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On Calculating Matrix Elements of Slater-Determinant Wave Functions in the Cluster Model

R. Beck
Institut für Angewandte Kernphysik

Kernforschungszentrum Karlsruhe

KERNFORSCHUNGSZENTRUM KARLSRUHE

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R. Beck

Kernforschungszentrum Karlsruhe GmbH, Karlsruhe

Kernforschungszentrum Karlsruhe GmbH
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Abstract

This report is concerned with the calculation of matrix elements of Slater-determinant wave functions. These matrix elements are the basic input to any calculation with the Generator Coordinate Method (GCM). The main emphasis lies upon the projection of angular momentum and parity. The projection method is an analytical one making extensive use of Racah algebra and leads to closed expressions of these matrix elements in terms of 3-j, 6-j and 9-j symbols. It is shown that matrix elements of the kinetic energy operator may be obtained in a simple way from those of the normalization. The spurious contribution of the kinetic energy operator to the center-of-mass energy is eliminated by projecting the linear momentum of the states.

ZUR BERECHNUNG VON MATRIXELEMENTEN VON VIELTEILCHENWELLENFUNKTIONEN IM CLUSTER MODELL

Zusammenfassung

Das Ziel der Arbeit ist die Berechnung von Matrixelementen des Identitätsoperators, sowie der Operatoren der kinetischen Energie und der Zweiteilchenwechselwirkung zwischen Vielteilchenwellenfunktionen. Diese Matrixelemente sind die Eingabedaten für jede Rechnung mit der Generator Koordinaten Methode. Das Hauptgewicht liegt dabei auf der Projektion von Drehimpuls und Parität. Die Projektionsmethode ist eine analytische, welche geschlossene Ausdrücke für diese Matrixelemente in Termen von 3-j, 6-j und 9-j Symbolen liefert. Es wird gezeigt, daß sich die Matrixelemente der kinetischen Energie in einfacher Weise auf diejenigen der Normierung zurückführen lassen. Die Translationsinvarianz der Zustände wird durch Projektion auf guten linearen Impuls sichergestellt.

Contents

1. Introduction

2. Specification of the Generator Coordinate (GC) Wave Function for Coupled Two- and Three-Cluster Structures

3. The Channel Representation of GC Wave Functions

4. Projection of Eigenstates of the Total Linear Momentum

5. Some Properties of Matrix Elements of Slater-Determinant Wave Functions

6. Expansion of Matrix Elements of a Scalar Spin-Isospin Independent Operator O between Two-Center Shell Model (SM) Functions into Spherical Tensors

7. Expansion of Matrix Elements of O between Two- and Three-Center SM Functions into Spherical Tensors

8. Expansion of Matrix Elements of O between Three-Center SM Functions into Spherical Tensors

9. Projection of Spin Angular Momentum

10. Discussion

1. Introduction

The cluster Model[1] of the nucleus has been fairly successful in explaining many features of nuclear phenomena in the low energy region. In most of these studies[2,3] the dominance of two-cluster structures is assumed. Simple arguments based on the binding energies of clusters suggest, however, that also three-cluster configurations might play an essential role in providing a simple model for some light nuclei. Recently the interplay of two- and three-cluster structures was studied in a calculation[4] of some low-lying states in ^{7}Li.

The aim of this report is to present in detail the method of calculating matrix elements of many body wave functions which are needed in applications of the cluster model to systems where two- and three-cluster structures are dominant.

In sec. 2 we specify the generator coordinate (GC) wave function for a system in which two- and three-cluster structures are dominant and introduce multipole expansions with respect to certain generator coordinates. In sec. 3 these wave functions are expressed in terms of another set of coordinates ("channel coordinates") which lead to an identification of the quantum numbers specifying the spherical tensors of sec. 2 with the quantum numbers of nuclear systems. Section 4 deals with the handling of the spurious contribution of the kinetic energy operator to matrix elements of Slater-determinant wave functions. Section 5 contains a collection of formulas for matrix elements of Slater-determinant wave functions which proved useful in numerical calculations. Some of these formulas were already derived by D.M. Brink in his article[5] on the α-particle model of light nuclei. In sections 6-8 the expansion of matrix elements of a scalar spin-isospin independent operator O between two- and three-center SM functions in terms of spherical tensors is worked out using Racah algebra. In sec. 9 the method of projecting spin angular momentum is outlined and applied to the nucleus ^{7}Li.

2. Specification of the Generator Coordinate Wave Function for Coupled Two- and Three-Cluster Structures

In order to describe a nucleus with N nucleons in which two- and three-cluster configurations with mass numbers $A^{(2)}$, $B^{(2)}$ $(A^{(2)}+B^{(2)} = N)$

and $A^{(3)}$, $B^{(3)}$, $C^{(3)}$ $(A^{(3)}+B^{(3)}+C^{(3)} = N)$ are predominant, we take a set of single-particle wave functions

$$\psi(\underset{\sim}{x},\underset{\sim}{s}) = (\beta/\pi)^{3/4} \exp[-\frac{\beta}{2}(\underset{\sim}{x}-\underset{\sim}{s})^2]\chi. \tag{2.1}$$

The function (2.1) describes the motion of a single nucleon in a 1s harmonic oscillator orbit centered at the point $\underset{\sim}{s}$. The spin-isospin part of the wave function is denoted by χ, the quantity β is the oscillator parameter. We then construct products of $A^{(2)}$, $B^{(2)}$, $A^{(3)}$ etc. single particle functions (2.1) with oscillator orbits centered at $\underset{\sim}{s}_A(2)$, $\underset{\sim}{s}_B(2)$, $\underset{\sim}{s}_A(3)$ etc. which correspond to the clusters $A^{(2)}$, $B^{(2)}$, $A^{(3)}$ etc.

$$\phi_A(2)\ (\{\underset{\sim}{x}_A(2)\},\ \underset{\sim}{s}_A(2)) = \prod_{i=1}^{A^{(2)}} \psi_i(\underset{\sim}{x}_i,\underset{\sim}{s}_A(2)) \tag{2.2}$$

where

$$\{\underset{\sim}{x}_A(2)\} = (\underset{\sim}{x}_1,\ \underset{\sim}{x}_2,\ldots\ \underset{\sim}{x}_A(2)).$$

From the functions (2.2) we form the two sets of antisymmetrized ($\mathcal{A}$ = antisymmetrizer) N-particle functions

(i) two-cluster functions

$$\phi^{(2)}_{I_i I\nu}(\{\underset{\sim}{x}\},\underset{\sim}{s}) = [\mathcal{A}\phi_A(2)(\{\underset{\sim}{x}\}_A(2),\ \underset{\sim}{s}_A(2))\phi_B(2)(\{\underset{\sim}{x}\}_B(2),\ \underset{\sim}{s}_B(2))]_{I\nu} \tag{2.3a}$$

where

$$\underset{\sim}{s} = \underset{\sim}{S}_A(2)-\underset{\sim}{S}_B(2),\ A^{(2)}\underset{\sim}{S}_A(2)+B^{(2)}\underset{\sim}{S}_B(2) = 0 \tag{2.4a}$$

and

$$\{\underset{\sim}{x}\} = (\underset{\sim}{x}_1\ldots\underset{\sim}{x}_N).$$

(ii) three-cluster functions

$$\phi^{(3)}_{I_i I\nu}(\{\underset{\sim}{x}\},\ \underset{\sim}{s}_1,\ \underset{\sim}{s}_2)$$

$$= [\mathcal{A}\phi_A(3)\ (\{\underset{\sim}{x}\}_A(3),\ \underset{\sim}{S}_A(3))\phi_B(3)\ (\{\underset{\sim}{x}\}_B(3),\ \underset{\sim}{S}_B(3))$$
$$* \ \phi_C(3)\ (\{\underset{\sim}{x}\}_C(3),\ \underset{\sim}{S}_C(3))]_{I\nu} \tag{2.3b}$$

where

$$\underset{\sim}{s}_1 = \underset{\sim}{s}_A(3)-\underset{\sim}{s}_B(3),\ \underset{\sim}{s}_2 = \underset{\sim}{s}_C(3)-(A^{(3)}\underset{\sim}{s}_A(3)+B^{(3)}\underset{\sim}{s}_B(3))/(A^{(3)}+B^{(3)})$$

$$A^{(3)}\underset{\sim}{s}_A(3)+B^{(3)}\underset{\sim}{s}_B(3)+C^{(3)}\underset{\sim}{s}_C(3) = 0. \tag{2.4b}$$

The symbol $[\quad]_{I\nu}$ means that the spins of all particles are coupled to the total spin I and projection ν on the Z axis, whereas the symbol I_i stands for all intermediate spin quantum numbers which are necessary for this coupling. We observe that both sets of functions (2.3a) and (2.3b) form a spherical tensor of rank I in spin space.

It will prove useful later on to expand the two-cluster functions (2.3a) in terms of spherical harmonics

$$\phi^{(2)}(\{\underset{\sim}{x}\},\ \underset{\sim}{s}) = \sum_{LM} \frac{1}{s}\, \phi^{(2)}(\{\underset{\sim}{x}\},\ LMs)\ Y^{*}_{LM}(\hat{s}). \tag{2.5a}$$

In a similar way the three-cluster function (2.3b) can be written in a bipolar basis[6)]

$$\phi^{(3)}(\{\underset{\sim}{x}\},\ \underset{\sim}{s}_1,\ \underset{\sim}{s}_2,) = \sum_{L_1L_2LM} \frac{1}{s_1s_2}\, \phi^{(3)}(\{\underset{\sim}{x}\},\ L_1L_2LMs_1s_2)$$

$$*\ B^{*}(L_1L_2LM\hat{s}_1,\hat{s}_2) \tag{2.5b}$$

where

$$B(L_1L_2LM\hat{s}_1,\hat{s}_2) = \sum_{M_1M_2} (L_1M_1,L_2M_2|LM)Y_{L_1M_1}(\hat{s}_1)Y_{L_2M_2}(\hat{s}_2) \tag{2.6a}$$

For simplicity we suppressed all spin quantum numbers in eqs. (2.5a, 2.5b). The bipolar harmonics (2.6a) enjoy the following properties

$$\int d\hat{s}_1 d\hat{s}_2\ B^{*}(L_1L_2LM\hat{s}_1,\ \hat{s}_2)\ B(L_1'L_2'L'M'\ \hat{s}_1,\hat{s}_2)$$

$$= \delta_{L_1L'_1}\delta_{L_2L'_2}\delta_{LL'}\delta_{MM'} \tag{2.6b}$$

$$B(L_1L_2LM-\hat{s}_1,-\hat{s}_2) = (-)^{L_1+L_2}\ B(L_1L_2LM\hat{s}_1,\hat{s}_2) \tag{2.6c}$$

In order to study the tensor properties of the wave functions (2.5a) and (2.5b) in coordinate space, we observe that a simultaneous rotation of the basis of both the spatial coordinates $\underset{\sim}{x}_i$ and the vectors $\underset{\sim}{s}_A(2)$, $\underset{\sim}{s}_B(2)$ etc. specifying the positions of the corresponding harmonic oscillator wells leave the wave functions unchanged. This is a consequence of the fact that relative 1s orbits only are involved. By virtue of eqs. (2.4a) and (2.4b) it follows that the rotation of the basis of vectors $\tilde{s}_A(2)$, $\tilde{s}_B(2)$ etc. may be replaced by a rotation of the basis of the generator coordinates $\tilde{s}$, $\tilde{s}_1$ and $\tilde{s}_2$.

$$R_{\tilde{x}}(\Omega)\ R_{\tilde{s}}(\Omega)\ \phi^{(2)}(\{\tilde{x}\},\ \tilde{s}) = \phi^{(2)}(\{\tilde{x}\},\ \tilde{s}) \tag{2.7a}$$

$$R_{\tilde{x}}(\Omega)\ R_{\tilde{s}_1,\tilde{s}_2}(\Omega)\ \phi^{(3)}(\{x\},\ \tilde{s}_1,\ \tilde{s}_2) = \phi^{(3)}(\{\tilde{x}\},\ \tilde{s}_1,\ \tilde{s}_2), \tag{2.7b}$$

where $R(\Omega)$ is a unitary rotation operator which rotates the basis through Euler angles Ω. If we insert the expansions (2.5) into eqs. (2.7) we find

$$R_x(\Omega)\phi^{(2)}(\{\tilde{x}\},\mathcal{L}\mathcal{M}s) = \sum_{\mathcal{M}'} D^{\mathcal{L}}_{\mathcal{M}'\mathcal{M}}(\Omega)\phi^{(2)}(\{\tilde{x}\},\mathcal{L}\mathcal{M}'s) \tag{2.8a}$$

$$R_x(\Omega)\phi^{(3)}(\{\tilde{x}\},L_1L_2\mathcal{L}\mathcal{M}s_1s_2) = \sum_{\mathcal{M}'} D^{\mathcal{L}}_{\mathcal{M}'\mathcal{M}}(\Omega)\phi^{(3)}(\{\tilde{x}\},L_1L_2\mathcal{L}\mathcal{M}'s_1s_2) \tag{2.8b}$$

where

$$D^{\mathcal{L}}_{\mathcal{M}'\mathcal{M}}(\Omega) = (\mathcal{L}\mathcal{M}'|R(\Omega)|\mathcal{L}\mathcal{M})$$

is the usual rotation matrix.

The last two equations imply that both sets of wave functions $\phi^{(2)}_{I_i I\nu}(\{\tilde{x}\},\mathcal{L}\mathcal{M}s)$ and $\phi^{(3)}_{I_i I\nu}(\{\tilde{x}\},\ L_1L_2\mathcal{L}\mathcal{M}s_1s_2)$ form a spherical tensor of rank $\mathcal{L}$ in coordinate space. Upon coupling the spin and coordinate tensors in $\phi^{(2)}$ and $\phi^{(3)}$ we may obtain wave functions which are eigenfunctions of the total angular momentum

$$\phi^{(2)}_{I_i I}(\{\tilde{x}\},\ \mathcal{L}s,\ JM) = \sum_{\nu\mathcal{M}} (I\nu,\mathcal{L}\mathcal{M}|JM)\phi^{(2)}_{I_i I\nu}(\{\tilde{x}\},\mathcal{L}\mathcal{M}s) \tag{2.9a}$$

$$\phi^{(3)}_{I_i I}(\{x\},L_1L_2\mathcal{L}s_1s_2,JM) = \sum_{\nu\mathcal{M}} (I\nu,\mathcal{L}\mathcal{M}|JM)\phi^{(3)}_{I_i I\nu}(\{\tilde{x}\},L_1L_2\mathcal{L}\mathcal{M}s_1s_2) \tag{2.9b}$$

where $M = \nu+\mathcal{M}$.

The properties of these tensors under the parity transformation $\tilde{x}_i \rightarrow -\tilde{x}_i$ may be derived from the relations

$$\phi^{(2)}(\{-\tilde{x}\},\tilde{s}) = \phi^{(2)}(\{\tilde{x}\},-\tilde{s}) \tag{2.10a}$$

and

$$\phi^{(3)}(\{-\underset{\sim}{x}\};\underset{\sim}{s}_1,\underset{\sim}{s}_2) = \phi^{(3)}(\{\underset{\sim}{x}\},-\underset{\sim}{s}_1,-\underset{\sim}{s}_2) \qquad (2.10b)$$

which follow from the fact that all particle coordinates occur in the combination $(\underset{\sim}{x}_i-\underset{\sim}{s}_A(2))^2$ etc.
Inserting the expansions (2.5) into eqs. (2.10), we obtain

$$\phi^{(2)}(\{-\underset{\sim}{x}\},\mathcal{L}s,JM) = (-)^{\mathcal{L}}\phi^{(2)}(\{\underset{\sim}{x}\},\mathcal{L}s,JM) \qquad (2.11a)$$

$$\phi^{(3)}(\{-\underset{\sim}{x}\},L_1L_2\mathcal{L}s_1s_2,JM) = (-)^{L_1+L_2}\phi^{(3)}(\{\underset{\sim}{x}\},L_1L_2\mathcal{L}s_1s_2,JM) \qquad (2.11b)$$

where we used $Y_{\mathcal{L}M}(-\hat{s}) = (-)^{\mathcal{L}}Y_{\mathcal{L}M}(\hat{s})$ together with eq. (2.6c).
Finally, a trial function of the GC type with fixed total angular momentum and parity is constructed by superposing the functions (2.9)

$$\psi(\{\underset{\sim}{x}\}JM\pi) = \sum_{I_iIL}\int_0^\infty ds f^{(2)}_{I_iI}(LsJM)\phi^{(2)}_{I_iI}(\{\underset{\sim}{x}\},Ls,JM)$$

$$+\sum_{I_iIL_1L_2\mathcal{L}}\int_0^\infty ds_1ds_2 f^{(3)}_{I_iI}(L_1L_2\mathcal{L}s_1s_2JM)\phi^{(3)}_{I_iI}(\{x\},L_1L_2\mathcal{L}s_1s_2,JM) \qquad (2.12)$$

where the parity relations (2.11) restrict the possible orbital angular momenta

$$(-)^L = (-)^{L_1+L_2} = \pi \qquad (2.13a)$$

whereas the triangular rules in eqs. (2.6a) and (2.9) imply

$$|I - L| \le J \le |I - L| \qquad (2.13b)$$

$$|L_1-L_2| \le \mathcal{L} \le |L_1+L_2| \qquad (2.13c)$$

$$|I - \mathcal{L}| \le J \le |I + \mathcal{L}| \qquad (2.13d)$$

3. The Channel Representation of GC Wave Functions

In the last section we expressed the N-particle wave functions of the GC type in terms of the coordinates $\underset{\sim}{x}_i$ (i = 1..N) of all nucleons.

There is an alternative choice of coordinates which is convenient if we want to use these wave functions in a scattering calculation. For brevity, we shall call this set of coordinates the channel coordinates. Rewriting the wave functions in terms of channel coordinates also leads to a simple physical interpretation of the orbital angular momenta L, L_1, L_2 and $\mathcal{L}$ defined in the last section. In addition, the spurious contribution of the kinetic energy operator to the total center-of-mass energy is easily studied in this representation.

We define channel coordinates as follows

(i) two-cluster systems

Let $\underset{\sim}{R}_A(2)$ and $\underset{\sim}{R}_B(2)$ denote the centers of mass of the clusters $A^{(2)}$ and $B^{(2)}$

$$\underset{\sim}{R}_A(2) = 1/A^{(2)} \sum_{i=1}^{A^{(2)}} \underset{\sim}{x}_i$$
$$\underset{\sim}{R}_B(2) = 1/B^{(2)} \sum_{i=A^{(2)}+1}^{N} \underset{\sim}{x}_i . \qquad (3.1)$$

We then define N-2 intrinsic coordinates,

$$\underset{\sim}{\xi}_i^{(2)} = \begin{cases} \underset{\sim}{x}_i - \underset{\sim}{R}_A(2) \\ \underset{\sim}{x}_i - \underset{\sim}{R}_B(2) \end{cases} \quad \text{for } i \doteq \begin{cases} 1,\dots(A^{(2)}-1) \\ (A^{(2)}+1)\dots(N-1) \end{cases} \qquad (3.2a)$$

The distance $\underset{\sim}{r}$ between clusters $A^{(2)}$ and $B^{(2)}$ and their center-of-mass coordinate $\underset{\sim}{R}$ are chosen as the remaining two coordinates

$$\underset{\sim}{r} = \underset{\sim}{R}_A(2) - \underset{\sim}{R}_B(2) \qquad (3.2b)$$

$$\underset{\sim}{R} = (A^{(2)}\underset{\sim}{R}_A(2) + B^{(2)}\underset{\sim}{R}_B(2))/N. \qquad (3.2c)$$

If we insert the N coordinates (3.2) into the two-cluster function (2.3a) we obtain

$$\phi^{(2)}_{I_i I\nu}(\{\underset{\sim}{x}\},\underset{\sim}{s}) = (\beta/\pi)^{3/4N} \exp(-\tfrac{1}{2}\beta N \underset{\sim}{R}^2)$$
$$* [\mathcal{A} \exp\{-\tfrac{1}{2}\beta[\sum_{i=1}^{N} \underset{\sim}{\xi}_i^{(2)2} + \frac{A^{(2)}B^{(2)}}{N} \quad (\underset{\sim}{r} - \underset{\sim}{s})^2]\} * \prod_{i=1}^{N} \chi_i \;]_{I_i I\nu} \qquad (3.3)$$

where we used the abbreviations

$$\underset{\sim}{\xi}^{(2)}_{A^{(2)}} = -\sum_{i=1}^{A^{(2)}-1} \underset{\sim}{\xi}_i^{(2)} \quad \text{and} \quad \underset{\sim}{\xi}_N^{(2)} = -\sum_{i=A^{(2)}+1}^{N-1} \underset{\sim}{\xi}_i^{(2)}$$

Expanding eq. (3.3) in terms spherical harmonics we have

$$\phi^{(2)}_{I_i I\nu}(\{\underset{\sim}{x}\},\underset{\sim}{s}) = (\beta/\pi)^{3/4N} \exp(-\tfrac{1}{2}\beta N R^2)$$

$$* \; [A \exp\{-\tfrac{1}{2}\beta[\sum_{i=1}^{N} \xi_i^{(2)2} + \frac{A^{(2)}B^{(2)}}{N} \quad (r^2+s^2)]\}$$

$$* \; 4\pi \sum_{LM} i_L \, (\beta\frac{A^{(2)}B^{(2)}}{N} \, r\, s) \quad Y_{LM} \; (\hat{r}) \, Y^*_{LM}(\hat{s}) \, [\prod_{i=1}^{N} \chi_i]_{I_i I\nu}$$

where i_L is a modified spherical Bessel function.
A comparison with eq. (2.5a) gives

$$\phi^{(2)}(\{\underset{\sim}{x}\}, LMs) = (\beta/\pi)^{3/4N} \exp(-\tfrac{1}{2}\beta N R^2)$$

$$*[A \exp\{-\tfrac{1}{2}\beta[\sum_{i=1}^{N} \xi_i^{(2)2} + \frac{A^{(2)}B^{(2)}}{N} \quad (r^2+s^2)]\}$$

$$*4\pi s \, i_L(\beta \, \frac{A^{(2)}B^{(2)}}{N} \; r\, s) \quad Y_{LM}(\hat{r} \quad) \, [\prod_{i=1}^{N} \chi_i]_{I_i I\nu} \qquad (3.4)$$

which shows that L is the orbital angular momentum related to the relative motion of the clusters $A^{(2)}$ and $B^{(2)}$.

<u>(ii) three-cluster systems</u>

Let $\underset{\sim}{R}_A(3)$, $\underset{\sim}{R}_B(3)$ and $\underset{\sim}{R}_C(3)$ be the centers of mass of the clusters $A^{(3)}$, $B^{(3)}$ and $C^{(3)}$, respectively

$$\underset{\sim}{R}_A(3) = 1/A^{(3)} \sum_{i=1}^{A^{(3)}} \underset{\sim}{x}_i$$

$$\underset{\sim}{R}_B(3) = 1/B^{(3)} \sum_{i=A^{(3)}+1}^{A^{(3)}+B^{(3)}} \underset{\sim}{x}_i \qquad (3.5)$$

$$\underset{\sim}{R}_C(3) = 1/C^{(3)} \sum_{A^{(3)}+B^{(3)}+1}^{N} \underset{\sim}{x}_i$$

When then define N-3 intrinsic coordinates

$$\underset{\sim}{\xi}_i^{(3)} = \begin{cases} \underset{\approx}{x}_i - \underset{\approx}{R}_A(3) \\ \underset{\approx}{x}_i - \underset{\approx}{R}_B(3) \\ \underset{\approx}{x}_i - \underset{\approx}{R}_C(3) \end{cases} \quad \text{for} \quad \begin{cases} i = 1 \ldots (A^{(3)}-1) \\ i = (A^{(3)}+1) \ldots (A^{(3)}+B^{(3)}-1) \\ i = (A^{(3)}+B^{(3)}+1) \ldots (N-1) \end{cases} \tag{3.6a}$$

The remaining three coordinates are chosen in accordance with the usual definition of Jacobi coordinates of the three body system (compare with eq. (2.4b)

$$\underset{\approx}{r}_1 = \underset{\approx}{R}_A(3) - \underset{\approx}{R}_B(3) \tag{3.6b}$$

$$\underset{\approx}{r}_2 = \underset{\approx}{R}_C(3) - (A^{(3)}\underset{\approx}{R}_A(3) + B^{(3)}\underset{\approx}{R}_B(3))/(A^{(3)}+B^{(3)}) \tag{3.6c}$$

$$\underset{\approx}{R} = \left(A^{(3)}\underset{\approx}{R}_A(3) + B^{(3)}\underset{\approx}{R}_B(3) + C^{(3)}\underset{\approx}{R}_C(3)\right)/N \tag{3.6d}$$

If we insert the N coordinates (3.6) in the three-cluster function (2.3b) we obtain

$$\phi^{(3)}_{I_i I\nu}(\{\underset{\approx}{x}\}, \underset{\approx}{s}_1, \underset{\approx}{s}_2)$$

$$= (\beta/\pi)^{3/4N} \exp(-\tfrac{1}{2}\beta N R^2)[\mathcal{A} \exp\{-\tfrac{1}{2}\beta[\sum_{i=1}^{N} \xi_i^{(3)2}$$

$$+ \frac{A^{(3)}B^{(3)}}{A^{(3)}+B^{(3)}}(\underset{\approx}{r}_1-\underset{\approx}{s}_1)^2 + \frac{(A^{(3)}+B^{(3)})C^{(3)}}{N}(\underset{\approx}{r}_2-\underset{\approx}{s}_2)^2\}$$

$$* \prod_{i=1}^{N} \chi_i]_{I_i I\nu} \tag{3.7}$$

where we used the abbreviations

$$\underset{\sim}{\xi}^{(3)}_{A^{(3)}} = -\sum_{i=1}^{A^{(3)}-1} \underset{\sim}{\xi}_i^{(3)}, \quad \underset{\sim}{\xi}^{(3)}_{A^{(3)}+B^{(3)}} = -\sum_{i=A^{(3)}+1}^{A^{(3)}+B^{(3)}-1} \underset{\sim}{\xi}_i^{(3)}$$

and

$$\underset{\sim}{\xi}_N^{(3)} = -\sum_{i=A^{(3)}+B^{(3)}+1}^{N-1} \underset{\sim}{\xi}_i^{(3)}$$

Expanding eq. (3.7) in terms of bipolar harmonics (2.6a) we have

$$\phi^{(3)}_{I_i I\nu}(\{x\},s_1,s_2)$$

$$= (\beta/\pi)^{3/4N} \exp(-\tfrac{1}{2}\beta NR^2)[A \exp\{-\tfrac{1}{2}\beta[\sum_{i=1}^{N} \xi_i^{(3)2}$$

$$+ \frac{A^{(3)}B^{(3)}}{A^{(3)}+B^{(3)}}(r_1^2+s_1^2)+\frac{(A^{(3)}+B^{(3)})C^{(3)}}{N}(r_2^2+s_2^2)\}$$

$$* \sum_{L_1L_2LM}(4\pi)^2 i_{L_1}(\beta\frac{A^{(3)}B^{(3)}}{A^{(3)}+B^{(3)}} r_1s_1) i_{L_2}(\beta\frac{(A^{(3)}+B^{(3)})C^{(3)}}{N} r_2s_2)$$

$$* B(L_1L_2LM\hat{r}_1,\hat{r}_2)B^*(L_1L_2LM\hat{s}_1,\hat{s}_2) \prod_{i=1}^{N}\chi_i]_{I_i I\nu}$$

A comparison with eq. (2.5b) gives

$$\phi^{(3)}_{I_i I\nu}(\{x\},L_1L_2LMs_1\ s_2)$$

$$= (\beta/\pi)^{3/4N} \exp(-\tfrac{1}{2}\beta NR^2)[A \exp\{-\tfrac{1}{2}\beta[\sum_{i=1}^{N} \xi_i^{(3)2}$$

$$+ \frac{A^{(3)}B^{(3)}}{A^{(3)}+B^{(3)}}(r_1^2+s_1^2)+\frac{(A^{(3)}+B^{(3)})C^{(3)}}{N}(r_2^2+s_2^2)\}$$

$$* s_1s_2(4\pi)^2 i_{L_1}(\beta\frac{A^{(3)}B^{(3)}}{A^{(3)}+B^{(3)}} r_1s_1) i_{L_2}(\beta\frac{(A^{(3)}+B^{(3)})C^{(3)}}{N} r_2s_2)$$

$$* B(L_1L_2LM\hat{r}_1,\hat{r}_2)\prod_{i=1}^{N}\chi_i]_{I_i I\nu} \qquad (3.8)$$

Refering to the definition (2.6a) of the bipolar harmonics, we see that L_1 and L_2 are the orbital angular momenta related to the Jacobi coordinates r_1 and r_2, respectively. These two angular momenta are then coupled to the total orbital angular momentum L. We conclude that the decomposition of the N-particle functions $\phi^{(2)}$ and $\phi^{(3)}$ into spherical tensors with definite angular momenta is especially useful if there is information available - either from experiment or from theory - on angular momenta of the cluster involved. In this way one may restrict the summation over angular momenta in the ansatz (2.12) of the trial function to those which dominate in a specific state. To illustrate this point, let us consider a three cluster model[4) of ^7Li assuming a clusterization into ^4He, ^2H and neutron. The ground state $3/2^-$ and the first excited state $1/2^-$(0.48 MeV) may be described in a L-S coupling scheme by $L_1 = 0$ (relative motion between ^4He and ^2H), $L_2 = 1$ (relative motion between the neutron and ^6Li), $L = 1$ (total orbital angular momentum) and $I_n = 1/2$ (spin of neutron), $I_\alpha = 0$ (spin of ^4He), $I_d = (0,1)$ (spin of ^2H), $I = 1/2$ (total spin). The excited state $5/2^-$(7.46 MeV) may be characterized by the same set of orbital angular momentum quantum numbers while the spin quantum numbers are $I_n = 1/2$, $I_\alpha = 0$, $I_d = 1$ and $I = 3/2$.

4. Projection of Eigenstates of the Total Linear Momentum

If a nuclear state is represented by a shell-model wave function (or by a product of shell-model wave functions centered at different positions as in our case) the center of mass of the system is confined to a small region in space (see eqs. (3.3) and (3.7)). As a consequence, the center-of-mass energy is not zero but has some finite positive value. We therefore project this state onto the eigenspace of the operator of total linear momentum[7) by introducing the following linear combinations

(i) two-cluster functions

$$\Phi^{(2)}(\{\underset{\sim}{x}\}\underset{\sim}{K},\underset{\sim}{s}) = \int d^3S e^{i\underset{\sim}{K}\cdot\underset{\sim}{S}}\, \Phi^{(2)}(\{\underset{\sim}{x}\}\underset{\sim}{S},\underset{\sim}{s}) \tag{4.1a}$$

where we used in eq. (2.3a) the relations

$$\underset{\sim}{s} = \underset{\sim}{S}_A(2)-\underset{\sim}{S}_B(2), \underset{\sim}{S} = (A^{(2)}\underset{\sim}{S}_A(2)+B\underset{\sim}{S}_B(2))/N$$

instead of eq. (2.4a).

(ii) three-cluster functions

$$\phi^{(3)}(\{\underset{\sim}{x}\}\underset{\sim}{K},\underset{\sim}{s}_1,\underset{\sim}{s}_2) = \int d^3S\ e^{i\underset{\sim}{K}\cdot\underset{\sim}{S}}\phi^{(3)}(\{\underset{\sim}{x}\}\underset{\sim}{S},\underset{\sim}{s}_1,\underset{\sim}{s}_2) \tag{4.1b}$$

Again the mean position of the cluster centers

$$\underset{\sim}{S} = [A^{(3)}\underset{\sim}{S}_A(3)+B^{(3)}\underset{\sim}{S}_B(3)+C^{(3)}\underset{\sim}{S}_C(3)]/N$$

is not fixed at the origin as in eq. (2.4b) but is used as generator coordinate. The quadratic forms in the particle coordinates appearing in the functions $\phi^{(2)}$ and $\phi^{(3)}$ may now be evaluated in terms the channel coordinates and the generator coordines $\underset{\sim}{s}$, $\underset{\sim}{S}$ and $\underset{\sim}{s}_1, \underset{\sim}{s}_2, \underset{\sim}{S}$. One then obtains

$$\sum_{i=1}^{A^{(2)}} (\underset{\sim}{x}_i - \underset{\sim}{S}_A(2))^2 + \sum_{i=A^{(2)}+1}^{N} (\underset{\sim}{x}_i - \underset{\sim}{S}_B(2))^2$$

$$= \sum_{i=1}^{N} (\xi_i^{(2)})^2 + A^{(2)} (\underset{\sim}{R}_A(2) - \underset{\sim}{S}_A(2))^2 + B^{(2)} (\underset{\sim}{R}_B(2) - \underset{\sim}{S}_B(2))^2$$

$$= \sum_{i=1}^{N} (\xi_i^{(2)})^2 + N(\underset{\sim}{R} - \underset{\sim}{S})^2 + \frac{A^{(2)} B^{(2)}}{N} (\underset{\sim}{r} - \underset{\sim}{s})^2 \tag{4.2a}$$

and

$$\sum_{i=1}^{A^{(3)}} (\underset{\sim}{x}_i - \underset{\sim}{S}_A(3))^2 + \sum_{i=A^{(3)}+1}^{A^{(3)}+B^{(3)}} (\underset{\sim}{x}_i - \underset{\sim}{S}_B(3))^2 + \sum_{i=A^{(3)}+B^{(3)}+1}^{N} (\underset{\sim}{x}_i - \underset{\sim}{S}_C(3))^2$$

$$= \sum_{i=1}^{N} (\xi_i^{(3)})^2 + A^{(3)} (\underset{\sim}{R}_A(3) - \underset{\sim}{S}_A(3))^2 + B^{(3)} (\underset{\sim}{R}_B(3) - \underset{\sim}{S}_B(3))^2 + C^{(3)} (\underset{\sim}{R}_C(3) - \underset{\sim}{S}_C(3))^2$$

$$= \sum_{i=1}^{N} (\xi_i^{(3)})^2 + N(\underset{\sim}{R} - \underset{\sim}{S})^2 + \frac{A^{(3)} B^{(3)}}{A^{(3)} + B^{(3)}} (\underset{\sim}{r}_1 - \underset{\sim}{s}_1)^2$$

$$+ C^{(3)} (A^{(3)} + B^{(3)}) / N \cdot (\underset{\sim}{r}_2 - \underset{\sim}{s}_2)^2 \tag{4.2b}$$

In both cases the dependence on the center-of-mass coordinate is through $(\underset{\sim}{R} - \underset{\sim}{S})^2$, leading to a factorization of the wave functions

$$\phi = \phi_{int} \exp[-\frac{\beta}{2} N (\underset{\sim}{R} - \underset{\sim}{S})^2] \tag{4.3}$$

where ϕ_{int} is an intrinsic wave function depending only on the relative coordinates of the nucleons. Using eqs. (4.1) and (4.3) we may then write for the scalar product of two many body wave funcitons with linear momentum $\underset{\sim}{K}$ and $\underset{\sim}{K}'$

$$<\phi(\underset{\sim}{K})|\phi'(\underset{\sim}{K}')>$$

$$= (2\pi)^3\delta^3(\underset{\sim}{K}-\underset{\sim}{K}')(\frac{4\pi}{\beta N})^{3/2}\ e^{-K^2/(\beta N)} \tag{4.4}$$

$$* <\phi(\underset{\sim}{S} = 0)|\phi'(\underset{\sim}{S}' = 0)>$$

In order to eliminate the spurious contribution to the energy when calculating matrix elements of the Hamiltonian between shell-model wave functions, we calculate matrix elements of the kinetic energy operator of the center-of-mass motion $T_{CM} = -\hbar^2/(2M)\Delta_{\underset{\sim}{R}}$, where $M = Nm$ is the total mass of the nucleus (m is the nucleon mass) between wave functions (4.1). Using the separation (4.3) of the wave functions, we obtain

$$<\phi(\underset{\sim}{K})|\ H\ |\phi'(\underset{\sim}{K}')>$$

$$= \int d^3S\ d^3S'\ \exp\ [i(\underset{\sim}{K}\cdot\underset{\sim}{S}'-\underset{\sim}{K}\cdot\underset{\sim}{S})]$$

$$* \int d^3R\ \exp\ [-\tfrac{1}{2}\beta N(\underset{\sim}{R}-\underset{\sim}{S})^2]<\phi_{int}|\ H-T_{CM}$$

$$-\frac{\hbar^2}{2M}\Delta_R\ |\phi'_{int}>\ \exp\ [-\tfrac{1}{2}\beta N(\underset{\sim}{R}-\underset{\sim}{S}')^2]$$

We notice that $(H-T_{CM})$ is independent of the center-of-mass coordinate $\underset{\sim}{R}$. The integration over $\underset{\sim}{R}$ may then be carried out easily.

$$<\phi(\underset{\sim}{K})|\ H\ |\phi(\underset{\sim}{K}')>$$

$$= \int d^3S\ d^3S'\ \exp\ [i(\underset{\sim}{K}\cdot\underset{\sim}{S}'-\underset{\sim}{K}\cdot S)]$$

$$* (\frac{\pi}{\beta N})^{3/2}\ \exp\ [-\frac{\beta N}{4}(\underset{\sim}{S}-\underset{\sim}{S}')^2]$$

$$* <\phi_{int}|\ H-T_{CM}-\frac{\beta\hbar^2}{4m}\ [-3+\frac{\beta N}{2}\ (\underset{\sim}{S}-\underset{\sim}{S}')^2]|\phi'_{int}>$$

$$= (2\pi)^3\delta^3(\underset{\sim}{K}-\underset{\sim}{K}')(\frac{2\pi}{\beta N})^3\ e^{-K^2/(\beta N)}$$

(continued next page)

$$* \langle\phi_{int}|H-T_{CM}+\frac{(\hbar K)^2}{2M}|\phi'_{int}\rangle$$

$$= (2\pi)^3\delta^3(\underset{\sim}{K}-\underset{\sim}{K}')(\frac{4\pi}{\beta N})^{3/2}e^{-K^2/(\beta N)}$$

$$* \langle\phi(\underset{\sim}{S}=0)|H-T_{CM}+\frac{(\hbar K)^2}{2M}|\phi'(\underset{\sim}{S}=0)\rangle$$

$$= (2\pi)^3\delta^3(\underset{\sim}{K}-\underset{\sim}{K}')(\frac{4\pi}{\beta N})^{3/2}e^{-K^2/(\beta N)}$$

$$* \langle\phi(\underset{\sim}{S}=0)|H-\frac{3\beta\hbar^2}{4m}+\frac{(\hbar K)^2}{2M}|\phi'(\underset{\sim}{S}'=0)\rangle \quad (4.5)$$

In the sequel we shall use the wave functions (2.9) with a fixed center of clusters ($\underset{\sim}{S}$ = 0)instead of the functions (4.1) with a fixed center-of-mass momentum $\underset{\sim}{K}$. In calculating matrix elements between wave functions (2.9) we must not forget, however, to subtract the spurious contribution to the center-of-mass energy $3\beta\hbar^2/(4m)$.

5. Some Properties of Matrix Elements of Slater-Determinant Wave Functions

In this section we derive explicit formulas for matrix elements of the kinetic energy operator and the two-body interaction operator between Slater-determinant wave functions. The derivation here is based on the work by D.M. Brink[5]. Our first objective is to show that once the overlap of two Slater determinants is known it is trivial to calculate matrix elements of the kinetic energy operator. In the remainder of this section we calculate matrix elements of a spin-isospin independent two-body interaction and derive some useful symmetry relations for them.

(i) Normalization

Let $\psi_1\ldots\psi_N$ and $\psi'_1\ldots\psi'_N$ be two sets of single particle functions. Let Φ_o and Φ'_o be products of N single particle functions

$$\Phi_o = \prod_{i=1}^{N} \psi_i(x_i) \ , \ \Phi'_o = \prod_{i=1}^{N} \psi'_i(x_i) \quad (5.1a)$$

The corresponding antisymmetrized Slater-determinant wave functions are defined by

$$\Phi = \sqrt{N!}\ \mathcal{A}\Phi_o \ , \ \Phi' = \sqrt{N!}\ \mathcal{A}\Phi'_o \quad (5.1b)$$

with the antisymmetrization operator A satisfying

$$A\Phi(x_1 \dots x_N) = \frac{1}{N!} \sum_P \varepsilon(\alpha\beta\dots\zeta)\Phi(x_\alpha, x_\beta \dots x_\zeta) \tag{5.1c}$$

where the symbol x_i comprises spatial and spin coordinates of particle i. The sum in eq. (5.1c) goes over all N! permutations of the particle coordinates, and $\varepsilon(\alpha\beta\dots\zeta)$ is the signature of the permutation which transforms $\{1,2\dots n\}$ into $\{\alpha,\beta\dots\zeta)$. Thus

$$\begin{aligned}
<\Phi|\Phi'> &= <\Phi_o|A\Phi'_o>N! \\
&= \sum_P <\psi_1(1)\dots\psi_N(N)|\varepsilon(\alpha\beta\dots\zeta)\psi'_\alpha(1)\psi'_\beta(2)\dots\psi'_\zeta(N)> \\
&= \det\{<\psi_i|\psi'_j>\}
\end{aligned} \tag{5.2a}$$

For later reference we quote also the results when we expand the determinant in (5.2a) into cofactors of one or two rows

$$<\Phi|\Phi'> = \sum_{k=1}^{N} <\psi_i|\psi'_k>C_{ik} \tag{5.2b}$$

and

$$<\Phi|\Phi'> = \sum_{\substack{k,l=1 \\ k \neq l}}^{N} <\psi_i|\psi'_k><\psi_j|\psi'_l>C_{ijkl} \tag{5.2c}$$

with the cofactors

$$C_{ik} = (-)^{i+k} A_{ik} \tag{5.3a}$$

$$C_{ijkl} = \pm (-)^{i+j+k+l} A_{ijkl} \qquad \text{if} \begin{Bmatrix} i \lessgtr j,\ k \lessgtr l \\ i \lessgtr j,\ k \gtrless l \end{Bmatrix} \tag{5.3b}$$

The minors A_{ik} (A_{ijkl}) are defined as the determinants of the normalization matrix $<\psi_i|\psi'_k>$ when the i-th column and the k-th row (the i-th and j-th columns and the k-th and l-th rows) are left out.

(ii) Kinetic Energy

The kinetic energy operator is $T = \sum_{i=1}^{N} t_i$ where $t_i = -\hbar^2/(2m)\nabla_i^2$ acts only on the spatial coordinates of nucleon i.

$$<\Phi|T|\Phi'> = \sum_{i=1}^{N} <t_i\Phi_o|A\Phi'_o>N! \qquad (5.4)$$

The wave function $t_i\Phi_o$ is obtained from Φ_o by replacing ψ_i by $t_i\psi_i$. If we use the single particle functions (2.1) then

$$<\psi_i|\psi'_j> = <\chi_i|\chi'_j> \exp[-\frac{\beta}{4}(\underset{\sim}{s}_i-\underset{\sim}{s}'_j)^2] \qquad (5.5)$$

$$<t_i\psi_i|\psi'_j> = [\frac{3\beta\hbar^2}{4m} + \frac{\hbar^2\beta^2}{2m}\frac{d}{d\beta}] <\psi_i|\psi'_j> \qquad (5.6)$$

The modified determinants in eq. (5.4) may be evaluated using the cofactor expansion (5.2b)

$$<\Phi|T|\Phi'> = \sum_{i,j=1}^{N} <t_i\psi_i|\psi'_j> C_{ij}$$

together with the relation

$$\sum_{i,j=1}^{N} C_{ij}(\beta)\frac{d}{d\beta}<\psi_i|\psi'_j> = \frac{d}{d\beta}\det\{<\psi_i|\psi'_j>\} \qquad (5.7)$$

$$<\Phi|T-T_{CM}|\Phi'> = [\frac{3\beta\hbar^2(N-1)}{4m} + \frac{\hbar^2\beta^2}{2m}\frac{d}{d\beta}]<\Phi|\Phi'> \qquad (5.8)$$

The proof of the relation (5.7) requires the expansion theorem of determinants. Let $D(\beta) = \det\{a_{ij}(\beta)\}$ where the matrix elements a_{ij} depend on the parameter β.

Then for ε infinitesimally small

$$D(\beta+\varepsilon) = \det\{a_{ij}(\beta) + \varepsilon\frac{d}{d\beta}a_{ij}(\beta)\}$$

$$= \begin{vmatrix} a_{11}(\beta)\ldots\ldots & a_{1N}(\beta) \\ \cdot & \\ \cdot & \\ \cdot & \\ a_{N1}(\beta)\ldots\ldots & a_{NN}(\beta) \end{vmatrix} + \varepsilon\sum_{j=1}^{N}\begin{vmatrix} a_{11}(\beta)\ldots\frac{d}{d\beta}a_{1j}(\beta)\ldots a_{1N}(\beta) \\ \cdot \\ \cdot \\ \cdot \\ a_{N1}(\beta)\ldots\frac{d}{d\beta}a_{Nj}(\beta)\ldots a_{NN}(\beta) \end{vmatrix}$$

Using the cofactor expansion (5.2b) yields the desired result

$$D'(\beta) = \frac{1}{\varepsilon}\,[D(\beta+\varepsilon) - D(\beta)]$$
$$= \sum_{ij} \frac{da_{ij}(\beta)}{d\beta}\, C_{ij}(\beta)\ .$$

(iii) Two-Body Interaction

The spin-isospin independent interaction is $V = \frac{1}{2}\sum_{i\neq j} V_{ij}$ where V_{ij} acts only on the spatial coordinates $\underset{\sim}{x}_i$ and $\underset{\sim}{x}_j$ of the nucleons i and j. Let $\varphi(\underset{\sim}{x})$ denote the spatial part of ψ, then

$$<\Phi|V|\Phi'> = \frac{1}{2}\sum_{i\neq j} <V_{ij}\Phi_o|A\Phi_o'>\ N!$$

$$= \frac{1}{2}\sum_{i\neq j}\ \sum_{\alpha\beta\ldots\zeta} \varepsilon(\alpha\beta\ldots\zeta) \int d^3x_1\ldots d^3x_N \varphi^*{}_1(\underset{\sim}{x}_1)<\chi_1(1)|\ldots$$

$$\ldots\varphi_N^*(\underset{\sim}{x}_N)<\chi_N(N)|V_{ij}\varphi_\alpha'(\underset{\sim}{x}_1)|\chi_\alpha'(1)>\ldots|\varphi_\zeta'(\underset{\sim}{x}_N)|\chi_\zeta'(N)>$$

$$= \frac{1}{2}\sum_{i\neq j} \int d^3x_i d^3x_j\ V_{ij} \sum_{\alpha\beta..\zeta} \varepsilon(\alpha\beta\ldots\zeta)$$

$$* <\psi_1|\psi_\alpha'><\psi_2|\psi_\beta'>\ldots<\chi_i|\chi_\rho'>\varphi_i^*(\underset{\sim}{x}_i)\varphi_\rho'(\underset{\sim}{x}_i)$$

$$\ldots<\chi_j|\chi_\sigma'>\varphi_j^*(\underset{\sim}{x}_j)\varphi_\sigma'(\underset{\sim}{x}_j)\ldots.<\psi_N|\psi_\zeta'>$$

$$= \frac{1}{2}\sum_{i\neq j} \int d^3x_i d^3x_j\ V_{ij}\ \det\{\ b^{(ij)}\} \qquad (5.9)$$

The matrix $b^{(ij)}$ has elements identical to those of the normalization matrix except for the i-th and j-th row. The elements of the i-th row read

$$<\chi_i|\chi_k'>\varphi_i^*(\underset{\sim}{x}_i)\varphi_k'(\underset{\sim}{x}_i) \qquad ,\ k = 1\ldots N$$

and similarly for the j-th row. Expanding det$'$ $\{b^{(ij)}\}$ in terms of the matrix elements of the i-th and j-th row

$$\det\{b^{(ij)}\} = \sum_{k \neq l} \langle\chi_i|\chi_k'\rangle\langle\chi_j|\chi_l'\rangle \varphi_i^*(\underset{\sim}{x}_i)\varphi_k'(\underset{\sim}{x}_i)$$

$$* \; \varphi_j^*(\underset{\sim}{x}_j)\varphi_l'(\underset{\sim}{x}_j) C_{ijkl} \tag{5.10}$$

where the generalized cofactors are defined in eq. (5.3b). By means of eq. (5.10) we obtain from eq. (5.9)

$$\langle\Phi|V|\Phi'\rangle = \frac{1}{2} \sum_{i \neq j, k \neq l} \langle\chi_i|\chi_k'\rangle\langle\chi_j|\chi_l'\rangle \int d^3x_i d^3x_j$$

$$* \; \varphi_i^*(\underset{\sim}{x}_i)\varphi_j^*(\underset{\sim}{x}_j) V_{ij} \varphi_k'(\underset{\sim}{x}_i)\varphi_l'(\underset{\sim}{x}_j) C_{ijkl} \tag{5.11}$$

If we compare this equation with the expression (5.2c) of the normalization matrix element we realize that all relations with respect to spin-isospin quantum numbers of $\langle\Phi|\Phi'\rangle$ remain true for matrix elements $\langle\Phi|V|\Phi'\rangle$ of a spin-isospin independent two-body interaction V. In sec. 9 when dealing with the projection of spin angular momentum, we shall make use of this property. Equation (5.11) may be simplified by noting the symmetry relations

$$C_{ijkl} = - C_{ijlk} = - C_{jikl}$$

$$C_{ijkl} = C_{jilk}$$

with follow from eq. (5.3b)

$$\langle\Phi|V|\Phi'\rangle = \frac{1}{2} \sum_{i \neq j, k \neq l} V_{ijkl} \, C_{ijkl}$$

$$= \frac{1}{2} \sum_{i<j, k<l} \bar{V}_{ijkl} \, C_{ijkl} \tag{5.12}$$

where

$$\bar{V}_{ijkl} = V_{ijkl} - V_{jikl} - V_{ijlk} + V_{jilk} \tag{5.13}$$

$$V_{ijkl} = \langle\chi_i|\chi_k'\rangle\langle\chi_j|\chi_l'\rangle\int d^3x_1 d^3x_2 \psi_i^*(\underset{\sim}{x}_1)\psi_j^*(\underset{\sim}{x}_2)$$

$$V_{12}\psi_k'(\underset{\sim}{x}_1)\psi_l'(\underset{\sim}{x}_2) \tag{5.14}$$

Suppose the two-body interaction V_{12} can be approximated by a sum of Gaussians

$$V_{12} = V(\underset{\sim}{x}_1-\underset{\sim}{x}_2) = \sum_k V_k \exp[-\frac{\alpha_k}{2}(\underset{\sim}{x}_1-\underset{\sim}{x}_2)^2](1-m_k+m_k P_{12}^x) \tag{5.15}$$

where P_{12}^x is the space exchange operator, then the two-body matrix elements of the direct interaction are

$$V_{ijkl} = \langle\chi_i|\chi_k'\rangle\langle\chi_j|\chi_l'\rangle(\frac{\beta}{\alpha+\beta})^{3/2}\exp\{-\frac{\alpha\beta}{8(\alpha+\beta)}(\underset{\sim}{s}_i+\underset{\sim}{s}_k'$$

$$-\underset{\sim}{s}_j-\underset{\sim}{s}_l')^2-\frac{\beta}{4}[(\underset{\sim}{s}_i-\underset{\sim}{s}_k')^2+(\underset{\sim}{s}_j-\underset{\sim}{s}_l')^2]\}$$

$$= (\frac{\beta}{\alpha+\beta})^{3/2}\exp[-\frac{\alpha\beta}{8(\alpha+\beta)}(\underset{\sim}{s}_i+\underset{\sim}{s}_k'-\underset{\sim}{s}_j-\underset{\sim}{s}_l')^2]$$

$$* \langle\psi_i|\psi_k'\rangle\langle\psi_j|\psi_l'\rangle \tag{5.16}$$

while those of the space-exchange interaction V^x are

$$V_{ijkl}^x = \langle\chi_i|\chi_k'\rangle\langle\chi_j|\chi_l'\rangle(\frac{\beta}{\alpha+\beta})^{3/2}$$

$$* \exp\{-\frac{\alpha\beta}{8(\alpha+\beta)}(\underset{\sim}{s}_i+\underset{\sim}{s}_l'-\underset{\sim}{s}_j-\underset{\sim}{s}_k')^2$$

$$-\frac{\beta}{4}[(\underset{\sim}{s}_i-\underset{\sim}{s}_l')^2+(\underset{\sim}{s}_j-\underset{\sim}{s}_k')^2]\} \tag{5.17}$$

where the single particle functions are those of eq. (2.1).

6. Expansion of Matrix Elements of a Scalar Spin-Isospin Independent Operator O between Two-Center Shell Model (SM) Functions into Spherical Tensors

Owing to the simple structure (5.5) of the single-particle overlaps, the overlap of two two-center SM functions has the general form

$$\langle\Phi^{(2)}(\underset{\sim}{s})|\Phi^{(2)}(\underset{\sim}{s}')\rangle$$

$$= \sum_i v^{(i)}\exp[-\beta(u^{(i)}s^2+u'^{(i)}s'^2)+\beta w^{(i)}\underset{\sim}{s}\cdot\underset{\sim}{s}']$$

$$= \sum_i v^{(i)}\exp[-\beta(u^{(i)}s^2+u'^{(i)}s'^2)]4\pi\sum_{LM} i_L(\beta w^{(i)}ss')Y_{LM}(\hat{s})Y^*_{LM}(\hat{s})$$

The overlap of the spherical tensors defined in eq. (2.5a) has the form

$$\langle\Phi^{(2)}(LMs)|\Phi^{(2)'}(L'M's')\rangle = \delta_{LL'}\delta_{MM'}\langle\Phi^{(2)}(Ls)|\Phi^{(2)'}(Ls')\rangle \qquad (6.1a)$$

with

$$\langle\Phi^{(2)}(Ls)|\Phi^{(2)'}(Ls')\rangle = \sum_i v^{(i)}\exp[-\beta(u^{(i)}s^2+u'^{(i)}s'^2)]4\pi ss' i_L(\beta w^{(i)}ss') \qquad (6.1b)$$

which is diagonal in L and M and independent of M, as expected.

To calculate matrix elements of the kinetic-energy operator T, we use eq. (5.8)

$$\langle\Phi^{(2)}(Ls)|T-T_{CM}|\Phi^{(2)}(Ls')\rangle$$

$$= \left(\frac{\hbar^2\beta}{4m}\right)\sum_i v^{(i)}\exp[-\beta(u^{(i)}s^2+u'^{(i)}s'^2)]4\pi ss'$$

$$* \{[3(N-1)+2L-2\beta(u^{(i)}s^2+u'^{(i)}s'^2)]i_L(\beta w^{(i)}ss')$$

$$+ 2\beta w^{(i)}ss' i_{L+1}(\beta w^{(i)}ss')\} \qquad (6.2)$$

where the relation

$$Z i'_L(Z) = Z i_{L+1}(Z)+L i_L(Z)$$

was used.

Matrix elements of the two-body interaction (5.15) have the same structure (6.1) as those of the normalization.

7. Expansion of Matrix Elements of a Scalar Spin-Isospin Independent Operator O between Two- and Three-Center SM Functions into Spherical Tensors

The overlap of a two- and a three-center SM function has the structure

$$\langle\Phi^{(2)}(\underset{\sim}{s})|\Phi^{(3)}(\underset{\sim}{s}'_1,\underset{\sim}{s}'_2)\rangle$$

$$=\sum_i v^{(i)}\exp[-\beta(u^{(i)}s^2+u_1^{(i)}s_1'^2+u_2^{(i)}s_2'^2)+\beta(w_1^{(i)}\underset{\sim}{s}\cdot\underset{\sim}{s}'_1+w_2^{(i)}\underset{\sim}{s}\cdot\underset{\sim}{s}'_2)]$$

$$=\sum_i v^{(i)}\exp[-\beta(u^{(i)}s^2+u_1^{(i)}s_1'^2+u_2^{(i)}s_2'^2)](4\pi)^2\sum_{L_1L_2}$$

$$*\, i_{L_1}(\beta w_1^{(i)}ss'_1)\, i_{L_2}(\beta w_2^{(i)}ss'_2)$$

$$*\{\sum_{M_1M_2} Y_{L_1M_1}(\hat{s})Y_{L_2M_2}(\hat{s})Y^*_{L_1M_1}(\hat{s}'_1)Y^*_{L_2M_2}(\hat{s}'_2)\}$$

The term in curly brackets may be simplified by expanding the product of the first two spherical harmonics into a series of spherical harmonics and by coupling the last two spherical harmonics to bipolar harmonics, eq. (2.6a)

$$\{\ \ \} = \sum_{\mathcal{L}\mathcal{M}\mathcal{L}'\mathcal{M}'M_1M_2} \frac{\hat{L}_1\hat{L}_2\hat{\mathcal{L}}}{\sqrt{4\pi}}\begin{pmatrix}L_1 & L_2 & \mathcal{L}\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}L_1 & L_2 & \mathcal{L}\\ M_1 & M_2 & \mathcal{M}\end{pmatrix} Y^*_{\mathcal{L}\mathcal{M}}(\hat{s})$$

$$*(L_1M_1,L_2M_2|\mathcal{L}'\mathcal{M}')\ B^*(L_1L_2\mathcal{L}'\mathcal{M}'\hat{s}'_1,\hat{s}'_2)$$

$$=\sum_{\mathcal{L}\mathcal{M}} \frac{\hat{L}_1\hat{L}_2}{\sqrt{4\pi}}\begin{pmatrix}L_1 & L_2 & \mathcal{L}\\ 0 & 0 & 0\end{pmatrix}(-)^{\mathcal{L}}Y_{\mathcal{L}\mathcal{M}}(\hat{s})\ B^*(L_1L_2\mathcal{L}\mathcal{M}\hat{s}'_1,\hat{s}'_2)$$

In the derivation of the last equation we used the unitarity of the Clebsch Gordan coefficients. The symbol $\begin{pmatrix}L_1 & L_2 & \mathcal{L}\\ M_1 & M_2 & \mathcal{M}\end{pmatrix}$ is the 3-j symbol, and $\hat{L} = \sqrt{2L-1}$. Thus

$$<\Phi^{(2)}(LMs)|\Phi^{(3)}(L_1'L_2'L'M's_1',s_2')>$$

$$= \delta_{LL'}\ \delta_{MM'}\ <\Phi^{(2)}(Ls)|\Phi^{(3)}(L_1'L_2'Ls_1',s_2')>$$

where

$$<\Phi^{(2)}(Ls)|\Phi^{(3)}(L_1'L_2'Ls_1',s_2')$$

$$= \sum_i v^{(i)} \exp\{-\beta[u^{(i)}s^2+u_{1'}^{(i)}s_1'^2+u_{2'}^{(i)}\ s_2'^2]\}$$

$$* \ (4\pi)^{3/2} ss_1'\ s_2' i_{L_1'}(\beta w_{1'}^{(i)} ss_1') i_{L_2'}(\beta w_{2'}^{(i)} ss_2')$$

$$* \ \hat{L}_1'\ \hat{L}_2' \begin{pmatrix} L_1' & L_2' & L \\ 0 & 0 & 0 \end{pmatrix} (-)^L \tag{7.1}$$

Parity conservation is contained in $\begin{pmatrix} L_1' & L_2' & L \\ 0 & 0 & 0 \end{pmatrix}$ which is zero unless $L_1'+L_2'+L=$ even, or

$$(-)^L = (-)^{L_1'+L_2'}$$

The calculation of matrix elements of the kinetic energy operator is again based on eq. (5.8)

$$<\Phi^{(2)}(Ls)|T-T_{CM}|\Phi^{(3)}(L_1'L_2'Ls_1's_1')$$

$$= \sum_i v^{(i)} \exp\{-\beta[u^{(i)}s\ +u_{1'}^{(i)}s_1'^2+u_{2'}^{(i)}s_2'^2]\}$$

$$* \ (4\pi)^{3/2} ss_1's_2'\{i_{L_1'}(\beta w_{1'}^{(i)} ss_1') i_{L_2'}(\beta w_{2'}^{(i)} ss_2')$$

$$* \ [\frac{3\hbar^2\beta(N-1)}{4m} - \frac{\hbar^2\beta^2}{2m}(u^{(i)}s^2+u_{1'}^{(i)}s_1'^2+u_{2'}^{(i)}s_2'^2)+\frac{\hbar^2\beta}{2m}(L_1'+L_2')]$$

$$+ \ [(\beta w_{1'}^{(i)} ss_1') i_{L'+1}(\beta w_{1'}^{(i)} ss_1') i_{L_2'}\ \ (\beta w_{2'}^{(i)} ss_2')$$

$$+ \ (\beta w_{2'}^{(i)} ss_2') i_{L_1'}(\beta w_{1'}^{(i)} ss_1') i_{L_2'+1}(\beta w_{2'}^{(i)} ss_2')](\frac{\hbar^2\beta}{2m})\}$$

$$* \ \hat{L}_1'\ \hat{L}_2' \begin{pmatrix} L_1' & L_2' & L \\ 0 & 0 & 0 \end{pmatrix} (-)^L \tag{7.2}$$

In the matrix element of the two-body interaction (5.15) there are also terms $\sim \underset{\sim}{s}_1'\cdot\underset{\sim}{s}_2'$ in the exponential functions, i.e.

$$\langle\Phi^{(2)}(\underset{\sim}{s})|V|\Phi^{(3)}(\underset{\sim}{s}'_1,\underset{\sim}{s}'_2)\rangle$$

$$= \sum_i v^{(i)} \exp\{-\beta[u^{(i)}s^2 + u^{(i)}_{1'}s_1'^2 + u^{(i)}_{2'}s_2'^2]\}$$

$$* \exp\{\beta[w^{(i)}_{1'}\underset{\sim}{s}\cdot\underset{\sim}{s}'_1 + w^{(i)}_{2'}\underset{\sim}{s}\cdot\underset{\sim}{s}'_2 + w^{(i)}_{1'2'}\underset{\sim}{s}'_1\cdot\underset{\sim}{s}'_2]\}$$

$$= \sum_i v^{(i)} \exp\{\quad\}(4\pi)^3 \sum_{l_1 l_2 l_3 m_1 m_2 m_3} i_{l_1}(\beta w^{(i)}_{1'} s s_1')\, i_{l_2}(\beta w^{(i)}_{2'} s s_2')\, i_{l_3}(\beta w^{(i)}_{1'2'} s_1' s_2')$$

$$* \{Y^*_{l_1 m_1}(\hat{s}) Y_{l_1 m_1}(\hat{s}'_1) Y^*_{l_2 m_2}(\hat{s}) Y_{l_2 m_2}(\hat{s}'_2) Y_{l_3 m_3}(\hat{s}'_1) Y^*_{l_3 m_3}(\hat{s}'_2)\} \qquad (7.3)$$

Upon coupling of spherical harmonics in the indicated way we obtain for the term in curly brackets

$$\{\quad\} = (4\pi)^{-3/2} \sum_{\mathcal{L}\mathcal{M}L_1'M_1'L_2'M_2'} (2l_1+1)(2l_2+1)(2l_3+1)\hat{\mathcal{L}}\hat{L}_1'\hat{L}_2'$$

$$* \begin{pmatrix} l_1 & l_2 & \mathcal{L} \\ m_1 & m_2 & \mathcal{M} \end{pmatrix} \begin{pmatrix} l_1 & l_2 & \mathcal{L} \\ 0 & 0 & 0 \end{pmatrix} Y_{\mathcal{L}\mathcal{M}}(\hat{s})$$

$$* \begin{pmatrix} l_1 & l_3 & L_1' \\ m_1 & m_3 & M_1' \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_1' \\ 0 & 0 & 0 \end{pmatrix} Y^*_{L_1'M_1'}(\hat{s}'_1)$$

$$* \begin{pmatrix} l_2 & l_3 & L_2' \\ m_2 & -m_3 & M_2' \end{pmatrix} \begin{pmatrix} l_2 & l_3 & L_2' \\ 0 & 0 & 0 \end{pmatrix} Y^*_{L_2'M_2'}(\hat{s}'_2)\ (-)^{m_3}$$

$$= (4\pi)^{-3/2} \sum_{\mathcal{L}\mathcal{M}\mathcal{L}'\mathcal{M}'L_1'M_1'L_2'M_2'} (2l_1+1)(2l_2+1)(2l_3+1)\hat{\mathcal{L}}\hat{\mathcal{L}}'\hat{L}_1'\hat{L}_2'(-)^{L_1'-L_2'}$$

$$* \begin{pmatrix} l_1 & l_2 & \mathcal{L} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_1' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_3 & L_2' \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \left[\begin{pmatrix} l_1 & l_2 & \mathcal{L} \\ m_1 & m_2 & \mathcal{M} \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_1' \\ m_1 & m_3 & M_1' \end{pmatrix} \begin{pmatrix} l_2 & l_3 & L_2' \\ m_2 & -m_3 & M_2' \end{pmatrix} \right.$$

$$\left. * \begin{pmatrix} L_1' & L_2' & \mathcal{L}' \\ M_1' & M_2' & -\mathcal{M}' \end{pmatrix} (-)^{m_3+\mathcal{M}'} \right] Y_{\mathcal{L}\mathcal{M}}(\hat{s})\ B^*(L_1'L_2'\mathcal{L}'\mathcal{M}'\hat{s}'_1,\hat{s}'_2)$$

The summation over magnetic quantum numbers in the quantity contained in the square brackets is carried out in terms of 9-j symbols[6)]

$$\sum_{m_1m_2m_3M_1'M_2'} [\quad]$$

$$= \sum_{m_1m_2m_3M_1'M_2'} \begin{pmatrix} L & l_1 & l_2 \\ M & m_1 & m_2 \end{pmatrix} \begin{pmatrix} L' & L_1' & L_2' \\ -M' & M_1' & M_2' \end{pmatrix} \begin{pmatrix} L_1' & l_3 & l_1 \\ M_1' & m_3 & m_1 \end{pmatrix} \begin{pmatrix} L_2' & l_3 & l_2 \\ M_2' & -m_3 & m_2 \end{pmatrix} (-)^{m_3+M'}$$

$$* (-)^{l_1+l_3+L_1'}(-)^{l_2+l_3+L_2'}$$

$$= \sum_{\lambda\mu m_3} (2\lambda+1) \begin{pmatrix} L' & \lambda & L \\ -M' & \mu & M \end{pmatrix} \begin{pmatrix} \lambda & l_3 & l_3 \\ \mu & m_3 & -m_3 \end{pmatrix} (-)^{m_3+M'}$$

$$* (-)^{l_1+l_2+L_1'+L_2'} \begin{Bmatrix} L' & \lambda & L \\ L_1' & l_3 & l_1 \\ L_2' & l_3 & l_2 \end{Bmatrix}$$

$$= \begin{pmatrix} L' & 0 & L \\ -M' & 0 & M \end{pmatrix} \hat{l}_3 (-)^{l_1+l_2+l_3+L_1'+L_2'} \begin{Bmatrix} L & 0 & L \\ L_1' & l_3 & l_1 \\ L_2' & l_3 & l_2 \end{Bmatrix}$$

$$= \delta_{LL'}\delta_{MM'}(-)^{L} \frac{1}{2L+1} (-)^{l_1+l_2+l_3+L_1'+L_2'+l_2+L_1'+L+l_3}$$

$$* \begin{Bmatrix} l_1 & l_2 & L \\ L_2' & L_1' & l_3 \end{Bmatrix} \tag{7.4}$$

where we used eqs. (3.7.9) and (6.4.14) of ref.(8) together with the relation

$$\sum_{m} (-)^{l-m} \begin{pmatrix} l & l & L \\ m & -m & 0 \end{pmatrix} = \hat{l}\delta_{L0} \tag{7.5}$$

From eqs. (7.3), (7.4) and the symmetry relation

$$\begin{Bmatrix} l_1 & l_2 & L \\ L_2' & L_1' & l_3 \end{Bmatrix} = \begin{Bmatrix} L & l_1 & l_2 \\ l_3 & L_2' & L_1' \end{Bmatrix} = \begin{Bmatrix} L & L_2' & L_1' \\ l_3 & l_1 & l_2 \end{Bmatrix} = \begin{Bmatrix} L_1' & L_2' & L \\ l_2 & l_1 & l_3 \end{Bmatrix}$$

we get

$$\langle\Phi^{(2)}(\underset{\sim}{s})|V|\Phi^{(3)}(\underset{\sim}{s}'_1,\underset{\sim}{s}'_2)\rangle$$

$$= \sum_i v^{(i)}\exp\{\quad\}(4\pi)^{3/2}\sum_{l_1l_2l_3} i_{l_1}i_{l_2}i_{l_3}\sum_{LML'_1L'_2}(2l_1+1)(2l_2+1)(2l_3+1)$$

$$* \hat{L}'_1\hat{L}'_2(-)^{l_1+L'_1}\begin{pmatrix}l_1 & l_2 & L\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_3 & L'_1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2 & l_3 & L'_2\\ 0 & 0 & 0\end{pmatrix}$$

$$* \begin{Bmatrix}L'_1 & L'_2 & L\\ l_2 & l_1 & l_3\end{Bmatrix} Y_{LM}(\hat{s})\; B^*_{L'_1L'_2LM}(\hat{s}'_1,\hat{s}'_2) \tag{7.6}$$

If we introduce the expansions (2.5a) and (2.5b) of the many-body wave functions in terms of spherical and bipolar harmonics into this equation then

$$\langle\Phi^{(2)}(LMs)|V|\Phi^{(3)}(L'_1L'_2LMs'_1s'_2)\rangle = \delta_{LL}\delta_{MM}\langle\Phi^{(2)}(Ls)|V|\Phi^{(3)}(L'_1L'_2Ls_1s_2)\rangle$$

where

$$\langle\Phi^{(2)}(Ls)|V|\Phi^{(3)}(L'_1L'_2Ls_1s_2)\rangle$$

$$= \sum_i v^{(i)}\exp\{-\beta[u^{(i)}s^2+u^{(i)}_{1'}s'^2_1+u^{(i)}_{2'}s'^2_2]\}(4\pi)^{3/2}ss'_1s'_2$$

$$* \sum_{l_1l_2l_3} i_{l_1}(\beta w^{(i)}_{1'}ss'_1)\,i_{l_2}(\beta w^{(i)}_{2'}ss'_2)\,i_{l_3}(\beta w^{(i)}_{1'2'}s'_1s'_2)$$

$$* (2l_1+1)(2l_2+1)(2l_3+1)\hat{L}'_1\hat{L}'_2(-)^{l_1+L'_1}$$

$$* \begin{pmatrix}l_1 & l_2 & L\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_3 & L'_1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2 & l_3 & L'_2\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}L'_1 & L'_2 & L\\ l_2 & l_1 & l_3\end{Bmatrix} \tag{7.7}$$

Parity conservation follows from the CG-coefficients, i.e.

$$l_1 + l_2 + L = \text{even}$$
$$l_1 + l_3 + L'_1 = \text{even}$$
$$l_2 + l_3 + L'_2 = \text{even}$$

which imply $(-)^L = (-)^{L'_1+L'_2}$

8. Expansion of Matrix Elements of a Scalar Spin-Isospin Indpendent Operator O between Three-Center SM Functions into Spherical Tensors

The overlap of two three-cluster functions containing only 1s single-particle orbits reads

$$\langle\Phi^{(3)}(\underset{\sim}{s}_1,\underset{\sim}{s}_2)|\Phi^{(3)}(\underset{\sim}{s}_1',\underset{\sim}{s}_2')\rangle$$

$$= \sum_i v^{(i)} \exp\{-\beta[u_1^{(i)}(s_1^2+s_1'^2)+u_2^{(i)}(s_2^2+s_2'^2)]$$

$$+ \beta[w_{11'}^{(i)}\underset{\sim}{s}_1\cdot\underset{\sim}{s}_1'+w_{12'}^{(i)}\underset{\sim}{s}_1\cdot\underset{\sim}{s}_2'+w_{21'}^{(i)}\underset{\sim}{s}_2\cdot\underset{\sim}{s}_1'+w_{22'}^{(i)}\underset{\sim}{s}_2\cdot\underset{\sim}{s}_2']\}$$

$$= \sum_i v^{(i)} \exp\{-\beta[u_1^{(i)}(s_1^2+s_1'^2)+u_2^{(i)}(s_2^2+s_2'^2)]\}$$

$$* (4\pi)^4 \sum_{l_1\ldots l_4\; m_1\ldots m_4} i_{l_1}(\beta w_{11'}^{(i)}s_1s_1')\, i_{l_2}(\beta w_{12'}^{(i)}s_1s_2')\, i_{l_3}(\beta w_{21'}^{(i)}s_2s_1')$$

$$* i_{l_4}(\beta w_{22'}^{(i)}s_2s_2')\{Y_{l_1m_1}^*(\hat{s}_1)Y_{l_1m_1}(\hat{s}_1')Y_{l_2m_2}^*(\hat{s}_1)Y_{l_2m_2}(\hat{s}_2')$$

$$* Y_{l_3m_3}^*(\hat{s}_2)Y_{l_3m_3}(\hat{s}_1')Y_{l_4m_4}^*(\hat{s}_2)Y_{l_4m_4}(\hat{s}_2')\} \qquad (8.1)$$

As in the previous cases, we proceed by coupling the spherical harmonics to obtain for the expression in curly brackets

$$\{\;\} = (4\pi)^{-2} \sum_{\substack{L_1M_1L_2M_2\\ L_1'M_1'L_2'M_2'}} \hat{l}_1^2\ldots\hat{l}_4^2\hat{L}_1\hat{L}_2\hat{L}_1'\hat{L}_2' \begin{pmatrix} l_1 & l_2 & L_1 \\ m_1 & m_2 & M_1 \end{pmatrix}$$

$$* \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ m_3 & m_4 & M_2 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_1' \\ m_1 & m_3 & M_1' \end{pmatrix}$$

$$* \begin{pmatrix} l_1 & l_3 & L_1' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_2' \\ m_2 & m_4 & M_2' \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_2' \\ 0 & 0 & 0 \end{pmatrix}$$

(continued next page)

$$* \; Y_{L_1M_1}(\hat{s}_1)Y_{L_2M_2}(\hat{s}_2)Y^*_{L_1'M_1'}(\hat{s}_1')Y^*_{L_2'M_2'}(\hat{s}_2')$$

$$= (4\pi)^{-2} \sum_{\substack{L_1M_1L_2M_2\mathcal{L}\mathcal{M} \\ L_1'M_1'L_2'M_2'\mathcal{L}'\mathcal{M}'}} \hat{l}_1^2 \ldots \hat{l}_4^2 \hat{L}_1 \hat{L}_2 \hat{L}_1' \hat{L}_2' \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \begin{pmatrix} l_3 & l_4 & L_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_1' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_2' \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \; (L_1M_1, L_2M_2|\mathcal{L}\mathcal{M})(L_1'M_1', L_2'M_2'|\mathcal{L}'\mathcal{M}') \; B(L_1L_2\mathcal{L}\mathcal{M}\hat{s}_1, \hat{s}_2)$$

$$* \; B^*(L_1'L_2'\mathcal{L}'\mathcal{M}'\hat{s}_1', \hat{s}_2') \left[\begin{pmatrix} l_1 & l_2 & L_1 \\ m_1 & m_2 & M_1 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ m_3 & m_4 & M_2 \end{pmatrix} \right.$$

$$\left. * \begin{pmatrix} l_1 & l_3 & L_1' \\ m_1 & m_3 & M_1' \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_2' \\ m_2 & m_4 & M_2' \end{pmatrix} \right] \qquad (8.2)$$

Again the summation over magnetic quantum numbers in the quantity contained in the square brackets is carried out in terms of 9-j symbols

$$\sum_{m_1 \ldots m_4} [\quad] = \sum_{m_1 \ldots m_4} \begin{pmatrix} L_1 & l_1 & l_2 \\ M_1 & m_1 & m_2 \end{pmatrix} \begin{pmatrix} L_2 & l_3 & l_4 \\ M_2 & m_3 & m_4 \end{pmatrix} \begin{pmatrix} l_3 & L_1' & l_1 \\ m_3 & M_1' & m_1 \end{pmatrix} \begin{pmatrix} l_4 & L_2' & l_2 \\ m_4 & M_2' & m_2 \end{pmatrix}$$

$$= \sum_{LM} (2L+1) \begin{pmatrix} L_2 & L & L_1 \\ M_2 & M & M_1 \end{pmatrix} \begin{pmatrix} L & L_1' & L_2' \\ M & M_1' & M_2' \end{pmatrix} \begin{Bmatrix} L_2 & L & L_1 \\ l_3 & L_1' & l_1 \\ l_4 & L_2' & l_2 \end{Bmatrix}$$

$$= \sum_{LM} (-)^{(L_1-L_2)-(L_1'-L_2')} (L_1M_1, L_2M_2|L-M)(L_1'M_1', L_2'M_2'|L-M)\{\quad\} \qquad (8.3)$$

Inserting eqs. (8.2) and (8.3) into eq. (8.1) we are left with

$$<\Phi^{(3)}(\underset{\sim}{s}_1, \underset{\sim}{s}_2)|\Phi^{(3)}(\underset{\sim}{s}_1', \underset{\sim}{s}_2')>$$

$$= \sum_i v^{(i)} \exp\{-\beta[u_1^{(i)}(s_1^2+s_1'^2)+u_2^{(i)}(s_2^2+s_2'^2)]\}(4\pi)^2$$

$$* \sum_{l_1l_2l_3l_4L_1L_2L_1'L_2'\mathcal{L}\mathcal{M}} i_{l_1}(\beta w_{11}^{(i)}, s_1 s_1') \, i_{l_2}(\beta w_{12}^{(i)}, s_1 s_2')$$

(continued next page)

$$* \; i_{l_3}(\beta w_{21}^{(i)} s_2 s_1') i_{l_4}(\beta w_{22}^{(i)} s_2 s_2') \hat{l}_1^2 \ldots \hat{l}_4^2 \hat{L}_1 \hat{L}_2 \hat{L}_1' \hat{L}_2'$$

$$* \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_1' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_2' \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \; (-)^{(L_1-L_2)-(L_1'-L_2')} \begin{Bmatrix} L_2 & L & L_1 \\ l_3 & L_1' & l_1 \\ l_4 & L_2' & l_2 \end{Bmatrix} B(L_1 L_2 LM \hat{s}_1, \hat{s}_2)$$

$$* \; B^*(L_1' L_2' LM \hat{s}_1', \hat{s}_2')$$

From eq. (2.5b) we conclude that

$$<\Phi^{(3)}(L_1 L_2 LM s_1 s_2) | \Phi^{(3)}(L_1' L_2' L' M' s_1' s'_2)>$$

$$= \delta_{LL'} \delta_{MM'} <\Phi^{(3)}(L_1 L_2 L s_1 s_2) | \Phi^{(3)}(L_1' L_2' L s_1' s_2')>$$

where

$$<\Phi^{(3)}(L_1 L_2 L s_1 s_2) | \Phi^{(3)}(L_1' L_2' L s_1' s_2')>$$

$$= s_1 s_2 s_1' s_2' \sum_i v^{(i)} \exp\{-\beta[u_1^{(i)}(s_1^2 + s_1'^2) + u_2^{(i)}(s_2^2 + s_2'^2)]\} \; (4\pi)^2$$

$$* \sum_{l_1 l_2 l_3 l_4} i_{l_1}(\beta w_{11}^{(i)} s_1 s_1') i_{l_2}(\beta w_{12}^{(i)} s_1 s_2') i_{l_3}(\beta w_{21}^{(i)} s_2 s_1')$$

$$* \; i_{l_4}(\beta w_{22}^{(i)} s_2 s_2') \hat{l}_1^2 \ldots \hat{l}_4^2 \hat{L}_1 \hat{L}_2 \hat{L}_1' \hat{L}_2' \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \begin{pmatrix} l_1 & l_3 & L_1' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_2' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} L_2 & L & L_1 \\ l_3 & L_1' & l_1 \\ l_4 & L_2' & l_2 \end{Bmatrix} \qquad (8.4)$$

Again parity conservation follows from CG-coefficients, i.e.

$l_1 + l_2 + L_1$ = even
$l_3 + l_4 + L_2$ = even
$l_1 + l_3 + L_1'$ = even
$l_2 + l_4 + L_2'$ = even

thus

$$(-)^{L_1+L_2} = (-)^{L_1'+L_2'}$$

Matrix elements of the kinetic energy operator are calculated using eq.(5.8)

$$<\Phi^{(3)}(L_1L_2\mathcal{L}\mathcal{M}s_1s_2)|T-T_{CM}|\Phi^{(3)}(L_1'L_2'\mathcal{L}'\mathcal{M}'s_1's_2')>$$

$$= \delta_{\mathcal{L}\mathcal{L}'}\delta_{\mathcal{M}\mathcal{M}'}<\Phi^{(3)}(L_1L_2\mathcal{L}s_1s_2)|T-T_{CM}|\Phi^{(3)}(L_1'L_2'\mathcal{L}s_1's_2')>$$

where

$$<\Phi^{(3)}(L_1L_2\mathcal{L}s_1s_2)|T-T_{CM}|\Phi^{(3)}(L_1'L_2'\mathcal{L}s_1's_2')>$$

$$= s_1s_2s_1's_2' \sum_i v^{(i)}\exp\{-\beta[u_1^{(i)}(s_1^2+s_1'^2)+u_2^{(i)}(s_2^2+s_2'^2)]\}\ (4\pi)^2$$

$$* \sum_{l_1l_2l_3l_4}\Bigg\{\Bigg[\frac{3\hbar^2\beta(N-1)}{4m} - \frac{\hbar^2\beta^2}{2m}[u_1^{(i)}(s_1^2+s_1'^2)+u_2^{(i)}(s_2^2+s_2'^2)]$$

$$+\frac{\hbar^2\beta}{2m}(l_1+l_2+l_3+l_4)\Bigg]i_{l_1}i_{l_2}i_{l_3}i_{l_4}$$

$$+\frac{\hbar^2\beta}{2m}\Bigg[(\beta w_{11'}^{(i)}s_1s_1')i_{l_1+1}i_{l_2}i_{l_3}i_{l_4}+(\beta w_{12'}^{(i)}s_1s_2')i_{l_1}i_{l_2+1}i_{l_3}i_{l_4}$$

$$+(\beta w_{21'}^{(i)}s_2s_1')i_{l_1}i_{l_2}i_{l_3+1}i_{l_4}+(\beta w_{22'}^{(i)}s_2s_2')i_{l_1}i_{l_2}i_{l_3}i_{l_4+1}\Bigg]\Bigg\}\hat{l}_1^2\hat{l}_2^2\hat{l}_3^2\hat{l}_4^2$$

$$* \hat{L}_1\hat{L}_2\hat{L}_1'\hat{L}_2'\begin{pmatrix}l_1 & l_2 & L_1\\0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_3 & l_4 & L_2\\0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_3 & L_1'\\0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2 & l_4 & L_2'\\0 & 0 & 0\end{pmatrix}\begin{Bmatrix}L_2 & \mathcal{L} & L_1\\l_3 & L_1' & l_1\\l_4 & L_2' & l_2\end{Bmatrix} \quad (8.5)$$

In the case of two three-cluster wave functions the matrix elements of the two-body interaction (5.15) also contain terms $\sim \underset{\sim}{s}_1'\cdot\underset{\sim}{s}_2'$ and $\underset{\sim}{s}_1\cdot\underset{\sim}{s}_2$ in the exponentials, i.e.

$$<\Phi^{(3)}(\underset{\sim}{s}_1,\underset{\sim}{s}_2)|V|\Phi^{(3)}(\underset{\sim}{s}_1',\underset{\sim}{s}_2')>$$

$$= \sum_i v^{(i)}\exp\{-\beta[u_1^{(i)}s_1^2+u_2^{(i)}s_2^2+u_{1'}^{(i)}s_1'^2+u_{2'}^{(i)}s_2'^2]$$

$$+\beta[w_{11'}^{(i)}\underset{\sim}{s}_1\cdot\underset{\sim}{s}_1'+w_{12'}^{(i)}\underset{\sim}{s}_1\cdot\underset{\sim}{s}_2'+w_{21'}^{(i)}\underset{\sim}{s}_2\cdot\underset{\sim}{s}_1'+w_{22'}^{(i)}\underset{\sim}{s}_2\cdot\underset{\sim}{s}_2'$$

$$+w_{12}^{(i)}\underset{\sim}{s}_1\cdot\underset{\sim}{s}_2+w_{1'2'}^{(i)}\underset{\sim}{s}_1'\cdot\underset{\sim}{s}_2']\} \quad (8.6)$$

$$= \sum_i v^{(i)} \exp\{-\beta[u_1^{(i)} s_1^2 + u_2^{(i)} s_2^2 + u_{1'}^{(i)} s_1'^2 + u_{2'}^{(i)} s_2'^2]\}$$

$$* (4\pi)^6 \sum_{l_1..l_6 m_1..m_6} i_{l_1}(\beta w_{11'}^{(i)} s_1 s_1') i_{l_2}(\beta w_{12'}^{(i)} s_1 s_2') i_{l_3}(\beta w_{21'}^{(i)} s_2 s_1')$$

$$* i_{l_4}(\beta w_{22'}^{(i)} s_1 s_2') i_{l_5}(\beta w_{12}^{(i)} s_1 s_2) i_{l_6}(\beta w_{1'2'}^{(i)} s_1' s_2')$$

$$* \{Y_{l_1 m_1}(\hat{s}_1) Y^*_{l_1 m_1}(\hat{s}_1') Y_{l_2 m_2}(\hat{s}_1) Y^*_{l_2 m_2}(\hat{s}_2')$$

$$* Y_{l_3 m_3}(\hat{s}_2) Y^*_{l_3 m_3}(\hat{s}_1') Y_{l_4 m_4}(\hat{s}_2) Y^*_{l_4 m_4}(\hat{s}_2')$$

$$* Y_{l_5 m_5}(\hat{s}_1) Y^*_{l_5 m_5}(\hat{s}_2) Y^*_{l_6 m_6}(\hat{s}_1') Y_{l_6 m_6}(\hat{s}_2')\}$$

Coupling of spherical harmonics in the indicated way gives

$$\{\ \} = (4\pi)^{-2} \sum_{\substack{L_1..L_4 \\ M_1..M_4}} (2l_1+1)\ldots(2l_4+1)\hat{L}_1\ldots\hat{L}_4$$

$$* \begin{pmatrix} l_1 & l_2 & L_1 \\ m_1 & m_2 & M_1 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix} Y^*_{L_1 M_1}(\hat{s}_1) Y_{l_5 m_5}(\hat{s}_1)$$

$$* \begin{pmatrix} l_3 & l_4 & L_2 \\ m_3 & m_4 & M_2 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ 0 & 0 & 0 \end{pmatrix} Y^*_{L_2 M_2}(\hat{s}_2) Y^*_{l_5 m_5}(\hat{s}_2)$$

$$* \begin{pmatrix} l_1 & l_3 & L_3 \\ m_1 & m_3 & M_3 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_3 \\ 0 & 0 & 0 \end{pmatrix} Y_{L_3 M_3}(\hat{s}_1') Y^*_{l_6 m_6}(\hat{s}_1')$$

$$* \begin{pmatrix} l_2 & l_4 & L_4 \\ m_2 & m_4 & M_4 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_4 \\ 0 & 0 & 0 \end{pmatrix} Y_{L_4 M_4}(\hat{s}_2') Y_{l_6 m_6}(\hat{s}_2')$$

$$= (4\pi)^{-4} \sum_{\substack{L_1...L_8 \\ M_1...M_8}} (2l_1+1)\ldots(2l_6+1)(2L_1+1)\ldots(2L_4+1)\hat{L}_5\ldots\hat{L}_8$$

(continued next page)

$$* \begin{pmatrix} l_1 & l_2 & L_1 \\ m_1 & m_2 & M_1 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_1 & l_5 & L_5 \\ M_1 & -m_5 & M_5 \end{pmatrix} \begin{pmatrix} L_1 & l_5 & L_5 \\ 0 & 0 & 0 \end{pmatrix} Y_{L_5M_5}(\hat{s}_1)(-)^{m_5}$$

$$* \begin{pmatrix} l_3 & l_4 & L_2 \\ m_3 & m_4 & M_2 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_2 & l_5 & L_6 \\ M_2 & m_5 & M_6 \end{pmatrix} \begin{pmatrix} L_2 & l_5 & L_6 \\ 0 & 0 & 0 \end{pmatrix} Y_{L_6M_6}(\hat{s}_2)$$

$$* \begin{pmatrix} l_1 & l_3 & L_3 \\ m_1 & m_3 & M_3 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_3 & l_6 & L_7 \\ M_3 & -m_6 & M_7 \end{pmatrix} \begin{pmatrix} L_3 & l_6 & L_7 \\ 0 & 0 & 0 \end{pmatrix} Y^*_{L_7M_7}(\hat{s}'_1)(-)^{m_6}$$

$$* \begin{pmatrix} l_2 & l_4 & L_4 \\ m_2 & m_4 & M_4 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_4 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_4 & l_6 & L_8 \\ M_4 & m_6 & M_8 \end{pmatrix} \begin{pmatrix} L_4 & l_6 & L_8 \\ 0 & 0 & 0 \end{pmatrix} Y^*_{L_8M_8}(\hat{s}'_2)$$

Upon coupling the spherical harmonics in the indicated way to bipolar harmonics, we obtain

$$\{ \;\; \} = (4\pi)^{-4} \sum_{\substack{L_1\ldots L_8 \\ M_1\ldots M_8}} \sum_{\mathcal{LML'M'}} (2l_1+1)\ldots(2l_6+1)(2L_1+1)\ldots(2L_4+1)\hat{L}_5\ldots\hat{L}_8$$

$$* \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_1 & l_5 & L_5 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_2 & l_5 & L_6 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_3 \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \begin{pmatrix} L_3 & l_6 & L_7 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_4 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_4 & l_6 & L_8 \\ 0 & 0 & 0 \end{pmatrix} \hat{\mathcal{L}}\hat{\mathcal{L}}'(-)^{L_5-L_6+\mathcal{M}}(-)^{L_7-L_8+\mathcal{M}'}$$

$$*\left[\begin{pmatrix} L_1 & l_1 & l_2 \\ M_1 & m_1 & m_2 \end{pmatrix} \begin{pmatrix} L_2 & l_3 & l_4 \\ M_2 & m_3 & m_4 \end{pmatrix} \begin{pmatrix} l_3 & L_3 & l_1 \\ m_3 & M_3 & m_1 \end{pmatrix} \begin{pmatrix} l_4 & L_4 & l_2 \\ m_4 & M_4 & m_2 \end{pmatrix} \right]$$

$$* \begin{pmatrix} L_1 & l_5 & L_5 \\ M_1 & -m_5 & M_5 \end{pmatrix} \begin{pmatrix} L_2 & l_5 & L_6 \\ M_2 & m_5 & M_6 \end{pmatrix} \begin{pmatrix} L_5 & L_6 & \mathcal{L} \\ M_5 & M_6 & -\mathcal{M} \end{pmatrix} (-)^{m_5+m_6}$$

$$* \begin{pmatrix} L_3 & l_6 & L_7 \\ M_3 & -m_6 & M_7 \end{pmatrix} \begin{pmatrix} L_4 & l_6 & L_8 \\ M_4 & m_6 & M_8 \end{pmatrix} \begin{pmatrix} L_7 & L_8 & \mathcal{L}' \\ M_7 & M_8 & -\mathcal{M}' \end{pmatrix}$$

$$* \; B(L_5L_6\mathcal{LM}\hat{s}_1\hat{s}_2) \; B^*(L_7L_8\mathcal{L'M'}\hat{s}'_1\hat{s}'_2) \qquad (8.7)$$

Summing over magnetic quantum numbers in the term in square brackets gives

$$\sum_{m_1\ldots m_4} [\;\;] = \sum_{LM} (2L+1) \begin{pmatrix} L_2 & L & L_1 \\ M_2 & M & M_1 \end{pmatrix} \begin{pmatrix} L & L_3 & L_4 \\ M & M_3 & M_4 \end{pmatrix} \begin{Bmatrix} L_2 & L & L_1 \\ l_3 & L_3 & l_1 \\ l_4 & L_4 & l_2 \end{Bmatrix}$$

and

$$\sum_{M_1M_2M_5M_6m_5} \begin{pmatrix} L_1 & l_5 & L_5 \\ M_1 & -m_5 & M_5 \end{pmatrix} \begin{pmatrix} L_2 & l_5 & L_6 \\ M_2 & m_5 & M_6 \end{pmatrix} \begin{pmatrix} L_2 & L & L_1 \\ M_2 & M & M_1 \end{pmatrix} \begin{pmatrix} L_5 & L_6 & \mathcal{L} \\ M_5 & M_6 & -\mathcal{M} \end{pmatrix} (-)^{m_5}$$

$$= \sum_{M_1M_2M_5M_6m_5} \begin{pmatrix} l_5 & L_5 & L_1 \\ -m_5 & M_5 & M_1 \end{pmatrix} \begin{pmatrix} l_5 & L_6 & L_2 \\ m_5 & M_6 & M_2 \end{pmatrix} \begin{pmatrix} L_6 & \mathcal{L} & L_5 \\ M_6 & -\mathcal{M} & M_5 \end{pmatrix} \begin{pmatrix} L_2 & L & L_1 \\ M_2 & M & M_1 \end{pmatrix} (-)^{m_5}$$

$$= \sum_{\lambda\mu m_5} (2\lambda+1) \begin{pmatrix} l_5 & \lambda & l_5 \\ m_5 & \mu & -m_5 \end{pmatrix} \begin{pmatrix} \lambda & \mathcal{L} & L \\ \mu & -\mathcal{M} & M \end{pmatrix} \begin{Bmatrix} l_5 & \lambda & l_5 \\ L_6 & \mathcal{L} & L_5 \\ L_2 & L & L_1 \end{Bmatrix} (-)^{m_5}$$

$$= \hat{l}_5 (-)^{l_5} \begin{pmatrix} 0 & \mathcal{L} & L \\ 0 & -\mathcal{M} & M \end{pmatrix} \begin{Bmatrix} l_5 & 0 & l_5 \\ L_6 & \mathcal{L} & L_5 \\ L_2 & \mathcal{L} & L_1 \end{Bmatrix}$$

$$= \delta_{\mathcal{L}L} \delta_{\mathcal{M}M} \, \hat{l}_5/\hat{\mathcal{L}} \, (-)^{l_5+\mathcal{L}+\mathcal{M}} \begin{Bmatrix} l_5 & 0 & l_5 \\ L_6 & \mathcal{L} & L_5 \\ L_2 & \mathcal{L} & L_1 \end{Bmatrix}$$

where we used eq. (7.5).
Similarly

$$\sum_{M_3M_4M_7M_8m_6} \begin{pmatrix} L_3 & l_6 & L_7 \\ M_3 & -m_6 & M_7 \end{pmatrix} \begin{pmatrix} L_4 & l_6 & L_8 \\ M_4 & m_6 & M_8 \end{pmatrix} \begin{pmatrix} L_7 & L_8 & \mathcal{L}' \\ M_7 & M_8 & -\mathcal{M}' \end{pmatrix} \begin{pmatrix} L & L_3 & L_4 \\ M & M_3 & M_4 \end{pmatrix} (-)^{m_6}$$

$$= \sum_{M_3M_4M_7M_8m_6} \begin{pmatrix} l_6 & L_7 & L_3 \\ -m_6 & M_7 & M_3 \end{pmatrix} \begin{pmatrix} l_6 & L_8 & L_4 \\ m_6 & M_8 & M_4 \end{pmatrix} \begin{pmatrix} L_8 & \mathcal{L}' & L_7 \\ M_8 & -\mathcal{M}' & M_7 \end{pmatrix} \begin{pmatrix} L_4 & L & L_3 \\ M_4 & M & M_3 \end{pmatrix} (-)^{m_6}$$

$$= \sum_{\lambda\mu m_6} (2\lambda+1) \begin{pmatrix} l_6 & \lambda & l_6 \\ m_6 & \mu & -m_6 \end{pmatrix} \begin{pmatrix} \lambda & \mathcal{L}' & L \\ \mu & -\mathcal{M}' & M \end{pmatrix} \begin{Bmatrix} l_6 & \lambda & l_6 \\ L_8 & \mathcal{L}' & L_7 \\ L_4 & L & L_3 \end{Bmatrix}$$

$$= \hat{l}_6 \, (-)^{l_6} \begin{pmatrix} 0 & \mathcal{L}' & L \\ 0 & -\mathcal{M}' & M \end{pmatrix} \begin{Bmatrix} l_6 & 0 & l_6 \\ L_8 & L & L_7 \\ L_4 & L & L_3 \end{Bmatrix}$$

$$= \delta_{\mathcal{L}'L} \, \delta_{\mathcal{M}'-M} \, \hat{l}_6/\hat{\mathcal{L}}' \, (-)^{l_6+\mathcal{L}'+\mathcal{M}'} \begin{Bmatrix} l_6 & 0_1 & l_6 \\ L_8 & \mathcal{L}' & L_7 \\ L_4 & \mathcal{L}' & L_3 \end{Bmatrix} \qquad (8.9)$$

From eqs. (8.6)...(8.9) we obtain

$$<\Phi^{(3)}(\underset{\sim}{s}_1,\underset{\sim}{s}_2)|V|\Phi^{(3)}(\underset{\sim}{s}'_1,\underset{\sim}{s}'_2)>$$

$$= \sum_i v^{(i)} \exp\{-\beta[u_1^{(i)} s_1^2 + u_2^{(i)} s_2^2 + u_{1'}^{(i)} s_1'^2 + u_{2'}^{(i)} s_2'^2]\}(4\pi)^2$$

$$* \overline{\sum_{\substack{l_1..l_6 LM \\ L_1..L_8}}} i_{l_1}(\beta w_{11'}^{(i)} s_1 s_1') i_{l_2}(\beta w_{12'}^{(i)} s_1 s_2') i_{l_3}(\beta w_{21'}^{(i)} s_2 s_1')$$

$$* i_{l_4}(\beta w_{22'}^{(i)} s_2 s_2') i_{l_5}(\beta w_{12}^{(i)} s_1 s_2) i_{l_6}(\beta w_{1'2'}^{(i)} s_1' s_2')$$

$$* (2l_1+1)\ldots(2l_6+1)(2L_1+1)\ldots(2L_4+1)\hat{L}_5\ldots\hat{L}_8$$

$$* \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_1 & l_5 & L_5 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_2 & l_5 & L_6 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_3 \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \begin{pmatrix} L_3 & l_6 & L_7 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_4 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_4 & l_6 & L_8 \\ 0 & 0 & 0 \end{pmatrix} \hat{l}_5 \hat{l}_6 (-)^{l_5+l_6}$$

$$* \begin{Bmatrix} l_5 & 0 & l_5 \\ L_6 & \mathcal{L} & L_5 \\ L_2 & \mathcal{L} & L_1 \end{Bmatrix} \begin{Bmatrix} l_6 & 0 & l_6 \\ L_8 & \mathcal{L} & L_7 \\ L_4 & \mathcal{L} & L_3 \end{Bmatrix} \begin{Bmatrix} L_2 & \mathcal{L} & L_1 \\ l_3 & L_3 & l_1 \\ l_4 & L_4 & l_2 \end{Bmatrix} (2\mathcal{L}+1)$$

$$* (-)^{L_5+L_6+L_7+L_8} \; B(L_5L_6\mathcal{LM}\hat{s}_1\hat{s}_2) \; B^*(L_7L_8\mathcal{LM}\hat{s}'_1\hat{s}'_2)$$

Using the relation (6.4.14) of ref.(8)

$$\begin{Bmatrix} e & 0 & e \\ c & f & a \\ d & f & b \end{Bmatrix} = \frac{(-)^{b+c+e+f}}{\hat{e}\,\hat{f}} \begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix}$$

we get

$$<\Phi^{(3)}(\underset{\sim}{s}_1,\underset{\sim}{s}_2)|V|\Phi^{(3)}(\underset{\sim}{s}'_1,\underset{\sim}{s}'_2)>$$

$$= \sum_i v^{(i)} \exp\{\qquad\}(4\pi)^2 \overline{\sum_{\substack{l_1..l_6 LM \\ L_1...L_8}}} i_{l_1}\ldots i_{l_6}$$

$$* (2l_1+1)\ldots(2l_6+1)(2L_1+1)\ldots(2L_4+1)\;\hat{L}_5\ldots\hat{L}_8\;(-)^{l_5+l_6}$$

(continued next page)

$$* \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & L_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & L_4 \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \begin{pmatrix} L_1 & l_5 & L_5 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_2 & l_5 & L_6 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_3 & l_6 & L_7 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_4 & l_6 & L_8 \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \begin{Bmatrix} L_5 & L_1 & l_5 \\ L_2 & L_6 & L \end{Bmatrix} \begin{Bmatrix} L_7 & L_3 & l_6 \\ L_4 & L_8 & L \end{Bmatrix} \begin{Bmatrix} L_2 & L & L_1 \\ l_3 & L_3 & l_1 \\ l_4 & L_4 & l_2 \end{Bmatrix}$$

$$* \; B(L_5 L_6 L M \hat{s}_1 \hat{s}_2) \; B^*(L_7 L_8 L M \hat{s}'_1 \hat{s}'_2)$$

Upon comparing this equation with the expansion (2.5b)

$$<\Phi^{(3)}(L_1 L_2 L M s_1 s_2)|V|\Phi^{(3)}(L'_1 L'_2 L' M' s'_1 s'_2)>$$

$$= \delta_{LL'} \delta_{MM'} <\Phi^{(3)}(L_1 L_2 L s_1 s_2)|V|\Phi^{(3)}(L'_1 L'_2 L s'_1 s'_2)>$$

where

$$<\Phi^{(3)}(L_1 L_2 L s_1 s_2)|V|\Phi^{(3)}(L'_1 L'_2 L s'_1 s'_2)>$$

$$= (s_1 s_2 s'_1 s'_2) \sum_i v^{(i)} \exp\{-\beta[u_1^{(i)} s_1^2 + u_2^{(i)} s_2^2 + u_{1'}^{(i)} s_1'^2 + u_{2'}^{(i)} s_2'^2]\} (4\pi)^2$$

$$* \sum_{l_1 \cdots l_6} (2l_1+1) \ldots (2l_6+1) i_{l_1}(\beta w_{11'}^{(i)} s_1 s'_1) i_{l_2}(\beta w_{12'}^{(i)} s_1 s'_2)$$

$$* \; i_{l_3}(\beta w_{21'}^{(i)} s_2 s'_1) i_{l_4}(\beta w_{22'}^{(i)} s_2 s'_2) i_{l_5}(\beta w_{12}^{(i)} s_1 s_2) i_{l_6}(\beta w_{1'2'}^{(i)} s'_1 s'_2)$$

$$* \; \hat{L}_1 \hat{L}_2 \hat{L}'_1 \hat{L}'_2 (-)^{l_5 l_6}$$

$$* \sum_{\lambda_1 \lambda_2 \lambda'_1 \lambda'_2} (2\lambda_1+1)(2\lambda_2+1)(2\lambda'_1+1)(2\lambda'_2+1)$$

$$* \begin{pmatrix} l_1 & l_2 & \lambda_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & \lambda_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & \lambda'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & \lambda'_2 \\ 0 & 0 & 0 \end{pmatrix}$$

$$* \begin{pmatrix} \lambda_1 & l_5 & L_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_2 & l_5 & L_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda'_1 & l_6 & L'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda'_2 & l_6 & L'_2 \\ 0 & 0 & 0 \end{pmatrix}$$

(continued next page)

$$* \begin{Bmatrix} L_1 & L_2 & L \\ \lambda_2 & \lambda_1 & l_5 \end{Bmatrix} \begin{Bmatrix} L_1' & L_2' & L \\ \lambda_2' & \lambda_1' & l_6 \end{Bmatrix} \begin{Bmatrix} \lambda_2 & L & \lambda_1 \\ l_3 & \lambda_1' & l_1 \\ l_4 & \lambda_2' & l_2 \end{Bmatrix} \qquad (8.10)$$

Again parity conservation is contained in the CG-coefficients, i.e.

$$\begin{aligned} l_1 + l_2 + \lambda_1 &= \text{even} \\ l_3 + l_4 + \lambda_2 &= \text{even} \\ l_1 + l_3 + \lambda_1' &= \text{even} \\ l_2 + l_4 + \lambda_2' &= \text{even} \\ \lambda_1 + l_5 + L_1 &= \text{even} \\ \lambda_2 + l_5 + L_2 &= \text{even} \\ \lambda_1' + l_6 + L_1' &= \text{even} \\ \lambda_2' + l_6 + L_2' &= \text{even} \end{aligned}$$

thus $\quad (-)^{L_1+L_2} = (-)^{L_1'+L_2'}$.

9. Projection of Spin Angular Momentum

One way to project spin angular momentum from Slater-determinant wave functions is to start from their representation in terms of creation operators

$$|\Phi\rangle = \prod_{i=1}^{N} a^+_{\nu_i} |0\rangle \qquad (9.1)$$

where we left out all quantum numbers except the spin direction ν_i of particle i. The two operators $a^+_{-1/2}$ and $a^+_{1/2}$ form a spherical tensor operator of rank 1/2. The product $a^+_{-1/2} a^+_{1/2}$ is a scalar operator, i.e. is rotationally invariant.

Indeed, from the fact that $a^+_{-1/2}$ and $a^+_{1/2}$ anticommute we observe that $a^+_\nu \; a^+_{-\nu}$ is an odd function of ν. Upon rotating the basis of the spinors, we have

$$R a^+_\nu a^+_{-\nu} R^{-1}$$

$$= \sum_{\sigma\sigma'} D^{1/2}_{\sigma\nu} \, D^{1/2}_{\sigma-\nu} \, a^+_\sigma \, a^+_{\sigma'} ,$$

$$= \sum_{\sigma\sigma' I\rho\rho'} (2I+1) \begin{pmatrix} 1/2 & 1/2 & I \\ \sigma & \sigma' & \rho \end{pmatrix} \begin{pmatrix} 1/2 & 1/2 & I \\ \nu & -\nu & \rho' \end{pmatrix} \mathcal{D}^{I*}_{\rho\rho'} \, a^+_\sigma \, a^+_{\sigma'}$$

$$= -\sum_{\sigma\sigma' I\rho\rho'} (-)^I (2I+1) \begin{pmatrix} 1/2 & 1/2 & I \\ \sigma & \sigma' & \rho \end{pmatrix} \begin{pmatrix} 1/2 & 1/2 & I \\ -\nu & \nu & \rho' \end{pmatrix} \mathcal{D}^{I*}_{\rho\rho'} a^+_\sigma \, a^+_{\sigma'}$$

As this has to be an odd function of ν, we conclude $(-)^I$ = even, i.e. $I = 0$ and

$$R \, a^+_\nu \, a^+_{-\nu} R^{-1} = a^+_\nu \, a^+_{-\nu} \tag{9.2}$$

To be specific, we consider the case of ^{7}Li which was treated[4] as a superposition of a two- and a three-cluster wave function

$$|^7\text{Li}\rangle = |\alpha\text{-t}\rangle + |\alpha\text{-d-n}\rangle \; . \tag{9.3}$$

In the two-cluster wave function $|\Phi^{(2)}\rangle = |\alpha\text{-t}\rangle$, the only unpaired spin is that of the neutron in the triton, whereas in the case of the three-cluster functions $|\Phi^{(3)}\rangle = |\alpha\text{-d-n}\rangle$ we have three unpaired spins: The spins of proton and neutron in the deuteron cluster which are coupled to the spin I_d of the deuteron, and the spin of the extra neutron n.
Upon coupling the spins of the deuteron and that of the neutron we form a spherical tensor in spin space of rank I

$$\Phi^{(3)}_{I_d \, I\nu} = \sum_{\nu_{pd}\nu_{nd}\nu_n\nu_d} (1/2\nu_{pd}, 1/2\nu_{nd} | I_d\nu_d)(I_d\nu_d, 1/2\nu_n | I\nu) * \Phi^{(3)}_{\nu_{pd}\nu_{nd}\nu_n} \tag{9.4}$$

In the following we consider separately the overlaps between shell model wave functions with one or/and two unpaired spins.

(i) matrix elements between SM functions with one and two unpaired spins

$$\langle \Phi^{(2)}_{\nu_t} | \mathcal{O} | \Phi^{(3)\prime}_{I_d I\nu} \rangle = \sum_{\nu_{pd}\nu_{nd}\nu_n\nu_d} (1/2\nu_{pd}, 1/2\nu_{nd} | I_d\nu_d)(I_d\nu_d, 1/2\nu_n | I\nu) \langle \Phi^{(2)}_{\nu_t} | \mathcal{O} | \Phi^{(3)\prime}_{\nu_{pd}\nu_{nd}\nu_n} \rangle \tag{9.5}$$

An explicit calculation of the normalization matrix element $<\Phi^{(2)}_{\nu_t}|\Phi^{(3)'}_{I_d I\nu}>$ leads to the following relation which due to eqs. (5.8) and (5.11) is true for any spin-isospin independent operator O

$$<\Phi^{(2)}_{\nu_t}|O|\Phi^{(3)'}_{\nu_{pd}\nu_{nd}\nu_n}>$$

$$= \delta_{\nu_t\nu_{pd}}[\delta_{\nu_{nd}\ 1/2}\delta_{\nu_n -1/2} - \delta_{\nu_{nd} -1/2}\delta_{\nu_n\ 1/2}]<\Phi^{(2)}|O|\Phi^{(3)'}> \quad (9.6)$$

where the matrix element on the r.h.s. is spin independent. Using this relation in eq. (9.5) we find

$$<\Phi^{(2)}_{\nu_t}|O|\Phi^{(3)'}_{I_d I\nu}>$$

$$= \sum_{\nu_d}[(1/2\nu,\ 1/2\ 1/2|I_d\nu_d)(I_d\nu_d,\ 1/2 -1/2|I\nu)$$

$$-(1/2\nu,\ 1/2 -1/2|I_d\nu_d)(I_d\nu_d,\ 1/2\ 1/2|I\nu)]\ <\Phi^{(2)}|O|\Phi^{(3)'}>\delta_{\nu_t\nu}$$

$$= \sum_{\nu_d\nu_n} -(-)^{I_d}\left(\frac{2I_d+1}{2}\right)^{1/2}(I_d\nu_d,\ 1/2\nu_n|1/2\nu)$$

$$* \ (I_d\nu_d,\ 1/2\nu_n|I\nu)<\Phi^{(2)}|O|\Phi^{(3)'}>\delta_{\nu_t\nu}$$

$$= -(-)^{I_d}\left(\frac{2I_d+1}{2}\right)^{1/2}\delta_{I 1/2}\delta_{\nu_t\nu}<\Phi^{(2)}|O|\Phi^{(3)'}> \quad (9.7a)$$

In the special case where the spin of the deuteron $I_d=1$ we have

$$<\Phi^{(2)}_{\nu_t}|O|\Phi^{(3)'}_{I_d=1,I\nu}> = \sqrt{3/2}\ \delta_{I 1/2}\ \delta_{\nu_t\nu}<\Phi^{(2)}|O|\Phi^{(3)'}> \quad (9.7b)$$

(ii) matrix elements between SM functions with two unpaired spins

From eq. (9.4) we obtain

$$<\Phi^{(3)}_{I_d I\nu}|O|\Phi^{(3)'}_{I'_d I'\nu'}>$$

$$= \sum_{\substack{\nu_{pd}\nu_{nd}\nu_n\nu_d \\ \nu'_{pd}\nu'_{nd}\nu'_n\nu'_d}}(1/2\nu_{pd},1/2\nu_{nd}|I_d\nu_d)(I_d\nu_d,1/2\nu_n|I\nu)$$

(continued next page)

$$* \; (1/2\nu'_{pd}, 1/2\nu'_{nd}|I'_d\nu'_d)(I'_d\nu'_d, 1/2\nu'_n|I'\nu')$$

$$* \; <\Phi^{(3)}_{\nu_{pd}\nu_{nd}\nu_n}|O|\Phi^{(3)'}_{\nu'_{pd}\nu'_{nd}\nu'_n}> \qquad (9.8)$$

Again the structure of the matrix element in eq. (9.8) may be obtained from an explicit calculation of the normalization matrix element $<\Phi^{(3)}_{\nu_{pd}\nu_{nd}\nu_n}|\Phi^{(3)'}_{\nu'_{pd}\nu'_{nd}\nu'_n}>$ using eqs. (5.8) and (5.11)

$$<\Phi^{(3)}_{\nu_{pd}\nu_{nd}\nu_n}|O|\Phi^{(3)'}_{\nu'_{pd}\nu'_{nd}\nu'_n}>$$

$$= \delta_{\nu_{pd}\,\nu'_{pd}}\{[\delta_{\nu_{nd}1/2}\delta_{\nu_n 1/2}\delta_{\nu'_{nd}1/2}\delta_{\nu'_n 1/2}$$

$$+ \delta_{\nu_{nd}-1/2}\delta_{\nu_n -1/2}\delta_{\nu'_{nd}-1/2}\delta_{\nu'_n -1/2}]<\Phi^{(3)}_{++}|O|\Phi^{(3)'}_{++}>$$

$$+ [\delta_{\nu_{nd}1/2}\delta_{\nu_n -1/2}\delta_{\nu'_{nd}1/2}\delta_{\nu'_n -1/2}$$

$$+ \delta_{\nu_{nd}-1/2}\delta_{\nu_n 1/2}\delta_{\nu'_{nd}-1/2}\delta_{\nu_n 1/2}]<\Phi^{(3)}_{+-}|O|\Phi^{(3)'}_{+-}>$$

$$+ [\delta_{\nu_{nd}1/2}\delta_{\nu_n -1/2}\delta_{\nu'_{nd}-1/2}\delta_{\nu'_n 1/2}$$

$$+ \delta_{\nu_{nd}-1/2}\delta_{\nu_n 1/2}\delta_{\nu'_{nd}1/2}\delta_{\nu'_n -1/2}]<\Phi^{(3)}_{+-}|O|\Phi^{(3)'}_{-+}>\} \qquad (9.9)$$

and

$$<\Phi^{(3)}_{++}|O|\Phi^{(3)'}_{++}> = <\Phi^{(3)}_{+-}|O|\Phi^{(3)'}_{+-}> + <\Phi^{(3)}_{+-}|O|\Phi^{(3)'}_{-+}> \qquad (9.10)$$

where the signs in the matrix elements refer to the spin directions of the two neutrons, e.g.

$$<\Phi^{(3)}_{+-}|O|\Phi^{(3)'}_{+-}> = <\Phi^{(3)}_{\nu_{pd}\nu_{nd}=1/2\;\nu_n=-1/2}|O|\Phi^{(3)}_{\nu_{pd}\nu'_{nd}=1/2\;\nu'_n=-1/2}> .$$

Inserting eqs. (9.9) and (9.10) into eq. (9.8) we may carry out the summation over spin directions

$$<\Phi^{(3)}_{I_d I\nu}|O|\Phi^{(3)'}_{I'_d I'\nu'}>$$

$$= \sum_{\nu_{pd}\nu_d\nu'_d} \{[(1/2\nu_{pd},1/2\ 1/2|I_d\nu_d)(I_d\nu_d,1/2\ 1/2|I\nu)$$

$$* (1/2\nu_{pd},1/2\ 1/2|I'_d\nu'_d)(I'_d\nu'_d,1/2\ 1/2|I'\nu')$$

$$+ (1/2\nu_{pd},1/2-1/2|I_d\nu_d)(I_d\nu_d,1/2-1/2|I\nu)$$

$$* (1/2\nu_{pd},1/2-1/2|I'_d\nu'_d)(I'_d\nu'_d,1/2-1/2|I'\nu')]<\Phi^{(3)}_{++}|O|\Phi^{(3)'}_{++}>$$

$$+ [(1/2\nu_{pd},1/2\ 1/2|I_d\nu_d)(I_d\nu_d,1/2-1/2|I\nu)$$

$$* (1/2\nu_{pd},1/2\ 1/2|I'_d\nu'_d)(I'_d\nu'_d,1/2-1/2|I'\nu')$$

$$+ (1/2\nu_{pd},1/2-1/2|I_d\nu_d)(I_d\nu_d 1/2\ 1/2|I\nu)$$

$$* (1/2\nu_{pd},1/2-1/2|I'_d\nu'_d)(I'_d\nu'_d\ 1/2\ 1/2|I'\nu')]<\Phi^{(3)}_{+-}|O|\Phi^{(3)'}_{+-}>$$

$$+ [(1/2\nu_{pd},1/2\ 1/2|I_d\nu_d)(I_d\nu_d,1/2-1/2|I\nu)$$

$$* (1/2\nu_{pd},1/2-1/2|I'_d\nu'_d)(I'_d\nu'_d,1/2\ 1/2|I'\nu')$$

$$+ (1/2\nu_{pd},1/2-1/2|I_d\nu_d)(I_d\nu_d,1/2\ 1/2|I\nu)$$

$$* (1/2\nu_{pd},1/2\ 1/2|I'_d\nu'_d)(I'_d\nu'_d,1/2-1/2|I'\nu')]<\Phi^{(3)}_{+-}|O|\Phi^{(3)'}_{-+}>\}$$

$$= \sum_{\nu_{pd}\nu_d\nu'_d\mu\sigma} (1/2\nu_{pd},1/2\mu|I_d\nu_d)(I_d\nu_d,1/2\sigma|I\nu)$$

$$* (1/2\nu_{pd},1/2\mu|I'_d\nu'_d)(I'_d\nu'_d,1/2\sigma|I'\nu')<\Phi^{(3)}_{++}|O|\Phi^{(3)'}_{++}>$$

$$+ \sum_{\nu_{pd}\nu_d\nu_{d'}} [(1/2\nu_{pd},1/2\ 1/2|I_d\nu_d)(I_d\nu_d,1/2-1/2|I\nu)$$

$$* (1/2\nu_{pd},1/2-1/2|I'_d\nu'_d)(I'_d\nu'_d,1/2\ 1/2|I'\nu')$$

$$+ (1/2\nu_{pd},1/2-1/2|I_d\nu_d)(I_d\nu_d,1/2\ 1/2|I\nu)$$

(continued next page)

$* \; (1/2\nu_{pd}, 1/2\ 1/2|I_d'\nu_d')(I_d'\nu_d', 1/2 -1/2|I'\nu')$

$- \; (1/2\nu_{pd}, 1/2\ 1/2|I_d\nu_d)(I_d\nu_d, 1/2 -1/2|I\nu)$

$* \; (1/2\nu_{pd}, 1/2\ 1/2|I_d'\nu_d')(I_d'\nu_d', 1/2 -1/2|I'\nu')$

$- \; (1/2\nu_{pd}, 1/2 -1/2|I_d\nu_d)(I_d\nu_d, 1/2\ 1/2|I\nu)$

$* \; (1/2\nu_{pd}, 1/2 -1/2|I_d'\nu_d')(I_d'\nu_d', 1/2\ 1/2|I'\nu')]<\Phi_{+-}^{(3)}|o|\Phi_{-+}^{(3)'}>$

$$= \delta_{I_d\ I_d'} \sum_{\nu_d\sigma} (I_d\nu_d, 1/2\sigma|I\nu)(I_d\nu_d, 1/2\sigma|I'\nu')<\Phi_{++}^{(3)}|o|\Phi_{++}^{(3)'}>$$

$$- \sum_{\nu_{pd}\nu_d\nu_d'} [(1/2 -1/2, I_d\nu_d|1/2\nu_{pd})(1/2 -1/2, I_d\nu_d|I\nu)$$

$* \; (1/2\ 1/2, I_d'\nu_d'|1/2\nu_{pd})(1/2\ 1/2, I_d'\nu_d'|I'\nu')$

$+ \; (1/2\ 1/2, I_d\nu_d|1/2\nu_{pd})(1/2\ 1/2, I_d\nu_d|I\nu)$

$* \; (1/2 -1/2, I_d'\nu_d'|1/2\nu_{pd})(1/2 -1/2, I_d'\nu_d'|I'\nu')$

$+ \; (1/2 -1/2, I_d\nu_d|1/2\nu_{pd})(1/2 -1/2, I_d\nu_d|I\nu)$

$* \; (1/2 -1/2, I_d'\nu_d'|1/2\nu_{pd})(1/2 -1/2, I_d'\nu_d'|I'\nu')$

$+ \; (1/2\ 1/2, I_d\nu_d|1/2\nu_{pd})(1/2\ 1/2, I_d\nu_d|I\nu)$

$* \; (1/2\ 1/2, I_d'\nu_d'|1/2\nu_{pd})(1/2\ 1/2, I_d'\nu_d'|I'\nu')]$

$$* \sqrt{\frac{2I_d+1}{2}} \sqrt{\frac{2I_d'+1}{2}} \, (-)^{I_d+1/2-I} \, (-)^{I_d'+1/2-I'} <\Phi_{+-}^{(3)}|o|\Phi_{-+}^{(3)'}>$$

$$<\Phi_{I_dI\nu}^{(3)}|o|\Phi_{I_d'I'\nu'}^{(3)'}>$$

$$= \delta_{I_dI_d'} \delta_{II'} \delta_{\nu\nu'} <\Phi_{++}^{(3)}|o|\Phi_{++}^{(3)'}> \quad .$$

(continued next page)

$$- \sqrt{(2I_d+1)(2I_d'+1)}\ 1/2 \sum_{\nu_{pd}\nu_d\nu_d',\mu\mu'} (1/2\mu, I_d\nu_d | 1/2\nu_{pd})$$

$$* (1/2\mu, I_d\nu_d | I\nu)(1/2\mu', I_d'\nu_d' | 1/2\nu_{pd})(1/2\mu', I_d'\nu_d' | I'\nu')$$

$$* (-)^{I_d+1/2-I} (-)^{I_d'+1/2-I'} <\Phi_{+-}^{(3)} | O | \Phi^{(3)'}>$$

$$= \delta_{II'}\delta_{\nu\nu'} \{ \delta_{I_d I_d'} <\Phi_{++}^{(3)} | O | \Phi_{++}^{(3)'}>$$

$$- \delta_{I,1/2}\ 1/2 \sqrt{2I_d+1} \cdot \sqrt{2I_d'+1}\ (-)^{I_d+I_d'} <\Phi_{+-}^{(3)} | O | \Phi_{-+}^{(3)'}> \} \qquad (9.11a)$$

In the special case where $I_d=1$

$$<\Phi_{I\nu}^{(3)} | O | \Phi_{I'\nu'}^{(3)'}>$$

$$= \delta_{II'}\delta_{\nu\nu'} \{ <\Phi_{++}^{(3)} | O | \Phi_{++}^{(3)'}> - \delta_{I\ 1/2}\ 3/2\ <\Phi_{+-}^{(3)} | O | \Phi_{-+}^{(3)'}> \} \qquad (9.11b)$$

10. Discussion

In sections 7 und 8 we derived formulas for matrix elements between SM functions which describe two- or three-cluster structures. When three-cluster structures are involved, some of these formulas contain sums over modified spherical Bessel functions $i_l(x)$ where the order l runs from zero to infinity. Using the WKB approximation one can derive the following asymptotic expansion of the modified spherical Bessel functions

$$i_l(x) \simeq \frac{1}{2x} \left[1+\left(\frac{l+1/2}{x}\right)^2\right]^{-1/4} \exp\{-(l+1/2)[\ln(\tfrac{2}{x}(l+1/2))-1]\}$$

which holds in the limit $(l+1/2)^2 >> x^2$.
Roughly speaking, i_l vanishes exponentially with increasing order l, so that the sum over l converges rapidly. In a practical calculation[4)] it turned out that $l_{max}=3$ is usually sufficient to get an accuracy of 10^{-5} in the overlaps.

In this report the method of angular momentum projection was restricted twofold:

(i) Only those SM functions were considered which are constructed from nucleons occupying 1s orbits. In a present study[9] the projection method is extended to cope with situations where the wave functions contain also nucleons in 1p orbits.

(ii) The calculation of matrix elements was restricted to spin-isospin independent scalar operators O. In nuclei or clusters with open shells it might be necessary to take also more complicated interactions like tensor and spin-orbit interaction into account. The spherical representation of cluster wave functions is especially suited[9] to deal with these operators which have a simple structure when expressed in terms of spherical tensor operators[8].

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