{(2)}-\nabla_{(1)})\big]^{(\kappa)}\Big]^{(0)}\\
&\quad=\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\otimes\big[\nabla_{(2)}\otimes\nabla_{(2)}\big]^{(\kappa)}\Big]^{(0)}\\
&\qquad-2\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\otimes\big[\nabla_{(1)}\otimes\nabla_{(2)}\big]^{(\kappa)}\Big]^{(0)}\\
&\qquad+\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\otimes\big[\nabla_{(1)}\otimes\nabla_{(1)}\big]^{(\kappa)}\Big]^{(0)}\,. \qquad \text{(A.6.17)}
\end{aligned}$$

We have now to change the coupling scheme and separate the operators depending on the coordinates of the first particle, from the operators depending on the coordinates of the second one. Similarly, for an arbitrary even rank j, we have

$$\begin{aligned}
&\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\otimes\big[\nabla_{(2)}\otimes\nabla_{(2)}\big]^{(\kappa')}\Big]^{(j)}\\
&\quad=\sum_{k}(-)^{k_1+k_2+\kappa'+j}\sqrt{(2\kappa+1)(2k+1)}\begin{Bmatrix}k_1 & k_2 & \kappa\\ \kappa' & j & k\end{Bmatrix}\\
&\qquad\Big[C^{(k_1)}(\hat{r}_1)\otimes\Big[C^{(k_2)}(\hat{r}_2)\otimes\big[\nabla_{(2)}\otimes\nabla_{(2)}\big]^{(\kappa')}\Big]^{(k)}\Big]^{(j)}
\end{aligned} \qquad \text{(A.6.18)}$$

$$\begin{aligned}
&\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\otimes\big[\nabla_{(1)}\otimes\nabla_{(2)}\big]^{(\kappa')}\Big]^{(j)}\\
&\quad=\sum_{kk'}\sqrt{(2\kappa+1)(2\kappa'+1)(2k+1)(2k'+1)}\begin{Bmatrix}k_1 & k_2 & \kappa\\ 1 & 1 & \kappa'\\ k & k' & j\end{Bmatrix}\\
&\qquad\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes\nabla_{(1)}\Big]^{(k)}\otimes\Big[C^{(k_2)}(\hat{r}_2)\otimes\nabla_{(2)}\Big]^{(k')}\Big]^{(j)}
\end{aligned} \qquad \text{(A.6.19)}$$

$$\begin{aligned}
&\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\otimes\big[\nabla_{(1)}\otimes\nabla_{(1)}\big]^{(\kappa')}\Big]^{(j)}\\
&\quad=\sum_{k}(-)^{k_2+\kappa'-\kappa+k}\sqrt{(2\kappa+1)(2k+1)}\begin{Bmatrix}k_2 & k_1 & \kappa\\ \kappa' & j & k\end{Bmatrix}\\
&\qquad\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes\big[\nabla_{(1)}\otimes\nabla_{(1)}\big]^{(\kappa')}\Big]^{(k)}\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(j)}
\end{aligned} \qquad \text{(A.6.20)}$$

For the particular case when j is equal to zero, these reduce to:

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A.

$$\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\odot\big[\nabla_{(2)}\odot\nabla_{(2)}\big]^{(\kappa)}\Big]^{(0)}$$
$$=\Big[C^{(k_1)}(\hat{r}_1)\otimes\Big[C^{(k_2)}(\hat{r}_2)\otimes\big[\nabla_{(2)}\odot\nabla_{(2)}\big]^{(\kappa)}\Big]^{(k_1)}\Big]^{(0)} \qquad \text{(A.6.21)}$$

$$\Rightarrow \delta_{k_1\lambda}\frac{(-)^{k_1}}{\sqrt{2k_1+1}}F(l_1j_1;l_3j_3;\lambda)\,\langle l_1\parallel C^{(\lambda)}\parallel l_3\rangle\,F(l_2j_2;l_4j_4;\lambda)\,CGG_2(\lambda k_2\kappa,k_2\kappa\lambda) \qquad \text{(A.6.22)}$$

B.

$$\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\odot\big[\nabla_{(1)}\odot\nabla_{(2)}\big]^{(\kappa)}\Big]^{(0)}$$
$$=\sum_k(-)^{k+k_2+1}\sqrt{(2\kappa+1)(2k+1)}\begin{Bmatrix}k_1 & k_2 & \kappa\\ 1 & 1 & k\end{Bmatrix}$$
$$\Big[\Big[C^{(k_1)}(\hat{r}_1)\odot\nabla_{(1)}\Big]^{(k)}\odot\Big[C^{(k_2)}(\hat{r}_2)\odot\nabla_{(2)}\Big]^{(k)}\Big]^{(0)} \qquad \text{(A.6.23)}$$

$$\Rightarrow(-)^{k_2+1}\sqrt{2\kappa+1}$$
$$\begin{Bmatrix}k_1 & k_2 & \kappa\\ 1 & 1 & \lambda\end{Bmatrix}F(l_1j_1;l_3j_3;\lambda)\,F(l_2j_2;l_4j_4;\lambda)\,CGCG(k_1k_2\kappa,k_1\lambda k_2\lambda) \qquad \text{(A.6.24)}$$

C.

$$\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\odot\big[\nabla_{(1)}\odot\nabla_{(1)}\big]^{(\kappa)}\Big]^{(0)}$$
$$=\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes\big[\nabla_{(1)}\odot\nabla_{(1)}\big]^{(\kappa)}\Big]^{(k_2)}\odot C^{(k_2)}(\hat{r}_2)\Big]^{(0)} \qquad \text{(A.6.25)}$$

$$\Rightarrow\delta_{k_2\lambda}\frac{(-)^{k_2}}{\sqrt{2k_2+1}}F(l_1j_1;l_3j_3;\lambda)\,CGG_1(k_1\lambda\kappa,k_1\kappa\lambda)\,F(l_2j_2;l_4j_4;\lambda)\,\langle l_2\parallel C^{(\lambda)}\parallel l_4\rangle \qquad \text{(A.6.26)}$$

Here we have the notations

$$CGG_1(k_1k_2\kappa,kl\lambda)$$
$$=\langle n_1n_2\,;\,l_1\parallel u^{(k_1k_2,2\kappa)}(r_1,r_2)\,\Big[C^{(k)}(\hat{r}_1)\odot\big[\nabla_{(1)}\odot\nabla_{(1)}\big]^{(l)}\Big]^{(\lambda)}\parallel n_3n_4\,;\,l_3\rangle \qquad \text{(A.6.27)}$$

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$$CGG_2(k_1k_2\kappa, kl\lambda)$$
$$= \langle n_1n_2\,;\, l_2 \parallel u^{(k_1k_2,2\kappa)}(r_1,r_2)\ \left[C^{(k)}(\hat{r}_2)\odot[\nabla_{(2)}\otimes\nabla_{(2)}]^{(l)}\right]^{(\lambda)} \parallel n_3n_4\,;\, l_4\rangle \tag{A.6.28}$$

and

$$CGCG(k_1k_2\kappa, l_1l_2\lambda_1\lambda_2)$$
$$= \langle n_1l_1 \parallel u^{(k_1,2\kappa)}(r_1)\ \left[C^{(l_1)}(\hat{r}_1)\odot\nabla_{(1)}\right]^{(l_2)} \parallel n_3l_3\rangle$$
$$\langle n_2l_2 \parallel u^{(k_2,2\kappa)}(r_2)\ \left[C^{(\lambda_1)}(\hat{r}_2)\odot\nabla_{(2)}\right]^{(\lambda_2)} \parallel n_4l_4\rangle\,. \tag{A.6.29}$$

A.7 $L^2\ (\sigma_1\cdot\sigma_2)$ Interaction.

The $L^2\sigma\sigma$ interaction is given by:

$$V_{L2S} = V_{l2s}(r)\ L^2\ (\sigma_1\cdot\sigma_2) = \left(-\sqrt{3}\right)\ V_{l2s}(r)\ L^2\ [\sigma_1\odot\sigma_2]^{(0)}\,. \tag{A.7.1}$$

Since the $L^2\sigma\sigma$ interaction differs from the L^2 interaction only through the spin-space part, $(\sigma_1\cdot\sigma_2)$, we can derive everything starting with Eq. (A.6.10) and adding the corresponding spin-spin interaction

$$V_{l2s}(r)\ L^2\ (\sigma_1\cdot\sigma_2) = \frac{3}{2}\sum_{\kappa=0,2}\frac{1}{\sqrt{2\kappa+1}}\left\{\begin{array}{ccc}1&1&1\\1&\kappa&1\end{array}\right\}\langle 1\,0\,1\,0\mid\kappa\,0\rangle$$
$$\sum_{k_1k_2} i^{k_2-k_1-\kappa}(2k_1+1)(2k_2+1)\,\langle k_1\,0\,k_2\,0\mid\kappa\,0\rangle\ u^{(k_1k_2,\kappa 2)}(r_1,r_2)$$
$$\left[\left[C^{(k_1)}(\hat{r}_1)\odot C^{(k_2)}(\hat{r}_2)\right]^{(\kappa)}\odot\left[(\nabla_{(2)}-\nabla_{(1)})\odot(\nabla_{(2)}-\nabla_{(1)})\right]^{(\kappa)}\right]^{(0)}(\sigma_1\cdot\sigma_2)$$
$$-\frac{1}{\sqrt{3}}\sum_{k_1k_2} i^{k_2-k_1-1}(2k_1+1)(2k_2+1)\,\langle k_1\,0\,k_2\,0\mid 1\,0\rangle\ u^{(k_1k_2,11)}(r_1,r_2)$$
$$\left\{\left[\left[C^{(k_1)}(\hat{r}_1)\odot C^{(k_2)}(\hat{r}_2)\right]^{(1)}\odot\nabla_{(2)}\right]^{(0)}(\sigma_1\cdot\sigma_2)\right.$$
$$\left.-\left[\left[C^{(k_1)}(\hat{r}_1)\odot C^{(k_2)}(\hat{r}_2)\right]^{(1)}\odot\nabla_{(1)}\right]^{(0)}(\sigma_1\cdot\sigma_2)\right\}\,. \tag{A.7.2}$$

Accordingly, from Eqs (A.6.21,A.6.23,A.6.25,A.6.13,A.6.15) we obtain the five contributions to the *ph* matrix element $\langle n_1n_3\,;\,(l_1\tfrac{1}{2})_{j_1}(l_3\tfrac{1}{2})^-_{j_3}\,;\,\lambda\mu\mid V_{L2S}\mid n_4n_2\,;\,(l_4\tfrac{1}{2})_{j_4}(l_2\tfrac{1}{2})^-_{j_2}\,;\,\lambda\mu\rangle$

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A.

$$\Big[\Big[C^{(k_1)}(\hat{r}_1)\otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\otimes[\nabla_{(2)}\otimes\nabla_{(2)}]^{(\kappa)}\Big]^{(0)}\ (\sigma_1\cdot\sigma_2)$$
$$=\sum_k\frac{(-)^{k+1}}{\sqrt{2k_1+1}}$$
$$\left(\Big[C^{(k_1)}(\hat{r}_1)\otimes\sigma_1\Big]^{(k)}\odot\Big[\Big[C^{(k_2)}(\hat{r}_2)\otimes[\nabla_{(2)}\otimes\nabla_{(2)}]^{(\kappa)}\Big]^{(k_1)}\odot\sigma_2\Big]^{(k)}\right)\quad(A.7.3)$$

$$\Rightarrow\frac{(-)^{\lambda+1}}{\sqrt{2k_1+1}}\,G(l_1j_1;l_3j_3;k_1\lambda)\,\langle l_1\parallel C^{(k_1)}\parallel l_3\rangle\,G(l_2j_2;l_4j_4;k_1\lambda)\,CGG_2(k_1k_2\kappa,k_2\kappa k_1)\quad(A.7.4)$$

B.

$$\Big[\Big[C^{(k_1)}(\hat{r}_1)\odot C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\odot[\nabla_{(1)}\odot\nabla_{(2)}]^{(\kappa)}\Big]^{(0)}\ (\sigma_1\cdot\sigma_2)$$
$$=(-)^{k_2}\sqrt{2\kappa+1}\sum_k(-)^k\begin{Bmatrix}k_1&k_2&\kappa\\1&1&k\end{Bmatrix}\sum_l(-)^l$$
$$\left(\Big[\Big[C^{(k_1)}(\hat{r}_1)\odot\nabla_{(1)}\Big]^{(k)}\odot\sigma_1\Big]^{(l)}\odot\Big[\Big[C^{(k_2)}(\hat{r}_2)\odot\nabla_{(2)}\Big]^{(k)}\odot\sigma_2\Big]^{(l)}\right)\quad(A.7.5)$$

$$\Rightarrow(-)^{k_2+\lambda}\sqrt{2\kappa+1}$$
$$\sum_k(-)^k\begin{Bmatrix}k_1&k_2&\kappa\\1&1&k\end{Bmatrix}G(l_1j_1;l_3j_3;k\lambda)\,G(l_2j_2;l_4j_4;k\lambda)\,CGCG(k_1k_2\kappa,k_1kk_2k)\quad(A.7.6)$$

C.

$$\Big[\Big[C^{(k_1)}(\hat{r}_1)\odot C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)}\odot[\nabla_{(1)}\odot\nabla_{(1)}]^{(\kappa)}\Big]^{(0)}\ (\sigma_1\cdot\sigma_2)$$
$$=\sum_k\frac{(-)^{k+1}}{\sqrt{2k_2+1}}$$
$$\left(\Big[\Big[C^{(k_1)}(\hat{r}_1)\odot[\nabla_{(1)}\odot\nabla_{(1)}]^{(\kappa)}\Big]^{(k_2)}\odot\sigma_1\Big]^{(k)}\odot\Big[C^{(k_2)}(\hat{r}_2)\odot\sigma_2\Big]^{(k)}\right)\quad(A.7.7)$$

$$\Rightarrow\frac{(-)^{\lambda+1}}{\sqrt{2k_2+1}}\,G(l_1j_1;l_3j_3;k_2\lambda)\,CGG_1(k_1k_2\kappa,k_1\kappa k_2)\,G(l_2j_2;l_4j_4;k_2\lambda)\,\langle l_2\parallel C^{(k_2)}\parallel l_4\rangle\quad(A.7.8)$$

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D.

$$\left[\left[C^{(k_1)}(\hat{r}_1)\odot C^{(k_2)}(\hat{r}_2)\right]^{(1)}\odot\nabla_{(2)}\right]^{(0)}\ (\sigma_1\cdot\sigma_2)$$
$$=\frac{(-)}{\sqrt{2k_1+1}}\sum_k(-)^k\left(\left[C^{(k_1)}(\hat{r}_1)\odot\sigma_1\right]^{(k)}\odot\left[\left[C^{(k_2)}(\hat{r}_2)\odot\nabla_{(2)}\right]^{(k_1)}\right]^{(k)}\right) \tag{A.7.9}$$

$$\Rightarrow\frac{(-)^{\lambda+1}}{\sqrt{2k_1+1}}G(l_1j_1;l_3j_3;k_1\lambda)\ \langle l_1\parallel C^{(k_1)}\parallel l_3\rangle\ G(l_2j_2;l_4j_4;k_1\lambda)\ CG_2(k_1k_2,k_2k_1) \tag{A.7.10}$$

E.

$$\left[\left[C^{(k_1)}(\hat{r}_1)\odot C^{(k_2)}(\hat{r}_2)\right]^{(1)}\odot\nabla_{(1)}\right]^{(0)}\ (\sigma_1\cdot\sigma_2)$$
$$=\frac{(-)}{\sqrt{2k_2+1}}\sum_k(-)^k\left(\left[\left[C^{(k_1)}(\hat{r}_1)\odot\nabla_{(1)}\right]^{(k_2)}\odot\sigma_1\right]^{(k)}\odot\left[C^{(k_2)}(\hat{r}_2)\odot\sigma_2\right]^{(k)}\right) \tag{A.7.11}$$

$$\Rightarrow\frac{(-)^{\lambda+1}}{\sqrt{2k_2+1}}G(l_1j_1;l_3j_3;k_2\lambda)\ CG_1(k_1k_2,k_1k_2)\ G(l_2j_2;l_4j_4;k_2\lambda)\ \langle l_2\parallel C^{(k_2)}\parallel l_4\rangle \tag{A.7.12}$$

A.8 Quadrupole Spin-Orbit Interaction.

The quadrupole spin-orbit interaction, V_{LS2}, is given as the radial factor, $V_{ls2}(r)$, multiplying the operator

$$\begin{aligned}(L\cdot S)^2 &= (L\cdot S)\ (L\cdot S) = (-\sqrt{3})^2\left[\ [L\odot S]^{(0)}\odot[L\odot S]^{(0)}\ \right]^{(0)}\\ &= 3\sum_{jj'}\sqrt{2j+1}\sqrt{2j'+1}\begin{Bmatrix}1&1&0\\1&1&0\\j&j'&0\end{Bmatrix}\left[\ [L\odot L]^{(j)}\odot[S\odot S]^{(j')}\ \right]^{(0)}\\ &= \sum_j\sqrt{2j+1}\left[\ [L\odot L]^{(j)}\odot[S\odot S]^{(j)}\ \right]^{(0)}.\end{aligned} \tag{A.8.1}$$

A close inspection of the last expression 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, $\vec{L}$.

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- *Case* $j = 0$.

$$\left[\left[L \otimes L \right]^{(0)} \otimes \left[S \otimes S \right]^{(0)} \right]^{(0)} = \frac{1}{3} L^2 S^2 = \frac{1}{6} L^2 \left(3 + \sigma_1 \cdot \sigma_2 \right) . \qquad \text{(A.8.2)}$$

where we have used

$$S^2 = \frac{1}{4} \left(\sigma_1 + \sigma_2 \right)^2 = \frac{1}{2} \left(3 + \sigma_1 \cdot \sigma_2 \right) . \qquad \text{(A.8.3)}$$

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

$$\begin{aligned} \tilde{V}_{l2} &= V_{l2} + \frac{1}{2} V_{ls2} , \\ \tilde{V}_{l2ss} &= V_{l2ss} + \frac{1}{6} V_{ls2} . \end{aligned} \qquad \text{(A.8.4)}$$

- *Case* $j = 1$.

$$\begin{aligned} \sqrt{3} \left[\left[L \otimes L \right]^{(1)} \otimes \left[S \otimes S \right]^{(1)} \right]^{(0)} &= \sqrt{3} \frac{-1}{\sqrt{3}} \left(\frac{-i}{\sqrt{2}} \right)^2 \left(\left(\vec{L} \times \vec{L} \right) \cdot \left(\vec{S} \times \vec{S} \right) \right) \\ &= \frac{1}{2} \left(\left(i \vec{L} \right) \cdot \left(i \vec{S} \right) \right) = - \frac{1}{2} \vec{L} \cdot \vec{S} . \end{aligned} \qquad \text{(A.8.5)}$$

where we have used the Q.M. definition of the angular momentum:

$$\left[J_i, J_j \right] = i J_k \qquad \text{or} \qquad \vec{J} \times \vec{J} = i \vec{J} . \qquad \text{(A.8.6)}$$

Similarly, we introduce the effective radial amplitude for the spin-orbital interaction, as:

$$\tilde{V}_{ls} = V_{ls} - \frac{1}{2} V_{ls2} . \qquad \text{(A.8.7)}$$

- *Case* $j = 2$.

$$\begin{aligned} \sqrt{5} \left[\left[L \otimes L \right]^{(2)} \otimes \left[S \otimes S \right]^{(2)} \right]^{(0)} &= \frac{\sqrt{5}}{4} 2 \left[\left[L \otimes L \right]^{(2)} \otimes \left[\sigma_1 \otimes \sigma_2 \right]^{(2)} \right]^{(0)} \\ &= \frac{\sqrt{5}}{2} \left[\left[L \otimes L \right]^{(2)} \otimes \left[\sigma_1 \otimes \sigma_2 \right]^{(2)} \right]^{(0)} . \end{aligned} \qquad \text{(A.8.8)}$$

We can see that the only new component of the interaction that we have not addressed yet is the one corresponding to $j = 2$. However, for now we shall keep the discussion on a general level. The following steps come natural

$$\begin{aligned} \left[L \otimes L \right]^{(j)} &= - \frac{1}{2} \left[\left[r \otimes \left(p_2 - p_1 \right) \right]^{(1)} \otimes \left[r \otimes \left(p_2 - p_1 \right) \right]^{(1)} \right]^{(j)} \\ &= \frac{3}{2} r^2 \sum_{\kappa \kappa' = 0,2} \sqrt{2\kappa + 1} \sqrt{2\kappa' + 1} \begin{Bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ \kappa & \kappa' & j \end{Bmatrix} \langle 1\,0\,1\,0 \mid \kappa\, 0 \rangle \\ &\qquad \left[C^{(\kappa)}(\hat{r}) \otimes \left[\left(\nabla_{(2)} - \nabla_{(1)} \right) \otimes \left(\nabla_{(2)} - \nabla_{(1)} \right) \right]^{(\kappa')} \right]^{(j)} \\ &\quad - 3 r \left(- \right)^j \begin{Bmatrix} 1 & 1 & 1 \\ 1 & 1 & j \end{Bmatrix} \left[C^{(1)}(\hat{r}) \otimes \left(\nabla_{(2)} - \nabla_{(1)} \right) \right]^{(j)} . \end{aligned} \qquad \text{(A.8.9)}$$

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Again, we use lemma 1 in order to expand the unnormalized spherical harmonics $C^{(\kappa)}(\hat{r})$ and $C^{(1)}(\hat{r})$

$$
\begin{aligned}
V_{ls2}(r)\,[L \otimes L]^{(j)} \;=\; & \frac{3}{2}\, r^2 \sum_{\kappa\kappa'=0,2} \sqrt{\frac{2\kappa'+1}{2\kappa+1}} \begin{Bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ \kappa & \kappa' & j \end{Bmatrix} \langle 1\,0\,1\,0 \mid \kappa\,0\rangle \\
& \sum_{k_1 k_2} i^{k_2-k_1-\kappa}\,(2k_1+1)(2k_2+1)\,\langle k_1\,0\,k_2\,0 \mid \kappa\,0\rangle\, u^{(k_1 k_2,2\kappa)}(r_1,r_2) \\
& \Big[\Big[C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2)\Big]^{(\kappa)} \odot [(\nabla_{(2)}-\nabla_{(1)}) \odot (\nabla_{(2)}-\nabla_{(1)})]^{(\kappa')}\Big]^{(j)} \\
- r\,(-)^j & \begin{Bmatrix} 1 & 1 & 1 \\ 1 & 1 & j \end{Bmatrix} \\
& \sum_{k_1 k_2} i^{k_2-k_1-1}\,(2k_1+1)(2k_2+1)\,\langle k_1\,0\,k_2\,0 \mid 1\,0\rangle\, u^{(k_1 k_2,11)}(r_1,r_2) \\
& \Big[\Big[C^{(k_1)}(\hat{r}_1) \otimes C^{(k_2)}(\hat{r}_2)\Big]^{(1)} \odot (\nabla_{(2)}-\nabla_{(1)})\Big]^{(j)} \,. \qquad \text{(A.8.10)}
\end{aligned}
$$

Based on Eqs (A.6.18,A.6.19,A.6.20, A.6.11,A.6.12), 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. Similarly to the previous $\vec{L}$-dependent interactions, we get the various contributions to the *ph* coupled matrix element $\langle n_1 n_3 \,;\, (l_1 \tfrac{1}{2})_{j_1} (l_3 \tfrac{1}{2})^{-}_{j_3} \,;\, \lambda\mu \mid V_{LS2} \mid n_4 n_2 \,;\, (l_4 \tfrac{1}{2})_{j_4} (l_2 \tfrac{1}{2})^{-}_{j_2} \,;\, \lambda\mu\rangle$

A.

$$
\begin{aligned}
& \Big[\Big[C^{(k_1)}(\hat{r}_1) \odot \Big[C^{(k_2)}(\hat{r}_2) \odot [\nabla_{(2)} \odot \nabla_{(2)}]^{(\kappa')}\Big]^{(k)}\Big]^{(2)} \odot [\sigma_1 \,,\, \sigma_2]^{(2)}\Big]^{(0)} \\
& = (-)^{k+1}\sqrt{5} \sum_{l} \begin{Bmatrix} k_1 & k & 2 \\ 1 & 1 & l \end{Bmatrix} \\
& \Big(\Big[C^{(k_1)}(\hat{r}_1) \odot \sigma_1\Big]^{(l)} \odot \Big[\Big[C^{(k_2)}(\hat{r}_2) \odot [\nabla_{(2)} \odot \nabla_{(2)}]^{(\kappa')}\Big]^{(k)} \,,\, \sigma_2\Big]^{(l)}\Big) \qquad \text{(A.8.11)}
\end{aligned}
$$

$$
\begin{aligned}
& \Rightarrow (-)^{k+1}\sqrt{5} \\
& \begin{Bmatrix} k_1 & k & 2 \\ 1 & 1 & \lambda \end{Bmatrix} G(l_1 j_1; l_3 j_3; k_1 \lambda)\, \langle l_1 \,\|\, C^{(k_1)} \,\|\, l_3\rangle\, G(l_2 j_2; l_4 j_4; k\lambda)\, CGG_2(k_1 k_2 \kappa, k_2 \kappa' k) \qquad \text{(A.8.12)}
\end{aligned}
$$

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B.

$$\left[\left[\left[C^{(k_1)}(\hat{r}_1)\otimes\nabla_{(1)}\right]^{(k)}\odot\left[C^{(k_2)}(\hat{r}_2)\otimes\nabla_{(2)}\right]^{(k')}\right]^{(2)}\odot[\sigma_1\odot\sigma_2]^{(2)}\right]^{(0)}$$
$$=(-)^{k'+1}\sqrt{5}\sum_l\begin{Bmatrix}k & k' & 2\\ 1 & 1 & l\end{Bmatrix}$$
$$\left(\left[\left[C^{(k_1)}(\hat{r}_1)\otimes\nabla_{(1)}\right]^{(k)}\otimes\sigma_1\right]^{(l)}\odot\left[\left[C^{(k_2)}(\hat{r}_1)\odot\nabla_{(2)}\right]^{(k')}\odot\sigma_2\right]^{(l)}\right) \tag{A.8.13}$$

$$\Rightarrow(-)^{k'+1}\sqrt{5}$$
$$\begin{Bmatrix}k & k' & 2\\ 1 & 1 & \lambda\end{Bmatrix}G(l_1j_1;l_3j_3;k\lambda)\,G(l_2j_2;l_4j_4;k'\lambda)\,CGCG(k_1k_2\kappa.\,k_1kk_2k') \tag{A.8.14}$$

C.

$$\left[\left[\left[C^{(k_1)}(\hat{r}_1)\odot\left[\nabla_{(1)}\otimes\nabla_{(1)}\right]^{(\kappa')}\right]^{(k)}\otimes C^{(k_2)}(\hat{r}_2)\right]^{(2)}\odot[\sigma_1\odot\sigma_2]^{(2)}\right]^{(0)}$$
$$=(-)^{k_2+1}\sqrt{5}\sum_l\begin{Bmatrix}k & k_2 & 2\\ 1 & 1 & l\end{Bmatrix}$$
$$\left(\left[\left[C^{(k_1)}(\hat{r}_1)\otimes\left[\nabla_{(1)}\otimes\nabla_{(1)}\right]^{(\kappa')}\right]^{(k)}\otimes\sigma_1\right]^{(l)}\odot\left[C^{(k_2)}(\hat{r}_2)\odot\sigma_2\right]^{(l)}\right) \tag{A.8.15}$$

$$\Rightarrow(-)^{k_2+1}\sqrt{5}$$
$$\begin{Bmatrix}k & k_2 & 2\\ 1 & 1 & \lambda\end{Bmatrix}G(l_1j_1;l_3j_3;k\lambda)\,CGG_1(k_1k_2\kappa.\,k_1\kappa'k)\,G(l_2j_2;l_4j_4;k_2\lambda)\,\langle l_2\|C^{(k_2)}\|l_4\rangle \tag{A.8.16}$$

D.

$$\left[\left[C^{(k_1)}(\hat{r}_1)\otimes\left[C^{(k_2)}(\hat{r}_2)\odot\nabla_{(2)}\right]^{(k)}\right]^{(2)}\odot[\sigma_1\odot\sigma_2]^{(2)}\right]^{(0)}$$
$$=(-)^{k+1}\sqrt{5}\sum_l\begin{Bmatrix}k_1 & k & 2\\ 1 & 1 & l\end{Bmatrix}$$
$$\left(\left[C^{(k_1)}(\hat{r}_1)\otimes\sigma_1\right]^{(l)}\odot\left[\left[C^{(k_2)}(\hat{r}_2)\otimes\nabla_{(2)}\right]^{(k)}\odot\sigma_2\right]^{(l)}\right) \tag{A.8.17}$$

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$$\Rightarrow (-)^{k+1}\sqrt{5} \begin{Bmatrix} k_1 & k & 2 \\ 1 & 1 & \lambda \end{Bmatrix} G(l_1 j_1; l_3 j_3; k_1 \lambda)\ \langle l_1 \| C^{(k_1)} \| l_3 \rangle\ G(l_2 j_2; l_4 j_4; k\lambda)\ CG_2(k_1 k_2, k_2 k) \tag{A.8.18}$$

E.

$$\left[\left[\left[C^{(k_1)}(\hat{r}_1) \otimes \nabla_{(1)}\right]^{(k)} \odot C^{(k_2)}(\hat{r}_2)\right]^{(2)} \odot [\sigma_1 \odot \sigma_2]^{(2)}\right]^{(0)}$$
$$= (-)^{k_2+1}\sqrt{5} \sum_l \begin{Bmatrix} k & k_2 & 2 \\ 1 & 1 & l \end{Bmatrix}$$
$$\left(\left[\left[C^{(k_1)}(\hat{r}_1) \odot \nabla_{(1)}\right]^{(k)} \odot \sigma_1\right]^{(l)} \odot \left[C^{(k_2)}(\hat{r}_2) \odot \sigma_2\right]^{(l)}\right) \tag{A.8.19}$$

$$\Rightarrow (-)^{k_2+1}\sqrt{5} \begin{Bmatrix} k & k_2 & 2 \\ 1 & 1 & \lambda \end{Bmatrix} G(l_1 j_1; l_3 j_3; k\lambda)\ CG_1(k_1 k_2, k_1 k)\ G(l_2 j_2; l_4 j_4; k_2 \lambda)\ \langle l_2 \| C^{(k_2)} \| l_4 \rangle \tag{A.8.20}$$

A.9 Center-of-Mass Relevant Operators.

From the center-of-mass corrections we have two additional operators that must be included in the two-body matrix elements of the interaction. These are:

$$-\frac{1}{mA}\,\vec{p}_1 \cdot \vec{p}_2 = \frac{\hbar^2}{mA}\,\vec{\nabla}_1 \cdot \vec{\nabla}_2 \tag{A.9.1}$$

and

$$\frac{1}{mA}\,\vec{r}_1 \cdot \vec{r}_2 \tag{A.9.2}$$

The *ph* matrix elements contribute only for a multipolarity $\lambda = 1$. According to our lemma 2, we obtain

$$-\frac{1}{mA}\,\langle 1\bar{2}\,|\,\vec{p}_1 \cdot \vec{p}_2\,|\,3\bar{4}\rangle = \frac{\hbar^2}{mA}\,\frac{(-)^{k_1}}{\sqrt{3}}\,\langle 1 \| \nabla \| 2\rangle \frac{(-)^{k_4}}{\sqrt{3}}\,\langle 4 \| \nabla \| 3\rangle \tag{A.9.3}$$

and

$$\frac{1}{mA}\,\langle 1\bar{2}\,|\,\vec{r}_1 \cdot \vec{r}_2\,|\,3\bar{4}\rangle = \frac{1}{mA}\,\frac{(-)^{k_1}}{\sqrt{3}}\,\langle 1 \| \vec{r} \| 2\rangle \frac{(-)^{k_4}}{\sqrt{3}}\,\langle 4 \| \vec{r} \| 3\rangle\,. \tag{A.9.4}$$

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where the reduced matrix elements are calculated as

$$\frac{(-)^{k_1}}{\sqrt{3}}\langle 1 \| \vec{\nabla} \| 2\rangle = \frac{\sqrt{(2j_1+1)(2j_2+1)}}{3}$$
$$\times \langle j_1 \tfrac{1}{2} j_2 -\tfrac{1}{2} | 10\rangle \langle R_1(r) | \left\{ \frac{d}{dr} + \frac{1}{2}(l_2 - l_1)(3\ell_2 - \ell_1 + 1)\frac{1}{r} \right\} | R_2(r)\rangle \quad \text{(A.9.5)}$$

and

$$\frac{(-)^{k_1}}{\sqrt{3}}\langle 1 \| \vec{r} \| 2\rangle = \frac{\sqrt{(2j_1+1)(2j_2+1)}}{3}\langle j_1 \tfrac{1}{2} j_2 -\tfrac{1}{2} | 10\rangle \langle R_1(r) | r | R_2(r)\rangle \quad \text{(A.9.6)}$$

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Appendix B

Two-Body Matrix Elements Calculation in a Harmonic Oscillator Single-Particle Basis Using Moshinsky Transformation.

One key element of our nuclear structure calculation has to do with the reliability of the two-body matrix elements calculation for the basic interaction. We have chosen the Argonne $v18$ potential [Wi-95] as the most realistic nucleon-nucleon potential to date. The computation of the two-body matrix elements relies on the formalism presented in Appendix A. An independent check of those formulas is available when the radial part of the single-particle wave functions is described by the radial part of the harmonic oscillator wave functions. In this particular case the Moshinsky transformations allow the decoupling of the relative motion degree of freedom and we are not required to separate the $\vec{r}_1$ $\vec{r}_2$ such as in lemma 1.

B.1 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

$$\vec{r} = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2) \qquad \vec{R} = \frac{1}{\sqrt{2}}(\vec{r}_1 + \vec{r}_2)\,: \tag{B.1.1}$$

  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*

$$|n_1 n_2\,(l_1 l_2)\,\lambda\mu\rangle = \sum_{m_1 m_2} \langle l_1\, m_1\, l_2\, m_2 \mid \lambda\,\mu\rangle\; |n_1 l_1 m_1\rangle\; |n_2 l_2 m_2\rangle\,: \tag{B.1.2}$$

- *center-of-mass frame*

$$|nN\,(lL)\,\lambda\mu\rangle = \sum_{m,M} \langle l\, m\, L\, M \mid \lambda\,\mu\rangle\; |nlm\rangle\; |NLM\rangle\,. \tag{B.1.3}$$

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The transformation brackets (*Moshinsky brackets*) are then the coefficients which arise on developing the eigenket (B.1.2) in a series of eigenkets (B.1.3):

$$|n_1 n_2\,(l_1 l_2)\,\lambda\mu\rangle \;=\; \sum_{nlNL} \langle n\,l\,N\,L\,\lambda \mid n_1\,l_1\,n_2\,l_2\,\lambda\rangle\;|nN\,(lL)\,\lambda\mu\rangle\,. \tag{B.1.4}$$

It may be shown that this transformation is independent of the magnetic quantum number μ. The transformation bracket vanishes for all combinations of its parameters which do not satisfy the total angular momentum

$$\vec{\lambda} \;=\; \vec{l}_1 + \vec{l}_2 \;=\; \vec{l} + \vec{L}. \tag{B.1.5}$$

and energy

$$\begin{aligned} E \;&=\; (2n_1 + l_1 + 3/2) \;+\; (2n_2 + l_2 + 3/2) \\ &=\; (2n + l + 3/2) \;+\; (2N + L + 3/2) \end{aligned} \tag{B.1.6}$$

conservation laws. Therefore, the transformation bracket vanishes for all combinations of its parameters which do not satisfy the energy condition (B.1.6), and any summations over λ will be restricted to

$$\begin{aligned} |l_1 - l_2| \le \lambda \le l_1 + l_2\,. \\ |l - L| \le \lambda \le l + L\,. \end{aligned} \tag{B.1.7}$$

We shall next show how to calculate two-body matrix element in a harmonic oscillator single-particle basis using the Moshinsky brackets. First, we change the angular momentum coupling scheme, going from the **JJ** coupling scheme to the **LS** coupling scheme:

$$\begin{aligned} &\langle n_1 n_2\,(l_1 \tfrac{1}{2})_{j_1}(l_2 \tfrac{1}{2})_{j_2};\, J'M' \mid V(\vec{r}_1,\vec{r}_2) \mid n_3 n_4\,(l_3 \tfrac{1}{2})_{j_3}(l_4 \tfrac{1}{2})_{j_4};\, JM\rangle \\ &= \sum_{\lambda\lambda' SS'} \sqrt{(2j_1+1)(2j_2+1)(2\lambda'+1)(2S'+1)} \begin{Bmatrix} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ \lambda' & S' & J' \end{Bmatrix} \\ &\qquad \sqrt{(2j_3+1)(2j_4+1)(2\lambda+1)(2S+1)} \begin{Bmatrix} l_3 & \frac{1}{2} & j_3 \\ l_4 & \frac{1}{2} & j_4 \\ \lambda & S & J \end{Bmatrix} \\ &\qquad \langle n_1 n_2\,(l_1 l_2)\lambda'\,(\tfrac{1}{2}\,\tfrac{1}{2})S';\, J'M' \mid V \mid n_3 n_4\,(l_3 l_4)\lambda\,(\tfrac{1}{2}\,\tfrac{1}{2})S;\, JM\rangle\,. \end{aligned} \tag{B.1.8}$$

Secondly, we use the Moshinsky brackets and switch from the *laboratory frame* to the *center-of-mass frame*:

$$\begin{aligned} &\langle n_1 n_2\,(l_1 l_2)\lambda'\,(\tfrac{1}{2}\,\tfrac{1}{2})S';\, J'M' \mid V(\vec{r}_1,\vec{r}_2) \mid n_3 n_4\,(l_3 l_4)\lambda\,(\tfrac{1}{2}\,\tfrac{1}{2})S;\, JM\rangle \\ &= \sum_{nlNL;n'l'N'L'} \langle n_1\,l_1\,n_2\,l_2\,\lambda' \mid n'\,l'\,N'\,L'\,\lambda'\rangle\,\langle n_3\,l_3\,n_4\,l_4\,\lambda \mid n\,l\,N\,L\,\lambda\rangle \\ &\qquad \langle n'N'\,(l'L')\lambda'\,(\tfrac{1}{2}\,\tfrac{1}{2})S';\, J'M' \mid V(\vec{r}) \mid nN\,(lL)\lambda\,(\tfrac{1}{2}\,\tfrac{1}{2})S;\, JM\rangle\,. \end{aligned} \tag{B.1.9}$$

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Therefore, we obtain

$$\langle n_1 n_2 (l_1 \tfrac{1}{2})_{j_1} (l_2 \tfrac{1}{2})_{j_2}; J'M' \mid V(\vec{r}_1, \vec{r}_2) \mid n_3 n_4 (l_3 \tfrac{1}{2})_{j_3} (l_4 \tfrac{1}{2})_{j_4}; JM \rangle = \sqrt{(2j_1+1)(2j_2+1)}$$
$$\sum_{nlNL\lambda; n'l'N'L'\lambda'} \sqrt{(2\lambda+1)(2\lambda'+1)}\, \langle n_1 l_1\, n_2 l_2\, \lambda' \mid n' l'\, N' L'\, \lambda' \rangle \langle n_3 l_3\, n_4 l_4\, \lambda \mid n l\, N L\, \lambda \rangle$$
$$\sqrt{(2j_3+1)(2j_4+1)} \sum_{S,S'=0}^{1} \sqrt{(2S+1)(2S'+1)} \begin{Bmatrix} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ \lambda' & S' & J' \end{Bmatrix} \begin{Bmatrix} l_3 & \frac{1}{2} & j_3 \\ l_4 & \frac{1}{2} & j_4 \\ \lambda & S & J \end{Bmatrix}$$
$$\langle n'N' (l'L')\lambda' (\tfrac{1}{2}\tfrac{1}{2})S'; J'M' \mid V(\vec{r}) \mid nN (lL)\lambda (\tfrac{1}{2}\tfrac{1}{2})S; JM \rangle . \qquad \text{(B.1.10)}$$

Given a particular potential $V(\vec{r})$, all we have to do is to calculate the matrix element

$$\langle n'N' (l'L')\lambda' (\tfrac{1}{2}\tfrac{1}{2})S'; J'M' \mid V(\vec{r}) \mid nN (lL)\lambda (\tfrac{1}{2}\tfrac{1}{2})S; JM \rangle . \qquad \text{(B.1.11)}$$

We shall redo now the calculation of the matrix elements discussed in Appendix A.

B.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 ([Ed-65], Eq. 5.4.1a)

$$\langle n'N' (l'L')_{\lambda'} (\tfrac{1}{2}\tfrac{1}{2})_{S'}; J'M_{J'} \mid V_c(r) \mid nN (lL)_{\lambda} (\tfrac{1}{2}\tfrac{1}{2})_{S}; JM_J \rangle$$
$$= \frac{\delta_{JJ'}\delta_{M_J M_{J'}}}{\hat{J}} \langle n'N' (l'L')_{\lambda'} (\tfrac{1}{2}\tfrac{1}{2})_{S'}; JM_J \parallel V_c(r) \parallel nN (lL)_{\lambda} (\tfrac{1}{2}\tfrac{1}{2})_{S}; JM_J \rangle . \qquad \text{(B.2.1)}$$

The resulting reduced matrix element is evaluated using ([Ed-65], Eq. 7.1.7). We have

$$\langle n'N' (l'L')_{\lambda'} (\tfrac{1}{2}\tfrac{1}{2})_{S'}; JM_J \parallel V_c(r) \parallel nN (lL)_{\lambda} (\tfrac{1}{2}\tfrac{1}{2})_{S}; JM_J \rangle$$
$$= \delta_{SS'} (-)^{\lambda'+S+J+0} (2J+1) \begin{Bmatrix} \lambda' & J & S \\ J & \lambda & 0 \end{Bmatrix} \langle n'N' (l'L')_{\lambda'} \parallel V_c(r) \parallel nN (lL)_{\lambda} \rangle . \qquad \text{(B.2.2)}$$

We use ([Ed-65], Eq. 7.1.7) one more time for the reduced matrix element

$$\langle n'N' (l'L')_{\lambda'} \parallel V_c(r) \parallel nN (lL)_{\lambda} \rangle = \delta_{NN'}\delta_{LL'}$$
$$(-)^{l'+L+\lambda+0} \sqrt{(2\lambda+1)(2\lambda'+1)} \begin{Bmatrix} l' & \lambda' & L \\ \lambda & l & 0 \end{Bmatrix} \langle n'\, l' \parallel V_c(r) \parallel n\, l \rangle . \qquad \text{(B.2.3)}$$

The Wigner $6j$ symbols in Eqs. (B.2.2,B.2.3) are readily calculated as

$$\begin{Bmatrix} \lambda' & J & S \\ J & \lambda & 0 \end{Bmatrix} = \begin{Bmatrix} \lambda' & \lambda & 0 \\ J & J & S \end{Bmatrix} = \delta_{\lambda\lambda'} \frac{(-)^{\lambda+J+S}}{\sqrt{(2\lambda+1)(2J+1)}} . \qquad \text{(B.2.4)}$$

$$\begin{Bmatrix} l' & \lambda' & L \\ \lambda & l & 0 \end{Bmatrix} = \begin{Bmatrix} l' & l & 0 \\ \lambda & \lambda' & L \end{Bmatrix} = \delta_{ll'}\delta_{\lambda\lambda'} \frac{(-)^{l+\lambda+L}}{\sqrt{(2\lambda+1)(2l+1)}} . \qquad \text{(B.2.5)}$$

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Moreover, from the Wigner-Eckart theorem we have:

$$\delta_{ll'}\,\frac{\langle n'\,l'\,\|\,V_c(r)\,\|\,n\,l\rangle}{\sqrt{2l+1}} = \langle n'\,l'm_l\mid V_c(r)\mid n\,lm_l\rangle$$
$$= \delta_{ll'}\,\mathcal{RM}(n'l:\,nl)\,. \qquad \text{(B.2.6)}$$

Thus, plugging Eqs. (B.2.4), (B.2.5) and (B.2.6) into Eqs. (B.2.2) and (B.2.3), Eq. (B.2.1) becomes

$$\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\,J'M_{J'}\mid V_c(r)\mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\,JM_J\rangle$$
$$= \delta_{JJ'}\,\delta_{M_JM_{J'}}\,\delta_{SS'}\,\delta_{NN'}\,\delta_{LL'}\;\delta_{ll'}\;\delta_{\lambda\lambda'}\,\mathcal{RM}[V_c(r)](n'l:\,nl)\,, \qquad \text{(B.2.7)}$$

where

$$\mathcal{RM}[V(r)](n'l:\,nl) = \langle n'\,l'\,\|\,V(r)\,\|\,n\,l\rangle$$
$$= \int_0^\infty \mathrm{d}r\;r^2\,R_{n'l}(r)V(r)R_{nl}(r)\,. \qquad \text{(B.2.8)}$$

An alternative calculation of the central interaction matrix element, can be obtained by converting the matrix element to m representation and use the orthonormality properties of the angular momentum and spin eigenfunctions

$$\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\,J'M_{J'}\mid V_c(r)\mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\,JM_J\rangle$$
$$= \sum_{\mu'm_{S'};\mu m_S}\langle\lambda'\,\mu'\,S'\,m_{S'}\mid J'\,M_{J'}\rangle\,\langle\lambda\,\mu\,S\,m_S\mid J\,M_J\rangle$$
$$\langle n'N'\,\lambda'\mu'\,S'm_{S'}\mid V_c(r)\mid nN\,\lambda\mu\,Sm_S\rangle$$
$$= \sum_{\mu'm_{S'};\mu m_S}\langle\lambda'\,\mu'\,S'\,m_{S'}\mid J'\,M_{J'}\rangle\,\langle\lambda\,\mu\,S\,m_S\mid J\,M_J\rangle$$
$$\delta_{\lambda\lambda'}\delta_{\mu\mu'}\,\delta_{SS'}\delta_{m_Sm_{S'}}\,\langle n'N'\,(l'L')\lambda\mu\mid V_c(r)\mid nN\,(l'L')\lambda\mu\rangle$$
$$= \delta_{JJ'}\,\delta_{M_JM_{J'}}\,\delta_{NN'}\,\delta_{LL'}\,\delta_{ll'}\,\delta_{\lambda\lambda'}\,\delta_{SS'}\,\mathcal{RM}[V_c(r)](n'l:\,nl)\,. \qquad \text{(B.2.9)}$$

Here, in the last step, we have also used the unitary property of the Clebsch-Gordan coefficients.

B.3 Spin-Spin Interaction.

We shall carry out the spin-spin interaction matrix element calculation using the m representation approach outlined in the previous section

$$\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\,J'M_{J'}\mid V_s(r)\,\sigma_1\cdot\sigma_2\mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\,JM_J\rangle$$
$$= \sum_{m_{l'}M'm_{S'}\mu'}\langle l'\,m_{l'}\,L'\,M'\mid\lambda'\,\mu'\rangle\langle\lambda'\,\mu'\,S'\,m_{S'}\mid J'\,M_{J'}\rangle$$
$$\sum_{m_lMm_S\mu}\langle l\,m_l\,L\,M\mid\lambda\,\mu\rangle\langle\lambda\,\mu\,S\,m_S\mid J\,M_J\rangle$$
$$\langle n'N'\,l'm_{l'}\,L'M'\,S'm_{S'}\mid V_s(r)\,\sigma_1\cdot\sigma_2\mid nN\;nN\;lm_l\,LM\,Sm_S\rangle\,. \qquad \text{(B.3.1)}$$

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We have the matrix element

$$\begin{aligned}&\langle n'N'\, l'm_{l'}\, L'M'\, S'm_{S'} \mid V_s(r)\, \sigma_1\cdot\sigma_2 \mid nN\; nN\; lm_l\; LM\; Sm_S\rangle \\ &\quad = \delta_{NN'}\delta_{LL'}\delta_{MM'}\delta_{ll'}\delta_{m_l m_{l'}}\, \langle n'l \mid V_s(r) \mid nl\rangle\, \langle (\tfrac{1}{2}\tfrac{1}{2})_{S'} \mid \sigma_1\cdot\sigma_2 \mid (\tfrac{1}{2}\tfrac{1}{2})_S\rangle\,. \end{aligned} \quad \text{(B.3.2)}$$

The spin dependent factor in the last equation is given by

$$\langle (\tfrac{1}{2}\tfrac{1}{2})_{S'} \mid \sigma_1\cdot\sigma_2 \mid (\tfrac{1}{2}\tfrac{1}{2})_S\rangle \;=\; 2\left[S(S+1)-\frac{3}{2}\right]\delta_{SS'}\,. \quad \text{(B.3.3)}$$

where we used the fact that $\hat{s}_i = \frac{1}{2}\hat{\sigma}_i$. We put these results together and obtain

$$\begin{aligned}&\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\tfrac{1}{2})_{S'};\, J'M_{J'} \mid V_s(r)\,\sigma_1\cdot\sigma_2 \mid nN\,(lL)_\lambda(\tfrac{1}{2}\tfrac{1}{2})_S;\, JM_J\rangle \\ &\quad = \delta_{NN'}\delta_{LL'}\delta_{MM'}\delta_{ll'}\delta_{SS'}\delta_{\lambda\lambda'}\delta_{JJ'}\delta_{M_JM_{J'}}\, 2\left[S(S+1)-\frac{3}{2}\right]\, \mathcal{R}.\mathcal{M}[V_s(r)](n'l;\, nl)\,. \end{aligned} \quad \text{(B.3.4)}$$

B.4 Tensor Interaction.

We shall start the calculation of the tensor interaction matrix element. by using ([Ed-65], Eq. 7.1.6)

$$\begin{aligned}&\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\tfrac{1}{2})_{S'};\, J'M_{J'} \mid V_t(r)\, S_{12} \mid nN\,(lL)_\lambda(\tfrac{1}{2}\tfrac{1}{2})_S;\, JM_J\rangle \\ &= \delta_{JJ'}\delta_{M_JM_{J'}}(-)^{\lambda+S'+J}\left\{\begin{array}{ccc} J & S' & \lambda' \\ 2 & \lambda & S\end{array}\right\}\sqrt{\frac{2}{3}} \\ &\qquad \sum_{n''N''}\langle n'N'\,(l'L')_{\lambda'} \parallel V_t(r)\, C^{(2)}(\hat{r}) \parallel n''N''\,(lL)_\lambda\rangle \\ &\qquad\qquad \langle n''N''\,(\tfrac{1}{2}\tfrac{1}{2})_{S'} \parallel [\sigma_1 \otimes \sigma_2]^{(2)} \parallel nN\,(\tfrac{1}{2}\tfrac{1}{2})_S\rangle\,. \end{aligned} \quad \text{(B.4.1)}$$

where

$$\begin{aligned} S_{12} &= \frac{1}{r^2}(\sigma_1\cdot r)\,(\sigma_2\cdot r) \;-\; \frac{1}{3}\sigma_1\cdot\sigma_2 \\ &= \sqrt{\frac{2}{3}}\left(C^{(2)}(\hat{r}) \otimes [\sigma_1 \otimes \sigma_2]^{(2)}\right). \end{aligned} \quad \text{(B.4.2)}$$

We evaluate the reduced matrix elements in Eq. (B.4.1):

1. ([Ed-65], Eq. 7.1.5) - for S (S') = 0,1

$$\begin{aligned}&\langle (\tfrac{1}{2}\tfrac{1}{2})_{S'} \parallel [\sigma_1 \otimes \sigma_2]^{(2)} \parallel (\tfrac{1}{2}\tfrac{1}{2})_S\rangle \\ &\quad = \sqrt{5(2S+1)(2S'+1)}\left\{\begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & 1 \\ S' & S & 2\end{array}\right\}\langle \tfrac{1}{2} \parallel \sigma_1 \parallel \tfrac{1}{2}\rangle\langle \tfrac{1}{2} \parallel \sigma_2 \parallel \tfrac{1}{2}\rangle \\ &\quad = \frac{\sqrt{5}}{2}\delta_{S1}\delta_{SS'}\,, \end{aligned} \quad \text{(B.4.3)}$$

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where

$$\langle \tfrac{1}{2} \| \sigma_i \| \tfrac{1}{2} \rangle = 2 \langle \tfrac{1}{2} \| s_i \| \tfrac{1}{2} \rangle = \sqrt{6} . \tag{B.4.4}$$

and

$$\left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & 1 \\ S' & S & 2 \end{array} \right\} = \frac{7}{36} \delta_{S1} \delta_{SS'} : \tag{B.4.5}$$

2. ([Ed-65], Eq. 7.1.7)

$$\begin{aligned} \langle n'N' \, (l'L')_{\lambda'} \| \, V_t(r) \, C^{(2)}(\hat{r}) \, \| \, nN \, (lL)_{\lambda} \rangle &= \delta_{NN'} \delta_{LL'} (-)^{l'+L+\lambda+2} \\ & \sqrt{(2\lambda+1)(2\lambda'+1)} \left\{ \begin{array}{ccc} l' & \lambda' & L \\ \lambda & l & 2 \end{array} \right\} \langle n' \, l' \| \, V_t(r) \, C^{(2)}(\hat{r}) \, \| \, n \, l \rangle ; \end{aligned} \tag{B.4.6}$$

3.

$$\begin{aligned} \langle n' \, l' \| \, V_t(r) \, C^{(2)}(\hat{r}) \, \| \, n \, l \rangle &= \langle l' \| \, C^{(2)}(\hat{r}) \, \| \, l \rangle \, \mathcal{RM}[V_t(r)](n'l' : nl) . \\ &= \sqrt{(2l+1)} \, \langle l \, 0 \, 2 \, 0 \mid l' \, 0 \rangle \, \mathcal{RM}[V_t(r)](n'l' ; nl) . \end{aligned} \tag{B.4.7}$$

Thus, we get:

$$\begin{aligned} & \langle n'N' \, (l'L')_{\lambda'} (\tfrac{1}{2} \tfrac{1}{2})_{S'} ; \, J'M_{J'} \mid V_t(r) \, S_{12} \mid nN \, (lL)_{\lambda} (\tfrac{1}{2} \tfrac{1}{2})_{S} ; \, JM_J \rangle \\ &= \delta_{JJ'} \delta_{M_J M_{J'}} \delta_{NN'} \delta_{LL'} \delta_{SS'} \delta_{S1} (-)^{l'+L+J+1} \sqrt{(2\lambda+1)(2\lambda'+1)} \\ & \quad 7 \sqrt{\frac{5}{6}} \, \sqrt{(2l+1)} \, \langle l \, 0 \, 2 \, 0 \mid l' \, 0 \rangle \left\{ \begin{array}{ccc} J & S & \lambda' \\ 2 & \lambda & S \end{array} \right\} \left\{ \begin{array}{ccc} l' & \lambda' & L \\ \lambda & l & 2 \end{array} \right\} \mathcal{RM}[V_t(r)](n'l' ; nl) . \end{aligned} \tag{B.4.8}$$

B.5 Spin-Orbit Interaction.

Similarly to the tensor interaction case, we use ([Ed-65], Eq. 7.1.6)

$$\begin{aligned} & \langle n'N' \, (l'L')_{\lambda'} (\tfrac{1}{2} \tfrac{1}{2})_{S'} ; \, J'M_{J'} \mid V_{ls}(r) \, \vec{l} \cdot \vec{S} \mid nN \, (lL)_{\lambda} (\tfrac{1}{2} \tfrac{1}{2})_{S} ; \, JM_J \rangle \\ &= \delta_{JJ'} \delta_{M_J M_{J'}} (-)^{\lambda+S'+J} \left\{ \begin{array}{ccc} J & S' & \lambda' \\ 1 & \lambda & S \end{array} \right\} \\ & \quad \sum_{n''N''} \langle n'N' \, (l'L')_{\lambda'} \| \, V_{ls}(r) \, \vec{l} \, \| \, n''N'' \, (lL)_{\lambda} \rangle \langle n''N'' \, (\tfrac{1}{2} \tfrac{1}{2})_{S'} \| \vec{S} \| \, nN \, (\tfrac{1}{2} \tfrac{1}{2})_{S} \rangle . \end{aligned} \tag{B.5.1}$$

The resulting matrix elements are:

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1. ([Ed-65], Eq. 5.4.3) - for $S = 0, 1$

$$\begin{aligned}\langle(\tfrac{1}{2}\tfrac{1}{2})_{S'} \,\|\vec{S}\,\|\, (\tfrac{1}{2}\tfrac{1}{2})_S\rangle &= \delta_{SS'}\sqrt{S(S+1)(2S+1)} \\ &= \sqrt{6}\,\delta_{S1}\delta_{SS'}\,: \end{aligned} \tag{B.5.2}$$

2. ([Ed-65], Eq. 7.1.7)

$$\begin{aligned}&\langle n'N'\,(l'L')_{\lambda'} \,\|\, V_{ls}(r)\,\vec{l}\,\|\, nN\,(lL)_\lambda\rangle \\ &= \delta_{NN'}\delta_{LL'}(-)^{l'+L+\lambda+1}\sqrt{(2\lambda+1)(2\lambda'+1)}\left\{\begin{array}{ccc} l' & \lambda' & L \\ \lambda & l & 1\end{array}\right\}\langle n'\,l' \,\|\, V_{ls}(r)\,\vec{l}\,\|\, n\,l\rangle\,:\end{aligned} \tag{B.5.3}$$

3. ([Ed-65], Eq. 5.4.3)

$$\langle n'\,l' \,\|\, V_{ls}(r)\,\vec{l}\,\|\, n\,l\rangle = \delta_{ll'}\sqrt{l(l+1)(2l+1)}\;\mathcal{RM}[V_{ls}(r)](n'l\,:\,nl)\,. \tag{B.5.4}$$

Collecting terms, we find

$$\begin{aligned}&\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\; J'M_{J'} \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid nN\,(lL)_\lambda(\tfrac{1}{2}\,\tfrac{1}{2})_S;\; JM_J\rangle \\ &= \delta_{JJ'}\delta_{M_JM_{J'}}\delta_{NN'}\delta_{LL'}\delta_{ll'}\delta_{SS'}\delta_{S1}(-)^{l+L+J}\sqrt{(2\lambda+1)(2\lambda'+1)} \\ &\quad \sqrt{6}\,\sqrt{l(l+1)(2l+1)}\left\{\begin{array}{ccc} J & S & \lambda' \\ 1 & \lambda & S\end{array}\right\}\left\{\begin{array}{ccc} l & \lambda' & L \\ \lambda & l & 1\end{array}\right\}\mathcal{RM}[V_{ls}(r)](n'l\,:\,nl)\,.\end{aligned} \tag{B.5.5}$$

It is interesting going about re-deriving the spin-orbit matrix element by converting the matrix element to m representation. As a first step, we use the fact that the matrix element is rotationally invariant, i.e. M_J independent

$$\begin{aligned}&\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\; JM_J \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid nN\,(lL)_\lambda(\tfrac{1}{2}\,\tfrac{1}{2})_S;\; JM_J\rangle \\ &= \frac{1}{2J+1}\sum_{M_J}\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\; JM_J \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid nN\,(lL)_\lambda(\tfrac{1}{2}\,\tfrac{1}{2})_S;\; JM_J\rangle \\ &= \frac{1}{2J+1}\sum_{M_J}\sum_{m_{l'}M'm_{S'}\mu'}\langle l'\,m_{l'}\,L'\,M' \mid \lambda'\,\mu'\rangle\langle\lambda'\,\mu'\,S'\,m_{S'} \mid J\,M_J\rangle \\ &\qquad \sum_{m_lMm_S\mu}\langle l\,m_l\,L\,M \mid \lambda\,\mu\rangle\langle\lambda\,\mu\,S\,m_S \mid J\,M_J\rangle \\ &\qquad \langle n'N'\,l'm_{l'}\,L'M'\,S'm_{S'} \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid nN\,lm_l\,LM\,Sm_S\rangle\,.\end{aligned} \tag{B.5.6}$$

The spin-orbit matrix element in the m representation can be greatly simplified as

$$\begin{aligned}&\langle n'N'\,l'm_{l'}\,L'M'\,S'm_{S'} \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid nN\,lm_l\,LM\,Sm_S\rangle \\ &= \delta_{NN'}\delta_{LL'}\delta_{MM'}\langle n'\,l'm_{l'}\,S'm_{S'} \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid n\,lm_l\,Sm_S\rangle\,.\end{aligned} \tag{B.5.7}$$

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For the remainder matrix element, we couple the relative angular momentum $\vec{l}$ and the total spin $\vec{S}$ to a total angular momentum $\vec{K}$

$$\begin{aligned}
&\langle n' l' m_{l'} S' m_{S'} \mid V_{ls}(r)\, \vec{l}\cdot\vec{S} \mid n\, l m_l\, S m_S\rangle \\
&= \sum_{K\kappa;K'\kappa'} \langle l' m_{l'} S' m_{S'} \mid K'\kappa'\rangle\langle l\, m_l\, S\, m_S \mid K\,\kappa\rangle\langle n' (l'S') K'\kappa' \mid V_{ls}(r)\, \vec{l}\cdot\vec{S} \mid n\,(lS)\, K\kappa\rangle \\
&= \sum_{K\kappa} \langle l' m_{l'} S' m_{S'} \mid K\,\kappa\rangle\langle l\, m_l\, S\, m_S \mid K\,\kappa\rangle\langle n' (l'S') K\kappa \mid V_{ls}(r)\, \vec{l}\cdot\vec{S} \mid n\,(lS)\, K\kappa\rangle\,.
\end{aligned} \tag{B.5.8}$$

The matrix element $\langle n' (l'S') K'\kappa' \mid V_{ls}(r)\, \vec{l}\cdot\vec{S} \mid n\,(lS)\, K\kappa\rangle$ is diagonal in the K-space and κ-independent

$$\begin{aligned}
&\langle n' (l'S') K'\kappa' \mid V_{ls}(r)\, \vec{l}\cdot\vec{S} \mid n\,(lS)\, K\kappa\rangle \\
&\quad = \delta_{KK'}\,\delta_{\kappa\kappa'}\,\frac{1}{2}\,[K(K+1) - l(l+1) - S(S+1)]\;\mathcal{RM}[V_{ls}(r)](n'l\,;\,nl)\,.
\end{aligned} \tag{B.5.9}$$

Then, we have

$$\begin{aligned}
&\langle n'N' (l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\, JM_J \mid V_{ls}(r)\, \vec{l}\cdot\vec{S} \mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\, JM_J\rangle \\
&= \delta_{NN'}\delta_{LL'}\,\frac{1}{2J+1}\sum_{K}\sum_{m_l m_S \mu}\sum_{m_{l'} m_{S'} \mu'} \langle n' (l'S') K \mid V(r)\, \vec{l}\cdot\vec{S} \mid n\,(lS)\, K\rangle \\
&\sum_{M}\langle l' m_{l'}\, L\, M \mid \lambda'\mu'\rangle\langle l\, m_l\, L\, M \mid \lambda\,\mu\rangle \sum_{M_J}\langle \lambda'\mu'\, S' m_{S'} \mid J\, M_J\rangle\langle \lambda\,\mu\, S\, m_S \mid J\, M_J\rangle \\
&\sum_{\kappa}\langle l' m_{l'}\, S' m_{S'} \mid K\,\kappa\rangle\langle l\, m_l\, S\, m_S \mid K\,\kappa\rangle
\end{aligned}$$

$$\begin{aligned}
&= \delta_{NN'}\delta_{LL'}\,\frac{1}{2J+1}\sum_{K}\sum_{m_l m_S \mu}\sum_{m_{l'} m_{S'} \mu'} \langle n' (l'S') K \mid V_{ls}(r)\, \vec{l}\cdot\vec{S} \mid n\,(lS)\, K\rangle \\
&\sum_{M}(-)^{l'-m_{l'}}\sqrt{\frac{2\lambda'+1}{2L+1}}\langle \lambda'\mu'\, l'\, -m_{l'} \mid L\, M\rangle(-)^{l-m_l}\sqrt{\frac{2\lambda+1}{2L+1}}\langle \lambda\,\mu\, l\, -m_l \mid L\, M\rangle \\
&\sum_{\sigma m_\sigma}(-)^{S'-m_{S'}-S-\mu-J}(2J+1)\begin{Bmatrix} \lambda' & S' & J \\ S & \lambda & \sigma \end{Bmatrix} \\
&\qquad\qquad \langle \lambda'\mu'\, \lambda\, -\mu \mid \sigma\, m_\sigma\rangle\langle S\, m_S\, S'\, -m_{S'} \mid \sigma\, m_\sigma\rangle \\
&\sum_{\sigma' m_{\sigma'}}(-)^{S'-m_{S'}-S-m_l-K}(2K+1)\begin{Bmatrix} l' & S' & K \\ S & l & \sigma' \end{Bmatrix} \\
&\qquad\qquad \langle l'\, m_{l'}\, l\, -m \mid \sigma'\, m'_\sigma\rangle\langle S\, m_S\, S'\, -m_{S'} \mid \sigma'\, m'_\sigma\rangle
\end{aligned}$$

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$$= \delta_{NN'}\delta_{LL'} \frac{1}{2J+1} \sum_K \sum_{m_l m_S \mu} \sum_{m_{l'} m_{S'} \mu'} \langle n'\,(l'S')\,K \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid n\,(lS)\,K\rangle$$

$$(-)^{l'-m_{l'}+l-m_l} \frac{\sqrt{(2\lambda'+1)(2\lambda+1)}}{2L+1}$$

$$\sum_{\sigma'' m''_{\sigma'}} (-)^{l'+m_{l'}-l-\mu-L}(2L+1) \left\{ \begin{array}{ccc} \lambda' & l' & L \\ l & \lambda & \sigma'' \end{array} \right\}$$

$$\langle \lambda' \mu' \lambda\ -\mu \mid \sigma'' m''_\sigma\rangle \langle l\ -m_l\, l'\, m_{l'} \mid \sigma''\, m''_\sigma\rangle$$

$$\sum_{\sigma m_\sigma} (-)^{S'-m_{S'}-S-\mu-J}(2J+1) \left\{ \begin{array}{ccc} \lambda' & S' & J \\ S & \lambda & \sigma \end{array} \right\}$$

$$\langle \lambda' \mu' \lambda\ -\mu \mid \sigma\, m_\sigma\rangle \langle S\, m_S\, S'\ -m_{S'} \mid \sigma\, m_\sigma\rangle$$

$$\sum_{\sigma' m_{\sigma'}} (-)^{S'-m_{S'}-S-m_l-K}(2K+1) \left\{ \begin{array}{ccc} l' & S' & K \\ S & l & \sigma' \end{array} \right\}$$

$$\langle l'\, m_{l'}\, l\ -m_l \mid \sigma'\, m'_\sigma\rangle \langle S\, m_S\, S'\ -m_{S'} \mid \sigma'\, m'_\sigma\rangle\,.$$

(B.5.10)

All sums involving the Clebsch-Gordon coefficients can be reduced by token of the orthogonality relationships, which yields

$$\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\, JM_J \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid nN\,(lL)_\lambda(\tfrac{1}{2}\,\tfrac{1}{2})_S;\, JM_J\rangle$$

$$= \delta_{NN'}\delta_{LL'} \sum_K (-)^{-J-K-L}(2K+1)\sqrt{(2\lambda'+1)(2\lambda+1)}$$

$$\langle n'\,(l'S')\,K \mid V(r)\,\vec{l}\cdot\vec{S} \mid n\,(lS)\,K\rangle$$

$$\sum_{\sigma m_\sigma} (-)^{l+l'-\sigma} \left\{ \begin{array}{ccc} \lambda' & S' & J \\ S & \lambda & \sigma \end{array} \right\} \left\{ \begin{array}{ccc} l' & S' & K \\ S & l & \sigma \end{array} \right\} \left\{ \begin{array}{ccc} \lambda' & l' & L \\ l & \lambda & \sigma \end{array} \right\}$$

$$= \delta_{NN'}\delta_{LL'} \sum_K (-)^{-J-K-L}(2K+1)\sqrt{(2\lambda'+1)(2\lambda+1)}$$

$$(-)^{l+l'}\langle n'\,(l'S')\,K \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid n\,(lS)\,K\rangle$$

$$\sum_\sigma (-)^{-\sigma}(2\sigma+1) \left\{ \begin{array}{ccc} \lambda' & S' & J \\ S & \lambda & \sigma \end{array} \right\} \left\{ \begin{array}{ccc} l' & S' & K \\ S & l & \sigma \end{array} \right\} \left\{ \begin{array}{ccc} \lambda' & l' & L \\ l & \lambda & \sigma \end{array} \right\}.$$

(B.5.11)

Using the identity ([Sh-74], p 929: 2.91)

$$\sum_\sigma (-)^{\lambda'+\lambda+\sigma}(2\sigma+1) \left\{ \begin{array}{ccc} S & S' & \sigma \\ \lambda' & \lambda & J \end{array} \right\} \left\{ \begin{array}{ccc} S & S' & \sigma \\ l' & l & K \end{array} \right\} \left\{ \begin{array}{ccc} l & l' & \sigma \\ \lambda' & \lambda & L \end{array} \right\}$$

$$= (-)^{l'+S'+l+S+L+K+J} \left\{ \begin{array}{ccc} l & \lambda & L \\ J & K & S \end{array} \right\} \left\{ \begin{array}{ccc} l' & \lambda' & L \\ J & K & S' \end{array} \right\} \qquad \text{(B.5.12)}$$

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we evaluate the σ sum of Wigner $6j$ symbols, and obtain

$$\begin{aligned}
&\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\ JM_J \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\ JM_J\rangle \\
&\quad = \delta_{NN'}\delta_{LL'}\,\sqrt{(2\lambda'+1)(2\lambda+1)}\,(-)^{\lambda'+\lambda+S'+S} \\
&\qquad \sum_K (2K+1)\begin{Bmatrix} l & \lambda & L \\ J & K & S \end{Bmatrix}\begin{Bmatrix} l' & \lambda' & L \\ J & K & S' \end{Bmatrix}\langle n'\,(l'S')\,K \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid n\,(lS)\,K\rangle\,.
\end{aligned} \tag{B.5.13}$$

The only missing link now is that the matrix element $\langle n'\,(l'S')\,K'\kappa' \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid n\,(lS)\,K\kappa\rangle$ shown in Eq. (B.5.9) has a $\delta_{ll'}\delta_{SS'}$ built-in condition in addition to the fact that the matrix is diagonal in K-space. This fact, together with Eq. (B.5.9), gives

$$\begin{aligned}
&\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\ JM_J \mid V_{ls}(r)\,\vec{l}\cdot\vec{S} \mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\ JM_J\rangle \\
&\quad = \delta_{JJ'}\delta_{M_JM_{J'}}\delta_{NN'}\delta_{LL'}\delta_{ll'}\delta_{SS'}\,(-)^{\lambda'+\lambda}\,\sqrt{(2\lambda'+1)(2\lambda+1)}\;\mathcal{R}\mathcal{M}[V_{ls}(r)](n'l\,;\,nl) \\
&\qquad \sum_K \frac{2K+1}{2}\,[K(K+1)-l(l+1)-S(S+1)]\begin{Bmatrix} l & \lambda & L \\ J & K & S \end{Bmatrix}\begin{Bmatrix} l & \lambda' & L \\ J & K & S \end{Bmatrix}.
\end{aligned} \tag{B.5.14}$$

B.6 l^2 Interaction.

The matrix element of the l^2 interaction can be easily calculated when the matrix element is written in the m representation

$$\begin{aligned}
&\langle n'N'\,l'm_{l'}\,L'M'\,S'm_{S'} \mid V_{l2}(r)\,l^2 \mid nN\,lm_l\,LM\,Sm_S\rangle \\
&\quad = \delta_{NN'}\,\delta_{LL'}\,\delta_{MM'}\,\delta_{ll'}\,\delta_{m_lm_{l'}}\;\;\delta_{SS'}\,\delta_{m_Sm_{S'}}\;\;l(l+1)\;\;\mathcal{R}\mathcal{M}(n'l:\,nl)\,.
\end{aligned} \tag{B.6.1}$$

As we already have done many times before, we use the transformation

$$\begin{aligned}
&\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\ J'M_{J'} \mid V_{l2}(r)\,l^2 \mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\ JM_J\rangle \\
&\quad = \sum_{m_{l'}M'm_{S'}\mu'} \langle l'\,m_{l'}\,L'\,M' \mid \lambda'\,\mu'\rangle\langle\lambda'\,\mu'\,S'\,m_{S'} \mid J'\,M_{J'}\rangle \\
&\qquad \sum_{m_lMm_S\mu} \langle l\,m_l\,L\,M \mid \lambda\,\mu\rangle\langle\lambda\,\mu\,S\,m_S \mid J\,M_J\rangle \\
&\qquad\qquad \langle n'N'\,l'm_{l'}\,L'M'\,S'm_{S'} \mid V_{l2}(r)\,l^2 \mid nN\,lm_l\,LM\,Sm_S\rangle\,,
\end{aligned} \tag{B.6.2}$$

substitute Eq. (B.6.1) and apply the orthogonality of the Clebsch-Gordon coefficients in order to reduce the sums over the magnetic moments. We have

$$\begin{aligned}
&\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\ J'M_{J'} \mid V_{l2}(r)\,l^2 \mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\ JM_J\rangle \\
&\quad = \delta_{NN'}\,\delta_{LL'}\,\delta_{ll'}\,\delta_{SS'}\;\;l(l+1)\;\;\mathcal{R}\mathcal{M}[V_{l2}(r](n'l\,;\,nl) \\
&\qquad \sum_{m_S\mu\mu'} \langle\lambda'\,\mu'\,S\,m_S \mid J'\,M_{J'}\rangle\langle\lambda\,\mu\,S\,m_S \mid J\,M_J\rangle \sum_{m_lM} \langle l\,m_l\,L\,M \mid \lambda'\,\mu'\rangle\langle l\,m_l\,L\,M \mid \lambda\,\mu\rangle
\end{aligned}$$

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$$= \delta_{NN'}\,\delta_{LL'}\,\delta_{ll'}\,\delta_{SS'}\quad l(l+1)\;\;\mathcal{RM}(n'l\,;\,nl)$$
$$\delta_{\lambda\lambda'}\sum_{m_S\mu\mu}\langle\lambda\,\mu\,S\,m_S\mid J'\,M_{J'}\rangle\langle\lambda\,\mu\,S\,m_S\mid J\,M_J\rangle$$

Finally, we get

$$\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\,J'M_{J'}\mid V_{l2}(r)\,l^2\mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\,JM_J\rangle$$
$$= \delta_{JJ'}\,\delta M_JM_{J'}\,\delta_{\lambda\lambda'}\,\delta_{NN'}\,\delta_{LL'}\,\delta_{ll'}\,\delta_{SS'}\quad l(l+1)\;\;\mathcal{RM}(n'l\,:\,nl)\,. \qquad \text{(B.6.3)}$$

B.7 $l^2\;\sigma_1\cdot\sigma_2$ Interaction.

The derivation of the matrix element for the $l^2\;\sigma_1\cdot\sigma_2$ interaction follows closely the calculation of the matrix element corresponding to the l^2 interaction. Again, we go to the m representation where the calculation of the matrix element is particularly simple, even though a little more involved that the one in the previous section: we have now a spin-space part in addition to the angular part

$$\langle n'N'\,\lambda'\mu'\,S'm_{S'}\mid V_{l2s}(r)\,l^2\;\sigma_1\cdot\sigma_2\mid nN\,\lambda\mu\,Sm_S\rangle$$
$$= \delta_{\lambda\lambda'}\,\delta_{\mu\mu'}\quad\delta_{SS'}\,\delta_{m_Sm_{S'}}\quad 2\Big[S(S+1)-\frac{3}{2}\Big]\quad\langle n'N'\,\lambda\mu\mid V_{l2s}(r)\,l^2\mid nN\,\lambda\mu\rangle$$
$$= \delta_{\lambda\lambda'}\,\delta_{\mu\mu'}\quad\delta_{SS'}\,\delta_{m_Sm_{S'}}\quad 2\Big[S(S+1)-\frac{3}{2}\Big]$$
$$\sum_{m_lM;m_{l'}M'}\langle l'\,m_{l'}\;L'\,M'\mid\lambda\,\mu\rangle\langle l\,m_l\;L\,M\mid\lambda\,\mu\rangle\;\langle n'N'\,l'm_{l'}\;L'M'\mid V_{l2s}(r)\,l^2\mid nN\,lm_l\;LM\rangle$$
$$= \delta_{\lambda\lambda'}\,\delta_{\mu\mu'}\,\delta_{SS'}\,\delta_{m_Sm_{S'}}\,2\Big[S(S+1)-\frac{3}{2}\Big]\,\delta_{ll'}\,\delta_{m_lm_{l'}}\;l(l+1)\;\mathcal{RM}[V_{l2s}(r)](n'l\,:\,nl)$$
$$\sum_{m_lM;m_{l'}M'}\langle l'\,m_{l'}\;L'\,M'\mid\lambda\,\mu\rangle\langle l\,m_l\;L\,M\mid\lambda\,\mu\rangle\,\delta_{NN'}\,\delta_{LL'}\,\delta_{MM'}$$
$$= \delta_{\lambda\lambda'}\,\delta_{\mu\mu'}\,\delta_{SS'}\,\delta_{m_Sm_{S'}}\,\delta_{NN'}\,\delta_{LL'}\,\delta_{ll'}\,2\Big[S(S+1)-\frac{3}{2}\Big]\quad l(l+1)\;\;\mathcal{RM}[V_{l2s}(r)](n'l\,:\,nl)\,. \qquad \text{(B.7.1)}$$

Then, we have

$$\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\,J'M_{J'}\mid V_{l2s}(r)\,l^2\;\sigma_1\cdot\sigma_2\mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\,JM_J\rangle$$
$$= \sum_{m_S\mu;m_{S'}\mu'}\langle\lambda'\,\mu'\,S'\,m_{S'}\mid J'\,M_{J'}\rangle\langle\lambda\,\mu\,S\,m_S\mid J\,M_J\rangle$$
$$\langle n'N'\,l'm_{l'}\;L'M'\,S'm_{S'}\mid V_{l2s}(r)\,l^2\;\sigma_1\cdot\sigma_2\mid nN\,lm_l\;LM\,Sm_S\rangle$$
$$= \delta_{\lambda\lambda'}\,\delta_{SS'}\,\delta_{NN'}\,\delta_{LL'}\,\delta_{ll'}\,2\Big[S(S+1)-\frac{3}{2}\Big]\quad l(l+1)\;\;\mathcal{RM}[V_{l2s}(r)](n'l\,:\,nl)$$
$$\sum_{m_S\mu}\langle\lambda\,\mu\,S\,m_S\mid J'\,M_{J'}\rangle\langle\lambda\,\mu\,S\,m_S\mid J\,M_J\rangle$$
$$= \delta_{JJ'}\delta_{M_JM_{J'}}\delta_{\lambda\lambda'}\,\delta_{SS'}\,\delta_{NN'}\,\delta_{LL'}\,\delta_{ll'}\,2\Big[S(S+1)-\frac{3}{2}\Big]\;l(l+1)\;\mathcal{RM}[V_{l2s}(r)](n'l\,;\,nl)\,. \qquad \text{(B.7.2)}$$

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B.8 Quadrupole Spin-Orbit Interaction.

The second procedure used to derive the spin-orbit matrix element, Eq (B.5.14) allows us to write down immediately the matrix element of the quadrupole spin-orbit interaction

$$\begin{aligned}
&\langle n'N'\,(l'L')_{\lambda'}(\tfrac{1}{2}\,\tfrac{1}{2})_{S'};\ JM_J \mid V_{ls2}(r)\,(\vec{l}\cdot\vec{S})^2 \mid nN\,(lL)_{\lambda}(\tfrac{1}{2}\,\tfrac{1}{2})_{S};\ JM_J\rangle \\
&\quad = \delta_{NN'}\delta_{LL'}\delta_{ll'}\delta_{SS'}\,(-)^{\lambda'+\lambda}\,\sqrt{(2\lambda'+1)(2\lambda+1)}\ \mathcal{RM}[V_{ls2}(r)](n'l:\,nl) \\
&\qquad \sum_K \frac{2K+1}{4}[K(K+1)-l(l+1)-S(S+1)]^2 \begin{Bmatrix} l & \lambda & L \\ J & K & S \end{Bmatrix} \begin{Bmatrix} l & \lambda' & L \\ J & K & S \end{Bmatrix}.
\end{aligned} \tag{B.8.1}$$

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Appendix C

Three-Body Matrix Elements Calculation.

We shall consider the case of tensor products of spherical tensors of the form

$$\left(X_1^{(k)} \odot \left[Y_2^{(k_1)} \otimes Z_3^{(k_2)}\right]^{(k)}\right) . \tag{C.0.1}$$

Then, we calculate expectation values of the operator (C.0.1). between 3-body states where the angular momentum of the first particle is coupled by particle-hole coupling to the total angular momentum of the second and third particles. This can be shown to be equal to

$$\begin{aligned}
&\langle (j_1 \overline{j_6})_\lambda \mid \left(X_1^{(k)} \odot \left[Y_2^{(k_1)} \otimes Z_3^{(k_2)}\right]^{(k)}\right) \mid \left((j_5 j_4)_{j_{54}} (j_2 j_3)_{\overline{j_{23}}}\right)_\lambda \rangle \\
&= \delta_{k\lambda} (-)^{j_{23}+j_{54}} \frac{\hat{j}_{23}\hat{j}_{54}}{\hat{\lambda}} \begin{Bmatrix} j_2 & j_5 & k_1 \\ j_3 & j_4 & k_2 \\ j_{23} & j_{54} & \lambda \end{Bmatrix} \\
&\quad \langle j_1 \| X^{(\lambda)} \| j_6 \rangle \langle j_2 \| Y^{(k_1)} \| j_5 \rangle \langle j_3 \| Z^{(k_2)} \| j_4 \rangle \ .
\end{aligned} \tag{C.0.2}$$

The corresponding three-body matrix element in the m-representation can be obtained as:

$$\begin{aligned}
&\langle l_1 j_1 l_2 j_2 l_3 j_3 \mid \left(X_1^{(k)} \odot \left[Y_2^{(k_1)} \otimes Z_3^{(k_2)}\right]^{(k)}\right) \mid l_6 j_6 l_5 j_5 l_4 j_4 \rangle \\
&= \sum_\lambda \delta_{k\lambda} \sum_{j_{23}\ j_{54}} (-)^{j_6+j_{54}} \frac{\hat{j}_{23}\hat{j}_{54}}{\hat{\lambda}} \begin{Bmatrix} j_2 & j_5 & k_1 \\ j_3 & j_4 & k_2 \\ j_{23} & j_{54} & \lambda \end{Bmatrix} \\
&\quad \langle j_1 \| X^{(\lambda)} \| j_6 \rangle \langle j_2 \| Y^{(k_1)} \| j_5 \rangle \langle j_3 \| Z^{(k_2)} \| j_4 \rangle \\
&\quad \sum_{m_{23}\, m_{54}} (-)^{-m_6-m_{23}} \langle j_2 m_2 j_3 m_3 \mid j_{23} m_{23} \rangle \langle j_5 m_5 j_4 m_4 \mid j_{54} m_{54} \rangle \\
&\quad \sum_\mu \langle j_1 m_1 j_6 - m_6 \mid \lambda\mu \rangle \langle j_{54} m_{54} j_{23} - m_{23} \mid \lambda\mu \rangle \\
&= \langle j_1 \| X^{(k)} \| j_6 \rangle \langle j_2 \| Y^{(k_1)} \| j_5 \rangle \langle j_3 \| Z^{(k_2)} \| j_4 \rangle \\
&\quad \sum_{j_{23}\ j_{54}} (-)^{j_6+j_{54}} \frac{\hat{j}_{23}\hat{j}_{54}}{\hat{k}} \begin{Bmatrix} j_2 & j_5 & k_1 \\ j_3 & j_4 & k_2 \\ j_{23} & j_{54} & k \end{Bmatrix} \\
&\quad \sum_{m_{23}\, m_{54}} (-)^{-m_6-m_{23}} \langle j_2 m_2 j_3 m_3 \mid j_{23} m_{23} \rangle \langle j_5 m_5 j_4 m_4 \mid j_{54} m_{54} \rangle \\
&\quad \sum_\kappa \langle j_1 m_1 j_6 - m_6 \mid k\kappa \rangle \langle j_{54} m_{54} j_{23} - m_{23} \mid k\kappa \rangle
\end{aligned} \tag{C.0.3}$$

In any actual calculation we shall only encounter three-body matrix elements in the m-representation, summed over all the magnetic quantum numbers (m_1, m_2, m_3, m_4, m_5, m_6).

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Note. The following reduced matrix element is particularly important ([Ed-65], Eq. 7.1.5):

$$\langle (l'\tfrac{1}{2})j' \,|\, \left[C^{(k_1)} \otimes \sigma\right]^{(k_2)} \,|\, (l\tfrac{1}{2})j\rangle = \hat{j}\hat{j}'\hat{k}_2 \begin{Bmatrix} l' & l & k_1 \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j' & j & k_2 \end{Bmatrix} \langle l' \,\|\, C^{(k_1)} \,\|\, l\rangle \langle \tfrac{1}{2} \,\|\, \sigma \,\|\, \tfrac{1}{2}\rangle$$

$$= \sqrt{6}\,\hat{j}\hat{j}'\hat{k}_2 \begin{Bmatrix} l' & l & k_1 \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j' & j & k_2 \end{Bmatrix} \langle l' \,\|\, C^{(k_1)} \,\|\, l\rangle\,, \quad \text{(C.0.4)}$$

where we have

$$\langle l' \,\|\, C^{(k)} \,\|\, l\rangle = \hat{l}\,\langle l0\,k0 \,|\, l'0\rangle \quad \text{(C.0.5)}$$

with $l + l' + k = even$. Note that, if $k_2 = 0$ and $l = l'$, then $k_1 = 1$, and the reduced matrix element (C.0.4) vanishes.

C.1 Radial Part of the Three-Body Matrix Elements.

Based on the experience gained in dealing with the two-body matrix elements, we shall now address the calculation of the radial part of the three-body matrix elements:

$$R^{k_1 k_2, \kappa_1 \kappa_2; kl}_{n_1 l_1\, n_2 l_2\, n_3 l_3 : n_6 l_6\, n_5 l_5\, n_4 l_4} = \int_0^\infty r_1^2\, dr_1\, \mathcal{R}_{n_1 l_1}(r_1)\, \mathcal{R}_{n_6 l_6}(r_1) \int_0^\infty r_2^2\, dr_2\, \mathcal{R}_{n_2 l_2}(r_2)\, \mathcal{R}_{n_5 l_5}(r_2)\, u(r_1, r_2) \int_0^\infty r_3^2\, dr_3\, \mathcal{R}_{n_3 l_3}(r_3)\, \mathcal{R}_{n_4 l_4}(r_3)\, v(r_1, r_3)\,. \quad \text{(C.1.1)}$$

where we have

$$u(r_1, r_2) = u^{(k_1 k_2; k)}(r_1, r_2) = \frac{2}{\pi} \int_0^\infty p^2\, dp\, \tilde{a}^{(k)}(p)\, j_{k_1}(pr_1)\, j_{k_2}(pr_2)$$

$$v(r_1, r_3) = v^{(\kappa_1 \kappa_2; l)}(r_1, r_3) = \frac{2}{\pi} \int_0^\infty q^2\, dq\, \tilde{b}^{(l)}(q)\, j_{\kappa_1}(qr_1)\, j_{\kappa_2}(qr_3)\,. \quad \text{(C.1.2)}$$

with

$$\tilde{a}^{(k)}(p) = \int_0^\infty r^2\, dr\, \mathcal{A}(r)\, j_k(pr)$$

$$\tilde{b}^{(l)}(q) = \int_0^\infty r^2\, dr\, \mathcal{B}(r)\, j_l(qr)\,. \quad \text{(C.1.3)}$$

Similarly to Eqs. (A.1.8) and (A.1.10), we have

$$\int_0^\infty r_2^2\, dr_2\, \mathcal{R}_{n_2 l_2}(r_2)\, \mathcal{R}_{n_5 l_5}(r_2)\, j_{k_2}(pr_2) = \frac{1}{(\sqrt{2})^3} \sum_n A^{n k_2}_{n_2 l_2\, n_5 l_5} \left[\sqrt{\frac{\pi}{2}}\, \widetilde{HO}_{n k_2}(p')\right]$$

$$\int_0^\infty r_3^2\, dr_3\, \mathcal{R}_{n_3 l_3}(r_3)\, \mathcal{R}_{n_4 l_4}(r_3)\, j_{\kappa_2}(qr_3) = \frac{1}{(\sqrt{2})^3} \sum_m A^{m \kappa_2}_{n_3 l_3\, n_4 l_4} \left[\sqrt{\frac{\pi}{2}}\, \widetilde{HO}_{m \kappa_2}(q')\right], \quad \text{(C.1.4)}$$

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where we have $p' = \frac{b}{\sqrt{2}}p$ and $q' = \frac{b}{\sqrt{2}}q$, and the expansion coefficients are defined as

$$\begin{aligned} A^{nk_2}_{n_2 l_2\, n_5 l_5} &= \int_0^\infty x'^2_2\, dx'_2\; R_{n_2 l_2}(\tfrac{1}{\sqrt{2}}x'_2)\; R_{n_5 l_5}(\tfrac{1}{\sqrt{2}}x'_2)\; \mathcal{HO}_{nk_2}(x'_2) \\ A^{m\kappa_2}_{n_3 l_3\, n_4 l_4} &= \int_0^\infty x'^3_2\, dx'_3\; R_{n_3 l_3}(\tfrac{1}{\sqrt{2}}x'_3)\; R_{n_4 l_4}(\tfrac{1}{\sqrt{2}}x'_3)\; \mathcal{HO}_{m\kappa_2}(x'_3)\,. \end{aligned} \qquad \text{(C.1.5)}$$

with $x' = \frac{\sqrt{2}}{b}r$. Therefore, the radial piece $R^{k_1 k_2,\kappa_1\kappa_2;kl}_{n_1 l_1\, n_2 l_2\, n_3 l_3\,;\, n_6 l_6\, n_5 l_5\, n_4 l_4}$ becomes

$$\begin{aligned} &\frac{2}{\pi}\left(\frac{1}{\sqrt{2}}\right)^6 \sum_n A^{nk_2}_{n_2 l_2\, n_5 l_5} \sum_m A^{m\kappa_2}_{n_3 l_3\, n_4 l_4} \int_0^\infty x_1^2\, dx_1\; R_{n_1 l_1}(x_1)\; R_{n_6 l_6}(x_1) \\ &\int_0^\infty p^2\, dp\; \tilde{a}^{(k)}(p)\; \widetilde{\mathcal{HO}}_{nk_2}(p')\; j_{k_1}(pr_1) \int_0^\infty q^2\, dq\; \tilde{b}^{(l)}(q)\; \widetilde{\mathcal{HO}}_{m\kappa_2}(q')\; j_{\kappa_1}(qr_1)\;. \end{aligned} \qquad \text{(C.1.6)}$$

The integral

$$\int_0^\infty p^2\, dp\; \tilde{a}^{(k)}(p)\; \widetilde{\mathcal{HO}}_{nk_2}(p')\; j_{k_1}(pr_1) \qquad \text{(C.1.7)}$$

can be calculated by changing variable from p to $p' = \frac{b}{\sqrt{2}}p$

$$\left(\frac{\sqrt{2}}{b}\right)^3 \int_0^\infty p'^2\, dp'\; \tilde{a}^{(k)}(\tfrac{\sqrt{2}}{b}p')\; \widetilde{\mathcal{HO}}_{nk_2}(p')\; j_{k_1}(p'x'_1) \qquad \text{(C.1.8)}$$

and expanding out part of the integrand in a harmonic oscillator basis

$$\tilde{a}^{(k)}(\tfrac{\sqrt{2}}{b}p')\; \widetilde{\mathcal{HO}}_{nk_2}(p') = \sum_s B^{sk_1}_{k,nk_2}\; \widetilde{\mathcal{HO}}_{sk_1}(p')\,. \qquad \text{(C.1.9)}$$

where the new expansions coefficients, $B^{sk_1}_{k,nk_2}$, are

$$B^{sk_1}_{k,nk_2} = \int_0^\infty p'^2\, dp'\; \tilde{a}^{(k)}(\tfrac{\sqrt{2}}{b}p')\; \widetilde{\mathcal{HO}}_{nk_2}(p')\; \widetilde{\mathcal{HO}}_{sk_1}(p')\,. \qquad \text{(C.1.10)}$$

Then, the integral (C.1.7) is readily calculated

$$\begin{aligned} &\int_0^\infty p^2\, dp\; \tilde{a}^{(k)}(p)\; \widetilde{\mathcal{HO}}_{nk_2}(p')\; j_{k_1}(pr_1) \\ &= \left(\frac{\sqrt{2}}{b}\right)^3 \sum_s B^{sk_1}_{k,nk_2} \int_0^\infty p'^2\, dp'\; \widetilde{\mathcal{HO}}_{sk_1}(p')\; j_{k_1}(p'x'_1) \\ &= \left(\frac{\sqrt{2}}{b}\right)^3 \sum_s B^{sk_1}_{k,nk_2} \left[\sqrt{\frac{\pi}{2}}\; \mathcal{HO}_{sk_1}(x'_1)\right]\,. \end{aligned} \qquad \text{(C.1.11)}$$

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In a similar manner, we also obtain

$$\int_0^\infty q^2\,dq\;\tilde{b}^{(l)}(q)\;\widetilde{HO}_{m\kappa_2}(q')\;j_{\kappa_1}(qr_1) \;=\; \left(\frac{\sqrt{2}}{b}\right)^3 \sum_t B^{t\kappa_1}_{l,m\kappa_2}\;\left[\sqrt{\frac{\pi}{2}}\;HO_{t\kappa_1}(x'_1)\right]. \tag{C.1.12}$$

with

$$B^{t\kappa_1}_{l,m\kappa_2} \;=\; \int_0^\infty q'^2\,dq'\;\tilde{b}^{(l)}(\tfrac{\sqrt{2}}{b}q')\;\widetilde{HO}_{m\kappa_2}(q')\;\widetilde{HO}_{t\kappa_1}(q')\,. \tag{C.1.13}$$

The substitution of the p and q integrals in Eq. (C.1.6), using Eqs. (C.1.11) and (C.1.12), plus one more change of variable ($x_1 \rightarrow \frac{1}{\sqrt{2}}x'_1$), lead to the final form of the radial part of the three-body matrix element

$$\begin{aligned} R^{k_1k_2,\kappa_1\kappa_2;kl}_{n_1l_1\,n_2l_2\,n_3l_3\,:\,n_6l_6\,n_5l_5\,n_4l_4} \;=\; & \left(\frac{1}{\sqrt{2}\,b^2}\right)^3 \sum_n A^{nk_2}_{n_2l_2\,n_5l_5} \sum_m A^{m\kappa_2}_{n_3l_3\,n_4l_4} \\ & \sum_s B^{sk_1}_{k,nk_2} \sum_t B^{t\kappa_1}_{l,m\kappa_2}\;\mathcal{I}^{k_1\kappa_1\,:\,st}_{n_1l_1\,n_6l_6}\,. \end{aligned} \tag{C.1.14}$$

where we have introduced the notation

$$\mathcal{I}^{k_1\kappa_1\,:\,st}_{n_1l_1\,n_6l_6} \;=\; \int_0^\infty x'^2_1\,dx'_1\;R_{n_1l_1}(\tfrac{1}{\sqrt{2}}x'_1)\;R_{n_6l_6}(\tfrac{1}{\sqrt{2}}x'_1)\;HO_{sk_1}(x'_1)\;HO_{t\kappa_1}(x'_1) \tag{C.1.15}$$

C.2 Two-Pion-Exchange Interaction.

$V_{2\pi 3N}$ such as presented in Equation (2.3.1) is not a convenient form to be implemented in a many-body calculation. What we actually need is an operator form, where tensor operators are coupled as in Eq. (C.0.1)

$$\left(X^{(k)}_1 \odot \left[Y^{(k_1)}_2 \odot Z^{(k_2)}_3\right]^{(k)}\right). \tag{C.2.1}$$

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Therefore, in order to transform $V_{2\pi 3N}$ given in Eq. (2.3.1) and obtain the required operator format, we shall make use of the following identities ([Ca-83])

$$\sigma_2 \cdot \sigma_3 = \frac{1}{2}\{\sigma_1 \cdot \sigma_2 \,.\, \sigma_1 \cdot \sigma_3\} \tag{C.2.2}$$

$$(\sigma_2 \cdot \hat{r}_{12})\,(\sigma_3 \cdot \hat{r}_{12}) = \frac{1}{6}\{(S_{12} + \sigma_1 \cdot \sigma_2) \,.\, \sigma_1 \cdot \sigma_3\} \tag{C.2.3}$$

$$(\sigma_2 \cdot \hat{r}_{13})\,(\sigma_3 \cdot \hat{r}_{13}) = \frac{1}{6}\{\sigma_1 \cdot \sigma_2 \,.\, (S_{13} + \sigma_1 \cdot \sigma_3)\} \tag{C.2.4}$$

$$(\sigma_2 \cdot \hat{r}_{12})\,(\sigma_3 \cdot \hat{r}_{13})\,(\hat{r}_{12} \cdot \hat{r}_{13}) = \frac{1}{18}\{(S_{12} + \sigma_1 \cdot \sigma_2) \,.\, (S_{13} + \sigma_1 \cdot \sigma_3)\} \tag{C.2.5}$$

$$\sigma_1 \cdot \sigma_2 \times \sigma_3 = \frac{1}{2\,i}[\sigma_1 \cdot \sigma_2 \,.\, \sigma_1 \cdot \sigma_3] \tag{C.2.6}$$

$$(\sigma_2 \cdot \hat{r}_{12})\,(\sigma_3 \cdot \sigma_1 \times \hat{r}_{12}) = \frac{1}{6\,i}[(S_{12} + \sigma_1 \cdot \sigma_2) \,.\, \sigma_1 \cdot \sigma_3] \tag{C.2.7}$$

$$(\sigma_2 \cdot \hat{r}_{13})\,(\sigma_1 \cdot \sigma_3 \times \hat{r}_{13}) = \frac{1}{6\,i}[\sigma_1 \cdot \sigma_2 \,.\, (S_{13} + \sigma_1 \cdot \sigma_3)] \tag{C.2.8}$$

$$(\sigma_2 \cdot \hat{r}_{12})\,(\sigma_3 \cdot \hat{r}_{13})\,(\sigma_1 \cdot \hat{r}_{12} \times \hat{r}_{13}) = \frac{1}{18\,i}[(S_{12} + \sigma_1 \cdot \sigma_2) \,.\, (S_{13} + \sigma_1 \cdot \sigma_3)] \,. \tag{C.2.9}$$

The inclusion of the two-pion-exchange interaction $V_{2\pi 3N}$, reduces then to the computation of three-body matrix elements of the operators

1. $\sigma_2 \cdot \sigma_3$

$$= \sum_k (2k+1)\; u^{(kk;0)}(r_1, r_2) \sum_l (-)^l\,(2l+1)\; v^{(ll;0)}(r_1, r_3) \sum_\lambda \langle k0\, l0 \mid \lambda 0\rangle$$
$$\sum_{j_{23}} (-)^{j_{23}}\,\hat{j}_{33} \sum_{k_{23}} \hat{k}_{23} \begin{Bmatrix} l & k & \lambda \\ k_{23} & j_{23} & 1 \end{Bmatrix}$$
$$\left(C_1^{(\lambda)} \odot \left[\left[C_2^{(k)} \otimes \sigma_2\right]^{(k_{23})} \otimes \left[C_3^{(l)} \otimes \sigma_3\right]^{(j_{23})}\right]^{(\lambda)}\right) \tag{C.2.10}$$

2. $(\sigma_2 \cdot \hat{r}_{12})\,(\sigma_3 \cdot \hat{r}_{12})$

$$= \sum_j \langle 10\,10 \mid j0\rangle \sum_{k_1 k_2} i^{k_2+k_1-j}\,(2k_1+1)\,(2k_2+1)\,\langle k_1 0\, k_2 0 \mid j0\rangle\; u^{(k_1 k_2; j)}(r_1, r_2)$$
$$\sum_{j_{23}} (-)^{j_{23}}\,\hat{j}_{23} \sum_{k_{23}} (-)^{k_{23}}\,\hat{k}_{23} \sum_k (2k+1)\; v^{(kk;0)}(r_1, r_3) \begin{Bmatrix} k_1 & k_2 & j \\ 1 & 1 & k_{23} \end{Bmatrix}$$
$$\sum_\lambda (-)^\lambda \langle k0\, k_1 0 \mid \lambda 0\rangle \begin{Bmatrix} k & k_1 & \lambda \\ k_{23} & j_{23} & 1 \end{Bmatrix}$$
$$\left(C_1^{(\lambda)} \odot \left[\left[C_2^{(k_2)} \otimes \sigma_2\right]^{(k_{23})} \otimes \left[C_3^{(k)} \otimes \sigma_3\right]^{(j_{23})}\right]^{(\lambda)}\right) \tag{C.2.11}$$

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3. $(\sigma_2 \cdot \hat{r}_{13})\,(\sigma_3 \cdot \hat{r}_{13})$

$$= \sum_j \langle 10\,10 \mid j0\rangle \sum_{k_1 k_2} i^{k_2+k_1-j}\,(2k_1+1)\,(2k_2+1)\,\langle k_1 0\,k_2 0 \mid j0\rangle\; v^{(k_1 k_2 j)}(r_1, r_3)$$
$$\sum_{k_{23}} \hat{k}_{23} \sum_{j_{23}} \hat{j}_{23} \sum_k (2k+1)\; u^{(kk0)}(r_1, r_2) \begin{Bmatrix} k_1 & k_2 & j \\ 1 & 1 & j_{23} \end{Bmatrix}$$
$$\sum_\lambda \langle k0\,k_1 0 \mid \lambda 0\rangle \begin{Bmatrix} k & k_1 & \lambda \\ j_{23} & k_{23} & 1 \end{Bmatrix}$$
$$\left(C_1^{(\lambda)} \odot \left[\left[C_2^{(k)} \otimes \sigma_2 \right]^{(k_{23})} \otimes \left[C_3^{(k_2)} \otimes \sigma_3 \right]^{(j_{23})} \right]^{(\lambda)} \right) \qquad \text{(C.2.12)}$$

4. $(\sigma_2 \cdot \hat{r}_{12})\,(\sigma_3 \cdot \hat{r}_{13})\,(\hat{r}_{12} \cdot \hat{r}_{13})$

$$= \sum_k \langle 10\,10 \mid k0\rangle \sum_j \langle 10\,10 \mid j0\rangle$$
$$\sum_{k_1 k_2} i^{k_2-k_1-k}\,(2k_1+1)\,(2k_2+1)\,\langle k_1 0\,k_2 0 \mid k0\rangle\; u^{(k_1 k_2 k)}(r_1, r_2)$$
$$\sum_{\kappa_1 \kappa_2} i^{\kappa_2+\kappa_1-j}\,(2\kappa_1+1)\,(2\kappa_2+1)\,\langle \kappa_1 0\,\kappa_2 0 \mid j0\rangle\; v^{(\kappa_1 \kappa_2 j)}(r_1, r_3)$$
$$\sum_{k_{23}} (-)^{k_{23}}\,\hat{k}_{23} \begin{Bmatrix} k_1 & k_2 & k \\ 1 & 1 & k_{23} \end{Bmatrix} \sum_{j_{23}} \hat{j}_{23} \begin{Bmatrix} \kappa_1 & \kappa_2 & j \\ 1 & 1 & j_{23} \end{Bmatrix}$$
$$\sum_\lambda \langle k_1 0\,\kappa_1 0 \mid \lambda 0\rangle \begin{Bmatrix} k_1 & \kappa_1 & \lambda \\ j_{23} & k_{23} & 1 \end{Bmatrix}$$
$$\left(C_1^{(\lambda)} \odot \left[\left[C_2^{(k_2)} \otimes \sigma_2 \right]^{(k_{23})} \otimes \left[C_3^{(\kappa_2)} \otimes \sigma_3 \right]^{(j_{23})} \right]^{(\lambda)} \right) \qquad \text{(C.2.13)}$$

5. $\sigma_1 \cdot \sigma_2 \times \sigma_3$

$$= -\sqrt{6}\,i \sum_k (2k+1)\; u^{(kk0)}(r_1, r_2) \sum_l (2l+1)\; v^{(ll0)}(r_1, r_3)$$
$$\sum_j (-)^j\,\hat{j}\,\langle k0\,l0 \mid j0\rangle \sum_\lambda (-)^\lambda \sum_{k_{23}} \hat{k}_{23} \sum_{j_{23}} \hat{j}_{23} \begin{Bmatrix} k & l & j \\ 1 & 1 & 1 \\ k_{23} & j_{23} & \lambda \end{Bmatrix}$$
$$\left(\left[C_1^{(j)} \otimes \sigma_1 \right]^{(\lambda)} \odot \left[\left[C_2^{(k)} \otimes \sigma_2 \right]^{(k_{23})} \otimes \left[C_3^{(l)} \otimes \sigma_3 \right]^{(j_{23})} \right]^{(\lambda)} \right) \qquad \text{(C.2.14)}$$

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6. $(\sigma_2 \cdot \hat{r}_{12})\,(\sigma_3 \cdot \sigma_1 \times \hat{r}_{12})$

$$= -\sqrt{6}\,i \sum_j \langle 10\,10 \mid j0\rangle \sum_{k_1 k_2} i^{k_2-k_1-j}\,(2k_1+1)\,(2k_2+1)\,\langle k_1 0\, k_2 0 \mid j0\rangle$$
$$u^{(k_1 k_2 j)}(r_1, r_2) \sum_k (2k+1)\; v^{(kk0)}(r_1, r_3) \sum_l (-)^l \hat{l}\,\langle k_1 0\, k0 \mid l0\rangle$$
$$\sum_{k_{23}} (-)^{k_{23}} \hat{k}_{23} \begin{Bmatrix} k_1 & k_2 & j \\ 1 & 1 & k_{23} \end{Bmatrix} \sum_{j_{23}} \hat{j}_{23} \sum_\lambda (-)^\lambda \begin{Bmatrix} k_1 & k & l \\ 1 & 1 & 1 \\ k_{23} & j_{23} & \lambda \end{Bmatrix}$$
$$\left(\left[C_1^{(l)} \odot \sigma_1 \right]^{(\lambda)} \odot \left[\left[C_2^{(k_2)} \odot \sigma_2 \right]^{(k_{23})} \odot \left[C_3^{(k)} \odot \sigma_3 \right]^{(j_{23})} \right]^{(\lambda)} \right) \qquad \text{(C.2.15)}$$

7. $(\sigma_2 \cdot \hat{r}_{13})\,(\sigma_1 \cdot \sigma_3 \times \hat{r}_{13})$

$$= -\sqrt{6}\,i \sum_j \langle 10\,10 \mid j0\rangle \sum_{k_1 k_2} i^{k_2-k_1-j}\,(2k_1+1)\,(2k_2+1)\,\langle k_1 0\, k_2 0 \mid j0\rangle$$
$$v^{(k_1 k_2 j)}(r_1, r_3) \sum_k (2k+1)\; u^{(kk0)}(r_1, r_2) \sum_l (-)^l \hat{l}\,\langle k0\, k_1 0 \mid l0\rangle$$
$$\sum_{k_{23}} \hat{k}_{23} \sum_{j_{23}} (-)^{j_{23}} \hat{j}_{23} \begin{Bmatrix} k_1 & k_2 & j \\ 1 & 1 & j_{23} \end{Bmatrix} \sum_\lambda (-)^\lambda \begin{Bmatrix} k & k_1 & l \\ 1 & 1 & 1 \\ k_{23} & j_{23} & \lambda \end{Bmatrix}$$
$$\left(\left[C_1^{(l)} \odot \sigma_1 \right]^{(\lambda)} \odot \left[\left[C_2^{(k)} \odot \sigma_2 \right]^{(k_{23})} \odot \left[C_3^{(k_2)} \odot \sigma_3 \right]^{(j_{23})} \right]^{(\lambda)} \right) \qquad \text{(C.2.16)}$$

8. $(\sigma_2 \cdot \hat{r}_{12})\,(\sigma_3 \cdot \hat{r}_{13})\,(\sigma_1 \cdot \hat{r}_{12} \times \hat{r}_{13})$

$$= -\sqrt{6}\,i \sum_k \langle 10\,10 \mid k0\rangle \sum_j \langle 10\,10 \mid j0\rangle$$
$$\sum_{k_1 k_2} i^{k_2-k_1-k}\,(2k_1+1)\,(2k_2+1)\,\langle k_1 0\, k_2 0 \mid k0\rangle\; u^{(k_1 k_2 k)}(r_1, r_2)$$
$$\sum_{\kappa_1 \kappa_2} i^{\kappa_2-\kappa_1-j}\,(2\kappa_1+1)\,(2\kappa_2+1)\,\langle \kappa_1 0\, \kappa_2 0 \mid j0\rangle\; v^{(\kappa_1 \kappa_2 j)}(r_1, r_3)$$
$$\sum_l (-)^l \hat{l}\,\langle k_1 0\, \kappa_1 0 \mid l0\rangle \sum_{k_{23}} (-)^{k_{23}} \hat{k}_{23} \begin{Bmatrix} k_1 & k_2 & k \\ 1 & 1 & k_{23} \end{Bmatrix}$$
$$\sum_{j_{23}} (-)^{j_{23}} \hat{j}_{23} \begin{Bmatrix} \kappa_1 & \kappa_2 & j \\ 1 & 1 & j_{23} \end{Bmatrix} \sum_\lambda (-)^\lambda \begin{Bmatrix} k_1 & \kappa_1 & l \\ 1 & 1 & 1 \\ k_{23} & j_{23} & \lambda \end{Bmatrix}$$
$$\left(\left[C_1^{(l)} \odot \sigma_1 \right]^{(\lambda)} \odot \left[\left[C_2^{(k_2)} \odot \sigma_2 \right]^{(k_{23})} \odot \left[C_3^{(\kappa_2)} \odot \sigma_3 \right]^{(j_{23})} \right]^{(\lambda)} \right)$$
$$\text{(C.2.17)}$$

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C.3 Repulsive Three-Nucleon Interaction.

Similarly to the two-pion-exchange interaction $V_{2\pi 3N}$ treatment above, we need to transform the short-range interaction part of the three-nucleon potential, $V^I_{3N\,R}$, and obtain the required operator form (C.0.1) of the interaction, as

$$V^I_{3N\,R} = \sum_k (-)^k (2k+1)\; u^{(kk;0)}(r_1, r_2) \sum_l (-)^l (2l+1)\; v^{(ll;0)}(r_1, r_3)$$
$$\sum_\lambda (-)^\lambda \langle k0\, l0 \mid \lambda 0\rangle \left(C_1^{(\lambda)} \odot \left[C_2^{(k)} \odot C_3^{(l)} \right]^{(\lambda)} \right) . \qquad \text{(C.3.1)}$$

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Appendix D

Isospin Matrix Elements Calculation.

The isospin dependence of the matrix elements is worked out in m_τ representation. We introduce the isospin operator in terms of the usual Pauli matrices

$$\tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \tau_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{D.0.1}$$

We introduce the proton/neutron creation/destruction operators in terms of the Cartesian components of the isospin operator

$$\tau_+ = \frac{1}{2}(\tau_x + i\tau_y) \tag{D.0.2}$$

$$\tau_- = \frac{1}{2}(\tau_x - i\tau_y) \tag{D.0.3}$$

such that

$$\begin{aligned} \tau_+ |p\rangle &= 0 \qquad & \tau_+ |n\rangle &= |p\rangle \\ \tau_- |n\rangle &= 0 \qquad & \tau_- |p\rangle &= |n\rangle . \end{aligned}$$

Reciprocally, we have

$$\tau_x = \tau_+ + \tau_- \tag{D.0.4}$$

$$\tau_y = \frac{1}{i}(\tau_+ - \tau_-) \tag{D.0.5}$$

With these definitions, the expectation values of the various operators in m_τ representation, are computed in terms of the matrices

$$\langle \tau' | \tau_+ | \tau \rangle = \begin{cases} 1 & \text{if } |\tau\rangle = |n\rangle \text{ and } |\tau'\rangle = |p\rangle \\ 0 & \text{otherwise} \end{cases} \tag{D.0.6}$$

$$\langle \tau' | \tau_- | \tau \rangle = \begin{cases} 1 & \text{if } |\tau\rangle = |p\rangle \text{ and } |\tau'\rangle = |n\rangle \\ 0 & \text{otherwise} \end{cases} \tag{D.0.7}$$

$$\langle \tau' | \tau_z | \tau \rangle = \begin{cases} 1 & \text{if } |\tau\rangle = |\tau'\rangle = |p\rangle \\ -1 & \text{if } |\tau\rangle = |\tau'\rangle = |n\rangle \\ 0 & \text{otherwise} \end{cases} \tag{D.0.8}$$

The following two-operators are relevant for the calculation of two- and three-body matrix elements:

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- $\tau_1 \cdot \tau_2$: appears in the calculation of both two- and three-body matrix elements. In terms of the proton/neutron creation/destruction operators, $\tau_\pm$, this operator can be expressed as

$$\tau_1 \cdot \tau_2 = 2(\tau_{1+}\tau_{2-} + \tau_{1-}\tau_{2+}) + \tau_{10}\tau_{20} \tag{D.0.9}$$

- $\tau_1 \cdot (\tau_2 \times \tau_3)$: appears in the calculation of three-body matrix elements. We first introduce the spherical tensor components of the isospin operator:

$$\tau_1^{(1)} = -\frac{1}{\sqrt{2}}(\tau_x + i\tau_y) \tag{D.0.10}$$

$$\tau_{-1}^{(1)} = +\frac{1}{\sqrt{2}}(\tau_x - i\tau_y) \tag{D.0.11}$$

$$\tau_0^{(1)} = \tau_z \tag{D.0.12}$$

Note the relationship: $\tau_{\pm 1}^{(1)} = \mp\sqrt{2}\tau_\pm$. In terms of their spherical tensor components, we have

$$\begin{aligned}
&\tau_1 \cdot (\tau_2 \times \tau_3) \\
&= -i\sqrt{2}\left\{-\tau_{1\,1}^{(1)}[\tau_2 \otimes \tau_3]_{-1}^{(1)} - \tau_{1\,-1}^{(1)}[\tau_2 \otimes \tau_3]_{1}^{(1)} + \tau_{1\,0}^{(1)}[\tau_2 \otimes \tau_3]_{0}^{(1)}\right\} \qquad \text{(D.0.13)} \\
&= -i\sqrt{2}\sum_{m_{\tau 2} m_{\tau 3}} \tau_{2\,m_{\tau 2}}^{(1)} \tau_{3\,m_{\tau 3}}^{(1)} \left\{-\langle 1 m_{\tau 2}\, 1 m_{\tau 3} \mid 1\,-1\rangle \tau_{1\,1}^{(1)}\right. \\
&\qquad \left. -\langle 1 m_{\tau 2}\, 1 m_{\tau 3} \mid 1\,1\rangle \tau_{1\,-1}^{(1)} + \langle 1 m_{\tau 2}\, 1 m_{\tau 3} \mid 1\,0\rangle \tau_{1\,0}^{(1)}\right\} \qquad \text{(D.0.14)}
\end{aligned}$$

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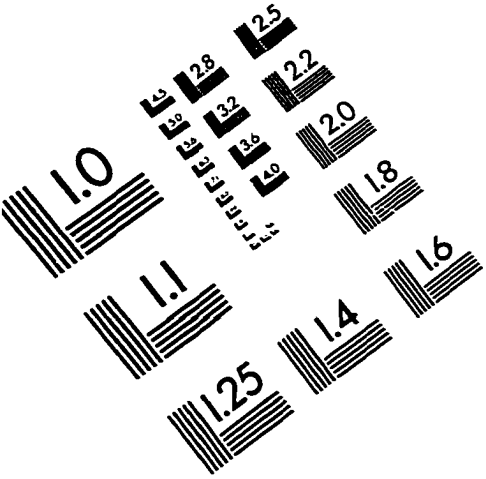
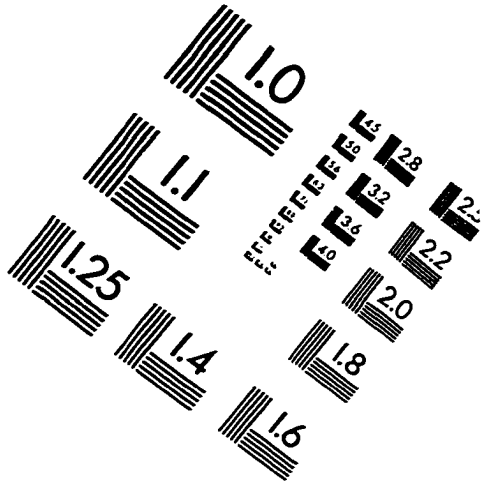
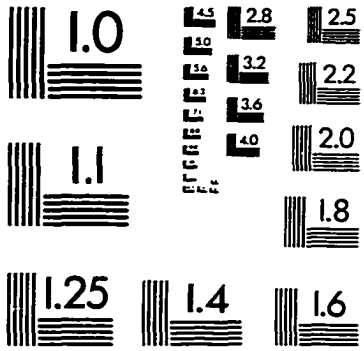
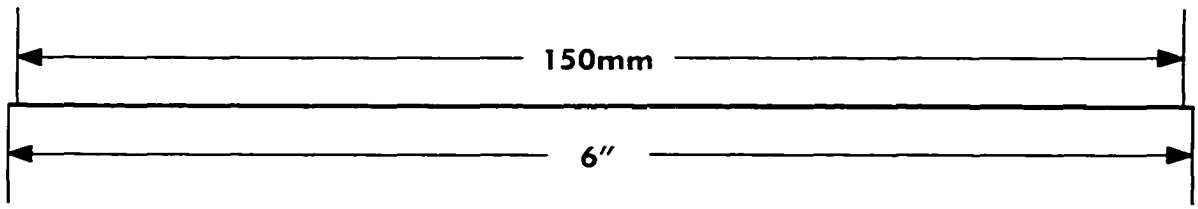
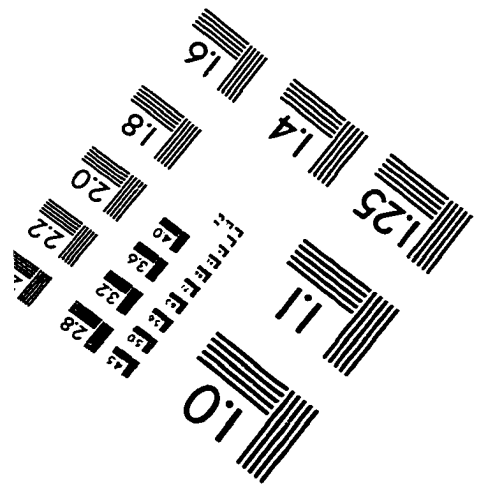
IMAGE EVALUATION TEST TARGET (QA-3)

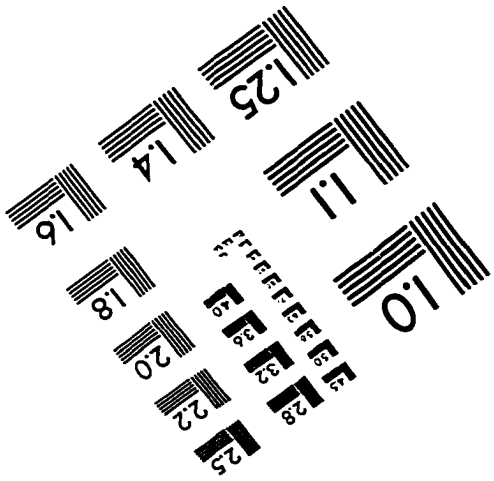












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