# NOTES ON DWBA98/DWBB98

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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:

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

where $\sigma$ is the spin projection of the in going plane wave on an arbitrary axis and $\sigma'$ 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 $\lambda$ instead of $\sigma$:

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

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 $\phi_r, \theta_r$ and $\psi_r$ 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:

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

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

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

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:

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

where $|\sigma>$ is the spin eigenfunction with a projection $\sigma$ along the axis of quantisation and $f_{lj}(r)$ is a radial function normalised according to:

$$\int_0^\infty r^2 f_{lj}^2(r)dr = 1. \qquad \text{(I – 6)}$$

Projecting $|\sigma>$ on $\vec{r}$, using the relation between spherical harmonics and rotation matrix elements, we get:

$$|jm>= \frac{\sqrt{2j+1}}{4\pi}\sum_\lambda \phi_\lambda^j(r) R^{(j)}_{m,\lambda}{}^\star(\phi,\theta,\psi)|\lambda> \qquad \text{(I – 7)}$$

with

$$\phi^j_{\frac{1}{2}}(r) = (-)^{l+j-\frac{1}{2}} f_{ij}(r) \qquad \phi^j_{-\frac{1}{2}}(r) = f_{ij}(r) \qquad \text{(I – 8)}$$

**All references to the orbital angular momentum have disappeared** from the description of the bound state, **but there are now two radial functions** $\phi^j_{\pm\frac{1}{2}}$ which are equal within a sign for a state of well-defined parity.

**It should be noted that a helicity state as defined here has no direct physical significance: there must be always two helicity states.**

## 1.2. – MULTIPOLE EXPANSION IN THE HELICITY FORMALISM

If no spins are involved, the interaction can be expanded around the origin as follows:

$$V(|\vec{r}_1 - \vec{r}_2|) = \sum_L (2L+1) V_L(r_1, r_2) P_L(\cos\theta) \qquad \text{(I – 9)}$$

and there are relations between multipoles, related to the Fourier transform of V:

$$\begin{aligned} W(q) &= \int \exp(i\vec{q}.\vec{r})\ V(r)\ d^3r, \\ V_L(r_1,r_2) &= \frac{2}{\pi}\int_0^\infty q^2 W(q) j_L(qr_1) j_L(qr_2) dq \end{aligned} \qquad \text{(I – 10)}$$

The recurrences between the Bessel functions can be used to obtain relations between multipoles.

For spin $\frac{1}{2}$ particles, it can be written:

$$\begin{aligned} V(1,2) = &\sum_{J,\lambda_1,\lambda_2,\lambda_1',\lambda_2'} (2J+1)|\lambda_1'><\lambda_2'| V^J_{\lambda_1'\lambda_2',\lambda_1\lambda_2}(1,2) <\lambda_1|<\lambda_2| \\ &\times \sum_\mu (-)^\mu R^{(J)}_{\mu,\lambda_1-\lambda_1'}(\phi_1,\theta_1,\psi_1) R^{(J)}_{-\mu,\lambda_2-\lambda_2'}(\phi_2,\theta_2,\psi_2) \end{aligned} \qquad \text{(I – 11)}$$

where $\phi_1, \theta_1, \psi_1$ describes a co-ordinate system with $z$-axis along $\vec{r}_1$ and $\phi_2, \theta_2, \psi_2$ another one with its $z$-axis along $\vec{r}_2$. The total expression is independent of $\psi_1$ and $\psi_2$.

### 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:

$$V_{\lambda'_1\lambda'_2,\lambda_1\lambda_2}(1,2) = \sum_J V^J_{\lambda'_1\lambda'_2,\lambda_1\lambda_2}(1,2)(-)^{\lambda'_1-\lambda_1} r^{(J)}_{\lambda'_1-\lambda_1,\lambda_2-\lambda'_2}(\theta) \qquad \text{(I – 12)}$$

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

$$V^J_{\lambda'_1\lambda'_2,\lambda_1\lambda_2}(1,2) = V^J_{-\lambda'_1-\lambda'_2,-\lambda_1-\lambda_2}(1,2) \qquad \text{(I – 13)}$$

Time reversal invariance depends on the nature of the operators:

$$V^J_{\lambda'_1\lambda'_2,\lambda_1\lambda_2}(1,2) = \eta V^J_{-\lambda_1-\lambda_2,-\lambda'_1-\lambda'_2}(1,2) \qquad \text{(I – 14)}$$

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

When the two nucleons are identical:

$$V^J_{\lambda'_1\lambda'_2,\lambda_1\lambda_2}(1,2) = V^J_{\lambda'_2\lambda'_1,\lambda_2\lambda_1}(2,1) \qquad \text{(I – 15)}$$

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 $2\times 2$ matrices. They are two even matrices:

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

and two odd ones:

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

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

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

and an odd part:

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

If the two particle are identical:

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

If time-reversal applies, $a, c, d, e$ and $f$ must be expressed in terms of time-reversal invariant operators, and $b$ must change sign; consequently, $b$ vanishes for a local interaction.

As the absolute value of the magnetic quantum numbers of the reduced matrix element must be less or equal to $J$, some two-body form factors vanish for $J = 0$:

$$\begin{aligned} &a^0(1,2) \neq 0, \qquad b^0(1,2) = b'^0(1,2) = c^0(1,2) = 0, \\ &d^0(1,2) \neq 0, \qquad e^0(1,2) = e'^0(1,2) = f^0(1,2) = 0, \end{aligned} \tag{I – 21}$$

## 1.2.2. – MULTIPOLE EXPANSION OF CENTRAL AND TENSOR INTERACTIONS

When the usual multipole expansion of the form factor of the interaction is given by:

$$V(|\vec{r}_1 - \vec{r}_2|) = \sum_L (2L+1) V_L(r_1, r_2) P_L(\cos\theta) \tag{I – 22}$$

**with the central interaction** $V(|\vec{r}_1 - \vec{r}_2|)$ we get for the even part:

$$\begin{aligned} a^J &= V_J(r_1, r_2) \\ b^J &= c^J = 0 \end{aligned} \tag{I – 23}$$

and for the odd part:

$$d^J = e^J = f^J = 0 \tag{I – 24}$$

**with the central interaction** $V(|\vec{r}_1 - \vec{r}_2|)(\vec{\sigma}_1.\vec{\sigma}_2)$ we get for the even part:

$$\begin{aligned} a^J &= b^J = 0 \\ c^J &= -V_J(r_1, r_2) \end{aligned} \tag{I – 25}$$

and for the odd part:

$$\begin{aligned} d^J &= \frac{1}{2J+1}\{J V_{J-1}(r_1, r_2) + (J+1) V_{J+1}(r_1, r_2)\} \\ e^J &= \frac{\sqrt{J(J+1)}}{2J+1}\{V_{J-1}(r_1, r_2) - V_{J+1}(r_1, r_2)\} \\ f^J &= \frac{1}{2J+1}\{(J+1) V_{J-1}(r_1, r_2) + J V_{J+1}(r_1, r_2)\} \end{aligned} \tag{I – 26}$$

To be able to do the multipole expansion of a tensor interaction, we use:

$$V(|\vec{r}_1 - \vec{r}_2|)\Big[3\big\{(\vec{\sigma}_1.(\vec{r}_1 - \vec{r}_2)\big\}\big\{(\vec{\sigma}_2.(\vec{r}_1 - \vec{r}_2)\big\} - (\vec{r}_1 - \vec{r}_2)^2 \vec{\sigma}_1.\vec{\sigma}_2\Big] \tag{I – 27}$$

which is the usual tensor interaction multiplied by: $(\vec{r}_1 - \vec{r}_2)^2$. We get for its even part:

$$\begin{aligned} &a^J(1,2) = b^J(1,2) = 0, \\ &c^J(1,2) = (r_1^2 + r_2^2) V_J(r_1, r_2) - r_1 r_2 \Big\{\frac{2J+3}{2J+1} V_{J-1}(r_1, r_2) + \frac{2J-1}{2J+1} V_{J+1}(r_1, r_2)\Big\} \end{aligned} \tag{I – 28}$$

and for its odd part:

$$
\begin{aligned}
d^J(1,2) &= 2(r_1^2+r_2^2)\Big\{\frac{J}{2J+1}V_{J-1}(r_1,r_2)+\frac{(J+1)}{2J+1}V_{J+1}(r_1,r_2)\Big\} - r_1r_2 \\
&\Big\{\frac{J(J-1)}{(2J-1)(2J+1)}V_{J-2}(r_1,r_2)+\frac{14J^2+14J-10}{(2J-1)(2J+3)}V_J(r_1,r_2)+\frac{(J+1)(J+2)}{(2J+1)(2J+3)}V_{J+2}(r_1,r_2)\Big\} \\
e^J(1,2) &= (2r_1^2-r_2^2)\frac{\sqrt{J(J+1)}}{2J+1}\Big\{V_{J-1}(r_1,r_2)-V_{J+1}(r_1,r_2)\Big\} + r_1r_2\sqrt{J(J+1)} \\
&\Big\{\frac{J-1}{(2J-1)(2J+1)}V_{J-2}(r_1,r_2)+\frac{1}{(2J-1)(2J+3)}V_J(r_1,r_2)-\frac{J+2}{(2J+1)(2J+3)}V_{J+2}(r_1,r_2)\Big\} \\
f^J(1,2) &= -(r_1^2+r_2^2)\Big\{\frac{(J+1)}{2J+1}V_{J-1}(r_1,r_2)+\frac{J}{2J+1}V_{J+1}(r_1,r_2)\Big\} - r_1r_2 \\
&\Big\{\frac{(J-1)(J+1)}{(2J-1)(2J+1)}V_{J-2}(r_1,r_2)-\frac{10J^2+10J-9}{(2J-1)(2J+3)}V_J(r_1,r_2)+\frac{J(J+2)}{(2J+1)(2J+3)}V_{J+2}(r_1,r_2)\Big\}
\end{aligned}
\qquad \text{(I – 29)}
$$

## 1.3. – MATRIX ELEMENT BETWEEN BOUND STATES

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

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

where

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

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

The antisymmetrised particle-particle matrix element is:

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

The antisymmetrised particle-hole matrix element is:

$$\begin{aligned}
&< j_1'\ j_1^{-1}; JM|V(1,2)|j_2\ j_2'^{-1}; JM >= \\
\sum_{m_1',m_2',m_1,m_2} (-)^{j_1-m_1+j_2'-m_2'} &< j_1'\ j_1\ m_1'\ -m_1|J\ M >< j_2\ j_2'\ m_2\ -m_2'|J\ M > \\
&\times \{< j_1'm_1'| < j_2'm_2'|V(1,2)(|j_1m_1 > |j_2m_2 > -|j_2m_2 > |j_1m_1 >)\} \\
&= f^J_{j_1'j_2',j_1j_2} - \sum_{J'}(-)^{j_1+j_2+J+J'}(2J'+1)\Big\{\begin{matrix} j_1 & j_1' & J \\ j_2 & j_2' & J' \end{matrix}\Big\} f^{J'}_{j_1'j_2',j_2j_1}
\end{aligned} \qquad (\text{I}-33)$$

The matrix element $f^J$ is the direct particle-hole term and it involves only multipoles with the $J$-value to which the particle and the hole are coupled.

In order to evaluate it, let us perform successively the integration and the summation on the helicities of particle 1 to obtain a one-body form factor:

$$\begin{aligned}
F^{Jj_1j_1'}_{\lambda_2'\lambda_2}(2) = &\sum_{\lambda_1',\lambda_1}(-)^{j_1-\lambda_1}\frac{1}{2}\sqrt{\frac{(2j_1+1)(2j_1'+1)}{2J+1}}\begin{pmatrix} j_1' & J & j_1 \\ \lambda_1' & \lambda_1-\lambda_1' & -\lambda_1 \end{pmatrix} \\
&\times \int V^J_{\lambda_1'\lambda_2',\lambda_1\lambda_2}(1,2)\phi^{j_1'\star}_{\lambda_1'}(r_1)\phi^{j_1}_{\lambda_1}(r_1)r_1^2dr_1
\end{aligned} \qquad (\text{I}-34)$$

and then the same operation on particle 2:

$$\begin{aligned}
f^J_{\lambda_1'\lambda_2',\lambda_1\lambda_2} = &\sum_{\lambda_2',\lambda_2}(-)^{j_2'-\lambda_2}\frac{1}{2}\sqrt{\frac{(2j_2+1)(2j_2'+1)}{2J+1}}\begin{pmatrix} j_2' & J & j_2 \\ \lambda_2' & \lambda_2-\lambda_2' & -\lambda_2 \end{pmatrix} \\
&\times \int F^{Jj_1'j_1}_{\lambda_2'\lambda_2}\phi^{j_2'\star}_{\lambda_2'}(r_2)\phi^{j_2}_{\lambda_2}(r_2)r_2^2dr_2
\end{aligned} \qquad (\text{I}-35)$$

The one-body form factor can be expressed with the elementary matrices:

$$\begin{aligned}
F^{Jj_1j_1'}(2) = &A^{Jj_1j_1'}\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} + B^{Jj_1j_1'}\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \\
&+ C^{Jj_1j_1'}\begin{vmatrix} -1 & 0 \\ 0 & 1 \end{vmatrix} + D^{Jj_1j_1'}\begin{vmatrix} 0 & -1 \\ 1 & 0 \end{vmatrix}\lambda
\end{aligned} \qquad (\text{I}-36)$$

## 1.3.2. – PARTICLE-HOLE GEOMETRICAL COEFFICIENT

When the matrix for the particle 1 is diagonal in the helicity space, the geometrical coefficient becomes:

$$G^J_{j_1j_1'} = (-)^{j_1+\frac{1}{2}}\sqrt{(2j_1+1)(2j_1'+1)}\begin{pmatrix} j_1' & J & j_1 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \qquad (\text{I}-37)$$

instead of the usual expression:

$$G^J_{j_1j_1'} = (-)^{j_1-\frac{1}{2}}\sqrt{(2j_1+1)(2j_1'+1)(2l_1+1)(2l_1'+1)}\begin{pmatrix} l_1 & l_1' & J \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} l_1 & l_1' & J \\ j_1' & j_1 & \frac{1}{2} \end{Bmatrix} \qquad (\text{I}-38)$$

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

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

Recurrence relations between Clebsh-Gordon coefficients gives:

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

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

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

or with the quantum number $\kappa$ 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:

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

where

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

## 1.3.3. – PARTICLE-HOLE MATRIX ELEMENT

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

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

where $\eta$ 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:

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

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

$$\begin{aligned} C^{Jj_1j'_1} &= G^J_{j_1j'_1}\int [d^J(1,2) + \alpha^J_{j_1j'_1} e'^J(2,1)]\phi^\star_{l'_1j'_1}(r_1)\phi_{l_1j_1}(r_1)r_1^2 dr_1 \\ D^{Jj_1j'_1} &= G^J_{j_1j'_1}\int [e^J(1,2) + \alpha^J_{j_1j'_1} f^J(1,2)]\phi^\star_{l'_1j'_1}(r_1)\phi_{l_1j_1}(r_1)r_1^2 dr_1 \end{aligned} \qquad (\text{I}-46)$$

Here we used the usual wave functions. $G^J_{jj'}$ and $\alpha^J_{jj'}$ are the geometrical coefficients given above.

The matrix element is:

$$f^J_{j'_1j'_2j_1j_2} = (-)^{j'_2-j_2} G^J_{j_2j'_2}\int \Big[\begin{pmatrix} A \\ C \end{pmatrix} + \alpha^J_{j_2j'_2}\begin{pmatrix} B \\ D \end{pmatrix}\Big]\phi^\star_{l'_2j'_2}(r_2)\phi_{l_2j_2}(r_2)r_2^2 dr_2 \qquad (\text{I}-47)$$

where $A$ and $B$ are used for the natural parity case and $C$ and $D$ are used for the unnatural parity case.

## 1.4. – SPIN-ORBIT INTERACTION

**The relative spin orbit interaction introduces more form factors in the computation of the particle-hole matrix elements.** Nevertheless, it can be also obtained in the same formalism. For the relative spin-orbit interaction, we used:

$$\begin{aligned} V(|\vec{r}_1 - \vec{r}_2|)\ (2\vec{L}.\vec{S}) &= V(|\vec{r}_1 - \vec{r}_2|)\Big[(\vec{r}_1 - \vec{r}_2) \times \frac{\vec{\nabla}_1 - \vec{\nabla}_2}{i}.(\vec{\sigma}_1 + \vec{\sigma}_2)\Big] \\ = V(|\vec{r}_1 - \vec{r}_2|)\{\vec{L}_1 + \vec{L}_2 + i\vec{r}_1 \times \vec{r}_2\Big(\frac{1}{r_2}\frac{d}{dr_2} - \frac{1}{r_1}\frac{d}{dr_1}\Big) \\ + \frac{1}{r_2^2}\vec{r}_1 \times (\vec{r}_2 \times \vec{L}_2) + \frac{1}{r_1^2}\vec{r}_2 \times (\vec{r}_1 \times \vec{L}_1)\}(\vec{\sigma}_1 + \vec{\sigma}_2) \end{aligned} \qquad (\text{I}-48)$$

**There is a factor 4 between these results and the usual notations ( a factor 2 in the definition and a factor 2 in the transformation to absolute coordinates.)**

### 1.4.1. – MULTIPOLES OF THE SPIN-ORBIT INTERACTION

The expression of the multipoles have been given in [4] J. RAYNAL, *Symposium sur les Mécanismes de Réactions Nucléaires et phénoménes de Polarisation* Université Laval, Québec, (1969).

For the even part, the multipoles invariant for time reversal are:

$$\begin{aligned} a^J(1,2) &= -2V_J - \frac{1}{2}\Big(\frac{r_1}{r_2} + \frac{r_2}{r_1}\Big)\Big\{\frac{J(J-1)}{2J+1}V_{J-1} - \frac{(J+1)(J+2)}{2J+1}V_{J+1}\Big\} \\ &+ \frac{J(J+1)}{2(2J+1)}\Big\{\frac{r_1}{r_2}\Big(\alpha^J_{j_2j'_2}\Big)^2 + \frac{r_2}{r_1}\Big(\alpha^J_{j_1j'_1}\Big)^2\Big\}(V_{J-1} - V_{J+1}) \\ c^J(1,2) &= V_J - \frac{1}{2(2J+1)}\Big(\frac{r_1}{r_2} + \frac{r_2}{r_1}\Big)\Big\{(J+1)V_{J-1} + JV_{J+1}\Big\} \end{aligned} \qquad (\text{I}-49)$$

and for the odd part, the multipoles are:

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

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

$$b^J_1(1,2) = \frac{\sqrt{J(J+1)}}{2J+1}\Big[\big(V_{J-1}-V_{J+1}\big)\big(r_2\frac{d}{dr_1}-r_1\frac{d}{dr_2}\big)+\frac{1}{2}\big(\frac{r_2}{r_1}-\frac{r_1}{r_2}\big)\big(c_1V_{J-1}+c_2V_{J+1}\big)\Big] \qquad \text{(I – 51)}$$

(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 $j_2'$**:

$$\begin{aligned} b^J_2(1,2) &= \frac{(j_1+\frac{1}{2})^2-(j_1'+\frac{1}{2})^2}{2\sqrt{J(J+1)}}\Big[-V_J+\frac{r_2}{r_1}\big\{\tfrac{J+1}{2J+1}V_{J-1}+\tfrac{J}{2J+1}V_{J+1}\big\}\Big] \\ &+\frac{(j_2+\frac{1}{2})-(-)^{j_2+j_2'+J}(j_2'+\frac{1}{2})}{2\alpha^J_{j_2j_2'}}\Big[V_J-\frac{r_1}{r_2}\big\{\tfrac{J}{2J+1}V_{J-1}+\tfrac{J+1}{2J+1}V_{J+1}\big\}\Big] \end{aligned} \qquad \text{(I – 52)}$$

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

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

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

an only three for unnatural parity excitation:

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

## 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:

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

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

**for non identical particles, $V_{(T=0)}$ and $V_{(T=1)}$ are divided by 2 and the sign of $V_{(T=0)}$ is changed in the exchange term.**

In the zero range limit, **all the multipoles $V_J(r_1, r_2)$ are replaced by** $\delta(r_1 - r_2)/r_1^2$. The spin-orbit and the tensor interactions vanish. For the central interaction, the exchange term, which includes sums of products of a 6j coefficient and $(-)^{j_2'-j_1} G^J_{j_2 j_1'} G^J_{j_1 j_2'}$ is equal or opposite to the direct term. In fact:

$$V_{(S=0,T=0)} = 0, \qquad V_{(S=1,T=1)} = 0 \tag{I – 56}$$

An expansion of the interaction with respect to its range can be performed:

$$V(r) = \sum_{n=0}^{\infty} C_n \, \delta^{(2n)}(r) \tag{I – 57}$$

where $C_n$ can be defined from the Fourier transform:

$$W(q) = \int e^{iqr} V(r) dr = \sum_{n=0}^{\infty} C_n \int e^{iqr} \delta^{(2n)}(r) dr = \sum_{n=0}^{\infty} (-)^n C_n q^{2n} \tag{I – 58}$$

Using the Fourier transform of the $\delta$ function, we obtain:

$$\delta^{(2n)}(r) \Rightarrow \delta(r_1 - r_2) \Big\{ \frac{1}{r_1} \frac{d^2}{dr_1^2} r_1 - \frac{J(J+1)}{r_1^2} \Big\}^n f_{j_1'}(r_1) f_{j_1}(r_1) \tag{I – 59}$$

where the derivation acts on all the functions of $r_1$.

## 1.4.3. – ZERO-RANGE LIMIT OF THE INTERACTIONS

An interaction of range $\mu$ and intensity V corresponds to a zero-range interaction of intensity $V\mu^3$. When the zero-range interaction does not exist, the related zero-range limit interaction has an intensity $V\mu^5$.

This approximation can be applied to the one body form factor of the $\vec{L}.\vec{S}$ interaction. Let us consider a particle-hole excitation with radial functions $f_p(r)$ and $f_h(r)$. With the transition form factor:

$$V_J(r) = G^J_{j_p j_h} \, f_p(r) \, f_h(r) \tag{I – 60}$$

the zero-range limit is:

$$\begin{aligned} V_{LS}(r) = & \Big[ J(J+1) \big( (\alpha^J_{j_p j_h})^2 + (\alpha^J_{j_i j_f})^2 - 2 \big) - 1 \Big] \frac{V_J(r)}{r^2} \\ & + \Big[ 1 - (-)^{l_p + l_h + J} \alpha^J_{j_p j_h} \alpha^J_{j_i j_j} \Big] \Big[ - (\gamma_i + \gamma_f + 1) \frac{V_J(r)}{r^2} \\ & + (\gamma_p + \gamma_h - \gamma_i - \gamma_f) \frac{1}{r} \Big\{ \frac{d}{dr} V_J(r) \Big\} \Big] + \Big[ 1 + (-)^{l_p + l_h + J} \Big] \Big[ (\gamma_i + \gamma_p + 1) \frac{V_J(r)}{r^2} \\ & + (\gamma_h - \gamma_p - \gamma_i + \gamma_f) \Big( \frac{V_J(r)}{r} \frac{d}{dr} + G^J_{j_p j_h} \frac{1}{r} f_p(r) \Big\{ \frac{d}{dr} f_h(r) \Big\} \Big) \Big] \end{aligned} \tag{I – 61}$$

which includes natural parity excitations for which $\Big[ 1 + (-)^{l_p + l_h + J} \Big] = 2$ and unnatural parity excitations for which $\Big[ 1 + (-)^{l_p + l_h + J} \Big] = 0$. **This expression is invariant under antisymmetrisation**: direct and exchange terms add for $T = 1$ and cancel for $T = 0$.

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 $\gamma_p$ and $\gamma_h$ which must cancel out. $V_J(r)$ is the transition form factor. Using:

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

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**:

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

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 $\gamma_p$ 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 $\vec{k}_i$ with the helicity $\sigma_i$ on a nucleus without spin described by $\Psi^{I_i}$ and an outcoming particle in the direction $\vec{k}_f$ with an helicity $\sigma_f$, the residual nucleus having the helicity $\mu_f$ described by a particle $j_p$ and a hole $j_h$, $\Psi^{I_f}_{\mu_f}$ the reaction is described by the helicity amplitudes:

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

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:

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

for an unpolarised beam. The polarisation of the outcoming particle and of the residual nucleus, and their correlations are described by the matrix:

$$F_{\sigma_f\mu_f;\sigma'_f\mu'_f} = \left[2\frac{d\sigma}{d\Omega}(\vec{k}_i,\vec{k}_f)\right]^{-1}\sum_{\sigma_i} f_{\sigma_f\mu_f;\sigma_i}(\vec{k}_i,\vec{k}_f)f^{\star}_{\sigma'_f\mu'_f;\sigma_i}(\vec{k}_i,\vec{k}_f) \qquad \text{(I – 69)}$$

## 1.5.1. – HELICITY AMPLITUDES IN TERMS OF THE INTEGRALS

With the axis of quantisation along $\vec{k}_f$ and $\theta$ the angle between $\vec{k}_i$ and $\vec{k}_f$:

$$\begin{aligned} f_{\sigma_f\mu_f;\sigma_i}(\theta) = &-\frac{m}{\hbar^2}\sqrt{\frac{v_f}{v_i}}\frac{1}{k_f k_i}\sum_{j_i,j_f,m_i}(-)^{j_i-\sigma_i}\sqrt{(2j_i+1)(2j_f+1)(2I_f+1)} \\ &\times \begin{pmatrix} j_i] & j_f & I_f \\ m_i & -\sigma_f & \mu_f \end{pmatrix} \quad r^{(j_i)}_{m_i,\sigma_i}(\theta) \quad f^{I_f}_{j_p(j_f\sigma_f),j_h(j_i\sigma_i)} \end{aligned} \qquad \text{(I – 70)}$$

where the $f^J$ are defined as between bound-states as far as the first particle is concerned. Noting the integrals between the usual radial wave functions by:

$$F_{\pm,\pm} = \int F(2)\Xi_{l_f=j_f\pm\frac{1}{2}}\Xi_{l_i=j_i\pm\frac{1}{2}} \qquad \text{(I – 71)}$$

the following expressions are obtained for natural parity excitations:

$$\begin{aligned} f^J_{j_p(j_f\frac{1}{2});j_h(j_i\pm\frac{1}{2})} =& i^{j_i-j_f+1}G^J_{j_1j'_1}\left\{(A+\alpha^J_{j_1j'_1}B)_{+,-} \mp (A-\alpha^J_{j_1j'_1}B)_{-,+}\right\} \\ &\text{if } j_i+j_f+J\text{is even} \\ f^J_{j_p(j_f\frac{1}{2});j_h(j_i\pm\frac{1}{2})} =& i^{j_i-j_f}G^J_{j_1j'_1}\left\{(A-\alpha^J_{j_1j'_1}B)_{-,-} \pm (A+\alpha^J_{j_1j'_1}B)_{+,+}\right\} \\ &\text{if } j_i+j_f+J\text{is odd} \end{aligned} \qquad \text{(I – 72)}$$

and for unnatural parity excitations, $A$ and $B$ are replaced by $C$ and $D$ and the conditions on $j_i+j_f+J$ exchanged.

For the exchange, the same calculation has to be done for all the transfer of $J$ possible, with the initial distorted wave instead of the hole function. For each value of $J$, the matrix elements are natural parity or unnatural parity according to the angular momentum of the incoming particle.

**This formalism has been used by** [5] R. SCHAEFFER, *Un modéle microscopique pour la diffusion inelastique de protons a basse et moyenne energie*, Thesis, Orsay, (1969).**for the inelastic scattering of protons exciting low lying collective states of $^{40}$Ca and some other nuclei with a real static interaction. It has also be used for charge exchange reaction.**

## 1.5.2. – CODE DWBA70

This code [6] R. SCHAEFFER and J. RAYNAL, DWBA70 (*unpublished*). and Ref[2] takes into account particle-hole excitations with many configurations. The interaction is real, density independent and must have Yukawa form-factors. A superposition of Yukawa form factors can be used. The interactions are the coulomb interaction, a scalar, $(\vec{\sigma}_1.\vec{\sigma}_2)$, tensor and

$(\vec{L}.\vec{S})$ 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:

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

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

## 2. – DWBA82

Even increased with the possibility to sum over more than one $J$-transfer, the code DWBA70 had to be modified for the use of a complex G-matrix instead of a real interaction. The code was rewritten with the same structure used in ECIS, which avoid any internal limitations.

### 2.1. – PRESENTATION OF THE INTERACTION

Beside the possibility to use macroscopic transition form factors, the interaction is introduced in a more conventional way, using $S$ and $T$ notations. The projectors on the value of $S$ are:

$$P_{S=0} = \frac{1-(\vec{\sigma}_1.\vec{\sigma}_2)}{4}, \qquad P_{S=1} = \frac{3+(\vec{\sigma}_1.\vec{\sigma}_2)}{4} \tag{II – 1}$$

**The finite range interactions are central, tensor and spin-orbit**:

$$\begin{array}{llll} V_{(S=0,T=0)}, & V_{(S=0,T=1)}, & V_{(S=1,T=0)}, & V_{(S=1,T=1)}, \\ V^{LS}_{(S=1,T=0)}, & V^{LS}_{(S=1,T=1)}, & V^{T}_{(S=1,T=0)}, & V^{T}_{(S=1,T=1)} \end{array} \tag{II – 2}$$

**The zero range interactions are**:

$$V_{(S=0,T=1)}, \qquad V_{(S=1,T=0)}, \qquad V^{LS}_{(S=1,T=1)} \tag{II – 3}$$

**and zero-range limits of the scalar interaction which are identical to some part of the Skyrme force and zero range limit of the tensor interaction**:

$$\begin{array}{llll} V^{Skyrme}_{(S=0,T=0)}, & V^{Skyrme}_{(S=0,T=1)}, & V^{Skyrme}_{(S=1,T=0)}, & V^{Skyrme}_{(S=1,T=1)}, \\ & V^{T,0-limit}_{(S=1,T=0)}, & V^{T,0-limit}_{(S=1,T=1)} & \end{array} \tag{II – 4}$$

All these interactions can be complex and density dependent. The density dependence can be:

$$V_J(r_1,r_2) \Rightarrow V_J(r_1,r_2)\sqrt{g(r_1)g(r_2)} \tag{II – 5}$$

or

$$V_J(r_1,r_2) \Rightarrow V_J(r_1,r_2)\frac{1}{2}\big[g(r_1)+g(r_2)\big] \tag{II – 6}$$

### 2.2. – THE SKYRME INTERACTION

The Skyrme force introduced by [7] T. H. R. SKYRME, Phil. Mag. **1**, 1043 (1956); Nucl. Phys. **9**, 615 (1959). is:

$$\begin{aligned} V(\vec{r}_1-\vec{r}_2) = t_0(1+x_0P^\sigma)\delta(\vec{r}_1-\vec{r}_2) + \frac{t_1}{2}\big[\delta(\vec{r}_1-\vec{r}_2)\vec{k}^2 + \vec{k'}^2\delta(\vec{r}_1-\vec{r}_2)\big] + \\ + t_2\vec{k'}.\delta(\vec{r}_1-\vec{r}_2)\vec{k} + iw_0(\sigma_1+\sigma_2)\vec{k'}\times\delta(\vec{r}_1-\vec{r}_2)\vec{k} \end{aligned} \tag{II – 7}$$

is a zero-range limit interaction; consequently, as shown by [8] J. P. BLAIZOT and J. RAYNAL, Lettere al Nuovo Cim. **12**, 508 (1975). its particle-hole matrix elements are products of quite simple geometrical coefficients with zero range radial integrals involving derivatives of the radial functions. The first term is the zero range scalar interaction and the last term is the zero range limit of the spin orbit interaction as they were used in DWBA70. Notations for Skyrme force are usually $4\pi$ 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:

$$t_1 \Rightarrow V^{Skyrme}_{(S=0,T=1)} + V^{Skyrme}_{(S=1,T=0)} \qquad \text{(II – 8)}$$

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:

$$t_2 \Rightarrow V^{Skyrme}_{(S=0,T=0)} + V^{Skyrme}_{(S=1,T=1)} \qquad \text{(II – 9)}$$

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 $T = 0$:

$$V^T \Rightarrow V^{T,0-limit}_{(S=1,T=0)} + V^{T,0-limit}_{(S=1,T=1)} \qquad \text{(II – 10)}$$

**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. – DWBA90

This new code has been developed to include $\vec{L}^2$ and $(\vec{L}.\vec{S})^2$ terms in the two-body interaction.

The interaction used in such calculation is obtained by a $\chi^2$ fit of the phase shifts of nucleon nucleon potentials like those of Paris or Bonn. Introduction of other interaction like $(\vec{L}.\vec{S})^2$ and $\vec{L}^2$ or $Q_{12} = (\vec{L}.\vec{S})^2 - \vec{L}^2$ reduces largely the $\chi^2$. For this reason, it appeared useful to add such interactions in the code.

### 3.1. – COMPUTATION OF THE MULTIPOLES OF $\vec{L}^2$ AND $(\vec{L}.\vec{S})^2$ INTERACTIONS

**The number of two-body and one-body form factors is quite large ( twenty one body form factors for natural parity, eighteen for unnatural parity ) and leads to some drastic changes in the notations.**

#### 3.1.1. – NEW NOTATIONS

Instead of $\alpha^J_{jj'}$, we define now:

$$\begin{aligned}\alpha^J_{jj'} &= (\gamma+1) - (-)^{l+l'+J}(\gamma'+1)\\ \beta^J_{jj'} &= (\gamma+1) + (-)^{l+l'+J}(\gamma'+1)\end{aligned} \qquad \text{(III – 1)}$$

which is the old definition of $\alpha^J_{jj'}$ multiplied by $\sqrt{J(J+1)}$, $\beta^J_{jj'}$ being the coefficient of opposite parity, as it appears already in some form factors of the spin orbit interaction.

We define the following eleven coefficients $X_i$ for particle 1 and the following eleven coefficients $Y_i$ for particle 2:

| | |
|---|---|
| $X_1 = \alpha^J_{j_1 j'_1}$ | $Y_1 = \alpha^J_{j_2 j'_2}$ |
| $X_2 = (\alpha^J_{j_1 j'_1})^2$ | $Y_2 = (\alpha^J_{j_2 j'_2})^2$ |
| $X_3 = \alpha^J_{j_1 j'_1}\beta^J_{j_1 j'_1}$ | $Y_3 = \alpha^J_{j_2 j'_2}\beta^J_{j_2 j'_2}$ |
| $X_4 = \beta^J_{j_1 j'_1}$ | $Y_4 = \beta^J_{j_2 j'_2}$ |
| $X_5 = \big[(\alpha^J_{j_1 j'_1})^2 - 1\big]\beta^J_{j_1 j'_1}$ | $Y_5 = \big[(\alpha^J_{j_2 j'_2})^2 - 1\big]\beta^J_{j_2 j'_2}$ |
| $X_6 = (\beta^J_{j_1 j'_1})^2$ | $Y_6 = (\beta^J_{j_2 j'_2})^2$ |
| $X_7 = (\alpha^J_{j_1 j'_1})^3$ | $Y_7 = (\alpha^J_{j_2 j'_2})^3$ |
| $X_8 = \alpha^J_{j_1 j'_1}(\beta^J_{j_1 j'_1})^2$ | $Y_8 = \alpha^J_{j_2 j'_2}(\beta^J_{j_2 j'_2})^2$ |
| $X_9 = \big[(\alpha^J_{j_1 j'_1})^2 - 1\big](\beta^J_{j_1 j'_1})^2$ | $Y_9 = \big[(\alpha^J_{j_2 j'_2})^2 - 1\big](\beta^J_{j_2 j'_2})^2$ |
| $X_{10} = \alpha^J_{j_1 j'_1}\big[(\alpha^J_{j_1 j'_1})^2 - 1\big](\beta^J_{j_1 j'_1})^2$ | $Y_{10} = \alpha^J_{j_2 j'_2}\big[(\alpha^J_{j_2 j'_2})^2 - 1\big](\beta^J_{j_2 j'_2})^2$ |
| $X_{11} = \alpha^J_{j_1 j'_1}\big[(\alpha^J_{j_1 j'_1})^2 - 1\big]\beta^J_{j_1 j'_1}$ | $Y_{11} = \alpha^J_{j_2 j'_2}\big[(\alpha^J_{j_2 j'_2})^2 - 1\big]\beta^J_{j_2 j'_2}$ |

Already in DWBA82, the zero range limit interactions involved for natural parity matrix elements

1) two second derivative form factors, with constant and $X_1$
2) five first derivative form factors, with constant and $X_1$ to $X_4$
3) nine form factors without derivatives, with constant and $X_1$ to $X_8$

### 3.1.2. – STRUCTURE OF THE MULTIPOLES

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

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

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:

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

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 $r_1 \to -r_1$ 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 $\beta^J_{j_2 j_2'}$) separately. 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 $Y_i$).

### 3.1.3. – COMPUTATION OF INTERACTIONS FROM SIMPLER ONES

We want to compute the particle hole matrix elements of the interaction:

$$V(|\vec{r}_1 - \vec{r}_2|)V_x(1,2)V_y(1,2) \qquad \text{(III – 7)}$$

where $V_x(1,2)$ and $V_y(1,2)$ are two interactions of which we know:

$$\begin{aligned} g^J_{j'_1 j'_2, j_1 j_2} = & \sum_{m'_1, m'_2, m_1, m_2} (-)^{j_1 - m_1 + j'_2 - m'_2} < j'_1\ j_1\ m'_1\ -m_1 | J\ M > \\ & \times < j_2\ j'_2\ m_2\ -m'_2 | J\ M >< j'_1 m'_1 j'_2 m'_2 | V(|\vec{r}_1 - \vec{r}_2|) V_x(1,2) | j_1 m_1 j_2 m_2 > \end{aligned} \qquad \text{(III – 8)}$$

with the radial dependence $V(|\vec{r}_1 - \vec{r}_2|)$ and

$$\begin{aligned} h^J_{j'_1 j'_2, j_1 j_2} = & \sum_{m'_1, m'_2, m_1, m_2} (-)^{j_1 - m_1 + j'_2 - m'_2} < j'_1\ j_1\ m'_1\ -m_1 | J\ M > \\ & \times < j_2\ j'_2\ m_2\ -m'_2 | J\ M >< j'_1 m'_1 j'_2 m'_2 | V_y(1,2) | j_1 m_1 j_2 m_2 > \end{aligned} \qquad \text{(III – 9)}$$

where there is no radial dependence, that is particle hole matrix elements limited to $L = 0$. Therefore, **for given $|j_1 m_1 >$ and $|j_2 m_2 >$, the possible $|j'_1 m'_1 >$ and $|j'_2 m'_2 >$ are very limited**.

Writing:

$$\begin{aligned} & < j'_1 m'_1 j'_2 m'_2 | V(|\vec{r}_1 - \vec{r}_2|) V_x(1,2) V_y(1,2) | j_1 m_1 j_2 m_2 > = \\ & \sum_{j''_1, m''_1, j''_2, m''_2} < j'_1 m'_1 j'_2 m'_2 | V(|\vec{r}_1 - \vec{r}_2|) V_x(1,2) | j''_1 m''_1 j''_2 m''_2 > \\ & \times < j''_1 m''_1 j''_2 m''_2 | V_y(1,2) | j_1 m_1 j_2 m_2 > \end{aligned} \qquad \text{(III – 10)}$$

we get:

$$\begin{aligned} f^J_{j'_1 j'_2, j_1 j_2} = & \sum_{J', J'', j''_1, j''_2} (-)^{j_2 + j'_2 + j_1 + j'_1 + J + J' + J''} (2J' + 1)(2J'' + 1) \\ & \times \left\{ \begin{matrix} J'' & J' & J \\ j'_1 & j_1 & j''_1 \end{matrix} \right\} \left\{ \begin{matrix} J'' & J' & J \\ j'_2 & j_2 & j''_2 \end{matrix} \right\} g^{J'}_{j'_1 j'_2, j''_1 j''_2} h^{J''}_{j''_1 j''_2, j_1 j_2} \end{aligned} \qquad \text{(III – 11)}$$

### 3.1.4. – COMPUTATION OF $\vec{L}^2$ AND $(\vec{L}.\vec{S})^2$

With the matrix elements of $(\vec{L}.\vec{\sigma}_1)$ and $(\vec{L}.\vec{\sigma}_2)$, one obtain:

$$\begin{aligned} \vec{L}^2 &= (\vec{L}.\vec{\sigma}_1)^2 - (\vec{L}.\vec{\sigma}_1) \\ (\vec{L}.\vec{S})^2 &= \frac{1}{4}\Big[(\vec{L}.\vec{\sigma}_1)(\vec{L}.\vec{\sigma}_2) + (\vec{L}.\vec{\sigma}_2)(\vec{L}.\vec{\sigma}_1)\Big] + \frac{1}{2}\Big[\vec{L}^2 - (\vec{L}.\vec{S})\Big] \end{aligned} \qquad \text{(III – 12)}$$

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

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

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 $\alpha$ and $\beta$ which multiply each power of $J$ in $P(J,\ldots)$
3) by identifying these polynomials in $\alpha$ and $\beta$.

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

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

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

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

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

### 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

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

There are relations between these multipoles:

1) due to the absence of these interactions in the relative $S$–state and the equality of the multipoles for a zero–range interaction, the following sums vanish:

$$\sum_L C_1^L = \sum_L C_2^L - C_3^L = \sum_{L'} C_4^{L'} = \sum_L C_5^L + C_6^L + C_7^L + \sum_{L'} C_8^{L'} + C_9^{L'} = 0 \qquad \text{(III – 17)}$$

2) there is a kind of "mirror" symmetry (invariance of geometrical coefficients when any quantum number $j \to -j-1$ [9] A. P. YUTSIS and A. A. BANDZAITIS, *The Theory of Angular Momenta in Quantum Mechanics*, Vilnius, 1965) which is a relation between the multipole for $L = J + n$ and the multipole for $L = J - n$:

$$C_i^{J+n} = f_{n,i}(J, X, Y) \qquad C_i^{J-n} = -f_{n,i}(-J-1, X, Y) \qquad \text{(III – 18)}$$

3) and the symmetry between the two particles by permutation of the $X$'s and the $Y$'s:

$$C_1^L \to C_1^L, \qquad C_2^L \to C_3^L, \qquad C_4^{L'} \to -C_4^{L'}, \qquad C_5^L \to C_7^L, \qquad C_6^L \to C_6^L, \qquad C_8^{L'} \to C_9^{L'} \qquad \text{(III – 19)}$$

The sum on $L$ or $L'$ involves the non negative values:

$$L = J-2,\ J\ , J+2, \qquad L' = J-1, J+1$$

for the three interactions and natural parity

$$L = J-1, J+1, \qquad L' = J-2,\ J\ , J+2$$

for $(\vec{L}.\vec{S})^2$ and unnatural parity

$$L = J-3, J-1, J+1, J+3, \qquad L' = J-2,\ J\ , J+2$$

for $\vec{L}^2(\vec{\sigma}_1.\vec{\sigma}_2)$ and unnatural parity.

We shall give the list of the multipoles $C_1$, $C_2$, $C_4$, $C_5$, $C_6$ and $C_8$, including those which can be obtained by the symmetry $J \to -J-1$. The other multipoles can be obtain by exchange of the $X$'s with the $Y$'s. For $J = 0$, the denominators $J(J+1)$ are replaced by 1; in this case, all the $X$'s vanish except for $X_4 = -X_5$ and $X_6 = -X_9$ and the same happens for the $Y$'s. Sometimes a different expression is needed to avoid division by $J = 0$.

### 3.2.2. – EVEN PARITY MULTIPOLE EXPANSIONS

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

1) the central interaction has only one multipole:

$$C_6^J = 1 \qquad \text{(III – 20)}$$

2) the $(\vec{\sigma}_1.\vec{\sigma}_2)$ has only one multipole:

$$C_6^J = -\frac{X_1 Y_1}{J(J+1)} \qquad \text{(III – 21)}$$

3) the spin orbit interaction has only:

$$\begin{aligned} C_4^{J-1} &= -C_4^{J+1} = \frac{1}{4(2J+1)}[X_1 - Y_1] \\ C_6^J &= -\frac{1}{8}\Big[4 - X_4 - Y_4 + \frac{(X_3 - X_1)Y_1 + (Y_3 - Y_1)X_1}{J(J+1)}\Big] \\ C_8^{J-1} &= -\frac{1}{8(2J+1)}\Big[(J-1)(J + X_1 - Y_1) - X_2 + JX_4 + \frac{1}{J}(X_1 - X_3)Y_1\Big] \\ C_8^{J+1} &= \frac{1}{8(2J+1)}\Big[(J+2)(J+1-X_1+Y_1) - X_2 - (J+1)X_4 - \frac{1}{J+1}(X_1 - X_3)Y_1\Big] \end{aligned} \qquad \text{(III – 22)}$$

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

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

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

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

$$\begin{aligned} C_2^{J-2} &= \frac{J-1}{4(2J-1)(2J+1)}\Big[J(J-2) - Y_1 + Y_3\Big] \\ C_2^J &= -\frac{1}{4(2J-1)(2J+3)}\Big[J(J+1) + Y_1 - Y_3\Big] \\ C_2^{J+2} &= -\frac{J+2}{4(2J+1)(2J+3)}\Big[(J+1)(J+3) - Y_1 + Y_3\Big] \\ C_4^{J-1} &= -C_4^{J+1} = -\frac{1}{4(2J+1)}\big[X_1 - X_3 - Y_1 + Y_3\big] \end{aligned} \qquad \text{(III – 25)}$$

$$\begin{aligned} C_5^{J-2} &= \frac{1}{16(2J-1)(2J+1)}\Big[(J-1)\{(J-3)[J(J-2) - 2Y_1 + 2Y_3] - Y_2 + 2Y_4 - Y_6\} - 2Y_5 + Y_9\Big] \\ C_5^J &= -\frac{1}{8(2J-1)(2J+3)}\Big[(J-1)(J+2)\{J(J+1) + 2Y_1 - 2Y_3\} - 2(J^2+J-1)(Y_2 - 2Y_4 + Y_6) \\ &\quad - 2Y_5 + Y_9\Big] \\ C_5^{J+2} &= \frac{1}{16(2J+1)(2J+3)}\Big[(J+2)\{(J+4)[(J+1)(J+3) - 2Y_1 + 2Y_3] + Y_2 - 2Y_4 + Y_6\} - 2Y_5 + Y_9\Big] \end{aligned} \qquad \text{(III – 26)}$$

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

$$
\begin{aligned}
C_8^{J-1} =& \frac{1}{8(2J+1)}\Big[(J-1)\{J(J+1)-X_1+X_3+Y_1-Y_3\}-J(Y_2-2Y_4+Y_6)\\
&+\frac{1}{J}(X_1-X_3)(Y_1-Y_3)\Big]\\
C_8^{J+1} =& \frac{1}{8(2J+1)}\Big[(J+2)\{J(J+1)-X_1+X_3+Y_1-Y_3\}-(J+1)(Y_2-2Y_4+Y_6)\\
&+\frac{1}{J+1}(X_1-X_3)(Y_1-Y_3)\Big]
\end{aligned}
\qquad \text{(III – 28)}
$$

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

$$
\begin{aligned}
&C_1^0 = -\,C_1^2 = -\frac{1}{6} \qquad C_2^2 = -\frac{1}{2}\\
&C_5^0 = -\,\frac{2Y_4-Y_6}{24} \qquad C_5^2 = \frac{24-2Y_4+Y_6}{48}\\
&C_6^0 = -\,\frac{32+6(X_4+Y_4)-3(X_6+Y_6)}{48} \qquad C_6^2 = -\frac{1}{3}\\
&C_8^1 = \frac{2Y_4-Y_6}{8}
\end{aligned}
\qquad \text{(III – 29)}
$$

without division by $J=0$.

**3.2.2.2. – EVEN PARITY MULTIPOLE EXPANSION OF $(\vec{L}.\vec{\sigma}_1)(\vec{L}.\vec{\sigma}_2)$**

$$
C_1^{J-2} = -\frac{(J-1)X_1Y_1}{4J(2J-1)(2J+1)} \quad C_1^J = \frac{(2J^2+2J-3)X_1Y_1}{4J(J+1)(2J-1)(2J+3)} \quad C_1^{J+2} = -\frac{(J+2)X_1Y_1}{4(J+1)(2J+1)(2J+3)}
\qquad \text{(III – 30)}
$$

$$
\begin{aligned}
C_2^{J-2} =& -\frac{X_1}{8J(2J-1)(2J+1)}\Big[(J-1)\{(J-2)(J+2Y_1)+(J-1)Y_4-Y_2\}+Y_5\Big]\\
C_2^{J} =& \frac{X_1}{8(2J-1)(2J+3)}\Big[2J(J+1)-\frac{1}{J(J+1)}\{2(J^2+J-3)Y_1+(2J^2+2J-3)Y_2+3(J^2+J-1)Y_4\\
&-3Y_5\}\Big]\\
C_2^{J+2} =& -\frac{X_1}{8(J+1)(2J+1)(2J+3)}\Big[(J+2)\{(J+3)(J+1-2Y_1)-(J+2)Y_4-Y_2\}-Y_5\Big]\\
C_4^{J-1} =& -\,C_4^{J+1} = -\frac{1}{8(2J+1)}\Big[3(X_1-Y_1)+\frac{1}{J(J+1)}\{(J^2+J-1)(X_4Y_1-X_1Y_4)+X_5Y_1-X_1Y_5\}\Big]
\end{aligned}
\qquad \text{(III – 31)}
$$

$$
\begin{aligned}
C_5^{J-2} =& -\frac{X_1}{16J(2J-1)(2J+1)}\Big[(J-1)\{(J-3)[J(J-2)-Y_2+(J-1)Y_4]+(J^2-6J+6)Y_1 \\
&+(J-1)Y_3+Y_8\}+(J-3)Y_5-Y_{11}\Big] \\
C_5^{J} =& \frac{X_1}{16(2J-1)(2J+3)}\Big[3(J-1)(J+2)-2Y_8+\frac{1}{J(J+1)}\{(J-1)(J+2)[3Y_2-(2J^2+2J-3)Y_4] \\
&-(2J^4+4J^3-J^2-3J+6)Y_1+3(3J^2+3J-2)Y_3-2(J^2+J+3)Y_5-3Y_{11}\}\Big] \\
C_5^{J+2} =& \frac{X_1}{16(J+1)(2J+1)(2J+3)}\Big[(J+2)\{(J+4)[(J+1)(J+3)-Y_2-(J+2)Y_4]-(J^2+8J+13)Y_1 \\
&+(J+2)Y_3-Y_8\}-(J+4)Y_5-Y_{11}\Big]
\end{aligned}
\qquad \text{(III – 32)}
$$

$$
\begin{aligned}
C_6^{J-2} =& \frac{1}{16(2J-1)(2J+1)}\Big[(J-1)\{2J(J^2-J+1)+(J-1)(J-2)(X_1+Y_1)-(2J-1)(X_2 \\
&+Y_2)+(2J^2+1)(X_4+Y_4)\}-(J+1)(X_5+Y_5)+\frac{1}{J}\{(J-1)\Big((J-1)[(J-1)(2X_1Y_1+X_4Y_1 \\
&+X_1Y_4)-X_2Y_1-X_1Y_2]+2(J^2+J+1)X_4Y_4-(2J+1)(X_4Y_2+X_2Y_4)+X_5Y_1+X_1Y_5 \\
&+2X_2Y_2\Big)-(J+2)(X_5Y_4+X_4Y_5)+X_5Y_2+X_2Y_5\}+\frac{2X_5Y_5}{J(J-1)}\Big] \\
C_6^{J} =& \frac{1}{16}\Big[X_2+Y_2+\frac{1}{J(J+1)}\{(3X_3-X_8)Y_1+X_1(3Y_3-Y_8)\}-\frac{1}{(2J-1)(2J+3)}\{4(J^4+2J^3 \\
&-8J^2-9J+6)+(7J^2+7J-6)(X_1+Y_1)+3(6J^2+6J-5)(X_4+Y_4)-3X_5-3Y_5 \\
&-2(2J^2+2J-1)X_1Y_1-(2J^2+2J-1)(X_4Y_1+X_1Y_4)-(X_2+2X_5)Y_1-X_1(Y_2+2Y_5)\} \\
&-\frac{1}{J(J+1)(2J-1)(2J+3)}\{2(2J^2+2J-3)X_2Y_2-6(2J^4+4J^3-J^2-3J+2)X_4Y_4 \\
&+6(J-1)(J+2)(X_5Y_4+X_4Y_5)+3[(X_4+X_5)Y_2+X_2(Y_4+Y_5)-4X_5Y_5]\}\Big] \\
C_6^{J+2} =& \frac{1}{16(2J+1)(2J+3)}\Big[(J+2)\{2(J+1)(J^2+3J+3)-(J+2)(J+3)(X_1+Y_1)-(2J+3)(X_2 \\
&+Y_2)-(2J^2+4J+3)(X_4+Y_4)\}+J(X_5+Y_5)+\frac{1}{J+1}\{(J+2)\Big((J+2)[(J+2)(2X_1Y_1+X_4Y_1 \\
&+X_1Y_4)+X_2Y_1+X_1Y_2]+2(J^2+J+1)X_4Y_4+(2J+1)(X_4Y_2+X_2Y_4)+X_5Y_1+X_1Y_5 \\
&+2X_2Y_2\Big)-(J-1)(X_5Y_4+X_4Y_5)-X_5Y_2-X_2Y_5\}+\frac{2X_5Y_5}{(J+1)(J+2)}\Big]
\end{aligned}
\qquad \text{(III – 33)}
$$

$$
\begin{aligned}
C_8^{J-1} =& \frac{1}{16(2J+1)}\Big[(J-1)\{(3J-3X_1+3Y_1-(2J+1)X_4\}+3JY_4-3Y_2+X_5 \\
&+\frac{3}{J}X_1Y_1-\frac{1}{J(J+1)}\{(J-1)[(J^2+J+1)(X_4Y_1-X_1Y_4)+X_5Y_1-X_1Y_5] \\
&-(2J^2+2J-1)X_4Y_2-(J^2-5J-5)X_1Y_3+(2J^3+3J^2-2)X_4Y_4 \\
&-(J+2)(X_5Y_4+X_4Y_5)-(2J+1)X_1Y_8+X_5Y_2+X_1Y_{11}\}-\frac{2X_5Y_5}{J(J-1)(J+1)}\Big] \\
C_8^{J+1} =& -\frac{1}{16(2J+1)}\Big[(J+2)\{(3J+3+3X_1-3Y_1-(2J+1)X_4\}-3(J+1)Y_4-3Y_2+X_5 \\
&-\frac{3}{J+1}X_1Y_1+\frac{1}{J(J+1)}\{(J+2)[(J^2+J+1)(X_4Y_1-X_1Y_4)+X_5Y_1-X_1Y_5] \\
&+(2J^2+2J-1)X_4Y_2+(J^2+7J+1)X_1Y_3+(2J^3+3J^2+1)X_4Y_4 \\
&-(J-1)(X_5Y_4+X_4Y_5)-(2J+1)X_1Y_8-X_5Y_2-X_1Y_{11}\}+\frac{2X_5Y_5}{J(J+1)(J+2)}\Big]
\end{aligned}
\qquad \text{(III – 34)}
$$

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 $C_6^0$ and $C_8^1$.

### 3.2.2.3. – EVEN PARITY MULTIPOLE EXPANSION OF $\vec{L}^2(\vec{\sigma}_1.\vec{\sigma}_2)$

$$
C_1^{J-2}=-\frac{(J-1)X_1Y_1}{4(J+1)(2J-1)(2J+1)} \quad C_1^J=\frac{(J^2+J-1)X_1Y_1}{2J(J+1)(2J-1)(2J+3)} \quad C_1^{J+2}=-\frac{(J+2)X_1Y_1}{4J(2J+1)(2J+3)} \qquad \text{(III – 36)}
$$

$$
\begin{aligned}
C_2^{J-2} =& -\frac{(J-1)X_1}{4J(J+1)(2J-1)(2J+1)}\Big[J(J-2)Y_1-Y_2+Y_4+Y_5\Big] \\
C_2^{J} =& \frac{X_1}{4J(J+1)(2J-1)(2J+3)}\Big[J(J+1)Y_1+Y_2-Y_4-Y_5\Big] \\
C_2^{J+2} =& \frac{(J+2)X_1}{4J(J+1)(2J+1)(2J+3)}\Big[(J+1)(J+3)Y_1-Y_2+Y_4+Y_5\Big] \\
C_4^{J-1} =& -C_4^{J+1}=-\frac{1}{4J(J+1)(2J+1)}\Big[X_1(Y_2-Y_4-Y_5)-Y_1(X_2-X_4-X_5)\Big]
\end{aligned}
\qquad \text{(III – 37)}
$$

$$
\begin{aligned}
C_5^{J-2} =& -\frac{X_1}{16J(J+1)(2J-1)(2J+1)}\Big[(J-1)\{(J-3)[J(J-2)Y_1-2Y_2+2Y_4+2Y_5]\\
&+2Y_3-Y_7-Y_8\}+Y_{10}-2Y_{11}\Big]\\
C_5^{J} =&\frac{X_1}{8J(J+1)(2J-1)(2J+3)}\Big[(J-1)(J+2)\{(J(J+1)Y_1+2Y_2-2Y_4-2Y_5\}\\
&+2(J^2+J-1)(2Y_3-Y_7-Y_8)+Y_{10}-2Y_{11}\Big]\\
C_5^{J+2} =& -\frac{X_1}{16J(J+1)(2J+1)(2J+3)}\Big[(J+2)\{(J+4)[(J+1)(J+3)Y_1-2Y_2+2Y_4+2Y_5]\\
&-2Y_3+Y_7+Y_8\}+Y_{10}-2Y_{11}\Big]
\end{aligned}
\qquad \text{(III – 38)}
$$

$$
\begin{aligned}
C_6^{J-2} =&\frac{1}{8(2J+1)}\Big[(J-1)\{J^2-X_2-Y_2+(J+1)(X_4+Y_4)\}-X_5-Y_5+\frac{1}{(J+1)(2J-1)}\{(J-1)\\
&[(J-1)^2X_1Y_1-(2J+3)(X_4Y_2+X_2Y_4)]+2X_5Y_2+2X_2Y_5\}-\frac{1}{J(J+1)(2J-1)}\{(J-1)\\
&\Big((J-1)[(X_2-X_4-X_5)Y_1+X_1(Y_2-Y_4-Y_5)]-(2J^3+5J^2+3J-1)X_4Y_4-(2J+1)X_2Y_2\Big)\\
&+(2J^2+3J-1)(X_5Y_4+X_4Y_5)\}+\frac{3J-1}{J(J-1)(J+1)(2J-1)}X_5Y_5\Big]\\
C_6^{J} =&\frac{1}{8}\Big[J^2+J+2-X_2-X_4-Y_2-Y_4+\frac{1}{2J(J+1)}\{(2X_3-X_7-X_8)Y_1+X_1(2Y_3-Y_7-Y_8)\}\\
&+\frac{1}{J(J+1)(2J-1)(2J+3)}\{(6J^4+12J^3+23J^2+17J-16)X_1Y_1+(4J^2+4J-1)X_2Y_2\\
&+(4J^4+8J^3-3J^2-7J+5)X_4Y_4-2(J^2+J-1)[(X_2-X_4-X_5)Y_1+X_1(Y_2-Y_4-Y_5)]\\
&-(4J^2+4J-5)(X_5Y_4+X_4Y_5)-2(X_4+X_5)Y_2-2X_2(Y_4+Y_5)\}\\
&+\frac{10(J^2+J-1)X_5Y_5}{(J-1)J(J+1)(J+2)(2J-1)(2J+3)}\Big]\\
C_6^{J+2} =&\frac{1}{8(2J+1)}\Big[(J+2)\{(J+1)^2-X_2-Y_2-J(X_4+Y_4)\}+X_5+Y_5+\frac{1}{J(2J+3)}\{(J+2)\\
&[(J+2)^2X_1Y_1+(2J-1)(X_4Y_2+X_2Y_4)]-2X_5Y_2-2X_2Y_5\}-\frac{1}{J(J+1)(2J+3)}\{(J+2)\\
&\Big((J+2)[(X_2-X_4-X_5)Y_1+X_1(Y_2-Y_4-Y_5)]-(2J^3+J^2-J+1)X_4Y_4-(2J+1)X_2Y_2\Big)\\
&+(2J^2+J-2)(X_5Y_4+X_4Y_5)\}+\frac{(3J+4)X_5Y_5}{J(J+1)(J+2)(2J+3)}\Big]
\end{aligned}
\qquad \text{(III – 39)}
$$

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

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:

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

3) the spin orbit interaction has only:

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

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

$$
\begin{aligned}
C^{J-2} &= -r_1 r_2 \, \frac{(J-1)(J-X_1)(J-Y_1)}{J(2J-1)(2J+1)} \\
C^{J+2} &= -r_1 r_2 \, \frac{(J+2)(J+1+X_1)(J+1+Y_1)}{(J+1)(2J+1)(2J+3)} \\
C^{J} &= (-4+2\frac{X_1 Y_1}{J(J+1)}) r_1 r_2 - C^{J-2} - C^{J+2} \\
C^{J-1} &= r_1^2 \, \frac{(2J+X_1)(J-Y_1)}{J(2J+1)} + r_2^2 \, \frac{(2J+Y_1)(J-X_1)}{J(2J+1)} \\
C^{J+1} &= r_1^2 \, \frac{(2J+2-X_1)(J+1+Y_1)}{(J+1)(2J+1)} + r_2^2 \, \frac{(2J+2-Y_1)(J+1+X_1)}{(J+1)(2J+1)}
\end{aligned}
\qquad \text{(III – 44)}
$$

5) the $\vec{L}^2$ interaction reduces to:

$$
C_6^{J-1} = C_6^{J+1} = -C_8^J = \frac{J(J+1)}{8}\Big(1+\frac{X_1-X_2}{J(J+1)}\Big)\Big(1+\frac{Y_1-Y_2}{J(J+1)}\Big) \qquad \text{(III – 45)}
$$

**3.2.3.1. – ODD PARITY MULTIPOLE EXPANSION OF $(\vec{L}.\vec{\sigma}_1)(\vec{L}.\vec{\sigma}_2)$**

$$
C_1^{J-1} = -C_1^{J+1} = -\frac{X_1 Y_1}{4J(J+1)(2J+1)} \qquad \text{(III – 46)}
$$

$$
\begin{aligned}
C_2^{J-1} =& -\frac{X_1}{8J(J+1)(2J+1)}\Big[2(J-1)Y_1 - Y_3 + (J^2+J-1)Y_4 - Y_5\Big] \\
C_2^{J+1} =& -\frac{X_1}{8J(J+1)(2J+1)}\Big[2(J+1)Y_1 + Y_3 - (J^2+J-1)Y_4 + Y_5\}\Big] \\
C_4^{J-2} =& -\frac{1}{8(2J-1)(2J+1)}\Big[(J^2-1)(X_4-Y_4) - X_5 + Y_5 + \frac{1}{J}\{(J^2-1)(X_4Y_1 - X_1Y_4) - X_5Y_1 \\
&+ X_1Y_5\}\Big] \\
C_4^{J} =& \frac{1}{8(2J-1)(2J+3)}\Big[(2J^2+2J-3)(X_4-Y_4) - 2X_5 + 2Y_5 \\
&+ \frac{1}{J(J+1)}\{(J^2+J-3)(X_4Y_1 - X_1Y_4) - 3X_5Y_1 + 3X_1Y_5\}\Big] \\
C_4^{J+2} =& -\frac{1}{8(2J+1)(2J+3)}\Big[J(J+2)(X_4-Y_4) - X_5 + Y_5 - \frac{1}{J+1}\{J(J+2)(X_4Y_1 - X_1Y_4) - X_5Y_1 \\
&+ X_1Y_5\}\Big]
\end{aligned}
\qquad \text{(III – 47)}
$$

$$
\begin{aligned}
C_5^{J-1} =& -\frac{X_1}{16(2J+1)}\Big[(J-2)(J-1) + \frac{1}{J(J+1)}\{(J-1)(J^2+2J-2)Y_1 - (J^2-2J-1)Y_2 \\
&+ (J-2)[(J^2+J-1)Y_4 - Y_3 - Y_5] - (J^2+J-1)Y_6 - JY_7 + Y_9\Big] \\
C_5^{J+1} =& \frac{X_1}{16(2J+1)}\Big[(J+2)(J+3) - \frac{1}{J(J+1)}\{(J+2)(J^2-3)Y_1 + (J^2+4J+2)Y_2 \\
&+ (J+3)[(J^2+J-1)Y_4 - Y_3 - Y_5] + (J^2+J-1)Y_6 - (J+1)Y_7 - Y_9\Big]
\end{aligned}
\qquad \text{(III – 48)}
$$

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

$$
\begin{aligned}
C_8^{J-2} =& \frac{1}{16(2J-1)(2J+1)}\Big[(J-1)\{(J-2)[J(J+X_1)-Y_2-(J+1)(X_4-Y_4)]\\
&+J(J+X_1)Y_1-(J+1)Y_6-Y_7\}+(J-2)(X_5-Y_5)+Y_9\\
&-\frac{1}{J}\{(J-1)\Big((J-2)[(J+1)(X_4Y_1-X_1Y_4)+X_1Y_2]+(J+1)(X_4Y_3-X_4Y_4+X_1Y_6)+X_1Y_7\Big)\\
&-(J-2)(X_5Y_1-X_1Y_5)+(J+1)X_4Y_5-X_5(Y_3-Y_4)-X_1Y_9\}+\frac{X_5Y_5}{J(J-1)}\Big]\\
C_8^{J} =& -\frac{1}{16(2J-1)(2J+3)}\Big[J(J+1)(2J^2+2J-1-2Y_2)+(13J^2+13J-9)X_1+(J^2+J-1)Y_1\\
&+(J^2+J-3)(X_4-Y_4)-(2J^2+2J-3)Y_6-3X_5+3Y_5+Y_7+2Y_9+\frac{1}{J(J+1)}\{(2J^4+4J^3\\
&-2J-3)(X_4Y_1-X_1Y_4)-(6J^4+12J^3-10J^2-16J+9)X_1Y_1-(19J^2+19J-12)X_1Y_2\\
&+(5J^2+5J-6)X_4Y_4-(2J^2+2J+3)(X_5Y_1-X_1Y_5)+2(2J^2+2J-3)X_5Y_4\\
&+3(2J^2+2J-1)X_1Y_7-(J^2+J-3)(X_4Y_3-2X_4Y_5+X_1Y_6)+3X_5Y_3-6X_5Y_5+3X_1Y_9\}\Big]\\
C_8^{J+2} =& \frac{1}{16(2J+1)(2J+3)}\Big[(J+2)\{(J+3)[(J+1)(J+1-X_1)-Y_2+J(X_4-Y_4)]\\
&-(J+1)(J+1-X_1)Y_1-JY_6+Y_7\}-(J+3)(X_5-Y_5)+Y_9\\
&-\frac{1}{J+1}\{(J+2)\Big((J+3)[J(X_4Y_1-X_1Y_4)-X_1Y_2]-J(X_4Y_3-X_4Y_4+X_1Y_6)+X_1Y_7\Big)\\
&-(J+3)(X_5Y_1-X_1Y_5)+JX_4Y_5+X_5(Y_3-Y_4)+X_1Y_9\}+\frac{X_5Y_5}{(J+1)(J+2)}\Big]
\end{aligned}
\qquad \text{(III – 50)}
$$

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

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

with special formulae for $C_4^0$, $C_6^1$ and $C_8^0$.

### 3.2.3.2. – ODD PARITY MULTIPOLE EXPANSION OF $\vec{L}^2(\vec{\sigma}_1.\vec{\sigma}_2)$

$$
\begin{aligned}
C_1^{J-3} =& \frac{(J-1)(J-2)(J+X_1)(J+Y_1)}{4J(2J-3)(2J-1)(2J+1)} \\
C_1^{J-1} =& -\frac{1}{4(2J-3)(2J+1)(2J+3)}\Big[J(J^2-3)+(3J^2-J-6)(X_1+Y_1)+\frac{X_1Y_1}{J}(J^2+2J-6)\Big] \\
C_1^{J+1} =& -\frac{1}{4(2J-1)(2J+1)(2J+5)}\Big[(J+1)(J^2+2J-2)-(3J^2+7J-2)(X_1+Y_1)+\frac{X_1Y_1}{J+1}(J^2-7)\Big] \\
C_1^{J+3} =& \frac{(J+2)(J+3)(J+1-X_1)(J+1-Y_1)}{4(J+1)(2J+1)(2J+3)(2J+5)}
\end{aligned}
\qquad \text{(III – 52)}
$$

$$
\begin{aligned}
C_2^{J-3} =& \frac{(J-2)(J+X_1)}{4J(2J-3)(2J-1)(2J+1)}\Big[(J-1)\{(J-3)(J+Y_1)+Y_3-Y_4\}+Y_5\Big] \\
C_2^{J-1} =& \frac{1}{4(2J-3)(2J+1)(2J+3)}\Big[(J-1)\{J[J^2-J-3-J(X_1+Y_1)]+(J-3)X_1Y_1\} \\
& +(J^2+J-3)(Y_3-Y_4)-(J-3)Y_5-\frac{1}{J(J+1)}\{(J^3-J^2-4J+3)X_1(Y_3-Y_4) \\
& -(J^2-J+3)X_1Y_5\}\Big] \\
C_2^{J+1} =& -\frac{1}{4(2J-1)(2J+1)(2J+5)}\Big[(J+2)\{(J+1)[J^2+3J-1+(J+1)(X_1+Y_1)]+(J+4)X_1Y_1\} \\
& +(J^2+J-3)(Y_3-Y_4)+(J+4)Y_5+\frac{1}{J(J+1)}\{(J^3+4J^2+J-5)X_1(Y_3-Y_4) \\
& +(J^2+3J+5)X_1Y_5\}\Big] \\
C_2^{J+3} =& -\frac{(J+3)(J+1-X_1)}{4(J+1)(2J+1)(2J+3)(2J+5)}\Big[(J+2)\{(J+4)(J+1-Y_1)+Y_3-Y_4\}-Y_5\Big] \\
C_4^{J-2} =& \frac{1}{4(2J-1)(2J+1)}\Big[(J-1)(X_3-X_4-Y_3+Y_4)+X_5-Y_5+\frac{1}{J}\{(J-1)[(X_3-X_4)Y_1 \\
& -X_1(Y_3-Y_4)]+X_5Y_1-X_1Y_5\}\Big] \\
C_4^{J} =& \frac{1}{4(2J-1)(2J+3)}\Big[X_3-X_4-2X_5-Y_3+Y_4+2Y_5-\frac{1}{J(J+1}\{(2J^2+2J-3)[(X_3-X_4)Y_1 \\
& -X_1(Y_3-Y_4)]+3X_5Y_1-3X_1Y_5\}\Big] \\
C_4^{J+2} =& -\frac{1}{4(2J+1)(2J+3)}\Big[(J+2)(X_3-X_4-Y_3+Y_4)-X_5+Y_5-\frac{1}{J+1}\{(J+2)[(X_3-X_4)Y_1 \\
& -X_1(Y_3-Y_4)]-X_5Y_1+X_1Y_5\}\Big]
\end{aligned}
\qquad \text{(III – 53)}
$$

$$
\begin{aligned}
C_5^{J-3} =& \frac{J+X_1}{16J(2J-3)(2J-1)(2J+1)}\Big[(J-1)\{(J-2)\Big((J-4)[J(J-3)+2Y_3-2Y_4] \\
& -Y_2-Y_6\Big)+(J^3-9J^2+28J-24)Y_1-Y_7-3Y_8\}+(J-2)[2(J-4)Y_5+Y_9]+Y_{10}\Big] \\
C_5^{J-1} =& -\frac{1}{16(2J-3)(2J+1)(2J+3)}\Big[(J-2)\{J(J-1)(J+1)(J+3+3X_1)-2(3J^2+2J-6)(Y_3-Y_4) \\
& -2(J+6)Y_5\}+(3J^4+2J^3-5J^2-10J+6)Y_1+(J^3+11J^2-14J-6)X_1Y_1 \\
& -(4J^3-9J^2-10J+21)Y_2-(4J^3-J^2-10J+3)Y_6-(4J^2+J-9)Y_7-(4J^2+3J-9)Y_8 \\
& +(J-3)Y_9+3Y_{10}-\frac{X_1}{J}\{(4J^3-7J^2-7J+12)Y_2+(4J^2-J-6)Y_7\} \\
& -\frac{X_1}{J(J+1)}\{2(J-2)[(J^3+4J^2+2J-6)(Y_3-Y_4)+(3J^2+4J+6)Y_5]+(4J^4+5J^3-14J^2 \\
& -13J+12)Y_6+(4J^3+9J^2-3J-18)Y_8-(3J^2+J-12)Y_9-(J+6)Y_{10}\}\Big] \\
C_5^{J+1} =& -\frac{1}{16(2J-1)(2J+1)(2J+5)}\Big[(J+3)\{J(J+1)(J+2)(J-2-3X_1)-2(3J^2+4J-5)(Y_3-Y_4) \\
& +2(J-5)Y_5\}-(3J^4+10J^3+7J^2+6J+12)Y_1+(J^3-8J^2-33J-18)X_1Y_1 \\
& -(4J^3+21J^2+20J-18)Y_2-(4J^3+13J^2+4J-8)Y_6+(4J^2+7J-6)Y_7+(4J^2+5J-8)Y_8 \\
& +(J+4)Y_9-3Y_{10}+\frac{X_1}{J+1}\{(4J^3+19J^2+19J-8)Y_2-(4J^2+9J-1)Y_7\} \\
& +\frac{X_1}{J(J+1)}\{2(J+3)[(J^3-J^2-3J+5)(Y_3-Y_4)-(3J^2+2J+5)Y_5]+(4J^4+11J^3-5J^2 \\
& -14J+10)Y_6-(4J^3+3J^2-9J+10)Y_8-(3J^2+5J-10)Y_9+(J-5)Y_{10}\}\Big] \\
C_5^{J+3} =& \frac{J+1-X_1}{16(J+1)(2J+1)(2J+3)(2J+5)}\Big[(J+2)\{(J+3)\Big((J+5)[(J+1)(J+4)+2Y_3-2Y_4] \\
& +Y_2+Y_6\Big)-(J^3+12J^2+49J+62)Y_1-Y_7-3Y_8]\}-(J+3)[2(J+5)Y_5-Y_9]-Y_{10}\Big]
\end{aligned}
\qquad (\text{III}-54)
$$

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

$$
\begin{aligned}
C_6^{J+1} = &- \frac{1}{8(2J-1)(2J+1)(2J+5)}\Big[(J+1)(7J^4+34J^3+66J^2+45J-42)-(5J^4+21J^3+42J^2\\
&+37J-37)(X_1+Y_1)+(3J^3+11J^2+5J-9)(X_3+Y_3-X_4-Y4)-(J^2-7)(X_5+Y_5)+\frac{1}{J+1}\\
&\{(7J^4+28J^3+51J^2+51J-27)X_1Y_1+(J^2-7)(X_4Y_3+X_3Y_4)-(5J+11)(X_5Y_3+X_3Y_5)\}\\
&+\frac{1}{J(J+1)}\{(8J^5+28J^4+9J^3-27J^2+4J+5)X_4Y_4-(J^4+4J^3+2J^2-2J+5)(X_3Y_1\\
&-X_4Y_1+X_1Y_3-X_1Y_4)+(7J^3+20J^2+5J-5)X_3Y_3+(3J^3+9J^2+5J+5)(X_5Y_1+X_1Y_5)\\
&-(8J^3+15J^2-13J-5)(X_5Y_4+X_4Y_5)\}+\frac{5X_5Y_5}{J(J+1)(J+2)}(3J^2+8J+2)\Big]\\
&+\frac{1}{16(J+1)}\Big[(J+1-X_1)\{(J+3)Y_2+(J+1)Y_6-Y_7-Y_8\}\\
&+(J+1-Y_1)\{(J+3)X_2+(J+1)X_6-X_7-X_8\}\Big]\\
C_6^{J+3} = &- \frac{J+3}{8(J+1)(J+2)(2J+1)(2J+3)(2J+5)}\Big[(J+2)\{(J+3)(J+1-X_1)+X_3-X_4\}-X_5\Big]\\
&\Big[(J+2)\{(J+3)(J+1-Y_1)+Y_3-Y_4\}-Y_5\Big]
\end{aligned}
\qquad \text{(III – 55)}
$$

$$
\begin{aligned}
C_8^{J-2} = &\frac{1}{8(2J-1)(2J+1)}\Big[(J-1)(J+X_1)\{J(J-2+Y_1)-Y_6\}+\frac{1}{J}\{(J-2)\Big((J-1)\\
&[(X_3-X_4)(J+Y_1)-(J+X_1)(Y_2+Y_3-Y_4)]+X_5(J+Y_1)-(J+X_1)Y_5\Big)\\
&+(J-1)[(X_3-X_4)(Y_3-Y_4)-(J+X_1)(Y_7+Y_8)]+X_5(Y_3-Y_4)+(X_3-X_4)Y_5\}\\
&+\frac{X_5Y_5}{J(J-1)}\Big]\\
C_8^{J} = &\frac{1}{8(2J-1)(2J+3)}\big[J(J+1)\{2J^2+2J-2-X_1\}+(2J^2+2J-1)(X_1Y_1-Y_6)+(2J^2+2J-3)\\
&\{X_3-X_4-Y_2-Y_3+Y_4\}+(3J^2+3J-2)Y_1+3X_5+3X_1Y_2+2X_3Y_3\\
&-3Y_5-X_1Y_6-(1+2X_1)(Y_7+Y_8)+\frac{1}{J(J+1)}\{(J^2+J-3)[(X_3-X_4)Y_1-X_1(Y_3-Y_4)]\\
&+(2J^2+2J+3)(X_5Y_1-X_1Y_5)+(4J^4+8J^3-5J^2-9J+6)X_4Y_4+(2J^2+2J-3)\\
&(X_4Y_3+X_3Y_4-2X_5Y_4-2X_4Y_5)-3X_5Y_3-3X_3Y_5+6X_5Y_5\}\big]\\
C_8^{J+2} = &\frac{1}{8(2J+1)(2J+3)}\Big[(J+2)(J+1-X_1)\{(J+1)(J+3-Y_1)-Y_6\}+\frac{1}{J+1}\{(J+3)\Big((J+2)\\
&[(X_3-X_4)(J+1-Y_1)-(J+1-X_1)(Y_2+Y_3-Y_4)]-X_5(J+1-Y_1)+(J+1-X_1)Y_5\Big)\\
&+(J+2)[(X_3-X_4)(Y_3-Y_4)+(J+1-X_1)(Y_7+Y_8)]-X_5(Y_3-Y_4)-(X_3-X_4)Y_5\}\\
&+\frac{X_5Y_5}{(J+1)(J+2)}\Big]
\end{aligned}
\qquad \text{(III – 56)}
$$

For $J = 0$, thirteen coefficients cannot be obtained from the formulae above. They are:

$$
\begin{aligned}
&C_1^1 = -\,C_1^3 = -\frac{1}{10} \qquad C_2^1 = -\frac{2+Y_4}{20} \qquad C_2^3 = -\frac{8-Y_4}{20}\\
&C_4^0 = -\,C_4^2 = -\frac{X_4-Y_4}{12} \qquad C_5^1 = \frac{Y_6}{20} \qquad C_5^3 = \frac{40-10Y_4+Y_6}{80}
\end{aligned}
$$

$$C_6^1 = -\frac{84 - 4(X_4 + Y_4) - 5(X_6 + Y_6) + 9X_4Y_4}{16} \qquad C_6^3 = -\frac{(6 - X_4)(6 - Y_4)}{80}$$
$$C_8^0 = \frac{X_4Y_4 - Y_6}{24} \qquad C_8^2 = \frac{12 - 6(X_4 - Y_4) + X_4Y_4 - 4Y_6}{48} \qquad \text{(III – 57)}$$

with special formulae for $C_6^1$ and $C_8^0$.

## 4. – ZERO RANGE

### 4.1. – ZERO RANGE LIMITS

The zero range limit is obtained by replacing the multipole $V_L$ in the matrix element:

$$\int_0^\infty f_1(r_1)f_2(r_2)r_1^m r_2^n V_L \frac{d^p}{r_1^p} f_3(r_1)\frac{d^q}{r_2^q} f_4(r_2) r_1^2 r_2^2 dr_1 dr_2 \qquad \text{(IV – 1)}$$

by the multipole of the function $\delta(r)$ which is $\frac{1}{r_1^2}\delta(r_1 - r_2)$ or, if the result vanishes, by the next term $\delta''(r)$ which is:

$$\delta''(r) \Rightarrow \frac{1}{r_1^2}\delta(r_1 - r_2)\Big\{\frac{1}{r_1}\frac{d^2}{dr_1^2}r_1 - \frac{L(L+1)}{r_1^2}\Big\} r_1^m \frac{d^p}{r_1^p} f_1(r_1)f_3(r_1) \qquad \text{(IV – 2)}$$

or by higher terms if the result still vanishes as it is the case for the tensor potential. In this expression, the derivation acts on the product of functions of $r_1$, except for $r_1^2 dr_1$.

**Note that in a finite range matrix elements, only the functions $f_3(r_1)$ and $f_4(r_2)$ are derived and in a zero range matrix element, the function $f_1(r_1)$ also can be derived.**

#### 4.1.1. – LIMIT OF THE DIFFERENT KINDS OF MULTIPOLES

For the second derivative terms, the sum of the coefficients of the different multipoles vanishes, so the derivative part of the limit of the multipole does not contribute. Consequently, we get:

$$C_1 \Rightarrow k_1 \int_0^\infty f_1(r)f_2(r)\Big[f_3(r)f_4''(r) - 2f_3'(r)f_4'(r) + f_3''(r)f_4(r)\Big] r^2 dr \qquad \text{(IV – 3)}$$

where:

$$k_1 = -\sum_L L(L+1)C_1^L \qquad \text{(IV – 4)}$$

For the first derivative terms, taking into account the relations between the multipoles,

1) the triple derivatives cancel out,
2) a double derivative remains,
3) first derivative terms add with those depending on the angular momentum:

$$\begin{aligned} &C_2, C_3, C_4, D_2, D_3, D_4 \Rightarrow \\ &k_2' \int_0^\infty \Big\{ f_1(r)f_2(r)\Big[f_3'(r)f_4'(r) - f_3''(r)f_4(r)\Big] + f_1'(r)f_2(r)\Big[f_3(r)f_4'(r) - f_3'(r)f_4(r)\Big]\Big\} r^2 dr \\ &+k_3' \int_0^\infty \frac{1}{r} f_1(r)f_2(r)f_3(r)f_4'(r) r^2 dr + k_4' \int_0^\infty \frac{1}{r} f_1(x)f_2(x)f_3'(r)f_4(r) r^2 dr \end{aligned} \qquad \text{(IV – 5)}$$

where:

$$\begin{aligned} k'_2 &= 4\sum_L C_2^L \\ k'_3 &= 6\sum_L C_2^L + \sum_L L(L+1)(C_1^L - C_2^L + C_3^L) - \sum_{L'} L'(L'+1)C_4^{L'} \\ k'_4 &= -2\sum_L C_2^L + \sum_L L(L+1)(C_1^L + C_2^L - C_3^L) + \sum_{L'} L'(L'+1)C_4^{L'} \end{aligned} \qquad \text{(IV – 6)}$$

For all the interactions which we consider, $k'_2 = 2k_1$ and $k'_4 = -k'_3$ and the sum of the two terms can be written as:

$$\begin{aligned} &k_1 \int_0^\infty \Big\{ f_1(r) f_2(r) \Big[ f_3(r) f''_4(r) - f''_3(r) f_4(r) \Big] + 2 f'_1(r) f_2(r) \Big[ f_3(r) f'_4(r) - f'_3(r) f_4(r) \Big] \Big\} r^2 dr \\ &+k_2 \int_0^\infty \frac{1}{r} f_1(r) f_2(r) \Big[ f_3(r) f'_4(r) - f'_3(r) f_4(r) \Big] r^2 dr \end{aligned} \qquad \text{(IV – 7)}$$

For the non derivative terms, taking into account the relations between the multipoles, the same occurs:

$$\begin{aligned} &C_5, C_6, C_7, C_8, C_9 \Rightarrow \\ &k_3 \int_0^\infty \frac{1}{r} f_2(r) f_4(r) \Big[ f'_1(r) f_3(r) + f_1(r) f'_3(r) \Big] dr + k_4 \int_0^\infty \frac{1}{r^2} f_1(r) f_2(r) f_3(r) f_4(r) dr \end{aligned} \qquad \text{(IV – 8)}$$

where:

$$\begin{aligned} k_3 &= 4\sum_L (C_5^L - C_7^L) + 2\sum_{L'} (C_8^{L'} - C_9^{L'}) \\ k_4 &= \sum_L (6C_5^L + 2C_7^L) + 2\sum_{L'} C_8^{L'} - \sum_L L(L+1)(C_5^L + C_6^L + C_7^L) \\ &\quad - \sum_{L'} L'(L'+1)(C_8^{L'} + C_9^{L'}) \end{aligned} \qquad \text{(IV – 9)}$$

The total matrix element is:

$$\begin{aligned} &k_1 \int_0^\infty \Big\{ f_1(r) f_2(r) \Big[ f_3(r) f''_4(r) - f''_3(r) f_4(r) \Big] + 2 f'_1(r) f_2(r) \Big[ f_3(r) f'_4(r) - f'_3(r) f_4(r) \Big] \Big\} r^2 dr \\ &+ \int_0^\infty \frac{1}{r} f_2(r) \Big[ k_2 f_1(r) f_3(r) f'_4(r) + (k_3 - k_2) f_1(r) f'_3(r) f_4(r) + k_3 f'_1(r) f_3(r) f_4(r) \Big] r^2 dr \\ &+k_4 \int_0^\infty \frac{1}{r^2} f_1(r) f_2(r) f_3(r) f_4(r) r^2 dr \end{aligned} \qquad \text{(IV – 10)}$$

### 4.1.2. – ZERO RANGE LIMIT EVEN PARITY

for $\vec{L}^2$:

$$k_1 = -(2J+1)$$

$$k_2 = -2(2J+1)$$

$$k_3 = 0$$

$$k_4 = \frac{2J+1}{4}\Big[ -6J(J+1) + X_2 - 2X_4 + X_6 + Y_2 - 2Y_4 + Y_6 + \frac{2}{J(J+1)}(X_1 - X_3)(Y_1 - Y_3)\Big]$$

for $(\vec{L}.\vec{\sigma}_1)(\vec{L}.\vec{\sigma}_2)$:

$$k_1 = \frac{2J+1}{2J(J+1)} X_1 Y_1$$

$$k_2 = \frac{2J+1}{4}\Big[X_1 - Y_1 + \frac{1}{J(J+1)}(X_2 Y_1 - X_1 Y_2)\Big]$$

$$k_3 = \frac{2J+1}{4}\Big[X_1 - Y_1 + \frac{1}{J(J+1)}(X_2 Y_1 - X_1 Y_2)\Big]$$

$$\begin{aligned} k_4 = \frac{2J+1}{8}\Big[ & -2(J^2+J+3) + X_1 - Y_1 + 2X_2 + 2Y_2 + 3X_4 + 3Y_4 + 4X_1Y_1 - 2X_4Y_4 \\ & -\frac{1}{J(J+1)}\{3X_1Y_1 + X_1(Y_2 - 3Y_3 + Y_8) - (X_2 + 3X_3 - X_8)Y_1 + 2X_2Y_2 - X_4Y_4 - X_5Y_4 - X_4Y_5 \\ & + 2X_5Y_5\}\Big] \end{aligned}$$

for $\vec{L}^2(\vec{\sigma}_1.\vec{\sigma}_2)$:

$$k_1 = \frac{2J+1}{J(J+1)} X_1 Y_1$$

$$k_2 = 2\frac{2J+1}{J(J+1)} X_1 Y_1$$

$$k_3 = 0$$

$$\begin{aligned} k_4 = & \frac{2J+1}{4}\Big[ -2(J^2+J+2) + 2X_2 + 2Y_2 + 2X_4 + 2Y_4 + 6X_1Y_1 - 2X_4Y_4 \\ & + \frac{1}{J(J+1)}\{(2X_3 - X_7 - X_8)Y_1 + X_1(2Y_3 - Y_7 - Y_8) - 2X_2Y_2 + 2X_4Y_4 + 2X_5Y_4 + 2X_4Y_5\} \\ & - \frac{4X_5Y_5}{(J-1)J(J+1)(J+2)}\Big] \end{aligned}$$

### 4.1.3. – ZERO RANGE LIMIT ODD PARITY

for $\vec{L}^2$:

$$k_1 = k_2 = k_3 = 0$$

$$k_4 = 2\Big(1 - \frac{X_1 - X_2}{J(J+1)}\Big)\Big(1 - \frac{Y_1 - Y_2}{J(J+1}\Big)$$

for $(\vec{L}.\vec{\sigma}_1)(\vec{L}.\vec{\sigma}_2)$:

$$k_1 = -\frac{2J+1}{2J(J+1)} X_1 Y_1$$

$$k_2 = \frac{2J+1}{4}\Big[X_4 - Y_4 + \frac{1}{J(J+1)}(X_1 Y_3 - X_3 Y_1)\Big]$$

$$k_3 = \frac{2J+1}{4}\Big[2X_1 - 2Y_1 + X_4 - Y_4 + \frac{1}{J(J+1)}(X_1 Y_3 - X_3 Y_1)\Big]$$

$$k_6 = \frac{2J+1}{8}\Big[ -6(J^2+J+1) + 7X_1 + X_2 + X_4 + X_6 + 3Y_1 + Y_2 - Y_4 + Y_6 - 2X_1Y_1$$
$$+ \frac{1}{J(J+1)}\{3X_1Y_1 - X_1(3Y_2 - Y_3 - Y_7) - (3X_2 + X_3 - X_7)Y_1 + 2X_3Y_3 - X_4Y_4 - X_5Y_4 - X_4Y_5\}$$
$$+ \frac{2X_5Y_5}{(J-1)J(J+1)(J+2)}\Big]$$

for $\vec{L}^2(\vec{\sigma}_1.\vec{\sigma}_2)$:

$$k_1 = -\frac{2J+1}{J(J+1)}\Big[J(J+1) + X_1Y_1\Big]$$

$$k_2 = -2\frac{2J+1}{J(J+1)}\Big[J(J+1) + X_1Y_1\Big]$$

$$k_3 = 0$$

$$k_4 = \frac{2J+1}{4}\Big[ -6(J^2+J+2) + 10X_1 + X_2 + X_6 + 10Y_1 + Y_2 + Y_6 - 6X_1Y_1 + 2X_4Y_4$$
$$- \frac{1}{J(J+1)}\{X_1(2Y_2 - Y_7 - Y_8) + (2X_2 - X_7 - X_8)Y_1 - 2X_3Y_3 + 2X_4Y_4 + 2X_5Y_4 + 2X_4Y_5\}$$
$$+ \frac{4X_5Y_5}{(J-1)J(J+1)(J+2)}\Big]$$

### 4.1.4. – ZERO RANGE LIMIT OF $\vec{L}^2$ AND $(\vec{L}.\vec{S})^2$

The coefficients of the two body form factors are given by a subroutine of 400 lines for the natural parity interaction and another one of 480 lines for the unnatural parity ones.

There are a maximum of twenty one body form factors

1) two with second derivative of the free wave function, with constant coefficient and $Y_1$
2) six with first derivative of the free wave function, with constant coefficient and from $Y_1$ to $Y_5$
3) twelve without derivative of the free wave function, with constant coefficient and from $Y_1$ to $Y_{11}$ (only eleven in unnatural parity cases).

As these operators do not contribute in the relative $L = 0$ state, their zero range limit is for the relative $L = 1$ state. There are only the zero range limits of $\vec{L}^2_{(S=0,T=0)}$, $\vec{L}^2_{(S=1,T=1)}$ and $(\vec{L}.\vec{S})^2_{(S=1,T=1)}$. The other vanish to higher order.

As can be seen by writing down these interactions in the relative coordinates, the zero range limits of $\vec{L}^2$ are identical to the Skyrme interactions $V^{Skyrme}_{(S=0,T=0)}$ and $V^{Skyrme}_{(S=1,T=1)}$.

The zero range limit of $(\vec{L}.\vec{S})^2$ cannot be independent of the zero range limit of $\vec{L}^2$, $(\vec{L}.\vec{S})$ and the tensor interaction because there are only three substates $J = 0, 1, 2$ for the relative state $L = 1$. The relation is:

$$(\vec{L}.\vec{S})^2 = \frac{4}{5}\,\vec{L}^2 + \frac{1}{60}V^T_{(T=1)} \qquad \text{(IV – 11)}$$

## 5. – DWBA98/DWBB98

The code DWBA91 added the possibility to compute the distorted waves from the two-body interaction and a description of the target in terms of occupation numbers. The potential is the one of a natural parity transition with $J = 0$. The direct term is very simple but the exchange terms include first derivative coming from the spin–orbit interaction and double derivatives when $\vec{L}^2$ or quadratic spin–orbit interactions are present. For a spin–zero target, there is a single integro–differential equation, which can be solved after an approximate discretisation by an iteration technique described in the subroutine INTE.

There was two versions of DWBA91: one for computers with high precision like the CRAY's, called CDC version and one for computers for which double precision is often necessary as the SUN's or the VAX's, called IBM version. In these last version, distorted waves and interactions are handled with single precision as the knowledge of their value is not so good. But this turned out to be insufficient to obtain the distorted waves from the two body interaction in some cases. A double precision IBM version has been used for studies of elastic scattering [10] P. J. DORTMANS, K. AMOS and S. KARATAGLIDIS, Journal of Physics **G23**, 183 (1997), [11] P. J. DORTMANS, K. AMOS, S. KARATAGLIDIS and J. RAYNAL, Phys. Rev. **C58**, 2249 (1998).

### 5.1. – ELASTIC SCATTERING

The computation of elastic scattering taking into account exchange interaction is very time consuming. For each value of the angular momentum and of the total spin, the matrix of the interaction must be computed. These matrices can be written on a file; computation for another energy with the same interaction, the same description of the target and the same integration points takes a negligible time in comparison if the matrices are read on a file. The name of the file is fort.8 if no other number is specified. Specification of the file allows to keep and to use different ones for the initial and the final state.

The elastic scattering can be considered as a particle-hole excitation of natural parity with $J = 0$. The quantum numbers of the particle and the hole are the same and the quantity $-\sqrt{2j+1}Z^0_{jj}$ where $Z$ is a particle-hole amplitude, is the occupation number.

In the direct term, in the expression given by Equ (I–53), the form factor $B^0$ vanishes; with a spin–orbit interaction, the derivative terms disappear, but the form factor $B^O_2(r)$ remains and is multiplied by the eigenvalue of $2\kappa = 2(\vec{l}.\vec{s}+1)$: it is the spin–orbit potential and a small contribution to the central potential. There is no difficulty to solve a Schrödinger equation with this two potentials. With quadratic spin-orbit two body interactions, there are three other form-factors $V_0(r), V_1(r), V_2(r)$ : a quadratic spin orbit with the factor $\kappa^2$, a first derivative and a second derivative. The equation to solve is then :

$$\Big\{\frac{d^2}{dr^2} - \big[E - \frac{l(l+1)}{r^2} + A(r) + 2\kappa B^0_2(r) + 4\kappa^2 V_0(r)\big] - V_1(r)\frac{d}{dr} - V_2(r)\frac{d^2}{dr^2}\Big\} f_{lj}(r) = 0 \qquad (\mathrm{V}-1)$$

This equation is written :

$$\Big\{\frac{d^2}{dr^2} - \frac{\big[E - \frac{l(l+1)}{r^2} + A(r) + 2\kappa B^0_2(r) + 4\kappa^2 V_0(r)\big]}{1 - V_2(r)}\Big\} f_{lj}(r) = 0 \qquad (\mathrm{V}-2)$$

If the DWBA error due to the absence of first derivatives :

$$\Delta C_{lj} = \int_0^{Rm} f_{lj}(r)\frac{V_1(r)}{1-V_2(r)}\frac{d}{dr} f_{lj}(r) dr \qquad (\mathrm{V}-3)$$

is too large, the equation is solved as explained below when there are exchange term.

For the exchange term, one can built the two kernels $K(x,y)$, $K'(x,y)$ and $K"(x,y)$ such that the DWBA approximation is given by :

$$C_{lj}^{(0)} = \int_0^{Rm} g_{lj}(x)dx \int_0^{Rm} \big\{K(x,y)g_{lj}(y) + K'(x,y)\frac{d}{dr}g_{lj}(y) + K"(x,y)\frac{d^2}{dr^2}g_{lj}(y)\big\}dy \qquad (V-4)$$

where $Rm$ is some matching radius beyond which the interaction vanishes. These kernels are strongly dependents upon the quantum numbers $l$ and $j$ and they have to be computed for each of their values. For each particle-hole component defined by $(l_p,j_p),(l_h,j_h),($ (here with $l_h = l_p, j_h = j_p$, the values of $J$ range from $|j-j_p|$ to $j+j_p$ with alternate natural and unnatural parity following the value of $J+l+l_p$. The two special Clebsch–Gordan coefficients are the same and the $6j-$symbol of the last part of Equ (I–33) reduces to $-(2J+1)/\sqrt{(2j+1)(2j'+1)}$.

The equation to solve is then :

$$\begin{aligned}&\Big\{\frac{d^2}{dr^2} - \big[E - \frac{l(l+1)}{r^2} + A(r) + 2\kappa B_2^0(r) + 4\kappa^2 V_0(r)\big] - V_1(r)\frac{d}{dr} - V_2(r)\frac{d^2}{dr^2}\Big\}f_{lj}(r)\\ &- \int_0^{Rm}\big\{K(r,r')f_{lj}(r') + K'(r,r')\frac{d}{dr'}f_{lj}(r') + K"(r,r')\frac{d^2}{dr'^2}f_{lj}(r')\big]dr' = 0\end{aligned} \qquad (V-5)$$

With the values $f(nh)$ of a function at equidistant points $nh$ up to the point $Nh$, the first and second derivatives are obtained by :

$$\begin{aligned}\frac{d}{dr}f(nh) &= \frac{1}{60h}\Big\{f(nh+3h) - f(nh-3h) - 9\big[f(nh+2h) - f(nh-2h)\big]\\ &\quad + 45\big[f(nh+h) - f(nh-h)\big]\Big\} - \frac{h^6}{420}\frac{d^7}{dr^7}f(nh)\\ \frac{d^2}{dr^2}f(nh) &= \frac{1}{180h^2}\Big\{2\big[f(nh+3h) + f(nh-3h)\big] - 27\big[f(nh+2h) + f(nh-2h)\big]\\ &\quad + 270\big[f(nh+h) + f(nh-h)\big] - 490f(nh)\Big\} - \frac{h^6}{560}\frac{d^8}{dr^8}f(nh)\end{aligned} \qquad (V-6)$$

for $3 < n < N-2$. For $n \le 3$ other formulae are used, involving the values $f(ih)$ for $i = 1\ldots6$ with the assumption that $f(0) = 0$. For $n \ge N-2$ other formulae are used involving $f(ih)$ for $i = N-6\ldots N$. These formulae can be used to extract the first or second derivative for a known function but cannot be introduced to replace the derivatives by the function itself, because they will act as recurrence relations for these derivatives. To see this effect, one can compute the roots of there recurrences, which shows how they propagate the errors. For that we replace $f(nh)$ by $x^n$ and we obtain :

$$\begin{aligned}x^6 - 9x^5 + 45x^4 - 45x^2 + 9x - 1 &= (x^2-1)x^2\Big[(x+\frac{1}{x})^2 - 9(x+\frac{1}{x}) + 44\Big]\\ 2x^6 - 27x^5 + 270x^4 - 490x^3 + 270x^2 - 27x + 2 &= (x-1)^2x^2\Big[2(x+\frac{1}{x})^2 - 23(x+\frac{1}{x}) + 218\Big]\end{aligned} \qquad (V-7)$$

The roots of the first equation are $x = \pm1$, $x = 4.400499678 \pm i4.986139479$ and the inverses of these two last ones. The roots of the second equations are twice $x = 1$, $x = 5.698108515 \pm i8.794300388$ and the inverses of these two last ones. If after some recurrence steps an error has been made, the errors related to $|x| < 1$ disappear, the errors related to $|x| = 1$ stay constant but the errors related to $|x| > 1$ grow tremendously. It is only possible to use :

$$\begin{aligned}\frac{d}{dr}f(nh) &= \frac{1}{2h}\big[f(nh+h) - f(nh-h)\big]\\ \frac{d^2}{dr^2}f(nh) &= \frac{1}{h^2}\big[f(nh+h) - 2f(nh) + f(nh-h)\big]\end{aligned} \qquad (V-8)$$

of which all the characteristic roots are $\pm 1$.

By a choice of equidistant points with step $h$ from the origin to the matching point $R_m$, the integro differential equation of is replaced by a set of linear equation. Noting by ;

$$\begin{aligned}
\mathcal{K}_{i,j} &= \frac{\Big[E - \frac{l(l+1)}{r_i^2} + A(r_i) + 2\kappa B_2^0(r_i) + 4\kappa^2 V_0(r_i)\Big]\delta_{i,j} + K(r_i, r_j)}{1 - V_2(r_i)}, \\
\mathcal{K}'_{i,j} &= \frac{V_1(r_i)\delta_{i,j} + K'(r_i, r_j)}{1 - V_2(r_i)}, \\
\mathcal{K}"_{i,j} &= \frac{K"(r_i, r_j)(1 - \delta_{i,j})}{1 - V_2(r_i)}, \qquad \mathcal{D}_i = 1 - \frac{K"(r_i, r_i))}{1 - V_2(r_i)}
\end{aligned} \tag{V – 9}$$

where $1 \leq (i, j) \leq N$. Using low order expressions for the derivatives, this linear system is ;

$$\mathcal{D}_i \frac{d^2}{dr^2} f(ih) - \sum_j \mathcal{M}_{i,j} f(jh) = 0 \tag{V – 10}$$

with :

$$\mathcal{M}_{i,j} = \Big\{ \mathcal{K}_{i,j} + \frac{1}{2h}\big[\mathcal{K}'_{i,j-1} - \mathcal{K}'_{j+1}\big] + \frac{1}{h^2}\big[\mathcal{K}"_{i,j-1} - 2\mathcal{K}"_{i,j} + \mathcal{K}"_{i,j+1}\big] \Big\} \tag{V – 11}$$

For the first point, the first and second derivatives are replaced by $l + 1$ and $l(l + 1)$, values expected at the first point with respect to the angular momentum $l$ of the function.

The linear system is rewritten :

$$\sum_j \mathcal{D}_i(\delta_{i,j+1} - 2\delta_{i,j} + \delta_{i,j-1}) + \frac{1}{12}(\mathcal{M}_{i,j+1} + 10\mathcal{M}_{i,j} + \mathcal{M}_{i,j-1}) f_j = \sum_j M_{i,j} f_j = 0 \tag{V – 12}$$

with the assumption that $f_0 = 0$, $\mathcal{M}_{i,0} = 0$ and $\mathcal{M}_{i,N+1} = 0$. The term $\delta_{N,N+1}$ is absent in the last equation, so the solution is :

$$f_i = \Big(M^{-1}\Big)_{i,N}, \qquad f_{N+1} = 1 \tag{V – 13}$$

Then $\frac{d}{dr} f_i$ and $\frac{d^2}{dr^2} f_i$ are computed using the precise expressions and their variants for the three first and the three last points. The "errors on the equations" $\Delta f_i$ are the residual values for each point, using the matrices $\mathcal{K}$, $\mathcal{K}'$ and $\mathcal{K}"$ with the precise derivatives. They are ;

$$\Delta f_i = \mathcal{D}_i \frac{d^2}{dr^2} f_i - \sum_j \mathcal{M}_{i,j} f_j \tag{V – 14}$$

The corresponding errors $\delta f_i$ on $f_i$ are obtained by :

$$\delta g_i = \sum_j \Big(M^{-1}\Big)_{i,j} \Delta f_j \tag{V – 15}$$

The criterion of convergence is ;

$$S = \sum_i |\delta g_i|^2 \tag{V – 16}$$

If $S \leq \epsilon$, the system is considered as solved (default value $\epsilon = 10^{-6}$. If $S \geq \epsilon$, $\Delta g_j$ is subtracted to $g_i$ and the process done again up to four times.

## 5.2. – DENSITY DEPENDENCE

The density dependence for a given target is in fact a variation of the strength of the interaction in function of the distance to the center of mass of the target. It can be given directly at different radii or as a function of the density of protons or neutrons. The density can be given as a profile defined by a Fermi form–factor with a given diffuseness and a reduced radius to multiply by the cubic root of the mass of the target. The density can also be computed from the description of the target. Proton density is used for the excitation of particle–hole proton states, the sum of the two densities or the neutron density for the excitation of neutron states.

But the multipole expansion involves the radii $r_1$ and $r_2$ whereas the density is a function of only one radius $r$. Three possibilities can be used :

1) the geometric mean approximation, which is the use of the product of square roots of the strengths defined at $r_1$ and at $r_2$. The square roots are computed after the obtaining the value of the interaction at each point and must be continuous. This method is excluded for a real interaction with a change of sign.
2) the arithmetic mean approximation which is the use of the half sum of the strengths defined at $r_1$ and at $r_2$.
3) the middle distance approximation which is the use of the strength at the point $\frac{1}{2}(r_1 + r_2)$. In this case, the advantage of using three successive single integrations for a Yukawa form factor is lost.

   This last possibility has been added in DWBA98.

## 5.3. – OBSERVABLES AND DWBB98

In the codes DWBA82 and DWBA91, there was the possibility to sum on $J$-transfers. No amplitudes were kept and the cross-sections, polarisations or analysing powers were summed for different $J$. This method can be extended to the spin–transfer coefficients, which are also an incoherent sum on spin–transfer but not for spin–correlation coefficients (polarised beam on a polarised target) for which there are also coherent effects. There was not possible to add $J$–transfer results to the elastic scattering for a target with spin non zero.

The need of such results is quite exceptional. The codes ECISxx include since a long time the computation of many kinds of observables. DWBB98, beside the input of the results of DWBA98 consists in s small number of simplified subroutines of ECIS; the definition and the diversity is the same.

The number of standard observables, which can be defined by a positive value, has been increased. It involves all the observables which can be measured with a polarised beam on a polarised target and all the spin–transfer observables.

## 6. – DESCRIPTION of DWBA98/DWBB98

The structure of the codes DWBAxx, starting with DWBA82 is the same as the structure of the codes ECISxx. A large array is used to store every quantities with no limitation to any peculiar dimension. The limitation is the maximum size of this array available on the computer.

We shall describe the subroutines in the order of their appearance in the code. The Table of Contents of these paragraph will reproduce a flow chart of the program.

The subroutine are stored separately in data sets "*xy_zzzz.f*" in which "*xy*" are chosen such the alphabetical order reproduces the order of appearance and "*zzzz*" are the four characters of the name of the subroutine or function "ZZZZ". In "*xy*", "*x*" is "*a*" for time and memory control subroutines which can be more or less machine dependent, "*b*" for input or distorted waves subroutines, "*c*" for main computation and results, "*d*" for DWBB98 and "*y*" is "*1, 2, ..., 9, a, b, ...*".

**SUBROUTINES OF DWBA98**

### 6.1. – a1 dwba.f

The main subroutine is CALC, from which the calculation never returns. The MAIN defines only the working array and calls CALC. It is the unique subroutine to compile if the working array must be increased. This subroutine and the other "*ay_zzzz.f*" subroutines are the almost the same as those used in the codes ECISxx and have the same old story [12] J. RAYNAL, Notes on ECIS94, CEA Report CEA-N-2772 (1994).

#### 6.1.1. – a2 memo.f

The subroutine MEMO is called from anywhere to check that the size of the working array is enough. If this size is insufficient, this subroutine returns LO(19)=.TRUE. and the calculation is stopped.

#### 6.1.2. – a3 hora.f

The subroutine HORA is called from different places to give the elapsed CPU time for the Job. It uses the subroutine STIM to get the allowed remaining CPU time. It prints the CPU time elapsed since the first call in hours, minutes, seconds and milliseconds and the time elapsed since last call in milliseconds.

### 6.1.3. – a4 stim.f,a5 etim.c

This subroutine STIM is very machine dependent and is the same as for ECIS. However, as there is no automatic search, any subroutine which gives the elapsed time of the job can be used instead of STIM. This version of STIM uses the system function ETIME of UNIX. The subroutine written in C, "*a5_etim.c*" replace ETIME in the LINUX system; it comes from a SLACKWARE distribution.

*Except for the change mentioned above for the subroutine MEMO, all the possibilities described in the Notes on ECIS to use the code on various computer can be used for DWBA. The only difference is that this code does not need the remaining time of the job.*

## 6.2. – b1 calc.f

Comment cards of this subroutine give the signification of many quantities in use, in peculiar of the logical LO and of the addresses in the large array. There is no return from this subroutine. The code can stop only on the input of the control word "FIN" in the subroutine LECT.

The operations done in this subroutine are:

1) set to .TRUE. the controls LO(1) to LO(7) before the first input.
2) call the subroutine LECT to read input.
3) call the subroutine DIRA for the direct calculation.
4) call the subroutine SCEF to print results without exchange.
5) if exchange is requested ( LO(17)=.FALSE. ) call the subroutine ECHA to do the exchange calculation. If exchange is not requested ( LO(17)=.TRUE. ), go back to 2) and call again LECT for a new input.
6) call the subroutine SCEF to print results with exchange.
7) call again the subroutine LECT to stop, get the input of another run or the data for another J-transfer.

## 6.3. – b2 lect.f

This subroutine reads all the input. This input stream is grouped into categories preceded by an integer ILECT which runs from 1 to 7. **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. Then, a new **title card** is read.
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.

#### 6.3.1. – b3 inpa.f,b4 inpb.f

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. There are 968 lines in 16 pages generated by "L̂" characters. This is the description of input for DWBA98 followed by the description of input for DWBB98.

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

#### 6.3.2. – 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.

#### 6.3.2.1. – b5 lec1.f

Reads data and sets up the single particle bound states by calling the subroutine STDP. Eventually, sums the harmonic oscillator functions with different radial quantum numbers. Computes the 'u' parameter of BCS one particle states from the value of the parameter 'v', which is read. If wanted, orthogonalises solutions of Woods-Saxon potential with the same non radial quantum numbers.

#### 6.3.2.2. – b6 stdp.f

This subroutine computes the Laguerre polynomials or a bound state in a Woods-Saxon potential. In this case, a search on the depth of the real potential is performed to find the bound state with a given binding energy.

#### 6.3.3. – ILECT=2: Description of two body interaction.

The subroutine LECT reads only the number of range and some storage requirements and the number of configurations describing the target. This number of configurations is required

for a density dependent interaction computed from the occupations number of the target. For an exchange reaction, these data can have to be read three times: for the initial state, for the final state and for the transition; if the storage needed for the first set of data, the storage requirement must be larger or equal to the largest one.

If the number of configuration is not zero, go to ILECT=6 data before calling LEC2.

#### 6.3.3.1. – b7 lec2.f

There are two arrays, KTF(7,7,KV) and CVF(7,6,KV), where KV is the number of different ranges. In a first part, after some logicals, the subroutine reads for each range J, the value of the range in CMU(1,J) and the code key of each interactions in KTF(I,K,J) for I=1 to 7 and K=1,2 which must be identical for K=1 and K=2 (that is T=0 and T=1, remnant of old versions in which they could be different). The subroutine determines how many form factors are present with this interaction. This number is the element ILL(I,J) of an array ILL(3,4):

I=1 for non derivative form factors,
I=2 for first derivative form factors,
I=3 for second derivative form factors,

J=1 for natural parity in the direct calculation,
J=2 for unnatural parity in the direct calculation,
J=3 for natural parity in the exchange calculation,
J=4 for unnatural parity in the exchange calculation.

The Coulomb potential is read or settled to its default value.

For each non zero interaction ( code key not 0 ), the code key is read again with the description of the interaction. The code key 4 of the previous version (complex density dependent interaction with a real form factor has been suppressed) but kept equivalent to 5. Any error on code key, double input or lack of input stops the code.

1) in any case the real strengths for T=0 and T=1 are read in CVF(K,1,J), CVF(K,2,J) and eventually ( code key 3, 4 or 5 ), the imaginary strengths in CVF(K,4,J), CVF(K,5,J), where K is the kind of interaction and J the range. KTF(K,I,J) are addresses and other informations, kind of density dependence for I=7.
2) if there is an interaction density dependent ( code key 2, 4 or 5), the density of protons and of neutrons are calculated at each point of integration. The form factor of the density can be given
   a) as a function of the radius ( XM=0 ), at increasing values of the radius,
   b) as a function of the density ( XM≠0 ) at decreasing values of the density; the density of the nucleus is described by a Woods-Saxon form factor, of which the parameters are read. It must be normalised to the units used for the input of the densities.
   c) or by the occupation numbers of the target.
3) for each interaction, instead of T=0 and T=1, are computed
   a) the proton-proton direct and exchange interaction
   b) the proton-neutron direct interaction
   c) the proton-neutron exchange interaction

and the density dependent form factors are interpolated by a four points Lagrange formula:

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

where $x$ is the density at the integration point and the $x_i$ the density at which the interaction is given. Note that the result of the interpolation of the three interactions written above is not exactly the same as the one of the interpolation of T=0 and T=1 in the previous versions if the geometric mean is requested.

4) the square root of the form factor is calculated if the use of the geometric mean is requested ( I5=1 ), it is divided by 2 for the use of arithmetic mean ( I5¿0 ) or is twice longer if value at middle point is requested ( I5¡0). I5 is stored in KTF(K,7,J) as $0, \pm 1$. 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.
5) the tables KTF(K,I,J) and CVF(K,I,J) are the address and the strength of the interaction K with range J, the real parts in I=1,2,3 and the imaginary parts in I=4,5,6.

### 6.3.4. – ILECT=3: Presentation of the results.

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

### 6.3.5. – 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.

#### 6.3.5.1. – b8 fdis.f

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. Write number of partial waves, masses, ... on fort.7 if requested for use in DWBB98.
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. ) and write the phase-shifts on fort.7 if requested for use in DWBB98.

4) after this DO LOOP:
   a) restore some informations if the free wave functions are computed with the two body interaction ( LO(37)=.TRUE. ).
   b) if requested ( LO(11)=.TRUE. ) and if the free wave functions are not computed with the two body interaction, ( LO(37)=.FALSE. ) applies non-locality corrections.
5) for the final state ( IG=2 ), if requested ( LO(10)=.TRUE. ), the Coulomb integrals for Coulomb corrections are computed by calling the subroutine CORI.
6) if requested ( LO(35)=.TRUE.), the results of elastic scattering can be printed by calling the subroutine SCEL for the initial state as well as for the final state.

#### 6.3.5.2. – b9 pote.f

This subroutine computes an array VR(I,K) in which there are:

- the real central potential ( including Coulomb potential ) for K=1,
- the imaginary central potential for K=2,
- the real spin orbit potential for K=3,
- the imaginary spin orbit potential for K=4.

If the free wave functions are computed ( LO(37)=.TRUE. ) with a two body interaction which includes $\vec{L}^2$ and/or $(\vec{L}.\vec{S})^2$ terms, there are five complex form factors in the working array VS(I,K):

- a non derivative complex form-factor for K=3 and 4,
- a non derivative complex form-factor to be multiplied by $\beta$ for K=11 and 12,
- a non derivative complex form-factor to be multiplied by $\beta^2$ for K=15 and 16,
- a first derivative complex form-factor for K=27 and 28,
- a second derivative complex form-factor for K=39 and 40.

These addresses are those used in other subroutines in more general cases. In the absence of $\vec{L}^2$ and $(\vec{L}.\vec{S})^2$ terms in the two body interactions, the three last form factor vanish. In these case:

VR(I,1)=−VS(I,3)−2VS(I,11)
VR(I,2)=−VS(I,4)−2VS(I,12)
VR(I,3)=−2VS(I,11)
VR(I,4)=−2VS(I,12)

and VR is computed in this way in all cases.

**If the free wave functions are not computed ( LO(37)=.FALSE. ) with the two body interaction**

1) this subroutine returns immediately for the final state if the potential is the same as in the initial state ( IG=2 and LO(32)=.TRUE. ).
2) for external potentials ( LO(36)=.TRUE. ):
   a) reads the ones given by points ( IEXT≤0 ).
   b) computes the ones given has sums of Woods-Saxon for factors ( IEXT>0 ).
3) for standard potentials ( LO(32)=.FALSE. ): computes the four form factors.
4) adds the Coulomb potential to VR(I,1) in cases 2) and 3).

**If the free wave functions are computed ( LO(37)=.TRUE. ) with the two body interaction**

1) if it is not for the final state ( IG=2 ) with the same potential as for the initial state ( LO(32)=.TRUE. ) saves the two body Coulomb interaction, and eventually reads

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.**

#### 6.3.5.3. – ba inte.f

This subroutine is called for a fixed total angular momentum and parity. The logical controls used in this subroutine are:

LOX(4)=.TRUE. to write potentials on a tape,
LOX(5)=.TRUE. to read potentials from a tape,
LOX(6)=.TRUE. if there is no microscopic exchange potential and
LO(8)=.TRUE. which indicates a plain computation with only central and spin orbit potentials.

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 multiplied 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. ): $\alpha$) if there is no derivative terms, the code returns; $\beta$) 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 and only 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.

3) the third part is the approximate resolution of the integro differential equations:

a) if needed, the non local potentials are multiplied by the inverse of the coefficient of the second derivative computed in 1) a),

b) the direct potential is added to the matrix of exchange potential,

c) the non derivative, first derivative and second derivative terms are added in XA(I,J,K) for K=7 and 8, using lowest order of difference on neighbouring functions for first derivatives and second derivatives but not for the diagonal second derivatives. These differences involve one point before and one point after: the potentials are taken to be zero at the origin and the last point is neglected.

d) the matrix XA(I,J,K) for K=7 and 8 is transformed into Numerov system of linear equations and inverted without any pivot research ( we presume that the next diagonal element is the largest ). The last row of the inverted matrix is the approximate solution normalised to a real value unity at the first step beyond the matching radius.

4) the last part is the refinement of the solution by doing at most four times the following operations:

a) the approximate solution is derived once by calling DERI and twice by calling DER2, taking into account in this second operation the value unity beyond the matching point,

b) the error is computed, using the non derivative, the first and second derivative potentials kept in XA(I,J,K) for K=1 to 6,

c) the approximate solution is corrected, using the inverted matrix in XA(I,J,K) for K=7 and 8; if the norm of the correction is very small, the process is stopped.

5) the solution is normalised as usual and the phase shift computed. If the norm of the difference between this solution and the one obtained in 1) is small enough, the computation of exchange is stopped by setting LOX(6)=LOX(8)=.TRUE. .

#### 6.3.5.4. – bb ptiv.f

This subroutine is called by the subroutines PTIP and PTII when they are called by the subroutine INTE to build the matrices for the exchange terms of a microscopic potential, instead of executing the DO LOOP which computes the form factors for inelastic scattering. The 250 or 334 complex coefficients XX and all the indications for the operations are transmitted by argument from the calling subroutines.

The differences with the subroutines PTCP and PTCI are:

1) the multipoles are explicitly built in the array XA(I,J,K) for K=7, including the correction term present in Eq (VI – 12)
2) the non derivative, first derivative and second derivative terms are summed in XA(I,J,K) for K=1,2, K=3,4 and K=5,6 respectively after multiplication by the geometrical coefficients for the second particle; this geometrical coefficients differ from those of the first particle, which are in the array XG, by the change $\alpha \rightarrow -\alpha$ for natural parity and $\beta \rightarrow -\beta$ for unnatural parity ( these indications are transmitted by the array XH from the calling subroutines ).

There is no two body Coulomb interaction in this subroutine.

#### 6.3.5.5. – bc fcou.f

This subroutine and the subroutines called by it are a small modification of those written at the Department de Calcul Electronique Saclay by: [13] BARDIN, C., DANDEU, Y., GAUTIER, L., GUILLERMIN, J., LENA, T., PERNET, J.M., Note CEA-N-906 (1968) and [14] 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 $\eta$ and $\rho$ 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.

##### 6.3.5.5.1. – bd fcz0.f

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 $\rho_m$ 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: $\alpha$) between the origin and $\rho = m$ if $\eta < 2.5$ ( Clenshaw expansion ), $\beta$) in the asymptotic region between $\rho_m$ and $\infty$ if $\eta > 2.5$ and normalises by computing the regular function at $\rho_m$ by calling the subroutine YFAS for this value.

#### 6.3.5.5.2. – be psi .f,bf sigm.f

These functions compute respectively the Coulomb phase-shift for L=0 and the real part of the logarithmic derivative of the gamma function for a complex argument.

#### 6.3.5.5.3. – bg yfri.f

This subroutine uses:
1) a Riccati method at the origin if $\eta > 0$, $\rho < 2\eta$ and $\eta\rho > 12$.
2) an asymptotic Riccati method $\eta > 0$, $\rho > 2\eta + 20\eta^{\frac{1}{4}}$ or $-14.0625 < \eta < 0$.
3) calls the subroutine YFCL for the asymptotic Clenshaw method if $\eta > 0$ and $2\eta < \rho < 2\eta + 20\eta^{\frac{1}{4}}$.
4) calls the subroutine YFCL for series at the origin if $\eta > 0$, $\rho < 2\eta$ and $\eta\rho < 12$ or $\eta < -14.0625$.

#### 6.3.5.5.4. – bh yfcl.f

This subroutine is called by YFRI. It uses an expansion on Chebyschev polynomials in the asymptotic region or a MacLaurin series expansion near the origin for which it needs the function PSI.

#### 6.3.5.5.5. – bi yfir.f

Computes irregular Coulomb functions by Taylor expansion around the origin or around the point $R = 7.5 + 4/3\eta$ at which the functions and their derivatives are obtained with the subroutine YFAS. For the expansion around the origin, this subroutine calls the function PSI.

#### 6.3.5.5.6. – bj yfas.f

Computes Coulomb functions with the asymptotic expansions.

#### 6.3.5.6. – bk cori.f,bl corh.f

The subroutine CORI is called by FDIS only for ILECT=5, when the coulomb functions are known for the initial and the final channel for long range Coulomb interaction. These subroutines are taken from the code ECIS79 and are valid only if the product of

the Coulomb parameter with the wave number is the same in the initial and in the final state ( the subroutines with the same name used in ECIS88 are generalised to different values of this product between the initial and the final state ).

The different part of this subroutine are:

1) first, the subroutine CORI calls the subroutine CORH to compute the integrals from 0 to $\infty$ of the product of two different regular Coulomb functions with the same angular momentum divided by r ( see [15] RAYNAL, J., Phys. Rev. **C23** (1981) 2571 ) .
2) then, the integrals of the product of two different Coulomb functions with L=0 and L=1 divided by $r$ are computed with the method described in: [16] RAWITSCHER, G. H., RASMUSSEN, C. H., Comput. Phys. Commun. **11** (1955) 183. A backwards integration can be needed.
3) the integrals from 0 to the matching radius of two different regular Coulomb functions divided by $r$ are computed by backward recurrence. The integrals between the matching radius and $\infty$ are obtained by difference with the results of the subroutine CORH. The values obtained in this way for L=0 and L=1 and the results of the direct calculation using the method of RAWITSCHER and RASMUSSEN are printed to check the accuracy of the calculation:

```
> 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.

#### 6.3.5.7. – bo scel.f

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.

### 6.3.6. – 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. ).

### 6.3.7. – 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.

#### 6.3.7.1. – bn lec6.f

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.

#### 6.3.7.2. – bo xyis.f

This subroutine performs different transformations on the amplitudes for different values of its argument ID which can have the values of 1 to 4. For ID=2 and ID=3, it is a change of notations for particle hole creation operators to

$$A^{JM}_{j_p j_h} = (-)^{j_h - m_h} < j_p j_h m_p - m_h | JM > a^{+}_{j_p m_p} a_{j_h m_h} \qquad (\text{VI} - 2)$$

used in the code as given in Ref [2].

ID=1 transformation from isospin formalism, assuming that there are as many particle states of proton and of neutron, with identical quantum numbers, the first half being particles identical to the incoming one.

ID=2 transformation from 'phase 1 of Gillet': the amplitudes must be multiplied by $(-)^{j_p+\frac{1}{2}}$.

ID=3 transformation from 'phase 2 of Gillet': the amplitudes must be multiplied by $(-)^{\text{Integer part of } [(l_p - l_h)/2]}$.

ID=4 transformation from BCS description of the particles.

### 6.3.8. – ILECT=7: End of the input stream for this calculation.

The subroutine LECT computes storage requirements, print maximum storage and calls the subroutine DIRZ. This set of data, which involves only the input of ILECT must be read even when reading data for a new J transfer.

#### 6.3.8.1. – c1 dirz.f

This subroutine is called with ILECT=7, but also with ILECT=4 or 5 if the free wave functions have to be computed with a microscopic potential ( LO(37)=.TRUE. ) .

1) It prepares the working array VS(I,K) where the first dimension is the number of steps and the second one is 68. It stores $r = Ih$ in VS(I,1), $r^2$ in VS(I,2) and 0 in VS(I,K) for K=3 to 42 and returns if there are no macroscopic contribution ( LO(26)=.FALSE. ).
2) If there are macroscopic contributions ( LO(26)=.TRUE. ), they are computed and stored in VS(I,K) for the adequate value of K, from the data read in the arrays V and NV in the subroutine LEC6. They can be:
   a) interpolation on a form factor given by points by the same method already used in subroutine LEC2,
   b) Woods-Saxon form factors to some power or their derivatives,
   c) for the Coulomb potential, the one of an uniformly charged sphere or the one of a Woods-Saxon distribution of charge,
   d) for the spin orbit potential, terms similar to those of the deformed spin orbit potential in ECIS ( LO(28)=.TRUE. ).

### 6.4. – c2 dira.f

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.

#### 6.4.1. – c3 mult.f

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 $V_{\mathrm{J}-3}$ to $V_{\mathrm{J}+3}$ in K=1 to 7,
2) regular multipoles ( Bessel functions for the variable $ir$ ) for $V_{\mathrm{J}-3}$ to $V_{\mathrm{J}+7}$ 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,
3) floating values of J, (2J+1) and square root of J(J+1) are stored in a common.

#### 6.4.2. – ONE–BODY FORM FACTORS

There are three subroutines: PTIP, PTII and PTI0 to compute the one body form factors, respectively for natural parity transition, unnatural parity transitions with a finite range interaction and zero range interaction for both parity. Each of them calls a subroutine, respectively PTCP, PTCI and PTC0, which returns coefficients. When called from the subroutine INTE, to compute exchange in a microscopic potentials, the subroutines PTIP and PTII call the subroutine PTIV to build the matrix for the integro differential equation.

#### 6.4.2.1. – c4 ptip.f

First, if called from ECHA, this subroutine sets to zero the form factors. Then, it calls the subroutine PTCP to obtain coefficients for $\vec{L}^2$, $\vec{L}^2$ $(\vec{\sigma}_1.\vec{\sigma}_2)$ and $(\vec{L}.\vec{\sigma}_1)(\vec{L}.\vec{\sigma}_2)$ interactions. After, there are two nested DO LOOP's on the radial dependences and the ranges ( no radial dependence is considered as the same radial dependence ). Inside them:

1) a DO LOOP on the 14 interaction selects 7 complex strengths VA, taking into account the isospin and if exchange calculation is going on or not,
2) if some value VA were found, 250 complex coefficients are computed, with expressions in this subroutine for the scalar, the tensor and the spin orbit interaction or with results of the subroutine PTCP for the other interactions,
3) if called from the subroutine INTE for the exchange term of a microscopic potential, this subroutine calls the subroutine PTIV and ends the LOOP's,
4) if not, the 250 complex coefficients are divided into 42 groups involving the same operations, but with their results related to different form factors. These operations are performed twice for a radial dependence with arithmetic mean. Indication for

each group are DATA: beginning and end in the 250 array, which input to use ( product of functions or derivative ), power of $r_1$ and $r_2$, which multipole to use and where to store the result ( non derivative, first derivative or second derivative form factor ). There are six successive steps with results in different working arrays in such a way that the steps of which the result is already obtained are skipped:

a) choice of the product of wave functions, or product of one wave function with a derivative of the other and multiplication by the $r_1$ radial dependence,
b) multiplication by a power of $r_1$ ( positive or negative ),
c) product with a multipole; to obtain the integral for a multipole $L$ of range $\mu$:

$$f(r) = \int_0^{Nh} h_L^{(+)}(i\mu\ r_>) j_L(i\mu\ r_<) g(r') dr' \qquad \text{(VI – 3)}$$

where $r_<$ is the smaller of $(r, r')$ and $r_>$ the larger, three successive sums are done:

$$\begin{aligned} F(nh) &= \sum_{j=1}^{n} j_L(i\mu\ jh) g(jh) \\ G(nh) &= \sum_{j=n+1}^{N} \frac{1}{h} h_L^{(+)}(i\mu\ jh) g(jh) \\ f(r) &= j_L(i\mu\ r) G(r) + \frac{1}{h} h_L^{(+)}(i\mu\ r) F(r) \end{aligned} \qquad \text{(VI – 4)}$$

but the scalar interaction needs a correction:

$$f_{\text{scalar}}(r) = f(r) - \frac{h^2 \mu}{12 r^2} g(r) \qquad \text{(VI – 5)}$$

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. ).

#### 6.4.2.2. – c5 ptcp.f

This subroutine returns if no $\vec{L}^2$ or $(\vec{L}.\vec{S})^2$ 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 $\vec{L}^2$ interaction,
I =2 for the $\vec{L}^2$ $(\vec{\sigma}_1.\vec{\sigma}_2)$ interaction,
I =3 for the $(\vec{L}.\vec{\sigma}_1)(\vec{L}.\vec{\sigma}_2)$ 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).

**6.4.2.3. – c6 ptii.f**

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 $\vec{L}^2$ $(\vec{\sigma}_1.\vec{\sigma}_2)$ and $(\vec{L}.\vec{\sigma}_1)(\vec{L}.\vec{\sigma}_2)$ 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 $\vec{L}^2$ 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.

**6.4.2.4. – c7 ptci.f**

Like the subroutine PTCP, this subroutine returns if no $\vec{L}^2$ or $(\vec{L}.\vec{S})^2$ 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 $\vec{L}^2$ $(\vec{\sigma}_1.\vec{\sigma}_2)$ interaction,
I =2 for the $(\vec{L}.\vec{\sigma}_1)(\vec{L}.\vec{\sigma}_2)$ interaction,

J stands for the geometrical dependence on the other particle ( J=1 to 11 for S0, J=1 to 6 for S1, J=1 to 2 for S2 ),

K stands for the multipole involved ( K=1 to 18 for S0, K=1 to 19 for S1, K=1 to 4 for S2 ), but S1(I,J,10)=−S1(I,J,9)−S1(I,J,11), S1(I,J,K+11)=−S1(I,J,K) with contribution of S2 for K=1 to 8.

**6.4.2.5. – c8 pti0.f**

This subroutine computes the form factors of a zero range interaction for natural and unnatural parity transitions. As the exchange is equal to the direct contribution, this subroutine is called only for the direct term, by the subroutine DIRA for a transition or by the subroutine POTE for a macroscopic potential. The input value of the interaction must take into account this point.

The structure of this subroutine is the same as the structure of subroutines PTCP and PTIP. After a call to the subroutine PTI0 which returns the geometrical coefficients for all the interactions, there is a DO LOOP on the radial dependences, in which 25 complex coefficients X0 are computed. They are divided into 9 groups of operations involving:

1) operation on the product of wave functions for the six first groups, or on the particle wave function for the three last ones,
2) eventually, multiplication by the radial dependence,
3) division by $r^2$ for the four first groups and by $r$ for the others,
4) simple or double derivation, using the subroutine DERI or the subroutine DER2 for the last five groups and multiplication by the hole function for the last three groups,

5) eventually, multiplication by the radial dependence,
6) division by $r^2$ for the groups 4,6 and 9 and by $r$ for the groups 3, 5, 7 and 8,
5) addition to the form factors.

#### 6.4.2.6. – c9 ptc0.f

This subroutine returns the coefficients needed in the subroutine PTI0.

### 6.4.3. – ca cora.f

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.

### 6.4.4. – DERIVATION

The two subroutines DERI and DER2 computes first and second derivatives, without dividing the result by the step size or its square. In fact, through the code, the coefficients of first and second derivative form factors are divided by this power of the step size.

#### 6.4.4.1. – cb deri.f

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:

$$x_i = \frac{1}{60}\big[45(y_{i+1} - y_{i-1}) - 9(y_{i+2} - y_{i-2}) + y_{i+3} - y_{i-3}\big] \qquad \text{(VI – 6)}$$

but for the first three points:

$$\begin{aligned} x_1 &= \frac{1}{60}\big[-77y_1 + 150y_2 - 100y_3 + 50y_4 - 15y_5 + 2y_6\big] \\ x_2 &= \frac{1}{60}\big[-24y_1 - 35y_2 + 80y_3 - 30y_4 + 8y_5 - y_6\big] \\ x_3 &= \frac{1}{60}\big[45(y_4 - y_2) - 9(y_5 - y_1) + y_6\big] \end{aligned} \qquad \text{(VI – 7)}$$

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

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

#### 6.4.4.2. – cc der2.f

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:

$$x_i = \frac{1}{180}\big[270(y_{i+1}+y_{i-1}) - 27(y_{i+2}+y_{i-2}) + 2y_{i+3} + 2y_{i-3} - 490y_i\big] \qquad \text{(VI – 9)}$$

but for the first three points:

$$\begin{aligned} x_1 &= \frac{1}{180}\big[-147y_1 - 255y_2 + 470y_3 - 285y_4 + 93*y_5 - 13y_6\big] \\ x_2 &= \frac{1}{180}\big[228y_1 - 420y_2 + 200y_3 + 15y_4 - 12y_5 + 2y_6\big] \\ x_3 &= \frac{1}{180}\big[270(y_4+y_2) - 27(y_5+y_1) + 2y_6) - 490y_3\big] \end{aligned} \qquad \text{(VI – 10)}$$

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

$$\begin{aligned} x_{n-2} &= \frac{1}{180}(2y_{n-6} - 12y_{n-5} + 15y_{n-4} + 200y_{n3} - 420y_{n-2} + 228y_{n-1} - 13y_n) \\ x_{n-1} &= \frac{1}{180}(-13y_{n-6} + 93y_{n-5} - 285y_{n-4} + 470y_{n3} - 255y_{n-2} - 147y_{n-1} + 137y_n) \\ x_n &= \frac{1}{180}(137y_{n-6} - 972y_{n-5} + 2970y_{n-4} - 5080y_{n3} + 5265y_{n-2} - 3132y_{n-1} + 812y_n) \end{aligned} \qquad \text{(VI – 11)}$$

### 6.4.5. – GEOMETRICAL COEFFICIENTS

Besides the function DCGS already called by INTE and the subroutine GEOM, there is also the function DJ6J, called only in the subroutine ECHA.

#### 6.4.5.1. – cd dcgs.f

This subroutine computes special Clebsch-Gordan coefficients for which the formula involves no summation. They are the ones with magnetic quantum numbers all zeros or $\frac{1}{2}$, 0, $-\frac{1}{2}$. One of the arguments of the function is the array of logarithms of factorials. The quantum numbers are given by their integer double value.

#### 6.4.5.2. – ce geom.f

With the values AA= $\alpha$ and AB= $\beta$ computed in the calling subroutine POTE, INTE, DIRA or ECHA, passed in the common /GABJ/, computes the $X_i$ in the array XG(11) in the same common:

$$\begin{array}{lll} X_1 = \alpha & X_5 = (\alpha^2-1)\beta & X_8 = \alpha\beta^2 \\ X_2 = \alpha^2 & X_6 = \beta^2 & X_{10} = (\alpha^3-\alpha)\beta^2 \\ X_3 = \alpha\beta & X_7 = \alpha^3 & X_{11} = (\alpha^3-\alpha)\beta \\ X_4 = \beta & X_8 = \alpha\beta^2 & \end{array} \qquad \text{(VI – 12)}$$

#### 6.4.5.3. – cf dj6j.f

This function computes the 6-j coefficients needed for the exchange. Like the function DCGS, one of its argument is a table of logarithms of factorials and the quantum numbers are given by their integer double value. This subroutine is also used in DWBB98.

### 6.5. – cg echa.f

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.

### 6.6. – ch scef.f

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, this subroutine writes the amplitudes on fort.7 for DWBB98 if requested. Then there is:

1) the transformation to helicity amplitudes, which involves some 3-jm symbols. The one with magnetic quantum numbers $\frac{1}{2}, 0, -\frac{1}{2}$ are given by the function DCGS and the other computed from it by recurrence. The total cross section is computed in this part.
2) for equidistant angles:
   a) the reduced rotation matrix elements are given by the subroutine EMRO and half of the amplitudes are computed, taking parity into account,
   b) cross section, analysing power, polarisation, spin-flip and the observable Q are computed,
   c) if there is a sum on J transfers, the observables are added to the result of previous computations separately without and with exchange,
   d) these observables are printed.
3) the total cross section is printed and the subroutine GRAL is called.
4) for the last value of a sum on J transfer, the total observables are printed and the subroutine GRAL is called for them.

### 6.6.1. – ci emro.f

This subroutine computes a series of reduced rotation matrix elements with increasing angular momentum and the same magnetic quantum numbers. It uses upwards recurrence relations. In fact, there are three independent computations: one if none of the two magnetic quantum number s are zeros, the second if one of them is zero and the third if both of them are zeros.

This subroutine is also used by DWBB98.

### 6.6.2. – cj gral.f

This subroutine prints graphs of cross-sections or polarisations. It is called by the subroutine SCEL for the elastic scattering or by the subroutine SCEF for the transition. Indications read in subroutine LECT with ILECT=3 are transmitted by argument. There are two parts:

1) the logarithmic graph of the differential cross section, avoided if the number of logarithmic scales is zero or too large. For elastic scattering, the cross section divided by Rutherford's cross section is plotted ( cross section itself without charge ).
2) the graph of polarisations which can include the polarisation and the observable Q for elastic scattering, the asymmetry, polarisation, spin flip and observable Q for the transition. The choice is given in binary representation by a data.

## SUBROUTINES OF DWBB98

There are 11 subroutines in DWBB98, including *cf_dj6j.f* and *ci_emro.f* already used by DWBA98. Many of them are simplification of subroutines used in the code ECIS.

### 6.7. – d1 dwbb.f

This MAIN programme reads a title and two logical indicating to use or not relativistic kinematics and to give results in the laboratory or the center of mass system. It reads also angles for the result. Then

1) it calls DEPH to know parities and spins of the initial and final states and which observables to compute.
2) it calls OBSE to prepare the computation of observables.
3) it reads sets of phase shifts of which the two first must be for elastic scattering:

a) for elastic scattering, it reads masses, wave number coulomb parameter and phase–shift for $L = 0$, computes coulomb phase–shifts for $L \neq 0$ and calls LECA.
b) for inelastic scattering, it reads $J$–transfer, parity, dimension and calls LECB.

4) on end of data, the subroutine SCHE is called to transform the data into helicity formalism.
5) then the subroutine RESU is called and the computation is stopped on its return.

### 6.7.1. – d2 deph.f

There are two parts with comment cards before each to explain how are stored informations on each amplitude. The levels taken into account are those which are coupled plus those which are not coupled but of which an angular distribution is wanted.

1) In the first one, after reading spins and parities, the amplitudes are counted and arrays of quantum number stored. Indications to compute only once the reduced rotation matrix elements when they can be used for more than one amplitude to a sign are also stored.
2) In the second part, indications on the observables requested are read. There are 16 standard observable and any other can be requested by a negative number.

### 6.7.2. – d3 obse.f

This subroutine computes for all the observables the indications for the do-loops and the geometrical coefficients which will be needed in *d8_scat.f* to obtain the observables requested.

1) A first part reads indications for non standard observables identified by a negative number read in *d2_deph.f* and transform them into tensor notations.
2) A second part computes geometrical coefficients and do-loop limits. This part is run twice, the first time to obtain storage requirements, the second one for effective computation.

### 6.7.3. – d4 leca.f

This subroutine reads elastic phase shifts if some are given. They are stored only for the first set and if there are requested in the computation.

### 6.7.4. – d5 lecb.f

This subroutine reads inelastic results and adds to the ones previously read. The parity of the initial state is taken as positive. It uses the subroutine *cf_dj6j.f* to restore the quantum numbers from the notation as $J$–transfer.

### 6.7.5. – d6 sche.f

Then, for each total angular momentum and parity, the subroutine computes by recurrence the Clebsch-Gordan coefficients needed to go to the helicity formalism, transforms the scattering coefficients. Only the product of the parities of the initial and the final state is taken into account.

### 6.7.6. – d7 resu.f

This subroutine prints results after averaging on angles or transforming to laboratory system if requested. It calls the subroutine *d8_scat.f* for results at some angle and *d9_gral.f* to draw graphs of the cross–section or the polarisations.

### 6.7.7. – d8 scat.f

This subroutine computes the observables. In a first part it computes the helicity amplitudes with the reduced rotation matrix elements obtained by a call to subroutine *ci_emro.f*. A simple loop gives the cross-section in all cases and the vector polarisation and analysing power for spins 1/2 and 1. The other observables involve do-loops and coefficients which were computed in subroutine *d3_obse.f* and are used after transfer in some memories in equivalence. If observables are in the Laboratory system or with axis of quantification along the incoming direction, the collision matrix is rotated as indicated for the code ECIS or the angle $-\theta$.

### 6.7.8. – d9 gral.f

Subroutine very similar to *cj_gral.f*.

## 6.8. – SUMMARY

The main routine calls the assembler subroutine DWBA which calls the subroutine CALC, or the main routine calls directly CALC. There is no return from CALC. The calls between subroutines are given by the following table, in which the subroutines called by CALC are given in the first column and the names of the subroutines called by a subroutine are in the next column, on the same line or below:

**DWBA98:** DWBA calls CALC, which calls (beginning)

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

**DWBA98:** DWBA calls CALC, which calls (end)

```
DIRA        MULT
----        DCGS
----        GEOM
----        DERI
----        DER2
----        PTIP        PTCP
----        ----        PTIV
----        PTII        PTCI
----        ----        PTIV
----        PTIO        PTCO
----        ----        DERI
----        ----        DER2
----        CORA
----        HORA        STIM

ECHA        MULT
----        DCGS
----        GEOM
----        DJ6J
----        DERI
----        DER2
----        PTIP        PTCP
----        ----        PTIV
----        PTII        PTCI
----        ----        PTIV
----        HORA        STIM

SCEF        EMRO
----        GRAL
----        DCGS
HORA        STIM
```

**DWBB98:** DWBB calls

```
DWBB        DEPH
----        OBSE
----        LECA
----        LECB        DJ6J
----        SCHE
----        RESU        SCAT        EMRO
----        ----        GRAL
```

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## 8. – TABLE of CONTENTS