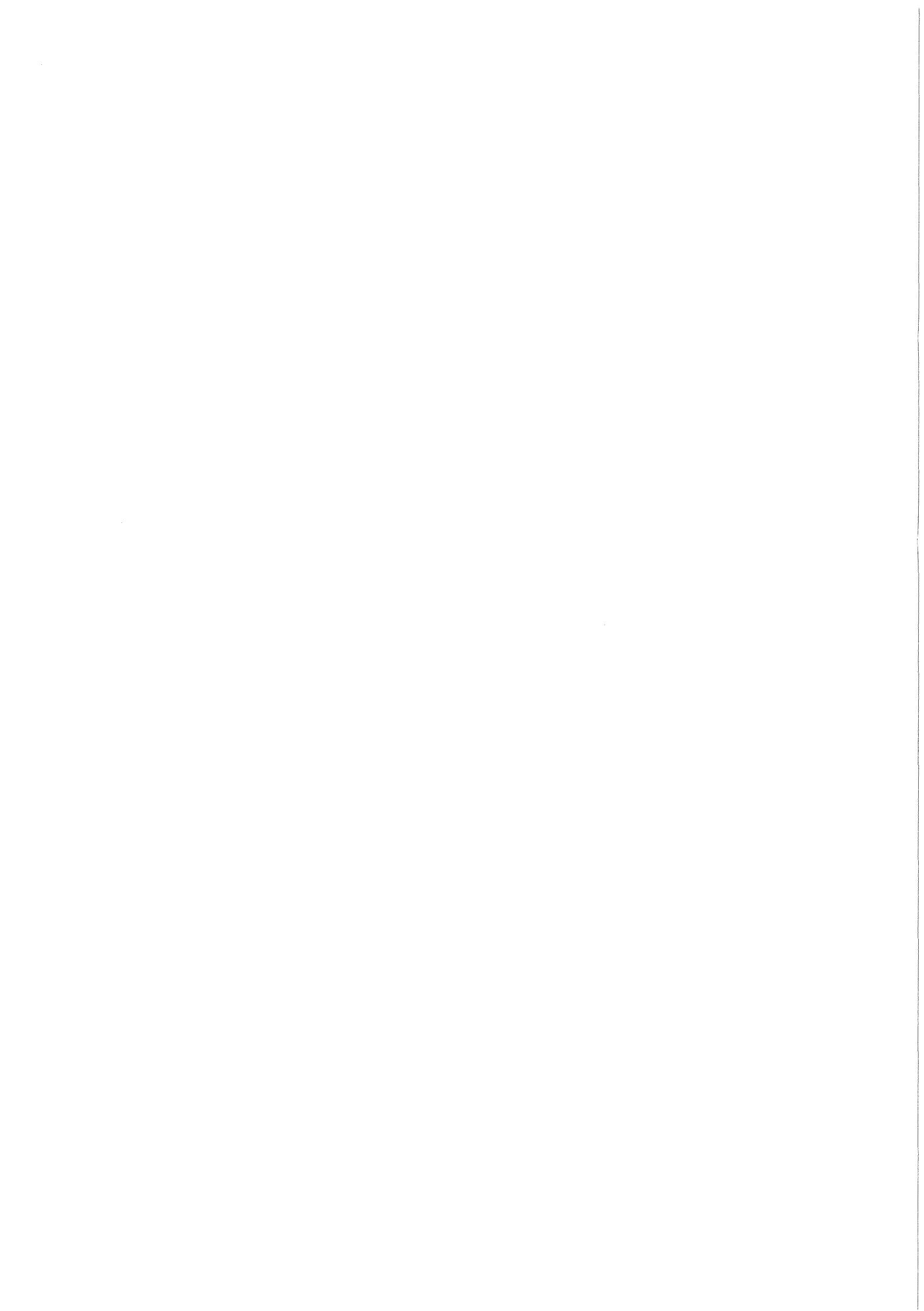


KfK 3539  
Mai 1983

# **Application of the Algebraic Programming System REDUCE 2 to Calculations in the Nuclear Cluster Model**

**R. Beck, F. Dickmann, J. Oehlschläger**  
**Institut für Angewandte Kernphysik**

**Kernforschungszentrum Karlsruhe**



KERNFORSCHUNGSZENTRUM KARLSRUHE

Institut für Angewandte Kernphysik

KFK 3539

Application of the Algebraic Programming System  
REDUCE 2 to Calculations in the Nuclear Cluster Model

R. Beck, F. Dickmann and J. Oehlschläger

Kernforschungszentrum Karlsruhe GmbH, Karlsruhe

Als Manuskript vervielfältigt  
Für diesen Bericht behalten wir uns alle Rechte vor

Kernforschungszentrum Karlsruhe GmbH  
ISSN 0303-4003

## Abstract

The paper shows to which extent algebraic calculations in the nuclear cluster model may be performed on a computer. After setting up the nuclear model, the calculation of relevant nuclear matrix elements is discussed. For simple cases, this is done by hand while more general examples are calculated analytically by the computer. Various REDUCE programs are presented to demonstrate the feasibility of the method.

Anwendung des Algebraischen Programmiersystems REDUCE 2 auf die Berechnung von Matrixelementen im Clustermodell des Atomkerns

## Zusammenfassung

Die Arbeit zeigt, in welchem Umfang sich die analytische Berechnung von Vielteilchenmatrixelementen, wie sie im Clustermodell des Atomkerns auftreten, mit Hilfe des algebraischen Programmiersystems REDUCE 2 auf einem Computer durchführen lässt. Anhand mehrerer Programmbeispiele werden die Einsatzmöglichkeiten des Systems REDUCE 2 auf den verschiedenen Stufen der Rechnung (Ein- und Zweiteilchenmatrixelemente, Vielteilchenmatrixelemente und Anknüpfung an ein FORTRAN Programm zur numerischen Berechnung) erläutert.

## CONTENTS

1. INTRODUCTION
2. FORMULATION OF THE NUCLEAR CLUSTER MODEL
  - 2.1 Model Space
  - 2.2 Model Hamiltonian
3. SINGLE-PARTICLE MATRIX ELEMENTS
  - 3.1 Overlap Matrix Elements
  - 3.2 Kinetic-Energy Matrix Elements
  - 3.3 Matrix Elements of the Charge Multipole Operator
4. TWO-PARTICLE MATRIX ELEMENTS
  - 4.1 Matrix Elements of the Central Interaction
  - 4.2 Matrix Elements of the Spin-Orbit Interaction
  - 4.3 Matrix Elements of the Tensor Interaction
5. MATRIX ELEMENTS OF SLATER-DETERMINANT WAVE FUNCTIONS
  - 5.1 The Overlap of Slater-Determinant Wave Functions
  - 5.2 Matrix Elements of One-Body Operators
  - 5.3 Matrix Elements of Two-Body Operators
6. INTERFACE BETWEEN SYMBOLIC AND NUMERICAL CALCULATIONS
7. DISCUSSION

## 1. INTRODUCTION

This paper is an attempt to interest people working with the nuclear cluster model<sup>1)</sup> in the application of the algebraic programming system REDUCE<sup>2)</sup>. In the nuclear cluster model one assumes that a given nucleus may be treated as an assembly of lighter nuclei (or clusters) having a relatively simple structure. The dynamics of the nuclear system is then determined by a variational equation allowing for different arrangements of these clusters.

The input to this equation are matrix elements of the nuclear Hamiltonian between few-cluster wave functions<sup>3)</sup>, usually of the Slater-determinant type, formed from single-particle oscillator wave functions. It is the calculation of these matrix elements using the algebraic programming system REDUCE which will be our main concern here. Although the reader is not supposed to be familiar with REDUCE, some basic knowledge of its application<sup>4)</sup> would be helpful.

We begin in section 2 by formulating the nuclear model, i.e. defining the model space and the model Hamiltonian.

In sections 3 and 4, we work out analytically the relevant one-and two-particle matrix elements. If only particles occupying s-waves are involved this can be done easily by hand. In the case when there are also particles in orbits with  $l > 0$  the calculation becomes rather tedious. The basic rule, however, is a very simple one, namely just a differentiation with respect to one or two parameters entering the s-wave matrix element. REDUCE offers the possibility to perform this differentiation analytically. We show how this works in practice giving a few examples of REDUCE programs.

Section 5 is devoted to the calculation of many-body matrix elements where - in addition to one - and two - particle matrix elements - also the determinant and various cofactors of the single-particle overlap matrix are needed. If all the single-particle states (or at least those within a given cluster) are characterized by a common oscillator parameter  $\beta$ , the analytical calculation of this determinant and the cofactor expansions reduces the number of terms considerably. REDUCE provides various operators

to perform these matrix manipulations analytically.

During these algebraic calculations we want to keep track of the analytic dependence of the matrix elements on certain quantum numbers of individual nucleons, e.g. the magnetic quantum number of a particle in a p-orbit. This information is needed when the many-body functions are projected onto the eigenspace of the operators of angular momentum and parity<sup>5)</sup>. This requirement is met by REDUCE through the possibility of introducing certain operators depending on symbolic variables.

The interface between algebraic and numerical processing of expressions is a rather critical part of the whole calculation which needs some careful analytical work prior to the application of REDUCE. Section 6 deals with boiling down the algebraic expressions obtained by REDUCE to a form suitable as input to a FORTRAN program. In section 7, we discuss some extensions and limitations of this work.

## 2. FORMULATION OF THE NUCLEAR CLUSTER MODEL

### 2.1 Model Space

We start from the set of single-particle functions ( $i = 1, 2$ )

$$\begin{aligned}\psi_{v\tau}(x \sim nlm \xi_i) &= \varphi(x \sim nlm \xi_i) \chi_{v\tau} \\ &= \varphi(x - \xi_i, nlm) \chi_{v\tau}\end{aligned}\quad (2.1)$$

whose spatial parts  $\varphi$  are eigenfunctions of the harmonic oscillator labelled by the radial quantum number  $n$ , the angular momentum quantum numbers  $l$  and  $m$  and by the vector  $\xi_i$  which specifies the center of the oscillator potential. The normalized oscillator functions are

$$\begin{aligned}\varphi(x \sim nlm) &= \left[ \frac{\beta^{l+3/2}}{\pi^{1/2}} \frac{2^{l+m+2}}{(2l+2m+1)!!} m! \right]^{1/2} L_n^{l+1/2}(\beta x^2) e^{-\frac{\beta}{2} x^2} Y_{lm}(x)\end{aligned}\quad (2.2)$$

expressed in terms of generalized Laguerre polynomials  $L_n^\alpha$  and solid spherical harmonics  $Y_{lm}$ . The quantity  $\beta = m\omega/\hbar$  is the oscillator parameter where  $m$  is the nucleon mass and  $\omega$  is the oscillator frequency. For later use we note that the functions (2.2) with  $l > 0$  may be obtained from those with  $l = 0$  by differentiation with respect to a spherical component of the vector  $x$ , e.g.

$$\varphi(x) = (\beta/\pi)^{3/4} \exp(-\frac{\beta}{2} x^2) \quad (2.3a)$$

$$\begin{aligned}\varphi(x \sim 1m) &= -(2/\beta)^{1/2} \nabla_m(x) \varphi(x) \\ &= -(2/\beta)^{1/2} \partial/\partial x_m^* \varphi(x)\end{aligned}\quad (2.3b)$$

$$\varphi(x \sim 2m) = \sqrt{2}/\beta \sum_{m_1 m_2} (1m_1, 1m_2 | 2m) \nabla_{m_1}(x) \nabla_{m_2}(x) \varphi(x) \quad (2.3c)$$

where we omitted all vanishing quantum numbers. The spin-isospin wave function  $\chi$  in eq. (2.1) is labelled by the spin projection  $v$  and isospin projection  $\tau$ . In order to simplify the notation we

collect all quantum numbers characterizing the single-particle wave functions  $\psi$  in a single letter  $i$

$$i = \{nlm\}_{\nu\tau}.$$

We construct products of  $A_1$  and  $A_2$  single-particle functions (2.1) with oscillator wells centered at  $S_{A_1}$  and  $S_{A_2}$  which correspond to the clusters  $A_1$  and  $A_2$ , respectively.

$$\begin{aligned}\phi_{A_1}(\{\tilde{x}\}_{A_1}, S_{A_1}) &= \prod_{i=1}^{A_1} \psi_i(x_i, S_{A_1}) \\ \phi_{A_2}(\{\tilde{x}\}_{A_2}, S_{A_2}) &= \prod_{i=A_1+1}^{A_1+A_2} \psi_i(x_i, S_{A_2})\end{aligned}\quad (2.4)$$

where

$$\begin{aligned}\{\tilde{x}\}_{A_1} &= (x_1, x_2, \dots, x_{A_1}) \\ \{\tilde{x}\}_{A_2} &= (x_{A_1+1}, \dots, x_A)\end{aligned}$$

From the functions (2.4) we form antisymmetrized ( $\mathcal{A}$  = anti-symmetrizer)  $A$ -particle functions ( $A = A_1 + A_2$ )

$$\phi_{A_1-A_2, I\nu}(\{\tilde{x}\}, \tilde{s}) = [\mathcal{A} \phi_{A_1}(\{\tilde{x}\}_{A_1}, S_{A_1}) \phi_{A_2}(\{\tilde{x}\}_{A_2}, S_{A_2})]_{I\nu} \quad (2.5)$$

where

$$\begin{aligned}\tilde{s} &= S_{A_1} - S_{A_2} \\ 0 &= A_1 S_{A_1} + A_2 S_{A_2}\end{aligned}\quad (2.6)$$

and

$$\{\tilde{x}\} = (x_1, \dots, x_A)$$

The vector  $\tilde{s}$  is the generator coordinate. The symbol  $[\ ]_{I\nu}$  means that the spins of all  $A$  particles are coupled to the total spin  $I$  and its projection  $\nu$  along the 3-axis.

The projection of the states (2.5) onto the eigenspace of the operators of angular momentum, parity and center-of-mass momentum may be found in refs. 3 and 5.

We choose the model I of  $^6\text{Li}$ , introduced by R. Krivec and M.V. Mihailović<sup>6)</sup> as an example to demonstrate the applicability of REDUCE to calculations in the nuclear cluster model. This cluster model describes  $^6\text{Li}$  as an interplay of the three cluster structures ( $^4\text{He}-^2\text{H}$ ), ( $^5\text{He}-\text{p}$ ) and ( $^5\text{Li}-\text{n}$ ), assuming that all clusters are constructed by filling nucleons into the lowest orbits of a harmonic oscillator well centered at some position. All harmonic oscillators are of the same size, i.e. are determined by the same oscillator parameter  $\beta$ .

We use the following ansatz for the trial wave function of the Generator Coordinate (GC) type with fixed total angular momentum and parity<sup>5)</sup>

$$\begin{aligned} \Psi(\{x_1, y_1, z_1, J, M, \pi\}) &= \sum_{IL} \int_0^\infty ds_1 f_{1I}(L J M s_1) \phi_{^{4\text{He}}-^2\text{H}, I}(x_1, y_1, z_1, L J M s_1) \\ &+ \sum_{ILK} \int_0^\infty ds_2 f_{2I}(L_1 K J M s_2) \phi_{^{3\text{He}}-\text{p}, I}(x_1, y_1, z_1, L_1 K J M s_2) \\ &+ \sum_{ILK} \int_0^\infty ds_3 f_{3I}(L_1 K J M s_3) \phi_{^{7\text{Li}}-\text{n}, I}(x_1, y_1, z_1, L_1 K J M s_3) \end{aligned} \quad (2.7)$$

where

$$f_1(s_1), f_2(s_2) \text{ and } f_3(s_3)$$

are the GC-amplitudes corresponding to the clusterizations  $^4\text{He}-^2\text{H}$ ,  $^5\text{He}-\text{p}$  and  $^5\text{Li}-\text{n}$ , respectively. In eq. (2.7), the vectors  $s_{A_i}$  specifying the various cluster centers are expressed in terms of the corresponding generator coordinates,  $x_1, y_1$  and  $z_1$ , eq. (2.6).

In the later development it will turn out useful to associate each particle  $i$  with the vector  $\tilde{s}_i$  (or the dimensionless vector  $\chi_i$ ) of its cluster center

$$\tilde{\chi}_i = (\beta/2)^{1/2} \tilde{s}_i = (\beta/2)^{1/2} C_i \tilde{s} \quad (2.8a)$$

where

$$C_i = B(CN(i)) \quad (2.8b)$$

$$B(1) = A_2/A$$

$$B(2) = -A_1/A \quad (2.8c)$$

and  $CN(1) = 1(2), i = 1 \dots 6$

if particle  $i$  belongs to the cluster  $A_1(A_2)$ .

In eq. (2.7), the quantity  $L$  results from a partial wave expansion with respect to the vector  $\tilde{s}$ . The clusters  ${}^5\text{He}$  ( ${}^5\text{Li}$ ) carry an intrinsic orbital angular momentum  $l = 1$  corresponding to a proton (neutron) in a p-orbit. The total orbital angular momentum  $\mathcal{L}$  (resulting from a coupling of  $L$  and  $l$ ) and the spin  $I$  are coupled to the total angular momentum  $\mathcal{J}$  and its 3-component  $M$ .

## 2.2 Model Hamiltonian

The model Hamiltonian is taken as

$$H = T - T_{CM} + V \quad (2.9a)$$

The operator of the kinetic energy

$$\begin{aligned} T &= \sum_{i=1}^A t_i; \\ t_i &= -(\hbar^2/2m_i) \nabla_i^2 \approx -(\hbar^2/2m) \nabla_i^2 \end{aligned} \quad (2.9b)$$

is approximated by using an averaged nucleon mass

$$m = [Z m_p + (A - Z) m_n]/A \quad (2.9c)$$

where  $Z$  stands for the number of protons while  $m_p$  and  $m_n$  are the masses of the proton and the neutron, respectively. The kinetic energy of the center-of-mass motion is denoted by  $T_{CM}$ .

The two-nucleon interaction  $V$  consists of a central (C), a spin-orbit (LS) and a tensor (T) part.

$$V = \sum_{i < j} (V_{ij}^{(C)} + V_{ij}^{(LS)} + V_{ij}^{(T)}) \quad (2.10a)$$

The radial dependence of each part is approximated by a sum of Gaussians<sup>7)</sup>.

$$V_{ij}^{(C)} = \sum_K (\omega_K^{(C)} + m_K^{(C)} P^{(M)} + b_K^{(C)} P^{(B)} + h_K^{(C)} P^{(H)}) V_K^{(C)} \exp(-\alpha_K^{(C)} x_{ij}^2/2) \quad (2.10b)$$

$$\begin{aligned} V_{ij}^{(LS)} &= \sum_K (\omega_K^{(LS)} + m_K^{(LS)} P^{(H)}) V_K^{(LS)} \exp(-\alpha_K^{(LS)} x_{ij}^2/2) \\ &\times [(x_i - x_j) \times (p_i - p_j)] \cdot (\xi_i + \xi_j) \hbar/2 \end{aligned} \quad (2.10c)$$

$$V_{ij}^{(T)} = \sum_k (m_k^{(T)} + m_k^{(T)} P^{(M)}) V_k^{(T)} x_{ij}^2 \exp(-\alpha_k^{(T)} x_{ij}^2/2) * \{ 3 [\xi_i \cdot (\tilde{x}_i - \tilde{x}_j)] [\xi_j \cdot (\tilde{x}_i - \tilde{x}_j)] x_{ij}^{-2} - \xi_i \cdot \xi_j \} \quad (2.10d)$$

$$\text{where } x_{ij} = | \tilde{x}_i - \tilde{x}_j |$$

The operator  $\xi_i$  and the matrix vector  $\xi_i$  denote the momentum and the three Pauli matrices of particle  $i$ , respectively. The exchange operators of space, spin and isospin are denoted by  $P^{(M)}$ ,  $P^{(B)}$  and  $P^{(H)}$ .

In order to test the validity of a nuclear model it is useful to calculate also elastic and inelastic form factors for electron scattering and compare them with the data. The elastic scattering of electrons from  ${}^6\text{Li}$  is mainly determined<sup>8)</sup> by the longitudinal C0 interaction. For inelastic scattering, whereby the nucleus  ${}^6\text{Li}$  is excited from its ground state ( $J_i^\pi = 1^+$ ) to the first excited state ( $J_f^\pi = 3^+$ ), the main contribution to the cross section comes from the longitudinal C2 interaction. This leads to the consideration of the charge multipole operator<sup>5)</sup>

$$M(c\lambda\mu q) = (4\pi i^\lambda)^{-1} \int d\hat{q} O(q) Y_{\lambda\mu}(\hat{q}) \quad (2.11a)$$

with

$$O(q) = \sum_{j=1}^A e_j \exp(iq \cdot \tilde{x}_j) \quad (2.11b)$$

and  $e_j = 1(0)$  for a proton (neutron). The vector  $\tilde{q}$  has the meaning of the momentum transferred from the electron to the nucleus.

In the following sections, we shall show in detail how matrix elements of the operators  $H$  and  $O(q)$  between many-body wave functions of the GC-type may be calculated utilizing the algebraic programming system REDUCE. The problem of solving the Schrödinger

equation with the Hamiltonian (2.9) in the subspace spanned by the function (2.7) and the calculation of charge form factors will be discussed elsewhere<sup>9)</sup>.

### 3. SINGLE-PARTICLE MATRIX ELEMENTS

#### 3.1 Overlap Matrix Elements

The overlap of two single-particle states (2.1) is the product of an orbital and a spin-isospin matrix element

$$\begin{aligned} & \langle \psi_{v\tau}(n'l'ms_i) | \psi_{v'\tau'}(n'l'm's'_{k'}) \rangle \\ &= \langle \varphi(n'l'ms_i) | \varphi(n'l'm's'_{k'}) \rangle \delta_{vv'} \delta_{\tau\tau'} \end{aligned} \quad (3.1)$$

The orbital overlap of two states with  $n = l = m = 0$  is given by

$$\begin{aligned} \langle \varphi(s_i) | \varphi(s'_{k'}) \rangle &= \exp[-\frac{\beta}{4}(s_i - s'_{k'})^2] \\ &= \exp[-\frac{1}{2}(y_i - y'_{k'})^2] \end{aligned} \quad (3.2)$$

Overlap matrix elements containing particles in p-waves may be obtained from eq. (3.2) by using eq. (2.3b)

$$\begin{aligned} & \langle \varphi(s_i) | \varphi(1m's'_{k'}) \rangle \\ &= \nabla_{m'}(y'_{k'}) \langle \varphi(s_i) | \varphi(s'_{k'}) \rangle \\ &= (y_i - y'_{k'})_{m'} \langle \varphi(s_i) | \varphi(s'_{k'}) \rangle \end{aligned} \quad (3.3a)$$

$$\begin{aligned} & \langle \varphi(1m's_i) | \varphi(s'_{k'}) \rangle \\ &= \nabla_m^*(y_i) \langle \varphi(s_i) | \varphi(s'_{k'}) \rangle \\ &= -(y'_i - y'_{k'})^* \langle \varphi(s_i) | \varphi(s'_{k'}) \rangle \end{aligned} \quad (3.3b)$$

$$\begin{aligned} & \langle \varphi(1m\tilde{s}_i) | \varphi(1m'\tilde{s}'_k) \rangle \\ &= - \partial/\partial(y'_{ik})^*_{m'} (y_i - y'_{ik})^*_{m'} \langle \varphi(s_i) | \varphi(s'_k) \rangle \\ &= [\delta_{mm'} - (y_i - y'_{ik})^*_{m'} (y_i - y'_{ik})_{m'}] \langle \varphi(s_i) | \varphi(s'_k) \rangle \end{aligned} \tag{3.3c}$$

In eqs. (3.3), the spherical component  $m$  of the vector  $\tilde{y}_i$  is denoted by  $(y_i)_m$ .

To have a simple example, we shall now demonstrate how the above calculation, i.e. the derivation of eq. (3.3c) may be done using REDUCE. Let us emphasize that we want to retain the analytic dependence of all matrix elements on the magnetic quantum numbers  $m$  and  $m'$ . In the later development of calculating many-body matrix elements (section 5), we shall see how this information may be kept, thus allowing to perform analytically all summations over magnetic quantum numbers which arise in projecting angular momentum<sup>5)</sup>.

The s-wave overlap (3.2), being an exponential function, remains the same in all expressions obtained by differentiation with respect to  $\chi$  or  $\chi'$  and therefore need not be kept explicitly at this stage of calculation. In the REDUCE program we define the operators  $YL$ ,  $YLC$ ,  $YR$ ,  $YRC$ ,  $KRON$ ,  $PHASE$ ,  $LL$ , and  $LR$  with the following meaning

$$\begin{aligned} YL(I,ML) &= (y_i)_m \\ YLC(I,ML) &= (y_i)^*_m = (y_i)_{-m} (-)^m \\ YR(K,MR) &= (y'_k)_m \\ YRC(K,MR) &= (y'_k)^*_m = (y'_k)_{-m} (-)^{m'} \\ KRON(ML,MR) &= \delta_{m,m'} \\ PHASE(ML) &= (-)^m \\ LL(I) &= l_i \\ LR(I) &= l'_i \end{aligned}$$

where  $l_i$  ( $l_i = 0, 1$  here) is the orbital angular momentum of particle  $i$ . In this section, we keep the particle indices  $i, j, k$  and  $l$  as symbolic variables (SCALARS in REDUCE), the reason being just a pedagogical one. The REDUCE program then reads:

```
COMMENT REDUCE PROGRAM 1
-----
THE PROCEDURE NORM(I,K) CALCULATES THE SINGLE-PARTICLE
NORMALIZATION MATRIX ELEMENTS (EQ.(3.3)) SUPPRESSING
THE S-WAVE MATRIX ELEMENT. THE DIFFERENTIATION RULES
OF THE EXPONENTIAL FUNCTION (EQS.(3.3A,3.3B)) ARE
IMPLEMENTED. $

OPERATOR YL, YLC, YR, YRC, KRON, PHASE, LL, LR$

COMMENT SPECIFICATION OF THE OPERATOR PHASE$

FOR ALL ML, MR MATCH
PHASE(ML)*PHASE(ML)=1,
PHASE(ML)*PHASE(MR)*KRON(-ML,-MR)=KRON(ML,MR)$

COMMENT
DIFFERENTIATION RULES FOR SPHERICAL VECTOR COMPONENTS$

FOR ALL ML, MR, I, J LET
DF(YL(I,ML),YL(J,MR))=0,
DF(YR(I,ML),YR(J,MR))=0,
DF(YL(I,ML),YR(J,MR))=0,
DF(YR(I,ML),YL(J,MR))=0,
DF(PHASE(ML),YL(I,MR))=0,
DF(PHASE(ML),YR(I,MR))=0$

FOR ALL ML, MR LET
DF(YL(I,ML),YL(I,MR))=KRON(ML,MR),
DF(YR(I,ML),YR(I,MR))=KRON(ML,MR),
DF(YL(K,ML),YL(K,MR))=KRON(ML,MR),
DF(YR(K,ML),YR(K,MR))=KRON(ML,MR)$

PROCEDURE NORM(I,K)$
BEGIN
R:=IF LL(I)=1 THEN (-YL(I,-ML)+YR(K,-ML))*PHASE(ML) ELSE 1$
IF LR(K)=1 THEN R:=R*(YL(I,MR)-YR(K,MR))
+DF(R,YR(K,-MR))*PHASE(MR)$
RETURN R$
END NORM$
```

```
COMMENT SPECIFICATION OF THE ORBITAL ANGULAR MOMENTUM OF
PARTICLES I ON THE LEFTHAND(L) AND K ON THE Righthand(R)
SIDE OF THE MATRIX ELEMENT$  
LET LL(I)=0,LR(K)=0$  
Z:=NORM(I,K);  
Z := 1  
  
LET LL(I)=0,LR(K)=1$  
Z:=NORM(I,K);  
Z := - YR(K,MR) + YL(I,MR)  
  
LET LL(I)=1,LR(K)=0$  
Z:=NORM(I,K);  
Z := PHASE(ML)*(YR(K,-ML) - YL(I,-ML))  
  
COMMENT  
TO SIMPLIFY COMPARISON WITH EQS.(3.3) WE INTRODUCE  
THE COMPLEX CONJUGATE VECTORS YLC AND YRC$  
FOR ALL ML, I MATCH  
YL(I,-ML)*PHASE(ML)=YLC(I,ML),  
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$  
  
Z:=Z;  
Z := - YLC(I,ML) + YRC(K,ML)  
  
FOR ALL ML, I CLEAR  
YL(I,-ML)*PHASE(ML),  
YR(I,-ML)*PHASE(ML)$  
  
ON LIST$  
LET LL(I)=1,LR(K)=1$  
  
Z:=NORM(I,K)$  
FOR ALL ML, I MATCH  
YL(I,-ML)*PHASE(ML)=YLC(I,ML),  
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$  
Z:=Z;  
Z := KRON(ML,MR)  
    + YLC(I,ML)*YR(K,MR)  
    - YLC(I,ML)*YL(I,MR)  
    - YRC(K,ML)*YR(K,MR)  
    + YRC(K,ML)*YL(I,MR)  
END$
```

### 3.2 Kinetic-Energy Matrix Elements

The kinetic-energy operator (2.9b) has the following single-particle matrix elements

$$\begin{aligned}
 & \langle \varphi(\tilde{s}_i) | t | \varphi(\tilde{s}'_k) \rangle \\
 &= (\hbar^2 \beta / 4m) \left[ 3 - \frac{\beta}{2} (\tilde{s}_i - \tilde{s}'_k)^2 \right] \langle \varphi(\tilde{s}_i) | \varphi(\tilde{s}'_k) \rangle \\
 &= \left[ \frac{3\hbar^2 \beta}{4m} + \frac{\hbar^2 \beta^2}{2m} \frac{d}{d\beta} \right] \langle \varphi(\tilde{s}_i) | \varphi(\tilde{s}'_k) \rangle
 \end{aligned} \tag{3.4a}$$

$$\begin{aligned}
 & \langle \varphi(\tilde{s}_i) | t | \varphi(1m \tilde{s}'_k) \rangle \\
 &= \left[ \frac{4\hbar^2 \beta}{4m} + \frac{\hbar^2 \beta^2}{2m} \frac{d}{d\beta} \right] \langle \varphi(\tilde{s}_i) | \varphi(1m \tilde{s}'_k) \rangle
 \end{aligned} \tag{3.4b}$$

$$\begin{aligned}
 & \langle \varphi(1m \tilde{s}_i) | t | \varphi(\tilde{s}'_k) \rangle \\
 &= \left[ \frac{4\hbar^2 \beta}{4m} + \frac{\hbar^2 \beta^2}{2m} \frac{d}{d\beta} \right] \langle \varphi(1m \tilde{s}_i) | \varphi(\tilde{s}'_k) \rangle
 \end{aligned} \tag{3.4c}$$

$$\begin{aligned}
 & \langle \varphi(1m \tilde{s}_i) | t | \varphi(1m \tilde{s}'_k) \rangle \\
 &= \left[ \frac{5\hbar^2 \beta}{4m} + \frac{\hbar^2 \beta^2}{2m} \frac{d}{d\beta} \right] \langle \varphi(1m \tilde{s}_i) | \varphi(1m \tilde{s}'_k) \rangle
 \end{aligned} \tag{3.4d}$$

We notice that matrix elements of the kinetic-energy operator may be obtained from the corresponding normalization matrix elements by differentiation with respect to the oscillator parameter  $\beta$  and adding an extra term  $(3+n_p)\hbar^2 \beta / 4m$  depending on the total number  $n_p$  of p-waves.

In section 5 we show that a similar relation also holds for many-body matrix elements. We therefore need not bother about the explicit calculation of the matrix elements (3.4) by REDUCE.

### 3.3 Matrix Elements of the Charge Multipole Operator

Matrix elements of the charge multipole operator  $M(c\lambda\mu q)$ , eq. (2.11a) may be obtained from those of the operator  $O(q)$ , eq. (2.11b). The s-wave single-particle matrix element of  $O(q)$  is

$$\begin{aligned} & \langle \varphi(\tilde{s}_i) | \exp(iq \cdot \tilde{x}) | \varphi(\tilde{s}'_k) \rangle \\ &= \exp\left[\frac{i}{2} \tilde{P} \cdot (\tilde{y}_i + \tilde{y}'_k) - \frac{q^2}{4\beta}\right] \langle \varphi(\tilde{s}_i) | \varphi(\tilde{s}'_k) \rangle \end{aligned} \quad (3.5a)$$

where we introduced the dimensionless vector  $\tilde{p} = (2/\beta)^{1/2} q$ . Matrix elements containing p-waves are calculated by REDUCE after implementing the differentiation rules

$$\begin{aligned} & \langle \varphi(\tilde{s}_i) | \exp(iq \cdot \tilde{x}) | \varphi(1m\tilde{s}'_k) \rangle \\ &= \nabla_{m1}(\tilde{y}'_k) \langle \varphi(\tilde{s}_i) | \exp(iq \cdot \tilde{x}) | \varphi(\tilde{s}'_k) \rangle \\ &= \left[ \frac{i}{2} \tilde{P} + (\tilde{y}_i - \tilde{y}'_k) \right]_{m1} \langle \varphi(\tilde{s}_i) | \exp(iq \cdot \tilde{x}) | \varphi(\tilde{s}'_k) \rangle \end{aligned} \quad (3.5b)$$

and

$$\begin{aligned} & \langle \varphi(1m\tilde{s}_i) | \exp(iq \cdot \tilde{x}) | \varphi(\tilde{s}'_k) \rangle \\ &= \nabla_m^*(\tilde{y}_i) \langle \varphi(\tilde{s}_i) | \exp(iq \cdot \tilde{x}) | \varphi(\tilde{s}'_k) \rangle \\ &= \left[ \frac{i}{2} \tilde{P} - (\tilde{y}_i - \tilde{y}'_k) \right]_m^* \langle \varphi(\tilde{s}_i) | \exp(iq \cdot \tilde{x}) | \varphi(\tilde{s}'_k) \rangle \end{aligned} \quad (3.5c)$$

The expressions on the right hand side of eqs. (3.5b) and (3.5c) contain the imaginary unit  $i$  which is one the reserved variables in REDUCE. The system replaces all powers of  $i$  by the appropriate combination of  $(-1)$  and  $i$ . In the following REDUCE program this happens in the last example when there are two p-waves.

COMMENT REDUCE PROGRAM 2

-----  
THE PROCEDURE FORM(I,K) CALCULATES THE SINGLE-PARTICLE  
MATRIX ELEMENTS OF THE OPERATOR O, EQ.(2.11B) SUPPRESSING  
THE S-WAVE MATRIX ELEMENT.  
THE DIFFERENTIATION RULES OF THE EXPONENTIAL FUNCTION  
(EQS.(3.5B,3.5C)) ARE IMPLEMENTED.\$

OPERATOR YL,YLC,YR,YRC,KRON,PHASE,LL,LR,P,PC\$  
OFF ALLFAC\$  
ON DIV\$

. . . . .  
COMMENT

THE SPECIFICATION OF THE OPERATOR PHASE AND THE  
DIFFERENTIATION RULES FOR SPHERICAL VECTOR COMPONENTS  
ARE THE SAME AS IN THE REDUCE PROGRAM 1 AND ARE  
SUPPRESSED IN THIS LISTING FOR BREVITY.\$

. . . . .  
PROCEDURE FORM(I,K)\$  
BEGIN  
R:=IF LL(I)=1  
  THEN (I\*P(-ML)/2-YL(I,-ML)+YR(K,-ML))\*PHASE(ML) ELSE 1\$  
IF LR(K)=1 THEN R:=R\*(I\*P(MR)/2+YL(I,MR)-YR(K,MR))  
  +DF(R,YR(K,-MR))\*PHASE(MR) \$  
RETURN R\$  
END FORM\$

LET LL(I)=0,LR(K)=1\$  
Z:=FORM(I,K);  
Z := 1/2\*I\*P(MR) - YR(K,MR) + YL(I,MR)

LET LL(I)=1,LR(K)=0\$  
Z:=FORM(I,K)\$  
FOR ALL ML,I MATCH  
YL(I,-ML)\*PHASE(ML)=YLC(I,ML),  
YR(I,-ML)\*PHASE(ML)=YRC(I,ML),  
P(-ML)\*PHASE(ML)=PC(ML)\$

Z:=Z;  
Z := 1/2\*I\*PC(ML) - YLC(I,ML) + YRC(K,ML)

FOR ALL ML,I CLEAR  
YL(I,-ML)\*PHASE(ML),  
YR(I,-ML)\*PHASE(ML),  
P(-ML)\*PHASE(ML)\$

ON LIST\$

LET LL(I)=1,LR(K)=1\$  
Z:=FORM(I,K)\$

```
FOR ALL ML,I MATCH
YL(I,-ML)*PHASE(ML)=YLC(I,ML),
YR(I,-ML)*PHASE(ML)=YRC(I,ML),
P(-ML)*PHASE(ML)=PC(ML)$
```

```
Z:=Z;
```

```
Z :=
```

```
- 1/2*I*YLC(I,ML)*P(MR)
+ 1/2*I*YRC(K,ML)*P(MR)
- 1/2*I*PC(ML)*YR(K,MR)
+ 1/2*I*PC(ML)*YL(I,MR)
+ KRON(ML,MR)
+ YLC(I,ML)*YR(K,MR)
- YLC(I,ML)*YL(I,MR)
- YRC(K,ML)*YR(K,MR)
+ YRC(K,ML)*YL(I,MR)
- 1/4*PC(ML)*P(MR)
```

```
END$
```

#### 4. TWO-PARTICLE MATRIX ELEMENTS

In this section, we calculate two-particle matrix elements of the phenomenological two-body interaction specified in section 2.2. The wave functions are those described in section 2.1. For computational ease, a Gaussian dependence of the interaction on the interparticle distance is adopted.

As in the previous cases, we shall follow our "canonical" procedure of first calculating by hand matrix elements with s-waves only and then writing a REDUCE program based on simple differentiation rules for those matrix elements which contain also particles in p-orbits.

##### 4.1 Matrix Elements of the Central Interaction

The spatial part of matrix elements  $V_{ijkl}$  of a central interaction with a Gaussian dependence on the interparticle distance

$$x_{12} = | \underline{x}_1 - \underline{x}_2 |$$

$$\mathcal{J}(x_{12}) = \exp(-\alpha x_{12}^2/2) \quad (4.1)$$

between s-wave single-particle functions is given by<sup>3)</sup>

$$\begin{aligned} & \int d\underline{x}_1 d\underline{x}_2 \varphi(\underline{x}_1 - \underline{s}_i) \varphi(\underline{x}_2 - \underline{s}_j) \mathcal{J}(x_{12}) \varphi(\underline{x}_1 - \underline{s}'_k) \varphi(\underline{x}_2 - \underline{s}'_l) \\ &= \left( \frac{\beta}{\alpha + \beta} \right)^{3/2} \exp \left[ -\frac{\delta}{2} (y_i - y_j + y'_k - y'_l)^2 \right. \\ & \quad \left. - \frac{1}{2} (y_i - y'_k)^2 - \frac{1}{2} (y_j - y'_l)^2 \right] \end{aligned} \quad (4.2a)$$

where  $\delta = \frac{\alpha}{2(\alpha + \beta)}$

In writing a REDUCE program for two-body matrix elements with particles in orbits with  $l > 0$  we have to implement the following

differentiation rules

$$\begin{aligned} \nabla_{m_1} (\tilde{y}'_{k(e)}) \exp \left[ -\frac{\delta}{2} (\tilde{y}_i - \tilde{y}_j + \tilde{y}'_k - \tilde{y}'_e)^2 \right. \\ \left. - \frac{1}{2} (\tilde{y}_i - \tilde{y}'_k)^2 - \frac{1}{2} (\tilde{y}_j - \tilde{y}'_e)^2 \right] \\ = \left[ (+) \delta(\tilde{y}_i - \tilde{y}_j + \tilde{y}'_k - \tilde{y}'_e) + (\tilde{y}_{i(j)} - \tilde{y}'_{k(e)}) \right]_{m_1} \exp [ ] \end{aligned} \quad (4.2b)$$

and

$$\begin{aligned} \nabla_m^* (\tilde{y}_{i(j)}) \exp [ ] \\ = \left[ (+) \delta(\tilde{y}_i - \tilde{y}_j + \tilde{y}'_k - \tilde{y}'_e) - (\tilde{y}_{i(j)} - \tilde{y}'_{k(e)}) \right]_m^* \exp [ ] \end{aligned} \quad (4.2c)$$

COMMENT REDUCE PROGRAM 3

-----  
THE PROCEDURE POT(I,J,K,L) CALCULATES THE SPATIAL PART  
OF THE TWO-BODY MATRIX ELEMENT OF A GAUSSIAN CENTRAL  
INTERACTION, EQ.(4.2), SUPPRESSING THE S-WAVE MATRIX  
ELEMENT. IT IS ASSUMED THAT AT MOST ONE OF THE  
PARTICLES OF EACH PAIR (I,J) AND (K,L) OCCUPIES A  
P-WAVE ORBIT WITH MAGNETIC QUANTUM NUMBERS ML AND MR.  
THE DIFFERENTIATION RULES FOR THE EXPONENTIAL  
FUNCTIONS, Eqs.(4.2B) AND (4.2C), ARE IMPLEMENTED.\$

OPERATOR YL, YLC, YR, YRC, KRON, PHASE, LL, LR\$  
OFF NAT\$  
ON LIST\$

.....  
COMMENT  
THE SPECIFICATION OF THE OPERATOR PHASE IS THE SAME  
AS IN THE REDUCE PROGRAM 1\$  
.....

COMMENT  
DIFFERENTIATION RULE FOR SPHERICAL VECTOR COMPONENTS\$

FOR ALL ML,MR,I,J LET  
DF(YL(I,ML),YL(J,MR))=0,  
DF(YR(I,ML),YR(J,MR))=0,  
DF(YL(I,ML),YR(J,MR))=0,  
DF(YR(I,ML),YL(J,MR))=0\$

```
FOR ALL ML,MR LET
DF(YL(I,ML),YL(I,MR))=KRON(ML,MR),
DF(YR(I,ML),YR(I,MR))=KRON(ML,MR),
DF(YL(J,ML),YL(J,MR))=KRON(ML,MR),
DF(YR(J,ML),YR(J,MR))=KRON(ML,MR),
DF(YL(K,ML),YL(K,MR))=KRON(ML,MR),
DF(YR(K,ML),YR(K,MR))=KRON(ML,MR),
DF(YL(L,ML),YL(L,MR))=KRON(ML,MR),
DF(YR(L,ML),YR(L,MR))=KRON(ML,MR)$

FOR ALL ML,MR,M,I LET
DF(KRON(ML,MR),YL(I,M))=0,
DF(KRON(ML,MR),YR(I,M))=0,
DF(PHASE(ML),YL(I,M))=0,
DF(PHASE(ML),YR(I,M))=0$

PROCEDURE POT(I,J,K,L)$
BEGIN
R:=1$
IF LL(I)=1 THEN
R:=R*PHASE(ML)*(-DELTA*(YL(I,-ML)-YL(J,-ML)+YR(K,-ML)
-YR(L,-ML))-(YL(I,-ML)-YR(K,-ML)))+DF(R,YL(I,ML))$
IF LL(J)=1 THEN
R:=R*PHASE(ML)*( DELTA*(YL(I,-ML)-YL(J,-ML)+YR(K,-ML)
-YR(L,-ML))-(YL(J,-ML)-YR(L,-ML)))+DF(R,YL(J,ML))$
IF LR(K)=1 THEN
R:=R*(-DELTA*(YL(I, MR)-YL(J, MR)+YR(K, MR)-YR(L, MR))
+(YL(I, MR)-YR(K, MR)))+DF(R,YR(K,-MR))*PHASE(MR)$
IF LR(L)=1 THEN
R:=R*( DELTA*(YL(I, MR)-YL(J, MR)+YR(K, MR)-YR(L, MR))
+(YL(J, MR)-YR(L, MR)))+DF(R,YR(L,-MR))*PHASE(MR)$
RETURN R$
END POT$

LET LL(I)=1,LL(J)=0,LR(K)=0,LR(L)=0$
Z:=POT(I,J,K,L)$

FOR ALL ML,I MATCH
YL(I,-ML)*PHASE(ML)=YLC(I,ML),
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$

Z:=Z;
Z :=
- YLC(I,ML)*DELTA
- YLC(I,ML)
+ YLC(J,ML)*DELTA
- YRC(K,ML)*DELTA
+ YRC(K,ML)
+ YRC(L,ML)*DELTA$

FOR ALL ML,I CLEAR
YL(I,-ML)*PHASE(ML),
YR(I,-ML)*PHASE(ML)$

LET LL(I)=0,LL(J)=0,LR(K)=1,LR(L)=0$
```

```
Z:=POT(I,J,K,L);
Z := YR(L,MR)*DELTA
- YR(K,MR)*DELTA
- YR(K,MR)
+ YL(J,MR)*DELTA
- YL(I,MR)*DELTA
+ YL(I,MR)$

FOR ALL ML,I CLEAR
YL(I,-ML)*PHASE(ML),
YR(I,-ML)*PHASE(ML)$

LET LL(I)=1,LL(J)=0,LR(K)=1,LR(L)=0$
Z:=POT(I,J,K,L)$

FOR ALL ML,I MATCH
YL(I,-ML)*PHASE(ML)=YLC(I,ML),
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$

Z:=Z;
Z :=
- KRON(ML,MR)*DELTA
+ KRON(ML,MR)
- YR(L,MR)*YLC(I,ML)*DELTA**2
- YR(L,MR)*YLC(I,ML)*DELTA
+ YR(L,MR)*YLC(J,ML)*DELTA**2
- YR(L,MR)*YRC(K,ML)*DELTA**2
+ YR(L,MR)*YRC(K,ML)*DELTA
+ YR(L,MR)*YRC(L,ML)*DELTA**2
+ YR(K,MR)*YLC(I,ML)*DELTA**2
+ 2*YR(K,MR)*YLC(I,ML)*DELTA
+ YR(K,MR)*YLC(I,ML)
- YR(K,MR)*YLC(J,ML)*DELTA**2
- YR(K,MR)*YLC(J,ML)*DELTA
+ YR(K,MR)*YRC(K,ML)*DELTA**2
- YR(K,MR)*YRC(K,ML)
- YR(K,MR)*YRC(L,ML)*DELTA**2
- YR(K,MR)*YRC(L,ML)*DELTA
- YL(J,MR)*YLC(I,ML)*DELTA**2
- YL(J,MR)*YLC(I,ML)*DELTA
+ YL(J,MR)*YLC(J,ML)*DELTA**2
- YL(J,MR)*YRC(K,ML)*DELTA**2
+ YL(J,MR)*YRC(K,ML)*DELTA
+ YL(J,MR)*YRC(L,ML)*DELTA**2
+ YL(I,MR)*YLC(I,ML)*DELTA**2
- YL(I,MR)*YLC(I,ML)
- YL(I,MR)*YLC(J,ML)*DELTA**2
+ YL(I,MR)*YLC(J,ML)*DELTA
+ YL(I,MR)*YRC(K,ML)*DELTA**2
- 2*YL(I,MR)*YRC(K,ML)*DELTA
+ YL(I,MR)*YRC(K,ML)
- YL(I,MR)*YRC(L,ML)*DELTA**2
+ YL(I,MR)*YRC(L,ML)*DELTA$
```

END\$

#### 4.2 Matrix Elements of the Spin-Orbit Interaction

We use a spherical representation<sup>10)</sup> and write the spin-orbit interaction (2.10c) as the scalar product of two spherical tensors

$$\mathcal{J}(x_{12}) \sum_m (-)^m L_{12}(1m) S_{12}(1-m) \quad (4.3a)$$

where

$$S_{12} = (\vec{s}_1 + \vec{s}_2) \hbar/2 \quad (4.3b)$$

is the total spin angular momentum of particles 1 and 2  
and

$$\vec{L}_{12} = -i\hbar (\vec{x}_1 - \vec{x}_2) \times (\vec{\nabla}_1 - \vec{\nabla}_2) \quad (4.3c)$$

is the relative orbital angular momentum of particles 1 and 2.

Reduced matrix elements of the spin tensor (4.3b) are given by<sup>11)</sup>

$$\langle I \parallel S(1) \parallel I' \rangle = \delta_{II'} \hbar [(2I+1)(I+1)I]^{1/2}$$

exhibiting the fact that the spin-orbit interaction acts only between triplet spin states ( $I = 1$ ), i.e.

$$\langle I=1 \parallel S(1) \parallel I=1 \rangle = \hbar \sqrt{6}$$

Matrix elements of the spatial tensor  $J(x_{12}) \vec{L}_{12}$  between harmonic oscillator s-wave functions (2.3a) read

$$\begin{aligned} & \int d\vec{x}_1 d\vec{x}_2 \varphi(\vec{x}_1 - \vec{s}_i) \varphi(\vec{x}_2 - \vec{s}_j) \mathcal{J}(x_{12}) \vec{L}_{12} \varphi(\vec{x}_1 - \vec{s}'_k) \varphi(\vec{x}_2 - \vec{s}'_l) \\ &= -i\hbar \left( \frac{\beta}{\alpha + \beta} \right)^{5/2} (\vec{y}_i - \vec{y}_j) \times (\vec{y}'_k - \vec{y}'_l) \\ & \quad * \exp \left[ -\frac{\delta}{2} (\vec{y}_i - \vec{y}_j + \vec{y}'_k - \vec{y}'_l)^2 \right. \\ & \quad \left. - \frac{1}{2} (\vec{y}_i - \vec{y}'_k)^2 - \frac{1}{2} (\vec{y}_j - \vec{y}'_l)^2 \right] \end{aligned} \quad (4.4)$$

In a spherical representation <sup>11)</sup> we get

$$\begin{aligned} & \int d\tilde{x}_1 d\tilde{x}_2 \varphi(\tilde{x}_1 - \tilde{s}_i) \varphi(\tilde{x}_2 - \tilde{s}_j) J(x_{12}) L_{12}(1\mu) \varphi(\tilde{x}_1 - \tilde{s}'_k) \varphi(\tilde{x}_2 - \tilde{s}'_l) \\ & = \hbar \sqrt{2} \left( \frac{\beta}{\alpha + \beta} \right)^{5/2} \sum_{m_1 m_2} (1m_1 1m_2 | 1\mu) (\tilde{y}_i - \tilde{y}_j)_{m_1} (\tilde{y}'_k - \tilde{y}'_l)_{m_2} \exp [ ] \end{aligned} \quad (4.5)$$

In order to calculate matrix elements with particles in  $l > 0$  orbits, we use again the property (2.3). The differentiations now include also the factor  $(\tilde{y}_i - \tilde{y}_j)_{m_1} (\tilde{y}'_k - \tilde{y}'_l)_{m_2}$  multiplying the exponential function. In the REDUCE program <sup>3</sup>, we simply replace the statement  $R := 1$  by

$$R := (\tilde{y}_i - \tilde{y}_j)_{m_1} (\tilde{y}'_k - \tilde{y}'_l)_{m_2}$$

The summation over the magnetic quantum numbers  $m_1$  and  $m_2$  (after multiplication by the Clebsch-Gordan coefficient  $(1m_1, 1m_2 | 1\mu)$ ) is not carried out at this level of the calculation. Treating  $m_1$  and  $m_2$  as SCALAR variables enables us to postpone this summation until the numerical processing in a FORTRAN program (see section 6).

COMMENT REDUCE PROGRAM 4

-----  
THE PROCEDURE GPOT(OPT,I,J,K,L) CALCULATES THE SPATIAL PART OF TWO-BODY MATRIX ELEMENTS OF A GAUSSIAN CENTRAL (OPT=1, EQ.(4.2)) AND A SPIN-ORBIT (OPT=2, EQ.(4.5)) INTERACTION SUPPRESSING THE S-WAVE MATRIX ELEMENT.\$

OPERATOR YL,YLC,YR,YRC,KRON,PHASE,LL,LR\$  
OFF NAT\$  
ON LIST\$

COMMENT

THE SPECIFICATION OF THE OPERATOR PHASE AND THE DIFFERENTIATION RULES FOR THE SPHERICAL VECTOR COMPONENTS ARE THE SAME AS IN THE REDUCE PROGRAM 3 AND ARE SUPPRESSED HERE FOR BREVITY.\$

```
PROCEDURE GPOT(OPT,I,J,K,L)$
BEGIN
R:=1$
IF OPT=2 THEN R:=(YL(I,M1)-YL(J,M1))*(YR(K,M2)-YR(L,M2))$
IF LL(I)=1 THEN
R:=R*PHASE(ML)*(-DELTA*(YL(I,-ML)-YL(J,-ML)+YR(K,-ML)
-YR(L,-ML))-(YL(I,-ML)-YR(K,-ML)))+DF(R,YL(I,ML))$
IF LL(J)=1 THEN
R:=R*PHASE(ML)*( DELTA*(YL(I,-ML)-YL(J,-ML)+YR(K,-ML)
-YR(L,-ML))-(YL(J,-ML)-YR(L,-ML)))+DF(R,YL(J,ML))$
IF LR(K)=1 THEN
R:=R*(-DELTA*(YL(I, MR)-YL(J, MR)+YR(K, MR)-YR(L, MR))
+(YL(I, MR)-YR(K, MR)))+DF(R,YR(K,-MR))*PHASE(MR)$
IF LR(L)=1 THEN
R:=R*( DELTA*(YL(I, MR)-YL(J, MR)+YR(K, MR)-YR(L, MR))
+(YL(J, MR)-YR(L, MR)))+DF(R,YR(L,-MR))*PHASE(MR)$
RETURN R$
END GPOT$

LET LL(I)=1,LL(J)=0,LR(K)=0,LR(L)=0$
Z:=GPOT(2,I,J,K,L)$

FOR ALL ML, I MATCH
YL(I,-ML)*PHASE(ML)=YLC(I,ML),
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$

Z:=Z;

Z := 
- YLC(I,ML)*YR(L,M2)*YL(J,M1)*DELTA
- YLC(I,ML)*YR(L,M2)*YL(J,M1)
+ YLC(I,ML)*YR(L,M2)*YL(I,M1)*DELTA
+ YLC(I,ML)*YR(L,M2)*YL(I,M1)
+ YLC(I,ML)*YR(K,M2)*YL(J,M1)*DELTA
+ YLC(I,ML)*YR(K,M2)*YL(J,M1)
- YLC(I,ML)*YR(K,M2)*YL(I,M1)*DELTA
- YLC(I,ML)*YR(K,M2)*YL(I,M1)
+ YLC(J,ML)*YR(L,M2)*YL(J,M1)*DELTA
- YLC(J,ML)*YR(L,M2)*YL(I,M1)*DELTA
- YLC(J,ML)*YR(K,M2)*YL(J,M1)*DELTA
+ YLC(J,ML)*YR(K,M2)*YL(I,M1)*DELTA
- YRC(K,ML)*YR(L,M2)*YL(J,M1)*DELTA
+ YRC(K,ML)*YR(L,M2)*YL(J,M1)
+ YRC(K,ML)*YR(L,M2)*YL(I,M1)*DELTA
- YRC(K,ML)*YR(L,M2)*YL(I,M1)
+ YRC(K,ML)*YR(K,M2)*YL(J,M1)*DELTA
- YRC(K,ML)*YR(K,M2)*YL(J,M1)
- YRC(K,ML)*YR(K,M2)*YL(I,M1)*DELTA
+ YRC(K,ML)*YR(K,M2)*YL(I,M1)
+ YRC(L,ML)*YR(L,M2)*YL(J,M1)*DELTA
- YRC(L,ML)*YR(L,M2)*YL(I,M1)*DELTA
- YRC(L,ML)*YR(K,M2)*YL(J,M1)*DELTA
+ YRC(L,ML)*YR(K,M2)*YL(I,M1)*DELTA
- KRON(M1,ML)*YR(L,M2)
+ KRON(M1,ML)*YR(K,M2)$
```

```
FOR ALL ML, I CLEAR
YL(I,-ML)*PHASE(ML),
YR(I,-ML)*PHASE(ML)$

LET LL(I)=0,LL(J)=0,LR(K)=1,LR(L)=0$
Z:=GPOT(2,I,J,K,L)$
FOR ALL ML, I MATCH
YL(I,-ML)*PHASE(ML)=YLC(I,ML),
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$

Z:=Z;

Z := 
- PHASE(MR)*KRON(M2, - MR)*YL(J,M1)
+ PHASE(MR)*KRON(M2, - MR)*YL(I,M1)
+ YR(L,MR)*YR(L,M2)*YL(J,M1)*DELTA
- YR(L,MR)*YR(L,M2)*YL(I,M1)*DELTA
- YR(L,MR)*YR(K,M2)*YL(J,M1)*DELTA
+ YR(L,MR)*YR(K,M2)*YL(I,M1)*DELTA
- YR(K,MR)*YR(L,M2)*YL(J,M1)*DELTA
- YR(K,MR)*YR(L,M2)*YL(J,M1)
+ YR(K,MR)*YR(L,M2)*YL(I,M1)*DELTA
+ YR(K,MR)*YR(L,M2)*YL(I,M1)
+ YR(K,MR)*YR(K,M2)*YL(J,M1)*DELTA
+ YR(K,MR)*YR(K,M2)*YL(J,M1)
- YR(K,MR)*YR(K,M2)*YL(I,M1)*DELTA
- YR(K,MR)*YR(K,M2)*YL(I,M1)
+ YL(J,MR)*YR(L,M2)*YL(J,M1)*DELTA
- YL(J,MR)*YR(L,M2)*YL(I,M1)*DELTA
- YL(J,MR)*YR(K,M2)*YL(J,M1)*DELTA
+ YL(J,MR)*YR(K,M2)*YL(I,M1)*DELTA
- YL(I,MR)*YR(L,M2)*YL(J,M1)*DELTA
+ YL(I,MR)*YR(L,M2)*YL(J,M1)
+ YL(I,MR)*YR(L,M2)*YL(I,M1)*DELTA
- YL(I,MR)*YR(L,M2)*YL(I,M1)
+ YL(I,MR)*YR(K,M2)*YL(J,M1)*DELTA
- YL(I,MR)*YR(K,M2)*YL(J,M1)
- YL(I,MR)*YR(K,M2)*YL(I,M1)*DELTA
+ YL(I,MR)*YR(K,M2)*YL(I,M1)$

FOR ALL ML, I CLEAR
YL(I,-ML)*PHASE(ML),
YR(I,-ML)*PHASE(ML)$

LET LL(I)=1,LL(J)=0,LR(K)=1,LR(L)=0$
Z:=GPOT(2,I,J,K,L)$
FOR ALL ML, I MATCH
YL(I,-ML)*PHASE(ML)=YLC(I,ML),
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$

Z:=Z;
```



- YR(K,MR)\*YLC(J,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA  
+ YR(K,MR)\*YLC(J,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
+ YR(K,MR)\*YLC(J,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA  
+ YR(K,MR)\*YLC(J,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YR(K,MR)\*YLC(J,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YR(K,MR)\*YLC(J,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
- YR(K,MR)\*YLC(J,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YR(K,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
- YR(K,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(J,M1)  
- YR(K,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(I,M1)  
- YR(K,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
+ YR(K,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(I,M1)  
- YR(K,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(J,M1)  
+ YR(K,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
- YR(K,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(I,M1)  
- YR(K,MR)\*YRC(L,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
- YR(K,MR)\*YRC(L,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA  
+ YR(K,MR)\*YRC(L,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA  
+ YR(K,MR)\*YRC(L,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YR(K,MR)\*YRC(L,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YR(K,MR)\*YRC(L,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
- YR(K,MR)\*YRC(L,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YR(K,MR)\*KRON(M1,ML)\*YR(L,M2)\*DELTA  
+ YR(K,MR)\*KRON(M1,ML)\*YR(L,M2)  
- YR(K,MR)\*KRON(M1,ML)\*YR(K,M2)\*DELTA  
- YR(K,MR)\*KRON(M1,ML)\*YR(K,M2)  
- YL(J,MR)\*YLC(I,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
- YL(J,MR)\*YLC(I,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA  
+ YL(J,MR)\*YLC(I,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
+ YL(J,MR)\*YLC(I,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA  
+ YL(J,MR)\*YLC(I,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YL(J,MR)\*YLC(I,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YL(J,MR)\*YLC(I,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
- YL(J,MR)\*YLC(I,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YL(J,MR)\*YLC(J,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
- YL(J,MR)\*YLC(J,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
- YL(J,MR)\*YLC(J,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
- YL(J,MR)\*YLC(J,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YL(J,MR)\*YLC(J,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
- YL(J,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YL(J,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA  
+ YL(J,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
- YL(J,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YL(J,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
+ YL(J,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YL(J,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA  
- YL(J,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA  
+ YL(J,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YL(J,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
- YL(J,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA  
+ YL(J,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YL(J,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
- YL(J,MR)\*YRC(K,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
- YL(J,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YL(J,MR)\*YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
- YL(J,MR)\*KRON(M1,ML)\*YR(L,M2)\*DELTA

```
+ YL(J,MR)*KRON(M1,ML)*YR(K,M2)*DELTA
+ YL(I,MR)*YLC(I,ML)*YR(L,M2)*YL(J,M1)*DELTA**2
- YL(I,MR)*YLC(I,ML)*YR(L,M2)*YL(J,M1)
- YL(I,MR)*YLC(I,ML)*YR(L,M2)*YL(I,M1)*DELTA**2
+ YL(I,MR)*YLC(I,ML)*YR(L,M2)*YL(I,M1)
- YL(I,MR)*YLC(I,ML)*YR(K,M2)*YL(J,M1)*DELTA**2
+ YL(I,MR)*YLC(I,ML)*YR(K,M2)*YL(J,M1)
+ YL(I,MR)*YLC(I,ML)*YR(K,M2)*YL(I,M1)*DELTA**2
- YL(I,MR)*YLC(I,ML)*YR(K,M2)*YL(I,M1)
- YL(I,MR)*YLC(J,ML)*YR(L,M2)*YL(J,M1)*DELTA**2
+ YL(I,MR)*YLC(J,ML)*YR(L,M2)*YL(J,M1)*DELTA
+ YL(I,MR)*YLC(J,ML)*YR(L,M2)*YL(I,M1)*DELTA**2
- YL(I,MR)*YLC(J,ML)*YR(L,M2)*YL(I,M1)*DELTA
+ YL(I,MR)*YLC(J,ML)*YR(K,M2)*YL(J,M1)*DELTA**2
- YL(I,MR)*YLC(J,ML)*YR(K,M2)*YL(J,M1)*DELTA
- YL(I,MR)*YLC(J,ML)*YR(K,M2)*YL(I,M1)*DELTA**2
+ YL(I,MR)*YLC(J,ML)*YR(K,M2)*YL(I,M1)*DELTA
+ YL(I,MR)*YRC(K,ML)*YR(L,M2)*YL(J,M1)*DELTA**2
- 2*YL(I,MR)*YRC(K,ML)*YR(L,M2)*YL(J,M1)*DELTA
+ YL(I,MR)*YRC(K,ML)*YR(L,M2)*YL(J,M1)
- YL(I,MR)*YRC(K,ML)*YR(L,M2)*YL(I,M1)*DELTA**2
+ 2*YL(I,MR)*YRC(K,ML)*YR(L,M2)*YL(I,M1)*DELTA
- YL(I,MR)*YRC(K,ML)*YR(L,M2)*YL(I,M1)
- YL(I,MR)*YRC(K,ML)*YR(K,M2)*YL(J,M1)*DELTA**2
+ 2*YL(I,MR)*YRC(K,ML)*YR(K,M2)*YL(J,M1)*DELTA
- YL(I,MR)*YRC(K,ML)*YR(K,M2)*YL(J,M1)
+ YL(I,MR)*YRC(K,ML)*YR(K,M2)*YL(I,M1)*DELTA**2
- 2*YL(I,MR)*YRC(K,ML)*YR(K,M2)*YL(I,M1)*DELTA
+ YL(I,MR)*YRC(K,ML)*YR(K,M2)*YL(I,M1)
- YL(I,MR)*YRC(L,ML)*YR(L,M2)*YL(J,M1)*DELTA**2
+ YL(I,MR)*YRC(L,ML)*YR(L,M2)*YL(J,M1)*DELTA
+ YL(I,MR)*YRC(L,ML)*YR(L,M2)*YL(I,M1)*DELTA**2
- YL(I,MR)*YRC(L,ML)*YR(L,M2)*YL(I,M1)*DELTA
+ YL(I,MR)*YRC(L,ML)*YR(K,M2)*YL(J,M1)*DELTA**2
- YL(I,MR)*YRC(L,ML)*YR(K,M2)*YL(J,M1)*DELTA
- YL(I,MR)*YRC(L,ML)*YR(K,M2)*YL(I,M1)*DELTA**2
+ YL(I,MR)*YRC(L,ML)*YR(K,M2)*YL(I,M1)*DELTA
+ YL(I,MR)*KRON(M1,ML)*YR(L,M2)*DELTA
- YL(I,MR)*KRON(M1,ML)*YR(L,M2)
- YL(I,MR)*KRON(M1,ML)*YR(K,M2)*DELTA
+ YL(I,MR)*KRON(M1,ML)*YR(K,M2)
- KRON(ML,MR)*YR(L,M2)*YL(J,M1)*DELTA
+ KRON(ML,MR)*YR(L,M2)*YL(J,M1)
+ KRON(ML,MR)*YR(L,M2)*YL(I,M1)*DELTA
- KRON(ML,MR)*YR(L,M2)*YL(I,M1)
+ KRON(ML,MR)*YR(K,M2)*YL(J,M1)*DELTA
- KRON(ML,MR)*YR(K,M2)*YL(J,M1)
- KRON(ML,MR)*YR(K,M2)*YL(I,M1)*DELTA
+ KRON(ML,MR)*YR(K,M2)*YL(I,M1)$
```

END\$

#### 4.3 Matrix Elements of the Tensor Interaction

As in the previous case of the spin-orbit interaction we use a spherical representation and write the tensor interaction in the scalar product form

$$J(x_{12}) \sum_m (-)^m L_{12}(2m) S_{12}(2-m) \quad (4.6a)$$

The spin tensor

$$S_{12}(2m) = \sum_{m_1 m_2} \delta_1(1m_1) \delta_2(1m_2) (1m_1 1m_2 | 2m) \quad (4.6b)$$

is a spherical tensor of rank 2 where  $\sigma_i(1m)$  is the Pauli matrix in a spherical representation referring to particle i. The spatial tensor  $L_{12}$  is proportional to the solid spherical harmonic function of rank 2

$$L_{12}(2m) = \left(\frac{8\pi}{15}\right)^{1/2} Y_{2m}(x_1 - x_2) \quad (4.6c)$$

Reduced matrix elements of the spin tensor  $S(2m)$  are nonvanishing only between triplet spin states

$$\langle I \| S(2) \| I' \rangle = \delta_{I1} \delta_{I'1} \sqrt{20} \quad (4.7)$$

It remains to calculate matrix elements of the spatial part of the tensor interaction

$$\begin{aligned} & \int dx_1 dx_2 \varphi(x_1 - s_i) \varphi(x_2 - s_j) J(x_{12}) L_{12}(2m) \\ & * \varphi(x_1 - s'_k) \varphi(x_2 - s'_l) \\ & = \left(\frac{8\pi}{15}\right)^{1/2} \left(\frac{\beta}{\pi}\right)^3 \exp\left\{-\frac{\delta}{2} (y_i - y_j + y'_k - y'_l)^2\right. \\ & \left. - \frac{1}{2} [(y_i - y'_k)^2 + (y_j - y'_l)^2]\right\} \end{aligned}$$

$$\begin{aligned} & * \int d\tilde{\rho}_1 \exp(-2\beta\tilde{\rho}_1^2) \int d\tilde{\rho}_2 \exp\left(-\frac{\alpha+\beta}{2}\tilde{\rho}_2^2\right) \\ & * Y_{2m} \left[ \tilde{\rho}_2 + \frac{\beta}{2(\alpha+\beta)} (\tilde{s}_i - \tilde{s}_j + \tilde{s}'_k - \tilde{s}'_l) \right] \\ & = \left(\frac{8\pi}{15}\right)^{1/2} \frac{1}{2\beta} \left(\frac{\beta}{\alpha+\beta}\right)^{7/2} \exp\left\{ 3Y_{2m} (y_i - y_j + y'_k - y'_l) \right\} \end{aligned} \quad (4.8a)$$

We note that there is no tensor interaction between pairs of nucleons belonging to the same s-wave clusters, i.e.

$$\tilde{y}_i = y_j \text{ and } \tilde{y}'_k = y'_l.$$

Matrix elements containing p-waves are calculated using again eq. (2.3) together with the expansion

$$Y_{2m}(\tilde{x}) = \left(\frac{10\pi}{3}\right)^{1/2} \sum_{m_1, m_2} (1m_1, 1m_2 | 2m) Y_{1m_1}(\tilde{x}) Y_{1m_2}(\tilde{x}) \quad (4.9)$$

In the REDUCE program 5, we simply add the statement

$$R := (y_i - y_j + y'_k - y'_l)_{m_1} (y_i - y_j + y'_k - y'_l)_{m_2}$$

to the procedure GPOT under opt = 3.

COMMENT REDUCE PROGRAM 5

SAME AS REDUCE PROGRAM 4 INCLUDING TWO-BODY MATRIX ELEMENTS OF THE TENSOR INTERACTION UNDER OPT=3\$

OPERATOR YL, YLC, YR, YRC, KRON, PHASE, LL, LR\$

```
PROCEDURE GPOT(OPT,I,J,K,L)$
BEGIN
R:=1$
IF OPT=2 THEN R:=(YL(I,M1)-YL(J,M1))*(YR(K,M2)-YR(L,M2))$
IF OPT=3 THEN R:=(YL(I,M1)-YL(J,M1)+YR(K,M1)-YR(L,M1))
           *(YL(I,M2)-YL(J,M2)+YR(K,M2)-YR(L,M2))$
IF LL(I)=1 THEN
R:=R*PHASE(ML)*(-DELTA*(YL(I,-ML)-YL(J,-ML)+YR(K,-ML)
- YR(L,-ML))-(YL(I,-ML)-YR(K,-ML)))+DF(R,YL(I,ML))$
IF LL(J)=1 THEN
R:=R*PHASE(ML)*( DELTA*(YL(I,-ML)-YL(J,-ML)+YR(K,-ML)
- YR(L,-ML))-(YL(J,-ML)-YR(L,-ML)))+DF(R,YL(J,ML))$
IF LR(K)=1 THEN
R:=R*(-DELTA*(YL(I,MR)-YL(J,MR)+YR(K,MR)-YR(L,MR))
+ (YL(I,MR)-YR(K,MR)))+DF(R,YR(K,-MR))*PHASE(MR)$
IF LR(L)=1 THEN
R:=R*( DELTA*(YL(I,MR)-YL(J,MR)+YR(K,MR)-YR(L,MR))
+ (YL(J,MR)-YR(L,MR)))+DF(R,YR(L,-MR))*PHASE(MR)$
RETURN R$
END GPOT$

LET LL(I)=1,LL(J)=0,LR(K)=0,LR(L)=0$
Z:=GPOT(3,I,J,K,L)$
FOR ALL ML,I MATCH
YL(I,-ML)*PHASE(ML)=YLC(I,ML),
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$
Z:=Z;
Z :=

- YLC(I,ML)*YR(L,M2)*YR(L,M1)*DELTA
- YLC(I,ML)*YR(L,M2)*YR(L,M1)
+ YLC(I,ML)*YR(L,M2)*YR(K,M1)*DELTA
+ YLC(I,ML)*YR(L,M2)*YR(K,M1)
- YLC(I,ML)*YR(L,M2)*YL(J,M1)*DELTA
- YLC(I,ML)*YR(L,M2)*YL(J,M1)
+ YLC(I,ML)*YR(L,M2)*YL(I,M1)*DELTA
+ YLC(I,ML)*YR(L,M2)*YL(I,M1)
+ YLC(I,ML)*YR(K,M2)*YR(L,M1)*DELTA
+ YLC(I,ML)*YR(K,M2)*YR(L,M1)
- YLC(I,ML)*YR(K,M2)*YR(K,M1)*DELTA
- YLC(I,ML)*YR(K,M2)*YR(K,M1)
+ YLC(I,ML)*YR(K,M2)*YL(J,M1)*DELTA
+ YLC(I,ML)*YR(K,M2)*YL(J,M1)
- YLC(I,ML)*YR(K,M2)*YL(I,M1)*DELTA
- YLC(I,ML)*YR(K,M2)*YL(I,M1)
- YLC(I,ML)*YL(J,M2)*YR(L,M1)*DELTA
- YLC(I,ML)*YL(J,M2)*YR(L,M1)
+ YLC(I,ML)*YL(J,M2)*YR(K,M1)*DELTA
+ YLC(I,ML)*YL(J,M2)*YR(K,M1)
- YLC(I,ML)*YL(J,M2)*YL(J,M1)*DELTA
- YLC(I,ML)*YL(J,M2)*YL(J,M1)
+ YLC(I,ML)*YL(J,M2)*YL(I,M1)*DELTA
+ YLC(I,ML)*YL(J,M2)*YL(I,M1)
+ YLC(I,ML)*YL(I,M2)*YR(L,M1)*DELTA
+ YLC(I,ML)*YL(I,M2)*YR(L,M1)
- YLC(I,ML)*YL(I,M2)*YR(K,M1)*DELTA
- YLC(I,ML)*YL(I,M2)*YR(K,M1)
+ YLC(I,ML)*YL(I,M2)*YL(J,M1)*DELTA
+ YLC(I,ML)*YL(I,M2)*YL(J,M1)
```

- YLC(I,ML)\*YL(I,M2)\*YL(I,M1)\*DELTA  
- YLC(I,ML)\*YL(I,M2)\*YL(I,M1)  
+ YLC(J,ML)\*YR(L,M2)\*YR(L,M1)\*DELTA  
- YLC(J,ML)\*YR(L,M2)\*YR(K,M1)\*DELTA  
+ YLC(J,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA  
- YLC(J,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA  
- YLC(J,ML)\*YR(K,M2)\*YR(L,M1)\*DELTA  
+ YLC(J,ML)\*YR(K,M2)\*YR(K,M1)\*DELTA  
- YLC(J,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
+ YLC(J,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YLC(J,ML)\*YL(J,M2)\*YR(L,M1)\*DELTA  
- YLC(J,ML)\*YL(J,M2)\*YR(K,M1)\*DELTA  
+ YLC(J,ML)\*YL(J,M2)\*YL(J,M1)\*DELTA  
- YLC(J,ML)\*YL(J,M2)\*YL(I,M1)\*DELTA  
- YLC(J,ML)\*YL(I,M2)\*YR(L,M1)\*DELTA  
+ YLC(J,ML)\*YL(I,M2)\*YL(K,M1)\*DELTA  
- YLC(J,ML)\*YL(I,M2)\*YL(J,M1)\*DELTA  
+ YLC(J,ML)\*YL(I,M2)\*YL(I,M1)\*DELTA  
- YRC(K,ML)\*YR(L,M2)\*YR(L,M1)\*DELTA  
+ YRC(K,ML)\*YR(L,M2)\*YR(L,M1)  
+ YRC(K,ML)\*YR(L,M2)\*YR(K,M1)\*DELTA  
- YRC(K,ML)\*YR(L,M2)\*YR(K,M1)  
- YRC(K,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA  
+ YRC(K,ML)\*YR(L,M2)\*YL(J,M1)  
+ YRC(K,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA  
- YRC(K,ML)\*YR(L,M2)\*YL(I,M1)  
+ YRC(K,ML)\*YR(K,M2)\*YR(L,M1)\*DELTA  
- YRC(K,ML)\*YR(K,M2)\*YR(L,M1)  
+ YRC(K,ML)\*YR(K,M2)\*YR(K,M1)  
+ YRC(K,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YRC(K,ML)\*YR(K,M2)\*YL(J,M1)  
- YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YRC(K,ML)\*YR(K,M2)\*YL(I,M1)  
- YRC(K,ML)\*YR(K,M2)\*YL(K,M1)\*DELTA  
+ YRC(K,ML)\*YR(K,M2)\*YL(K,M1)  
+ YRC(K,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YRC(K,ML)\*YR(K,M2)\*YL(J,M1)  
+ YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
- YRC(K,ML)\*YR(K,M2)\*YR(L,M1)\*DELTA  
+ YRC(K,ML)\*YR(K,M2)\*YR(L,M1)  
- YRC(K,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
+ YRC(K,ML)\*YR(K,M2)\*YL(J,M1)  
- YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YRC(K,ML)\*YR(K,M2)\*YL(I,M1)  
+ YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
- YRC(K,ML)\*YR(K,M2)\*YR(L,M1)\*DELTA  
+ YRC(K,ML)\*YR(K,M2)\*YR(L,M1)  
- YRC(K,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
+ YRC(K,ML)\*YR(K,M2)\*YL(J,M1)  
- YRC(K,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YRC(K,ML)\*YR(K,M2)\*YL(I,M1)  
+ YRC(L,ML)\*YR(L,M2)\*YR(L,M1)\*DELTA  
- YRC(L,ML)\*YR(L,M2)\*YR(K,M1)\*DELTA  
+ YRC(L,ML)\*YR(L,M2)\*YL(J,M1)\*DELTA  
- YRC(L,ML)\*YR(L,M2)\*YL(I,M1)\*DELTA  
- YRC(L,ML)\*YR(K,M2)\*YR(L,M1)\*DELTA  
+ YRC(L,ML)\*YR(K,M2)\*YR(K,M1)\*DELTA  
- YRC(L,ML)\*YR(K,M2)\*YL(J,M1)\*DELTA  
+ YRC(L,ML)\*YR(K,M2)\*YL(I,M1)\*DELTA

```
+ YRC(L,ML)*YL(J,M2)*YR(L,M1)*DELTA
- YRC(L,ML)*YL(J,M2)*YR(K,M1)*DELTA
+ YRC(L,ML)*YL(J,M2)*YL(J,M1)*DELTA
- YRC(L,ML)*YL(J,M2)*YL(I,M1)*DELTA
- YRC(L,ML)*YL(I,M2)*YR(L,M1)*DELTA
+ YRC(L,ML)*YL(I,M2)*YR(K,M1)*DELTA
- YRC(L,ML)*YL(I,M2)*YL(J,M1)*DELTA
+ YRC(L,ML)*YL(I,M2)*YL(I,M1)*DELTA
- KRON(M2,ML)*YR(L,M1)
+ KRON(M2,ML)*YR(K,M1)
- KRON(M2,ML)*YL(J,M1)
+ KRON(M2,ML)*YL(I,M1)
- KRON(M1,ML)*YR(L,M2)
+ KRON(M1,ML)*YR(K,M2)
- KRON(M1,ML)*YL(J,M2)
+ KRON(M1,ML)*YL(I,M2)$
FOR ALL ML, I CLEAR
YL(I,-ML)*PHASE(ML),
YR(I,-ML)*PHASE(ML)$
LET LL(I)=0,LL(J)=0,LR(K)=1,LR(L)=0$
Z:=GPOT(3,I,J,K,L)$
FOR ALL ML, I MATCH
YL(I,-ML)*PHASE(ML)=YLC(I,ML),
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$
Z:=Z;
Z :=
- PHASE(MR)*KRON(M2, - MR)*YR(L,M1)
+ PHASE(MR)*KRON(M2, - MR)*YR(K,M1)
- PHASE(MR)*KRON(M2, - MR)*YL(J,M1)
+ PHASE(MR)*KRON(M2, - MR)*YL(I,M1)
- PHASE(MR)*KRON(M1, - MR)*YR(L,M2)
+ PHASE(MR)*KRON(M1, - MR)*YR(K,M2)
- PHASE(MR)*KRON(M1, - MR)*YL(J,M2)
+ PHASE(MR)*KRON(M1, - MR)*YL(I,M2)
+ YR(L,MR)*YR(L,M2)*YR(L,M1)*DELTA
- YR(L,MR)*YR(L,M2)*YR(K,M1)*DELTA
+ YR(L,MR)*YR(L,M2)*YL(J,M1)*DELTA
- YR(L,MR)*YR(L,M2)*YL(I,M1)*DELTA
- YR(L,MR)*YR(K,M2)*YR(L,M1)*DELTA
+ YR(L,MR)*YR(K,M2)*YL(J,M1)*DELTA
- YR(L,MR)*YR(K,M2)*YL(I,M1)*DELTA
+ YR(L,MR)*YL(J,M2)*YR(L,M1)*DELTA
- YR(L,MR)*YL(J,M2)*YL(I,M1)*DELTA
- YR(L,MR)*YL(I,M2)*YR(L,M1)*DELTA
+ YR(L,MR)*YL(I,M2)*YR(K,M1)*DELTA
- YR(L,MR)*YL(I,M2)*YL(J,M1)*DELTA
+ YR(L,MR)*YL(I,M2)*YL(I,M1)*DELTA
- YR(K,MR)*YR(L,M2)*YR(L,M1)*DELTA
- YR(K,MR)*YR(L,M2)*YR(L,M1)
+ YR(K,MR)*YR(L,M2)*YR(K,M1)*DELTA
+ YR(K,MR)*YR(L,M2)*YR(K,M1)
- YR(K,MR)*YR(L,M2)*YL(J,M1)*DELTA
- YR(K,MR)*YR(L,M2)*YL(J,M1)
+ YR(K,MR)*YR(L,M2)*YL(I,M1)*DELTA
+ YR(K,MR)*YR(L,M2)*YL(I,M1)
```

+ YR(K,MR)\*YR(K,M2)\*YR(L,M1)\*DELTA  
+ YR(K,MR)\*YR(K,M2)\*YR(L,M1)  
- YR(K,MR)\*YR(K,M2)\*YR(K,M1)\*DELTA  
- YR(K,MR)\*YR(K,M2)\*YR(K,M1)  
+ YR(K,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA  
+ YR(K,MR)\*YR(K,M2)\*YL(J,M1)  
- YR(K,MR)\*YR(K,M2)\*YL(I,M1)\*DELTA  
- YR(K,MR)\*YR(K,M2)\*YL(I,M1)  
- YR(K,MR)\*YL(J,M2)\*YR(L,M1)\*DELTA  
- YR(K,MR)\*YL(J,M2)\*YR(L,M1)  
+ YR(K,MR)\*YL(J,M2)\*YR(K,M1)\*DELTA  
+ YR(K,MR)\*YL(J,M2)\*YR(K,M1)  
- YR(K,MR)\*YL(J,M2)\*YL(J,M1)\*DELTA  
- YR(K,MR)\*YL(J,M2)\*YL(J,M1)  
+ YR(K,MR)\*YL(J,M2)\*YL(I,M1)\*DELTA  
+ YR(K,MR)\*YL(J,M2)\*YL(I,M1)  
- YR(K,MR)\*YL(I,M2)\*YR(K,M1)\*DELTA  
- YR(K,MR)\*YL(I,M2)\*YR(K,M1)  
+ YR(K,MR)\*YL(I,M2)\*YL(J,M1)\*DELTA  
+ YR(K,MR)\*YL(I,M2)\*YL(J,M1)  
- YR(K,MR)\*YL(I,M2)\*YL(I,M1)\*DELTA  
- YR(K,MR)\*YL(I,M2)\*YL(I,M1)  
+ YL(J,MR)\*YR(L,M2)\*YR(L,M1)\*DELTA  
- YL(J,MR)\*YR(L,M2)\*YR(K,M1)\*DELTA  
+ YL(J,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA  
- YL(J,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA  
- YL(J,MR)\*YR(K,M2)\*YR(L,M1)\*DELTA  
+ YL(J,MR)\*YR(K,M2)\*YR(K,M1)\*DELTA  
- YL(J,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA  
+ YL(J,MR)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YL(J,MR)\*YL(J,M2)\*YR(L,M1)\*DELTA  
- YL(J,MR)\*YL(J,M2)\*YR(K,M1)\*DELTA  
- YL(J,MR)\*YL(I,M2)\*YR(L,M1)\*DELTA  
+ YL(J,MR)\*YL(I,M2)\*YR(K,M1)\*DELTA  
- YL(J,MR)\*YL(I,M2)\*YL(J,M1)\*DELTA  
- YL(J,MR)\*YL(I,M2)\*YL(I,M1)\*DELTA  
+ YL(I,MR)\*YR(L,M2)\*YR(L,M1)\*DELTA  
+ YL(I,MR)\*YR(L,M2)\*YR(K,M1)\*DELTA  
- YL(I,MR)\*YR(L,M2)\*YR(K,M1)  
- YL(I,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA  
+ YL(I,MR)\*YR(L,M2)\*YL(J,M1)  
+ YL(I,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA  
- YL(I,MR)\*YR(L,M2)\*YL(I,M1)  
+ YL(I,MR)\*YR(K,M2)\*YR(L,M1)\*DELTA  
- YL(I,MR)\*YR(K,M2)\*YR(L,M1)  
- YL(I,MR)\*YR(K,M2)\*YR(K,M1)\*DELTA  
+ YL(I,MR)\*YR(K,M2)\*YR(K,M1)  
+ YL(I,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YL(I,MR)\*YR(K,M2)\*YL(J,M1)  
- YL(I,MR)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YL(I,MR)\*YR(K,M2)\*YL(I,M1)  
- YL(I,MR)\*YL(J,M2)\*YR(L,M1)\*DELTA  
+ YL(I,MR)\*YL(J,M2)\*YR(L,M1)

```
+ YL(I,MR)*YL(J,M2)*YR(K,M1)*DELTA
- YL(I,MR)*YL(J,M2)*YR(K,M1)
- YL(I,MR)*YL(J,M2)*YL(J,M1)*DELTA
+ YL(I,MR)*YL(J,M2)*YL(I,M1)*DELTA
- YL(I,MR)*YL(J,M2)*YL(I,M1)
+ YL(I,MR)*YL(I,M2)*YR(L,M1)*DELTA
- YL(I,MR)*YL(I,M2)*YR(L,M1)
- YL(I,MR)*YL(I,M2)*YR(K,M1)*DELTA
+ YL(I,MR)*YL(I,M2)*YR(K,M1)
+ YL(I,MR)*YL(I,M2)*YL(J,M1)*DELTA
- YL(I,MR)*YL(I,M2)*YL(J,M1)
- YL(I,MR)*YL(I,M2)*YL(I,M1)*DELTA
+ YL(I,MR)*YL(I,M2)*YL(I,M1)$
```

FOR ALL ML, I CLEAR  
YL(I,-ML)\*PHASE(ML),  
YR(I,-ML)\*PHASE(ML)\$

```
LET LL(I)=1,LL(J)=0,LR(K)=1,LR(L)=0$
Z:=GPOT(3,I,J,K,L)$
FOR ALL ML, I MATCH
YL(I,-ML)*PHASE(ML)=YLC(I,ML),
YR(I,-ML)*PHASE(ML)=YRC(I,ML)$
Z:=Z;
```

```
Z := YLC(I,ML)*PHASE(MR)*KRON(M2, - MR)*YR(L,M1)*DELTA
+ YLC(I,ML)*PHASE(MR)*KRON(M2, - MR)*YR(L,M1)
- YLC(I,ML)*PHASE(MR)*KRON(M2, - MR)*YR(K,M1)*DELTA
- YLC(I,ML)*PHASE(MR)*KRON(M2, - MR)*YR(K,M1)
+ YLC(I,ML)*PHASE(MR)*KRON(M2, - MR)*YL(J,M1)*DELTA
+ YLC(I,ML)*PHASE(MR)*KRON(M2, - MR)*YL(J,M1)
- YLC(I,ML)*PHASE(MR)*KRON(M2, - MR)*YL(I,M1)*DELTA
- YLC(I,ML)*PHASE(MR)*KRON(M2, - MR)*YL(I,M1)
+ YLC(I,ML)*PHASE(MR)*KRON(M1, - MR)*YR(L,M2)*DELTA
+ YLC(I,ML)*PHASE(MR)*KRON(M1, - MR)*YR(L,M2)
- YLC(I,ML)*PHASE(MR)*KRON(M1, - MR)*YR(K,M2)*DELTA
- YLC(I,ML)*PHASE(MR)*KRON(M1, - MR)*YR(K,M2)
+ YLC(I,ML)*PHASE(MR)*KRON(M1, - MR)*YL(J,M2)*DELTA
+ YLC(I,ML)*PHASE(MR)*KRON(M1, - MR)*YL(J,M2)
- YLC(I,ML)*PHASE(MR)*KRON(M1, - MR)*YL(I,M2)*DELTA
- YLC(I,ML)*PHASE(MR)*KRON(M1, - MR)*YL(I,M2)
- YLC(I,ML)*YR(L,MR)*YR(L,M2)*YR(L,M1)*DELTA**2
- YLC(I,ML)*YR(L,MR)*YR(L,M2)*YR(L,M1)*DELTA
+ YLC(I,ML)*YR(L,MR)*YR(L,M2)*YR(K,M1)*DELTA**2
+ YLC(I,ML)*YR(L,MR)*YR(L,M2)*YR(K,M1)*DELTA
- YLC(I,ML)*YR(L,MR)*YR(L,M2)*YL(J,M1)*DELTA**2
- YLC(I,ML)*YR(L,MR)*YR(L,M2)*YL(J,M1)*DELTA
+ YLC(I,ML)*YR(L,MR)*YR(L,M2)*YL(I,M1)*DELTA**2
+ YLC(I,ML)*YR(L,MR)*YR(L,M2)*YL(I,M1)*DELTA
+ YLC(I,ML)*YR(L,MR)*YR(K,M2)*YR(L,M1)*DELTA**2
+ YLC(I,ML)*YR(L,MR)*YR(K,M2)*YR(L,M1)*DELTA
- YLC(I,ML)*YR(L,MR)*YR(K,M2)*YR(K,M1)*DELTA**2
- YLC(I,ML)*YR(L,MR)*YR(K,M2)*YR(K,M1)*DELTA
+ YLC(I,ML)*YR(L,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
+ YLC(I,ML)*YR(L,MR)*YR(K,M2)*YL(J,M1)*DELTA
- YLC(I,ML)*YR(L,MR)*YR(K,M2)*YL(I,M1)*DELTA**2
- YLC(I,ML)*YR(L,MR)*YR(K,M2)*YL(I,M1)*DELTA
```

```
- YLC(I,ML)*YR(L,MR)*YL(J,M2)*YR(L,M1)*DELTA**2
- YLC(I,ML)*YR(L,MR)*YL(J,M2)*YR(L,M1)*DELTA
+ YLC(I,ML)*YR(L,MR)*YL(J,M2)*YR(K,M1)*DELTA**2
+ YLC(I,ML)*YR(L,MR)*YL(J,M2)*YR(K,M1)*DELTA
- YLC(I,ML)*YR(L,MR)*YL(J,M2)*YL(J,M1)*DELTA**2
- YLC(I,ML)*YR(L,MR)*YL(J,M2)*YL(J,M1)*DELTA
+ YLC(I,ML)*YR(L,MR)*YL(J,M2)*YL(I,M1)*DELTA**2
+ YLC(I,ML)*YR(L,MR)*YL(J,M2)*YL(I,M1)*DELTA
+ YLC(I,ML)*YR(L,MR)*YL(I,M2)*YR(L,M1)*DELTA**2
+ YLC(I,ML)*YR(L,MR)*YL(I,M2)*YR(L,M1)*DELTA
- YLC(I,ML)*YR(L,MR)*YL(I,M2)*YR(K,M1)*DELTA**2
- YLC(I,ML)*YR(L,MR)*YL(I,M2)*YR(K,M1)*DELTA
+ YLC(I,ML)*YR(L,MR)*YL(I,M2)*YL(J,M1)*DELTA**2
+ YLC(I,ML)*YR(L,MR)*YL(I,M2)*YL(J,M1)*DELTA
- YLC(I,ML)*YR(L,MR)*YL(I,M2)*YL(I,M1)*DELTA**2
- YLC(I,ML)*YR(L,MR)*YL(I,M2)*YL(I,M1)*DELTA
+ YLC(I,ML)*YR(L,MR)*YL(I,M2)*YR(L,M1)*DELTA**2
+ 2*YLC(I,ML)*YR(K,MR)*YR(L,M2)*YR(L,M1)*DELTA
+ YLC(I,ML)*YR(K,MR)*YR(L,M2)*YR(L,M1)
- YLC(I,ML)*YR(K,MR)*YR(L,M2)*YR(K,M1)*DELTA**2
- 2*YLC(I,ML)*YR(K,MR)*YR(L,M2)*YR(K,M1)*DELTA
- YLC(I,ML)*YR(K,MR)*YR(L,M2)*YR(K,M1)
+ YLC(I,ML)*YR(K,MR)*YR(L,M2)*YL(J,M1)*DELTA**2
+ 2*YLC(I,ML)*YR(K,MR)*YR(L,M2)*YL(J,M1)*DELTA
+ YLC(I,ML)*YR(K,MR)*YR(L,M2)*YL(J,M1)
- YLC(I,ML)*YR(K,MR)*YR(L,M2)*YL(I,M1)*DELTA**2
- 2*YLC(I,ML)*YR(K,MR)*YR(L,M2)*YL(I,M1)*DELTA
- YLC(I,ML)*YR(K,MR)*YR(L,M2)
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YR(L,M1)*DELTA**2
- 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YR(L,M1)*DELTA
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YR(L,M1)
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YR(K,M1)*DELTA**2
+ 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YR(K,M1)*DELTA
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YR(K,M1)
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
- 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M1)*DELTA
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M1)
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M1)*DELTA**2
+ 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M1)*DELTA
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M1)
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YR(L,M1)*DELTA**2
+ 2*YLC(I,ML)*YR(K,MR)*YR(L,M2)*YR(L,M1)*DELTA
+ YLC(I,ML)*YR(K,MR)*YR(L,M2)*YR(L,M1)
- YLC(I,ML)*YR(K,MR)*YR(L,M2)*YR(K,M1)*DELTA**2
- 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YR(K,M1)*DELTA
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YR(K,M1)
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
+ 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M1)*DELTA
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M1)
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M1)*DELTA**2
- 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M1)*DELTA
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M1)
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M1)
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M2)*YR(L,M1)*DELTA**2
- 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M2)*YR(L,M1)*DELTA
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M2)*YR(L,M1)
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M2)*YL(J,M1)*DELTA**2
+ 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M2)*YL(J,M1)*DELTA
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M2)*YL(I,M1)
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M2)*YL(I,M1)*DELTA**2
- 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(J,M2)*YL(I,M1)*DELTA
- YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M2)*YR(L,M1)
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M2)*YR(K,M1)*DELTA**2
+ 2*YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M2)*YR(K,M1)*DELTA
+ YLC(I,ML)*YR(K,MR)*YR(K,M2)*YL(I,M2)*YR(K,M1)
```

- YLC(I,ML)\*YR(K,MR)\*YL(I,M2)\*YL(J,M1)\*DELTA\*\*2  
- 2\*YLC(I,ML)\*YR(K,MR)\*YL(I,M2)\*YL(J,M1)\*DELTA  
- YLC(I,ML)\*YR(K,MR)\*YL(I,M2)\*YL(J,M1)  
+ YLC(I,ML)\*YR(K,MR)\*YL(I,M2)\*YL(I,M1)\*DELTA\*\*2  
+ 2\*YLC(I,ML)\*YR(K,MR)\*YL(I,M2)\*YL(I,M1)\*DELTA  
+ YLC(I,ML)\*YR(K,MR)\*YL(I,M2)\*YL(I,M1)  
- YLC(I,ML)\*YL(J,MR)\*YR(L,M2)\*YR(L,M1)\*DELTA\*\*2  
- YLC(I,ML)\*YL(J,MR)\*YR(L,M2)\*YR(L,M1)\*DELTA  
+ YLC(I,ML)\*YL(J,MR)\*YR(L,M2)\*YR(K,M1)\*DELTA\*\*2  
+ YLC(I,ML)\*YL(J,MR)\*YR(L,M2)\*YR(K,M1)\*DELTA  
- YLC(I,ML)\*YL(J,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
- YLC(I,ML)\*YL(J,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA  
+ YLC(I,ML)\*YL(J,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
+ YLC(I,ML)\*YL(J,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA  
+ YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YR(L,M1)\*DELTA\*\*2  
+ YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YR(L,M1)\*DELTA  
- YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YR(K,M1)\*DELTA\*\*2  
- YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
+ YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YL(I,M1)\*DELTA  
+ YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
- YLC(I,ML)\*YL(J,MR)\*YR(K,M2)\*YL(I,M1)\*DELTA  
- YLC(I,ML)\*YL(J,MR)\*YL(J,M2)\*YR(L,M1)\*DELTA\*\*2  
- YLC(I,ML)\*YL(J,MR)\*YL(J,M2)\*YR(L,M1)\*DELTA  
+ YLC(I,ML)\*YL(J,MR)\*YL(J,M2)\*YL(I,M1)\*DELTA  
- YLC(I,ML)\*YL(J,MR)\*YL(J,M2)\*YL(I,M1)\*DELTA  
+ YLC(I,ML)\*YL(J,MR)\*YL(J,M2)\*YL(I,M1)\*DELTA

```

+ YLC(I,ML)*YL(I,MR)*YL(J,M2)*YL(J,M1)*DELTA**2
- YLC(I,ML)*YL(I,MR)*YL(J,M2)*YL(J,M1)
- YLC(I,ML)*YL(I,MR)*YL(J,M2)*YL(I,M1)*DELTA**2
+ YLC(I,ML)*YL(I,MR)*YL(J,M2)*YL(I,M1)
- YLC(I,ML)*YL(I,MR)*YL(I,M2)*YL(L,M1)*DELTA**2
+ YLC(I,ML)*YL(I,MR)*YL(I,M2)*YL(R,L,M1)
+ YLC(I,ML)*YL(I,MR)*YL(I,M2)*YL(K,M1)*DELTA**2
- YLC(I,ML)*YL(I,MR)*YL(I,M2)*YL(K,M1)
- YLC(I,ML)*YL(I,MR)*YL(I,M2)*YL(J,M1)*DELTA**2
+ YLC(I,ML)*YL(I,MR)*YL(I,M2)*YL(J,M1)
+ YLC(I,ML)*YL(I,MR)*YL(I,M2)*YL(I,M1)*DELTA**2
- YLC(I,ML)*YL(I,MR)*YL(I,M2)*YL(I,M1)
- YLC(J,ML)*PHASE(MR)*KRON(M2,-MR)*YR(L,M1)*DELTA
+ YLC(J,ML)*PHASE(MR)*KRON(M2,-MR)*YR(K,M1)*DELTA
- YLC(J,ML)*PHASE(MR)*KRON(M2,-MR)*YL(J,M1)*DELTA
+ YLC(J,ML)*PHASE(MR)*KRON(M2,-MR)*YL(I,M1)*DELTA
- YLC(J,ML)*PHASE(MR)*KRON(M1,-MR)*YR(L,M2)*DELTA
+ YLC(J,ML)*PHASE(MR)*KRON(M1,-MR)*YR(K,M2)*DELTA
- YLC(J,ML)*PHASE(MR)*KRON(M1,-MR)*YL(J,M2)*DELTA
+ YLC(J,ML)*PHASE(MR)*KRON(M1,-MR)*YL(I,M2)*DELTA
+ YLC(J,ML)*YR(L,MR)*YR(L,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YR(L,MR)*YR(L,M2)*YR(K,M1)*DELTA**2
+ YLC(J,ML)*YR(L,MR)*YR(L,M2)*YL(J,M1)*DELTA**2
- YLC(J,ML)*YR(L,MR)*YR(L,M2)*YL(I,M1)*DELTA**2
- YLC(J,ML)*YR(L,MR)*YR(K,M2)*YR(L,M1)*DELTA**2
+ YLC(J,ML)*YR(L,MR)*YR(K,M2)*YR(K,M1)*DELTA**2
- YLC(J,ML)*YR(L,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
+ YLC(J,ML)*YR(L,MR)*YR(K,M2)*YL(I,M1)*DELTA**2
+ YLC(J,ML)*YR(L,MR)*YL(J,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YR(L,MR)*YL(J,M2)*YR(K,M1)*DELTA**2
+ YLC(J,ML)*YR(L,MR)*YL(J,M2)*YL(J,M1)*DELTA**2
- YLC(J,ML)*YR(L,MR)*YL(J,M2)*YL(I,M1)*DELTA**2
- YLC(J,ML)*YR(L,MR)*YL(I,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YR(L,MR)*YL(I,M2)*YR(K,M1)*DELTA**2
- YLC(J,ML)*YR(L,MR)*YL(I,M2)*YL(J,M1)*DELTA**2
+ YLC(J,ML)*YR(L,MR)*YL(I,M2)*YL(I,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YR(L,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YR(L,M2)*YL(J,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YR(L,M2)*YL(J,M1)*DELTA
+ YLC(J,ML)*YR(K,MR)*YR(L,M2)*YR(K,M1)*DELTA**2
+ YLC(J,ML)*YR(K,MR)*YR(L,M2)*YR(K,M1)*DELTA
- YLC(J,ML)*YR(K,MR)*YR(L,M2)*YL(J,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YR(L,M2)*YL(J,M1)*DELTA
+ YLC(J,ML)*YR(K,MR)*YR(L,M2)*YR(L,M1)*DELTA
- YLC(J,ML)*YR(K,MR)*YR(K,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YR(K,M2)*YR(K,M1)*DELTA
+ YLC(J,ML)*YR(K,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
+ YLC(J,ML)*YR(K,MR)*YR(K,M2)*YL(J,M1)*DELTA
- YLC(J,ML)*YR(K,MR)*YR(K,M2)*YL(I,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YR(K,M2)*YL(I,M1)*DELTA
- YLC(J,ML)*YR(K,MR)*YL(J,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YL(J,M2)*YR(L,M1)*DELTA
+ YLC(J,ML)*YR(K,MR)*YL(J,M2)*YR(K,M1)*DELTA**2
+ YLC(J,ML)*YR(K,MR)*YL(J,M2)*YR(K,M1)*DELTA
- YLC(J,ML)*YR(K,MR)*YL(J,M2)*YL(J,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YL(J,M2)*YL(J,M1)*DELTA

```

```
+ YLC(J,ML)*YR(K,MR)*YL(J,M2)*YL(I,M1)*DELTA**2
+ YLC(J,ML)*YR(K,MR)*YL(J,M2)*YL(I,M1)*DELTA
+ YLC(J,ML)*YR(K,MR)*YL(I,M2)*YR(L,M1)*DELTA**2
+ YLC(J,ML)*YR(K,MR)*YL(I,M2)*YR(L,M1)*DELTA
- YLC(J,ML)*YR(K,MR)*YL(I,M2)*YR(K,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YL(I,M2)*YR(K,M1)*DELTA
+ YLC(J,ML)*YR(K,MR)*YL(I,M2)*YL(J,M1)*DELTA**2
+ YLC(J,ML)*YR(K,MR)*YL(I,M2)*YL(J,M1)*DELTA
- YLC(J,ML)*YR(K,MR)*YL(I,M2)*YL(I,M1)*DELTA**2
- YLC(J,ML)*YR(K,MR)*YL(I,M2)*YL(I,M1)*DELTA
+ YLC(J,ML)*YL(J,MR)*YR(L,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YL(J,MR)*YR(L,M2)*YR(K,M1)*DELTA**2
+ YLC(J,ML)*YL(J,MR)*YR(L,M2)*YR(K,M1)*DELTA**2
+ YLC(J,ML)*YL(J,MR)*YR(L,M2)*YL(J,M1)*DELTA**2
- YLC(J,ML)*YL(J,MR)*YR(L,M2)*YL(I,M1)*DELTA**2
- YLC(J,ML)*YL(J,MR)*YR(K,M2)*YR(L,M1)*DELTA**2
+ YLC(J,ML)*YL(J,MR)*YR(K,M2)*YR(K,M1)*DELTA**2
- YLC(J,ML)*YL(J,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
+ YLC(J,ML)*YL(J,MR)*YR(K,M2)*YL(I,M1)*DELTA**2
+ YLC(J,ML)*YL(J,MR)*YR(K,M2)*YL(L,M1)*DELTA**2
- YLC(J,ML)*YL(J,MR)*YR(K,M2)*YL(I,M1)*DELTA**2
+ YLC(J,ML)*YL(J,MR)*YR(K,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YL(J,MR)*YR(K,M2)*YR(K,M1)*DELTA**2
+ YLC(J,ML)*YL(I,MR)*YR(L,M2)*YR(L,M1)*DELTA
+ YLC(J,ML)*YL(I,MR)*YR(L,M2)*YR(K,M1)*DELTA**2
- YLC(J,ML)*YL(I,MR)*YR(L,M2)*YR(K,M1)*DELTA
- YLC(J,ML)*YL(I,MR)*YR(L,M2)*YL(I,M1)*DELTA
+ YLC(J,ML)*YL(I,MR)*YR(L,M2)*YR(K,M1)*DELTA
- YLC(J,ML)*YL(I,MR)*YR(L,M2)*YL(J,M1)*DELTA**2
- YLC(J,ML)*YL(I,MR)*YR(K,M2)*YR(L,M1)*DELTA
- YLC(J,ML)*YL(I,MR)*YR(K,M2)*YR(K,M1)*DELTA**2
+ YLC(J,ML)*YL(I,MR)*YR(K,M2)*YR(K,M1)*DELTA
+ YLC(J,ML)*YL(I,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
- YLC(J,ML)*YL(I,MR)*YR(K,M2)*YL(I,M1)*DELTA
- YLC(J,ML)*YL(I,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
+ YLC(J,ML)*YL(I,MR)*YR(I,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YL(I,MR)*YR(I,M2)*YR(K,M1)*DELTA
- YLC(J,ML)*YL(I,MR)*YR(I,M2)*YL(J,M1)*DELTA**2
+ YLC(J,ML)*YL(I,MR)*YR(I,M2)*YL(J,M1)*DELTA
+ YLC(J,ML)*YL(I,MR)*YR(I,M2)*YL(I,M1)*DELTA**2
- YLC(J,ML)*YL(I,MR)*YR(I,M2)*YL(I,M1)*DELTA
+ YLC(J,ML)*YL(I,MR)*YR(I,M2)*YR(L,M1)*DELTA**2
- YLC(J,ML)*YL(I,MR)*YR(I,M2)*YR(K,M1)*DELTA
+ YLC(J,ML)*YL(I,MR)*YR(I,M2)*YR(K,M1)*DELTA**2
- YLC(J,ML)*YL(I,MR)*YR(I,M2)*YL(J,M1)*DELTA**2
- YLC(J,ML)*YL(I,MR)*YR(I,M2)*YL(I,M1)*DELTA**2
+ YLC(J,ML)*YL(I,MR)*YR(I,M2)*YL(J,M1)*DELTA
- YLC(J,ML)*YL(I,MR)*YR(I,M2)*YL(I,M1)*DELTA
```

+ YRC(K,ML)\*PHASE(MR)\*KRON(M2, - MR)\*YR(L,M1)\*DELTA  
- YRC(K,ML)\*PHASE(MR)\*KRON(M2, - MR)\*YR(L,M1)  
- YRC(K,ML)\*PHASE(MR)\*KRON(M2, - MR)\*YR(K,M1)\*DELTA  
+ YRC(K,ML)\*PHASE(MR)\*KRON(M2, - MR)\*YR(K,M1)  
+ YRC(K,ML)\*PHASE(MR)\*KRON(M2, - MR)\*YL(J,M1)\*DELTA  
- YRC(K,ML)\*PHASE(MR)\*KRON(M2, - MR)\*YL(J,M1)  
- YRC(K,ML)\*PHASE(MR)\*KRON(M2, - MR)\*YL(I,M1)\*DELTA  
+ YRC(K,ML)\*PHASE(MR)\*KRON(M2, - MR)\*YL(I,M1)  
+ YRC(K,ML)\*PHASE(MR)\*KRON(M1, - MR)\*YR(L,M2)\*DELTA  
- YRC(K,ML)\*PHASE(MR)\*KRON(M1, - MR)\*YR(L,M2)  
- YRC(K,ML)\*PHASE(MR)\*KRON(M1, - MR)\*YR(K,M2)\*DELTA  
+ YRC(K,ML)\*PHASE(MR)\*KRON(M1, - MR)\*YR(K,M2)  
+ YRC(K,ML)\*PHASE(MR)\*KRON(M1, - MR)\*YL(J,M2)\*DELTA  
- YRC(K,ML)\*PHASE(MR)\*KRON(M1, - MR)\*YL(J,M2)  
- YRC(K,ML)\*PHASE(MR)\*KRON(M1, - MR)\*YL(I,M2)\*DELTA  
+ YRC(K,ML)\*PHASE(MR)\*KRON(M1, - MR)\*YL(I,M2)  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YR(L,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YR(L,M1)\*DELTA  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YR(K,M1)\*DELTA\*\*2  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YR(K,M1)\*DELTA  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(K,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(K,M1)\*DELTA  
+ YRC(K,ML)\*YR(L,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
- YRC(K,ML)\*YR(L,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YRC(K,ML)\*YR(L,MR)\*YR(K,M2)\*YL(K,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(L,MR)\*YR(K,M2)\*YL(K,M1)\*DELTA  
+ YRC(K,ML)\*YR(L,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
- YRC(K,ML)\*YR(L,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YRC(K,ML)\*YR(L,MR)\*YR(K,M2)\*YL(K,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(L,MR)\*YR(K,M2)\*YL(K,M1)\*DELTA  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(K,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(K,M1)\*DELTA  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA  
- YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(K,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(L,MR)\*YR(L,M2)\*YL(K,M1)\*DELTA  
+ YRC(K,ML)\*YR(K,MR)\*YR(L,M2)\*YR(L,M1)\*DELTA\*\*2  
- YRC(K,ML)\*YR(K,MR)\*YR(L,M2)\*YR(L,M1)  
- YRC(K,ML)\*YR(K,MR)\*YR(L,M2)\*YR(K,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(K,MR)\*YR(L,M2)\*YR(K,M1)  
+ YRC(K,ML)\*YR(K,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
- YRC(K,ML)\*YR(K,MR)\*YR(L,M2)\*YL(J,M1)  
- YRC(K,ML)\*YR(K,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(K,MR)\*YR(L,M2)\*YL(I,M1)  
- YRC(K,ML)\*YR(K,MR)\*YR(K,M2)\*YR(L,M1)\*DELTA\*\*2  
+ YRC(K,ML)\*YR(K,MR)\*YR(K,M2)\*YR(L,M1)



```
+ 2*YRC(K,ML)*YL(I,MR)*YR(L,M2)*YR(K,M1)*DELTA
- YRC(K,ML)*YL(I,MR)*YR(L,M2)*YR(K,M1)
+ YRC(K,ML)*YL(I,MR)*YR(L,M2)*YL(J,M1)*DELTA**2
- 2*YRC(K,ML)*YL(I,MR)*YR(L,M2)*YL(J,M1)*DELTA
+ YRC(K,ML)*YL(I,MR)*YR(L,M2)*YL(J,M1)
- YRC(K,ML)*YL(I,MR)*YR(L,M2)*YL(I,M1)*DELTA**2
+ 2*YRC(K,ML)*YL(I,MR)*YR(L,M2)*YL(I,M1)*DELTA
- YRC(K,ML)*YL(I,MR)*YR(L,M2)*YL(I,M1)
- YRC(K,ML)*YL(I,MR)*YR(K,M2)*YR(L,M1)*DELTA**2
+ 2*YRC(K,ML)*YL(I,MR)*YR(K,M2)*YR(L,M1)*DELTA
- YRC(K,ML)*YL(I,MR)*YR(K,M2)*YR(L,M1)
+ YRC(K,ML)*YL(I,MR)*YR(K,M2)*YR(K,M1)*DELTA**2
- 2*YRC(K,ML)*YL(I,MR)*YR(K,M2)*YR(K,M1)*DELTA
+ YRC(K,ML)*YL(I,MR)*YR(K,M2)*YR(K,M1)
- YRC(K,ML)*YL(I,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
+ 2*YRC(K,ML)*YL(I,MR)*YR(K,M2)*YL(J,M1)*DELTA
- YRC(K,ML)*YL(I,MR)*YR(K,M2)*YL(J,M1)
+ YRC(K,ML)*YL(I,MR)*YR(K,M2)*YL(J,M1)*DELTA**2
- 2*YRC(K,ML)*YL(I,MR)*YR(K,M2)*YL(J,M1)*DELTA
+ YRC(K,ML)*YL(I,MR)*YR(K,M2)*YL(I,M1)
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YR(L,M1)*DELTA**2
- 2*YRC(K,ML)*YL(I,MR)*YR(J,M2)*YR(L,M1)*DELTA
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YR(L,M1)
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YR(K,M1)*DELTA**2
+ 2*YRC(K,ML)*YL(I,MR)*YR(J,M2)*YR(K,M1)*DELTA
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YR(K,M1)
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(J,M1)*DELTA**2
- 2*YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(J,M1)*DELTA
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(J,M1)
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(J,M1)*DELTA**2
+ 2*YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(J,M1)*DELTA
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(J,M1)
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(J,M1)*DELTA
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(J,M1)*DELTA
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(J,M1)
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)*DELTA**2
- 2*YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)*DELTA
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)*DELTA**2
+ 2*YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)*DELTA
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)*DELTA
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)*DELTA
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)
- YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)*DELTA**2
- 2*YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)*DELTA
+ YRC(K,ML)*YL(I,MR)*YR(J,M2)*YL(I,M1)
- YRC(L,ML)*PHASE(MR)*KRON(M2, - MR)*YR(L,M1)*DELTA
+ YRC(L,ML)*PHASE(MR)*KRON(M2, - MR)*YR(K,M1)*DELTA
- YRC(L,ML)*PHASE(MR)*KRON(M2, - MR)*YL(J,M1)*DELTA
+ YRC(L,ML)*PHASE(MR)*KRON(M2, - MR)*YL(I,M1)*DELTA
- YRC(L,ML)*PHASE(MR)*KRON(M1, - MR)*YR(L,M2)*DELTA
+ YRC(L,ML)*PHASE(MR)*KRON(M1, - MR)*YR(K,M2)*DELTA
- YRC(L,ML)*PHASE(MR)*KRON(M1, - MR)*YL(J,M2)*DELTA
+ YRC(L,ML)*PHASE(MR)*KRON(M1, - MR)*YL(I,M2)*DELTA
+ YRC(L,ML)*YR(L,MR)*YR(L,M2)*YR(L,M1)*DELTA**2
- YRC(L,ML)*YR(L,MR)*YR(L,M2)*YR(K,M1)*DELTA**2
+ YRC(L,ML)*YR(L,MR)*YR(L,M2)*YL(J,M1)*DELTA**2
- YRC(L,ML)*YR(L,MR)*YR(L,M2)*YL(I,M1)*DELTA**2
- YRC(L,ML)*YR(L,MR)*YR(K,M2)*YR(L,M1)*DELTA**2
+ YRC(L,ML)*YR(L,MR)*YR(K,M2)*YR(K,M1)*DELTA**2
```



- YRC(L,ML)\*YL(I,MR)\*YR(L,M2)\*YR(L,M1)\*DELTA\*\*2  
+ YRC(L,ML)\*YL(I,MR)\*YR(L,M2)\*YR(L,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YR(L,M2)\*YR(K,M1)\*DELTA\*\*2  
- YRC(L,ML)\*YL(I,MR)\*YR(L,M2)\*YR(K,M1)\*DELTA  
- YRC(L,ML)\*YL(I,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YRC(L,ML)\*YL(I,MR)\*YR(L,M2)\*YL(J,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA\*\*2  
- YRC(L,ML)\*YL(I,MR)\*YR(L,M2)\*YL(I,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YR(K,M2)\*YR(L,M1)\*DELTA\*\*2  
- YRC(L,ML)\*YL(I,MR)\*YR(K,M2)\*YR(L,M1)\*DELTA  
- YRC(L,ML)\*YL(I,MR)\*YR(K,M2)\*YR(K,M1)\*DELTA\*\*2  
+ YRC(L,ML)\*YL(I,MR)\*YR(K,M2)\*YR(K,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA\*\*2  
- YRC(L,ML)\*YL(I,MR)\*YR(K,M2)\*YL(J,M1)\*DELTA  
- YRC(L,ML)\*YL(I,MR)\*YR(K,M2)\*YL(I,M1)\*DELTA\*\*2  
+ YRC(L,ML)\*YL(I,MR)\*YR(K,M2)\*YL(I,M1)\*DELTA  
- YRC(L,ML)\*YL(I,MR)\*YL(J,M2)\*YR(L,M1)\*DELTA\*\*2  
+ YRC(L,ML)\*YL(I,MR)\*YL(J,M2)\*YR(L,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YL(J,M2)\*YR(K,M1)\*DELTA\*\*2  
- YRC(L,ML)\*YL(I,MR)\*YL(J,M2)\*YR(K,M1)\*DELTA  
- YRC(L,ML)\*YL(I,MR)\*YL(J,M2)\*YR(K,M1)\*DELTA\*\*2  
+ YRC(L,ML)\*YL(I,MR)\*YL(J,M2)\*YR(K,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YL(J,M2)\*YL(I,M1)\*DELTA\*\*2  
- YRC(L,ML)\*YL(I,MR)\*YL(J,M2)\*YL(I,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YR(L,M1)\*DELTA\*\*2  
- YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YR(L,M1)\*DELTA  
- YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YR(L,M1)\*DELTA\*\*2  
+ YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YR(L,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YL(J,M1)\*DELTA\*\*2  
- YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YL(J,M1)\*DELTA  
- YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YL(J,M1)\*DELTA\*\*2  
+ YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YL(J,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YL(I,M1)\*DELTA  
- YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YL(I,M1)\*DELTA  
+ YRC(L,ML)\*YL(I,MR)\*YL(I,M2)\*YL(I,M1)\*DELTA  
+ PHASE(MR)\*KRON(M2,ML)\*KRON(M1, - MR)  
+ PHASE(MR)\*KRON(M2, - MR)\*KRON(M1,ML)  
- KRON(M2,ML)\*YR(L,MR)\*YR(L,M1)\*DELTA  
+ KRON(M2,ML)\*YR(L,MR)\*YR(K,M1)\*DELTA  
- KRON(M2,ML)\*YR(L,MR)\*YL(J,M1)\*DELTA  
+ KRON(M2,ML)\*YR(L,MR)\*YL(I,M1)\*DELTA  
+ KRON(M2,ML)\*YR(K,MR)\*YR(L,M1)\*DELTA  
+ KRON(M2,ML)\*YR(K,MR)\*YR(L,M1)  
- KRON(M2,ML)\*YR(K,MR)\*YR(K,M1)\*DELTA  
- KRON(M2,ML)\*YR(K,MR)\*YR(K,M1)  
+ KRON(M2,ML)\*YR(K,MR)\*YL(J,M1)\*DELTA  
+ KRON(M2,ML)\*YR(K,MR)\*YL(J,M1)  
- KRON(M2,ML)\*YR(K,MR)\*YL(I,M1)\*DELTA  
- KRON(M2,ML)\*YR(K,MR)\*YL(I,M1)  
- KRON(M2,ML)\*YL(J,MR)\*YR(L,M1)\*DELTA  
+ KRON(M2,ML)\*YL(J,MR)\*YR(K,M1)\*DELTA  
- KRON(M2,ML)\*YL(J,MR)\*YL(J,M1)\*DELTA  
+ KRON(M2,ML)\*YL(J,MR)\*YL(I,M1)\*DELTA  
+ KRON(M2,ML)\*YL(I,MR)\*YR(L,M1)\*DELTA  
- KRON(M2,ML)\*YL(I,MR)\*YR(L,M1)  
- KRON(M2,ML)\*YL(I,MR)\*YR(K,M1)\*DELTA  
+ KRON(M2,ML)\*YL(I,MR)\*YR(K,M1)  
+ KRON(M2,ML)\*YL(I,MR)\*YL(J,M1)\*DELTA  
- KRON(M2,ML)\*YL(I,MR)\*YL(J,M1)  
- KRON(M2,ML)\*YL(I,MR)\*YL(I,M1)\*DELTA  
+ KRON(M2,ML)\*YL(I,MR)\*YL(I,M1)

```
- KRON(M1,ML)*YR(L,MR)*YR(L,M2)*DELTA
+ KRON(M1,ML)*YR(L,MR)*YR(K,M2)*DELTA
- KRON(M1,ML)*YR(L,MR)*YL(J,M2)*DELTA
+ KRON(M1,ML)*YR(L,MR)*YL(I,M2)*DELTA
+ KRON(M1,ML)*YR(K,MR)*YR(L,M2)*DELTA
+ KRON(M1,ML)*YR(K,MR)*YR(L,M2)
- KRON(M1,ML)*YR(K,MR)*YR(K,M2)*DELTA
- KRON(M1,ML)*YR(K,MR)*YR(K,M2)
+ KRON(M1,ML)*YR(K,MR)*YL(J,M2)*DELTA
+ KRON(M1,ML)*YR(K,MR)*YL(J,M2)
- KRON(M1,ML)*YR(K,MR)*YL(I,M2)*DELTA
- KRON(M1,ML)*YR(K,MR)*YL(I,M2)
- KRON(M1,ML)*YL(J,MR)*YR(L,M2)*DELTA
+ KRON(M1,ML)*YL(J,MR)*YR(K,M2)*DELTA
- KRON(M1,ML)*YL(J,MR)*YL(J,M2)*DELTA
+ KRON(M1,ML)*YL(J,MR)*YL(I,M2)*DELTA
+ KRON(M1,ML)*YL(I,MR)*YR(L,M2)*DELTA
- KRON(M1,ML)*YL(I,MR)*YR(L,M2)
- KRON(M1,ML)*YL(I,MR)*YR(K,M2)*DELTA
+ KRON(M1,ML)*YL(I,MR)*YR(K,M2)
+ KRON(M1,ML)*YL(I,MR)*YL(J,M2)*DELTA
- KRON(M1,ML)*YL(I,MR)*YL(J,M2)
- KRON(M1,ML)*YL(I,MR)*YL(I,M2)*DELTA
+ KRON(M1,ML)*YL(I,MR)*YL(I,M2)
- YR(L,M2)*YR(L,M1)*KRON(ML,MR)*DELTA
+ YR(L,M2)*YR(L,M1)*KRON(ML,MR)
+ YR(L,M2)*YR(K,M1)*KRON(ML,MR)*DELTA
- YR(L,M2)*YR(K,M1)*KRON(ML,MR)
- YR(L,M2)*YL(J,M1)*KRON(ML,MR)*DELTA
+ YR(L,M2)*YL(J,M1)*KRON(ML,MR)
+ YR(L,M2)*YL(I,M1)*KRON(ML,MR)*DELTA
- YR(L,M2)*YL(I,M1)*KRON(ML,MR)
+ YR(K,M2)*YR(L,M1)*KRON(ML,MR)*DELTA
- YR(K,M2)*YR(L,M1)*KRON(ML,MR)
- YR(K,M2)*YL(J,M1)*KRON(ML,MR)*DELTA
+ YR(K,M2)*YL(J,M1)*KRON(ML,MR)
+ YR(K,M2)*YL(I,M1)*KRON(ML,MR)*DELTA
- YR(K,M2)*YL(I,M1)*KRON(ML,MR)
- YR(K,M2)*YL(I,M1)*KRON(ML,MR)*DELTA
+ YR(K,M2)*YL(I,M1)*KRON(ML,MR)
- YL(J,M2)*YR(L,M1)*KRON(ML,MR)*DELTA
+ YL(J,M2)*YR(L,M1)*KRON(ML,MR)
+ YL(J,M2)*YR(K,M1)*KRON(ML,MR)*DELTA
- YL(J,M2)*YR(K,M1)*KRON(ML,MR)
- YL(J,M2)*YL(J,M1)*KRON(ML,MR)*DELTA
+ YL(J,M2)*YL(J,M1)*KRON(ML,MR)
+ YL(J,M2)*YL(I,M1)*KRON(ML,MR)*DELTA
- YL(J,M2)*YL(I,M1)*KRON(ML,MR)
+ YL(I,M2)*YR(L,M1)*KRON(ML,MR)*DELTA
- YL(I,M2)*YR(L,M1)*KRON(ML,MR)
- YL(I,M2)*YR(K,M1)*KRON(ML,MR)*DELTA
+ YL(I,M2)*YR(K,M1)*KRON(ML,MR)
+ YL(I,M2)*YL(J,M1)*KRON(ML,MR)*DELTA
- YL(I,M2)*YL(J,M1)*KRON(ML,MR)
- YL(I,M2)*YL(I,M1)*KRON(ML,MR)*DELTA
+ YL(I,M2)*YL(I,M1)*KRON(ML,MR)$
```

END\$

## 5. MATRIX ELEMENTS OF SLATER-DETERMINANT WAVE FUNCTIONS

In this Section, we recast the formulas<sup>3)</sup> for matrix elements of various operators between Slater-determinant wave functions in such a manner as to make them suitable for an evaluation by REDUCE. In this connection let us just mention that it turned out essential to work with integer powers of the quantities  $B_3 \dots$ , defined below.

### 5.1 The Overlap of Slater-Determinant Wave Functions

The overlap of two A-particle Slater-determinant wave functions is proportional to the determinant of the  $A \times A$  matrix of overlaps  $\tilde{n}_{ik} = \langle \psi_i | \psi_k' \rangle$  of single-particle wave functions  $\psi_i$ , eq. (2.1)

$$\langle \phi | \phi' \rangle = \det \{ \tilde{n}_{ik} \} \quad (5.1)$$

where we left out an overall normalization constant. If we substitute eq. (2.8a) into eqs. (3.1, (3.2) and (3.3) we find that the matrix elements  $\tilde{n}_{ik}$  take the form

$$\tilde{n}_{ik} = B_1^{c_i^2} B_2^{c_k'^2} B_3^{c_i c_k'} g_{ik} \quad (5.2)$$

where

$$\begin{aligned} B_1 &= \exp(-\beta s^2/4) \\ B_2 &= \exp(-\beta s'^2/4) \\ B_3 &= \exp(\beta s \cdot s'/2) \end{aligned} \quad (5.3)$$

The matrix  $g_{ik}$  is a polynomial in  $s$  and  $s'$  which is zero unless the spin and isospin projections of particles  $i$  and  $k$  are the same.

From eq. (5.2) we see that the determinant (5.1) may be

$$\begin{aligned} &\text{reduced to } \det \{ \tilde{n}_{ik} \} \\ &= B_1^{\sum_i c_i^2} B_2^{\sum_k c_k'^2} \det \{ B_3 [(c_i - d)(c_k' - d') + c_i d' + c_k' d - dd'] g_{ik} \} \\ &= F \det \{ n_{ik} \} \end{aligned} \quad (5.4)$$

where

$$n_{ik} = B_3 (c_i - d)(c'_k - d') \quad (5.5)$$

$$= \tilde{n}_{ik} B_1^{-c_i^2} B_2^{-c_k'^2} B_3 (-c_i d' - c'_k d + dd')$$

$$F = B_1^{\sum_i c_i^2} B_2^{\sum_k c_k'^2} B_3^{-Add'} \quad (5.6)$$

In deriving eq. (5.4), we used

$$\sum_i c_i = \sum_k c'_k = 0$$

which follows from eqs. (2.8). The reason for introducing the constants  $d$  and  $d'$  in eq. (5.4) is the following:

If we identify  $d$  with a member of the set  $\{c_i\}$  and similarly  $d'$  with a member of the set  $\{c'_k\}$ , we find that the matrix

$$M_{ik} = (c_i - d)(c'_k - d') \quad (5.7)$$

takes the values 0 and 1 only. Thus the matrix element  $n_{ik}$  contains the variable  $B_3$  in powers of 0 and 1 only. The calculation of  $\det \{n_{ik}\}$ , eq. (5.4) is now reduced to the trivial calculation of the factor  $F$ , eq. (5.6) and the evaluation of  $\det \{n_{ik}\}$ . The latter one is done by the REDUCE program 6. In writing the REDUCE program, we have to specify the 6 nucleons in  ${}^6\text{Li}$  in the various clusterizations. The table I contains the necessary information.

Table I

Specification of the 6 nucleons in  ${}^6\text{Li}$  in the clusterizations ( ${}^4\text{He} - {}^2\text{H}$ ), ( ${}^5\text{He} - \text{p}$ ) and ( ${}^5\text{Li} - \text{n}$ ) by their isospin-3-component  $T_3(i)$ , their spin-3-component  $S_3(i)$ , their cluster center  $CN(i)$  and orbital angular momentum  $L(i)$ .  $CN(i) = 1(2)$  means that the particle  $i$  belongs to the heavy (light) clusters  ${}^4\text{He}$ ,  ${}^5\text{He}$ ,  ${}^5\text{Li}$  ( ${}^2\text{H}$ ,  $\text{p}$ ,  $\text{n}$ ), respectively.

clusterization	particle number	1	2	3	4	5	6
$^4\text{He} - ^2\text{H}$	$T_3(i)$	1/2	1/2	1/2	-1/2	-1/2	-1/2
	$S_3(i)$	1/2	-1/2	1/2	1/2	-1/2	1/2
	$CN(i)$	1	1	2	1	1	2
	$L(i)$	0	0	0	0	0	0
$^5\text{He}-p$	$CN(i)$	1	1	2	1	1	1
	$L(i)$	0	0	0	0	0	1
$^5\text{Li}-n$	$CN(i)$	1	1	1	1	1	2
	$L(i)$	0	0	1	0	0	0

As an example, we show the REDUCE program 6 which calculates the overlap  $\langle \Phi_5\text{He-p}(1m) | \Phi_5\text{Li-n}(1m') \rangle$ , keeping the magnetic quantum numbers  $m$  and  $m'$  as analytical variables. We have to implement table I specifying the 6 nucleons in  $^6\text{Li}$  on the lefthand and righthand side of the matrix element. All quantum numbers are declared arrays with  $LL(i)$  and  $LR(i)$  specifying the orbital angular momentum  $l$  of particle  $i$  on the left- and right-hand side, respectively, etc. The particle coordinates  $i$  and  $k$  are now treated as integers ranging from 1 to 6. In the procedure  $NRM(i,k)$ , the factor  $B_3^{(c_i-d)(c_k'-d')}$ , eq. (5.5), is included now.

The coefficients  $c_i$  and  $c'_k$  are calculated from eq. (2.8). We choose  $d = d' = c_1$ .

COMMENT REDUCE PROGRAM 6

MANY-BODY OVERLAP ( 5HE-P,1M,S | 5LI-N,1M',S' )\$

OPERATOR YL,YR,KRON,PHASE\$

COMMENT

THE SPECIFICATION OF THE OPERATOR PHASE IS THE SAME AS  
IN THE REDUCE PROGRAM 1\$

COMMENT

DIFFERENTIATION RULE FOR SPHERICAL VECTOR COMPONENTS\$

```
FOR I:=1:6 DO
BEGIN
FOR ALL ML,MR LET
DF(YL(I,ML),YL(I,MR))=KRON(ML,MR),
DF(YR(I,ML),YR(I,MR))=KRON(ML,MR),
DF(YL(I,ML),YR(I,MR))=0,
DF(YR(I,ML),YL(I,MR))=0$
FOR J:=1:6 DO
BEGIN
IF I=J THEN GOTO NEXTJ$
FOR ALL ML,MR LET
DF(YL(I,ML),YL(J,MR))=0,
DF(YR(I,ML),YR(J,MR))=0,
DF(YL(I,ML),YR(J,MR))=0,
DF(YR(I,ML),YL(J,MR))=0$
NEXTJ:
END$
END$
```

COMMENT IMPLEMENTATION OF TABLE I\$

```
ARRAY
B(2),CNL(6),CNR(6),CL(6),CR(6),T3(6),S3(6),LL(6),LR(6)$
COMMENT EQ.(2.8)$
B(1):=1/6$
B(2):=-5/6$
FOR I:=1:6 DO
BEGIN
CNL(I):=CNR(I):=1$
END$
CNL(3):=CNR(6):=2$
FOR I:=1:6 DO
BEGIN
CL(I):=B(CNL(I))$
CR(I):=B(CNR(I))$
END$
DL:=DR:=CL(1)$
T3(1):=T3(2):=T3(3):=1$
T3(4):=T3(5):=T3(6):=0$
S3(1):=S3(3):=S3(4):=S3(6):=1$
S3(2):=S3(5):=0$
```

```
FOR I:=1:6 DO
LL(I):=LR(I):=0$
LL(6):=LR(3):=1$

PROCEDURE NRM(I,K)$
COMMENT THE PROCEDURE NRM(I,K) CALCULATES THE
MATRIX ELEMENTS N(I,K), EQ(5.5)$
BEGIN
R:=IF LL(I)=1 THEN (-YL(I,-ML)+YR(K,-ML))*PHASE(ML) ELSE 1$
IF LR(K)=1 THEN R:=R*(YL(I,MR)-YR(K,MR))
+DF(R,YR(K,-MR))*PHASE(MR)$
IF CL(I)-DL =0 OR CR(K)-DR=0 THEN RETURN R ELSE RETURN R*B3$
END NRM$

COMMENT CALCULATION OF DET(N(I,K))$
MATRIX N(6,6)$
FOR I:=1:6 DO
FOR K:=1:6 DO
N(I,K):=IF T3(I)=T3(K) AND S3(I)=S3(K) THEN NRM(I,K) ELSE 0$

Z:=DET(N)$

OPERATOR SL,SR,SLC,SRC$

FOR I:=1:6 DO
FOR ALL M LET
YL(I,M)=CL(I)*SL(M),
YR(I,M)=CR(I)*SR(M)$

FOR ALL M MATCH
SL(-M)*PHASE(M)=SLC(M),
SR(-M)*PHASE(M)=SRC(M)$

Z:=Z;
Z := SRC(ML)*SL(MR)

END$
```

## 5.2 Matrix Elements of One-Body Operators

### (i) The kinetic-energy matrix element:

It has been shown (see eq. (5.8) of ref. 3) that matrix elements of the kinetic-energy operator between Slater-Determinant wave functions may be obtained in a simple way from overlap matrix elements if particles in s-waves only are involved. We generalize this result to matrix elements containing in addition to particles in s-waves also particles in p-waves.

We start from the cofactor expansion <sup>3)</sup> of the kinetic-energy matrix element

$$\langle \phi | \tau | \phi' \rangle = \sum_{ik=1}^A \tilde{C}_{ik} \langle \psi_i | \tau | \psi'_k \rangle \quad (5.8)$$

and assume that there are  $n$  particles in the function  $\phi$  which occupy p-orbits ( $i = i_1, i_2 \dots i_n$ ) and  $n'$  particles in the function  $\phi'$  which occupy p-orbits ( $k = k_1, k_2 \dots k_{n'}$ ), all other particles filling s-orbits. If we substitute the single-particle matrix elements (3.4) of the kinetic-energy operator into eq. (5.8) we get

$$\begin{aligned} \langle \phi | \tau | \phi' \rangle &= \left( \frac{\hbar^2 \beta}{4m} \right) \sum_{ik=1}^A \tilde{C}_{ik} \left[ 3 + \sum_{\alpha=1}^A (\delta_{ii_\alpha} + \delta_{kk_\alpha}) \right. \\ &\quad \left. + 2\beta \frac{d}{d\beta} \right] \langle \psi_i | \psi'_k \rangle \\ &= \left( \frac{\hbar^2 \beta}{4m} \right) \left[ 3A \sum_{k=1}^A \tilde{C}_{ik} \langle \psi_i | \psi'_k \rangle + n \sum_{k=1}^A \tilde{C}_{ik} \langle \psi_i | \psi'_k \rangle \right. \\ &\quad \left. + n' \sum_{i=1}^A \tilde{C}_{ik} \langle \psi_i | \psi'_k \rangle + \sum_{i,k=1}^A \tilde{C}_{ik} 2\beta \frac{d}{d\beta} \langle \psi_i | \psi'_k \rangle \right] \\ &= \left( \frac{\hbar^2 \beta}{4m} \right) [3A + n_p + 2\beta \frac{d}{d\beta}] \langle \phi | \phi' \rangle \end{aligned} \quad (5.9)$$

where  $n_p = n + n'$  is the number of p-orbits in the matrix element.

The dependence of the matrix element  $\langle \phi | \phi' \rangle$  on the oscillator parameter  $\beta$  is known through eqs. (5.3). The differentiation with respect to  $\beta$  in eq. (5.9) may therefore be carried out analytically<sup>5)</sup>.

The resulting expression is included in the FORTRAN program for the numerical processing of  $\langle \phi | \phi' \rangle$  (see Section 6). Thus the kinetic-energy operator need not be considered on the level of REDUCE calculations provided the oscillator parameter  $\beta$  is the same for all orbits.

(ii) The charge multipole matrix element:

As in the previous case, we use the cofactor expansion

$$\langle \phi | O(q) | \phi' \rangle = \sum_{ik} \tilde{C}_{ik} \langle \psi_i | \exp(iq \cdot \vec{x}) | \psi_k' \rangle \equiv \sum_{ik} \tilde{C}_{ik} \tilde{O}_{ik}(q) \quad (5.10)$$

and study the exponential functions entering this expression. Inserting eq. (2.8a) into eq. (3.5a) we find that the single-particle matrix element  $\delta_{ik}(q)$  between s-wave single-particle states is proportional to

$$\begin{aligned} g_{ik} \exp \left[ \frac{i}{2} q \cdot \vec{s} c_i + \frac{i}{2} q \cdot \vec{s}' c'_k - \frac{q^2}{4\beta} - \frac{\beta}{4} (\delta^2 c_i^2 + \delta'^2 c_k'^2 - 2 \vec{s} \cdot \vec{s}' c_i c'_k) \right] \\ = g_{ik} \exp \left[ \frac{i}{2} q \cdot \vec{s} (c_i - c_0) + \frac{i}{2} q \cdot \vec{s}' (c'_k - c'_0) - \frac{q^2}{4\beta} \right. \\ \left. + \frac{i}{2} q \cdot \vec{s} c_0 + \frac{i}{2} q \cdot \vec{s}' c'_0 \right. \\ \left. - \frac{\beta^2}{4} (\delta^2 c_i^2 + \delta'^2 c_k'^2 - 2 \vec{s} \cdot \vec{s}' c_i c'_k) \right] \end{aligned}$$

The matrix  $g_{ik}$  contains Kronecker deltas in spin and isospin and - in the case of p-wave matrix elements - also polynomials in  $\vec{s}$  and  $\vec{s}'$ .

If we introduce

$$\begin{aligned} B_7 &= \exp\left(\frac{i}{2}q \cdot \hat{\alpha}\right) \\ B_8 &= \exp\left(\frac{i}{2}q \cdot \hat{\beta}\right) \end{aligned} \quad (5.11)$$

and choose  $c_o$  and  $c'_o$  such that  $c_i - c_o = (0, 1)$  and  $c'_k - c'_o = (0, 1)$  we conclude that

$$\langle \Phi | O(q) | \Phi' \rangle \sim \exp\left(\frac{q^2}{4\beta}\right) B_1^{-c_o} B_8^{-c'_o}$$

contains  $q$  only through terms  $(B_7)^a (B_8)^b$  where  $a$  and  $b$  may take the values zero or one. The dependence of  $\langle \Phi | O(q) | \Phi' \rangle$  on the quantities  $B_1$ ,  $B_2$  and  $B_3$ , eq. (5.3), is obtained from an expansion in terms of the cofactors  $c_{ik}$  of the matrix  $n_{ik}$ , eq. (5.5),

$$\begin{aligned} c_{ik} &= \tilde{C}_{ik} \prod_{\substack{\alpha \neq i \\ \beta \neq k}} B_1^{-c_\alpha^2} B_2^{-c_\beta^{12}} B_3^{-c_\alpha^{12}} [ -c_\alpha d^1 - c'_\beta d + dd' ] \\ &= F^{-1} \tilde{C}_{ik} B_1^{c_i^2} B_2^{c_k^{12}} B_3^{c_i^{12}} [ c_i d^1 + c'_k d - dd' ] \end{aligned} \quad (5.12)$$

where the factor  $F$  is given by eq. (5.6) and  $\tilde{c}_{ik}$  is the cofactor of the matrix  $\tilde{n}_{ik}$ , eq. (5.2).

If we define

$$O_{ik}(q) = B_3^{(c_i - d)(c'_k - d')} B_7^{(c_i - c_o)} B_8^{(c'_k - c'_o)} g_{ik} \quad (5.13)$$

we find

$$\begin{aligned} &\{ F \exp\left(-\frac{q^2}{4\beta}\right) B_7^{c_o} B_8^{c'_o} \} \sum_{ik} c_{ik} O_{ik}(q) \\ &= \sum_{ik} \tilde{C}_{ik} \tilde{O}_{ik}(q) \\ &= \langle \Phi | O(q) | \Phi' \rangle \end{aligned} \quad (5.14)$$

In the REDUCE program 7 the factor in curly brackets in eq. (5.14) is suppressed. It is taken into account at a later stage of the calculations, i.e. in a FORTRAN program.

As an example, we choose the ( ${}^5\text{He-p}$ )-clusterization and calculate the quantity

$$\langle \Phi_5^{\text{He-p}} | \underset{\sim}{O}(q) | \Phi'_5^{\text{He-p}} \rangle \{ F \exp \left( \frac{q^2}{4\beta} \right) B_7^{c_o} B_8^{c'_o} \}^{-1}$$

where  $c_o = c'_o = c_3 = -5/6$  (see table I).

COMMENT REDUCE PROGRAM 7

MANY-BODY MATRIX ELEMENT (5HE-P,1M,S|O(Q)|5HE-P,1M',S')\$

OPERATOR YL,YR,KRON,PHASE,P,PC\$  
OFF ALLFAC\$

COMMENT

THE SPECIFICATION OF THE OPERATOR PHASE, THE  
DIFFERENTIATION RULES FOR THE SPHERICAL VECTOR COMPOMENTS  
AND THE PROCEDURE NRM(I,K) ARE THE SAME AS IN THE  
REDUCE PROGRAM 6\$

COMMENT IMPLEMENTATION OF TABLE I\$

ARRAY

B(2),CN(6),CL(6),CR(6),T3(6),S3(6),LL(6),LR(6)\$

COMMENT EQ.(2.8)\$

B(1):=1/6\$

B(2):=-5/6\$

FOR I:=1:6 DO CN(I):=1\$

CN(0):=CN(3):=2\$

FOR I:=0:6 DO

CL(I):=CR(I):=B(CN(I))\$

DL:=DR:=CL(1)\$

T3(1):=T3(2):=T3(3):=1\$

T3(4):=T3(5):=T3(6):=0\$

S3(1):=S3(3):=S3(4):=S3(6):=1\$

S3(2):=S3(5):=0\$

FOR I:=1:5 DO

LL(I):=LR(I):=0\$

LL(6):=LR(6):=1\$

```
PROCEDURE FRM(J,K)$
COMMENT FRM CALCULATES THE ONE-BODY MATRIX
ELEMENT OF THE OPERATOR O, EQ.(5.13)$
BEGIN
R:=IF LL(J)=1 THEN (I*P(-ML)/2-YL(J,-ML)+YR(K,-ML))
    *PHASE(ML) ELSE 1$
IF LR(K)=1 THEN R:=R*(I*P(MR)/2+YL(J,MR)-YR(K,MR))
    +DF(R,YR(K,-MR))*PHASE(MR)$
IF CL(J)-CL(O)=1 THEN R:=R*B7$
IF CR(K)-CR(O)=1 THEN R:=R*B8$
IF CL(J)-DL=0 OR CR(K)-DR=0 THEN RETURN R ELSE RETURN R*B3$
END FRM$

COMMENT NORMALIZATION MATRIX N(I,K), EQ.(5.5)$

MATRIX N(6,6),W(5,5)$
OPERATOR SL,SR,SLC,SRC$
ARRAY SIG(6)$

SIG(O):=1$
FOR I:=1:6 DO SIG(I):=-SIG(I-1)$
FOR I:=1:6 DO
FOR K:=1:6 DO
N(I,K):=IF T3(I)=T3(K) AND S3(I)=S3(K) THEN NRM(I,K) ELSE 0$
A:=6$

PROCEDURE CF1(I,K)$
COMMENT CF1(I,K) CALCULATES THE COFACTORS
OF THE MATRIX N$
BEGIN
I2:=0$
FOR I1:=1:A DO
BEGIN
IF I1=I THEN GOTO MI$
I2:=I2+1$
K2:=0$
FOR K1:=1:A DO
BEGIN
IF K1=K THEN GOTO MK$
K2:=K2+1$
W(I2,K2):=N(I1,K1)$
MK:END$
MI:END$
RETURN DET(W)*SIG(I+K)$
END CF1$

O:=0$

FOR J:=1:3 DO
FOR K:=1:3 DO
BEGIN
```

```
COF:=CF1(J,K)$  
IF COF=0 OR S3(J) NEQ S3(K) THEN GOTO NEXTK$  
O:=O+FRM(J,K)*COF$  
NEXTK:END$  
  
FOR J:=1:6 DO  
FOR ALL M LET YL(J,M)=CL(J)*SL(M),YR(J,M)=CR(J)*SR(M)$  
  
O:=O;  
  
O := 2*KRON(ML,MR)*B8*B7*B3  
- KRON(ML,MR)*B8*B7  
- KRON(ML,MR)*B8  
- KRON(ML,MR)*B7  
+ KRON(ML,MR)*B3$  
  
END$
```

### 5.3 Matrix Elements of Two-Body Operators

To calculate matrix elements of the two-body interaction  $V$  we start from the two-body matrix elements  $\tilde{V}_{ijkl}$  discussed in Section 4 and use an expansion <sup>3)</sup> in terms of generalized cofactors  $\tilde{c}_{ijkl}$  of the matrix  $\tilde{n}_{ik}$

$$\langle \phi | V | \phi' \rangle = \frac{1}{2} \sum_{i \neq j, k \neq l} \tilde{V}_{ijlk} \tilde{c}_{ijkl} \quad (5.15)$$

and recast it into a form suitable for algebraic processing by REDUCE. As in the previous cases we study the various exponentials entering the above expression. Inserting eq. (2.8) into eq. (4.2a), we find that the two-particle matrix element  $\tilde{V}_{ijkl}^{(D)}$  of the central part of the direct interaction is proportional to

$$\begin{aligned} \exp \{ - \frac{\beta \delta}{4} [ & s^2 (c_i - c_j)^2 + s'^2 (c'_k - c'_l)^2 \\ & + 2 s \cdot s' (c_i - c_j)(c'_k - c'_l) ] \\ - \frac{\beta}{4} [ & s^2 (c_i^2 + c_j^2) + s'^2 (c_k'^2 + c_l'^2) \\ & - 2 s \cdot s' (c_i c'_k + c_j c'_l) ] \} g_{ijkl} \end{aligned} \quad (5.16)$$

The quantities  $g_{ijkl}$  contain Kronecker deltas in spin and isospin and - in the case of p-wave matrix elements - also polynomials in  $s$  and  $s'$ .

The term proportional to  $\delta$  is easily dealt with observing that

$$(c_i - c_j)^2 = 0, 1$$

and

$$(c_i - c_j)(c_k^1 - c_l^1) = 0, \pm 1$$

If we introduce

$$\begin{aligned} B_4 &= \exp\left(-\frac{\beta\delta}{4}s^2\right) \\ B_5 &= \exp\left(-\frac{\beta\delta}{4}s'^2\right) \\ B_6 &= \exp\left(-\frac{\beta\delta}{2}\tilde{s} \cdot \tilde{s}'\right) \end{aligned} \quad (5.17)$$

we conclude that  $\langle \Phi | v | \Phi' \rangle B_6$  contains terms proportional to  $(B_4)^a (B_5)^b (B_6)^c$  where  $a$  and  $b$  may take the values 0 and 1 while  $c$  may be 0, 1 and 2. The dependence of  $\langle \Phi | v | \Phi' \rangle$  on the quantities  $B_1$ ,  $B_2$  and  $B_3$ , eq. (5.3), may be studied by a cofactor expansion involving the matrix  $n_{ik}$ , eq. (5.5). Let  $c_{ijkl}$  denote the generalized cofactors of the matrix  $n_{ik}$ , then

$$\begin{aligned} c_{ijlk} &= \sum_{\alpha \neq i,j} \overline{(B_1^{-C_\alpha^2} B_3^{-C_\alpha d^1 + dd^1})} \overline{(B_2^{-C_\alpha^{12}} B_3^{-C_\alpha^1 d})} \\ &= F^{-1} \sum_{\alpha \neq i,j} B_1^{C_\alpha^2 + C_\alpha^{12}} B_2^{C_\alpha^{12} + C_\alpha^1} \\ &\quad * B_3 [(C_i + C_j)d^1 + (C_k^1 + C_l^1)d - 2dd^1] \end{aligned} \quad (5.18)$$

where the quantity  $F$  is defined in eq. (5.6). We note that the symmetry relations of the two sets of cofactors  $\tilde{c}_{ijkl}$  and  $c_{ijkl}$  are the same, i.e.

$$c_{ijlk} = -c_{jilk} = -c_{ijlk} = c_{jilk} \quad (5.19)$$

Let

$$V_{ijkl}^{(D)}(\delta) = B_4^{(C_i - C_j)^2} B_5^{(C_k' - C_l')^2} B_6^{(C_i - C_j)(C_k' - C_l')} \quad (5.20)$$

denote the  $\delta$ -dependent part of the two-body matrix element (5.16), then

$$\begin{aligned} & F \frac{1}{2} \sum_{i \neq j, k \neq l} V_{ijkl}^{(D)}(\delta) B_3^{[(C_i - d)(C_k' - d') + (C_j - d)(C_l' - d')]} g_{ijkl} c_{ijkl} \\ &= \frac{1}{2} \sum_{i \neq j, k \neq l} V_{ijkl}^{(D)}(\delta) B_1^{C_i^2 + C_j^2} B_2^{C_k'^2 + C_l'^2} B_3^{C_i C_k' + C_j C_l'} g_{ijkl} \tilde{c}_{ijkl} \\ &= \langle \phi | V^{(D)} | \phi' \rangle \end{aligned} \quad (5.21)$$

The symmetry relations (5.19) allow for a restriction of the summation in eq. (5.21) with the result

$$\begin{aligned} & \langle \phi | V^{(D)} | \phi' \rangle \\ &= F \frac{1}{2} \sum_{i < j, k < l} \bar{V}_{ijkl}^{(D)} c_{ijkl} \end{aligned} \quad (5.22a)$$

with

$$V_{ijkl} = V_{ijkl}(\delta) B_3^{[(C_i - d)(C_k' - d') + (C_j - d)(C_l' - d')]} \quad (5.22b)$$

$$* g_{ijkl} \quad (5.22c)$$

$$\bar{V}_{ijkl} = V_{ijkl} - V_{jikl} - V_{ijek} + V_{jile}$$

It remains to study matrix elements of the exchange interaction, the only case of interest being here the Majorana space exchange. From eq. (5.16) we find that the corresponding two-particle matrix element  $V_{ijkl}^{(M)}$  is proportional to

$$V_{ijkl}^{(M)}(\delta) B_1^{C_i^2 + C_j^2} B_2^{C_k'^2 + C_l'^2} B_3^{(C_i C_k' + C_j C_l')} g_{ijkl}^{(M)}$$

where the symbol (M) means exchange of the spatial coordinates  $k$  and  $l$ . Thus we find for the Majorana exchange contribution

$$\begin{aligned} & F \frac{1}{2} \sum_{i \neq j, k \neq l} V_{ijkl}^{(M)}(\delta) B_3^{[(C_i - d)(C_k' - d') + (C_j - d)(C_l' - d')]} g_{ijkl}^{(M)} c_{ijkl} \\ &= \frac{1}{2} \sum_{i \neq j, k \neq l} V_{ijkl}^{(M)}(\delta) B_1^{C_i^2 + C_j^2} B_2^{C_k'^2 + C_l'^2} B_3^{(C_i C_k' + C_j C_l')} g_{ijkl}^{(M)} c_{ijkl} \\ &= \langle \phi | V^{(M)} | \phi' \rangle \end{aligned}$$

or

$$\langle \phi | V^{(M)} | \phi' \rangle = F \frac{1}{2} \sum_{1 < i, j, k < e} \bar{V}_{ijkl}^{(M)} c_{ijkl} \quad (5.23a)$$

with

$$V_{ijkl}^{(M)} = V_{ijkl}^{(M)}(\delta) B_3 [(C_i - d)(C_j - d') + (C_j - d)(C_k - d')] * g_{ijkl}^{(M)} \quad (5.23b)$$

The REDUCE program for the calculation of matrix elements of the central two-body interaction (2.10b) consists of the following steps:

- (i) calculate the matrix elements  $n_{ik}$ , eq. (5.5)
- (ii) determine the generalized cofactors  $c_{ijkl}$  of the matrix  $n_{ik}$ . This is done by the procedure CF2(i,j,k,l) using the operator DET for the evaluation of determinants
- (iii) calculate matrix elements  $V_{ijkl}^{(D)} \cdot WD + V_{ijkl}^{(M)} \cdot WM$ , eqs. (5.22, 5.23) with weights WD and WM for the direct and the Majorana exchange part
- (iv) sum over (ijkl) taking into account Kronecker deltas in spin and isospin
- (v) substitute the generator coordinates  $\tilde{s}$  and  $\tilde{s}'$  for the vectors of the cluster centers, eq. (2.8)  
Actually the program substitutes the dimensionless quantities  $SL(m) = (\beta/2)^{1/2} s_m$  and  $SR(m) = (\beta/2)^{1/2} s'_m$ .

As an example, we quote the REDUCE program 8 for the calculation of

$$\langle \Phi_5^+ He-p (1ms) | V^{(D)} WD + V^{(M)} WM | \Phi_5^+ He-p (1m's') \rangle * B_6 / F$$

COMMENT REDUCE PROGRAM 8

MANY-BODY MATRIX ELEMENT OF THE CENTRAL INTERACTION  
( 5HE-P, 1M, S | V(D)\*WD+V(M)\*WM| 5HE-P, 1M', S' ),  
EQS. (5.22,5.23). WD AND WM ARE THE WEIGHTS OF THE  
DIRECT AND THE EXCHANGE INTERACTION, RESPECTIVELY.\$

OPERATOR YL, YR, KRON, PHASE\$  
OFF ALLFAC\$

COMMENT THE SPECIFICATION OF THE OPERATOR PHASE AND THE  
DIFFERENTIATION RULES FOR THE SPHERICAL VECTOR COMPONENTS  
ARE THE SAME AS IN THE REDUCE PROGRAM 6\$

PROCEDURE NRM(I,K)\$  
COMMENT NRM(I,K) CALCULATES THE ELEMENTS N(I,K), EQ.(5.5)\$  
BEGIN  
R:=IF LL(I)=1 THEN (-YL(I,-ML)+YR(K,-ML))\*PHASE(ML) ELSE 1\$  
IF LR(K)=1 THEN R:=R\*(YL(I,MR)-YR(K,MR))  
+DF(R,YR(K,-MR))\*PHASE(MR)\$  
IF CL(I)-DL=0 OR CR(K)-DR=0 THEN RETURN R ELSE RETURN R\*B3\$  
END NRM\$

PROCEDURE GPT(OPT,I,J,K,L)\$  
COMMENT GPT(OPT,I,J,K,L) CALCULATES THE SPATIAL PART OF  
THE TWO-BODY MATRIX ELEMENT V(I,J,K,L), ASSUMING THAT AT  
MOST ONE OF THE PARTICLES OF EACH PAIR (I,J) AND (K,L)  
OCCUPIES A P-WAVE ORBIT WITH MAGNETIC QUANTUM NUMBER  
ML AND MR.\$  
BEGIN  
R:=1\$  
IF OPT=2 THEN R:=(YL(I,M1)-YL(J,M1))\*(YR(K,M2)-YR(L,M2))\$  
IF OPT=3 THEN R:=(YL(I,M1)-YL(J,M1)+YR(K,M1)-YR(L,M1))  
\*(YL(I,M2)-YL(J,M2)+YR(K,M2)-YR(L,M2))\$  
IF LL(I)=1 THEN  
R:=R\*PHASE(ML)\*(-DELTA\*(YL(I,-ML)-YL(J,-ML)+YR(K,-ML)  
-YR(L,-ML))-(YL(I,-ML)-YR(K,-ML)))+DF(R,YL(I,ML))\$  
IF LL(J)=1 THEN  
R:=R\*PHASE(ML)\*( DELTA\*(YL(I,-ML)-YL(J,-ML)+YR(K,-ML)  
-YR(L,-ML))-(YL(J,-ML)-YR(L,-ML)))+DF(R,YL(J,ML))\$  
IF LR(K)=1 THEN  
R:=R\*(-DELTA\*(YL(I,MR)-YL(J,MR)+YR(K,MR)-YR(L,MR))  
+(YL(I,MR)-YR(K,MR)))+DF(R,YR(K,-MR))\*PHASE(MR)\$  
IF LR(L)=1 THEN  
R:=R\*( DELTA\*(YL(I,MR)-YL(J,MR)+YR(K,MR)-YR(L,MR))  
+(YL(J,MR)-YR(L,MR)))+DF(R,YR(L,-MR))\*PHASE(MR)\$  
IF CL(I) NEQ CL(J) THEN R:=R\*B4\$  
IF CR(K) NEQ CR(L) THEN R:=R\*B5\$  
CS:=1+(CL(I)-CL(J))\*(CR(K)-CR(L))\$  
IF CS=1 THEN R:=R\*B6\$  
IF CS=2 THEN R:=R\*B6\*B6\$  
R:=IF CL(I)-DL=0 OR CR(K)-DR=0 THEN R ELSE R\*B3\$  
R:=IF CL(J)-DL=0 OR CR(L)-DR=0 THEN R ELSE R\*B3\$  
RETURN R\$  
END GPT\$

```
COMMENT IMPLEMENTATION OF TABLE I$  
ARRAY B(2),CN(6),CL(6),CR(6),T3(6),S3(6),LL(6),LR(6)$  
COMMENT EQ.(2.8)$  
B(1):=1/6$  
B(2):=-5/6$  
FOR I:=1:6 DO CN(I):=1$  
CN(3):=2$  
FOR I:=1:6 DO  
CL(I):=CR(I):=B(CN(I))$  
DL:=DR:=CL(1)$  
T3(1):=T3(2):=T3(3):=1$  
T3(4):=T3(5):=T3(6):=0$  
S3(1):=S3(3):=S3(4):=S3(6):=1$  
S3(2):=S3(5):=0$  
FOR I:=1:5 DO  
LL(I):=LR(I):=0$  
LL(6):=LR(6):=1$  
  
COMMENT NORMALIZATION MATRIX N(I,K),EQ.(5.5)$  
MATRIX N(6,6),U(4,4)$  
OPERATOR SL,SR,SLC,SRC$  
ARRAY SIG(24)$  
SIG(0):=1$  
FOR I:=1:24 DO SIG(I):=-SIG(I-1)$  
FOR I:=1:6 DO  
FOR K:=1:6 DO  
N(I,K):=IF T3(I)=T3(K) AND S3(I)=S3(K) THEN NRM(I,K) ELSE 0$  
A:=6$  
  
PROCEDURE CF2(I,J,K,L)$  
COMMENT CF2(I,J,K,L) CALCULATES GENERALIZED COFACTORS  
OF THE MATRIX N$  
BEGIN  
I2:=0$  
FOR I1:=1:A DO BEGIN  
IF I1=I OR I1=J THEN GOTO MJ$  
I2:=I2+1$  
K2:=0$  
FOR K1:=1:A DO BEGIN  
IF K1=K OR K1=L THEN GOTO MK$  
K2:=K2+1$  
U(I2,K2):=N(I1,K1)$  
MK: END$  
MJ: END$  
RETURN DET(U)*SIG(I+J+K+L)$  
END CF2$  
  
COMMENT CALCULATION OF THE MANY-BODY MATRIX ELEMENT$  
V:=0$  
FOR J:=2:6 DO  
FOR I:=1:(J-1) DO  
FOR L:=2:6 DO  
FOR K:=1:(L-1) DO  
BEGIN  
COF:=CF2(I,J,K,L)$  
IF COF=0 THEN GOTO NEXT$
```

```
IF T3(I) NEQ T3(K) OR S3(I) NEQ S3(K)
OR T3(J) NEQ T3(L) OR S3(J) NEQ S3(L) THEN GOTO ANTI$
V:=V+(WD*GPT(1,I,J,K,L)+WM*GPT(1,I,J,L,K))*COF$
ANTI:
IF T3(J) NEQ T3(K) OR S3(J) NEQ S3(K)
OR T3(I) NEQ T3(L) OR S3(I) NEQ S3(L) THEN GOTO NEXT$
V:=V-(WD*GPT(1,J,I,K,L)+WM*GPT(1,J,I,L,K))*COF$
NEXT:
END$
FOR I :=1:6 DO
FOR ALL M LET YL(I,M)=CL(I)*SL(M),YR(I,M)=CR(I)*SR(M)$
FOR ALL M LET
PHASE(M)*SL(-M)=SLC(M),
PHASE(M)*SR(-M)=SRC(M)$
V:=V;
V := SR(MR)*WM*B6*B5*DELTA**2*SRC(ML)
- SR(MR)*WM*B6*B5*DELTA*SRC(ML)
+ SR(MR)*WM*B5*B4*DELTA**2*SLC(ML)
- SR(MR)*WM*B5*B4*DELTA**2*SRC(ML)
+ SR(MR)*WM*B5*B4*DELTA*SRC(ML)
+ SR(MR)*WD*B6**2*B5*B4*DELTA**2*B3*SLC(ML)
+ SR(MR)*WD*B6**2*B5*B4*DELTA**2*B3*SRC(ML)
- SR(MR)*WD*B6*B5*DELTA**2*SRC(ML)
+ SL(MR)*WM*B6*B4*DELTA**2*SLC(ML)
- SL(MR)*WM*B6*B4*DELTA*SLC(ML)
- SL(MR)*WM*B5*B4*DELTA**2*SLC(ML)
+ SL(MR)*WM*B5*B4*DELTA**2*SRC(ML)
+ SL(MR)*WM*B5*B4*DELTA*SLC(ML)
- 2*SL(MR)*WM*B5*B4*DELTA*SRC(ML)
+ SL(MR)*WM*B5*B4*SRC(ML)
+ SL(MR)*WD*B6**2*B5*B4*DELTA**2*B3*SLC(ML)
+ SL(MR)*WD*B6**2*B5*B4*DELTA**2*B3*SRC(ML)
- SL(MR)*WD*B6*B4*DELTA**2*SLC(ML)
- WM*B6**2*B5*B4*KRON(ML,MR)*B3
- WM*B6*B5*DELTA*KRON(ML,MR)
- 3*WM*B6*B5*KRON(ML,MR)
- WM*B6*B4*DELTA*KRON(ML,MR)
- 3*WM*B6*B4*KRON(ML,MR)
+ 5*WM*B6*DELTA*KRON(ML,MR)*B3
- 4*WM*B6*DELTA*KRON(ML,MR)
+ 5*WM*B6*KRON(ML,MR)*B3
- 2*WM*B6*KRON(ML,MR)
+ WM*B5*B4*DELTA*KRON(ML,MR)
+ 4*WM*B5*B4*KRON(ML,MR)
- WD*B6**2*B5*B4*DELTA*KRON(ML,MR)*B3
+ 5*WD*B6**2*B5*B4*KRON(ML,MR)*B3
+ WD*B6*B5*DELTA*KRON(ML,MR)
- 4*WD*B6*B5*KRON(ML,MR)
+ WD*B6*B4*DELTA*KRON(ML,MR)
- 4*WD*B6*B4*KRON(ML,MR)
- 5*WD*B6*DELTA*KRON(ML,MR)*B3
+ 4*WD*B6*DELTA*KRON(ML,MR)
+ 10*WD*B6*KRON(ML,MR)*B3
- 6*WD*B6*KRON(ML,MR)
- WD*B5*B4*KRON(ML,MR)$
END$
```

## 6. INTERFACE BETWEEN SYMBOLIC AND NUMERICAL CALCULATIONS

In this Section, we consider the conversion of the algebraic expressions for various nuclear matrix elements into such a form as to make them amenable to numerical processing. As an example, let us consider the matrix element

$$V = \langle \Phi_5^+ \text{He-p} (1ms) | V^{(D)} \cdot WD + V^{(M)} \cdot WM | \Phi_5^+ \text{He-p} (1m's') \rangle B_6/F$$

obtained in the REDUCE program 8. As far as the dependence of  $V$  on the magnetic quantum numbers  $m$  and  $m'$  is concerned, we recognize five different types, namely

$$S_{mm}, S_m^* S_{m'}, S_m'^* S_{m'}, S_m^* S_{m'}, \text{ and } S_m'^* S_{m'}.$$

In calculating the reduced (in the sense of RACAH algebra) matrix element <sup>11)</sup>

$$\langle \Phi_5^+ \text{He-p} (L1s) | V^{(D)} WD + V^{(M)} WM | \Phi_5^+ \text{He-p} (L'1s') \rangle$$

i.e. projecting angular momentum, these five types are treated differently <sup>5)</sup>. It is therefore desirable, in a first step, to collect all terms which belong to the same type. REDUCE provides the operator COEFF which assigns coefficients of the various powers of a kernel, e.g. the statement COEFF (V,KRON (ML, MR), XO) assigns the i-th element of the array XO to the coefficient of the i-th power of KRON (ML,MR) in the expression V. Thus XO(1) contains now all terms of the first type. To collect all terms in the expression V which are proportional to  $S_m^* S_m'$  we first implement a substitution law of the type

```
FOR ALL ML,MR  MATCH SLC(ML)*SR(MR) = SLR(ML,MR) $
```

Then we use again the operator COEFF in the following way

COEFF (V,SLR(ML,MR),X1) to collect all terms of the second type in V. The terms of the remaining types are extracted similarly. In the next step we analyze each term of a given type with respect to its dependence on the exponential functions  $B_3 \dots B_6$  and the range parameter  $\delta$ . The discussion in Section 5 shows that V

is a polynomial in all these variables. Thus the coefficients of the various powers of  $B_3 \dots B_6$  and  $\delta$  may be extracted by a repeated application of the operator COEFF in nested DO loops. In the innermost DO loop we separate the terms proportional to WD (direct interaction) from those proportional to WM (Majorana exchange interaction) using the differentiation operator DF(...,WD) and DF(...,WM), respectively). The result of these manipulations (which is now just a number) together with the information on the type, the various powers of  $B_3 \dots B_6$ ,  $\delta$ , WD and WM is stored in a two-dimensional array RES. REDUCE offers the necessary facilities to produce a FORTRAN compatible file which may serve as input to a FORTRAN program.

COMMENT REDUCE PROGRAM 9

-----  
REDUCE OUTPUT PROCESSING.

THIS PROGRAM TAKES AS INPUT THE NUMERICAL EXPRESSION  
FOR V OBTAINED IN THE REDUCE PROGRAM 8 AND EXTRACTS  
ALL INFORMATION WHICH IS THEN STORED IN THE TWO-  
DIMENSIONAL ARRAY RES.

```
RES(IC,0)=|COEFFICIENT|
RES(IC,1)=1(DIRECT), 2(EXCHANGE)
RES(IC,2)=TYPE
RES(IC,3)=POWER OF B3
RES(IC,4)=POWER OF B4
RES(IC,5)=POWER OF B5
RES(IC,6)=POWER OF B6
RES(IC,7)=POWER OF DELTA
RES(IC,8)=SIG(COEFFICIENT)$
```

```
ARRAY X(4),R3(1),R4(1),R5(1),R6(2),RDEL(2),
X0(1),X1(1),X2(1),X3(1),X4(1),RES(40,8)$
OPERATOR SLR,SRL,SLL,SRR$
```

```
FOR ALL ML,MR MATCH
SLC(ML)*SR(MR)=SLR(ML,MR),
SRC(ML)*SL(MR)=SRL(ML,MR),
SLC(ML)*SL(MR)=SLL(ML,MR),
SRC(ML)*SR(MR)=SRR(ML,MR)$
```

```
COEFF(V,KRON(ML,MR),X0)$
COEFF(V,SLR(ML,MR),X1)$
COEFF(V,SRL(ML,MR),X2)$
COEFF(V,SLL(ML,MR),X3)$
COEFF(V,SRR(ML,MR),X4)$
```

```
X(0):=X0(1)$
X(1):=X1(1)$
X(2):=X2(1)$
X(3):=X3(1)$
X(4):=X4(1)$

IC:=0$

FOR IT:=0:4 DO
BEGIN
H:=X(IT)$
IF H=0 THEN GOTO NXIT$
M3:=COEFF(H,B3,R3)$
FOR I3:=0:M3 DO
BEGIN
H:=R3(I3)$
IF H=0 THEN GOTO NXI3$
M4:=COEFF(H,B4,R4)$
FOR I4:=0:M4 DO
BEGIN
H:=R4(I4)$
IF H=0 THEN GOTO NXI4$
M5:=COEFF(H,B5,R5)$
FOR I5:=0:M5 DO
BEGIN
H:=R5(I5)$
IF H=0 THEN GOTO NXI5$
M6:=COEFF(H,B6,R6)$
FOR I6:=0:M6 DO
BEGIN
H:=R6(I6)$
IF H=0 THEN GOTO NXI6$
MD:=COEFF(H,DELTA,RDEL)$
FOR ID:=0:MD DO
BEGIN
H:=RDEL(ID)$
IF H=0 THEN GOTO NXID$
Z:=DF(H,WD)$
IF Z=0 THEN GOTO NXM$
RES(IC,1):=1$
RES(IC,2):=IT$
RES(IC,3):=I3$
RES(IC,4):=I4$
RES(IC,5):=I5$
RES(IC,6):=I6$
RES(IC,7):=ID$
RES(IC,8):=IF Z<0 THEN 1 ELSE 0$
IF Z<0 THEN Z:=-Z$
RES(IC,0):=Z$
IC:=IC+1$
NXM:Z:=DF(H,WM)$
IF Z=0 THEN GOTO NXID$
```

```
RES(IC,1):=2$  
RES(IC,2):=I1$  
RES(IC,3):=I3$  
RES(IC,4):=I4$  
RES(IC,5):=I5$  
RES(IC,6):=I6$  
RES(IC,7):=ID$  
RES(IC,8):=IF Z<0 THEN 1 ELSE 0$  
IF Z<0 THEN Z:=-Z$  
RES(IC,0):=Z$  
IC:=IC+1$  
NXID:END$  
NXI6:END$  
NXI5:END$  
NXI4:END$  
NXI3:END$  
NXIT:END$  
  
FOR I:=0:IC-1 DO  
  WRITE " ",RES(I,1)," ",RES(I,2)," ",RES(I,3)," ",  
        RES(I,4)," ",RES(I,5)," ",RES(I,6)," ",  
        RES(I,7)," ",RES(I,8)," ",RES(I,0);  
  
  1 0 0 0 0 1 0 1 6$  
  2 0 0 0 0 1 0 1 2$  
  1 0 0 0 0 1 1 0 4$  
  2 0 0 0 0 1 1 1 4$  
  1 0 0 0 1 1 0 1 4$  
  2 0 0 0 1 1 0 1 3$  
  1 0 0 0 1 1 1 0 1$  
  2 0 0 0 1 1 1 1 1$  
  1 0 0 1 0 1 0 1 4$  
  2 0 0 1 0 1 0 1 3$  
  1 0 0 1 0 1 1 0 1$  
  2 0 0 1 0 1 1 1 1$  
  1 0 0 1 1 0 0 1 1$  
  2 0 0 1 1 0 0 0 4$  
  2 0 0 1 1 0 1 0 1$
```

1 0 1 0 0 1 0 0 10\$  
2 0 1 0 0 1 0 0 5\$  
1 0 1 0 0 1 1 1 5\$  
2 0 1 0 0 1 1 0 5\$  
1 0 1 1 1 2 0 0 5\$  
2 0 1 1 1 2 0 1 1\$  
1 0 1 1 1 2 1 1 1\$  
2 1 0 1 1 0 2 0 1\$  
1 1 1 1 1 2 2 0 1\$  
2 2 0 1 1 0 0 0 1\$  
2 2 0 1 1 0 1 1 2\$  
2 2 0 1 1 0 2 0 1\$  
1 2 1 1 1 2 2 0 1\$  
2 3 0 1 0 1 1 1 1\$  
1 3 0 1 0 1 2 1 1\$  
2 3 0 1 0 1 2 0 1\$  
2 3 0 1 1 0 1 0 1\$  
2 3 0 1 1 0 2 1 1\$  
1 3 1 1 1 2 2 0 1\$  
2 4 0 0 1 1 1 1 1\$  
1 4 0 0 1 1 2 1 1\$  
2 4 0 0 1 1 2 0 1\$  
2 4 0 1 1 0 2 1 1\$  
1 4 1 1 1 2 2 0 1\$

END\$

## 7. DISCUSSION

The calculation of many-body matrix elements in the nuclear cluster model is a typical hybrid <sup>2)</sup> problem requiring a combination of both symbolic and numerical techniques for its solution. Going through the previous Sections, one realizes that all calculations except one might have been performed in a FORTRAN program by giving explicit values to the variables  $B_1 \dots B_6$  and  $\beta$ . In solving the Hill-Wheeler equation <sup>9)</sup>, however, one would have to repeat the same calculation for many values of these variables. From an economical point of view it is therefore desirable to know the general expression and run a "smaller" FORTRAN program.

The above mentioned exception is the determination of the analytical dependence of many-body matrix elements on magnetic quantum numbers of individual nucleons occupying p-wave orbits. The method of projecting angular momentum developed in ref. 5 is based on the assumption that this dependence is known analytically.

In a more sophisticated calculation <sup>12)</sup>, e.g. if the oscillator parameter  $\beta$  is not the same for all particles, it turns out that an algebraic processing of determinants, cofactors etc. does not lead to any essential simplifications. However, the application of REDUCE is still of great advantage for calculating many-body matrix elements containing particles in orbits with  $\ell > 0$  from those containing particles in  $\ell = 0$  orbits only. To summarize: It is worthwhile to apply symbolic algebra to problems in the nuclear cluster model - and it makes great fun.

We wish to thank Dr. A. Kruppa and R. Kupsch for many helpful discussions. Two of us (R.B. and F.D.) are indebted to W. Abel for helping us to use the computer facilities at KfK.

REFERENCES

- 1 K. Wildermuth and Y.C. Tang, A Unified Theory of the Nucleus (Vieweg, Braunschweig, 1977)
- 2 W.S. Brown and A.C. Hearn, Comput. Phys. Commun. 17 (1979) 207
- 3 R. Beck, KfK-Report 3261 (1981)
- 4 A.C. Hearn, REDUCE User's Manual, Second Edition, University of Utah (March 1973)
- 5 R. Beck and F. Dickmann  
KfK-Report 3402 (1982)
- 6 R. Krivec and M.V. Mihailović,  
J. Phys. G: Nucl. Phys. 8 (1982) 821
- 7 A. Hasegawa and S. Nagata,  
Prog. Theor. Phys. 45 (1971) 1786
- 8 L.R. Suelzle, M.R. Yearian and H. Crannell,  
Phys. Rev. 162 (1967) 992
- 9 R. Beck and F. Dickmann, preprint
- 10 D.M. Brink and G.R. Satchler, Angular Momentum (Oxford University Press, Oxford, 1962)
- 11 A.R. Edmonds, Angular Momentum in Quantum Mechanics (Princeton University Press, Princeton, 1957)
- 12 R. Beck, F. Dickmann and A. Kruppa,  
to be published