PSR-338
DWBA91

OAK RIDGE NATIONAL LABORATORY

managed by
LOCKHEED MARTIN ENERGY RESEARCH CORPORATION
for the
U.S. DEPARTMENT OF ENERGY

RSICC PERIPHERAL SHIELDING ROUTINE COLLECTION

DWBA91

Code System for Fully Microscopic Analyses

of Nucleon-Nucleus Scattering

Contributed by:

Service de Physique Theorique, Gif-sur-Yvette, France
and
Theoretische Kernphysik, University of Hamburg, Hamburg, Germany
through the
NEA Data Bank, Iss-ley-Moulineaux, France

RADIATION SAFETY INFORMATION COMPUTATIONAL CENTER

Documentation for PSR-338/DWBA91 Code Package

**Please note there are no even numbered pages in this section.

(November 1993)

RSIC CODE PACKAGE PSR-338

1. NAME AND TITLE

DWBA91: Code System for Fully Microscopic Analyses of Nucleon-Nucleus Scattering.

AUXILIARY PROGRAM

DWBA91 - Interaction: generates input data for DWBA91 for the two-body interaction for a given energy based on the energy and density dependent effective interaction table.

2. CONTRIBUTORS

Service de Physique Theorique, CEA Saclay, Gif-sur-Yvette, France, and Theoretische Kernphysik, University of Hamburg, Hamburg, Germany through the NEA Data Bank, Issy-les-Moulineaux, France.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; VAX, CRAY, and IBM mainframe (P00338/MNYCP/00).

4. NATURE OF PROBLEM SOLVED

Direct interaction reaction cross sections and angular distributions are calculated. The relativistic cinematics option is included.

5. METHOD OF SOLUTION

The distorted wave Born approximation is used. DWBA91 includes a fully microscopic nonlocal optical model obtained with the description of the target by its occupation numbers and with the two-body interaction for the initial and final distorted waves. The effective interaction is input as a quasi potential operator which generates plane wave t-/g-matrix elements equal to those generated from some nucleon nucleon potentials. The effective interaction may comprise central, tensor, (LS), L**2 and (LS)**2 operator components with Yukawa form factors and complex density dependent strengths.

Minimum relativity makes allowance for DWBA91 to be used for projectiles at low and medium energy.

6. RESTRICTIONS OR LIMITATIONS

None noted.

7. TYPICAL RUNNING TIME

Sample problem execution times on a VAX 6000-420 with a 20% load percentage:

Sample problem 1 4 minutes 46 seconds
Sample problem 2 19 minutes 9 seconds
Sample problem 3 26 minutes 39 seconds

8. COMPUTER HARDWARE REQUIREMENTS

The codes run on Vax, IBM, Cray and CDC computers. Sample problem 3 requires slightly more than 15000 blocks of free space for the creation of scratch file (logical unit 8 - FOR008.DAT).

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran compiler is required. DWBA91 was tested at RSICC using VAX Fortran on a VAX 6000-420 running VMS 5.5-2.

10. REFERENCES

J. Raynal and H. V. von Geramb, "A New Microcscopic DWBA Code Version and Some Applications" (1992).

J. Raynal, "Notes on DWBA91" (September 9, 1991).

11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and 1 DS/HD (1.2 MB) diskette which contains the source code, sample input/output, and a README.RSI file which describes the installation and operation of DWBA91 and DWBA91 - Interaction written in DOS compressed self-extracting files.

12. DATE OF ABSTRACT

October 1993.

KEYWORDS: NUCLEAR MODELS

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A New Microscopic DWBA Code Version and Some Applications

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A new level of fully microscopic analyses of nucleon–nucleus scattering has been reached with the version DWBA91[1]. As compared to versions prior to 1990, a fully microscopic nonlocal optical model for the initial and final distorted waves has been included which makes use of a complex, energy and medium dependent effective interaction. The effective interaction is input as a quasi potential operator which generates plane wave t–/g–matrix elements equal to those generated from some nucleon nucleon potentials. The effective interaction may comprise central, tensor, (LS), L^2 and $(LS)^2$ operator components with Yukawa form factors and complex density dependent strengths. All features of the older versions of DWBAxx are still available as options despite the fact that many parts of the program have been rewritten or restructured. Minimum relativity makes allowance for the code to be used for projectiles at low and medium energy.

In this contribution we distinguish studies of the elastic scattering with the nonlocal optical models as compared to others with local microscopic and phenomenological optical models and studies of inelastic scattering.

The computations show that elastic scattering differential cross sections and spin observables are better reproduced with the nonlocal optical model as compared with local equivalents. The major change comes from the inclusion of L^2 and $(LS)^2$ operators in the effective interaction. With the new parametrization scheme [2] we greatly improved the reproduction of reference half–off shell t–/g–matrices in all partial waves with $\ell \leq 5$ and eliminated problems with the unitarity which were present in older formulations of effective interactions. Inelastic scattering uses the same effective interaction as transition operator and we made applications to some benchmark transitions in ^{12}C. Cross sections and angular distributions of spin observables for ^{12}C(p,p'), 1^+, T=0,1 at 12.71 and 15.11 MeV were computed and compared with some data at 185, 200, 318 and 400 MeV. The contributions from the L^2 and $(LS)^2$ operators to the spin-flip transitions are unexpectedly large. We attribute this to malfunction in very high partial waves of the effective interaction which the program generates and whose limits are only determined from the cutoff in partial waves and exchange multipoles. Similar results and conclusions can be drawn from calculations done for ^{40}Ca and ^{208}Pb. The program is not restricted to the here used form of the effective interaction but other parameterizations, which may be favored by a user, can be used as well.

1. J.Raynal, for inquiries use the E–mail address:
   RAYNAL@POSEIDON.SACLAY.CEA.FR
2. H.V. von Geramb, K. Amos, L. Berge, S. Bräutigam, H. Kohlhoff and I. Ingemarsson, Phys.Rev. C44 (1991) 73.

SECTION 2

NOTES ON DWBA91

by

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1. – DWBA70

The codes DWBAxx computes the inelastic scattering of nucleons on a target of which the excited state is described microscopically by particle-hole configurations, with a two body interaction. It is based on the helicity formalism of the multipole expansion of this interaction.

1.1. – THE TWO HELICITY FORMALISMS

The expansion of a distorted wave is usually written as:

$$\Xi_{\sigma}^{(+)}(\vec{k},\vec{r}) = \frac{4\pi}{kr} \sum_{j,l,m,\mu,\mu',\sigma'} i^l\, \Xi_{lj}(kr) \quad < l\frac{1}{2}\mu\sigma|jm >< l\frac{1}{2}\mu'\sigma'|jm > Y_l^{\mu *}(\hat{k})Y_l^{\mu'}(\hat{r})\,|\sigma' > \qquad (I-1)$$

where σ is the spin projection of the in going plane wave on an arbitrary axis and σ' its projection at the point $\vec{r}$ on the same axis.

1.1.1. – DESCRIPTION OF A DISTORTED WAVE

If we choose this arbitrary axis along $\vec{k}$, we introduce the usual helicity defined in [1] M. JACOB and G. C. WICK, Ann. of Phys. 7 , 404 (1959). with λ instead of σ:

$$|\sigma >= \sum_{\lambda} R_{\sigma,\lambda}^{(\frac{1}{2})^*}(\hat{k})|\lambda > \qquad (I-2)$$

The helicity formalism for multipole expansion as defined in [2] J. RAYNAL, Nucl. Phys. A97, 593 (1967). and also described in [3] J. RAYNAL, in *The structure of Nuclei* (IAEA, Vienna, 1972). consists in a similar projection of $|\sigma' >$ along $\vec{r}$. If ϕ_r, θ_r and ψ_r are the Euler angles between a frame with its z-axis along $\vec{k}$ and a frame with its z-axis along $\vec{r}$, this wave function may be written as:

$$\Xi_{\lambda}^{(+)}(\vec{k},\vec{r}) = \frac{1}{2k\sqrt{2\pi}} \sum_{j,\lambda'} (2j+1)\Xi_{\lambda,\lambda'}^{j}(kr)R_{\lambda,\lambda'}^{(j)^*}(\phi_r,\theta_r,\psi_r)|\lambda' > \qquad (I-3)$$

where the helicity functions $\Xi_{\lambda,\lambda'}^{j}$ are:

$$\Xi_{\lambda,\lambda'}^{j} = \frac{i^{j-\frac{1}{2}}}{r}\{\Xi_{l=j-\frac{1}{2},j}(kr) + i(-)^{\lambda-\lambda'}\Xi_{l=j+\frac{1}{2},j}(kr)\} \qquad (I-4)$$

They do not have a well-defined parity.

1.1.2. – DESCRIPTION OF A BOUND STATE

The usual description of the bound state of a spin $\frac{1}{2}$ particle with orbital angular momentum l, a total angular momentum j and its projection m on the quantisation axis is:

$$|jm >= f_{lj}(r) \sum_{\mu,\sigma} < l\frac{1}{2}\mu\sigma|jm > Y_l^{\mu}(\theta,\phi)|\sigma > \qquad (I-5)$$

1.2.1. – SYMMETRIES OF THE MULTIPOLE EXPANSION

Some symmetry properties are also required, in general, of the two-body force. In order to study their consequences, it is simpler to choose the axis of quantisation along $\vec{r}_1$ together with a frame of reference for particle 2 given by the Euler angles $(0, \theta, 0)$ and obtain:

$$V_{\lambda_1'\lambda_2',\lambda_1\lambda_2}(1,2) = \sum_J V^J_{\lambda_1'\lambda_2',\lambda_1\lambda_2}(1,2)(-)^{\lambda_1'-\lambda_1} r^{(J)}_{\lambda_1'-\lambda_1,\lambda_2-\lambda_2'}(\theta) \qquad (I-12)$$

The action of the parity operator P is the same as for standard helicity because $\vec{r}$ and impulsion behave similarly:

$$V^J_{\lambda_1'\lambda_2',\lambda_1\lambda_2}(1,2) = V^J_{-\lambda_1'-\lambda_2',-\lambda_1-\lambda_2}(1,2) \qquad (I-13)$$

Time reversal invariance depends on the nature of the operators:

$$V^J_{\lambda_1'\lambda_2',\lambda_1\lambda_2}(1,2) = \eta V^J_{-\lambda_1-\lambda_2,-\lambda_1'-\lambda_2'}(1,2) \qquad (I-14)$$

where $\eta = -1$ for a derivative term or an expression odd in the permutation of λ and λ'.

When the two nucleons are identical:

$$V^J_{\lambda_1'\lambda_2',\lambda_1\lambda_2}(1,2) = V^J_{\lambda_2'\lambda_1',\lambda_2\lambda_1}(2,1) \qquad (I-15)$$

For a given value of J, the matrix $V_{\lambda_1'\lambda_2',\lambda_1\lambda_2}(1,2)$ can be written on the basis of Kronecker products of 2×2 matrices. They are two even matrices:

$$\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}, \qquad \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \qquad (I-16)$$

and two odd ones:

$$\begin{vmatrix} -1 & 0 \\ 0 & 1 \end{vmatrix}, \qquad \begin{vmatrix} 0 & -1 \\ 1 & 0 \end{vmatrix}. \qquad (I-17)$$

If parity conservation applies, the two-body interaction can be separated into an even part:

$$\begin{aligned} & a^J(1,2)\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \otimes \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} + b^J(1,2)\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \otimes \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \\ & + b'^J(1,2)\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \otimes \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} + c^J(1,2)\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \otimes \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \end{aligned} \qquad (I-18)$$

and an odd part:

$$\begin{aligned} & d^J(1,2)\begin{vmatrix} -1 & 0 \\ 0 & 1 \end{vmatrix} \otimes \begin{vmatrix} -1 & 0 \\ 0 & 1 \end{vmatrix} + e^J(1,2)\begin{vmatrix} -1 & 0 \\ 0 & 1 \end{vmatrix} \otimes \begin{vmatrix} 0 & -1 \\ 1 & 0 \end{vmatrix} \\ & + e'^J(1,2)\begin{vmatrix} 0 & -1 \\ 1 & 0 \end{vmatrix} \otimes \begin{vmatrix} -1 & 0 \\ 0 & 1 \end{vmatrix} + f^J(1,2)\begin{vmatrix} 0 & -1 \\ 1 & 0 \end{vmatrix} \otimes \begin{vmatrix} 0 & -1 \\ 1 & 0 \end{vmatrix} \end{aligned} \qquad (I-19)$$

If the two particle are identical:

$$\begin{aligned} & a^J(1,2) = a^J(2,1), \quad && b^J(1,2) = b'^J(2,1) \quad && c^J(1,2) = c^J(2,1), \\ & c^J(1,2) = c^J(2,1), \quad && e^J(1,2) = e'^J(2,1) \quad && f^J(1,2) = f^J(2,1), \end{aligned} \qquad (I-20)$$

and for its odd part:

$$d^J(1,2) = 2(r_1^2 + r_2^2)\Big\{\frac{J}{2J+1}V_{J-1}(r_1,r_2) + \frac{(J+1)}{2J+1}V_{J+1}(r_1,r_2)\Big\} - r_1r_2$$
$$-\Big\{\frac{J(J-1)}{(2J-1)(2J+1)}V_{J-2}(r_1,r_2) + \frac{14J^2+14J-10}{(2J-1)(2J+3)}V_J(r_1,r_2) + \frac{(J+1)(J+2)}{(2J+1)(2J+3)}V_{J+2}(r_1,r_2)\Big\}$$
$$\epsilon^J(1,2) = (2r_1^2 - r_2^2)\frac{\sqrt{J(J+1)}}{2J+1}\Big\{V_{J-1}(r_1,r_2) - V_{J+1}(r_1,r_2)\Big\} + r_1r_2\sqrt{J(J+1)}$$
$$\Big\{\frac{J-1}{(2J-1)(2J+1)}V_{J-2}(r_1,r_2) + \frac{1}{(2J-1)(2J+3)}V_J(r_1,r_2) - \frac{J+2}{(2J+1)(2J+3)}V_{J+2}(r_1,r_2)\Big\}$$
$$f^J(1,2) = -(r_1^2 + r_2^2)\Big\{\frac{(J+1)}{2J+1}V_{J-1}(r_1,r_2) + \frac{J}{2J+1}V_{J+1}(r_1,r_2)\Big\} - r_1r_2$$
$$\Big\{\frac{(J-1)(J+1)}{(2J-1)(2J+1)}V_{J-2}(r_1,r_2) - \frac{10J^2+10J-9}{(2J-1)(2J+3)}V_J(r_1,r_2) + \frac{J(J+2)}{(2J+1)(2J+3)}V_{J+2}(r_1,r_2)\Big\} \qquad (I-29)$$

1.3. - MATRIX ELEMENT BETWEEN BOUND STATES

After integration over angles, using the helicity formalism for the interaction and the bound states:

$$< j_1'm_1'| < j_2'm_2'|V(1,2)|j_1m_1 > |j_2m_2 >$$
$$= \sum_{J,\mu}(-)^{j_1-m_1+j_2'-m_2'}(2J+1)\begin{pmatrix} j_1' & J & j_1 \\ m_1' & \mu & -m_1\end{pmatrix}\begin{pmatrix} j_2' & J & j_2 \\ m_2' & \mu & -m_2\end{pmatrix} \; f^J_{j_1'j_2',j_1j_2} \qquad (I-30)$$

where

$$f^J_{j_1'j_2',j_1j_2} = \sum_{\lambda_1',\lambda_2',\lambda_1,\lambda_2}\frac{1}{4}\sqrt{(2j_1'+1)(2j_2'+1)(2j_1+1)(2j_2+1)}$$
$$\times(-)^{j_1-\lambda_1+j_2'-\lambda_2}\begin{pmatrix} j_1' & J & j_1 \\ \lambda_1' & \lambda_1-\lambda_1' & -\lambda_1\end{pmatrix}\begin{pmatrix} j_2' & J & j_2 \\ \lambda_2' & \lambda_2-\lambda_2' & -\lambda_2\end{pmatrix} \qquad (I-31)$$
$$\times\int\int V^J_{\lambda_1'\lambda_2',\lambda_1\lambda_2}(1,2)\phi^{j_1'*}_{\lambda_1'}(r_1)\phi^{j_2'*}_{\lambda_2'}(r_2)\phi^{j_1*}_{\lambda_1}(r_1)\phi^{j_2*}_{\lambda_2}(r_2)r_1^2r_2^2dr_1dr_2$$

1.3.1. - PARTICLE-PARTICLE AND PARTICLE-HOLE MATRIX ELEMENT

The antisymmetrised particle-particle matrix element is:

$$< j_1'\,j_2';JM|V(1,2)|j_1\,j_2;JM >$$
$$= \sum_{m_1',m_2',m_1,m_2} < j_1\,j_2\,m_1\,m_2|J\,M >< j_1'\,j_2'\,m_1'\,m_2'|J\,M >$$
$$\times\{< j_1'm_1'| < j_2'm_2'|V(1,2)(|j_1m_1 > |j_2m_2 > -|j_2m_2 > |j_1m_1 >)\} \qquad (I-32)$$
$$= \sum_{J'}(-)^{J+j_1+j_2}(2J'+1)\begin{Bmatrix} j_1 & j_2 & J \\ j_2' & j_1' & J'\end{Bmatrix}f^{J'}_{j_1'j_2',j_1j_2} - \sum_{J'}(2J'+1)\begin{Bmatrix} j_1 & j_2 & J \\ j_1' & j_2' & J'\end{Bmatrix}f^{J'}_{j_1'j_2',j_2j_1}$$

and when the matrix is non diagonal, the geometry is:

$$(-)^{l_1+1}\sqrt{(2j_1+1)(2j'_1+1)}\begin{pmatrix} j'_1 & J & j_1 \\ -\frac{1}{2} & 1 & -\frac{1}{2} \end{pmatrix} = \alpha^J_{j_1j'_1} G^J_{j_1j'_1} \qquad (\mathrm{I}-39)$$

Recurrence relations between Clebsh-Gordon coefficients gives:

$$\alpha^J_{j_1j'_1} = (-)^{l_1+j_1-\frac{1}{2}} \frac{(j_1+\frac{1}{2}) + (-)^{j_1+j'_1+J}(j'_1+\frac{1}{2})}{\sqrt{J(J+1)}} \qquad (\mathrm{I}-40)$$

which can be expressed whith the eigenvalue γ of $\vec{l}.\vec{\sigma}$ as follows:

$$\alpha^J_{j_1j'_1} = \begin{cases} \dfrac{\gamma_1-\gamma'_1}{\sqrt{J(J+1)}}, & \text{for a natural parity} \\ \dfrac{\gamma_1+\gamma'_1+2}{\sqrt{J(J+1)}}, & \text{for an unnatural parity} \end{cases} \qquad (\mathrm{I}-41)$$

or with the quantum number κ of Dirac equation because $\kappa = \gamma + 1$.

The coefficient $G^J_{j_1j'_1}$ is given by the summed formula which holds for 3-j coefficients of which the magnetic quantum numbers are zeros:

$$G^J_{jj'} = (-)^{In(\frac{J+j'-j+2}{2})} \frac{g(j+j'+J+1)}{g(J+j-j')g(J+j'-j)g(j+j'-J}. \qquad (\mathrm{I}-42)$$

where

$$g(n) = \frac{\sqrt{n!}}{n!!} = \begin{cases} \sqrt{\dfrac{2\times 4\times\ldots\times(n-1)}{3\times 5\times\ldots\times n}}, & \text{when n is odd} \\ \sqrt{\dfrac{2\times 4\times\ldots\times n}{3\times 5\times\ldots\times(n-1)}}, & \text{when n is even} \end{cases} \qquad (\mathrm{I}-43)$$

1.3.3. – PARITY OF THE PARTICLE-HOLE MATRIX ELEMENT

With the elementary matrices, the sum on the helicities of one particle involves two terms and the geometrical coefficient is:

$$\frac{1}{2}(-)^{j_1-\lambda_1}[1+\eta(-)^{l_1+l'_1+J}]\sqrt{(2j_1+1)(2j'_1+1)}\begin{pmatrix} j'_1 & j & j_1 \\ \lambda'_1 & \lambda_1-\lambda'_1 & -\lambda_1 \end{pmatrix} \qquad (\mathrm{I}-44)$$

where η is the symmetry of the matrix.

Therefore, there are two kind of particle-hole matrix elements

the "natural parity" matrix elements for which $l_1+l'_1+J$ is even. All the contribution of the interaction comes from its even part:

$$\begin{aligned} A^{Jj_1j'_1} &= G^J_{j_1j'_1}\int[a^J(1,2)+\alpha^J_{j_1j'_1}b'^J(2,1)]\phi^*_{l'_1j'_1}(r_1)\phi_{l_1j_1}(r_1)r_1^2dr_1 \\ B^{Jj_1j'_1} &= G^J_{j_1j'_1}\int[b^J(1,2)+\alpha^J_{j_1j'_1}c^J(1,2)]\phi^*_{l'_1j'_1}(r_1)\phi_{l_1j_1}(r_1)r_1^2dr_1 \end{aligned} \qquad (\mathrm{I}-45)$$

and for the odd part, the multipoles are:

$$
\begin{aligned}
d^J(1,2) &= -\frac{J(J+1)}{2(2J+1)}\Big\{2-\Big(\alpha^J_{j_1j_1'}\Big)^2-\Big(\alpha^J_{j_2j_2'}\Big)^2\Big\}(V_{J-1}-V_{J+1})\\
e^J(1,2) &= -\frac{\sqrt{J(J+1}}{2(2J+1)}\Big[\Big\{(J+2)V_{J-1}-(2J+1)\frac{r_2}{r_1}V_J+(J-1)V_{J+1}\Big\}\\
&\qquad -\Big(\alpha^J_{j_1j_1'}\Big)^2\Big\{(J+1)V_{J-1}-(2J+1)\frac{r_2}{r_1}V_J+JV_{J+1}\Big\}\Big]\\
f^J(1,2) &= -\frac{1}{2J+1}\Big\{(J+1)V_{J-1}+JV_{J+1}\Big\}+\frac{1}{2}\Big(\frac{r_1}{r_2}+\frac{r_2}{r_1}\Big)V_J
\end{aligned}
\qquad (I-50)
$$

In the even part, the multipole b is the sum of a derivative term:

$$
b_1^J(1,2)=\frac{\sqrt{J(J+1)}}{2J+1}\Big[(V_{J-1}-V_{J+1})\Big(r_2\frac{d}{dr_1}-r_1\frac{d}{dr_2}\Big)+\frac{1}{2(2J+1)}\Big(\frac{r_2}{r_1}-\frac{r_1}{r_2}\Big)(c_1V_{J-1}+c_2V_{J+1})\Big] \qquad (I-51)
$$

(where $c_1 = J+1$ and $c2 = J$, but where $c_1 = J-1$ and $c2 = J+2$ if the functions are multiplied by r as usual)

and a term odd for the permutation of j_1 and j_2 with j_1' and j_2':

$$
\begin{aligned}
b_2^J(1,2) &= \frac{(j_1+\frac{1}{2})^2-(j_1'+\frac{1}{2})^2}{2\sqrt{J(J+1)}}\Big[-V_J+\frac{r_2}{r_1}\Big\{\tfrac{J+1}{2J+1}V_{J-1}+\tfrac{J}{2J+1}V_{J+1}\Big\}\Big]\\
&+\frac{(j_2+\frac{1}{2})-(-)^{j_2+j_2'+J}(j_2'+\frac{1}{2})}{2\alpha^J_{j_2j_2'}}\Big[V_J-\frac{r_1}{r_2}\Big\{\tfrac{J}{2J+1}V_{J-1}+\tfrac{J+1}{2J+1}V_{J+1}\Big\}\Big]
\end{aligned}
\qquad (I-52)
$$

the departure from the previous geometry appears by this terms and the presence of α^2 in the "natural parity" two-body form factor a^J and in the "unnatural parity" ones c^J and ϵ^J.

There are five one body form factors for a natural parity excitation:

$$
\begin{aligned}
F_{LS} &= A(r)+B(r)\frac{(\gamma_i-\gamma_f)}{\sqrt{J(J+1)}}+A_1(r)\frac{(\gamma_i-\gamma_f)^2}{J(J+1)}+B_2(r)(\gamma_i+\gamma_f+2)\\
&+A_2(r)\frac{(\gamma_i-\gamma_f)(\gamma_i+\gamma_f+2)}{J(J+1)}+\Big\{A_3(r)+B_3(r)\frac{(\gamma_i-\gamma_f)}{\sqrt{J(J+1)}}\Big\}\frac{d}{dr}
\end{aligned}
\qquad (I-53)
$$

an only three for unnatural parity excitation:

$$
F_{LS}(r)=C(r)+D(r)\frac{(\gamma_i+\gamma_f+2)}{\sqrt{J(J+1)}}+C_1(r)\frac{(\gamma_i+\gamma_f+2)^2}{J(J+1)} \qquad (I-54)
$$

1.4.2. - EXPANSION FOR SMALL RANGES

In fact, the two body interaction is separated into four parts which are respectively $V_{(S=0,T=0)}$, $V_{(S=1,T=0)}$, $V_{(S=0,T=1)}$ and $V_{(S=1,T=1)}$. The tensor and the spin orbit interactions are pure $S=1$. For a central interaction:

$$
V_{(S=0)}=V\ \frac{1-\vec{\sigma}_1.\vec{\sigma}_2}{4},\qquad V_{(S=1)}=V\ \frac{3+\vec{\sigma}_1.\vec{\sigma}_2}{4} \qquad (I-55)
$$

for identical particles, $V_{T=0}$ do not contribute

This is easily understood in relative coordinates. For a relative angular momentum L, the symmetrised states are those with $L+S+T$ odd. The zero-range implies $L=0$ and the next term is $L=1$. As the spin orbit is $S=1$, its zero-range limit must be $T=1$ because it is for $L=1$.

1.4.4. – COMPARISON WITH MACROSCOPIC MODELS

When the excited state is collective, there are many contributions with different values of γ_p and γ_h which must cancel out. $V_J(r)$ is the transition form factor. Using:

$$\sum G^J_{j_pj_h}\frac{1}{r}f_p(r)\{\frac{d}{dr}f_h(r)\}=\frac{1}{2r}\{\frac{d}{dr}V_J(r)\},\qquad (\alpha^J_{j_pj_h})^2=\frac{1}{2} \tag{I - 62}$$

we get for a natural parity state, taking the Hermitian part:

$$V_{LS}(r)=\Big[(\gamma_i-\gamma_f)(\gamma_i-\gamma_f+1)-J(J+1)\Big]\frac{V_J(r)}{r^2}-2\gamma_i\frac{1}{r}\{\frac{1}{r}\frac{d}{dr}V_J(r)\}+2(\gamma_f-\gamma_i)\frac{V_J(r)}{r}\frac{d}{dr} \tag{I - 63}$$

to be compared to the macroscopic result:

$$\bar{\nabla}\{V_J(r)Y_J^M(\hat{r})\}\times\frac{\bar{\nabla}}{i}.\bar{\sigma}=\Big[\frac{1}{r}\{\frac{d}{dr}V_J(r)\}\gamma_i+\frac{V_J(r)}{r}(\gamma_i-\gamma_f)\frac{d}{dr}+\frac{V_J(r)}{2r^2}\{J(J+1)-(\gamma_i-\gamma_f)(\gamma_i-\gamma_f+1)\}\Big] \tag{I - 64}$$

and for an unnatural parity state:

$$V_{LS}(r)=\Big[(\gamma_i+\gamma_f+2)(\gamma_i+\gamma_f+1)-J(J+1)\Big]\frac{V_J(r)}{r^2}-(\gamma_i+\gamma_f)\frac{1}{r}\{\frac{1}{r}\frac{d}{dr}V_J(r)\} \tag{I - 65}$$

In the peculiar case $J=0$ and natural parity, summation over all the nucleons must lead to the optical model. The interaction is:

$$V_{LS}(r)=2\gamma_p\frac{V_0(r)\lambda}{r^2}+2(\gamma_p-\gamma_i)\frac{1}{r}\{\frac{d}{dr}V_0(r)\} \tag{I - 66}$$

where the factors γ_p disappear after summation on two complete shells with the same angular momentum l and the same radial functions.

1.5. – APPLICATION TO NUCLEAR REACTIONS AND CODE DWBA70

For an incoming particle in the direction $\bar{k}_i$ with the helicity σ_i on a nucleus without spin described by Ψ^{I_i} and an outcoming particle in the direction $\bar{k}_f$ with an helicity σ_f, the residual nucleus having the helicity μ_f described by a particle j_p and a hole j_h, $\Psi^{I_f}_{\mu_f}$ the reaction is described by the helicity amplitudes:

$$f_{\sigma_f\mu_f;\sigma_i}(\bar{k}_i,\bar{k}_f)=-\frac{m}{2\pi\hbar^2}\sqrt{\frac{v_f}{v_i}}<\Xi^{(-)}_{\sigma_f}(\bar{k}_f,\bar{r})\Psi^{I_f}_{\mu_f}|V|\Xi^{(+)}_{\sigma_i}(\bar{k}_f,\bar{r})\Psi^{I_i}> \tag{I - 67}$$

where v_i and v_f are the velocities in the initial and the final state. The normalisation has been chosen in such a way that:

$$\frac{d\sigma}{d\Omega}(\bar{k}_i,\bar{k}_f)=\frac{1}{2}\sum_{\sigma_i,\sigma_f,\mu_f}|f_{\sigma_f\mu_f;\sigma_i}(\bar{k}_i,\bar{k}_f)|^2 \tag{I - 68}$$

$(\vec{L}.\vec{S})$ for identical and different particles. Central and $(\vec{L}.\vec{S})$ interactions can have zero range limit.

In fact, in these calculations we use only Yukawa form factors because its multipole expansion:

$$\frac{\exp(-\lambda|\vec{r}_1-\vec{r}_2|)}{\lambda|r_1-r_2|}=\sum_{L=0}^{\infty}(2L+1)\; i\; j_L(i\lambda r_<)\; h_L^{(+)}(i\lambda r_>)\; P_L(\cos\theta) \qquad (I-73)$$

is such that the double integral over r_1 and r_2 reduces to three single integrals.

orbit interaction as they were used in DWBA70. Notations for Skyrme force are usually 4π those of DWBA70.

The t_1 term of the Skyrme force includes a double derivative on the wave function in relative coordinates. So, it acts in relative $L = 0$ state and is the next term to the zero range scalar interaction:

$$t_1 \Rightarrow V^{Skyrme}_{(S=0,T=1)} + V^{Skyrme}_{(S=1,T=0)} \qquad (II-7)$$

The t_2 term of the Skyrme force includes a single derivative on the wave function in relative coordinates on the right and on the left. So, it acts in relative $L = 1$ and:

$$t_2 \Rightarrow V^{Skyrme}_{(S=0,T=0)} + V^{Skyrme}_{(S=1,T=1)} \qquad (II-8)$$

Similar expressions are obtained for the zero range limit of the tensor interaction. There are two parts: the tensor interaction in relative $L = 1$ state, which is $T = 1$ and the tensor interaction between relative $L = 0$ and relative $L = 2$ state, which is $T = 0$:

$$V^T \Rightarrow V^{T,0-limit}_{(S=1,T=0)} + V^{T,0-limit}_{(S=1,T=1)} \qquad (II-9)$$

One has to take into account that this last interaction is the limit of $\frac{1}{r}\frac{d^4}{dr^4}r$ acting in relative coordinates.

3.1.2. - STRUCTURE OF THE MULTIPOLES

With these notations, the spin-orbit one body form factor reads:

$$F_{LS} = A(r) + B(r)Y_1 + A_1(r)Y_2 + A_2(r)Y_3 + B_2(r)Y_4 + \left\{A_3(r) + B_3(r)Y_1\right\}\frac{d}{dr} \qquad \text{(III - 2)}$$

for a natural parity excitation and:

$$F_{LS}(r) = C(r) + D(r)Y_1 + C_1(r)Y_2 \qquad \text{(III - 3)}$$

for an unnatural parity excitation. Note that there is a difference of a factor $\sqrt{J(J+1)}$ with the previous definition for the form factors $B(r)$, $B_3(r)$ and $D(r)$ and a factor $J(J+1)$ for $A_1(r)$, $A_2(r)$ and $C_1(r)$.

The multipoles of an interaction for the computation of a particle hole matrix element f^J involve terms:

$$U_{L,int} = r_1^m r_2^n \frac{d^{p+q}}{dr_1^p dr_2^q} V_L(r_1, r_2) \qquad \text{(III - 4)}$$

with $m + n - p - q = 0$ except for the tensor interaction in which $m + n = 2$, $p = q = 0$. The parity of such term for the change $r_1 \rightarrow -r_1$ is:

$$\eta = (-)^{m-p+L} = (-)^{n-q+L}$$

For a natural parity matrix element, $\eta = (-)^J$ and for an unnatural parity matrix element, $\eta = (-)^{J+1}$. So:

$$(-)^{m-p} = (-)^{n-q} = \begin{cases} (-)^{J-L}, & \text{for a natural parity} \\ (-)^{J-L+1}, & \text{for an unnatural parity} \end{cases} \qquad \text{(III - 5)}$$

The total geometrical coefficient for this term which exists only if $L \geq 0$ is:

$$(-)^{j_2'-j_2} G^J_{j_2 j_2'} G^J_{j_1 j_1'} \frac{P_{L,int}(J, \alpha^J_{j_1 j_1'}, \beta^J_{j_1 j_1'}, \alpha^J_{j_2 j_2'}, \beta^J_{j_2 j_2'})}{Q_{L,int}(J)} \qquad \text{(III - 6)}$$

where $P_{L,int}$ and $Q_{L,int}$ are polynomials.

For all the interactions which we have in mind:

1) The denominator polynomial $Q_{L,int}(J)$ is a product of terms
   a) like $(2J+1)$, $(2J-1)$, $(2J+3)$, $(2J-3)$ and so on,
   b) but also $(J+2)$, $(J+1)$, J and $(J-1)$ (these two last terms can give trouble when $J = 0$ or $J = 1$ if they appear for $L \geq J$ or $L \geq J-1$ respectively).
2) The numerator polynomial $P_{L,int}(J, \alpha^J_{j_1 j_1'}, \beta^J_{j_1 j_1'}, \alpha^J_{j_2 j_2'}, \beta^J_{j_2 j_2'})$ is of any degree in J and up to the third degree in $(\alpha^J_{j_1 j_1'}, \beta^J_{j_1 j_1'})$, $(\alpha^J_{j_2 j_2'}$ and $\beta^J_{j_2 j_2'})$ separetely. It has been found that this dependence can be rewritten in terms of the 11 X_i and 11 Y_i only.

The X_i and Y_i has been chosen such that the terms with a dangerous denominator does not exist.

1) For $J = 0$, $\alpha = 0, \beta \neq 0$, so $X_4 = -X_5$, $X_6 = -X_9$ and all the other X_i vanish (same behaviour for the Y_i).
2) For $J = 1$, $\alpha = \pm 1, \beta \neq 0$ or $\alpha \neq 0, \beta = 0$, so $X_5 = X_9 = X_{10} = X_{11} = 0$ (same behaviour for the Y_i).

The matrix element of $(\bar{L}.\bar{\sigma}_1)$ has been divided in four parts:

$$\begin{aligned}
&1) \quad i\Big(\bar{r}_1 \times \bar{r}_2\Big\{\frac{1}{r_2}\frac{d}{dr_1} - \frac{1}{r_1}\frac{d}{dr_2}\Big\}\Big).\bar{\sigma}_1\\
&2) \quad \frac{1}{r_2^2}\Big(\bar{r}_1 \times \Big\{\bar{r}_2 \times \bar{L}_2\Big\}\Big).\bar{\sigma}_1\\
&3) \quad \frac{1}{r_1^2}\Big(\bar{r}_2 \times \Big\{\bar{r}_1 \times \bar{L}_1\Big\}\Big).\bar{\sigma}_1\\
&4) \quad \Big(\bar{L}_1 + \bar{L}_2\Big).\bar{\sigma}_1
\end{aligned} \qquad \text{(III - 13)}$$

and the polynomials $Q(J)$ and $P(J,\ldots)$ obtained for each product. This job was done numerically for each term

1) by finding which is the polynomial $Q(J)$ which gives integer values of $P(J,\ldots)$
2) by finding by difference on J the polynomials in α and β which multiply each power of J in $P(J,\ldots)$
3) by identifying these polynomials in α and β.

A similar operation has to be done in order to separate $\bar{L}^2_{(S=0,T=0)}$, $\bar{L}^2_{(S=0,T=1)}$, $\bar{L}^2_{(S=1,T=0)}$ and $\bar{L}^2_{(S=1,T=1)}$ to obtain $\bar{L}^2(\bar{\sigma}_1.\bar{\sigma}_2)$ with $\bar{L}^2$ and $(\bar{\sigma}_1.\bar{\sigma}_2)$.

Three results have been obtained for natural parity matrix elements and three others for unnatural parity matrix elements. They are those of $\bar{L}^2$, $\bar{L}^2$ $(\bar{\sigma}_1.\bar{\sigma}_2)$ and $(\bar{L}.\bar{\sigma}_1)(\bar{L}.\bar{\sigma}_2)$.

3.2. – MULTIPOLES OF $\bar{L}^2$ AND $(\bar{L}.\bar{S})^2$ INTERACTIONS

Among six expressions needed, the $\bar{L}^2$ for unnatural parity is the only one manageable to be printed in one piece:

$$\bar{L}^2 = \frac{1}{8}\Big(V_{J-1} + V_{J+1} - (\frac{r_1}{r_2} + \frac{r_2}{r_1})V_J\Big)\Big(1 - \frac{X_1 - X_2}{J(J+1)}\Big)\Big(1 - \frac{Y_1 - Y_2}{J(J+1)}\Big) \qquad \text{(III - 14)}$$

3.2.1. – NUMBER OF MULTIPOLES AND SYMMETRIES

All the others five interactions are of the form

$$\begin{aligned}
&\sum_L C_1^L V_L\Big(r_1^2\frac{d^2}{dr_2^2} - 2r_1r_2\frac{d^2}{dr_1dr_2} + r_2^2\frac{d^2}{dr_1^2}\Big)\\
&+\sum_L C_2^L V_L\frac{r_1^2}{r_2}\frac{d}{dr_2} + \sum_L C_3^L V_L\frac{r_2^2}{r_1}\frac{d}{dr_1} + \sum_{L'} C_4^{L'} V_{L'} r_1\frac{d}{dr_2}\\
&+\sum_L D_2^L V_L r_1\frac{d}{dr_1} + \sum_L D_3^L V_L r_2\frac{d}{dr_2} + \sum_{L'} D_4^{L'} V_{L'} r_2\frac{d}{dr_1}\\
&+\sum_L C_5^L\frac{r_1^2}{r_2^2}V_L + \sum_L C_6^L V_L + \sum_L C_7^L\frac{r_2^2}{r_1^2}V_L + \sum_{L'} C_8^{L'}\frac{r_1}{r_2}V_{L'} + \sum_{L'} C_9^{L'}\frac{r_2}{r_1}V_{L'}
\end{aligned} \qquad \text{(III - 15)}$$

with

$$D_2^L = -C_2^L - C_1^L, \qquad D_3^L = -C_3^L - C_1^L, \qquad D_4^{L'} = -C_4^{L'} \qquad \text{(III - 16)}$$

4) the tensor interaction has different multipoles which we can write:

$$C^J = (r_1^2 + r_2^2)\frac{X_1 Y_1}{J(J+1)} \qquad C^{J-1} = -r_1 r_2 \frac{(2J+3)X_1Y_1}{(2J+1)J(J+1)} \qquad C^{J+1} = -r_1 r_2 \frac{(2J-1)X_1Y_1}{(2J+1)J(J+1)} \tag{III - 23}$$

3.2.2.1. – EVEN PARITY MULTIPOLE EXPANSION OF $\vec{L}^2$

$$C_1^{J-2} = \frac{J(J-1)}{4(2J-1)} \qquad C_1^J = -\frac{(2J+1)(J^2+J-1)}{2(2J-1)(2J+3)} \qquad C_1^{J+2} = \frac{(J+1)(J+2)}{4(2J+3)} \tag{III - 24}$$

$$\begin{aligned}
C_2^{J-2} =& \frac{J-1}{4(2J-1)}\left[J(J-2) - Y_1 + Y_3\right]\\
C_2^J =& -\frac{2J+1}{4(2J-1)(2J+3)}\left[J(J+1) + Y_1 - Y_3\right]\\
C_2^{J+2} =& -\frac{J+2}{4(2J+3)}\left[(J+1)(J+3) - Y_1 + Y_3\right]\\
C_4^{J-1} =& -C_4^{J+1} = -\frac{1}{4}\left[X_1 - X_3 - Y_1 + Y_3\right]
\end{aligned} \tag{III - 25}$$

$$\begin{aligned}
C_5^{J-2} =& \frac{1}{16(2J-1)}\left[(J-1)\{(J-3)[J(J-2) - 2Y_1 + 2Y_3] - Y_2 + 2Y_4 - Y_6\} - 2Y_5 + Y_9\right]\\
C_5^J =& -\frac{2J+1}{8(2J-1)(2J+3)}\left[(J-1)(J+2)\{J(J+1) + 2Y_1 - 2Y_3\} - 2(J^2+J-1)(Y_2 - 2Y_4 + Y_6)\right.\\
&\left. - 2Y_5 + Y_9\right]\\
C_5^{J+2} =& \frac{1}{16(2J+3)}\left[(J+2)\{(J+4)[(J+1)(J+3) - 2Y_1 + 2Y_3] + Y_2 - 2Y_4 + Y_6\} - 2Y_5 + Y_9\right]
\end{aligned} \tag{III - 26}$$

$$\begin{aligned}
C_6^{J-2} =& -\frac{J-1}{8J(2J-1)}\left[J(J-1) - X_1 + X_3\right]\left[J(J-1) - Y_1 + Y_3\right]\\
C_6^J =& \frac{2J+1}{16}\left[X_2 - 2X_4 + X_6 + Y_2 - 2Y_4 + Y_6 - \frac{2}{(2J-1)(2J+3)}\{6J^4 + 12J^3 + 23J^2 + 17J - 16\right.\\
&\left. - 2(J^2+J-1)(X_1 - X_3 + Y_1 - Y_3)\} - \frac{6(X_1 - X_3)(Y_1 - Y_3)}{J(J+1)(2J-1)(2J+3)}(2J^2 + 2J - 1)\right]\\
C_6^{J+2} =& -\frac{J+2}{8(J+1)(2J+3)}\left[(J+1)(J+2) - X_1 + X_3\right]\left[(J+1)(J+2) - Y_1 + Y_3\right]
\end{aligned} \tag{III - 27}$$

$$\begin{aligned}
C_8^{J-1} =& \frac{1}{8}\left[(J-1)\{J(J+1) - X_1 + X_3 + Y_1 - Y_3\} - J(Y_2 - 2Y_4 + Y_6)\right.\\
&\left. + \frac{1}{J}(X_1 - X_3)(Y_1 - Y_3)\right]
\end{aligned}$$

$$C_6^{J-2}=\frac{1}{16(2J-1)}\Big[(J-1)\{2J(J^2-J+1)+(J-1)(J-2)(X_1+Y_1)-(2J-1)(X_2+Y_2)$$
$$+(2J^2+1)(X_4+Y_4)\}-(J+1)(X_5+Y_5)+\frac{1}{J}\{(J-1)\Big((J-1)[(J-1)(2X_1Y_1+X_4Y_1$$
$$+X_1Y_4)-X_2Y_1-X_1Y_2]+2(J^2+J+1)X_4Y_4-(2J+1)(X_4Y_2+X_2Y_4)+X_5Y_1+X_1Y_5$$
$$+2X_2Y_2\Big)-(J+2)(X_5Y_4+X_4Y_5)+X_5Y_2+X_2Y_5\}+\frac{2X_5Y_5}{J(J-1)}\Big]$$

$$C_6^{J}=\frac{2J+1}{16}\Big[X_2+Y_2+\frac{1}{J(J+1)}\{(3X_3-X_8)Y_1+X_1(3Y_3-Y_8)\}-\frac{1}{(2J-1)(2J+3)}\{4(J^4+2J^3$$
$$-8J^2-9J+6)+(7J^2+7J-6)(X_1+Y_1)+3(6J^2+6J-5)(X_4+Y_4)-3X_5-3Y_5$$
$$-2(2J^2+2J-1)X_1Y_1-(2J^2+2J-1)(X_4Y_1+X_1Y_4)-(X_2+2X_5)Y_1-X_1(Y_2+2Y_5)\}$$
$$-\frac{1}{J(J+1)(2J-1)(2J+3)}\{2(2J^2+2J-3)X_2Y_2-6(2J^4+4J^3-J^2-3J+2)X_4Y_4$$
$$+6(J-1)(J+2)(X_5Y_4+X_4Y_5)+3[(X_4+X_5)Y_2+X_2(Y_4+Y_5)-4X_5Y_5]\}\Big]$$

$$C_6^{J+2}=\frac{1}{16(2J+3)}\Big[(J+2)\{2(J+1)(J^2+3J+3)-(J+2)(J+3)(X_1+Y_1)-(2J+3)(X_2+Y_2)$$
$$-(2J^2+4J+3)(X_4+Y_4)\}+J(X_5+Y_5)+\frac{1}{J+1}\{(J+2)\Big((J+2)[(J+2)(2X_1Y_1+X_4Y_1$$
$$+X_1Y_4)+X_2Y_1+X_1Y_2]+2(J^2+J+1)X_4Y_4+(2J+1)(X_4Y_2+X_2Y_4)+X_5Y_1+X_1Y_5$$
$$+2X_2Y_2\Big)-(J-1)(X_5Y_4+X_4Y_5)-X_5Y_2-X_2Y_5\}+\frac{2X_5Y_5}{(J+1)(J+2)}\Big]$$
(III - 33)

$$C_8^{J-1}=\frac{1}{16}\Big[(J-1)\{(3J-3X_1+3Y_1-(2J+1)X_4\}+3JY_4-3Y_2+X_5+\frac{3}{J}X_1Y_1$$
$$-\frac{1}{J(J+1)}\{(J-1)[(J^2+J+1)(X_4Y_1-X_1Y_4)+X_5Y_1-X_1Y_5]-(2J^2+2J-1)X_4Y_2$$
$$-(J^2-5J-5)X_1Y_3+(2J^3+3J^2-2)X_4Y_4-(J+2)(X_5Y_4+X_4Y_5)-(2J+1)X_1Y_8$$
$$+X_5Y_2+X_1Y_{11}\}-\frac{2X_5Y_5}{J(J-1)(J+1)}\Big]$$

$$C_8^{J+1}=-\frac{1}{16}\Big[(J+2)\{(3J+3+3X_1-3Y_1-(2J+1)X_4\}-3(J+1)Y_4-3Y_2+X_5-\frac{3}{J+1}X_1Y_1$$
$$+\frac{1}{J(J+1)}\{(J+2)[(J^2+J+1)(X_4Y_1-X_1Y_4)+X_5Y_1-X_1Y_5]+(2J^2+2J-1)X_4Y_2$$
$$+(J^2+7J+1)X_1Y_3+(2J^3+3J^2+1)X_4Y_4-(J-1)(X_5Y_4+X_4Y_5)-(2J+1)X_1Y_8$$
$$-X_5Y_2-X_1Y_{11}\}+\frac{2X_5Y_5}{J(J+1)(J+2)}\Big]$$
(III - 34)

For $J=0$, the non vanishing values of the coefficients above are:

$$C_6^0=\frac{(2-X_4)(2-Y_4)}{8}\qquad C_6^2=\frac{(2-X_4)(2-Y_4)}{16}\qquad C_8^1=-\frac{3(2-X_4)(2-Y_4)}{32}\qquad \text{(III - 35)}$$

with special formulae for C_8^0 and C_8^1.

$$C_6^{J+2} = \frac{1}{8}\Big[(J+2)\{(J+1)^2 - X_2 - Y_2 - J(X_4+Y_4)\} + X_5 + Y_5 + \frac{1}{J(2J+3)}\{(J+2)[(J+2)^2 X_1 Y_1$$
$$+ (2J-1)(X_4Y_2 + X_2Y_4)] - 2X_5Y_2 - 2X_2Y_5\} - \frac{1}{J(J+1)(2J+3)}\{(J+2)\Big((J+2)$$
$$[(X_2 - X_4 - X_5)Y_1 + X_1(Y_2 - Y_4 - Y_5)] - (2J^3 + J^2 - J + 1)X_4Y_4 - (2J+1)X_2Y_2\Big)$$
$$+ (2J^2 + J - 2)(X_5Y_4 + X_4Y_5)\} + \frac{(3J+4)X_5Y_5}{J(J+1)(J+2)(2J+3)}\Big] \qquad \text{(III - 39)}$$

$$C_8^{J-1} = -\frac{1}{8}\Big[(J-1)\{J^2 - X_2 - Y_2 + (J+1)(X_4+Y_4) + X_1Y_1\} - X_5 - Y_5 + \frac{1}{J+1}\{X_2Y_2 + X_1(2Y_3 - Y_7$$
$$- Y_8)\} - \frac{1}{J(J+1)}\{(J^2+J-1)(X_4Y_2 + X_2Y_4) - (J^3 + 2J^2 - 2)X_4Y_4 - (J-1)[X_1(Y_2 - Y_4$$
$$- Y_5) - (X_2 - X_4 - X_5)Y_1] + (J+2)(X_5Y_4 + X_4Y_5) - X_5Y_2 - X_2Y_5\} + \frac{2X_5Y_5}{J(J-1)(J+1)}\Big]$$
$$C_8^{J+1} = -\frac{1}{8}\Big[(J+2)\{(J+1)^2 - X_2 - Y_2 - J(X_4+Y_4) + X_1Y_1\} + X_5 + Y_5 + \frac{1}{J}\{X_2Y_2 + X_1(2Y_3 - Y_7$$
$$- Y_8)\} + \frac{1}{J(J+1)}\{(J^2+J-1)(X_4Y_2 + X_2Y_4) + (J^3 + J^2 - J + 1)X_4Y_4 + (J+2)[X_1(Y_2 - Y_4$$
$$- Y_5) - (X_2 - X_4 - X_5)Y_1] - (J-1)(X_5Y_4 + X_4Y_5) - X_5Y_2 - X_2Y_5\} + \frac{2X_5Y_5}{J(J+1)(J+2)}\Big] \qquad \text{(III - 40)}$$

For $J = 0$, the non vanishing values of the coefficients above are:

$$C_6^0 = C_6^2 = -C_8^1 = \frac{(2 - X_4)(2 - Y_4)}{16} \qquad \text{(III - 41)}$$

with special formulae for all.

3.2.3. – ODD PARITY MULTIPOLE EXPANSIONS

Let us give in these notations the multipoles of the other interactions:

1) the central interaction vanishes.
2) the $(\vec{\sigma}_1.\vec{\sigma}_2)$ has only two multipole:

$$C_6^{J-1} = \frac{(J + X_1)(J + Y_1)}{(2J+1)J} \qquad C_6^{J+1} = \frac{(J + 1 - X_1)(J + 1 - Y_1)}{(2J+1)(J+1)} \qquad \text{(III - 42)}$$

3) the spin orbit interaction has only:

$$C_6^{J-1} = -\frac{1}{8(2J+1)}\Big[2J(J+1) + (J+2)(X_1 + Y_1) - X_2 - Y_2 + \frac{1}{J}(2X_1Y_1 - X_2Y_1 - X_1Y_2)\Big]$$
$$C_6^{J-1} = \frac{1}{8(2J+1)}\Big[2J(J+1) - (J-1)(X_1 + Y_1) - X_2 - Y_2 + \frac{1}{(J+1)}(2X_1Y_1 - X_2Y_1 - X_1Y_2)\Big]$$
$$C_8^{J} = \frac{1}{8J(J+1)}\Big[J(J+1) + Y_1 - Y_2\Big]X_1 \qquad \text{(III - 43)}$$

$$C_6^{J-1} = \frac{1}{16}\Big[J\{4J-(J-1)(X_1+Y_1)\} - 3X_2 + X_7 - 3Y_2 + Y_7 - \frac{1}{J}(3X_2Y_1 + 3X_1Y_2 - X_7Y_1 - X_1Y_7) - \frac{1}{J+1}\{2(J^2+J+1)X_1Y_1 - (J^2+J-1)(X_4Y_1 + X_1Y_4) + (X_3+X_5)Y_1 + X_1(Y_3+Y_5)\} + \frac{1}{J(J+1)}\{(J^2+J-1)(X_4Y_3+X_3Y_4) - 2(J^2-2)X_4Y_4 + 2(J+2)(X_5Y_4+X_4Y_5) + 2X_3Y_3 - X_5Y_3 - X_3Y_5\} - \frac{4X_5Y_5}{J(J-1)(J+1)}\Big]$$

$$C_6^{J-1} = -\frac{1}{16}\Big[(J+1)\{4(J+1)-(J+2)(X_1+Y_1)\} - 3X_2 + X_7 - 3Y_2 + Y_7 + \frac{1}{J+1}(3X_2Y_1 + 3X_1Y_2 - X_7Y_1 - X_1Y_7) + \frac{1}{J}\{2(J^2+J+1)X_1Y_1 - (J^2+J-1)(X_4Y_1+X_1Y_4) + (X_3+X_5)Y_1 + X_1(Y_3+Y_5)\} + \frac{1}{J(J+1)}\{(J^2+J-1)(X_4Y_3+X_3Y_4) - 2(J^2+2J-1)X_4Y_4 - 2(J-1)(X_5Y_4+X_4Y_5) + 2X_3Y_3 - X_5Y_3 - X_3Y_5\} + \frac{4X_5Y_5}{J(J+1)(J+2)}\Big] \qquad \text{(III - 49)}$$

$$C_8^{J-2} = \frac{1}{16(2J-1)}\Big[(J-1)\{(J-2)[J(J+X_1) - Y_2 - (J+1)(X_4-Y_4)] + J(J+X_1)Y_1 - (J+1)Y_6 - Y_7\} + (J-2)(X_5-Y_5) + Y_9 - \frac{1}{J}\{(J-1)\Big((J-2)[(J+1)(X_4Y_1 - X_1Y_4) + X_1Y_2] + (J+1)(X_4Y_3 - X_4Y_4 + X_1Y_6) + X_1Y_7\Big) - (J-2)(X_5Y_1 - X_1Y_5) + (J+1)X_4Y_5 - X_5(Y_3-Y_4) - X_1Y_9\} + \frac{X_5Y_5}{J(J-1)}\Big]$$

$$C_8^{J} = -\frac{2J+1}{16(2J-1)(2J+3)}\Big[J(J+1)(2J^2+2J-1-2Y_2) + (13J^2+13J-9)X_1 + (J^2+J-1)Y_1 + (J^2+J-3)(X_4-Y_4) - (2J^2+2J-3)Y_6 - 3X_5 + 3Y_5 + Y_7 + 2Y_9 + \frac{1}{J(J+1)}\{(2J^4+4J^3 - 2J - 3)(X_4Y_1 - X_1Y_4) - (6J^4+12J^3-10J^2-16J+9)X_1Y_1 - (19J^2+19J-12)X_1Y_2 + (5J^2+5J-6)X_4Y_4 - (2J^2+2J+3)(X_5Y_1 - X_1Y_5) + 2(2J^2+2J-3)X_5Y_4 + 3(2J^2+2J-1)X_1Y_7 - (J^2+J-3)(X_4Y_3 - 2X_4Y_5 + X_1Y_6) + 3X_5Y_3 - 6X_5Y_5 + 3X_1Y_9\}\Big]$$

$$C_8^{J+2} = \frac{1}{16(2J+3)}\Big[(J+2)\{(J+3)[(J+1)(J+1-X_1) - Y_2 + J(X_4-Y_4)] - (J+1)(J+1-X_1)Y_1 - JY_6 + Y_7\} - (J+3)(X_5-Y_5) + Y_9 - \frac{1}{J+1}\{(J+2)\Big((J+3)[J(X_4Y_1 - X_1Y_4) - X_1Y_2] - J(X_4Y_3 - X_4Y_4 + X_1Y_6) + X_1Y_7\Big) - (J+3)(X_5Y_1 - X_1Y_5) + JX_4Y_5 + X_5(Y_3-Y_4) + X_1Y_9\} + \frac{X_5Y_5}{(J+1)(J+2)}\Big] \qquad \text{(III - 50)}$$

For $J = 0$, the non vanishing values of the coefficients above are:

$$C_4^0 = -C_4^2 = \frac{X_4 - Y_4}{24} \qquad C_6^1 = -\frac{4 - X_4Y_4}{16}$$
$$C_8^0 = -\frac{X_4Y_4 - Y_6}{48} \qquad C_8^2 = \frac{12 + 6(X_4 - Y_4) - X_4Y_4 - 2X_6}{96} \qquad \text{(III - 51)}$$

$$
\begin{aligned}
C_5^{J-3} = & \frac{J+X_1}{16J(2J-3)(2J-1)}\Big[(J-1)\{(J-2)\Big((J-4)[J(J-3)+2Y_3-2Y_4]-Y_2-Y_6\Big) \\
& +(J^3-9J^2+28J-24)Y_1-Y_7-3Y_8\}+(J-2)[2(J-4)Y_5+Y_9]+Y_{10}\Big] \\
C_5^{J-1} = & -\frac{1}{16(2J-3)(2J+3)}\Big[(J-2)\{J(J-1)(J+1)(J+3+3X_1)-2(3J^2+2J-6)(Y_3-Y_4) \\
& -2(J+6)Y_5\}+(3J^4+2J^3-5J^2-10J+6)Y_1+(J^3+11J^2-14J-6)X_1Y_1 \\
& -(4J^3-9J^2-10J+21)Y_2-(4J^3-J^2-10J+3)Y_6-(4J^2+J-9)Y_7-(4J^2+3J-9)Y_8 \\
& +(J-3)Y_9+3Y_{10}-\frac{X_1}{J}\{(4J^3-7J^2-7J+12)Y_2+(4J^2-J-6)Y_7\} \\
& -\frac{X_1}{J(J+1)}\{2(J-2)[(J^3+4J^2+2J-6)(Y_3-Y_4)+(3J^2+4J+6)Y_5]+(4J^4+5J^3-14J^2 \\
& -13J+12)Y_6+(4J^3+9J^2-3J-18)Y_8-(3J^2+J-12)Y_9-(J+6)Y_{10}\}\Big] \\
C_5^{J+1} = & -\frac{1}{16(2J-1)(2J+5)}\Big[(J+3)\{J(J+1)(J+2)(J-2-3X_1)-2(3J^2+4J-5)(Y_3-Y_4) \\
& +2(J-5)Y_5\}-(3J^4+10J^3+7J^2+6J+12)Y_1+(J^3-8J^2-33J-18)X_1Y_1 \\
& -(4J^3+21J^2+20J-18)Y_2-(4J^3+13J^2+4J-8)Y_6+(4J^2+7J-6)Y_7+(4J^2+5J-8)Y_8 \\
& +(J+4)Y_9-3Y_{10}+\frac{X_1}{J+1}\{(4J^3+19J^2+19J-8)Y_2-(4J^2+9J-1)Y_7\} \\
& +\frac{X_1}{J(J+1)}\{2(J+3)[(J^3-J^2-3J+5)(Y_3-Y_4)-(3J^2+2J+5)Y_5]+(4J^4+11J^3-5J^2 \\
& -14J+10)Y_6-(4J^3+3J^2-9J+10)Y_8-(3J^2+5J-10)Y_9+(J-5)Y_{10}\}\Big] \\
C_5^{J+3} = & \frac{J+1-X_1}{16(J+1)(2J+3)(2J+5)}\Big[(J+2)\{(J+3)\Big((J+5)[(J+1)(J+4)+2Y_3-2Y_4]+Y_2+Y_6\Big) \\
& -(J^3+12J^2+49J+62)Y_1-Y_7-3Y_8]\}-(J+3)[2(J+5)Y_5-Y_9]-Y_{10}\Big]
\end{aligned}
$$

(III – 54)

$$
\begin{aligned}
C_6^{J-3} = & -\frac{J-2}{8J(J-1)(2J-3)(2J-1)}\Big[(J-1)\{(J-2)(J+X_1)+X_3-X_4\}+X_5\Big] \\
& \Big[(J-1)\{(J-2)(J+Y_1)+Y_3-Y_4\}+Y_5\Big] \\
C_6^{J-1} = & -\frac{1}{8(2J-3)(2J+3)}\Big[J(7J^4-6J^3+6J^2+13J-48)+(5J^4-J^3+9J^2+4J-48) \\
& (X_1+Y_1)+(3J^3-2J^2-8J+6)(X_3+Y_3-X_4-Y_4)+(J^2+2J-6)(X_5+Y_5)+\frac{1}{J} \\
& \{(7J^4+9J^2-5J-48)X_1Y_1+(J^2+2J-6)(X_4Y_3+X_3Y_4)+(5J-6)(X_5Y_3+X_3Y_5)\} \\
& +\frac{1}{J(J+1)}\{(8J^5+12J^4-23J^3-34J^2+13J+15)X_4Y_4+(J^4-4J^2-2J+6)(X_3Y_1 \\
& -X_4Y_1+X_1Y_3-X_1Y_4)+(7J^3+J^2-14J-3)X_3Y_3+(3J^3-4J-6)(X_5Y_1+X_1Y_5) \\
& -(8J^3+9J^2-19J-15)(X_5Y_4+X_4Y_5)\}+\frac{5X_5Y_5}{J(J-1)(J+1)}(3J^2-2J-3)\Big] \\
& +\frac{1}{16J}\Big[(J+X_1)\{(J-2)Y_2+JY_6+Y_7+Y_8\} \\
& +\{(J-2)X_2+JX_6+X_7+X_8\}(J+Y_1)\Big]
\end{aligned}
$$

$$C_5^1 = -\frac{84 - 4(X_4 + Y_4) - 5(X_6 + Y_6) + 9X_4Y_4}{16} \qquad C_5^3 = -\frac{(6 - X_4)(6 - Y_4)}{80}$$
$$C_3^0 = \frac{X_4Y_4 - Y_6}{24} \qquad C_3^2 = \frac{12 - 6(X_4 - Y_4) + X_4Y_4 - 4Y_6}{48} \tag{III - 57}$$

with special formulae for C_6^1 and C_3^0.

4.3. - LECT

This subroutine reads all the input. This input stream is grouped into categories preceded by an integer ILECT which runs from 1 to 7. It allows part of the input stream to be changed in subsequent calculations. The first input stream must be read in the order of increasing ILECT. The different categories are

ILECT=1 Description of the single particle bound states.
ILECT=2 Description of two body interaction.
ILECT=3 Presentation of the results.
ILECT=4 Optical model of the initial channel.
ILECT=5 Optical model of the final channel.
ILECT=6 Description of the excited state.
ILECT=7 End of the input stream for this calculation.

For each category of data corresponding to ILECT=1 to 6, there is an upper limit of resident quantities in the array. Intermediate computation are performed beyond the upper limit already in use. If in a subsequent calculation the upper limit of new data is larger then the previous one, the data for larger values of ILECT must be read again.

If this calculation is not the first one and the previous calculation involved a summation on J-transfer (LO(8)=.TRUE.) and the has not been read (LO(18)=.TRUE. in the last input) the subroutine reads the description of the new J-transfer (in the category ILECT=6, but without reading ILECT).

In any other case, this input starts by a **title** card:

1) if this title is 'DESCRIPTION ' from column 1, the description of the input is printed by calling the subroutines INPA and INPB.
2) if this title is 'FIN ' from column 1, the calculation is stopped.
3) if the title card is neither 'FIN ' or 'DESCRIPTION ', the subroutine LECT reads a card of logical control.

4.3.1. - INPA-INPB

These two subroutine are called one after the other if the title is 'DESCRIPTION '. They include only WRITE statements and they have been generated from the text written on cards with a special program available with ECIS79. After the printing, a new **title** card is read in LECT.

The description of the subroutines called by LECT is given according to which value of ILECT uses them.

4.3.2. - ILECT=1: Description of the single particle bound states.

The subroutine LECT reads only the number of configurations and the number of steps of integration.

the parameters are read. It must be normalised to the units used for the input of the densities.

3) the form factors are interpolated by a four points Lagrange formula:

$$V(x) = \sum_{i=1}^{i=4} V(x_i) \prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \qquad (IV-1)$$

4) the square root of the form factor is calculated if the use of the geometric mean is requested (I4=1) or it is divided by 2 for the use of arithmetic mean (I4 is stored in KTF(K,3,J)). In order to be able to obtain the square root, a real form factor should be always positive. A continuous square root of a complex form factor is obtained by introducing a change of sign in the result when the real part of the form factor is negative and the sign of its imaginary part changes.

4.3.4. – ILECT=3: Presentation of the results.

After the input of these data, the table of logarithms of factorials used for geometrical coefficients is computed.

4.3.5. – ILECT=4: Optical model of the initial channel.

If the two body interaction is used to compute the free wave functions, and they are not read on a tape, the subroutine LEC6 described below with ILECT=6 is called for the input of the description of the target (note that the description of the target is in terms of occupation numbers, that is scalar products of creation and annihilation operators and not in term of their tensor coupling to zero) and the subroutine DIRZ is called to initialise the working array for microscopic potentials and, eventually, compute the macroscopic potential read in LEC6. In any case, some dimensions and reservations have to be computed. Then LECT calls the subroutine FDIS with IG=1.

4.3.5.1. – FDIS

This subroutine is called first for the initial state (IG=1) and after that for the final state (IG=2). This subroutine:

1) computes the center of mass energy and calls the subroutine POTE for the potentials.
2) computes wave number and Coulomb parameters and calls the subroutine FCOU for the Coulomb functions.
3) in a DO LOOP on the partial waves:
   a) computes the Coulomb functions at two different points from their value and the value of their derivative in a middle point. Formulae are obtained from a five points derivation formula and three Numerov steps of integration with half step size.
   b) calls the integration subroutine INTE.
   c) computes partial absorption and print them with the phase shifts if requested (LO(33)=.TRUE.).

a new one (LOX(3)=.TRUE.) and some other quantities (number of partial waves. limit of exchange) if LOX(6)=.TRUE. .

2) if the potentials are not to be read on a tape (LOX(5)=.FALSE.),
   a) computes them by calling the subroutines MULT and PTIP as done in subroutine DIRA for the transition to a 0^+ level in a loop on the configurations of the target (the subroutine GEOM, DERI and DER2 are also used in this computation); note that the geometrical factor given by the function DCGS in the subroutine DIRA reduces to unity in this case.
   b) computes the Coulomb potential if it is not requested from the two body interaction (LOX(2)=.FALSE.),
   c) computes the array VR from VS as described above,
   d) if requested (LOX(4)=.TRUE.), write on tape the number of steps, the step size and the arrays VS and VR (storage of about 14 times the number of steps, in single precision).
2) if requested (LOX(5)=.TRUE.), the potentials are read on a tape, but the program stops if the number of steps and the step size do not agree with those of the run.
3) if requested (LOX(7)=.TRUE.), the proton, neutron and total density are printed.

If requested (LO(34)=.TRUE.), the subroutine prints the potentials.

4.3.5.3. – FCOU

This subroutine and the subroutines called by it are a small modification of those written at the Department de Calcul Electronique Saclay by: [10] BARDIN, C., DANDEU, Y., GAUTIER, L., GUILLERMIN, J., LENA, T., PERNET, J.M., Note CEA-N-906 (1968) and [11] BARDIN, C., DANDEU, Y., GAUTHIER, C., GUILLERMIN, J., LENA, T., PERNET, J.-M., WOLTHER, H. H., TAMURA, T., Comp. Phys. Comm. 3 (1972) 72. They compute the regular and the irregular Coulomb functions and their derivatives for a given η and ρ for different values of the angular momentum L, starting from L=0. In the original subroutines, the calculation of phase-shifts has been suppressed except for L=0, the factorisation of some power of 10 has been changed from modulo 60 to modulo 15 in order to avoid overflow in the computation of Coulomb corrections on a VAX computer. This subroutine calls FCZ0 to obtain Coulomb functions for L=0 and computes the other ones by recurrence involving function and derivative at two values of L. For the regular function, upwards recurrence is used if $\rho < \eta + \sqrt{L(L+1)}$ and downwards recurrence in the other case. Upwards recurrence is used for the irregular function.

4.3.5.3.1. – FCZ0

This subroutine computes the Coulomb functions for L=0. It calls the function SIGM to obtain the phase-shift.

1) for $\eta = 0$, the subroutine returns sin and cos,
2) for $\eta > 28$ or $\eta < -8$, the subroutine calls YFRI to use Riccati methods.
3) for $\rho \geq \rho_m = 7.5 + 5|\eta|/3$, where ρ_m is the asymptotic limit, the subroutine calls YFAS to use asymptotic expansions.
4) for other values, the subroutine calls YFIR for the irregular function and:
   a) if $0 < \eta < 10$ and $\rho < 2$ or $\eta > 10$ and $\eta > (5\rho + 6)/7$, the subroutine uses regular series at the origin for the regular Coulomb functions.
   b) in all the other cases, it uses expansion in Chebyshev polynomials for the regular function: α) between the origin and $\rho = m$ if $\eta < 2.5$ (Clenshaw

This subroutine uses the working array VS only for the microscopic optical model (LO(37)=.TRUE.). The main operations are:

1) the first part is an usual solution of the Schrödinger equation:
   a) at the first call, for a microscopic potential including first and second derivative term, the inverse of the second derivative terms in the Schrödinger equation is computed. and the first derivative potential is multipied by it.
   b) the potential for this equation is computed in the memories reserved to return the wave function. It is obtained from the microscopic potential in VS or from VR if there are no derivatives. In the first case, it is multiplied by the inverse of first derivatives. For microscopic calculations, this potential is kept in VS(I,K) for K=37 and 38.
   c) $2 + h^2V/(1 - h^2V/12)$ is computed and the equation is solved by Numerov method.
   d) phase shift and normalised solution are obtained. The subroutine returns for a macroscopic potential.
2) the second part is the set up of the integro differential system of equations needed with a microscopic potential (LO(37)=.TRUE.):
   a) if the exchange is not included because it was not requested or because the angular momentum is higher than the limit (LOX(6)=.TRUE.): α) if there is no derivative terms, the code returns; β) if there are first derivative terms, the wave function is derived by calling the subroutine DERI and the DWBA effect of these derivative terms computed. If the effect is small, the subroutine returns and will return for higher angular momenta (LO(8) is set .TRUE.).
   a) if the potential has not to be read on a tape (LOX(5)=.FALSE.), the subroutine initialises to 0 the working array XA(I,J,K) of which the two first dimensions are the number of steps:
      - the non derivative terms will be in K=1 and 2,
      - the first derivative terms will be in K=3 and 4,
      - the second derivative terms will be in K=5 and 6,
      - K=7 is used as a working array in the subroutine PTIV,
      - the final system of integro differential equations will be built and solved in K=7 and 8.
   c) if exchange in the microscopic potential is requested (LOX(6)=.FALSE.) and if the angular momentum or the J transfer is not too large, there is a DO LOOP on the J transfer including a call to the subroutine MULT to compute the multipoles and a nested DO LOOP on the configurations with a call to the subroutine PTIP for the natural parity case or to the subroutine PTII for the unnatural parity case. In this use, the subroutines PTIP and PTII call the subroutine PTIV to build the matrices XA. The subroutine GEOM, DERI and DER2 are also used inside the nested DO LOOP. Note that the geometrical factor which is essentially in the subroutine ECHA the product of a 6-j symbol given by the function DJ6J and two 3-j symbols given by the function DCGS reduces here to the square of the 3-j symbol between the total angular momentum of the free wave j and the bound state j' and the value J of the transfer multiplied by $-(2J+1)/\{(2j+1)(2j'+1)\}$. If no contribution is found, the exchange is suppressed by setting LOX(6)=.TRUE. .
   d) if requested (LOX(4)=.TRUE.), the matrix XA is written on tape. This storage is very large: it involves six times the square of the number of steps in single precision for each total angular momentum and parity.
   e) if the potential has to be read on a tape (LOX(5)=.TRUE.), the subroutine reads it but set LOX(6)=.TRUE. if it finds a end of file.

```
> INTEGRALS WITH REGULAR FUNCTIONS: (L+1)       DIRECT          BACKWARDS RECURRENCE
>                                    1       0.9773035046D-02     0.9773035021D-02
>                                    2       0.9758158329D-02     0.9758158318D-02
```

The integrals of products of irregular functions between themselves and with the regular ones are obtained by upwards recurrence.

4.3.5.6. – SCEL

This subroutine is quite similar to the subroutine SCEF for which more details will be given but simpler:

1) it compute the helicity phase shifts and the partial absorptions which are summed to obtain the total reaction cross section,
2) for the angles given with ILECT=3, it computes the amplitudes with the reduced matrices of rotation given by the subroutine EMRO and obtains the cross section, the cross section divided by Rutherford's cross section for charged particles, the polarisation and the observable Q and print them,
3) it prints the total reaction cross section and calls the subroutine GRAL with indications read with ILECT=3 for the elastic scattering.

4.3.6. – ILECT=5: Optical model of the final channel.

Except for the input of Q instead of the laboratory energy, same as for ILECT=4 if the optical model is changed (LO(32)=.FALSE.), but the subroutine FDIS is called with IG=2 instead of 1 . If the optical potential is the same (LO(32)=.TRUE.) and is obtained from the two body interaction (LO(37)=.TRUE.) and the potential have been written on a tape for the initial state (LOX(4)=.TRUE., LOX(5)=.FALSE.), they will be read from the tape for the final state (LOX(4)=.FALSE., LOX(5)=.TRUE.).

4.3.7. – ILECT=6: Description of the excited state.

The subroutine reads number of configuration, angular momentum and parity and calls the subroutine LEC6 which uses subroutine XYIS.

4.3.7.1. – LEC6

This subroutine:

1) reads the description of the configurations (if called for the description of the target, this description is in terms of occupation numbers, that is $-\sqrt{(2j+1)}$ times the usual value) and checks the validity of angular quantum numbers,
2) with the use of BCS (LO(15)=.TRUE.), calls the subroutine XYIS with ID=4 to transform the data,
3) in case of different notation (LOO(K)=.TRUE.), calls the subroutine with ID=K,
4) with a macroscopic interaction (LO(26)=.TRUE.) reads the description of these macroscopic form factors.

4.4. – DIRA

This subroutine computes the transition amplitudes in SOM(I,J,K) for the direct term. After calling the subroutine MULT to obtain the multipole for the J of the transfer, there is:

1) a DO LOOP on the contribution of each of the configurations, successively for X and for Y. The geometrical coefficient is obtained with the function DCGS and the subroutine GEOM, the subroutines DERI and DER2 are used to derive the bound functions, the contribution of the zero range interaction is computed in the subroutine PTI0, the contribution of finite range interaction is computed in subroutine PTIP for natural parity transitions or subroutine PTII for unnatural parity transitions. The working array VS(I,K) is used for the product of bound waves functions and their derivative in K=43 to 48. Results are in the same array:
   a) twelve non derivative complex form factors in K=3 to 26 to be used without coefficient and with the 11 coefficients XG computed by the subroutine GEOM,
   b) six first derivative complex form factors in K=27 to 38 to be used without coefficient and with the 5 first coefficients XG,
   c) two second derivative complex form factors in K=39 to 42 to be used without coefficient and with the first coefficient XG.
2) if requested (LO(14)=.FALSE.) the subroutine DIRA print the existing form factors.
3) two nested DO LOOPs on the total angular momentum of the initial particle and the parity which include the computation in VS(I,K) for K=43 to 66 of the product of the form factors with the initial wave function and its derivatives obtained with the subroutine DERI and DER2, and a DO LOOP on the final waves with:
   a) the computation of geometrical coefficients with the function DCGS and the subroutine GEOM,
   b) if requested (LO(21)=.FALSE.) evaluation of the Coulomb corrections using the subroutine CORA,
   c) summation into VS(I,67) and VS (I,68) of the products of initial wave with form factors multiplied by the geometrical coefficients computed in the subroutine GEOM and integration of the result with the final wave.

4.4.1. – MULT

For a value of the transfer J, this subroutine computes the arrays of multipoles AM(J,K,L) of which the first dimension is the number of steps, the last one the number of ranges and the second one is 18:

1) irregular multipoles (Hankel functions of first kind for the variable ir) for V_{J-3} to V_{J+3} in K=1 to 7,
2) regular multipoles (Bessel functions for the variable ir) for V_{J-3} to V_{J+7} in K=8 to 18.

The subroutine is assumed to have been called already for a value J' given as argument (at the first time, J'=−1). This subroutine do:

1) if there is a two body Coulomb interaction, the subroutine computes the irregular and the regular Coulomb multipoles at the end of the array AM,
2) there are three nested DO LOOP's on the range, on the integration points and on the J values from the last one plus one (J'+1) to the one requested in which:
   a) if J=0, the multipoles for negative values are set to zero, the first regular multipole and the first four irregular multipoles are computed; a backwards recurrence is used to obtain the regular multipole, using the value for J=0 to normalise them,
   b) if J≠0, all the multipoles are shifted down: a new irregular multipole is easily obtained by upwards recurrence, a new regular multipole has to be obtained by backwards recurrence which has to be done only once for 5 values of J, due to the extra storage,

4.4.3.1. - DERI

Computes $h\frac{d}{dr}$ of a function where h is the step size. It assumes the value before the first to be zero and needs at least 7 values. It uses:

$$x_i = \frac{1}{60}\left[45(y_{i+1} - y_{i-1}) - 9(y_{i+2} - y_{i-2}) + y_{i+3} - y_{i-3}\right] \qquad \text{(IV - 4)}$$

but for the first three points:

$$\begin{aligned} x_1 &= \frac{1}{60}\left[-77y_1 + 150y_2 - 100y_3 + 50y_4 - 15y_5 + 2y_6\right] \\ x_2 &= \frac{1}{60}\left[-24y_1 - 35y_2 + 80y_3 - 30y_4 + 8y_5 - y_6\right] \\ x_3 &= \frac{1}{60}\left[45(y_4 - y_2) - 9(y_5 - y_1) + y_6\right] \end{aligned} \qquad \text{(IV - 5)}$$

and for the last three points (n being the last one):

$$\begin{aligned} x_{n-2} &= \frac{1}{60}\left[y_{n-6} - 8y_{n-5} + 30y_{n-4} - 80y_{n-3} + 35 * y_{n-2} + 24y_{n-1} - 2y_n\right] \\ x_{n-1} &= \frac{1}{60}\left[-2y_{n-6} + 15y_{n-5} - 50y_{n-4} + 100y_{n-3} - 150y_{n-2} + 77y_{n-1} + 10y_n\right] \\ x_n &= \frac{1}{60}\left[10y_{n-6} - 72y_{n-5} + 225y_{n-4} - 400y_{n-3} + 450y_{n-2} - 360y_{n-1} + 147y_n\right] \end{aligned} \qquad \text{(IV - 6)}$$

4.4.3.2. - DER2

Computes $h^2\frac{d^2}{dr^2}$ of a function where h is the step size. It assumes the value before the first to be zero and needs at least 7 values. It uses:

$$x_i = \frac{1}{180}\left[270(y_{i+1} + y_{i-1}) - 27(y_{i+2} + y_{i-2}) + 2y_{i+3} + 2y_{i-3} - 490y_i\right] \qquad \text{(IV - 7)}$$

but for the first three points:

$$\begin{aligned} x_1 &= \frac{1}{180}\left[-147y_1 - 255y_2 + 470y_3 - 285y_4 + 93 * y_5 - 13y_6\right] \\ x_2 &= \frac{1}{180}\left[228y_1 - 420y_2 + 200y_3 + 15y_4 - 12y_5 + 2y_6\right] \\ x_3 &= \frac{1}{180}\left[270(y_4 + y_2) - 27(y_5 + y_1) + 2y_6) - 490y_3\right] \end{aligned} \qquad \text{(IV - 8)}$$

and for the last three points (n being the last one):

$$\begin{aligned} x_{n-2} &= \frac{1}{180}(2y_{n-6} - 12y_{n-5} + 15y_{n-4} + 200y_{n3} - 420y_{n-2} + 228y_{n-1} - 13y_n) \\ x_{n-1} &= \frac{1}{180}(-13y_{n-6} + 93y_{n-5} - 285y_{n-4} + 470y_{n3} - 255y_{n-2} - 147y_{n-1} + 137y_n) \\ x_n &= \frac{1}{180}(137y_{n-6} - 972y_{n-5} + 2970y_{n-4} - 5080y_{n3} + 5265y_{n-2} - 3132y_{n-1} + 812y_n) \end{aligned} \qquad \text{(IV - 9)}$$

but the scalar interaction needs a correction:

$$f_{\text{scalar}}(r) = f(r) - \frac{h^2\mu}{12r^2}g(r) \qquad (\text{IV} - 12)$$

which cancels out for tensor, spin orbit and other interactions,

d) multiplication by the r_2 radial dependence,
e) multiplication by a power of r_2 (positive or negative),
f) addition to the form factor.

The subroutine returns if it is called by the subroutine INTE for the exchange term of the microscopic potential. In the other cases, the two body Coulomb contribution is computed, if requested (LO(16)=.TRUE.).

4.4.4.2. - PTCP

This subroutine returns if no $\bar{L}^2$ or $(\bar{L}.\bar{S})^2$ interaction is used. If they are used, the subroutine computes with the coefficients XG the arrays S0(I,J,K), S1(I,J,K) and S2(I,J,K) respectively for the non derivative, the first derivative and the second derivative form factors.

I =1 for the $\bar{L}^2$ interaction,
I =2 for the $\bar{L}^2$ $(\bar{\sigma}_1.\bar{\sigma}_2)$ interaction,
I =3 for the $(\bar{L}.\bar{\sigma}_1)(\bar{L}.\bar{\sigma}_2)$ interaction,
J stands for the geometrical dependence on the other particle (J=1 to 12 for S0, J=1 to 6 for S1, J=1 to 2 for S2),
K stands for the multipole involved (K=1 to 13 for S0, K=1 to 14 for S1, K=1 to 3 for S2), but S1(I,J,8)=−S1(I,J,7), S1(I,J,K+8)=−S1(I,J,K) with contribution of S2 for K=1 to 6 and S2(I,J,2)=−S2(I,J,1)−S2(I,J,3).

4.4.4.3. - PTII

This subroutine is very similar to the subroutine PTCI and is called from the same subroutines, except for the subroutine POTE. The differences with the subroutine PTCP are:

1) it calls the subroutine PTCI instead of the subroutine PTIP, to obtain coefficients for $\bar{L}^2$ $(\bar{\sigma}_1.\bar{\sigma}_2)$ and $(\bar{L}.\bar{\sigma}_1)(\bar{L}.\bar{\sigma}_2)$ interactions only.
2) if some value VA were found, 334 complex coefficients are computed, with expressions in this subroutine for the scalar, the tensor, the spin orbit and the $\bar{L}^2$ interaction or with results of the subroutine PTCI for the other interactions.
3) if not called from the subroutine INTE for the exchange term of a microscopic potential, this subroutine acts like the subroutine PTCP but there are 59 groups of operations instead of 42.
4) there is no Coulomb interaction.

4.4.4.4. - PTCI

Like the subroutine PTCP, this subroutine returns if no $\bar{L}^2$ or $(\bar{L}.\bar{S})^2$ interaction is used. If they are used, the subroutine computes with the coefficients XG the arrays

5) addition to the form factors.

4.4.4.7. – PTC0

This subroutine returns the coefficients needed in the subroutine PTI0.

4.4.5. – CORA

For given angular momenta, this subroutine returns the four coefficients needed in the asymptotic region, if its last argument is .TRUE. (see Ref [10]). When this last argument is .FALSE., it returns also the four other coefficients needed for finite integrals. This is limited to a transfer of angular momentum 4. There are special formulae for the on-shell corrections which are necessary only for dipole excitation.

4.5. – ECHA

Inside five nested DO LOOP's on the multipoles, on the configurations, on the contributions of the amplitude X and Y, on the total angular momentum of the initial wave and on its parity, there is:

1) the computation of the form factors:
   a) the geometrical coefficient is obtained with the function DCGS and the subroutine GEOM,
   b) the particle wave function is multiplied with the initial wave function or its derivatives obtained with the subroutines DERI and DER2,
   c) the form factors are obtained with the subroutine PTIP in the natural parity case and the subroutine PTII in the unnatural parity case,
   d) the form factors in VS(I,K) for K=3 to 26 (or less) are multiplied by the hole wave function; the other ones are multiplied by the first or the second derivative of the hole function obtained with the subroutine DERI or DER2 and the result added to VS(I,K) for K=3 to 14 for the first derivative, K=3 to 6 for the second derivative.
2) a DO LOOP on the final waves:
   a) the geometrical coefficient is obtained with the functions DJ6J and DCGS and the subroutine GEOM,
   b) the form factors are summed into VS(I,K) for K=43 and 44,
   c) the integrals with the final wave are done and the result added to SOM(I,J,K) which contains already the result of the direct calculation when this subroutine is called.

4.6. – SCEF

This subroutine prints results at equidistant angles. The input is the array of integrals SOM(I,J,K) in which K is the total angular momentum of the initial wave plus one half, J corresponds to the total angular momentum of the final wave, starting from one for the lowest one and the real parts are stored in I=1 and 3, the imaginary parts in I=2 and 4 for the two integrals. After the output of the title of the run, there is:

LECT	INPA					
----	INPB					
----	LEC1	STDP	MEMO			
----	----	MEMO				
----	LEC2	MEMO				
----	FDIS	POTE	DERI			
----	----	----	DER2			
----	----	----	GEOM			
----	----	----	MULT			
----	----	----	PTIP	PTCP		
----	----	----	----	PTIV		
----	----	----	PTIO	DERI		
----	----	----	----	DER2		
----	----	----	----	PTCO		
----	----	FCOU	FCZO	SIGM		
----	----	----	----	YFRI	YFCL	PSI
----	----	----	----	YFAS		
----	----	----	----	YFIR	PSI	
----	----	----	----	----	YFAS	
----	----	INTE	DCGS			
----	----	----	DERI			
----	----	----	DER2			
----	----	----	GEOM			
----	----	----	MULT			
----	----	----	PTIP	PTCP		
----	----	----	----	PTIV		
----	----	----	PTII	PTCI		
----	----	----	----	PTIV		
----	----	CORI	CORH			
----	----	----	MEMO			
----	----	SCEL	EMRO			
----	----	----	GRAL			
----	----	----	MEMO			
----	----	MEMO				
----	LEC6	XYIS				
----	----	MEMO				
----	DIRZ	DERI				
----	HORA	STIM				
----	MEMO					

DIRA	MULT	
----	DCGS	
----	GEOM	
----	DERI	
----	DER2	
----	PTIP	PTCP
----	----	PTIV
----	PTII	PTCI
----	----	PTIV
----	PTIO	PTCO
----	----	DERI
----	----	DER2

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