NOTES ON ECIS94

Jacques Raynal
Service de Physique Théorique,
Laboratoire de la Direction des Sciences de la Matière du Commissariat à l'Energie Atomique,
CE–Saclay, F-91190 Gif-sur-Yvette CEDEX, France

Summary :

This report includes all the "Notes" written on different versions of the Code `ECIS`. The Chapter I relates the evolution of these codes since the first study of how to solve coupled-channel equations by the method of "Equations Couplées en Itérations Séquentielles". The Chapter II indicates how these codes have been used on various computers, because such indications can help to solve future problems.

Chapter III presents the "generalised optical model" in the Dirac and the Schrödinger formalism and the numerical methods. Chapter IV deals with the special treatment of long range interaction. Possibilities to describe excitation of particle and target are the subject of Chapter V and zero-range transfer reactions are presented in Chapter VI. Miscellaneous topics are gathered in Chapter VII and Chapter VIII is a description of the last version of the code, called `ECIS94`.

Sommaire :

Ce rapport reprend toutes les "Notes" écrites sur les différentes version du programme `ECIS`. Le Chapitre I retrace l'évolution de ces programmes depuis la première étude de la résolution des équations de voies couplées par la méthode des "Equations Couplées en Itérations Séquentielles". Le Chapitre II montre comment ces programmes ont été utilisés sur différents ordinateurs car ces indications peuvent être précieuses pour l'avenir.

Le Chapitre III présente le "modèle optique généralisé" dans le formalisme de Dirac et de Schrödinger ainsi que les méthodes numériques. Le sujet du Chapitre IV est le traitement des intéractions à longue portée. La possibilité de décrire l'excitation de la particule et de la cible est étudiée dans le Chapitre V et celle de réaction de transfert avec portée nulle dans le Chapitre VII. Divers sujets sont rassemblés dans le Chapitre VIII et le Chapitre IX est la description de la dernière version du programme, appelée `ECIS94`.

Contents

Chapter I

Introduction - History

The name "ECIS" is made of the first letters of "Equations Couplées en Itérations Séquentielles", by reference to the method of solution used in the codes, although the usual method of solution is also present and has been written with as much care.

A Numerical methods

The numerical methods are a generalisation of those studied for the optical model in : [1] MELKANOFF, M.A., SAWADA, T. and RAYNAL, J., *"Nuclear Optical Model Calculations"*, published in "Methods in Computational Physics.**6**: Nuclear Physics" ALDER, B., FERNBACH, S. and ROTENBERG, M., eds. (Academic Press, New York, 1966) page 1. The application to coupled equations has been presented in : [2] RAYNAL, J., *"Optical-Model and Coupled-Channel Calculations in Nuclear Physics"*, published in "Computing as a Language of Physics", ICTP International Seminar Course, Trieste, Italy, Aug.2-10, 1971 (IAEA, 1972), page 281.

A.1 Integration methods

The programme uses integration methods related to the Numerov method described in : [3] NOUMEROV, B. V., *"A Method of Extrapolation of Perturbations"*, Monthly Notices Roy. Astr. Soc. **84** (1924) page 592. The Numerov method do not deal with the function but with a combination of the function and its second derivative depending on the step size.

Unhappily, the name of Numerov method is used in many Numerical Analysis books, in many articles of Journal of Computational Physics and of Computational Physics Communications for another method which deals only with the functions and which is named Cowell method in Ref. [1] and [2] as it can been found in : [4] COWELL, P. H. and CROMMELIN, A. C. D., Appendix to Greenwich Observations for 1909, Edinburgh (1910) page 84.

The text of Ref. [3] is unambiguous on this point. NOUMEROV presents his method for an inhomogeneous equation (see Equation (20) of Ref. [2]) and begins by :

> "I have pointed out in my previous work* the advantage which is to be got in the numerical integration of the equations of perturbed motion by the introduction of special rectangular co-ordinates. In fact, if we denote by $\overline{x}$, $\overline{y}$, $\overline{z}$ the special co-ordinates connected with ordinary heliocentric rectangular co-ordinates by the equations
>
> $$\overline{x} = x\Big(1 + \frac{k^2\omega^2}{12r^3}\Big); \qquad \overline{y} = y\Big(1 + \frac{k^2\omega^2}{12r^3}\Big); \qquad \overline{z} = z\Big(1 + \frac{k^2\omega^2}{12r^3}\Big) \tag{I.1}$$

*B. Noumerov, "Méthode nouvelle de la détermination des orbites et le calcul des éphémerides en tenant compte des perturbations",*Publications de l'Observatoire Central de Russie*, vol. ii., Moscou, 1923.

where k is the Gaussian constant, ω the interval of integration, and r the radius vector,..."

The reference [5] given above by NOUMEROV himself is quite difficult to find, but Ref. [3] can be found in any Astronomy library.

In astronomical problems, NOUMEROV had to solve a third order equation at each step. In coupled channel calculations, the use of his method leads to solve a system of linear equations at each step. In Ref. [1] was presented a method which replaces this resolution by a matrix multiplication. This "Modified Numerov method" has a truncation error of the same order, but of reversed sign for a constant potential. Details, comparison with methods used by other authors and discussions can be found in Ref. [2].

The programme `ECIS` uses the "Modified Numerov method" of integration with the usual methods of coupled channels calculations (`LO(21)=.TRUE.`), but only in the Schrödinger formalism. With iterations (`LO(21)=.FALSE.`), which are compulsory with deformed spin-orbit and in Dirac formalism, it uses the "Modified Numerov method" if `LO(27)=.FALSE.` or the Numerov method if `LO(27)=.TRUE.`. The option `LO(26)=.TRUE.` (`LO(30)=.TRUE.` in `ECIS79`) given as "integration stabilised for long range potentials" means the inclusion of the truncation error as described in Ref. [2], assuming a constant potential; for usual coupled equations (`LO(21)=.TRUE.`), only the diagonal potential is taken into account; no improvement of the inelastic scattering has to be expected from that and it effects mainly the elastic result.

More details will be given in section (III.C).

A.2 Iteration methods

The iteration methods are described Ref.[2]. The first description was in : [6] RAYNAL, J., *"Equations couplées et D.W.B.A."*, published in "Sur quelques Méthodes de Physique Nucléaire Théorique" Aussois (France) Feb 26 - March 2 1968 (Institut de Physique Nucléaire de Lyon) (LYCEN-6804) pages 179 and another one can be found in : [7] RAYNAL, J., *"Recurrence relations for distorted-wave Born approximation Coulomb excitation integrals and their use in coupled channel calculations"*, Phys. Rev. **C23** (1981) page 2571.

A.2.a Scheme of iterations

The principle of the iterations is to write all the non-diagonal terms as inhomogeneous terms of single equations. The procedure is obtained by considering an expansion of the solution in powers of the strength of these inhomogeneous terms and by setting a recurrence relation between different powers. However, this notion of power expansion is not respected because the last known solution is used to compute the inhomogeneous term with the hope to obtain a quicker result. The computation will depend upon the order of equations: it is why these iterations are called "sequential".

In `ECIS79`, if `LO(26)=.FALSE.`, the inhomogeneous differential equations are solved: ("Differential method"). If `LO(26)=.TRUE.`, an irregular solution of the single inhomogeneous equations is obtained, a Green's function is built with it and the "optical" solution and its integral with the inhomogeneous term computed ("Integral method"). There is no noticeable difference of time between these two methods. However, the solution by the "Differential method" can involve differences of large numbers and fail to give the good result: it is the case when there is a closed channel with a large Q value, for which the "Integral method" gives good results.

However, since the code `ECIS88` as described by [8] RAYNAL, J., *"Coupled Channel Calculations and Computer Code* `ECIS`*"*, published in "Workshop on Applied Nuclear Theory and Nuclear Model Calculations for Nuclear Technology Applications", Trieste, Italy, Feb. 15-March 18, 1988,(Trieste, 1988), MEHTA, M., K. and SCHMIDT, J., J., eds. (World Scientific, 1989) page 506, the generalisation of the Optical Model in the Dirac phenomenology introduced by [9] ARNOLDS, L. C., CLARK, B. C., MERCER, R. L. and SCWANDT, F., *Dirac potential model analysis of* $\vec{p}$*–*^{40}*Ca elastic scattering at 180 MeV and the wine-bottle-bottom shape"*, Phys. Rev. **C23** (1981) page 1949 can be used. The equations to solve have been described in : [10] RAYNAL, J., *"Coupled Channels Description of Inelastic Scattering*

with a Dirac Equation", published in "Proceedings of the 6th International Symposium on Polarization Phenomena in Nuclear Physics", Osaka, Japan, Aug. 26-30, 1985, KONDO, M., KOBAYASHI, S. and TANIFUJI, M., eds., J. Phys. Soc. Japan **55** (Suppl.) (1986) page 922, in : [11] RAYNAL, J., *"Formalisme des Voies Couplées et Programmes* `ECIS`*"*, published in "Réunion des Spécialistes sur l'Utilisation du Modéle Optique pour le Calcul des Sections Efficaces Neutroniques au-dessous de 20MeV", NEANDC-222 "U", Paris, France, Nov. 13-15, 1985 (OCDE, 1986) page 63 and in : [12] RAYNAL, J., *"Ambiguity on the imaginary potentials in the Dirac formalism for the elastic and the inelastic scattering of nucleons"*, Phys. Lett. **B196** (1987) page 7. If these equations are correctly solved and not approximated as described in : [13] RAYNAL, J. and SHERIF, H., S., *"Comparison between Dirac Equation and its Equivalent Schrödinger Equation for Inelastic Scattering"*, published in "Proceedings of the 6th International Symposium on Polarization Phenomena in Nuclear Physics", Osaka, Japan, Aug. 26-30, 1985, KONDO, M., KOBAYASHI, S. and TANIFUJI, M., eds., J. Phys. Soc. Japan **55** (Suppl.) (1986) page 924, it is difficult to include the reorientation terms in the left side (uncoupled equations) of the iteration procedure. So, since `ECIS88`, the reorientation terms are not used in the calculation of the uncoupled solutions, except if `LO(29)=.TRUE.`, which can be used only in the Schrödinger formalism.

Because the "Differential method" of iterations has no practical equivalent for Dirac equations and no clear advantage in the Schrödinger formalism, there is only the "Integral method" (Green's function) since the code `ECIS88`. (The option `LO(29)` of `ECIS79`, "matching with derivatives" has also been discarded).

A.2.b Pade approximants

This iteration procedure is not converging in all cases. Problems arise chiefly for neutron scattering at very low energy or for heavy ions scattering for the "grazing" J-value. After four iterations, the code looks after the convergence of Pade approximants (see in : [14] PADE, H., *"Sur la représentation approchée d'une fonction par des fractions rationnelles*, Ann. Sci. Ec. Norm. Sup. Paris **9** (1892) page 1 and **16** (1899) page 395 and in : [15] WALL, H. S., *"Continued Fractions"*, Van Nostrand, New York 1948) built with the results already obtained.

To explain the role of the Pade approximants let us multiply the inhomogeneous terms by some factor x. There are some values (complex) of x for which there are solutions of the system which are purely outgoing for all the equations: there are the **Weinberg states**, and the x's are the Weinberg eigenvalues. The solution of the system of coupled equations can be expressed with Weinberg eigenfunctions and eigenvalues. If one does not use the "sequential" method but does an exact power expansion, this expansion converge only when the smallest $|x|$ is smaller than unity. The Pade approximant generates poles which are the Weinberg eigenvalues and can be smaller than unity. It can be verified, in case of non-convergence that the poles of the Pade approximants with small absolute value are the same for all the equations. The use of the sequential approach do not change this situation.

The ability of Pade approximants to construct the poles from the power series depends drastically of the precision of the intermediate calculations. The limit is about $|x| > 1/6$ and is better with the `CDC` version of the programme than with the `IBM` version. It can be useful to use the `CDC` version on an `IBM` after doubling its precision. However, for low energy neutrons, the computation with the usual methods (`LO(21)=.TRUE.`) can be quite quick and can be used if one is not interested by spin-orbit deformation.

If `LO(22)=.TRUE.` , Pade approximants are not used. If `LO(22)=.FALSE.` Pade approximants are computed after the fourth iteration if there is no natural convergence and if convergence has been obtained for all the precedent equations in this iteration. There is convergence when two Pade approximants differ by less than the precision required, even if there are not the ones evaluated with the maximum number of parameters. The iteration procedure stops when the maximum number of iterations is reached or when a phase-shift in the last iteration was larger than 10^{10} because there is no more hope to find a precise result.

When convergence has not been obtained with Pade approximants, if `LO(23)=.TRUE.`, the equations for this J-value and parity are solved by usual methods as if `LO(21)=.TRUE.` and a warning printed. On the contrary, if `LO(23)=.FALSE.`, in the last iteration, the Pade approximants are computed even if the precedent equations did not converge and the mean value of the two nearest results is kept as the solution. The shift to usual methods of integration is forbidden in Dirac formalism.

See also section (III.D.4).

A.2.c Increase of the imaginary potential

In low energy neutron scattering on a target with $0^+ - 2^+ - 4^+$ rotational band, there are usually convergence problems which come from a large difference between coupled and uncoupled solutions of the Schrödinger equations: the imaginary potential needed in coupled channel equations is weaker than the one needed to describe elastic scattering. An attempt to avoid this problem is to use a stronger imaginary potential and to introduce the difference as a reorientation term. For that, the reorientation terms must be in the second member (`LO(29)=.FALSE.`). The ratio of increase is a data of the input. Some examples are given in Ref. [8] and Ref. [11].

Advantages of this process in heavy-ion inelastic scattering have not been studied.

B History of different versions

The Buck and Hill's code `INCH` for coupled channels was the starting point of `ECIS`. Some features remains, chiefly in the input of data. The names given to the different versions are those with which they have been kept on a tape for the oldest one, and those which have been explicitly introduced into the code for the latest ones.

B.1 Earlier codes

B.1.a Code `ECIS68`

In `ECIS68` the integration method of the code `INCH` was changed into the Numerov Method with matching at two points as described in Ref. [2] in order to get more precise results. The geometrical coefficients were replaced by those written at the Département de Calcul Electronique of Saclay by : [16] LAFON, R., *"Sous-Programmes* `DFCG-DFC3J`*,* `DFR6J` *et* `DFR9J` *(IBM 360)"*, Report DCE-Saclay No. 326 (1967). There was only the "Differential `ECIS` method", including Pade approximants. The use of a large working space cut into arrays by calls to subroutines to avoid fixed dimensions, was already introduced. This code was used to compare the `ECIS` method to the usual methods. There was no comparison with experimental data. Results can be found in Ref. [6] and in : [17] RAYNAL, J., *"An iterative procedure for coupled channel calculations"*, Communication IV-129 in "Dubna publication D-3893" International Symposium on Nuclear Structure, Dubna, URSS (1968).

B.1.b Code `ECIS69`

In `ECIS69`, the Coulomb functions for the open channels were replaced by those written at the Department de Calcul Electronique Saclay by : [18] BARDIN, C., DANDEU, Y., GAUTIER, L., GUILLERMIN, J., LENA, T. and PERNET, J.M., Note CEA-N-906 (1968) and [19] BARDIN, C., DANDEU, Y., GAUTHIER, C., GUILLERMIN, J., LENA, T., PERNET, J.-M., WOLTHER, H. H. and TAMURA, T., *"Coulomb functions in entire (η, ρ)-plane "*, Comp. Phys. Comm. **3** (1972) page 72. The code was largely rewritten to take into account the full Thomas form for the spin-orbit deformation. In peculiar, the helicity formalism as in : [20] JACOB, M. and WICK, G. C., *"On the General Theory of Collisions for Particles with Spin"*, Annals of Physics **7** (1959) page 404 or in : [21] RAYNAL, J., *"Aspects Géometriques des Réactions"*, Note CEA-N-l529 (1972) (see also in : [22] RAYNAL, J., *"Utilisation de Faisceaux de Deutons Polarisés et Détermination des Paramètres du Modèle Optique"*, Thesis, Faculté d'Orsay, June 24 1964 (Rapport CEA-N-2511-1964) and translation ANL-TRANS-258, the Chapter II.) was introduced for the amplitudes. A 20 points Gauss-Legendre integration was used for the form factors of the rotational model. Results obtained were reported in : [23] RAYNAL, J., *"Couplage LS dans les descriptions macroscopiques et microscopiques des réactions nucléaires"*, published in "Symposium sur les

Mécanismes de Réaction Nucléaire et Phénomenes de Polarisation" Québec, Canada, Sept. 1-2, 1969 (Les Presses de l'Université Laval, 1970) page 75 and in : [24] RAYNAL, J., *"Potentiel spin-orbite déformé en équations couplées (abstract)"*, published in "International Conference on Properties of Nuclear States", Montreal, Canada, Aout 25-30, 1969 HARVEY, M., CUSSON, R. Y., GEIGER, J., S. and PEARSON, J., M. eds. (Les Presses de l'Université de Montréal, 1969) page 771.

B.1.c Code ECIS70

The version ECIS70 is shortly described in Ref. [2]. The asymmetric rotational model is added: the form factors are calculated by integration on the sphere with 36 points, the weights of which were obtained once for all by the inversion of the matrix of rotation matrix elements at these points (this procedure means that the potential is supposed to be expanded only with 36 rotation matrix elements, the coefficients of which are obtained by solving a set of 36 linear equations). The number of multipoles is limited to 15 (id est $\lambda = 8$, whereas 36 is $\lambda = 14$). In the usual method to solve coupled equations, a Schmidt's orthogonalisation procedure is introduced every n points to avoid a loss of independence between the solutions. There was also an attempt to write on a scratch tape the couplings between equations. These couplings are sums of form factors multiplied by a geometrical coefficient: if they are computed before for the iteration method, the time can be divided by two in the rotational model. The use of a scratch tape turned out to be worse than the computation at each iteration. Results obtained at that time were presented in : [25] RAYNAL, J., *"Effets de l'interaction L.S nucléon-nucléon sur l'asymétrie de la diffusion inélastique de protons"*, Colloque sur les Mécanismes des Réactions Nucléaires, Grenoble, France, March 16-18, 1970, GUGENBERGER, P., eds. J. Physique **31C2** (1970) page 92, in : [26] LOMBARD, R., M., MAYER, B. and RAYNAL, J., *"Calculs d'asymétrie de protons polarisés de 20,3 MeV sur* ^{24}Mg, ^{26}Mg *et* ^{28}Si*"*, Colloque sur les Mécanismes des Réactions Nucléaires, Grenoble, France, March 16-18, 1970, GUGENBERGER, P., eds. J. Physique **31C2** (1970) page 90 and in : [27] RAYNAL, J., *"Nuclear structure effects on asymmetry of proton scattering"*, published in "Polarization Phenomen a in Nuclear Reactions: Proceedings of the 3rd International Symposium", Madison, USA, Aug.31 - Sept.4, 1970 BARSCHALL, H., H. and HAEBERLI W., eds. (The University of Wisconsin Press, 1971) page 798.

ECIS70 **was given to Karlsruhe where Dr. G. SCHWEIMER adapted it for automatic search on alpha inelastic scattering.** In this code the spin orbit deformation was limited to spin one half, only cross-section, polarisation, analysing power and spin-flip were computed.

B.1.d Code ECIS71

The ECIS71 code was an attempt to introduce automatic search in ECIS70. The integral version of the ECIS method was added and turned out to be equivalent to the differential version at the point of view of time. The spin orbit deformation is extended to any spin. The different attempts of automatic search are described in Ref. [2].

With ECIS71 began the rewriting of the subroutines for integration, geometrical coefficients and reduced rotation matrix element in IBM Assembler language. A subroutine written by RENARDY defines as working array all the region left free by the programme and allows the use of a LOAD MODULE with different sizes. At that time were written Ref. [2] and [28] RAYNAL, J., *"Spin-Orbit Interaction in Inelastic Nucleon Scattering"*, published in "The Structure of Nuclei", International Course on Nuclear Theory, Trieste, Jan. 13 - March 12, 1971, (IAEA,1972) page 75. Results can be found in : [29] RAYNAL, J., *"Interaction spin-orbite dans la diffusion inélastique de nucléons"*, published in "Sur Certains Aspects Microscopiques des Réactions Nucléaires", La Toussuire, France, Feb. 15-19, 1971 (IPN, Univérsité Claude Bernard, Lyon I) LYCEN 7104, page C7.1 and in : [30] De SWINIARSKI, R. and RAYNAL, J., *"Déformations dans la couche s-d et diffusion inélastique de protons polarisés"*, published in "Sur Certains Aspects Microscopiques des Réactions Nucléaires", La Toussuire, France, Feb. 15-19, 1971 (IPN, Univérsité Claude Bernard, Lyon I) LYCEN 7104, page S9.1.

B.1.e Code ECIS72

In ECIS72, there were further attempts of automatic search in the same approach as in ECIS71. The vibrational model is generalised to mixtures of one phonon and two phonons states. Publications of 1972 are in : [31] LOMBARD, R., KAMITSUBO, H., RAYNAL, J. and GOSSET, J., *"Etude des états collectifs de ^{32}S et de ^{34}S par diffusion inélastique de protons polarisés"*, C. R. Acad. Sci. **B274** (1972) page 761, in : [32] De SWINIARSKI, R., BACHER, A., D., RESMINI, F., G., PLATTNER, G., R., HENDRIE, D., L. and RAYNAL, J., *"Determination of deformation parameters od ^{20}Ne and ^{22}Ne by inelastic scattering of polarized protons"*, Phys. Rev. Lett. **28** (1972) page 1139 and in : [33] RAYNAL, J., *"Sur l'infuence de l'interaction spin-orbite à haute énergie"*, published in "Compte-Rendu de la Conférence Européenne de Physique Nucléaire. Vol 2", Aix-en-Provence, France, June 26 - July 1, 1972, page 149.

B.1.f Code ECIS73

In ECIS73, the observables which can be taken into account for automatic search are generalised to any one, in the notations of Ref. [21]. They can be defined in the laboratory system or with an axis of quantification perpendicular to the reaction plane. Publications of 1973 are in : [34] De SWINIARSKI, R., GENOUX-LUBAIN, A., BAGIEU, G., CAVAIGNAC, J., F., WORLEDGE, D., H. and RAYNAL, J., *"A coupled-channels analysis of 30 MeV proton scattering from low-lying positive-parity states in ^{19}F, ^{20}Ne, ^{21}Ne"*, Phys. Lett. **43B** (1973) page 27, in : [35] KUREPIN, A., B., LOMBARD, R., M. and RAYNAL, J., *"Method for identification of the nuclear collective modes"*, Phys. Lett. **45B** (1973) page 184 and in : [36] LOMBARD, R., M. and RAYNAL, J., *"Polarized-proton inelastic scattering on ^{32}S and possible evidence for an hexadecapole phonon state"*, Phys. Rev. Lett. **31** (1973) page 1015.

In the same time, Dr G. SCHWEIMER used ECIS in Karlsruhe and introduced an automatic search on parameters, using methods very different of those of Ref. [1] and [2]. He introduced also :

- the folding model,
- angular distribution which are sums of levels

but he was not interested in polarisation effects and could deal only with one cross-section for each level. He used different subroutines with the same name to treat different problems: for example, the difference between rotational and vibrational model is obtained by loading different subroutines for nuclear matrix elements and for form factors.

B.1.g Code ECIS75

In June 1973, in collaboration with Dr. G. SCHWEIMER, best points of the the Karlsruhe version were included to the code, giving ECIS75. Each subroutine includes many comment cards, and in peculiar explanation of inputs and outputs at their beginning. This was already done by Dr. G. SCHWEIMER in his KARLSRUHE version of ECIS. All the cards are identified by the four first characters of the subroutine and a sequence number in columns 73-80.

All personal attempts of automatic searches were stopped: the subroutines developed by Dr. G. SCHWEIMER in KARLSRUHE were introduced in the code. However, the use of different modules instead of loading different models at the same time with overlay, was not adopted. The folding model was introduced, after generalisation to the spin-orbit potential. Its meaning is the folding of a nucleon-nucleus potential with the intrinsic wave function of the incoming particle (the meaning of the KARLSRUHE version was the folding of the density distribution of the target with an alpha-nucleon interaction). The folding distribution can be Gaussian, the sum of two Yukawa or a Woods-Saxon distribution.

Other features from the KARLSRUHE version intruced in ECIS75 are :

- unresolved angular distributions,

- constrained asymmetric rotational model,
- anharmonic vibrational model,
- use of the mean value of the two nearest Pade results.

Some other details were added independently:

- J-dependence of imaginary potentials (dropped since ECIS78),
- symmetrised χ^2 for the cross-sections,
- factorisation of $(1 - x\cos\theta)$ in the amplitudes,
- possibility to save a search on a tape, if limited by the time.

A description of the INPUT was written on cards (681 cards). All these cards images were inserted in FORMATs in a programme, which could be used to reproduce the listing of these cards. However, this description was not inserted in the programme itself.

Publications of 1975 are in : [37] RAYNAL, J., *"Application des équations couplées"*, published in "3éme Session d'Etudes Biennale de Physique Nucléaire", La Toussuire, France, Feb. 10-15, 1975 (IPN, Univérsité Claude Bernard, Lyon I) LYCEN 7502, page C7.1 and in : [38] RAYNAL, J., *"Inelastic Scattering (Coupled Channels)"*, published in "Proceedings of the 4th International Symposium on Polarisation Phenomena in Nuclear Reactions", Zurich, Switzerland, Aug. 25-29 1975, GRUEBLER, W. and KONIG, V., eds., (Birkhauser, 1976) page 677.

B.1.h Code ECIS76

The code ECIS was adapted on a CDC computer by Dr. Marek SIEMASKO, from Katowice. At the same time, Dr. M. SIEMASKO introduced Hauser-Feshbach corrections for compound nucleus. To do that in the IBM versions, eight subroutines had to be modified, one of which was also translated into Assembler language. The resulting programme is ECIS76, with his two mean versions, one for low precision computers as the IBM and the other for large precision computers as CDC. However, due to the use of LOGICAL*1 and INTEGER*2, the IBM version cannot be run on other computers as UNIVAC, IRIS or Japanese FACCOM : some modifications had to be done on an IRIS computer at Bordeaux, a SIEMENS in Berlin, a FACCOM in Japan and an UNIVAC in Copenhagen, leading to a third version, the UNIVAC one.

B.2 Codes with Coulomb corrections

B.2.a Code ECIS78

With the introduction of Coulomb corrections for heavy ions, as described in Ref. [7], the code has been enlarged. In peculiar, in collaboration with Prof. H. V. von GERAMB, the possibility to use external form factors has been added, but these form factors can be read only by points. Publication of 1978 in : [39] RAYNAL, J., *"Déformation de l'interaction spin-orbite: relations avec la structure nucléaire et effets possibles sur la section efficace de diffusion inélastique"*, published in "La Physique Neutronique et les Données Nucléaires: Compte-Rendu", Harwell, GB, Sept. 1978 (OCDE, 1978) page 372.

B.2.b Code ECIS79

In ECIS79, the management of memories on CDC or UNIVAC computers has been changed. In the previous versions, it was possible to use a LOAD MODULE with different sizes with respect to the problem, but this size had to be known beforehand. In ECIS79, the core is requested when it is needed, as long as it is available. However, such procedure cannot be used on an IBM computer on which this management of memories must stay dummy.

The possibility of external potentials has been extended by the use of standard form factors as Woods-Saxon and its derivatives, rotational form factors, Laguerre polynomials and bound states in a potential.

The code `ECIS79` was given to the Nuclear Data Bank of the OCDE in 1982.

Publications obtained with it are in : [40] RAYNAL, J., *"Coupled channel calculations of heavy ion inelastic scattering with DWBA approximation for Coulomb interaction (communicated paper)"*, International Conference on Nuclear Physics, Berkeley, USA, Aug. 24-30 1980, in : [41] RAYNAL, J., *"Coulomb effects in proton inelastic scattering on heavy target (communicated paper)"*, International Conference on Nuclear Physics, Berkeley, USA, Aug. 24-30 1980 and in : [42] RAYNAL, J., *"Strong channel coupling method for cross-section calculations (lecture notes)"*, Workshop on Nuclear Model Computer Codes, Trieste, Italy, Jan. 16 - Feb. 3, 1984. For heavy ions problems, they are in : [43] BILWES, B., BILWES, R., BAEZA, A., DIAZ, J., FERRERO, J., L. and RAYNAL, J., *"Inelastic scattering of ^{32}S on ^{28}Si"*, 12th Winter Meeting on Nuclear Physics, Bormio, Italy, Jan. 23-27 1984, Ricerca Scientifica ed Educazione Permanente **35** (Suppl.) (1984) page 422, in : [44] BAEZA, A., DIAZ, J., FERRERO, J., L., BILWES, B., BILWES, R. and RAYNAL, J., *"Mutual excitations of $^{32}S + ^{28}Si$ at 90 and 97.09 MeV"*, Phys. Lett. **149B** (1984) page 73 and in : [45] BAEZA, A., BILWES, B., BILWES, R., DIAZ, J., FERRERO, J., L. and RAYNAL, J., *"Inelastic scattering of ^{32}S on ^{28}Si"*, Nucl. Phys. **A437** (1985) page 93.

B.3 Codes with Dirac formalism

B.3.a Codes `ECIS85` to `ECIS87`

In the Spring 1984 began some attempt to extend the Dirac phenomenology to inelastic scattering with the collaboration of Pr. H. SHERIF who, for instance, provided comparison with other codes for the elastic scattering. One of the points was to avoid the use of relativistic Coulomb functions by using Coulomb corrections as described in Ref. [7]; anyway, relativistic Coulomb functions do not take into account the effect of the anomalous magnetic moment. There was no difficulty to compute these corrections as long as they were used only for elastic scattering. The formalism was presented in Ref. [11] and earliest results were reported in Ref. [10] and Ref. [13]. Difference between `ECIS86` and `ECIS87` is essentially external form-factors generalised in Hamburg with Pr. H. V. von GERAMB in November 1986. During the Spring of 1987, `ECIS87` was left in various places in Canada and United-States. Results are presented in Ref. [12], in : [46] De SWINIARSKI, R., PHAM, D., L. and RAYNAL, J., *"Analyse of 800 MeV inelastic polarized proton scattering from ^{16}O and ^{54}Fe through the coupled Schrödinger or Dirac equations formalism (abstract)"*, published in "Conference on Nuclear Physics and Particle Physics", Birmingham, GB, April 6-8 1987 (The Institute of Physics) page 26 and in : [47] SHIM, S., CLARK, B., C., COOPER, E., D., HAMA, S., MERCER, R., L., RAY, L., RAYNAL, J. and SHERIF, H., S., *"Comparison of relativistic and nonrelativistic approaches to the collective model treatment of $p+^{40}Ca$ inelastic scattering"*, Phys. Rev. **C42** (1990) 1592.

B.3.b Code `ECIS88`

After completion of the relativistic Coulomb corrections, this code was described in Ref. [8] and given to the Nuclear Data Bank of the OCDE. However, some points were still missing, as the Bessel expansion of the form factors.

Results obtained in Dirac formalism or their comparison to results of the Schrödinger formalism can be found in : [48] RAYNAL, J., SHERIF, H., S., KOBOS, A., M., COOPER, E., D. and JOHANSSON, J., I., *"Dirac coupled channel calculations and nucleon scattering at large momentum transfer"*, Phys. Lett. **B218** (1989) page 403, in : [49] De SWINARSKI, R., PHAM, D., L. and RAYNAL, J., *"Dirac coupled-channels analysis of inelastic scattering of 800 MeV polarized protons from ^{16}O, ^{24}Mg and ^{26}Mg"*, Phys. Lett. **B213** page 247, in : [50] RAYNAL, J., *"Which potentials have to be surface peaked to reproduce large angle proton scattering at high energy"*, Australian J. Phys. **43** (1990) page 9, in : [51] RAYNAL, J., *"Inelastic scattering of protons at 800 MeV on ^{40}Ca at large angles"*, 7th International Conference on Polarization Phenomena in Nuclear Physics, Paris, France, July 9-13 1990, Abstracts of contributed papers, page 32F and in : [52] De SWINIARSKI, R., PHAM, D., L. and RAYNAL, J., *"Comparison*

of higher order deformations in several s-d shell nuclei obtained through Schrödinger and Dirac coupled-channel analysis of 900 MeV polarized protons inelastic scattering experiments", Z. Physik **A343** (1992) page 179.

Results related to heavy ions are given in : [53] KIENER, J., GSOTTSCHNEIDER, G., GILS, H., J., REBEL, H., CORCIALCIUC, V., BASU, S., K., BAUR, G. and RAYNAL, J., *"Investigation of the sequential break-up* $^6Li \rightarrow {}^6Li^*(3_1+) \rightarrow \alpha + d$ *of 156 MeV* ^6Li *projectiles on* ^{208}Pb *in the very forward angle hemisphere"*, Z. Phys. **A339** (1991) page 489 and in : [54] CORCIALCIUC, V., REBEL, H., KIENER, J., GSOTTSCHNEIDER, G., GILS, H., J., RAYNAL, J. and BAUR, G., *"Analysis of the sequential break-up* $^6Li \rightarrow {}^6Li^*(3_1+) \rightarrow \alpha + d$ *of 156 MeV* ^6Li *projectiles on* ^{208}Pb *observed in the very forward angle hemisphere (abstract)"*, Frühjahrstagung Darmstadt 1991 - Physik der Hadronen und Kerne, Darmstadt, Germany, March 11-15 1991, Verh. Dtsch. Phys. Ges. **6** (1991) page 6. But they still used primarily `ECIS79`.

B.3.c Codes `ECIS89` to `ECIS90`

At the end of 1988, Dr A. Ventura of the Centro di Calcolo ENEA at Bologna, Italy, was interested by the Bessel expansion of form factors. This part of the code has been completed with him. Some other changes have been done :

- use of the deformation lengths instead of the deformations when fixed relative deformations lengths are wanted,
- use of "symmetrised" Woods-Saxon form factors.

These codes have been given to some laboratories.

B.3.d Code `ECIS94`

This version will be the third given to the Nuclear Data Bank of the OCDE. Besides the use of Bessel expansion for form factors, the use of deformation lengths and the use of "symmetrised" Woods-Saxon potentials, it includes :

- two bound states transitions for particle hole excitations, with the possibility of the particle in the continuum,
- expansion of cross-sections in terms of Legendre polynomials,
- possibility of angular distribution for uncoupled states without giving explicitly all the reduced nuclear matrix elements,
- for Coulomb excitation, use of a magnetic multipole.

Chapter II

Use on various computers

The code ECIS involves two versions with respect to the internal precision of the computer on which it is used :

I If this precision is smaller than 10^{-8}, potentials and wave functions are stored in single precision but many quantities are in double precision: this happens for IBM, UNIVAC, VAX, PR1ME computers.

II If this precision is larger than 10^{-8}, as it is for the CDC and CRAY computers, the code is completely in single precision.

Some subroutines are identical between the two versions; for some others, the only difference is the change of the card DOUBLE PRECISION into comment card by adding C in column 1.

Note that it is possible to run the two versions on a CONVEX computer, using the "-cfc" option for the CDC version. In fact, it is the CDC version used this way which turns out to be the faster on a CONVEX computer.

The code ECIS79 involved about 14250 FORTRAN cards, including 2300 COMMENT cards. It was intended to be run with an OVERLAY structure. The code ECIS88 involved about 16700 FORTRAN cards, including 2500 COMMENT cards and the code ECIS94 involves about 18500 FORTRAN cards, including 3340 COMMENT cards. Most of the topics related in this Chapter are related to the code ECIS79.**As their knowledge can help to solve future problem, these topics are not obsolete**.

Even if the use of OVERLAY is no more of interest, there are two topics very machine dependent in the code ECIS: the management of the working array and the control of the time limit of the job. How to by-pass these two points is explained on comment cards in the MAIN subroutine. For example, the IBM version of the MAIN subroutine of ECIS79, ECIS88 and ECIS94 is :

```
|C 24/09/79  IBM                                                        MAIN-000
|C THE ASSEMBLER SUBROUTINE ECIS(I) DEFINES THE DOUBLE PRECISION ARRAY W MAIN-001
|C AND CALLS CALC(W,W,W,IDMX) WHERE IDMX IS THE LENGTH OF W             MAIN-002
|C W IS ALL THE REGION LEFT FREE BY THE PROGRAM EXCEPT 2*I K FOR BUFFERS MAIN-003
|C THE SUBROUTINE ECIS CAN BE ELIMINATED WITH THE FOLLOWING MAIN:       MAIN-004
|C     REAL*8 W(10000)                                                  MAIN-005
|C     CALL CALC(W,W,W,10000)                                           MAIN-006
|C     STOP                                                             MAIN-007
|C     END                                                              MAIN-008
|C THE ASSEMBLER SUBROUTINE STIM(I) HAS NO FORTRAN EQUIVALENT           MAIN-009
|C IT GIVES THE REMAINING TIME FOR THE JOB IN UNITS OF 26 MICROSECONDS  MAIN-010
|C IT CAN BE REPLACED BY:    (ANY USE OF TIME WILL BE SENSELESS)        MAIN-011
|C     SUBROUTINE STIM(I)                                               MAIN-012
|C     DATA K /0/                                                       MAIN-013
```

```
|C     K=K-1                                                                MAIN-014
|C     I=K                                                                  MAIN-015
|C     RETURN                                                               MAIN-016
|C     END                                                                  MAIN-017
|C*********************************************************************MAIN-018
|      CALL ECIS(3)                                                         MAIN-019
|      STOP                                                                 MAIN-020
|      END                                                                  MAIN-021
```

As shown above, each subroutine begins by a comment card giving the date of last revision and on which computer it can be used. All the cards are identified by the name of the subroutine in columns 73-76, a "–" in column 77 and by a number in columns 78-80, starting by 000.

A The IBM version

The dynamic allocation of memory is not possible on IBM.

A.1 Use on IBM360/370 - AMDHAL- SIEMENS-FUJITSU

The FORTRAN subroutines of ECIS79 for integration and for geometrical coefficients has been translated into ASSEMBLER language. These subroutines involved around 7000 cards and only the 1200 cards of geometrical coefficients and reduced matrix element can still be used in ECIS88 and ECIS94. The translation into ASSEMBLER language was done for an IBM360/91 or a similar computer, on which DO LOOP smaller than 16 machine instructions are very quick. These ASSEMBLER subroutines can be used on other computers: their output statements do not work on a SIEMENS-FUJITSU. However, the ASSEMBLER subroutines ECIS and STIM are very machine dependent and cannot be replaced everywhere.

A.1.a Use with JCL

The subroutine ECIS defines as working array all the space available for the JOB in its region, except for twice its argument 'K' for BUFFERS. It is :

```
|ECIS     TITLE '15/06/79-ECIS-CREATION DE ZONE DE TRAVAIL-ECIS79'       ECIS-000
|ECIS     CSECT                                                          ECIS-001
|* APPEL PAR CALL ECIS(N) OU N EST LA TAILLE EN DOUBLES K RESERVEE       ECIS-002
|* AUX BUFFERS.                                                          ECIS-003
|* CE SOUS PROGRAMME CREE UNE ZONE DE TRAVAIL DE TAILLE MAXIMUM          ECIS-004
|* ET APPELE CALC EN LUI PASSANT TROIS FOIS LA ZONE CREEE ET SA TAILLE   ECIS-005
|* EN DOUBLE MOTS.                                                       ECIS-006
|         SAVE  (14,12),T,*                                              ECIS-007
|         USING  ECIS,12                                                 ECIS-008
|         LR    12,15                                                    ECIS-009
|         SR    15,15                                                    ECIS-010
|         SPM   15                                                       ECIS-011
|         LA    4,SAVE                                                   ECIS-012
|         ST    13,4(4)                                                  ECIS-013
|         ST    4,8(13)                                                  ECIS-014
|         LR    13,4                                                     ECIS-015
|         L     1,0(1)                                                   ECIS-016
|         L     1,0(1)                                                   ECIS-017
|         SLL   1,11                                                     ECIS-018
|         ST    1,MIN                                                    ECIS-019
```

```
|         GETMAIN VU,A=ADGET,LA=MIN,SP=2                                  ECIS-020
|FREE     L     0,MIN                                                     ECIS-021
|         O     0,=X'02000000'    W IN SUBPOOL 2                          ECIS-022
|         FREEMAIN R,LV=(0),A=ADGET                                       ECIS-023
|         L     0,ADGET+4                                                 ECIS-024
|         S     0,MIN                                                     ECIS-025
|         SRL   0,3                                                       ECIS-026
|         ST    0,LONG                                                    ECIS-027
|         L     1,ADGET                                                   ECIS-028
|         A     1,MIN                                                     ECIS-029
|         ST    1,ARG                                                     ECIS-030
|         ST    1,ARG+4                                                   ECIS-031
|         ST    1,ARG+8                                                   ECIS-032
|         LA    1,ARG                                                     ECIS-033
|         L     15,=V(CALC)                                               ECIS-034
|         BALR  14,15         CALL CALC(W,W,W,INT)                      ECIS-035
|         L     13,4(13)                                                  ECIS-036
|         RETURN (14,12),T                                                ECIS-037
|ADGET    DS    D                                                         ECIS-038
|MIN      DC    A(0,MAX)                                                  ECIS-039
|ARG      DC    A(0,0,0,LONG)                                             ECIS-040
|LONG     DS    A                                                         ECIS-041
|SAVE     DS    18A                                                       ECIS-042
|MAX      EQU   X'400000'     4000K                                       ECIS-043
|         END                                                             ECIS-044
```

Use the indication at the end of a JOB to know the best REGION. If data are read with a large BLOCKSIZE, from a tape for example, this argument has to be changed into :

```
|      CALL ECIS(10)                                                      MAIN-019
```

instead of :

```
|      CALL ECIS(3)                                                       MAIN-019
```

The subroutine STIM gives the remaining time for the JOB in units of 1/38500 seconds. It is :

```
|STIM     TITLE '15/06/79-STIM-TEMPS D UNITE CENTRALE RESTANT-ECIS79'     STIM-000
|** CALL STIM(N)    N TEMPS RESTANT EN UNITES DE 26 MICROSECONDES         STIM-001
|**      N/384 TEMPS RESTANT EN CENTIEMES DE SECONDES                     STIM-002
|** VERSION COMPATIBLE MVT/VS2/TSO                                        STIM-003
|STIM     CSECT                                                           STIM-004
|         USING *,15                                                      STIM-005
|         STM   0,12,20(13)                                               STIM-006
|         L     RCVT,16               ->CVT                             STIM-007
|         L     RSHPC,88(,RCVT)       ->SHPC(MVT)                       STIM-008
|         L     RW,0(,RCVT)           ->TCBWORDS                        STIM-009
|         TM    X'74'(RCVT),X'12'     VS2?                              STIM-010
|         BO    VS2                                                     STIM-011
|         L     RTCB,4(,RW)           ->CURRENT TCB                     STIM-012
|         L     RTCB,X'7C'(,RTCB)     ->JOB STEP TCB                    STIM-013
|         L     RTCB,X'84'(,RTCB)     ->TCB DE L'INIT                   STIM-014
|         L     RTME,120(,RTCB)       TCBTME                            STIM-015
|         SR    RN,RN                                                   STIM-016
|LTIM     L     RTOX,12(,RTME)        TOX                               STIM-017
```

```
|         LR    RN,RTOX                                                  STIM-018
|         S     RN,0(,RSHPC)            TOX-SHPC                       STIM-019
|         SLL   RN,1          UNITES 13,... MICROSECONDES              STIM-020
|         A     RN,80         TOX-SHPC+TIMER,EN 13 MICROSECONDES       STIM-021
|         C     RTOX,12(,RTME)          SHPC MODIFIEE?                 STIM-022
|         BNE   LTIM                                                     STIM-023
|         SRL   RN,1      26,... MICROSECONDES                         STIM-024
|         B     STORE                                                    STIM-025
|         SPACE 2                                                        STIM-026
|VS2      DS    0H                                                       STIM-027
|         L     RA,12(,RW)              ->ASCB                         STIM-028
|         L     RW,X'50'(,RA)           JOB STEP TIME LIMIT,SECONDES   STIM-029
|         MH    RW,=H'100'              CENTIEMES DE S                 STIM-030
|         LM    RP,RI,X'40'(RA)         ELAPSED STEP TIME EN STCK      STIM-031
|         SRDL  RP,12         BIN(63) MICROSECONDES                    STIM-032
|         D     RP,=F'10000'            =>RP=MICROSECONDES,RI=1/100 DE S STIM-033
|         SR    RI,RW        -TEMPS RESTANT A L'ETAPE EN 1/100 DE S    STIM-034
|         M     RP,=F'384'              TIMER UNITS                    STIM-035
|         LPR   RN,RI                                                    STIM-036
|STORE    L     2,0(1)                                                   STIM-037
|         ST    RN,0(,2)                                                 STIM-038
|RETOUR   LM    0,12,20(13)                                              STIM-039
|         BR    14                                                       STIM-040
|         LTORG                                                          STIM-041
|RN       EQU   0                                                        STIM-042
|RTOX     EQU   2                                                        STIM-043
|RCVT     EQU   3                                                        STIM-044
|RTCB     EQU   3                                                        STIM-045
|RTME     EQU   3                                                        STIM-046
|RSHPC    EQU   4                                                        STIM-047
|RW       EQU   5                                                        STIM-048
|RA       EQU   6             ->ASCB                                     STIM-049
|RP       EQU   8             REGISTRE PAIR                              STIM-050
|RI       EQU   RP+1                                                     STIM-051
|         END                                                            STIM-052
```

It can have to be changed by a local subroutine.

The `OVERLAY` cards are not the same for the different codes. Those of `ECIS79` were :

```
| OVERLAY A                                                              OVLY-001
| INSERT CALX                                                            OVLY-002
| OVERLAY B                                                              OVLY-003
| INSERT LECT,LECD,DEPH,OBSE                                             OVLY-004
| OVERLAY B                                                              OVLY-005
| INSERT INPA                                                            OVLY-006
| OVERLAY B                                                              OVLY-007
| INSERT INPB                                                            OVLY-008
| OVERLAY A                                                              OVLY-009
| INSERT COLF,FCOU,FCZ0,PSI,YFRI,YFCL,YFAS,YFIR,COCL,SIGM,CORI,CORH      OVLY-010
| OVERLAY A                                                              OVLY-011
| INSERT VARI,FIT1,FIT2,FITE,REST,EVAL                                   OVLY-012
| OVERLAY A                                                              OVLY-013
| INSERT DJ6J                                                            OVLY-014
| OVERLAY C                                                              OVLY-015
| INSERT DJCG,REDM,VIBM,ROAM,ROTM                                        OVLY-016
```

```
| OVERLAY C                                                                    OVLY-017
| INSERT CAL1                                                                  OVLY-018
| OVERLAY D                                                                    OVLY-019
| INSERT POTE,DERI,COPO                                                        OVLY-020
| OVERLAY E                                                                    OVLY-021
| INSERT VIBP,ROTD,ROTP                                                        OVLY-022
| OVERLAY E                                                                    OVLY-023
| INSERT FOLD,HULT,FINT                                                        OVLY-024
| OVERLAY E                                                                    OVLY-025
| INSERT EXTP,INTP,STDP                                                        OVLY-026
| OVERLAY D                                                                    OVLY-027
| INSERT QUAN,DJ9J,DCGS,SCAM,CORA,CORB                                         OVLY-028
| OVERLAY F                                                                    OVLY-029
| INSERT INTI,INSI,INSH,COUP,SECM,PADE                                         OVLY-030
| OVERLAY F                                                                    OVLY-031
| INSERT INCH,CPCC,LINS                                                        OVLY-032
| OVERLAY D                                                                    OVLY-033
| INSERT SCHE,RESU,SCAT,GRAL,EMRO,RESC,CPSF                                    OVLY-034
```

Those of ECIS88 are :

```
| OVERLAY A                                                                    OV88-000
| INSERT CALX                                                                  OV88-001
| OVERLAY B                                                                    OV88-002
| INSERT LECL,LECT,LECD,DEPH,OBSE                                              OV88-003
| OVERLAY B                                                                    OV88-004
| INSERT INPA,INPB,INPC                                                        OV88-005
| OVERLAY A                                                                    OV88-006
| INSERT COLF,FCOU,FCZO,PSI,YFRI,YFCL,YFAS,YFIR,COCL,SIGM,CORI,CORO,CORZ OV88-007
| OVERLAY A                                                                    OV88-008
| INSERT VARI,FIT1,FIT2,FITE,REST,EVAL,EXTP                                    OV88-009
| OVERLAY A                                                                    OV88-010
| INSERT DJ6J                                                                  OV88-011
| OVERLAY C                                                                    OV88-012
| INSERT DJCG,REDM,VIBM,ROAM,ROTM                                              OV88-013
| OVERLAY C                                                                    OV88-014
| INSERT CAL1                                                                  OV88-015
| OVERLAY D                                                                    OV88-016
| INSERT POTE,DERI,COPO,ROTZ,ROTD,ROTP,FOLD,INTP,STDP,STBF                     OV88-017
| OVERLAY D                                                                    OV88-018
| INSERT QUAN,DJ9J,DCGS,SCHE,CORA,MTCH,CONU,PADE,DIAG                          OV88-019
| OVERLAY E                                                                    OV88-020
| INSERT INTI,INSI,INSH                                                        OV88-021
| OVERLAY E                                                                    OV88-022
| INSERT INTR,INRI,INRH                                                        OV88-023
| OVERLAY E                                                                    OV88-024
| INSERT INCH,LINS                                                             OV88-025
| OVERLAY D                                                                    OV88-026
| INSERT SCIN,RESU,SCAT,GRAL,EMRO,RESC                                         OV88-027
```

and none have been written for ECIS94. The difference is SCAM instead of SCHE in OV88-17 and SCHE,LCSP instead of SCIN in OV88-27.

A.1.b Use with MTS

This system do not allow OVERLAY, control of working space and of time. Follow indications in COMMENT cards of the MAIN routine.

A.2 Use on UNIVAC

At the first attempt to run the code ECIS79 on an UNIVAC computer, the following indications are inserted at the top of the MAIN subroutine

```
|C 30/01/80   MAIN FOR UNIVAC                                    ECIS79  ECIS-000
|C THIS PROGRAM IS LIMITED TO 126K PLUS 5 TIMES THE PARAMETER OF          ECIS-001
|C @XQT,X WHERE X IS TRANSFORMED TO 1 FOR A TO 26 FOR Z BY IOPTF.         ECIS-002
|C THE SUBROUTINE PMARZ AVOIDS THE AUTOMATIC CHANGES OF PAGE.             ECIS-003
|C****** TO BE ABLE TO USE A BLANK FOR .FALSE. THE USER OF UNIVAC MUS     ECIS-004
|C  INTRODUCE:                                                           ECIS-005
|C     DO 29 I=1,100                AND                                 ECIS-006
|C  29 LO(I)=.FALSE.              BEFORE CALX-123                        ECIS-007
|C     LX=.FALSE.                 BEFORE LECD-033                        ECIS-008
|C     LT1=.FALSE.                  AND                                  ECIS-009
|C     LT2=.FALSE.                BEFORE OBSE-097                        ECIS-010
|C     LO(37)=.FALSE.             BEFORE EVAL-033                        ECIS-011
|C     LO(35)=.FALSE.             BEFORE REST-038                        ECIS-012
|C*************************************************************************ECIS-013
|      REAL*8 W(2048)                                                     ECIS-014
|      COMMON /LARGE/ W                                                   ECIS-015
|      CALL PMARZ(66,0,66)                                                ECIS-016
|      CALL MEMINI(126+IOPTF(0)*5)                                        ECIS-017
|      CALL CALC(W,W,W,2048)                                              ECIS-018
|      STOP                                                               ECIS-019
|      END                                                                ECIS-020
```

Without these modifications, a LOGICAL read previously as .TRUE. cannot be read with a blank but must be read with a F. After ECIS79, the logicals are set .FALSE. before being read.

The use of files is done with :

```
| N$TAB 21,1,1,1,1,0 6 7 5 0          .                                  NTAB-000
|      END                            .                                  NTAB-001
```

The subroutine IOPTF, written in Copenhagen, allows to run jobs with a larger core in special cases, for instance overnight.

```
|          AXR$                       .                                  IOPT-000
|$(1), IOPTF*  ER     OPT$             .                                  IOPT-001
|          JZ        A0,2,X11         .                                  IOPT-002
|          LSC       A1,A0            .                                  IOPT-003
|          ANA,U     A2,8             .                                  IOPT-004
|          LA        A0,A2            .                                  IOPT-005
|          J         2,X11            .                                  IOPT-006
|          END                        .                                  IOPT-007
```

There is a dynamic allocation of core by the FORTRAN subroutine MEMO which is more similar to the one used on CDC than to the one used on IBM. This allocation is obtained by :

```
|C 14/05/80 UNIVAC                                                ECIS79  MEMO-000
|      SUBROUTINE MEMO(IDMT,NPLACE,NQ,IX,W,LO)                             MEMO-001
|C THIS SUBROUTINE GETS THE WORKING SPACE.                                 MEMO-002
|C IDMT     PREVIOUS SPACE                                                 MEMO-003
|C NPLACE   REQUESTED SPACE                                                MEMO-004
|C NQ       SPACE TO BE UPDATED                                            MEMO-005
|C IX: CONTROL NUMBER IX=1     FIRST CALL   STORE MINIMUM SIZE IN ID       MEMO-006
|C                    IX=2     DIMINUTION OF SPACE                        MEMO-007
|C                    IX=3     REQUEST NPLACE+ISTART, AT LEAST NPLACE     MEMO-008
|C                    IX=4     REQUEST NPLACE                             MEMO-009
|C                    IX=5     ABSOLUTE REQUEST                           MEMO-010
|C W:  WORKING SPACE                                                       MEMO-011
|C LO: LOGICAL CONTROLS  IF LO(94)=.TRUE. PRINT THE SIZE OF W              MEMO-012
|C OUTPUT VARIABLES: IDMT  SIZE OF WORKING SPACE                           MEMO-013
|C                   LO(216)=.TRUE. IF COMPUTATION CANNOT CONTINUE         MEMO-014
|C*************************************************************************MEMO-015
|      DIMENSION W(1)                                                      MEMO-016
|      LOGICAL LO(250)                                                     MEMO-017
|      DATA ISTART,IMOD /512,64/                                           MEMO-018
|      IF (IX-2) 1 , 2 , 3                                                 MEMO-019
|    1 ID=IDMT                                                             MEMO-020
|      NT=MAX0(-IMOD,ISTART-IDMT)                                          MEMO-021
|      NPLACE=0                                                            MEMO-022
|      GO TO 4                                                             MEMO-023
|    2 NT=MAX0(NPLACE,ID)-IDMT                                             MEMO-024
|      GO TO 5                                                             MEMO-025
|    3 NT=NPLACE-IDMT                                                      MEMO-026
|      IF (IX.NE.3) GO TO 4                                                MEMO-027
|      NT=NT+ISTART                                                        MEMO-028
|    4 NT=IMOD*(NT/IMOD+1)                                                 MEMO-029
|    5 CALL MEMORY(NT,NX,IR)                                               MEMO-030
|      IDMT=IDMT+NT+IR                                                     MEMO-031
|      LO(216)=(IDMT.LT.NPLACE).AND.((IX-5)*(IX-3).EQ.0)                   MEMO-032
|      NQ=NQ+NT+IR                                                         MEMO-033
|      IF (LO(94)) WRITE (6,1000) IX,NT,IR,NPLACE,IDMT,NX                  MEMO-034
|      IF (.NOT.LO(216)) RETURN                                            MEMO-035
|      WRITE (6,1001) IX,IDMT,NPLACE                                       MEMO-036
|      WRITE (6,1002)                                                      MEMO-037
|      RETURN                                                              MEMO-038
| 1000 FORMAT (/8H REQUEST,I2,4H FOR,I9,9H MEMORIES,I6,25H ARE MISSING.    MEMO-039
|     1  NPLACE =,I9,7H SIZE =,I9,15H  TOTAL LENGTH ,I10/)                 MEMO-040
| 1001 FORMAT (33H NOT ENOUGH PLACE .....   REQUEST,I2,I10,8H ALLOWED,I10MEMO-041
|     1,10H REQUESTED/)                                                    MEMO-042
| 1002 FORMAT (/34H ...STOP...  NEXT TIME, USE @XQT,Z/)                    MEMO-043
|      END                                                                 MEMO-044
```

with the machine language subroutine :

```
|          AXR$                      . SUBROUTINE WRITTEN IN STRASBOURGMEMI-000
|$(1)                                .  ON THE 23/01/80                MEMI-001
|MEMORY*                             .                                 MEMI-002
|          L         A1,*0,X11       . CALL MEMORY(I,J,K)              MEMI-003
|          SZ        *2,X11          .   I NUMBER OF MEMORIES REQUESTEDMEMI-004
|          L         A0,LASTD        .   J RETURNS THE SIZE OF THE     MEMI-005
|          JZ        A1,RETOUR       .         PROGRAM                 MEMI-006
|          A         A0,A1           .   K RETURNS DIFFERENCE BETWEEN  MEMI-007
```

```
|          JP        A1,MORE          .         NUMBER OF MEMORIES GIVENMEMI-008
|          ER        LCORE$           .         AND NUMBER OF MEMORIES  MEMI-009
|          J         LMCORE           .         REQUESTED               MEMI-010
|MORE      TLE       A0,MAXCOR        .                                 MEMI-011
|          J         ERMCORE          .                                 MEMI-012
|          ANU       A0,MAXCOR        .                                 MEMI-013
|          SN        A1,*2,X11        .                                 MEMI-014
|          L         A0,MAXCOR        .                                 MEMI-015
|ERMCORE   ER        MCORE$           .                                 MEMI-016
|LMCORE    S         A0,LASTD         .                                 MEMI-017
|RETOUR    S         A0,*1,X11        .                                 MEMI-018
|          J         4,X11            .                                 MEMI-019
|MEMINI*   L         A0,*0,X11        .  ENTRY USED TO STORE THE MAXIMUMMEMI-020
|          LSSL      A0,10            .    SIZE FOR THE RUN             MEMI-021
|          AN,U      A0,1             .                                 MEMI-022
|          S         A0,MAXCOR        . CALL  MEMINI(IMAX)             MEMI-023
|          J         2,X11            .  IMAX MAXIMUM SIZE IN K         MEMI-024
|$(0)                                 .                                 MEMI-025
|MAXCOR    +         0                .                                 MEMI-026
|LASTD     +         LASTD$           .                                 MEMI-027
|          END                        .                                 MEMI-028
```

The subroutine `STIM` has been also written in Copenhagen :

```
|          AXR$                       .                                 STIM-000
|$(1),STIM*  LXI,U   A1,PCTBD$        .                                 STIM-001
|          LA,U      A2,RPCTA$        .                                 STIM-002
|          LDJ       A1,$+1           .                                 STIM-003
|          LA        A0,03,A2         .                                 STIM-004
|          ANA       A0,013,A2        .                                 STIM-005
|          LDJ       A1,$+1           .                                 STIM-006
|          MI,U      A0,77            .                                 STIM-007
|          DI,U      A0,10            .                                 STIM-008
|          SA        A0,*0,X11        .                                 STIM-009
|          J         2,X11            .                                 STIM-010
|          END                        .                                 STIM-011
```

The programme `ECIS79` had to be used with following `OVERLAY` :

```
|SEG S1
|IN ECISR.ECIS,.CALC,.HORA,.STIM,.NTAB$,.MEMO,.MEMORY
|SEG A1*
|IN ECISR.CALX
|SEG B1*
|IN ECISR.LECT,.LECD,.IOPTF
|SEG B2*,B1
|IN ECISR.DEPH,.OBSE
|SEG A2*,A1
|IN ECISR.COLF,.FCOU,.FCZ0,.PSI,.YFRI,.YFCL,.YFAS,.YFIR,.COCL,.SIGM
|IN ECISR.CORI,.CORH
|SEG A3*,A1
|IN ECISR.VARI,.FIT1,.FIT2,.FITE,.REST,.EVAL
|SEG A4*,A1
|IN ECISR.DJ6J
|SEG C1*
```

```
|IN ECISR.DJCG,.REDM,.VIBM,.ROAM,.ROTM
|SEG C2*,C1
|IN ECISR.CAL1
|SEG D1*
|IN ECISR.POTE
|SEG E1*
|IN ECISR.ROTP,.ROTX
|SEG E2*,E1
|IN ECISR.VIBP
|SEG E3*,E1
|IN ECISR.DERI,.COPO
|SEG G1*
|IN ECISR.FOLD,.HULT,.FINT
|SEG G2*,G1
|IN ECISR.EXTP,.INTP,.STDP
|SEG D2*,D1
|IN ECISR.QUAN,.DJ9J,.DCGS,.SCAM,.CORA,.CORB
|SEG F1*
|IN ECISR.INTI,.INSI,.INSH,.COUP,.SECM,.PADE
|SEG F2*,F1
|IN ECISR.INCH,.CPCC,.LINS
|SEG D3*,D1
|IN ECISR.SCHE,.RESU,.SCAT,.GRAL,.EMRO,.CPSF
|SEG L1*,()
|IN LARGE
|SEG B3*,B1
|IN ECISR.INPA
|SEG B4*,B1
|IN ECISR.INPB
```

A.3 Use on VAX

Around 50 FORTRAN cards have to be changed in ECIS79, to deal with the larger floating value which is 10^{38}. The IBM versions of ECIS88 and ECIS94 need no change. There is no use of OVERLAY on this computer and the working array can be taken the largest possible. At the Washington State University, it has been possible to use as MAIN routine:

```
|C 26/11/81  VAX                                                    MAIN-000
|C THE ASSEMBLER SUBROUTINE ECIS(I) DEFINES THE DOUBLE PRECISION ARRAY W MAIN-001
|C AND CALLS CALC(W,W,W,IDMX) WHERE IDMX IS THE LENGTH OF W          MAIN-002
|C W IS ALL THE REGION LEFT FREE BY THE PROGRAM EXCEPT 2*I K FOR BUFFERS MAIN-003
|C THE SUBROUTINE ECIS CAN BE ELIMINATED WITH THE FOLLOWING MAIN:    MAIN-004
|      REAL*8 W(400000)                                             MAIN-005
|      CALL CALC(W,W,W,400000)                                      MAIN-006
|      STOP                                                         MAIN-007
|      END                                                          MAIN-008
```

There is no control of the time allowed for the JOB. The CPU elapsed time is given by following subroutine STIM :

```
|C 12/10/81  VAX                                                    STIM-000
|      SUBROUTINE STIM(I)                                           STIM-001
|C RETURNS INTEGER VALUE OF CURRENT CPU TIME IN HUNDREDTH OF SECONDS STIM-002
|C               ACCUMULATED BY PROCESS                             STIM-003
|C               RJS       12-OCT-81    (WASHINGTON STATE UNIVERSITY) STIM-004
```

```
|      IMPLICIT INTEGER*4 (A-Z)                                          STIM-005
|      PARAMETER JPI$_CPUTIM='0407'X                                     STIM-006
|      INTEGER*2 LIST(8)                                                 STIM-007
|      DATA LIST/4,JPI$_CPUTIM,6*0/                                      STIM-008
|      EQUIVALENCE (TIMELOC,LIST(3))                                     STIM-009
|      TIMELOC=%LOC(TIME)                                                STIM-010
|      STAT=SYS$GETJPI(,,,LIST,,,)                                       STIM-011
|      I=TIME                                                            STIM-012
|      RETURN                                                            STIM-013
|      END                                                               STIM-014
```

The subroutine HORA has been modified to suppress the transformation from IBM units.

A.4 Use on PR1ME

The code ECIS79 could not be used with F77, due to compilation errors found in the function SIGM and the strange behaviour of equivalences. With FTN, in which there is no DASIN and no DSINH, the two following subroutines must be added to the coulomb functions:

```
|      FUNCTION DASIN(X)
|      IMPLICIT REAL*8 (A-H,O-Z)
|      DASIN=DATAN2(X,DSQRT(1-X*X))
|      RETURN
|      END
|      FUNCTION DSINH(X)
|      IMPLICIT REAL*8 (A-H,O-Z)
|      DSINH=0.5D0*(DEXP(X)-DEXP(-X))
|      RETURN
|      END}
```

Further modifications had to be done : DFLOAT has to be replaced by DBLE(FLOAT( )) and a statement had to be modified in subroutine FITE. The OVERLAY is not needed. The MAIN routine is :

```
|C 27/01/82  PRIME                                                      MAIN-000
|C THE ASSEMBLER SUBROUTINE ECIS(I) DEFINES THE DOUBLE PRECISION ARRAY W MAIN-001
|C AND CALLS CALC(W,W,W,IDMX) WHERE IDMX IS THE LENGTH OF W             MAIN-002
|C W IS ALL THE REGION LEFT FREE BY THE PROGRAM EXCEPT 2*I K FOR BUFFERS MAIN-003
|C THE SUBROUTINE ECIS CAN BE ELIMINATED WITH THE FOLLOWING MAIN:       MAIN-004
|      REAL*8 W(160000)                                                 MAIN-005
|      COMMON W                                                         MAIN-006
|      CALL CALC(W,W,W,160000)                                          MAIN-007
|      STOP                                                             MAIN-008
|      END                                                              MAIN-009
```

The STIM subroutine is :

```
|C 17/01/82  PRIME                                                      STIM-000
|      SUBROUTINE STIM(I)                                               STIM-001
|C RETURNS INTEGER VALUE OF CURRENT CPU TIME IN HUNDREDTH OF SECONDS     STIM-002
|      CALL CTIM$A(I)                                                   STIM-003
|      RETURN                                                           STIM-004
|      END                                                              STIM-005
```

The compilation is :

```
| FTN  XX  -SA -L -X -INTL -BIG -64V
```

A.5 Use on BURROUGH

The code ECIS79 has been run on the BURROUGH 7700 of the Technische Hogeschool in Eindhoven, Netherlands.

Some errors without effect on other computers have been found:

- in subroutine HORA, M0 and M2 must be put on data,
- in subroutine CORH the array SP was not declared as single precision: add REAL*4 SP after IMPLICIT or change SP into OP and use IMPLICIT REAL*8 (A-H,P-Z),
- in the subroutine CAL1, in calls to CORB, an argument was of wrong type; use :

```
|     1,DW(NXC1),DW(NX1),NC,ISM,KAB,NW(NNIV),NW(NT),NW(NIVQ),DW(NFG),LMAXCAL1-075
|     21,LMAX3,INC,NW(NWR),LO)                                          CAL1-076
|     1DW(NXC1),DW(NX),NCXN,ISM,LMAX2,NW(NNIV),NW(NT),NW(NIVQ),DW(NFG),LMCAL1-137
|     2AX1,LMAX3,INC,NW(NML),LO)                                        CAL1-138
```

- in subroutine SCAT, the subroutine EMRO was not called with an array as argument; use :

```
|     1),X2,X3,SQX,MX,B(1),1)                                           SCAT-073
|     1),X2,X3,SQX,MX,B(2),1)                                           SCAT-075
|      W1=B(1)*B(2)                                                     SCAT-076
```

- an error was found in subroutine HULT.

These changes have been done to the programme on the 10/05/82. Furthermore, the parity of the levels cannot be read on this computer unless one uses :

```
|      IF (SPI.IS.SIGM) IPI(IV,1)=1                                     LECT-109
```

A.6 Use on SUN

This version of ECIS88 was run on a SUN computer without difficulty. As the system was UNIX, the subroutine STIM described for a CONVEX computer was used.

B The CDC version

The object deck of ECIS79 was conveniently handled as a SOURCE file for UPDATE. Using UPDATE,D., the identification of the cards appears in the compilation. The UPDATE identification is the name of the subroutine and the sequence number is the number of the card plus 2.

Due to the relative small size of CDC computers, the code must be used with segmentation (SEGLOAD). These segmentation cards for ECIS79 are :

```
|ECIS   GLOBAL  AZ,DBLPR,DECOU,TITR,FCL.C.                              OVCD-001
|RESU   GLOBAL  RESC                                                   OVCD-002
|ECIS   INCLUDE CALC                                                   OVCD-003
|LECT   INCLUDE LECD,DEPH,OBSE                                         OVCD-004
|FITE   INCLUDE VARI,REST,EVAL                                         OVCD-005
|QUAN   INCLUDE CORB,SCAM                                              OVCD-006
|ROTP   INCLUDE VIBP,EXTP,COPO                                         OVCD-007
|RESU   INCLUDE SCHE,CPSF                                              OVCD-008
|A      TREE    ECIS-(CALX-(INPA,INPB,LECT),COLF,DJ6J-(REDM,B),FITE)   OVCD-009
|B      TREE    CAL1-(POTE-(ROTP,FOLD),QUAN-(INTI,INCH),RESU)          OVCD-010
|       END                                                            OVCD-011
```

The time control is obtained by the CDC subroutine SECOND and a call to the CERN subroutine TIMING at the beginning of the JOB.

The CDC version uses the dynamic allocation of memories, using the MACRO instruction MEMORY. For that, the working array must be extended without overlapping the programme. The CERN subroutines MEMORY and INCLCM, used previously, include the size of the local computer. The maximum core can depend on the user, the hour of computation, or on the JOB card. A COMPASS subroutine INCM calling the MACRO MEMORY has been written by LE FUR, in order to get the maximum core allowed by the installation :

```
|          IDENT    INCM                                          INCM-000
|          ENTRY    INCM                                          INCM-001
|          VFD  36/4HINCM,24/INCM                                 INCM-002
| SVA0     DATA 0                                                 INCM-003
| SVX1     DATA 0                                                 INCM-004
| TAIL     DATA 0                                                 INCM-005
| INCM     DATA 0                                                 INCM-006
|          SB7  1                                                INCM-007
|          SX6  A0                                               INCM-008
|          BX7  X1                                               INCM-009
|          SA6  SVA0                                             INCM-010
|          SA7  A6+B7                                            INCM-011
|          SA4  X1                                               INCM-012
|          LX4  30                                               INCM-013
|          BX6  X4                                               INCM-014
|          SA6  TAIL                                             INCM-015
|          MEMORY  SCM,TAIL,RECALL,,NABORT                       INCM-016
|          SB7  1                                                INCM-017
|          SA1  SVX1                                             INCM-018
|          SA2  TAIL                                             INCM-019
|          AX2  30                                               INCM-020
|          BX6  X2                                               INCM-021
|          SA6  X1                                               INCM-022
|          SA2  A1-B7                                            INCM-023
|          SA0  X2                                               INCM-024
|          EQ   INCM                                             INCM-025
|          END                                                   INCM-026
```

called by the FORTRAN subroutine:

```
|      SUBROUTINE MEMORY(N,NTOT,IER)                             INCM-027
|      DATA KX /0/                                               INCM-028
|      IF (KX.EQ.0) CALL INCM(KX)                                INCM-029
|      N2=N                                                      INCM-030
|      KZ=KX+N2                                                  INCM-031
|      DO 1 I=1,1000                                             INCM-032
|      KX=KX+N2                                                  INCM-033
|      KY=KX                                                     INCM-034
|      CALL INCM(KX)                                             INCM-035
|      IF (KX.GE.KY.AND.N2.EQ.N) GO TO 2                         INCM-036
|      N2=(2*N2)/3                                               INCM-037
|      IF (N2.EQ.0) GO TO 2                                      INCM-038
|    1 CONTINUE                                                  INCM-039
|    2 NTOT=KX                                                   INCM-040
|      IER=KX-KZ                                                 INCM-041
|      RETURN                                                    INCM-042
|      END                                                       INCM-043
```

B.1 Use on CDC 7600

The working array can be in the SCM or in the LCM.

B.1.a Using SCM

The OVERLAY structure on a CDC 7600 puts the BLANK COMMON at the top of the root. In these circumstances, if the working array is in it, it cannot be extended without overlapping the programme.

The solution chosen (for ECIS79) is to add two cards before the END of the OVERLAY cards to create a second level:

```
|B      TREE    CAL1-(POTE-(ROTP,FOLD),QUAN-(INTI,INCH),RESU)            OVCD-010
|       LEVEL                                                            OVCD-011
|       TREE    CALS                                                     OVCD-012
|       END                                                              OVCD-013
```

and the subroutine CALS is :

```
|CDC 15/06/79                                                  ECIS79  CALS-000
|      SUBROUTINE CALS                                                   CALS-001
|C WITHOUT THE SUBROUTINE MEMORY TO GET THE SPACE, THIS SUBROUTINE MUST  CALS-002
|C BE REPLACED BY                                                        CALS-003
|C     DIMENSION W(10000)                                                CALS-004
|C     IDMX=10000                                                        CALS-005
|C     CALL CALC(W,W,IDMX)                                               CALS-006
|C*************************************************************************CALS-007
|      DIMENSION W(10)                                                   CALS-008
|      CALL CALC(W,W,10)                                                 CALS-009
|      RETURN                                                            CALS-010
|      END                                                               CALS-011
```

The MAIN programme is:

```
|      CALL CALS                                                         ECIS-008
|      STOP                                                              ECIS-009
|      END                                                               ECIS-010
```

The subroutine CALS and the second level are overwritten by the working array but the computation never go out of the subroutine CALC. The UPDATE instruction is :

```
|*COMPILE ECIS.CALS
```

B.1.b Using LCM

The code ECIS in its CDC version has been written in such a way that a quantity in the working array never appears in the call of a subroutine except as an array. All the working array can be shifted into the LCM by inserting :

```
|      LEVEL,A1,A2,A3.....}
```

in each subroutine, where A1,A2,A3... are the parts of the working array which are used. The MAIN programme is then :

```
|      COMMON W(512)                                                    LEV2-002
|      LEVEL 2,W                                                        LEV2-003
|      CALL CALC(W,W,512)                                               LEV2-004
|      STOP                                                             ECIS-009
|      END                                                              ECIS-010
```

The UPDATE (still for ECIS79) instruction is :

```
|*ID LEV2                                                              -ECIS79-
|*D ECIS.10                                                            LEV2-001
|      COMMON W(512)                                                    LEV2-002
|      LEVEL 2,W                                                        LEV2-003
|      CALL CALC(W,W,512)                                               LEV2-004
|.....................................................................
|*D INCM.018                                                           LEV2-013
|          MEMORY  LCM,TAIL,RECALL,,NABORT                              LEV2-014
|.....................................................................
|*I FIT1.39                                                            LEV2-125
|      LEVEL 2,I,W                                                      LEV2-126
|*I FIT2.55                                                            LEV2-127
|      LEVEL 2,A,D,IP                                                   LEV2-128
|*C ECIS.FIT2                                                          LEV2-129
```

B.2 Use on CDC 6600

On a CDC 6600, it is convenient to reduce the size of the BUFFER in the first card of the MAIN routine.

In some places, ECIS can be run as on a CDC 7600 with SCM. In some other places, the use of the MACRO MEMORY is inhibited unless the compilation is STATIC. The working array can be in the BLANK COMMON and the use of the subroutine CALS and of the second level of OVERLAY avoided.

The size of the working array can be controlled by the CM parameter of the JOB card with the following MAIN routine :

```
|CDC 16/10/78                                                          ECIS-000
|      PROGRAM ECIS(INPUT,OUTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT,TAPE7=PUNECIS-001
|     1CH,TAPE1)                                                       ECIS-002
|C                                                                     ECIS-003
|C    THE MAIN SUBROUTINE DEFINES THE WORKING SPACE W AND CALL THE     ECIS-004
|C SUBROUTINE CALC WITH THE LENGTH OF W AS  LAST ARGUMENT.             ECIS-005
|C                                                                     ECIS-006
|C*********************************************************************ECIS-007
|      COMMON // W(1)                                                   ECIS-008
|      CALL CALC(W,W,LENGTHB(W))                                        ECIS-009
|      STOP                                                            ECIS-010
|      END                                                             ECIS-011
```

and the COMPASS subroutine written in Amsterdam :

```
|          IDENT  LENGTHB                                              LENGTHB2
|          ENTRY  LENGTHB                                              LENGTHB3
| MEMREPLY BSSZ   1                                                    LENGTHB4
| LENGTHB  BSS    1                                                    LENGTHB5
|          SX7    X1                                                   LENGTHB6
|          SYSTEM MEM,R,MEMREPLY                                       LENGTHB7
```

```
|          SA1    MEMREPLY                                                LENGTHB8
|          AX1    30                                                      LENGTHB9
|          IX6    X1-X7                                                   LENGTH10
|          EQ     LENGTHB                                                 LENGTH11
|          END                                                            LENGTH12
```

The indication at the end of a JOB can be used to choose the best CM in a similar computation.

B.3 Use on CRAY

The code ECIS79 has been run on a CRAY computer. Due to the large size, the OVERLAY structure is not needed. No information on time and memory management.

The code ECIS88 has been used with memory management. The MAIN subroutine is then :

```
|CRAY 21/03/88                                                  ECIS88  ECIS-000
|      PROGRAM ECIS(INPUT,OUTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT,TAPE7=PUNECIS-001
|     1CH,TAPE8)                                                         ECIS-002
|      COMMON W(10)                                                      ECIS-003
|      CALL CALC(W,W,10)                                                 ECIS-004
|      STOP                                                              ECIS-005
|      END                                                               ECIS-006
```

and the subroutine MEMO is :

```
|CRAY 07/06/86                                                  ECIS88  MEMO-000
|      SUBROUTINE MEMO(IDMT,NPLACE,NQ,IX,LO)                             MEMO-001
|C THIS SUBROUTINE GETS THE WORKING SPACE.                               MEMO-002
|C IDMT     PREVIOUS SPACE                                               MEMO-003
|C NPLACE   REQUESTED SPACE                                              MEMO-004
|C NQ       SPACE TO BE UPDATED                                          MEMO-005
|C IX: CONTROL NUMBER IX=1     FIRST CALL   STORE MINIMUM SIZE IN ID     MEMO-006
|C                    IX=2     DIMINUTION OF SPACE                       MEMO-007
|C                    IX=3     REQUEST NPLACE+ISTART, AT LEAST NPLACE    MEMO-008
|C                    IX=4     REQUEST NPLACE                            MEMO-009
|C                    IX=5     ABSOLUTE REQUEST                          MEMO-010
|C LO: LOGICAL CONTROLS  IF LO(94)=.TRUE. PRINT THE SIZE OF W            MEMO-011
|C OUTPUT VARIABLES: IDMT  SIZE OF WORKING SPACE                         MEMO-012
|C                   LO(216)=.TRUE. IF COMPUTATION CANNOT CONTINUE       MEMO-013
|C*********************************************************************MEMO-014
|      LOGICAL LO(250)                                                   MEMO-015
|      DATA ISTART,IMOD /4096,1024/                                      MEMO-016
|      IF (IX-2) 1 , 2 , 3                                               MEMO-017
|    1 ID=IDMT                                                           MEMO-018
|      NT=MAX0(IDMT,ISTART)                                              MEMO-019
|      NPLACE=0                                                          MEMO-020
|      CALL MEMORY('MAXFL',IDMAX)                                        MEMO-021
|      CALL MEMORY('CURFL',NX)                                           MEMO-022
|      IDMAX=IDMAX-NX+IDMT                                               MEMO-023
|      GO TO 4                                                           MEMO-024
|    2 NT=MAX0(NPLACE,ID)-IDMT                                           MEMO-025
|      CALL MEMORY('UC',NT)                                              MEMO-026
|      IR=0                                                              MEMO-027
|      GO TO 5                                                           MEMO-028
|    3 NT=NPLACE-IDMT                                                    MEMO-029
```

```
|       IF (IX.NE.3) GO TO 4                                                  MEMO-030
|       NT=NT+ISTART                                                          MEMO-031
|     4 NT=IMOD*(NT/IMOD+1)                                                   MEMO-032
|       NV=MIN0(NT,IDMAX-IDMT)                                               MEMO-033
|       IR=NV-NT                                                             MEMO-034
|       CALL MEMORY('UC',NV)                                                 MEMO-035
|     5 CALL MEMORY('CURFL',NX)                                              MEMO-036
|       IDMT=IDMT+NT+IR                                                      MEMO-037
|       LO(216)=(IDMT.LT.NPLACE).AND.((IX-5)*(IX-3).EQ.0)                    MEMO-038
|       NQ=NQ+NT+IR                                                          MEMO-039
|       IF (LO(94)) WRITE (6,1000) IX,NT,IR,NPLACE,IDMT,NX,NX                MEMO-040
|       IF (.NOT.LO(216)) RETURN                                             MEMO-041
|       WRITE (6,1001) IX,IDMT,NPLACE                                        MEMO-042
|       WRITE (6,1002)                                                       MEMO-043
|       RETURN                                                               MEMO-044
| 1000 FORMAT (/8H REQUEST,I2,4H FOR,I9,9H MEMORIES,I6,25H ARE MISSING.      MEMO-045
|      1  NPLACE =,I9,7H SIZE =,I9,15H  TOTAL LENGTH ,I8,4X,O8,1HB/)         MEMO-046
| 1001 FORMAT (33H NOT ENOUGH PLACE .....   REQUEST,I2,I10,8H ALLOWED,I10MEMO-047
|     1,10H REQUESTED/)                                                      MEMO-048
| 1002 FORMAT (/48H ...STOP...  NEXT TIME, USE LARGER MFL PARAMETER/)        MEMO-049
|       END                                                                  MEMO-050
```

The subroutine `STIM` is :

```
|CRAY 09/01/88                                                  ECIS88  STIM-000
|       SUBROUTINE STIM(K)                                                 STIM-001
|       CALL TREMAIN(T)                                                    STIM-002
|       K=38500.*T                                                         STIM-003
|       RETURN                                                             STIM-004
|       END                                                                STIM-005
```

without changing the `IBM` subroutine `HORA`.

C Use on a CONVEX

On a `CONVEX` computer, the two versions can be used. As there can be only control of the elapsed time, a subroutine `STIM`, identical for the two versions, was written to stop the `JOB` just before an hour (the allowed time of the `QUEUE` for long `JOB`). This subroutine is :

```
|C 15/12/87  CONVEX  IBM AND CDC VERSIONS                       ECIS88  STIM-000
|       SUBROUTINE STIM(I)                                                STIM-001
|C RETURNS INTEGER VALUE OF CPU ELAPSED TIME IN HUNDREDTHS OF SECONDS      STIM-002
|       DIMENSION A(2)                                                     STIM-003
|       B=ETIME(A)                                                         STIM-004
|       I=38500*(3300.-B)                                                  STIM-005
|       RETURN                                                             STIM-006
|       END                                                                STIM-007
```

It can be used on any computer with the `UNIX` system.

The `IBM` version has to be compile with "fc –72" and the `CDC` version with "fc –cfc –72". Even if all the subroutines has been compiled beforehand and "fc" is used only to create a `LOAD MODULE`, one must use "fc –cfc" to get the right answer from the subroutine `STIM`.

Chapter III

Coupled channels

The inelastic scattering of nucleons exciting low lying collective states of the nuclei is usually described by coupled channel calculations using a collective model. A Dirac phenomenology using a scalar and a vector potential has been introduced in Ref. [9] to describe elastic scattering at quite large energies. Strictly speaking, these calculations are only valid for infinite mass targets because the center-of-mass is separable in non relativistic Schrödinger equation and not in Dirac equation. In the same approximation, deformation or vibration can be introduced in the scalar and in the vector potential of the Dirac formalism to study the inelastic scattering in the collective model.

For elastic scattering, there is a fully equivalent Schrödinger equation for the Dirac equation. The presence of some $1/r^2$ terms for charged particles do not affect strongly the results. For inelastic scattering, this transformation has to be done on the tri-dimensional Dirac equation. Then, the spin orbit potential appears as the cross product of the gradient of the potential with a gradient acting on the wave function. Such expression for the spin-orbit is used since a long time in the description of nucleon inelastic scattering by : [55] SHERIF, H., BLAIR, J. S., *"Inelastic proton scattering and the deformed spin dependent optical potential"*, Physics Letters **26B** (1968) 489. and : [56] SHERIF, H., *"Spin-dependent effects in proton inelastic scattering"*, Thesis University of Washington (1968). However, to write the Schrödinger equation, the wave function has been multiplied by the square root of the potential. As long as the potential is a given function of the radius, it is the only difference between Dirac and Schrödinger formalism. The potential used has usually Woods-Saxon form-factors in the two formalisms; the Schrödinger potential equivalent to the Dirac one gets a *wine-bottle-bottom* shape as said in the title of Ref. [9].

Coupled channel calculations are necessary even at large energies as 500 or 800 MeV as shown in Ref. [48] and [50]. At these energies, the elastic scattering of protons to backwards angles is well described when the strong low-lying collective states are taken into account. The difference between Schrödinger and Dirac approaches seems limited to the influence of the shape of the potential as shown in : [57] COOPER, E., D., *"Are the Dirac imaginary potentials surface peaked?"*, Nucl. Phys. **A495** (1989) page 483 and in Ref. [50].

A Dirac and Schrödinger formalisms

In order to describe inelastic nucleon scattering, we must start from Dirac equation because spin-orbit effects can not be understood without it.

A.1 The Dirac equation

To describe the scattering of a nucleon with "magnetic anomalous moment" in a Coulomb field $V_C(\vec{r})$, the Dirac equation is :

$$\Big(\frac{\hbar}{i}\vec{\alpha}.\vec{\nabla} + \beta m + V_C(\vec{r})\frac{i\mu\hbar}{2m}\beta\vec{\alpha}.\{\vec{\nabla}V_C(\vec{r})\}\Big)\psi(\vec{r}) = E\psi(\vec{r}). \tag{III.1}$$

More generally, this equation can be generalised to describe the scattering of this nucleon by a nucleus into the equation :

$$\Big(\frac{\hbar}{i}\vec{\alpha}.\vec{\nabla} + \beta\{m + V_S(\vec{r})\} + V_V(\vec{r}) + \frac{i\hbar}{2m}\beta\vec{\alpha}.\{\vec{\nabla}V_T(\vec{r})\}\Big)\psi(\vec{r}) = E\psi(\vec{r}) \tag{III.2}$$

where $V_S(\vec{r}), V_V(\vec{r}), V_T(\vec{r})$ are three finite range complex potentials of which the real and the imaginary part are approximated by a Woods-Saxon form factor but can be replaced by any other form factor given by a theory.

The Equ. (III.1) is valid in the laboratory system and the Equ. (III.2) can be used only for a target with an infinite mass with respect to the nucleon, so that the laboratory system is also the center of mass system and m is the rest mass of the nucleon.

We consider the mass m as a parameter which can be :

- the rest mass if `LO(98)=.TRUE.`,
- the reduced mass if `LO(98)=.FALSE.`, which allows a correct limit at low energy.

In this equation, the vector potential $V_V(\vec{r})$ and the tensor potential $V_T(\vec{r})$ include the Coulomb potential $V_C(\vec{r})$; in fact, for a nucleon with an "anomalous magnetic moment" μ_n, the tensor potential is reduced here to the Coulomb potential multiplied (at the low energy limit) by $\mu_n + \frac{1}{2}z$ where z is the charge of the nucleon.

The $\vec{\alpha}$ and β are four-dimensional Dirac matrices. They can be expressed in terms of two-dimensional unit matrix and Pauli matrices $\vec{\sigma}$ as follows and allow to write the wave function :

$$\vec{\alpha} = \begin{vmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{vmatrix}, \qquad \beta = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}, \qquad \psi(\vec{r}) = \begin{pmatrix} F(\vec{r}) \\ iG(\vec{r}) \end{pmatrix} \tag{III.3}$$

in terms of the **large component** $F(\vec{r})$ and the **small component** $G(\vec{r})$. They allow to write a set of two linear coupled equations with the Pauli matrices :

$$\begin{aligned} \hbar\vec{\sigma}.\vec{\nabla}\ G(\vec{r}) &= [E - m - V_V(\vec{r}) - V_S(\vec{r})]F(\vec{r}) + \frac{\hbar}{2m}\vec{\sigma}.[\vec{\nabla}V_T(\vec{r})]G(\vec{r}) \\ -\hbar\vec{\sigma}.\vec{\nabla}\ F(\vec{r}) &= [E + m - V_V(\vec{r}) + V_S(\vec{r})]G(\vec{r}) + \frac{\hbar}{2m}\vec{\sigma}.[\vec{\nabla}V_T(\vec{r})]F(\vec{r}) \end{aligned} \tag{III.4}$$

A.2 Reduction to Schrödinger equation

The terms $[\vec{\nabla}V_T(\vec{r})]$ are almost eliminated by the substitution :

$$G(\vec{r}) = \exp\Big(\frac{V_T(\vec{r})}{2m}\Big)\hat{G}(\vec{r}), \qquad F(\vec{r}) = \exp\Big(-\frac{V_T(\vec{r})}{2m}\Big)\hat{F}(\vec{r}), \tag{III.5}$$

respectively, to get :

$$\begin{aligned} \hbar\vec{\sigma}.\vec{\nabla}\ \hat{G}(\vec{r}) &= \exp\Big(-\frac{V_T(\vec{r})}{m}\Big)\big[E - m - V_V(\vec{r}) - V_S(\vec{r})\big]\hat{F}(\vec{r}) \\ -\hbar\vec{\sigma}.\vec{\nabla}\ \hat{F}(\vec{r}) &= \exp\Big(\frac{V_T(\vec{r})}{m}\Big)\big[E + m - V_V(\vec{r}) + V_S(\vec{r})\big]\hat{G}(\vec{r}) \end{aligned} \tag{III.6}$$

From the second equation, using :

$$D(\vec{r}) = E + m - V_V(\vec{r}) + V_S(\vec{r}), \qquad D_T(\vec{r}) = \exp\Big(\frac{V_T(\vec{r})}{m}\Big)D(\vec{r}) \tag{III.7}$$

we get :

$$\hat{G}(\vec{r}) = -\frac{1}{D_T(\vec{r})}\hbar\vec{\sigma}.\vec{\nabla}\ \hat{F}(\vec{r}) \tag{III.8}$$

which gives in the first equation, using :

$$(\vec{\sigma}.\vec{A})(\vec{\sigma}.\vec{B}) = (\vec{A}.\vec{B}) + i\vec{\sigma}.(\vec{A}\times\vec{B}) \tag{III.9}$$

and after multiplication by $D_T(\vec{r})$:

$$-\hbar^2\Big\{\Delta - \frac{1}{D_T(\vec{r})}\big[\vec{\nabla}D_T(\vec{r})\big].\vec{\nabla} - i\vec{\sigma}.\big[\vec{\nabla}D_T(\vec{r})\big]\times\vec{\nabla}\Big\}\hat{F}(\vec{r}) = D(\vec{r})[E-m-V_V(\vec{r})-V_S(\vec{r})]\hat{F}(\vec{r}) \tag{III.10}$$

This equation include first derivatives of $\hat{F}(\vec{r})$ which can be eliminated by using :

$$f(\vec{r}) = D_T(\vec{r})^{-\frac{1}{2}}\hat{F}(\vec{r}) = D(\vec{r})^{-\frac{1}{2}}F(\vec{r}) \tag{III.11}$$

to obtain :

$$\begin{aligned}\hbar^2\Big\{\Delta - \frac{3}{4}\Big(\frac{\vec{\nabla}D_T(\vec{r})}{D_T(\vec{r})}\Big)^2 + \frac{1}{2}\,\frac{\Delta D_T(\vec{r})}{D_T(\vec{r})} - i\vec{\sigma}.\big[\vec{\nabla}\ln D_T(\vec{r})\big]\times\vec{\nabla}\Big\}f(\vec{r})\\ +\Big\{-2EV_V(\vec{r}) - 2mV_S(\vec{r}) + V_V^2(\vec{r}) - V_S^2(\vec{r}) + \hbar^2k^2\Big\}f(\vec{r}) = 0\end{aligned} \tag{III.12}$$

with $\hbar^2k^2 = E^2 - m^2$.

This equation can be written :

$$\Big\{-\frac{\hbar^2}{2m}\big[\Delta + k^2\big] + V_1(\vec{r}) - \vec{\sigma}\big[\nabla\ln V_2(\vec{r})\big]\times\frac{\vec{\nabla}}{i}\Big\}f(\vec{r}) = 0 \tag{III.13}$$

with :

$$\begin{aligned}V_1(\vec{r}) &= \frac{\hbar^2}{2m}\Big\{\frac{3}{4}\Big(\frac{\vec{\nabla}D_T(\vec{r})}{D_T(\vec{r})}\Big)^2 - \frac{1}{2}\,\frac{\Delta D_T(\vec{r})}{D_T(\vec{r})}\Big\} + \frac{1}{2m}\Big\{2EV_V(\vec{r}) + 2mV_S(\vec{r}) - V_V(\vec{r})^2 + V_S(\vec{r})^2\Big\}\\ V_2(\vec{r}) &= D_T(\vec{r})\end{aligned} \tag{III.14}$$

A.3 The Schrödinger formalism

As long as there is only elastic scattering, the potentials have no angular dependence. Using :

$$\vec{\nabla} = \frac{\vec{r}}{r}\,\frac{d}{dr} - i\frac{1}{r^2}\,\vec{r}\times\vec{L} \tag{III.15}$$

the spin term of the Dirac equation for $D_T(\vec{r})$ independent of $\hat{r}$ reduces to :

$$-i\vec{\sigma}.\Big[\frac{\vec{r}}{r}\frac{d}{dr}\ \ln D_T(r)\Big]\times\vec{\nabla} = \frac{1}{r}\frac{d}{dr}\ln D_T(r)(\vec{\sigma}.\vec{L}) \tag{III.16}$$

and Equ. (III.13) can be written :

$$\Big\{-\frac{\hbar^2}{2m}\big[\Delta + k^2\big] + V_1(r) + \frac{1}{r}\big[\frac{d}{dr}V_2(r)\big](\vec{\sigma}.\vec{L})\Big\}f(\vec{r}) = 0 \tag{III.17}$$

The Schrödinger formalism is the use of Equ. (III.17).

An important difference is the use of the Coulomb potential $V_C(r)$ directly as a part of $V_1(r)$; it does not contribute to the spin-orbit potential. This allows the use of nonrelativistic coulomb functions. In the equivalent Schrödinger equation, the Coulomb potential is multiplied by the ratio E/m which is larger than 1 and its square appears also in $V_1(r)$ and $V_2(r)$ at large distances. This terms in $1/r^2$ are taken into account with the relativistic Coulomb functions. However, taking into account an "anomalous magnetic moment", terms in $1/r^2$ appears into the spin-orbit potential in both formalisms. The elastic scattering in the Dirac formalism cannot allow to determine a tensor potential, as shown in : [58] CLARK, B., C., HAMA, S., KALBERMANN, S., G., COOPER, E., D. and MERCER, R., L., *"Equivalent local Dirac potentials"*, Phys. Rev. **C31** (1985) page 694, because it depends only upon the two potentials $V_1(r)$ and $V_2(r)$ defined in Equ. (III.14). Nevertheless, it does not means that a known tensor potential has not to be used.

A.4 Radial dependence of potentials

The potentials $V_S(\vec{r})$, $V_V(\vec{r})$ and $V_V(\vec{r})$ in Dirac equation, $V_1(\vec{r})$ and $V_2(\vec{r})$ in Schrödinger equation are usually complex with a real and an imaginary parts parametrised by a depth V multiplying a Woods Saxon form factor :

$$f(r,a,R) = \frac{1}{1+\exp\left(\frac{r-R'}{a}\right)} \qquad \text{where} \qquad R' = RA^{1/3} \tag{III.18}$$

where A is the mass of the target. **These are called volume potentials.**

The imaginary part of V_1 can include also **a surface potential** with the form factor :

$$f'(r,a,R) = \frac{1}{4a}\frac{d}{dR'}\Big\{\frac{1}{1+\exp\left(\frac{r-R'}{a}\right)}\Big\} \qquad \text{where} \qquad R' = RA^{1/3} \tag{III.19}$$

and we generalise that to its real part. So, the two formalism deals with the same number of potentials.

Instead of the Woods-Saxon potential defined by Equ. (III.18), one can use a "symmetrised" Woods-Saxon potential which is :

$$f_s(r,a,R) = \Big[\frac{1}{1+\exp\left(\frac{r-R'}{a}\right)}\Big]\Big[\frac{1}{1+\exp\left(\frac{r+R'}{a}\right)}\Big] \tag{III.20}$$

The potentials $V_V(\vec{r})$ and $V_1(\vec{r})$ include the Coulomb potential $V_C(\vec{r})$ which is :

$$V_C(\vec{r}) = \begin{cases} \frac{1}{2}Ze^2\big(3-(r/R'_c)^2\big)/R'_c, & \text{for} \quad r < R'_c \\ Ze^2/r, & \text{for} \quad r > R'_c \end{cases} \tag{III.21}$$

where $R'_c = R_c A^{1/3}$ and Z is the product of charges of the particle and the target. $V_C(\vec{r})$ can also be computed from a diffuse charge with a density distribution given by a Woods-Saxon form factor, eventually multiplied by a factor $(1+cr^2)$ where c is a "third Coulomb parameter".

The potential can also be obtain from a microscopic description or replaced by a Fourier expansion on Bessel functions.

B The generalised optical model

In the generalised optical model, the potential describes also the different states of the target nucleus. See for example in : [59] TAMURA, T., *"Analyse of the Scattering of Nuclear Particles by Collective Nuclei in Terms of the Coupled-Channel Calculation"*, Rev. Mod. Phys. **37** (1965) 679 and in : [60] TAMURA, T., *"Coupled-channel approach to nuclear reactions"*, Ann. Rev. Nucl. Sci. **19** (1969) 99.

B.1 The macroscopic models

We give here the physical meaning of the macroscopic models used in `ECIS`.

B.1.a The symmetric rotational model

In the symmetric rotational model, the potentials are some functions $V(\vec{r},\hat{r}')$, where $\hat{r}'$ is the intrinsic axis of the nucleus. These potentials are parametrised by quadrupole and hexadecupole deformations β_2 and β_4,... using a radius $R(\theta)$ such that :

$$R(\theta) = R_0\big[1+\beta_2 Y_2^0(\theta)+\beta_4 Y_4^0(\theta)\dots\big] \tag{III.22}$$

where θ is the angle between $\vec{r}$ and $\hat{r}'$. There are only even deformations. This radius is used instead of R in the usual expressions of the optical model. The potential can be expanded into multipoles :

$$V(\vec{r},\hat{r}') = 4\pi \sum_{\lambda,\mu} V_\lambda(r) Y_\lambda^\mu(\hat{r}) Y_\lambda^{\mu\star}(\hat{r}'), \qquad V_\lambda(r) = \frac{1}{2}\int_0^\pi V(\vec{r},\hat{r}') P_\lambda(\cos\theta)\sin\theta d\theta, \tag{III.23}$$

where there are only even values of λ. This is obtained by a symmetric ten-points Legendre integral over θ of the potential multiplied by an adequate Legendre polynomial $P_\lambda(\cos\theta)$.

In this model, the target states are :

$$|\Phi_M^I >= \sqrt{\frac{2I+1}{16\pi^2}}\Big[\xi_K(r') R^{(J)}_{M,K}(\Omega) + (-)^{I-j}\xi_{-K}(r') R^{(J)}_{M,-K}(\Omega)\Big] \tag{III.24}$$

where $\xi_K(r')$ is the intrinsic function, Ω the rotation between the laboratory system and the intrinsic frame and j appears in the rotation of π around an axis perpendicular to the axis of symmetry for each component of the intrinsic state.

B.1.b The vibrational model

In the vibrational model, the radius is replaced by :

$$R = R_0\big[1 + \sum_{\lambda,\mu} \alpha_\lambda^\mu Y_\lambda^\mu(\theta,\phi)\big] \tag{III.25}$$

where :

$$\alpha_\lambda^\mu = \frac{\beta_\lambda^\mu}{\sqrt{2\lambda+1}}\Big(b_{\lambda,\mu} + (-)^\mu b^+_{\lambda,-\mu}\Big) \tag{III.26}$$

in which $b_{\lambda,\mu}$ are phonon creation operators and $b^+_{\lambda,\mu}$ are phonon annihilation operators. The potential is usually expanded in powers of the α's :

$$V(r,R_0) + \frac{d}{dR_0}V(r,R_0)R_0\sum_{\lambda,\mu}\alpha_\lambda^\mu Y_\lambda^\mu(\theta,\phi) + \frac{1}{2}\frac{d^2}{dR_0^2}V(r,R_0)R_0^2\Big(\sum_{\lambda,\mu}\alpha_\lambda^\mu Y_\lambda^\mu(\theta,\phi)\Big)^2 \tag{III.27}$$

with only the first derivative for the **first order vibrational model**, the first and the second derivatives for the **second order vibrational model**, but also the third derivative with nuclear matrix elements to be given in the **anharmonic vibrational model**.

In the harmonic vibrational model, the target states are :

$$|\Phi_M^I >= b_{IM}|0>, \qquad |\Phi_M^I >= |(L_1L_2)IM >= \frac{1}{\sqrt{1+\delta_{L_1,L_2}}}\Big[b_{L_1}b_{L_2}\Big]^I_M|0>, \tag{III.28}$$

for the 1-phonon and the 2-phonons states respectively.

B.1.c The vibration-rotational model

In the vibration-rotational model there is a static deformation like in the rotational model and a dynamical vibration α_L^M of the intrinsic state. Like in the vibrational model R_0 of Equ. (III.22) has to be replaced by R of the Equ. (III.25) but the expansion given by Equ. (III.27) is limited to the first derivative. Here, the value of M is important. The form factors are :

$$V_l^M(r) \propto \beta_L^M \int \frac{d}{dR}V(\vec{r},\hat{r}')\big[Y_L^M(\theta) - xY_l^M(\theta)\big]Y_l^{M^*}(\theta)d\theta \tag{III.29}$$

where the term $xY_l^M(\theta)$ is there only for the form factors with $l=0$ and $l=1$ to correct them for center of mass motion or translation and is defined by the condition that $\int V_l^M(r)r^{l+2}dr = 0$.

In the literature, the derivation of this model is presented with the summation of the two spherical harmonics, giving a sum with Clebsch-Gordan coefficients.

The nuclear states are those given by Equ. (III.24) with or without α_L^M acting on $\xi_K(r')$.

B.1.d The asymmetric rotational model

In the asymmetric rotational model, The radius is given by :

$$R(\theta) = R_0\Big(1 + \beta_2\big[\cos\gamma Y_2^0(\theta) + \frac{1}{\sqrt{2}}\sin\gamma\{Y_2^2(\theta) + Y_2^{-2}(\theta)\}\big] + \beta_4\cos\gamma' Y_4^0(\theta) + \dots\Big) \tag{III.30}$$

and the potential are :

$$V(\vec{r},\hat{r}') = V_0(\vec{r},\hat{r}') + V_2^0(\vec{r},\hat{r}')Y_2^0(\theta) + V_2^2(\vec{r},\hat{r}')\frac{1}{\sqrt{2}}\big[Y_2^2(\theta) + Y_2^{-2}(\theta)\big] + \dots \tag{III.31}$$

They are obtained by integration on the sphere with 36 points, the weights of which were obtained once for all by the inversion of the matrix of spherical harmonics at these points. This means that the potential is supposed to be expanded only with 36 terms, the coefficients of which are obtained by solving a set of 36 equations. The number of multipoles is limited to 15 (i. e. $L = 8$, whereas 36 is $L = 14$).

The nuclear states, as described in : [61] DAVYDOV, A., S. and FILIPPOV, G. F., *"Rotational states in even atomic nuclei"*, Nucl. Phys. **8** (1958) page 237, can be written :

$$\begin{aligned} |\Phi_M^{I_n}> \;=\; & \sqrt{\frac{2I+1}{8\pi^2}}\xi(r')\Big[\cos\beta_n^1 R_{M,0}^{(J)}(\Omega) + \sin\beta_n^1\cos\beta_n^2\frac{R_{M,2}^{(J)} + R_{M,-2}^{(J)}}{\sqrt{2}} \\ & + \sin\beta_n^1\sin\beta_n^2\cos\beta_n^3\frac{R_{M,4}^{(J)} + R_{M,-4}^{(J)}}{\sqrt{2}} + \dots\Big] \end{aligned} \tag{III.32}$$

for $I = 2m$ even with the possibility of $1 + m$ different states and :

$$|\Phi_M^{I_n}> = \sqrt{\frac{2I+1}{8\pi^2}}\xi(r')\Big[\cos\beta_n^2\frac{R_{M,2}^{(J)} - R_{M,-2}^{(J)}}{\sqrt{2}} + \sin\beta_n^2\cos\beta_n^3\frac{R_{M,4}^{(J)} - R_{M,-4}^{(J)}}{\sqrt{2}} + \dots\Big] \tag{III.33}$$

for $I = 2m + 1$ odd with the possibility of only m different states.

If the asymmetric rotational model is "constrained", the first state must be the 0^+ and the second state must be the first 2^+. If there is a third state, it must be the second 2^+. There is no protection in the code against using only elastic scattering, but no γ will be taken into account. The value read as β_1^1 for the first 2^+ is taken as the value of the γ in Equ. (III.30). The result given in Ref. [61] can be written :

$$\tan\beta_1^1 = -\frac{3\sin\gamma\cos 3\gamma - \cos\gamma\sin 3\gamma}{\sin\gamma\sin 3\gamma + 3\cos\gamma\cos 3\gamma + \sqrt{9 - 8\sin^2 3\gamma}}, \qquad \beta_2^1 = \beta_1^1 + \frac{\pi}{2} \tag{III.34}$$

because a sign does not matter.

B.2 The coupled equations

We shall take as example the rotational model. The equation to solve is :

$$\big[T + V - E\big]\Psi = 0 \tag{III.35}$$

where T is the kinetic energy and V the generalised optical potential.

B.2.a Schrödinger formalism

The total wave function is written :

$$\Psi(\vec{r}) = \frac{1}{r}\sum_{l,j,I,J} f_{ljIJ}(r)Y_{lsjIJM} \tag{III.36}$$

where :

$$Y_{lsjIJM} = i^l \sum_{\mu,\sigma,m,m'} < j,I,m,m'|J,M > \Big(< l,s,\mu,\sigma|j,m > Y_l^\mu(\hat{r})|s\sigma > \Big)\Phi_I^{m'} \tag{III.37}$$

are the target-spin-angular functions involving the target state ϕ_I.

Projecting the total equation on all the functions Y_{lsjIJM}, we obtain a system of coupled second order differential equations :

$$\frac{\hbar^2}{2m_i}\Big[\frac{d^2}{dr^2} - \frac{2\eta_i k_i}{r} - \frac{l_i(l_i+1)}{r^2} + k_i^2\Big] f_i(r) = \sum_{i'} \Big\{ \sum_\lambda G_{ii'}^\lambda V^\lambda(r) \Big\}\ f_{i'}(r) \tag{III.38}$$

where i and i' stands for any set of quantum numbers (l,j,I,J), k_i and η_i are the wave number and the coulomb parameter for equation i and $G_{ii'}^\lambda$ is a geometrical coefficient for the transition form factor $V^\lambda(r)$. For $\lambda = 0$ and $i = i'$, the second member of Equ. (III.38) includes the optical model. In general, $G_{ii'}^\lambda$ is the product of a "nuclear" part, which is the "reduced matrix element" and a geometric coefficient of the partial waves. For example, in the rotational model, a state of the target, member of a rotational band starting with 0^+ is described by Equ. (III.24) with $K = 0$:

$$|\Phi_{I,M} >= \sqrt{\frac{2I+1}{8\pi^2}} R_{M0}^{(I)\star}(\Omega)\chi(r') \tag{III.39}$$

where $\chi(r')$ is the intrinsic wave function. The result of integration on the nuclear state is :

$$< \Phi_{I_f,M_f}|V(\vec{r},\hat{r}')|\Psi_{I_i,M_i} >= \sqrt{4\pi}\sum_\lambda V_\lambda(r) Y_\lambda^\mu(\hat{r}) \times (-)^{M_i}\sqrt{(2I_i+1)(2I_f+1)(2\lambda+1)}$$
$$\begin{pmatrix} I_i & I_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} I_i & I_f & \lambda \\ M_f & -M_i & \mu \end{pmatrix} \tag{III.40}$$

and the total result is :

$$\sum_\lambda V_\lambda(r)(-)^{J+\lambda+\frac{1}{2}}\sqrt{(2I_i+1)(2I_f+1)(2j_i+1)(2j_f+1)}$$
$$\begin{pmatrix} I_i & I_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} j_f & \lambda & j_i \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}\begin{Bmatrix} I_i & I_f & \lambda \\ j_f & j_i & J \end{Bmatrix} \tag{III.41}$$

where there is a part which depends only upon the target and a part which depends only upon the nucleon, the two of them related by a $6j$ coefficient.

If there are n channels and if the spin of the particle is s_i, the spin of the target I_i and the product of the intrinsic parities η_i for the channel i, the total number of coupled equations for a total spin J sufficiently large and a parity η is :

$$N = \sum_{i=1}^n N_i = \sum_{n=1}^n \frac{1}{2}\big[(2I_i+1)(2s_i+1) + \epsilon_i'(-)^{J+\eta}\big] \tag{III.42}$$

where $\epsilon_i' = 0$ if I_i or s_i is half integer and $\epsilon_i' = \epsilon_i(-)^{I_i+s_i}$ if I_i and s_i are integers.

For the scattering of protons on a $0^+ - 2^+ - 4^+ - 6^+$ rotational band, this number is 28. For the scattering of α particles on the same levels, there are 16 equations or 12 equations according to the parity.

In the most general problem, the interaction V can be written as the scalar product of a tensor operator Q^{I^t} acting on the target, a tensor operator Q^S acting on the spin of the particle and the tensor $i^L\ Y_L^M(\hat{r})$ multiplying a radial form factor $V_{LSI^t}(r)$. Taking into account a factor $1/\sqrt{4\pi}$ introduced in the form factor, the geometrical coefficient is :

$$\frac{1}{\sqrt{4\pi}} < \big[(l_f\ s_f)^{j_f} I_f\big]^J |\big[i^L\ Y_L^M(\hat{r})\ Q^S\big]^{I^t}.Q^{I^t}|\big[(l_i\ s_i)^{j_i} I_i\big]^J >=< s_f||Q^S||s_i >< I_f||Q^{I^t}||I_i > \tag{III.43}$$

$$\times (-)^{J+I_f+j_i+\frac{1}{2}(l_f+l_i+L)}\sqrt{(2I^t+1)(2L+1)(2l_f+1)(2l_i+1)(2j_f+1)(2j_i+1)}$$
$$\begin{pmatrix} l_f & l_i & L \\ 0 & 0 & 0 \end{pmatrix}\left\{ \begin{matrix} j_f & j_i & I^t \\ I_i & I_f & J \end{matrix} \right\}\left\{ \begin{matrix} l_f & l_i & L \\ s_f & s_i & S \\ j_f & j_i & I^t \end{matrix} \right\} \qquad \text{(III.44)}$$

where the part of the second member written in Equ. (III.43) is the **"reduced nuclear matrix element"** and the one written in Equ. (III.44) is the geometrical factor computed by the code. This expression has the advantage to reduce the geometrical factor to the usual one of macroscopic excitations when $S = 0$ but is not symmetric when particle and target are exchanged : the reduced matrix element for a given L and $S = L$, $I^t = 0$ is $\sqrt{2S+1}$ the one for the same L and $S = 0$, $I^t = L$. Nevertheless, Equ. (III.44) was used up to `ECIS88`. To reduce this disadvantage, a factor $\sqrt{2S+1}$ has been introduced in the geometrical coefficient (III.44) in the code `ECIS94`. This correspond to use operators coupled to a scalar instead of the scalar product because :

$$\begin{aligned}(-)^{I^t} &< \left[(l_f\ s_f)^{j_f} I_f\right]^J | \left[i^L\ Y_L^M(\hat{r})\ , Q^S\ , Q^{I^t}\right]_0^0 | \left[(l_i\ s_i)^{j_i} I_i\right]^J > \\ &= \sqrt{2I^t+1} < \left[(l_f\ s_f)^{j_f} I_f\right]^J | \left[i^L\ Y_L^M(\hat{r})\ Q^S\right]^{I^t} . Q^{I^t} | \left[(l_i\ s_i)^{j_i} I_i\right]^J > \end{aligned} \qquad \text{(III.45)}$$

is symmetric for the exchange of Q^S and Q^{I^t}. In fact, the separation between reduced matrix element and geometrical coefficient correspond to the use of the expression given in Equ. (III.45) divided by $\sqrt{(2S+1)(2I^t+1)}$ in order to coincide with the usual notations for the macroscopic models.

Deformed spin-orbit interaction and magnetic multipole Coulomb interaction need a different approach. In the macroscopic models, there is no Q^S and this coefficient can be simplified.

B.2.b Spin-orbit deformation

It has been shown by `DWBA` calculations in Ref. [55] and [56] that the spin-orbit interaction should be the "full Thomas form" which is :

$$\vec{\nabla}\ V(\vec{r})\ \times \frac{\vec{\nabla}}{i}.\vec{\sigma} \qquad \text{(III.46)}$$

derived from Dirac's equation by elimination of small components, in order to fit experimental data in proton elastic scattering.

B.2.b.i Spin-orbit deformation for spin one-half

For a multipole $V_\lambda(r)\ Y_\lambda^\mu(\hat{r})$ of the interaction $V(\overline{r})$, it can be shown by elementary manipulation of Pauli matrices as given by Equ. (III.9) and with the expression of the gradient gien by Equ. (III.15) that the expression above is :

$$\begin{aligned}&\vec{\nabla}\Big[V_\lambda(r)\ Y_\lambda^\mu(\hat{r})\Big] \times \frac{\vec{\nabla}}{i}.\vec{\sigma} = \frac{1}{r}\Big[\frac{d}{dr}V_\lambda(r)\Big]Y_\lambda^\mu(\hat{r})(\vec{\sigma}.\vec{L}) - \frac{V_\lambda(r)}{r}\Big[(\vec{\sigma}.\vec{L})Y_\lambda^\mu(\hat{r})\Big]\frac{d}{dr} \\ &+\frac{V_\lambda(r)}{r^2}\Big[(\vec{\sigma}.\vec{L})Y_\lambda^\mu(\hat{r})\Big](\vec{\sigma}.\vec{L}) - \frac{V_\lambda(r)}{r^2}\Big[\vec{L}Y_\lambda^\mu(\hat{r})\Big].\vec{L}\end{aligned} \qquad \text{(III.47)}$$

(see in Ref. [23] and [28]).

For any spin, the eigenvalue of $2(\vec{L}.\vec{s})$ is :

$$2(\vec{L}.\vec{s}) = \frac{1}{2}[j(j+1) - l(l+1) - s(s+1)] \qquad \text{(III.48)}$$

that is for spin $\frac{1}{2}$:

- $\vec{L}.\vec{\sigma} = l$ if $j = l + \frac{1}{2}$,

- $\vec{L}.\vec{\sigma} = -l - 1 \qquad \text{if} \quad j = l - \frac{1}{2}.$

When taken between partial waves $|l_f j_f >$ and $|l_i j_i >$, the operators $\vec{L}.\vec{\sigma}$ can be replaced by their eigenvalues γ_f on $|l_f j_f >$ or γ_i on $|l_i j_i >$. The same holds for $\Big[\vec{L}Y^{\mu}_{\lambda}(\hat{r})\Big].\vec{L}$. Taking carefully into account on what acts the operator, one gets the same geometrical factor G^{λ}_{if} as for a central term, multiplied by :

$$\frac{1}{r}\Big[\frac{d}{dr}V_\lambda(r)\Big]\gamma_i + \frac{V_\lambda(r)}{r}(\gamma_i - \gamma_f)\frac{d}{dr} + \frac{V_\lambda(r)}{r^2}\Big[\lambda(\lambda+1) - (\gamma_f - \gamma_i)(\gamma_f - \gamma_i \pm 1)\Big] \tag{III.49}$$

where ± 1 holds if the wave function is/is not multiplied by r. For the optical model, $\lambda = 0$ and $\gamma_i = \gamma_f$ and the expression (III.49) reduces to the usual one. This expression as been shown to be equivalent to the zero-range limit of a two-body spin-orbit interaction in Ref.[23] and [28] using the helicity formalism as defined in : [62] RAYNAL, J., *"Multipole expansion of a two-body interaction in helicity formalism and its application to nuclear structure and nuclear reaction calculations"*, Nucl. Phys. **A97** (1967) 572.

To compare with some earlier works using :

$$\frac{1}{r}\Big[\frac{d}{dr}V_\lambda(r)\Big]\ \frac{\gamma_i + \gamma_f}{2} \tag{III.50}$$

and to be able to study the effects of each terms in the above expressions, six parameters z_1, z_2, z_3, z_4, z_5 and z_6 have been introduced to get :

$$\begin{aligned}&\frac{1}{r}\Big[\frac{d}{dr}V_\lambda(r)\Big](z_1 + z_3\gamma_i + z_4\gamma_f) + \frac{V_\lambda(r)}{r}z_6(\gamma_i - \gamma_f)\frac{d}{dr}\\ &+z_5\frac{V_\lambda(r)}{r^2}\Big[z_2\lambda(\lambda+1) - r(\gamma_f - \gamma_i)(\gamma_f - \gamma_i \pm 1)\Big]\end{aligned} \tag{III.51}$$

These parameters allow also to increase the spin-orbit transition without changing anything else.

The deformed spin-orbit in the "full Thomas form" introduces a first derivative of the wave function in the Schrödinger equation. The quick integration methods cannot deal with first derivatives (one has to use some Runge-Kutta method). However, the derivative terms are non diagonal because they have a factor $\gamma_i - \gamma_f$.**The deformed spin-orbit can be used only with the iteration method**.

B.2.b.ii Behaviour of the spin-orbit deformation

The behaviour of the deformed spin orbit interaction is a vector behaviour: the difference $\gamma_i - \gamma_f$ is also found to be the ratio of the geometries for a transfer of spin and a scalar interaction :

$$\left\{\begin{array}{ccc} l_f & l_i & L \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_f & j_i & J \end{array}\right\} = \frac{\gamma_f - \gamma_i}{\sqrt{3J(J+1)}}\left\{\begin{array}{ccc} l_f & l_i & L \\ \frac{1}{2} & \frac{1}{2} & 0 \\ j_f & j_i & J \end{array}\right\} \tag{III.52}$$

To compare deformed spin-orbit and other interactions, let us write consider a $0^+ \rightarrow 2^+$ reaction. There is one equation for the 0^+ state and 5 equations for the 2+ state. Let us consider their behaviour when the angular momenta increase. Among the five geometrical coefficients, there are :

1. those between $l_i = j_i \pm \frac{1}{2}$ and $l_f = j_f \pm \frac{1}{2}$:
   - for a central interaction, we shall take them as reference,
   - for a $\Delta S = 1$ interaction, Equ. (III.52) shows that there are of the same order,
   - for a spin-orbit interaction, the factor γ_i increases linearly with l and the other are constant.
2. those between $l_i = j_i \pm \frac{1}{2}$ and $l_f = j_f \mp \frac{1}{2}$ which :
   - are a factor l smaller than the first ones for a central term,

- for a $\Delta S = 1$ interaction, the Equ. (III.52) shows that there are multiplied by a factor l and become of the same order as the central interaction (1);
- for a spin-orbit interaction, the factors γ_i and $\gamma_i - \gamma_f$ increase linearly with l and the factor $6 - (\gamma_i - \gamma_f)(\gamma_i - \gamma_f + 1)$ increases quadratically.

This behaviour shows that spin-orbit interaction should become predominant at high energy.

B.2.b.iii Spin-orbit deformation for any spin

The "full Thomas form" of the spin-orbit interaction is conserved when the nucleon-nucleus potential is folded with the intrinsic wave function of the particle if this wave function involves only relative S-states. This is well known for the optical model of deuteron (see for example Ref. [22] Chapter IV). If the nucleon-nucleus spin-orbit form factor is $\frac{1}{r}\frac{d}{dr}f(r)$, the deuteron spin-orbit form factor is $\frac{1}{r}\frac{d}{dr}F(r)$ where $F(r)$ is obtained from $f(r)$ by folding, only if the deuteron D-wave is neglected.

This property of the folding for a structureless incident particle allows to extend the "full Thomas form" of the spin-orbit to any spin as done in Ref. [38]. For a spin $\vec{s}$, $2\vec{s}$ can be replaced by the sum of 2 $|s|$ Pauli matrices σ_i in Equ. (III.9) and Equ. (III.47) derived for each Pauli matrix. In this result, the term without Pauli matrices is multiplied by 2 $|s|$, the terms with one Pauli matrix are summed up to $2\vec{s}$ and the terms with two Pauli matrices need some recoupling. The total result is :

$$\frac{1}{r}\frac{dV_\lambda}{dr}\gamma_i + (\gamma_i - \gamma_f)\frac{V_\lambda}{dr}\frac{d}{dr} + \frac{V_\lambda}{2r^2}\Big\{|s|\big[\lambda(\lambda+1) - l_i(l_i+1) - l_f(l_f+1)\big] + \gamma_f + \frac{\gamma_i\gamma_f}{2|s|} + F\Big\} \qquad \text{(III.53)}$$

with :

$$F = -2|s| f_{l_i s j_i} f_{l_f s j_f} \begin{Bmatrix} l_i & j_i & s-1 \\ j_f & l_f & \lambda \end{Bmatrix} \begin{Bmatrix} l_i & j_i & s \\ j_f & l_f & \lambda \end{Bmatrix}^{-1} \qquad \text{(III.54)}$$

and :

$$\begin{aligned} f_{lsj} &= < l\ s\ j|(\vec{\sigma}.\vec{L})|l\ s-1\ j > \\ &= -\frac{\sqrt{[l(l+1) - (j-s)(j-s+1)][(j+s)(j+s+1) - l(l+1)]}}{2|s|} \end{aligned} \qquad \text{(III.55)}$$

The parametrisation introduced for spin one-half has been extended to :

$$\begin{aligned} &\frac{1}{r}\frac{dV_\lambda}{dr}(z_1 + z_3\gamma_i + z_4\gamma_f) + z_6(\gamma_i - \gamma_f)\frac{V_\lambda}{r}\frac{d}{dr} \\ &+z_5\frac{V_\lambda}{2r^2}\Big\{|s|\big[z_2\lambda(\lambda+1) - l_i(l_i+1) - l_f(l_f+1)\big] + \gamma_f + \frac{\gamma_i\gamma_f}{2|s|} + F\Big\} \end{aligned} \qquad \text{(III.56)}$$

B.2.c Dirac formalism

The large and the small component have a different angular dependence. This point is taken into account by writing instead of Equ. (III.36) :

$$|\Psi(\vec{r}) >= \frac{1}{r}\sum_{l,j,I,J} \begin{pmatrix} F_{l,j,I,J}(r) \\ -iG_{l,j,I,J}(r)(\vec{\sigma}.\hat{r}\,) \end{pmatrix} Y_{lsjIJM} \qquad \text{(III.57)}$$

where Y_{lsjIJM} is the same as for Schrödinger equation and is given by Equ. (III.37). Here, l stands instead of the parity quantum number.

The operator $-(\vec{\sigma}.\hat{r})$ interchanges the spin angular functions of the large and the small components.

Projecting the total equation on all the function Y_{lsjIJM}, we obtain the set of linear coupled equations :

$$\begin{aligned}
\hbar\Big[\frac{d}{dr} - \frac{K_i}{r} - \frac{1}{2m}\frac{dV_T^0(r)}{dr}\Big]G_i(r) + \big[E_i - m - V_S^0 - V_V^0\big]F_i(r) &= S_i(r) \\
-\hbar\Big[\frac{d}{dr} + \frac{K_i}{r} + \frac{1}{2m}\frac{dV_T^0(r)}{dr}\Big]F_i(r) + \big[E_i + m + V_S^0 - V_V^0\big]G_i(r) &= T_i(r) \qquad \text{(III.58)}
\end{aligned}$$

where the suffix i stands for (l, s, j, I, J), V^0 indicates the monopole parts of the interactions and :

$$K_i = (-)^{l-j-\frac{1}{2}}(j + \frac{1}{2}) \qquad \text{(III.59)}$$

The second members are :

$$\begin{aligned}
S_i(r) &= \sum_{\lambda,j} G_{i,j}^{\lambda}\Big[\big\{V_S^{\lambda} + V_V^{\lambda}\big\}F_j(r) + \frac{\hbar}{2m}\big\{\big(\frac{d}{dr} + \frac{K_i - K_j}{r}\big)V_T^{\lambda}\big\}G_j(r)\Big] \\
T_i(r) &= \sum_{\lambda,j} G_{i,j}^{\lambda}\Big[\big\{V_S^{\lambda} - V_V^{\lambda}\big\}G_j(r) + \frac{\hbar}{2m}\big\{\big(\frac{d}{dr} + \frac{K_j - K_i}{r}\big)V_T^{\lambda}\big\}F_j(r)\Big] \qquad \text{(III.60)}
\end{aligned}$$

where V^{λ} are the multipoles of the interactions and the geometrical coefficients are the same as for the Schrödinger equation :

- between F_i and F_j, expressions are identical,
- between G_i and G_j, the operators $(\vec{\sigma}.\hat{r})$ commute with the expression and their product being unity, the result is the same as between F_i and F_j,
- between F_i and G_j, the operators $(\vec{\sigma}.\vec{\nabla})$ and $(\vec{\sigma}.\hat{r})$ are treated like the spin-orbit deformation in the Schrödinger equation.

There is no reason to limit the coupling to macroscopic ones ($\Delta S = 0$). For $\Delta S \neq 0$, the rules given above are no more valid and the coefficient of the central term in the second equation (III.60) is no more the same as the coefficient of the first one and must be computed separately.

The codes `ECIS88` and `ECIS94` offer two possibilities :

- **to solve exactly the Dirac equation** as described above with `LO(100)=.TRUE.`,
- **to write the equivalent Schrödinger equation and to solve it, neglecting the presence of $D(\vec{r})^{\frac{1}{2}}$ in the definition given by Equ. (III.11) of the function** if `LO(99)=.TRUE.`

The result is exactly the same for the elastic scattering.

B.3 Solutions and angular distributions

We assume that there is no long range interactions. They shall be explained in Chapter (IV).

B.3.a Solution of the equation

Beyond a matching point for which all the potentials except the Coulomb one vanish, the solution $f_i(r)$ of the Schrödinger equation is a superposition of the regular Coulomb function $F_{l_i}(\eta_i; k_i r)$ and the irregular Coulomb function $G_{l_i}(\eta_i; k_i r)$. For the equivalent Schrödinger equation of the Dirac equation, there are long range terms r^{-2} and r^{-3} which implies the use of *relativistic Coulomb functions* instead of the usual, non-relativistic ones.

Coulomb corrections described in Ref. [7] allow the use of the non-relativistic Coulomb functions in the Dirac phenomenology for nucleon scattering. They were derived for heavy-ion

scattering to reduce the matching radius to the point where nuclear interactions vanish and to correct the non relativistic Coulomb functions at this point for the effect of the long range Coulomb interaction which decrease only as r^{-l-1}. We consider here that the Coulomb functions are corrected for these long range effects.

The solution must vanish at the origin, due to the factor $1/r$ in the definition of the radial functions. They must have a plane wave incoming part for the initial channel i and an outgoing wave for all the channels, normalised to the same flux (that is divided by $\sqrt{k}$). Their asymptotic form is :

$$\begin{aligned} f_f(r)_{r\to\infty} &\Rightarrow \delta_{i,f}F_{l_f}(\eta_f;k_f r) + C_f^i\Big(\frac{k_i m_f}{k_f m_i}\Big)^{\frac{1}{2}}\big[G_{l_f}(\eta_f;k_f r) + iF_{l_f}(\eta_f;k_f r)\big] \\ &\Rightarrow \delta_{i,f}F_{l_f}(\eta_f;k_f r) + \overline{C}_f^i\big[G_{l_f}(\eta_f;k_f r) + iF_{l_f}(\eta_f;k_f r)\big] \end{aligned} \tag{III.61}$$

and numerical integration gives the coefficients $\overline{C}_f^i$ by linear combination of the n solutions which vanish at the origin. The $\overline{C}_f^i$ are multiplied by $\sqrt{k_f m_i/(k_i m_f)}$ to get the C_f^i with are symmetric for the exchange of i and f as will be shown by Equ. (III.86). The same relation holds in Dirac formalism for the solution of the equivalent Schrödinger equation. An equivalent definition of the C_f^i will be given by Equ. (III.104) and (III.105).

By identification we obtain :

$$\begin{aligned} f_{\mu_f\sigma_f\mu_i\sigma_i}(\theta) = \frac{4\pi}{k_i}\sum \exp(i\sigma_{l_i}+i\sigma_{l_f})C_f^i &< l_i,s,\nu_i,\sigma_i|j_i,m_i >< j_i,I_i,m_i,\mu_i|J,M > \\ \times &< l_f,s,\nu_f,\sigma_f|j_f,m_f >< j_f,I_f,m_f,\mu_f|J,M > Y_{l_i}^{\nu_i\star}(\hat{k}_i)Y_{l_f}^{\nu_f}(\hat{k}_f) \end{aligned} \tag{III.62}$$

where σ and μ are the projections of the spins of the particle and the target, σ_{l_i} and σ_{l_f} are the Coulomb phase-shifts.

B.3.b Helicity formalism and cross-section

These amplitude are simplified by the helicity formalism (defined in Ref. [20]; see also Ref. [21] and [22]) in which the spin of the particle is projected on its momentum and the spin of the target is projected on the inverse direction.

The axis of quantisation is along $\vec{k}_i$ for the initial state and along $\vec{k}_f$ for the final state and the helicity of the target is opposite of the projection of its spin.

The helicity amplitude involve only a reduced rotation matrix element $r^{(J)}_{m,m'}(\theta)$:

$$f^{hel.}_{\mu_f\sigma_f\mu_i\sigma_i}(\theta) = f^{(Coul)\ \ hel.}_{\mu_f\sigma_f\mu_i\sigma_i}(\theta)\delta_{if} + \sum_J f^{(J)\ \ hel.}_{\mu_f\sigma_f\mu_i\sigma_i} r^{(J)}_{\sigma_f-\mu_f,\sigma_i-\mu_i}(\theta) \tag{III.63}$$

with :

$$\begin{aligned} f^{(J)\ \ hel.}_{\mu_f\sigma_f\mu_i\sigma_i}(\theta) = \frac{1}{k_i}\sum \exp(i\sigma_{l_i}+i\sigma_{l_f})C_f^i\sqrt{(2l_i+1)(2l_f+1)} &< l_i,s_i,0,\sigma_i|j_i,\sigma_i > \\ \times &< j_i,I_i,\sigma_i,-\mu_i|J,M_i >< l_f,s_f,0,\sigma_f|j_f,\sigma_f >< j_f,I_f,\sigma_f,-\mu_f|J,M_f > \end{aligned} \tag{III.64}$$

The coulomb helicity amplitude, which appears only in the incident channel, is the usual coulomb amplitude multiplied by the reduced rotation matrix elements for the spin s_i of the particle and the spin I_i of the target :

$$f^{(Coul)\ \ hel.}_{\mu_f\sigma_f\mu_i\sigma_i}(\theta) = -\frac{\eta}{2k\sin^2\frac{\theta}{2}}\exp\big(-2i\eta\ln\sin\frac{\theta}{2} + 2i\sigma_0\big) r^{(s_i)}_{\sigma_f,\sigma_i}(\theta) r^{(I_i)}_{-\mu_f,-\mu_i}(\theta) \tag{III.65}$$

Note that in the codes `ECIS`, σ_0 is used only to compute Coulomb corrections and that the Coulomb phase-shift σ_l is replaced everywhere else by $\sigma_l - \sigma_0$, independently for each level.

The direct interaction differential cross-section is :

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{1}{(2s_i+1)(2I_i+1)} \sum_{\sigma_i\sigma_f\mu_i\mu_f} |f^{hel.}_{\mu_f\sigma_f\mu_i\sigma_i}(\theta)|^2\Phi \tag{III.66}$$

and the total differential cross-section is obtained by adding the **differential compound cross-section** which is computed from the coefficients C^i_f.

In the code ECIS, the compound differential cross-section is expressed as a sum of terms, each of them being a sum of squares of reduced rotation matrix elements; usually, these squares are expanded into sums of Legendre polynomials.

B.3.c Observables

The formalism used to express the observables as been described in Ref. [21]. All the observables P can be expresses as :

$$P(\theta) \quad \frac{d\sigma(\theta)}{d\Omega} = \sum_{\lambda_i\mu_i} x^{\lambda_3\mu_3\lambda_4\mu_4}_{\lambda_1\mu_1\lambda_2\mu_2} \qquad A^{\lambda_3\mu_3\lambda_4\mu_4}_{\lambda_1\mu_1\lambda_2\mu_2} \tag{III.67}$$

where :

$$A^{\lambda_3\mu_3\lambda_4\mu_4}_{\lambda_1\mu_1\lambda_2\mu_2} = \mathrm{Trace}\Big\{ f^{hel.}(\theta)\big[\tau^{s_i}_{\lambda_1\mu_1} \otimes \tau^{I_i}_{\lambda_2\mu_2}\big]\ f^{hel.}(\theta)^+\big[\tau^{s_f}_{\lambda_3\mu_3} \otimes \tau^{I_f}_{\lambda_4\mu_4}\big]\Big\} \tag{III.68}$$

and, in peculiar, A^{0000}_{0000} is the cross-section. Here, the τ are tensor operators in spin space defined for $0 \le \lambda \le 2s$ and $-\lambda \le \mu \le \lambda$ by :

$$< s\ q|\tau^s_{\lambda\mu}|s\ q' >= (-)^{s-q'}\sqrt{2s+1} < s, s, q-q', \lambda|\mu, ec69 \tag{III.69}$$

Due to the helicity formalism, the description of the polarisation of the outgoing particles is along the outgoing direction in the center of mass system. The description can be shortened, using the relations :

$$\begin{array}{cccc} \textbf{hermiticity} & \left(A^{\lambda_3\mu_3\lambda_4\mu_4}_{\lambda_1\mu_1\lambda_2\mu_2}\right)^\star & = & (-)^{\sum\mu} A^{\lambda_3-\mu_3\lambda_4-\mu_4}_{\lambda_1-\mu_1\lambda_2-\mu_2} \\ \textbf{parity} & A^{\lambda_3\mu_3\lambda_4\mu_4}_{\lambda_1\mu_1\lambda_2\mu_2} & = & (-)^{\sum\lambda+\mu} A^{\lambda_3-\mu_3\lambda_4-\mu_4}_{\lambda_1-\mu_1\lambda_2-\mu_2} \end{array} \tag{III.70}$$

As consequences :

1. if the sum on λ is even, A is real,
2. if the sum on λ is odd, A is pure imaginary,
3. for the same λ's and opposite μ's, the A differs by $(-)^{\sum\lambda+\sum\mu}$.

For example, the spin-flip SP is :

$$SP(\theta) \quad \frac{d\sigma(\theta)}{d\Omega} = \frac{1}{2}\big(A^{0000}_{0000} + A^{1100}_{1100} + A^{1100}_{1-100}\big) \tag{III.71}$$

Experiments are in the laboratory system; if some axis in the reaction plane is requested to describe the final polarisation, a small rotation of the spin is needed for the scattering matrix. These rotations will be explained in sectio (VIIA).

Some observables as Q are defined with only the incident direction :

$$Q(\theta) \quad \frac{d\sigma(\theta)}{d\Omega} = \sqrt{2}A^{1100}_{1000} \tag{III.72}$$

and need a rotation of angle θ on the scattering matrix.

There are many ways to define an observable for the codes `ECIS` (with an axis perpendicular to the scattering plane, using magnetic quantum numbers, usual tensors operators). The codes transform informations into A's, store information for necessity of rotation of the scattering matrix and compute do-loops to use Equ. (III.68).

C Integration methods

More details on these topics can be found in Ref. [1] for single equations, in Ref. [2] for coupled equations.

C.1 Single equation

The second order linear differential equation without first derivative :

$$f''(r) = V(r)\, f(r) \tag{III.73}$$

is easily solved, using the relation between the function and its second derivative at three equidistant points :

$$\xi(r+h) = f(r+h) - \frac{h^2}{12} f''(r+h) = 2f(r) + \frac{5h^2}{6} f''(r) - f(r-h) + \frac{h^2}{12} f''(r-h) \tag{III.74}$$

with the truncation error :

$$\Delta = -\frac{h^6 f^{(VI)}(r)}{240} \tag{III.75}$$

(it is called Cowell method in Ref. [1]). If there is no need of the function $f(r)$, the integration can be performed using :

$$\xi(r+h) = 2\xi(r) - \xi(r-h) + u(r), \qquad u(r) = \frac{h^2 V(r)}{1 - \frac{h^2}{12} V(r)} \xi(r) \tag{III.76}$$

which is the Numerov's method and has the same truncation error.

For coupled equations, $V(r)$ is a matrix and the computation of $u(r)$ involves the resolution of a linear system of equations. It is easier to use the **Modified Numerov method** by expanding the fraction up to the terms in h^4 :

$$u(r) = \left\{ h^2 V(r) + \frac{h^4}{12} V^2(r) \right\} \xi(r) \tag{III.77}$$

with a truncation error :

$$\Delta = \frac{h^6 V^3(r) f(r)}{144} - \frac{h^6 f^{(VI)}(r)}{240} \tag{III.78}$$

For a constant potential, this truncation error is $-\frac{2}{3}$ the previous one. Such an expansion in the Cowell method has been used in : [63] BEURTEY, R., GUILLOU and RAYNAL J., *"Etude de la diffusion élastique des particules chargées a l'aide du modèle optique"*, Le Journal de Physique et le Radium **21** (1960) page 402. If needed, the wave function can be obtained by one of the two expressions :

$$\begin{aligned} f(r) &= \xi(r) + \frac{1}{12} u(r) \\ f(r) &= \frac{1}{12} [\xi(r-h) + 10\xi(r) + \xi(r+h)] \end{aligned} \tag{III.79}$$

with an error of the same order.

Note that (see Ref. [1]) :

- the Schrödinger equation is easily solved numerically by these methods, starting from 0 at the origin and a small value ϵ at the point h,
- to have a precise result, the starting values have to be modified for the angular momentum $l = 1$,
- for high angular momenta, the first few points do not matter for the result,
- as the solution increases quickly, it has to be divided by a large number as soon as it becomes too large,

- for coupled equations (see Ref. [2]), the starting values are ϵ for only one component, but a Schmidt's orthogonalisation procedure can be needed from time to time to avoid that solutions align between them,
- the Schrödinger equivalent of the Dirac equation for the angular momentum $l = 0$ with Coulomb potential down to the origin can need a power expansion as starting values, but it is not used in `ECIS`.

Matching with the asymptotic expressions can be done by writing the matching conditions at the points $R \pm h$, using :

$$\mathcal{F}_\updownarrow(\eta;\nabla\pm\langle) = \mathcal{F}_\updownarrow(\eta;\nabla\pm\langle) - \frac{\langle^\in}{\infty\in}\mathcal{F}''_\updownarrow(\eta;\nabla\pm\langle), \qquad \mathcal{G}_\updownarrow(\eta;\nabla\pm\langle) = \mathcal{G}_\updownarrow(\eta;\|\nabla\pm\langle) - \frac{\langle^\in}{\infty\in}\mathcal{G}''_\updownarrow(\eta;\nabla\pm\langle) \quad \text{(III.80)}$$

where the values of $\mathcal{F}_\updownarrow(\eta;\|\nabla\pm\langle)$ are obtained by writing three Numerov integration between $r-h$ and $r+h$ with steps $h/2$ and :

$$7[f(r+h)-f(r-h)]+16[f(r+h/2)-f(r-h/2)]-3h^2[f''(r+h/2)-f''(r-h/2)] = 30hf'(r) \quad \text{(III.81)}$$

and eliminating the functions at $R \pm h/2$ between these four equations.

The linear system of matching conditions :

$$\begin{aligned}
\xi_i^k(R+h) &= \sum_j \alpha_j^k \Big\{ \mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}+\langle)\delta_{\rangle|} + \overline{\mathcal{C}}^{|}_\rangle \left[\mathcal{G}_\rangle(\eta_\rangle;\mathcal{R}+\langle) + \rangle\mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}+\langle)\right] \Big\} \\
\xi_i^k(R-h) &= \sum_j \alpha_j^k \Big\{ \mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}-\langle)\delta_{\rangle|} + \overline{\mathcal{C}}^{|}_\rangle \left[\mathcal{G}_\rangle(\eta_\rangle;\mathcal{R}-\langle) + \rangle\mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}-\langle)\right] \Big\}
\end{aligned} \quad \text{(III.82)}$$

is simplified by writing "pseudo-Wronskians" of the numerical solutions with the regular and the irregular Coulomb functions, that is, expressions giving Wronskians when h tends to 0. Writing the matrices :

$$\begin{aligned}
A_i^k &= \frac{\xi_i^k(R+h)\mathcal{G}_\rangle(\eta_\rangle;\mathcal{R}-\langle) - \xi_\rangle^{\|}(\mathcal{R}-\langle)\mathcal{G}_\rangle(\eta_\rangle;\mathcal{R}+\langle)}{\mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}+\langle)\mathcal{G}_\rangle(\eta_\rangle;\mathcal{R}-\langle) - \mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}-\langle)\mathcal{G}_\rangle(\eta_\rangle;\mathcal{R}+\langle)} \\
B_i^k &= \frac{\xi_i^k(R+h)\mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}-\langle) - \xi_\rangle^{\|}(\mathcal{R}-\langle)\mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}+\langle)}{\mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}+\langle)\mathcal{G}_\rangle(\eta_\rangle;\mathcal{R}-\langle) - \mathcal{F}_\rangle(\eta_\rangle;\mathcal{R}-\langle)\mathcal{G}_\rangle(\eta_\rangle;\mathcal{R}+\langle)}
\end{aligned} \quad \text{(III.83)}$$

the matching conditions become :

$$A_i^k = \sum_j \alpha_j^k\{\delta_{ij} + i\overline{C}_i^j\}, \qquad B_i^k = -\sum_j \alpha_j^k \overline{C}_i^j, \quad \text{(III.84)}$$

and the solution is given by the linear system :

$$B_i^k = -\sum_j \left(A_j^k + iB_j^k\right)\overline{C}_i^j. \quad \text{(III.85)}$$

It should be noted that the solution of these equation for only one set of second members B_i^k for fixed i gives the C_i^j for fixed i whereas the C_i^j are needed for fixed j. Wronskian relations give :

$$\frac{k_i}{m_i}\overline{C}_j^i = \frac{k_j}{m_j}\overline{C}_i^j \quad \text{(III.86)}$$

which can be used to obtain result from only one system of linear equations. This relation prove the symmetry of the matrix C defined in Equ. (III.61) for $m_i = m_j$.

The error on the collision matrix is of the order of h^4. They are equivalent to an error to the potential by a term :

$$\Delta V = \frac{h^4}{240}\frac{d^6}{dr^6}, \qquad \Delta V = \frac{h^4}{240}\frac{d^6}{dr^6} - \frac{h^4}{144}V^3(r), \quad \text{(III.87)}$$

for the Numerov method and for the Modified Numerov method respectively. **They have a coherent contribution.** The step size in kr can be as large as $\frac{\pi}{2}$ but smaller than the diffusenesses. A good value is $h = 0.5$.

C.2 Green function for Schrödinger equation

The differential equation written :

$$\Big\{ -\frac{\hbar^2}{2m_i}\Big[\frac{d^2}{dr^2} - \frac{2\eta_i k_i}{r} - \frac{l_i(l_i+1)}{r^2} + k_i^2\Big] - V_i^{opt}(r) + V_{ii}(r)\Big\} f_i(r) = -\sum_j V_{ij}(r) f_j(r) \tag{III.88}$$

and the boundary conditions for the solution :

$$f_i(r)_{r\to\infty} = \delta_{i,0} F_{l_i}(\eta_i; k_i r) + \overline{C}_i^0 \big[G_{l_i}(\eta_i; k_i r) + iF_{l_i}(\eta_i; k_i r)\big] \tag{III.89}$$

where $\delta_{i,0}$ means only in the incident channel, can be replaced by an integral equation built with two kinds of solution of the single equations of the right member:

1) the **regular** or **optical** solution completely defined as vanishing at the origin and by its asymptotic value :

$$f_i^{reg}(r)_{r\to\infty} = F_{l_i}(\eta_i; k_i r) + C_i^{opt}\big[G_{l_i}(\eta_i; k_i r) + iF_{l_i}(\eta_i; k_i r)\big] \tag{III.90}$$

obtained by numerical integration from the origin.

2) the **irregular** solution completely defined by its asymptotic value :

$$f_i^{irr}(r)_{r\to\infty} = G_{l_i}(\eta_i; k_i r) + iF_{l_i}(\eta_i; k_i r) \tag{III.91}$$

obtained by numerical backward integration from the matching point.

These solutions are such that the Wronskian is :

$$f_i^{irr}(r)\, f_i'^{reg}(r) - f_i'^{irr}(r)\, f_i^{reg}(r) = k_i \tag{III.92}$$

In practice, the irregular solution will be divided by k_i so that the Wronskian is unity. With these functions, the solution is :

$$\begin{aligned} f_i(r) = f_i^{reg}(r)\delta_{i,0} - \frac{2m_i}{\hbar^2 k_i}\Big\{ & f_i^{irr}(r)\int_0^r f_i^{reg}(r')\sum_j V_{ij}(r') f_j(r') dr' \\ & + f_i^{reg}(r)\int_r^\infty f_i^{irr}(r')\sum_j V_{ij}(r') f_j(r') dr'\Big\} \end{aligned} \tag{III.93}$$

and the coefficient of the outgoing wave is :

$$\overline{C}_i^0 = C_i^{opt}\delta_{i,0} - \frac{2m_i}{\hbar^2 k_i}\int_0^\infty f_i^{reg}(r)\sum_j V_{ij}(r) f_j(r) dr \tag{III.94}$$

The `DWBA` approximation is to replace $f_j(r)$ by $f_j^{reg}(r)$ in Equ. (III.94).

The derivative terms generated by the deformed spin orbit are in the second member of Equ. (III.88). In fact, it is $g(r) = rf'(r)$ which is needed because the form factor stored for the derivative term of Equ. (III.49) is $V_\lambda(r)/r^2$. It is obtained by numerical derivation related to the formulae giving the derivative x of the function y :

- for the 3 first points :

$$\begin{aligned} x_1 &= [147y_1 - 360y_2 + 450y_3 - 400y_4 + 225y_5 - 72y_6 + 10y_7]/(60h) \\ x_2 &= [10y_1 + 77y_2 - 150y_3 + 100y_4 - 50y_5 + 15y_6 - 2y_7]/(60h) \\ x_3 &= [-2y_1 + 24y_2 + 35y_3 - 80y_4 + 30y_5 - 8y_6 + y_7]/(60h) \end{aligned} \tag{III.95}$$

- from the 4th point to $N-3$ if there are N points :

$$x_i = [45(y_{i-1} - y_{i+1}) - 9(y_{i-2} - y_{i+2}) + y_{i-3} - y_{i+3}]/(60h) \tag{III.96}$$

- for the 3 last points :

$$\begin{aligned} x_{N-2} &= [y_{N-6} - 8y_{N-5} + 30y_{N-4} - 80y_{N-3} + 35y_{N-2} + 24y_{N-1} - 2y_N]/(60h) \\ x_{N-1} &= [-2y_{N-6} + 15y_{N-5} - 50y_{N-4} + 100y_{N-3} - 150y_{N-2} + 77y_{N-1} + 10y_N]/(60h) \\ x_N &= [10y_{N-6} - 72y_{N-5} + 225y_{N-4} - 400y_{N3} + 450y_{N-2} - 360y_{N-1} + 147y_N]/(60h) \end{aligned} \tag{III.97}$$

In fact, in this application, the formulae for the first three points are shifted, taking into account that the function to derive is zero at the origin.

Integrals with the Green function are not straightforward, due to the discontinuity of the integrand. With :

$$\int_0^h f(x)dx = \frac{h}{2}[f(0) + f(h)] + \frac{h^2}{12}[f'(0) - f'(h)] + \frac{h^5}{720}f^{(IV)}(r) \tag{III.98}$$

For Schrödinger equation, the integrand vanishes at the origin and at ∞ and its derivative has the discontinuity given by Equ. (III.92). Using :

$$F(nh) = \sum_{i=1}^{n} W(ih)f^{reg}(ih), \qquad G(nh) = \sum_{i=n+1}^{\infty} W(ih)f^{irr}(ih) \tag{III.99}$$

where $W(ih)$ is the second member of Equ. III.85, the integral is :

$$f(nh) \propto f^{irr}(nh)F(nh) + f^{reg}(nh)G(nh) - \frac{h^2k}{12}W(nh) \tag{III.100}$$

with an error of the order h^4. In this equation k is the Wronskian given by Equ. (III.92) and reduces to unity in actual calculation with a redefinition of the irregular functions.

C.3 Green function for Dirac equation

The Dirac equation can be written as :

$$\begin{aligned} \hbar[\frac{d}{dr} - A_i(r)]G_i(r) + E_i(r)F_i(r) &= S_i(r) \\ -\hbar[\frac{d}{dr} + A_i(r)]F_i(r) + D_i(r)G_i(r) &= T_i(r) \end{aligned} \tag{III.101}$$

with :

$$A_i(r) = \frac{K_i}{r} + \frac{1}{2m}\frac{dV_T^0(r)}{dr}, \qquad D_i(r) = E_i + m + V_S^0 - V_V^0, \qquad E_i(r) = E_i - m - V_S^0 - V_V^0. \tag{III.102}$$

$S_i(r)$ and $T_i(r)$ are given by Equ. (III.60).

Two independent solutions of uncoupled equations are obtained by :

1. the two linear coupled equations are replaced by the equivalent Schrödinger equation,
2. its regular solution $f^{reg}(r)$ defined by Equ. (III.90) and its irregular solution $f^{irr}(r)$ defined by Equ. (III.91) are obtained,
3. they are multiplied by $D(r)^{\frac{1}{2}}$ to obtain $F^{reg}(r)$ and $F^{irr}(r)$ (there is no difficulty to obtain continuous square root of the complex function $D(r)$ as long as we assume that the real part is very large with respect to its imaginary part),
4. the small components $G^{reg}(r)$ and $G^{irr}(r)$ are obtained from the Dirac equation by numerical derivation using Equ. (III.95) to Equ. (III.97).

Due to the number of operations and their difficulties, all the reorientation terms are shifted in the second member of Equ. (III.58) (this is also done in the Schrödinger formalism if `LO(29)=.TRUE.`) and these functions are kept if there are needed for the system with an higher total J.

With the relation (III.92) for $f_i^{reg}(r)$ and $f_i^{irr}(r)$ and the Dirac equation, one obtains the Wronskian :

$$F_i^{irr}(r)\,G_i^{reg}(r) - G_i^{irr}(r)\,F_i^{reg}(r) = \hbar k_i \tag{III.103}$$

Here also, the irregular solution will be normalised such that the Wronskian is unity. With these functions, the system of equations (III.58) and its boundary conditions can be replaced by the integral equation :

$$\begin{aligned} F_i(r) &= F_i^{reg}(r)\delta_{i,0} - \frac{1}{\hbar^2 k_i}\Big\{F_i^{irr}(r)\int_0^r [F_i^{reg}(r')S_i(r') + G_i^{reg}(r')T_i(r')]dr' \\ &\quad + F_i^{reg}(r)\int_r^\infty [F_i^{irr}(r')S_i(r') + G_i^{irr}(r')T_i(r')]dr'\Big\} \\ G_i(r) &= G_i^{reg}(r)\delta_{i,0} - \frac{1}{\hbar^2 k_i}\Big\{G_i^{irr}(r)\int_0^r [F_i^{reg}(r')S_i(r') + G_i^{reg}(r')T_i(r')]dr' \\ &\quad + G_i^{reg}(r)\int_r^\infty [F_i^{irr}(r')S_i(r') + G_i^{irr}(r')T_i(r')]dr'\Big\} \end{aligned} \tag{III.104}$$

and the coefficient of the outgoing wave is the coefficient of the regular functions at ∞ :

$$\overline{C}_i^0 = C_i^{opt}\delta_{i,0} - \frac{1}{\hbar^2 k_i}\int_0^\infty [F_i^{reg}(r')S_i(r') + G_i^{reg}(r')T_i(r')]dr' \tag{III.105}$$

It is more difficult to obtain a precise value of this integral than in the Schrödinger formalism. The two terms of Equ. (III.98) introduce corrections and Equ. (III.100) does not hold.

To find the error coming from the first term of Equ. (III.98) let us add two elementary step sizes around $r = r'$:

$$\begin{aligned} \frac{h}{2}\Big[F_i^{irr}(r)\,G_i^{reg}(r)\,T_i(r) + F_i^{reg}(r)G_i^{irr}(r)\,T_i(r)\Big] &= h\Big[F_i^{irr}(r)\,G_i^{reg}(r) - \frac{\hbar k_i}{2}\Big]\,T_i(r) \\ \frac{h}{2}\Big[G_i^{irr}(r)\,F_i^{reg}(r)\,S_i(r) + G_i^{reg}(r)F_i^{irr}(r)\,S_i(r)\Big] &= h\Big[G_i^{irr}(r)\,F_i^{reg}(r) + \frac{\hbar k_i}{2}\Big]\,S_i(r) \end{aligned} \tag{III.106}$$

which is an error of order h if this correction is neglected.

With the second term of Equ. (III.98), we obtain a correction :

$$\begin{aligned} &-\frac{h^2 k_i}{12}\Big[D_i(r)S_i(r) + \hbar\big\{A_i(r)T_i(r) + \frac{d}{dr}T_i(r)\big\}\Big], \\ &-\frac{h^2 k_i}{12}\Big[E_i(r)T_i(r) + \hbar\big\{A_i(r)S_i(r) + \frac{d}{dr}S_i(r)\big\}\Big], \end{aligned} \tag{III.107}$$

for $F_i(r)$ and $G_i(r)$ respectively. All these correction give an error of the order h^4. However, the derivatives of $S_i(r)$ and $T_i(r)$ are neglected in the code `ECIS` for the three first and the three last points.

C.4 Calculations

The actual calculations are quite different of what was presented here. In the Schrödinger formalism, the system of coupled equations (III.88) is replaced by :

$$\Big[\frac{d^2}{dr^2} - \frac{2\eta_i k_i}{r} - \frac{l_i(l_i+1)}{r^2} + k_i^2 + \frac{2m_i}{\hbar^2}\big\{V_i^{opt}(r) - V_{ii}(r)\big\}\Big]g_i(r) = \sum_j \mathcal{V}_{ij}(r)g_j(r) \tag{III.108}$$

with :

$$f_i(r) = m_i^{\frac{1}{2}} g_i(r), \qquad \mathcal{V}_{ij}(r) = \frac{2(m_i m_j)^{\frac{1}{2}}}{\hbar^2}V_{ij}(r) \tag{III.109}$$

The result differs from the $\overline{C}$ matrix defined by Equ. (III.61) : its matrix elements have to be multiplied by $\sqrt{k_f/k_i}$ to obtain the C_i^f.

Calculations are also simplified by using f_i^{irr} such that the Wronskian given by Equ. (III.92) and (III.103) is unity.

D Equations couplées en iterations séquentielles

The usual method of numerical integration of coupled differential equations can be applied only in the Schrödinger formalism without spin-orbit deformation. It needs a lot of computing time and involves all the solutions whereas we need only one or a few of them.

In the `ECIS` method (**Sequential Iteration for Coupled Equations**), we suppose the equations ordered in decreasing order of coupling. The equations for the initial channel for which there is an incoming wave are in front.

The first one is labelled $f_0(r)$.

If there are more than one, the other solutions are obtained from a circular permutation of the equations.

With compound nucleus, all solutions are needed to compute the transmission coefficients and, if requested, to diagonalise the scattering matrix.

In its first presentation, there was the "differential" `ECIS` method which consist to solve single inhomogeneous second order differential equations and the "integral" `ECIS` method which has been generalised to Dirac formalism. They gave same results and they need same computational time and storage. The "differential" `ECIS` method have been suppressed because :

- there is no simple extension to the Dirac formalism,
- result is obtained as a difference of two numbers and can be quite wrong with high energy close channel.

D.1 0th order of iteration

We assume a multiplicative factor λ in front of the second members of the equations and do a power expansion with respect to λ and take the result for $\lambda = 1$.

For :

$$\Big\{ -\frac{\hbar^2}{2m_i}\Big[\frac{d^2}{dr^2} - \frac{2\eta_i k_i}{r} - \frac{l_i(l_i+1)}{r^2} + k_i^2\Big] - V_i^{opt}(r) + V_{ii}(r)\Big\} f_i(r) = \lambda\, W_i(r) \tag{III.110}$$

the solution is :

$$f_i(r) = f_i^{reg}(r)\delta_{i,0} + \lambda \int_0^\infty \mathcal{G}_\rangle(\nabla,\nabla')\mathcal{W}_\rangle(\nabla')\lceil\nabla' \tag{III.111}$$

with :

$$\mathcal{G}_\rangle(\nabla,\nabla') = \frac{\in\Updownarrow_\rangle}{\langle^{\in}\|_\rangle}\{_\rangle^{\nabla\rceil\}}(\nabla_<)\{_\rangle^{\rangle\nabla\nabla}(\nabla_>) \tag{III.112}$$

the **0th order of iteration** is obtained with $\lambda = 0$. Therefore, it is :

$$f_0^{(0)}(r) = f_0^{reg}(r) \qquad C_0^{(0)} = C_0^{opt} \qquad f_i^{(0)}(r) = 0 \qquad \overline{C}_i^{(0)} = 0 \tag{III.113}$$

D.2 1st order iteration:

For $i = 1$

$$\begin{aligned} f_1^{(1)}(r) &= -\int_0^\infty \mathcal{G}_\infty(\nabla,\nabla')\mathcal{V}_{\infty\prime}\{_\prime^{(\prime)}(\nabla')\lceil\nabla' \\ \overline{C}_1^{(1)} &= -\frac{2m_i}{\hbar^2 k_i}\int_0^\infty f_1^{reg}(r')V_{10}(r')f_0^{(0)}(r')dr' \end{aligned} \tag{III.114}$$

which gives the DWBA result.

For $i = 2$

$$\begin{aligned} f_2^{(1)}(r) &= -\int_0^\infty \mathcal{G}_\in(\nabla,\nabla')\Big[\mathcal{V}_{\in\prime}\{_\prime^{(\prime)}(\nabla') + \mathcal{V}_{\in\infty}\{_\infty^{(\infty)}(\nabla')\Big]\lceil\nabla' \\ \overline{C}_2^{(1)} &= -\frac{2m_i}{\hbar^2 k_i}\int_0^\infty f_2^{reg}(r')\Big[V_{20}(r')f_0^{(0)}(r') + V_{21}(r')f_1^{(1)}(r')\Big]dr' \end{aligned} \tag{III.115}$$

which takes into account the result already obtained for $f_1^{(1)}(r)$.

and the same up to the last equation.

After the last equation go back to $i = 0$:

$$\begin{aligned} f_0^{(1)}(r) &= f_0^{reg}(r) - \int_0^\infty \mathcal{G}_\prime(\nabla,\nabla')\Big[\mathcal{V}_{\prime\prime}(\nabla')\{_\prime^{(\prime)}(\nabla') + \sum_\rangle \mathcal{V}_{\prime\rangle}(\nabla')\{_\rangle^{(\infty)}(\nabla')\Big]\lceil\nabla' \\ C_0^{(1)} &= C_0^{opt} - \frac{2m_0}{\hbar^2 k_0}\int_0^\infty f_0^{reg}(r')\Big[V_{00}(r')f_0^{(0)}(r') + \sum_i V_{0i}(r')f_i^{(1)}(r')\Big]dr' \end{aligned} \tag{III.116}$$

The result is obtained if $C_0^{(1)}$ and all the $\overline{C}_i^{(1)}$ are less than a given ϵ.

D.3 nth order iteration

For $1 \le i \le N$

$$\begin{aligned} f_i^{(n)}(r) &= -\int_0^\infty \mathcal{G}_\rangle(\nabla,\nabla')\Big[\mathcal{V}_{\rangle\prime}\{_\prime^{(\backslash-\infty)}(\nabla') + \sum_{|=\infty}^{\rangle-\infty}\mathcal{V}_{\rangle|}(\nabla')\{_|^{(\backslash)}(\nabla') + \sum_{|=\rangle}^{\mathcal{N}}\mathcal{V}_{\rangle|}(\nabla')\{_|^{(\backslash-\infty)}(\nabla')\Big]\lceil\nabla' \\ \overline{C}_i^{(n)} &= -\frac{2m_i}{\hbar^2 k_i}\int_0^\infty f_i^{reg}(r')\Big[V_{i0}(r')f_0^{(n-1)}(r') + \sum_{j=1}^{i-1}V_{ij}(r')f_j^{(n)}(r') \\ &\quad + \sum_{j=i}^{N}V_{ij}(r')f_j^{(n-1)}(r')\Big]dr' \end{aligned} \tag{III.117}$$

and for i=0

$$\begin{aligned} f_0^{(n)}(r) &= f_0^{reg}(r) - \int_0^\infty \mathcal{G}_\prime(\nabla,\nabla')\Big[\mathcal{V}_{\prime\prime}(\nabla')\{_\prime^{(\backslash-\infty)}(\nabla') + \sum_{|=\infty}^{\mathcal{N}}\mathcal{V}_{\prime|}\{_|^{(\backslash)}(\nabla')\Big]\lceil\nabla' \\ C_0^{(n)} &= C_0^{opt} - \frac{2m_0}{\hbar^2 k_0}\int_0^\infty f_0^{reg}(r')\Big[V_{00}(r')f_0^{(n-1)}(r') + \sum_{j=1}^{N}V_{0j}f_j^{(n)}(r')\Big]dr' \end{aligned} \tag{III.118}$$

The result is obtained if $|C_0^{(n)} - C_0^{(n-1)}|$ and all the $|\overline{C}_i^{(n)} - \overline{C}_i^{(n-1)}|$ are less than a given ϵ.

D.4 Convergence and padé approximation

This method of iteration can give divergent results. The convergence can be accelerated and the possibility of divergence avoided by Padé approximants.

From the fourth iteration, if convergence is not obtained for the current equation but was obtained for all the previous equations in this iteration, the results $C_i^{(m)}$ for $1 \leq m \leq n$ are considered as :

$$C_i^{(m)} = \sum_{j=1}^{m} a_i^j \lambda^j \qquad \text{for} \qquad \lambda = 1 \tag{III.119}$$

even if each iteration do not correspond to a definite power of the λ introduced in the equation.

The polynomial of coefficients a_i^j is replaced by the ratio of two polynomials $P(\lambda)/Q(\lambda)$ with the same number of coefficients. This ratio is obtained as a continued fraction in such a way that a new $C_i^{(n)}$ adds only a new coefficient. If the continued fraction evaluated with all the coefficients and the continued fraction evaluated without the last coefficient differ by less than ϵ, their value is assumed to be the result.

The smallest or the few smallest zeroes of the denominator polynomial $Q(\lambda)$ are the same for all the equations. There are complex values. If the coupling of the equations is multiplied by one of these zeroes, the coefficient of the outgoing wave of all the equations blows up. For this value, the set of coupled equations has a solution which is purely outgoing in all the channel: in an exact power expansion with respect to the coupling (that is without the sequential procedure) it is a **Weinberg state**. If λ_j are the Weinberg eigenvalues and x_i^j the amplitudes of the outgoing waves with a proper normalisation :

$$C_i(\lambda) = \sum_j x_i^j \frac{1}{\lambda_j - \lambda} \qquad C_i^{(n)} = \sum_j \frac{x_i^j}{\lambda_j} \sum_{m=1}^{n} \frac{1}{{\lambda_j}^m} \tag{III.120}$$

If λ_j is small, each iteration gives the result of last one multiplied by $1/\lambda_j$. Iterations are stopped if these results become too large, or by a maximum number of iterations.

The minimum value of $|\lambda_j|$ is the convergence radius of the Taylor expansion. **In practice, Padé approximants give good results up to 6 times the radius of convergence** : that is for 20 iterations, results as large as 10^{15}. Indications on the actions of the code were given in section (I.A.2.b).

Chapter IV

Long range interactions

The description of this topic in Ref. [7] applies only to `ECIS79`. From the code `ECIS88`, this method allows to use non relativistic Coulomb functions as already stated in Ref. [7] which needs no generalisation for that. The Coulomb excitation in the Dirac formalism needed a drastic change of formulae. The use of such methods for the Coulomb spin-orbit interaction of chargeless particles needs a completely different calculation, even in Schrödinger formalism. Note that, in the Schrödinger formalism, the integral related to Coulomb spin-orbit interaction cannot be computed by this method when the sum of the two angular momenta is equal to the angular momentum transfer; the code neglect this correction.

A Long range contributions

For large values of r with deformed Coulomb interaction, the coupling between equations is :

$$\frac{2m}{\hbar^2} V_{if}(r) = \sum_{\lambda} \alpha_{if}^{\lambda} r^{-\lambda-1} \tag{IV.1}$$

where α_{if}^{λ} is the geometrical coefficient G_{if}^{λ} multiplied by some constant.

A.1 Iterations in the Schrödinger formalism

In Equ. (III.117) and (III.118) describing the nth iteration of `ECIS`, for sufficiently large values of r, we can assume that :

$$\begin{aligned} f_i^{reg}(r) &\rightarrow F_{l_i}(\eta_i;k_ir) + C_i^{opt}\big[G_{l_i}(\eta_i;k_ir) + iF_{l_i}(\eta_i;k_ir)\big] \\ f_i^{irr}(r) &\rightarrow G_{l_i}(\eta_i;k_ir) + iF_{l_i}(\eta_i;k_ir) \\ f_i^{(n)}(r) &\rightarrow F_{l_i}(\eta_i;k_ir)\delta_{i0} + C_i^{(n)}\big[G_{l_i}(\eta_i;k_ir) + iF_{l_i}(\eta_i;k_ir)\big] \end{aligned} \tag{IV.2}$$

The long range contribution can be expressed with the integrals :

$$M(H,K,\overline{k}R)_{l_il_f}^{-\lambda-1} = \int_{\overline{k}R}^{\infty} \frac{1}{\rho^{\lambda+1}} H_{l_i}(\eta_i;\epsilon\rho) K_{l_f}(\eta_f;\epsilon^{-1}\rho) d\rho \tag{IV.3}$$

with $\overline{k} = \sqrt{k_ik_f}$, $\epsilon = \sqrt{k_i/k_f}$ and H and K are the regular or the irregular Coulomb function or any combination of them. We shall also use :

$$V(H,K)_{i,j} = \sum_{\lambda} \alpha_{i,j}^{\lambda} \frac{\overline{k}^{\lambda}}{k_i} M(H,K,\overline{k}R)_{l_il_f}^{-\lambda-1} \tag{IV.4}$$

The equations (III.117) and (III.118) can be replaced by :

$$\begin{aligned} f_i^{(n)}(r) &= f_i^{reg}(r)\delta_{i0} + \frac{1}{k_i} f_i^{reg}(r)\Big\{ \int_r^R f_i^{irr}(r') \sum_j V_{ij}(r') f_j^{(m)}(r') dr' + A \Big\} \\ &\quad + \frac{1}{k_i} f_i^{irr}(r)\Big\{ \int_0^r f_i^{reg}(r') \sum_j V_{ij}(r') f_j^{(m)}(r') dr' \Big\} \\ C_i^{(n)} &= C^{(0)}\delta_{i0} + \frac{1}{k_i}\Big\{ \int_0^R f_i^{reg}(r') \sum_j V_{ij}(r') f_j^{(m)}(r') dr' + B \Big\} \end{aligned} \tag{IV.5}$$

where $m = n$ if $j < i$ and $m = n-1$ if $j \geq i$, the equation 0 being the last one. The corrections A are :

$$A = k_i \sum_j V(H^{(+)}, F)_{i,j}\delta_{j0} + C_j^{(m)} V(H^{(+)}, H^{(+)})_{i,j} \tag{IV.6}$$

and the corrections B are :

$$\begin{aligned} B &= k_i \sum_j \big[V(F,F)_{i,j} + C_i^{opt} V(H^{(+)}, F)_{i,j} \big]\delta_{j0} \\ &\quad + C_j^{(m)} \big[V(F, H^{(+)})_{i,j} + C_i^{opt} V(H^{(+)}, H^{(+)}) \big] \end{aligned} \tag{IV.7}$$

where $H_{l_i}^{(+)}(\eta_i; k_i r) = G_{l_i}(\eta_i; k_i r) + iF_{l_i}(\eta_i; k_i r)$ is the Coulomb outgoing function.

All the integrals involved are for natural parity, that is with $l_i + l_f + \lambda$ even.

A.2 Usual coupled equations

For n equations and with $\mathcal{F}$ and $\mathcal{G}$ replaced by corrected values, the system of Equ. (III.82) cannot be solved as a system of n linear equations similar to Equ. (III.83). The linear system of equation would be of dimension $2n$. However, one can obtain the results solving successively two systems of n linear equations.

The first step is to obtain a $\overline{C}$-matrix by matching with the "uncorrected" Coulomb functions. In this step the values of $\mathcal{F}_{\updownarrow\rangle}(\eta_\rangle; \mathcal{R} \pm \langle)$ and $\mathcal{G}_{\updownarrow\rangle}(\eta_\rangle; \mathcal{R} \pm \langle)$ are obtained taking into account the long range term (IV.1) in the three Numerov integration steps and in Equ. (III.81). The method to use is described by Equ. (III.83) to (III.85). This is equivalent to the matching with Coulomb function and its derivative at the point R.

In the second step, the Equ. (III.61) at ∞ is rewritten at the matching point R. The Coulomb functions at ∞ are replaced by the values which they get at the point R, taking into account the coupling given by Equ. (IV.1), that is for equation j :

$$\begin{aligned} F_{l_i}(\eta_i;\infty) &\Rightarrow F_{l_j}(\eta_j; k_j R)\Big\{\delta_{ij} - M(H^{(+)}, F)_{l_j,l_i} F_{l_j}(\eta_j; k_j R)\Big\} + V(F,F)_{l_j,l_i} H_{l_j}^{(+)}(\eta_j; k_j R) \\ H_{l_i}^{(+)}(\eta_i;\infty) &\Rightarrow H_{l_j}^{(+)}(\eta_j; k_j R)\Big\{\delta ij + M(F, H^{(+)})_{l_j,l_i} H_{l_j}^{(+)}(\eta_j; k_j R)\Big\} - V(H^{(+)}, H^{(+)})_{l_j,l_i} F_{l_j}(\eta_j; k_j R) \end{aligned} \tag{IV.8}$$

In the result, replacing :

$$F_{l_i}(\eta_i; k_i R) \Rightarrow -\sum_j \overline{C}_j^i \, H^{(+)}(\eta_j; k_j R) \tag{IV.9}$$

one obtains the system of linear equations :

$$\sum_l \Big(\delta_{j,l} + V(F, H^{(+)})_{jl} + \sum_k \overline{C}_k^j V(H^{(+)}, H^{(+)})_{kl} \Big) C_i^l = -V(F,F)_{ji} + \sum_k \overline{C}_k^j \Big(\delta_{ki} - V(H^{(+)}, F)_{ki} \Big) \tag{IV.10}$$

which is also of dimension n.

The integrals involved are the same as with iterations.

A.3 Coulomb spin-orbit interaction

For this interaction, instead of Equ. (IV.1), the coupling between two equations is :

$$\begin{aligned}\frac{2m}{\hbar^2}V_{if}(r) &= \sum_\lambda \alpha_{if}^\lambda\big[x_1 r^{-\lambda-3}+x_2\frac{1}{r}\frac{d}{dr}(r^{-\lambda-1})+x_3 r^{-\lambda-2}\frac{d}{dr}\big]\\ &= \sum_\lambda \alpha_{if}^\lambda\big[\{x_1-(\lambda+1)x_2\}r^{-\lambda-3}+x_3 r^{-\lambda-2}\frac{d}{dr}\big]\end{aligned} \qquad \text{(IV.11)}$$

where x_1, x_2 and x_3 are the three coefficients which appear in Equ. (III.49) and (III.53) in front of the three form factors. The coefficient x_3 implies a derivation of the wave function which is a pure Coulomb function. One can use one of the two formulae :

$$\big(1+\frac{\eta^2}{l^2}\big)^{\frac{1}{2}}F_{l-1}(\eta;\rho)=\Big(\frac{d}{d\rho}+\frac{l}{\rho}+\frac{\eta}{l}\Big)F_l(\eta;\rho),\qquad \big(1+\frac{\eta^2}{l^2}\big)^{\frac{1}{2}}F_l(\eta;\rho)=\Big(-\frac{d}{d\rho}+\frac{l}{\rho}+\frac{\eta}{l}\Big)F_{l-1}(\eta;\rho), \quad \text{(IV.12)}$$

to express the derivative with the Coulomb function itself and another Coulomb function with the angular momentum increased by one unit (it could be decreased). The result involves three terms :

1. with the same angular momentum and a factor r^{-1} which can be summed with the contributions of x_1 and x_2,
2. with the same angular momentum and without power of r,
3. with angular momentum increased by one unit.

So, three integrals are needed for spin-orbit interaction, one with $r^{-\lambda-3}$ and two with $r^{\lambda-2}$.

The integrals involved are of natural parity and also of non natural parity, with $l_i+l_f+\lambda$ odd.

A.4 Dirac formalism

In this formalism, the multipoles of the scalar and the vector potentials act only between larges components or small components whereas the multipoles of a tensor potential acts between large and small components.

For the Coulomb potential, which is a vector potential, the geometrical coefficient for large components is the same as the geometrical coefficient between small components. However, there are quite different for a magnetic multipole excitation (in particular, one or the other can vanish). The coefficients between large and small components of equations i and j are multiplied by the normalisation factors :

$$N_F=\frac{1}{2}\Big[(1+\frac{E_i}{m})(1+\frac{E_j}{m})\Big]^{\frac{1}{2}},\qquad N_G=\frac{1}{2}\Big[(1-\frac{E_i}{m})(1-\frac{E_j}{m})\Big]^{\frac{1}{2}}, \qquad \text{(IV.13)}$$

respectively. The two integrals are computed independently because they involve different quantum numbers.

The tensor potential involve no derivative of the wave function. The two integrals are computed independently, with normalisations similar to those of Equ. (IV.13).

All the integral involved are of natural parity except for relativistic corrections of uncoupled equations.

In the Dirac formalism and in the iteration method for the Schrödinger formalism, the integrals M of Equ. (IV.3) must be corrected for finite step errors. For a step h, taking into account the numerical integration described by Equ. (III.99) and (III.100), the result is too large : in a next step between R and $R+h$, described by Equ. (III.98), the contribution at R has been already taken into account. The value needed is :

$$\begin{aligned}\overline{M}(H,K,\overline{k}R)^{-\lambda-1}_{l_i l_f} &= \int_{\overline{k}R}^\infty \frac{1}{\rho^{\lambda+1}}H_{l_i}(\eta_i;\epsilon\rho)K_{l_f}(\eta_f;\epsilon^{-1}\rho)d\rho-\frac{h}{2}\frac{1}{R^{\lambda+1}}H_{l_i}(\eta_i;\epsilon R)K_{l_f}(\eta_f;\epsilon^{-1}R)\\ &\quad -\frac{h^2}{12}\frac{d}{dr}\Big\{\frac{1}{R^{\lambda+1}}H_{l_i}(\eta_i;\epsilon R)K_{l_f}(\eta_f;\epsilon^{-1}R)\Big\}\end{aligned} \qquad \text{(IV.14)}$$

On the contrary, with usual coupled equations, no finite step correction is needed.

A.5 Asymptotic J-region

Using the integrals defined by Equ. (IV.3), we divided the r-space into :

- $r < R$, the coupled channels region in which a numerical integration of the coupled equations is needed,
- $r > R$, a region in which only `DWBA` results are used.

When the total angular momentum J of the system increases, the result of the numerical integrals become smaller and smaller. For some critical value J_m, it does no more contribute, but the integrals of Equ. (IV.3) are still important because their mean contribution comes from $r >> R$; the computation must be continued up to some $J = J_M$. So, in the J-space, there are also two regions :

- $J \leq J_m$, the coupled channels region in which a numerical integration of the coupled equations is needed,
- $J_m < J < J_M$, an asymptotic region in which the optical solutions of the diagonal equations are pure regular Coulomb functions.

In the asymptotic region, the integrals can be extended to the origin, keeping the expression given in Equ. (IV.1) because the wave functions are very small in the interior region. The result is :

$$C_i^{(1)} = \sum_\lambda \alpha_{i0}^\lambda \, M(F,F,0)_{i,0}^{-\lambda-1} \tag{IV.15}$$

These integrals are real. This first order does not respect unitarity. However, the coupled channel problem can be formulated differently, in terms of the reactance matrix K, which is the coefficient of the irregular function (instead of the outgoing function) in the solution, with the normalised regular function in one channel only. The matrix C is obtained, solving a linear system of equation :

$$K_{if} = \sum_\lambda \alpha_{if}^\lambda \, M(F,F,0)_{i,f}^{-\lambda-1}, \qquad C = \frac{K}{1 - i\,K} \tag{IV.16}$$

The value of J_M can be very large. Valuable results can be obtained with a smaller value of J_M, using factorisation of $(1 - \cos\theta)$ in the amplitudes. Details will be given in section (VII.C.3).

B Recurrence relations

In the Schrödinger formalism, the product of the wave number k_i and the Coulomb parameter η_i of a channel i is a constant $C_i = k_i\eta_i$ independent of the channel i. All the considerations of Ref. [7] are based on this properties; the same restrictions are present also in the previous studies of the integrals from 0 to infinity in : [64] BIEDENHARN, L. C., McHALE, J., L. and THALER, R., M., *"Quantum calculation of Coulomb excitation. I"*, Phys. Rev. **100** (1955) page 376 as well in : [65] ALDER, K., BOHR, A., HUUS, T., MOTTELSON, B. and WINTHER, A., *"Study of Nuclear Structure by Electromagnetic Excitation with Accelerated Ions"*, Rev. Mod. Phys. **28** (1956) page 432. In the Dirac formalism, the products $\eta_i k_i$ are proportional to the total energy and all the considerations of these references have to be extended. However, the approach is quite similar.

B.1 General recurrence

In the Dirac phenomenology, the product $\eta_i k_i$ is proportional to the total energy of the incident particle, which varies from level to level. Therefore, the formula (36) of Ref. [7], which was a generalisation to

integrals from R to ∞ with regular or irregular Coulomb functions of formula (2.B.64) of Ref. [65] (which was written for integrals from 0 to ∞ involving only regular Coulomb functions) has to be replaced by :

$$\begin{aligned}
&x_1\epsilon\,\frac{|l_f+1+i\eta_f|}{l_f+1}M(H,K,\overline{k}R)^{-\lambda-1}_{l_i,l_f+1}+x_2\epsilon^{-1}\frac{|l_i+i\eta_i|}{l_i}M(H,K,\overline{k}R)^{-\lambda-1}_{l_i-1,l_f}\\
&-x_3\epsilon^{-1}\frac{|l_i+1+i\eta_i|}{l_i+1}M(H,K,\overline{k}R)^{-\lambda-1}_{l_i+1,l_f}-x_4\epsilon\,\frac{|l_f+i\eta_f|}{l_f}M(H,K,\overline{k}R)^{-\lambda-1}_{l_i,l_f-1}\\
&-\Big(\epsilon\,\frac{x_1\eta_f}{l_f+1}+\epsilon^{-1}\frac{x_2\eta_i}{l_i}-\epsilon^{-1}\frac{x_3\eta_i}{l_i+1}-\epsilon\,\frac{x_4\eta_f}{l_f}\Big)M(H,K,\overline{k}R)^{-\lambda-1}_{l_i,l_f}\\
&-\big[x_1(l_f-1)+x_2l_i-x_3(l_i+1)-x_4(l_f+\lambda+1)\big]M(H,K,\overline{k}R)^{-\lambda-2}_{l_i,l_f}\\
&=(x_1+x_4)\frac{1}{(\overline{k}R)^{\lambda+1}}H_{l_i}(\eta_i,\epsilon\,\overline{k}R)\;K_{l_f}(\eta_f,\epsilon^{-1}\overline{k}R)\\
&+(x_1+x_2+x_3+x_4)\int_{\overline{k}R}^{\infty}\frac{1}{\rho^{\lambda+1}}\Big[\frac{d}{d\rho}H_{l_i}(\eta_i,\epsilon\,\rho)\Big]K_{l_f}(\eta_f,\epsilon^{-1}\rho)d\rho
\end{aligned}\tag{IV.17}$$

where ϵ has been given below Equ. (IV.3) and x_1, x_2, x_3 and x_4 are independent parameters. Independent recurrence relations can be obtained by using various values of the x's such that :

$$x_1+x_2+x_3+x_4=0\tag{IV.18}$$

This formula can be obtained from the Equ. (IV.12).

Other recurrence relations can be obtained by combining those obtained from Equ. (IV.13) with peculiar choices of the x's.

Of particular interest are the recurrence relations between integrals with the same values for λ and the difference $q=l_f-l_i$. There are :

- three terms relations for $\lambda=q=0$
- four terms relations for $\lambda=|q|=0$
- five terms relations for $\lambda\neq q$.

In the non relativistic case, for which $\eta_ik_i=\eta_fk_f$, with $\lambda=1$ and $l_f=l_i+1$, $x_1=x_2=0$, the coefficient of the fifth term $M(H,K,\overline{k}R)^{-\lambda-1}_{L_i,l_f}$ vanishes, allowing to express the dipole integral in terms of two monopole integrals. As the monopole integrals fulfill a three terms recurrence relation in all cases, the dipole integrals with $l_f=l_i+1$ fulfill also a three terms recurrence relation, but only in the non-relativistic case.

B.2 Stored recurrence

In practice, we are interested in integrals with $\lambda\leq 4$. The structure of recurrence relation is such that any of them can be expressed in terms of four other ones. The simplest approach is to express all of them through local recurrences in terms of integrals with some fixed value of λ and q. **Integrals with the chosen values for λ and q will be evaluated beforehand, also by recurrence, with the best precision possible.**

One cannot choose the monopole integrals $\lambda=q=0$, nor the integrals for which $\lambda=|q|$, because their recurrence involves less than five terms. Therefore, all the four integrals needed cannot be of one of these kinds.

For the stored integrals, we choose those with $q=0$ to obtain symmetric expressions for the local recurrences with respect to the exchange of l_i and l_f and $\lambda=1$ for simplicity of the expressions. Furthermore, the stored integrals used for diagonal terms are the corrections from non relativistic to relativistic Coulomb functions (for that, they can been obtained with equations much simpler than those needed in the general case and described below).

The five term recurrence relation for $\lambda = 1$, $q = 0$ is not easy to handle directly. It can be replaced by an inhomogeneous three terms recurrence relation involving the monopole integrals with $\lambda = 0$, $q = 0$ as inhomogeneous terms. This is similar to what was obtained for non relativistic corrections in Equ. (37a) and (37b) in Ref. [7], but the inhomogeneous terms $\lambda = 1$, $q = 1$ used in the non relativistic case have to be replaced by the monopole integrals because they do not have a three terms recurrence relation in the relativistic case.

The monopole integrals are given by :

$$\begin{aligned}
&\frac{2l+2}{2l+1}|l+i\eta_i||l+i\eta_f|M(H,K,\overline{k}R)^{-1}_{l-1,l-1} - \Big\{2\eta_i\eta_f + l(l+1)\big(\epsilon^2+\epsilon^{-2}\big)\Big\}M(H,K,\overline{k}R)^{-1}_{l,l}\\
&+\frac{2l}{2l+1}|l+1+i\eta_i||l+1+i\eta_f|M(H,K,\overline{k}R)^{-1}_{l+1,l+1}\\
&= -\frac{l+1}{\overline{k}R}\Big\{\frac{1}{k_i}|l+i\eta_f|H_l(\eta_i;k_iR)K_{l-1}(\eta_f;k_fR) + \frac{1}{k_f}|l+i\eta_i|H_{l-1}(\eta_i;k_iR)K_l(\eta_f;k_fR)\\
&-\frac{1}{(\overline{k}R)^2}\Big[l(2l+1)+\eta_ik_f+\eta_fk_i\Big]H_l(\eta_i;k_iR)K_l(\eta_f;k_fR)\Big\}
\end{aligned} \tag{IV.19}$$

The recurrence which replace formula (37a) of Ref. [7] is :

$$\begin{aligned}
&\frac{2l-1}{2l+1}|l+i\eta_i||l+i\eta_f|\big[(l+1)^2(k_i^2-k_f^2)+(k_i^2\eta_i^2-k_f^2\eta_f^2)\big]M(H,K,\overline{k}R)^{-2}_{l-1,l-1}\\
&-\Big[k_i^4\eta_i^4-k_f^4\eta_f^4+\frac{1}{k_ik_f}\big\{(k_i^4\eta_i^2-k_f^4\eta_f^2)(2l^2+2l+1)+(k_i^4-k_f^4)(l+1)^2l^2\big\}\Big]M(H,K,\overline{k}R)^{-2}_{l,l}\\
&+\frac{2l+3}{2l+1}|l+1+i\eta_i||l+1+i\eta_f|\big[l^2(k_i^2-k_f^2)+(k_i^2\eta_i^2-k_f^2\eta_f^2)\big]M(H,K,\overline{k}R)^{-2}_{l+1,l+1}\\
&= -\frac{1}{l}(k_i^2-k_f^2)(\eta_ik_f+\eta_fk_i)|l+i\eta_i||l+i\eta_f|M(H,K,\overline{k}R)^{-1}_{l-1,l-1} - \frac{1}{2l}(k_i^2-k_f^2)\\
&\Big[\{l^2+\eta_f^2\}\{l\eta_fk_f-(l+2)\eta_ik_i\}\frac{k_f}{k_i}+\{l^2+\eta_i^2\}\{l\eta_ik_i-(l+2)\eta_fk_f\}\frac{k_i}{k_f}\Big]M(H,K,\overline{k}R)^{-1}_{l,l}\\
&+\frac{1}{l^2\overline{k}R}(k_i^2\eta_i^2-k_f^2\eta_f^2)|l+i\eta_i||l+i\eta_f|H_{l-1}(\eta_i;k_iR)K_{l-1}(\eta_f;k_fR) - \frac{k_i^2(l^2+\eta_i^2)-k_f^2(l^2+\eta_f^2)}{2l^2(\overline{k}R)^3}\\
&\Big\{\eta_f|l+i\eta_f|[2l(l+1)^2+(l+2)\eta_ik_i-l\eta_fk_f]H_l(\eta_i;k_iR)K_{l-1}(\eta_f;k_fR)\\
&+\eta_i|l+i\eta_i|[2l(l+1)^2+(l+2)\eta_fk_f-l\eta_ik_i]H_{l-1}(\eta_i;k_iR)K_l(\eta_f;k_fR)\Big\}\\
&+\Big\{\frac{k_i^2(l^2+\eta_i^2)+k_f^2(l^2+\eta_f^2)}{2l^2(\overline{k}R)^3}[2l^2(l+1)^2(2l+1)+l(l+2)(2l+1)(\eta_ik_i+\eta_fk_f)\\
&+2(l+1)(\overline{k}R)^2\eta_i\eta_f] - \frac{1}{2l\overline{k}R}\big[(k_i^4\eta_i^4-k_f^4\eta_f^4)+l(l+2)(k_i^2\eta_i^2+k_f^2\eta_f^2)(k_i^2-k_f^2)\\
&-2\big(\frac{k_i^4\eta_i^2-k_f^4\eta_f^2}{k_ik_f}\big)l\big]\Big\}H_l(\eta_i;k_iR)K_l(\eta_f;k_fR)
\end{aligned} \tag{IV.20}$$

In practice, we introduced :

$$C_X = k_i^2\eta_i^2+k_f^2\eta_f^2 \qquad D_X = k_i^2\eta_i^2-k_f^2\eta_f^2 \qquad D_Y = \frac{k_i^4\eta_i^2-k_f^4\eta_f^2}{k_ik_f} \qquad D_T = k_i^2-k_f^2 \tag{IV.21}$$

The Equ. (IV.20) is homogeneous in D_T, D_X and D_Y, which can be multiplied by a common factor :

- if $DX = 0$, $DT = 1$ and $DY = \eta_i\eta_f$,
- if $DX \neq 0$ and if $DT \neq 0$, DX and DY are divided by DT and DT is replaced by 1.

With these notations, Equ. (IV.20) is :

$$\begin{aligned}
&\frac{2l-1}{2l+1}|l+i\eta_i||l+i\eta_f|\big[(l+1)^2D_T+D_X\big]M(H,K,\overline{k}R)^{-2}_{l-1,l-1}\\
&-\Big[D_X\ C_X+D_Y(2l^2+2l+1)+D_T(l+1)^2l^2(\epsilon^2+\epsilon^{-2})\Big]M(H,K,\overline{k}R)^{-2}_{l,l}\\
&+\frac{2l+3}{2l+1}|l+1+i\eta_i||l+1+i\eta_f|\big[l^2D_T+D_X\big]M(H,K,\overline{k}R)^{-2}_{l+1,l+1}\\
&=-\frac{1}{l}D_T(\eta_ik_f+\eta_fk_i)|l+i\eta_i||l+i\eta_f|M(H,K,\overline{k}R)^{-1}_{l-1,l-1}\\
&-\frac{1}{2l}D_T\Big[\{l^2+\eta_f^2\}\{l\eta_fk_f-(l+2)\eta_ik_i\}\epsilon^{-2}+\{l^2+\eta_i^2\}\{l\eta_ik_i-(l+2)\eta_fk_f\}\epsilon^2\Big]M(H,K,\overline{k}R)^{-1}_{l,l}\\
&+\frac{1}{l^2\overline{k}R}D_X|l+i\eta_i||l+i\eta_f|H_{l-1}(\eta_i;k_iR)K_{l-1}(\eta_f;k_fR)\\
&-\frac{1}{2l^2(\overline{k}R)^3}(l^2D_T+D_X)\Big\{\eta_f|l+i\eta_f|[2l(l+1)^2+(l+2)\eta_ik_i-l\eta_fk_f]H_l(\eta_i;k_iR)K_{l-1}(\eta_f;k_fR)\\
&+\eta_i|l+i\eta_i|[2l(l+1)^2+(l+2)\eta_fk_f-l\eta_ik_i]H_{l-1}(\eta_i;k_iR)K_l(\eta_f;k_fR)\Big\}\\
&+\frac{1}{2l^2(\overline{k}R)^3}\Big\{[l^2D_T+D_X][2l^2(l+1)^2(2l+1)+l(l+2)(2l+1)(\eta_ik_i+\eta_fk_f)+2(l+1)(\overline{k}R)^2\eta_i\eta_f]\\
&-l(\overline{k}R)^2[C_XD_X+l(l+2)C_XD_T-2lD_Y]\Big\}H_l(\eta_i;k_iR)K_l(\eta_f;k_fR) \qquad \text{(IV.22)}
\end{aligned}$$

The four integrals $M(H,K,\overline{k}R)^{-1}_{0,0}$, $M(H,K,\overline{k}R)^{-1}_{1,1}$, $M(H,K,\overline{k}R)^{-2}_{0,0}$ and $M(H,K,\overline{k}R)^{-2}_{1,1}$ are needed to start the recurrence. As in : [66] RAWITSCHER, G. H. and RASMUSSEN, C. H., *"Error analysis of code AROSA for quantal Coulomb excitation calculations"*, Comput. Phys. Commun. **11** (1976) page 183, they can be obtained by integration of the product of the asymptotic expansions from the matching point to ∞. For the asymptotic expansion, see for example in : [67] ABRAMOVITH, M. and STEGUN, I., A., *"Handbook of Mathematical Functions"* Dover, New-York, (1972) page 541. For $l=0$ and $\eta<30$, this asymptotic expansion can be used only (see Ref. [19]) for $kR>5\eta/3+7.5$; for larger values of η, a look on the asymptotic formula shows a quadratic behaviour of the lower radius; $kR>0.06\eta^2$ seems to be a safe limit. To use a smaller matching point than the larger value R_m of $k_iR_m=5\eta_i/3+7.5$, $k_fR_m=5\eta_f/3+7.5$ and $\overline{k}R_m=.06\eta_i\eta_f$, the integral between R and R_m is computed by 40 points Gauss integrations, each Gauss integration being for $\Delta\overline{k}R<20$. This allows results for any R whereas the method of Ref. [66] gives results for a R which increases with angular momentum.

This procedure is convenient for $M(G,G,\overline{k}R)^{-2}_{l,l}$, which increases quickly with l. For $M(G,F,\overline{k}R)^{-2}_{l,l}$ and $M(F,G,\overline{k}R)^{-2}_{l,l}$, which remain of the same order of magnitude when η_i and η_f are not very different. On the contrary, $M(F,F,\overline{k}R)^{-2}_{l,l}$, which decreases when l increases, is not given accurately. The downward recurrence, starting from zero values for the integrals and using the usual procedure of downward recurrence for the regular Coulomb function of the inhomogeneous terms, give a very accurate value of the integral from the origin to the matching point; then $M(F,F,\overline{k}R)^{-2}_{l,l}$ is obtained by taking the difference with $M(F,F,0)^{-2}_{l,l}$, which is needed anyway in the asymptotic region.

B.3 Local recurrence

Due to the complexity of the expressions in the general case, when $\eta_ik_j\neq\eta_jk_i$, the expression of the integrals had to be changed with respect to what was described in Ref. [7]. Any integral is expressed as :

$$\begin{aligned}
M(H,K,\overline{k}R)^{-\lambda-1}_{l_i,l_j} &= \alpha_1M(H,K,\overline{k}R)^{-2}_{n-1,n-1}+\alpha_2M(H,K,\overline{k}R)^{-2}_{n,n}\\
&+ \alpha_3M(H,K,\overline{k}R)^{-2}_{n+1,n+1}+\alpha_4M(H,K,\overline{k}R)^{-2}_{n+2,n+2}
\end{aligned}$$

$$+ \quad \beta_1 H_n(\eta_i; k_i R) K_n(\eta_f; k_f R) + \beta_2 H_n(\eta_i; k_i R) K_{n+1}(\eta_f; k_f R)$$

$$+ \quad \beta_3 H_{n+1}(\eta_i; k_i R) K_n(\eta_f; k_f R) + \beta_4 H_{n+1}(\eta_i; k_i R) K_{n+1}(\eta_f; k_f R) \quad \text{(IV.23)}$$

with :

$$n = \text{Integer part of } \frac{1}{2}(l_i + l_f - \lambda + 3) \quad \text{(IV.24)}$$

If l_i and l_j are decreased by the same amount down to the first values for which the integral from 0 to ∞ converges, the value of n is 1. The four coefficients α depend upon λ, $q = l_f - l_i$, n, the Coulomb parameters and the wave numbers; the coefficients β depend upon the same parameters and also upon the radius R.

Using $\overline{\eta} = \sqrt{\eta_i \eta_f}$, $\epsilon' = \sqrt{\eta_f / \eta_i}$ ($\epsilon = \epsilon'$ in the non relativistic case) Equ. (IV.23) can be written :

$$\int_R^\infty \frac{1}{r^\lambda} H_{l_i}(\epsilon'^{-1}\overline{\eta}; \epsilon r) K_{l_f}(\epsilon' \overline{\eta}; \epsilon^{-1} r) dr$$

$$= \sum_{i=1}^{4} \alpha_i \int_R^\infty \frac{1}{r^2} H_{n+i-2}(\epsilon'^{-1}\overline{\eta}; \epsilon r) K_{n+i-2}(\epsilon' \overline{\eta}; \epsilon^{-1}\epsilon^{-1} r) dr + \sum_{i=1}^{4} \beta_i(R) P_i(R) \quad \text{(IV.25)}$$

with :

$$\begin{aligned} P_1(R) &= H_n(\epsilon'^{-1}\overline{\eta}; \epsilon r) K_n(\epsilon^{-1}\overline{\eta}; \epsilon' r) \\ P_2(R) &= H_n(\epsilon'^{-1}\overline{\eta}; \epsilon r) K_{n+1}(\epsilon^{-1}\overline{\eta}; \epsilon' r) \\ P_3(R) &= H_{n+1}(\epsilon'^{-1}\overline{\eta}; \epsilon r) K_n(\epsilon^{-1}\overline{\eta}; \epsilon' r) \\ P_4(R) &= H_{n+1}(\epsilon'^{-1}\overline{\eta}; \epsilon r) K_{n+1}(\epsilon^{-1}\overline{\eta}; \epsilon' r) \end{aligned} \quad \text{(IV.26)}$$

Using the recurrence relation of the Coulomb functions :

$$(2l+1)\Big[\eta + \frac{l(l+1)}{\rho}\Big] F_l(\eta; \rho) = l|l+1+i\eta|\, F_{l+1}(\eta; \rho) + (l+1)|l+i\eta|\, F_{l-1}(\eta; \rho) \quad \text{(IV.27)}$$

to express all the H with H_n and H_{n+1} and all the K with K_n and K_{n+1} (the power of ρ^{-1} always increases), we obtain :

$$\int_R^\infty \sum_{i=1}^{4} C_i(r) P_i(r) dr = \sum_{i=1}^{4} \beta_i(R) P_i(R) \quad \text{(IV.28)}$$

where the $C_i(r)$ are known polynomials of r^{-1} and the $\beta_i(R)$ unknown polynomials in R^{-1}, that is :

$$C_i(r) = \sum_{n=2}^{N} C_i^{(n)} r^{-n}, \qquad \beta_i(R) = \sum_{n=1}^{N-1} \beta_i^{(n)} R^{-n} \quad \text{(IV.29)}$$

Differentiating with respect to R, we get :

$$\sum_{n=2}^{N} C_i^{(n)} R^{-n} = \sum_{n=1}^{N-1} \Big[P_i(n) \beta_i^{(n)} R^{-n-1} + \sum_{j=1}^{4} Q_{i,j} \beta_j^{(n)} R^{-n} \Big] \quad \text{(IV.30)}$$

with the diagonal matrix :

$$P(n) = \begin{vmatrix} n-2l-2 & 0 & 0 & 0 \\ 0 & n & 0 & 0 \\ 0 & 0 & n & 0 \\ 0 & 0 & 0 & n+2l+2 \end{vmatrix}, \quad \text{(IV.31)}$$

and with the diagonal matrix :

$$Q = \frac{1}{2l+1} \begin{vmatrix} -\eta_i\epsilon - \eta_f\epsilon^{-1} & -|l+1+i\eta_f|\epsilon^{-1} & -|l+1+i\eta_i|\epsilon & 0 \\ |l+1+\eta_f|\epsilon^{-1} & \eta_f\epsilon^{-1} - \eta_i\epsilon & 0 & -|l+1+i\eta_i|\epsilon \\ |l+1+i\eta_i|\epsilon & 0 & \eta_i\epsilon - \eta_f\epsilon^{-1} & -|l+1+\eta_f|\epsilon^{-1} \\ 0 & |l+1+i\eta_i|\epsilon & |l+1+\eta_f|\epsilon^{-1} & \eta_i\epsilon + \eta_f\epsilon^{-1} \end{vmatrix}, \qquad \text{(IV.32)}$$

If the highest power of r^{-1} in the $C_i(r)$ is m, Equ. (IV.30) allows to obtain first the coefficients of R^{-m+1} in the β_i and, then, those of all the lower degree. As :

C_1 includes $[(\ldots/r^2 + \ldots/r + \ldots)\alpha_1 + \alpha_2 + \ldots\alpha_4]/r^2$

C_2 includes $[(\ldots/r + \ldots)\alpha_1 + (\ldots/r + \ldots)\alpha_4]/r^2$

C_3 includes $[(\ldots/r + \ldots)\alpha_1 + (\ldots/r + \ldots)\alpha_4]/r^2$

C_4 includes $[\ldots\alpha_1 + \alpha_3 + (\ldots/r^2 + \ldots/r + \ldots)\alpha_4]/r^2$

the coefficients $\beta_i^{(n)}$ for $n > 3$ do not depends on the α's. The Equ. (IV.30) written for $n = 2$ and zero values for the $\beta_i^{(1)}$ is a linear system of equations giving the α's. The coefficients $\beta_i^{(2)}$, which are in this equation, involve a specific dependence of l_i, l_j and λ and a very simple dependence upon α_1 and α_4.

The dipoles integral are slightly different : in particular, when $\eta_i = \eta_j$ and $k_i = k_j$, a different formula has to be used to avoid a division by zero.

All the expressions are simpler in the non-relativistic case, when $X = \eta_i k_i - \eta_j k_j$ vanishes. They have been separated into a "non-relativistic" part, which is their value for $X = 0$, and a "relativistic" part, in which X can be factorised.

The linear system of equations expressing the α as functions of the $\beta_i^{(2)}$ can be inverted. The coefficients of the inverse system are quite complex when X do not vanish. The coefficients α_1 and α_4 depends only on $\beta_1^{(2)}$ and $\beta_4^{(2)}$ respectively, the coefficients α_2 and α_3 depends on all the $\beta^{(2)}$. A close expression of the coefficients α can be obtained only when some β vanish, that is for $l_j = l_i + 1$, $\lambda = 1$ and $l_i = l_j$, $\lambda = 2$. The subroutine `CORA` stores the values of the $\beta^{(2)}$ for the cases of interest and compute the coefficients α. It do not seem that this increase of intermediate computations decrease too much the precision of the results.

All these coefficients have been obtained up to $\lambda = 5$ for even parity integrals ($l_i + l_j + \lambda$ even) as well as odd parity integrals ($l_i + l_j + \lambda$ odd). For $\lambda = 6$, only the even parity integrals with $X = 0$ have been obtained except for $|l_i - l_j| = 6$. These last results allows the computation of $\lambda = 4$ for the Coulomb spin-orbit in the Schrödinger formalism. However, these results involve around 1100 cards and their use in `ECIS` is not absolutely needed. In `ECIS88` there are only the complete expressions for natural and unnatural parity up to $\lambda = 3$ and the expressions of natural parity integrals for $\lambda = 4$ with $X = 0$; this insure the use of Coulomb corrections up to $\lambda = 4$ for the central potential in any case, up to $\lambda = 2$ for the Coulomb spin-orbit in Schrödinger phenomenology and $\lambda = 3$ in Dirac phenomenology. In `ECIS94`, all the results obtained have been introduced, but the difference with `ECIS88` is on `COMMENT` cards which can easily been activated. In this domain, it is not possible to derive the expressions "by hand". They were obtained using symbolic calculations on computer with `AMP` ("Algebraic Manipulation Program") as described in : [68] DROUFFE, J.-M., *"AMP Language Reference Manual, Version 6"*, Note CEA-n-2297, (1982).

If $k_i = k_f$ and $\eta_i = \eta_f = \eta$, the matrix Q given by Equ. (IV.32) is singular of rank 2. If Equ. (IV.30) is used to compute some $\beta^{(1)}$, only two of them are independent because the coefficients of r^{-1} are :

$$\begin{aligned} &2\eta\beta_1^{(1)} + |l+1+i\eta|\left[\beta_2^{(1)} + \beta_3^{(1)}\right] = 0 \\ &\beta_1^{(1)} - \beta_4^{(1)} = 0 \\ &\beta_1^{(1)} - \beta_4^{(1)} = 0 \\ &2\eta\beta_4^{(1)} + |l+1+i\eta|\left[\beta_2^{(1)} + \beta_3^{(1)}\right] = 0 \end{aligned} \qquad \text{(IV.33)}$$

that is : $\beta_1^{(1)} = \beta_4^{(1)}$ and $\beta = \beta_2^{(1)} + \beta_3^{(1)}$ simple function of $\beta_1^{(1)}$. Consequently, Equ. (IV.23) holds with $\alpha_1 = \alpha_4 = 0$ and the first term of the polynomial expansion of the $\beta_i(r)$ is r^{-1}. In fact, the five terms recurrences reduce to three terms recurrence. This behaviour was used in `ECIS79` but has been dropped since `ECIS88`.

B.4 Integrals from 0 to ∞

The integrals from 0 to ∞ are quite similar to those published in Ref. [65]: in general, the variables of the generalised hypergeometric functions of two variables depend upon the wave numbers and their parameters depend upon the Coulomb parameters. The formula (IIB.62), of Ref. [65], valid if $|l_i - l_f|$ is not equal to λ, becomes when $k_i > k_f$:

$$
\begin{aligned}
&M(F,F,0)^{-\lambda-1}_{l_i,l_f} = \pi \frac{k_f}{k_i}^{l_f} (2k_i)^{\lambda-2} \frac{\exp \pi\frac{\xi}{2}}{\sinh \pi\xi} (iX)^{\lambda+l_i-l_f-1} \frac{|\Gamma(l_f+1+i\eta_f)|}{|\Gamma(l_i+1+i\eta_i)|} \frac{\Gamma(2l_i+1)}{\Gamma(2l_f+1)\Gamma(l_i-l_f+1)} \\
&\times F_2(l_f-l_i+\lambda-1, l_f+1+i\eta_f, -l_i-i\eta_i, 2l_f+2, -2l_i; \frac{k_i}{k_f}X, -X) \\
&-\pi \frac{k_i}{k_f}^{l_i} (2k_f)^{\lambda-2} \frac{\exp -\pi\frac{\xi}{2}}{\sinh \pi\xi} (i\frac{k_i}{k_f}X)^{\lambda+l_f-l_i-1} \frac{|\Gamma(l_i+1+i\eta_i)|}{|\Gamma(l_f+1+i\eta_f)|} \frac{\Gamma(2l_f+1)}{\Gamma(2l_i+1)\Gamma(l_f-l_i+1)} \\
&\times F_2(l_i-l_f+\lambda-1, l_i+1+i\eta_i, -l_f-i\eta_f, 2l_i+2, -2l_f; -X, \frac{k_i}{k_f}X) \\
&+\pi \frac{(k_i-k_f)^\lambda}{2k_ik_f} \frac{\exp -\pi\frac{\xi}{2}}{\sinh \pi\xi} \frac{|\Gamma(l_i+1+i\eta_i)|}{|\Gamma(l_f+1+i\eta_f)|} \\
&\times \Re\Big\{ \frac{\Gamma(l_f+1+i\eta_f)}{\Gamma(\lambda+1+i\xi)\Gamma(l_i+1+i\eta_i)} \, i^{l_f-l_i-\lambda-1} \, (-X)^{i\eta_i} \, (-\frac{k_i}{k_f}X)^{-i\eta_f} \\
&\times F_3(-l_i+i\eta_i, -l_f-i\eta_f, l_i+1+i\eta_i, l_f+1-i\eta_f, \lambda+1+i\xi; X, \frac{k_i}{k_f}X)\Big\}
\end{aligned}
\tag{IV.34}
$$

where :

$$
\xi = \eta_i - \eta_f \qquad\qquad X = \frac{k_i - k_f}{2k_f} \tag{IV.35}
$$

Similarly, the formula (IIB.58) of Ref. [65] valid for $l_f = l_i + \lambda$, becomes :

$$
\begin{aligned}
&M(F,F,0)^{-\lambda-2}_{l_i,l_i+\lambda} = \exp \pi\frac{\xi}{2} \frac{|\Gamma(l_i+1+i\eta_i)|}{|\Gamma(l_f+1+i\eta_f)|} \Big(\frac{k_i}{k_f}\Big)^{l_i} (2k_f)^{\lambda-2} \Big\{ \frac{|\Gamma(\lambda+i\xi)|^2}{\Gamma(2\lambda)} \\
&\times F_2(-2\lambda+1, l_i+1-i\eta_i, l_i+1+i\eta_i, -\lambda+1+i\xi, -\lambda+1-i\xi; X, X) \\
&+\Re\Big[2\, S\, X^{\lambda+i\xi} \frac{\Gamma(l_f+1-i\eta_f)\Gamma(-\lambda-i\xi)}{\Gamma(l_i+1+i\eta_i)} \\
&\times F_2(-\lambda+1+i\xi, l_f+1-i\eta_f, l_i+1-i\eta_i, \lambda+1+i\xi, -\lambda+1+i\xi; X, X)\Big]\Big\}
\end{aligned}
\tag{IV.36}
$$

where :

$$
\begin{aligned}
&S = -1, \qquad \text{if } (\eta_i - \eta_f)(k_f - k_i) < 0 \quad \text{and} \quad \lambda \quad \text{is odd;} \\
&S = 1, \qquad \text{otherwise}
\end{aligned}
\tag{IV.37}
$$

These formulae holds even if $k_i = k_f$, that is $X = 0$: in the first formula, Equ. (IV.34), only the highest degree terms of the two generalised hypergeometric functions of two variables $F2$ remain, all the others vanish; the generalised hypergeometric function $F3$ of the first formula and one of the two $F2$ of the Equ. (IV.25) reduce to unity; the second $F2$ of the Equ. (IV.36) disappears. If $\eta_i = \eta_f$, careful limits of the expressions have to be taken, with derivative of gamma function inserted in each term of the generalised hypergeometric series. The special case $\eta_i = \eta_f = 0$ will be discussed in next section.

The monopole integrals are given by a different formula, corresponding to formula (IIB.56) of Ref. [65] :

$$M(F,F,0)^{-1}_{l,l} = \Big[\frac{4k_ik_f}{k_i+k_f}\Big]^{l+1} \frac{1}{\sinh\pi\xi|\Gamma(l+1+i\eta_i)||\Gamma(l+1+i\eta_f)|}$$
$$\Re\Big\{\big(\frac{k_f-k_i}{k_i+k_f}\big)^{i\xi}\ \frac{\Gamma(l+1+i\eta_i)\Gamma(l+1-i\eta_f)}{\Gamma(1+i\xi)}\ {}_2F_1(l+1-i\eta_f, l+1+i\eta_i, 1+i\xi; \Big[\frac{k_f-k_i}{k_i+k_f}\Big]^2\Big\} \tag{IV.38}$$

This formula do not hold if $k_i = k_f$ and has to be modified if $\eta_i = \eta_f$ but not zero; for $\eta_i = \eta_f = 0$, see below. All these formulae and their limits have been used to check the Coulomb integrals.

Equ. (IV.38) and (IV.34) are used to obtain the integrals for $l = 0$, $l = 1$ and $\lambda = 0$, $\lambda = 1$. All the other are obtained with the recurrence equations Equ. (IV.19) and (IV.20) (without the products of Coulomb functions). In fact, as downward recurrence is used to obtain stored integrals, only the integrals for $l = 0$ are necessary. Any integral is obtain by Equ. (IV.23), without the β's.

If $\eta_i = \eta_f$ and $k_i = k_f$, the stored integrals are :

$$M(F,F,0)^{-2}_{l,l} = \frac{1}{4l+2}\Big\{\pi - \pi\frac{\cosh\pi\eta}{\sinh\pi\eta} - \frac{1}{\eta} + \sum_{n=0}^{l}\frac{2\eta}{n^2+\eta^2}\Big\} \tag{IV.39}$$

which is used instead of the recurrence relation.

B.5 Coulomb corrections for chargeless particles

If there is no charge, the recurrence relations do not relate natural parity and unnatural parity integral, that is those for which $l_i + l_j + \lambda$ is even with those for which $l_i + l_j + \lambda$ is odd. The Equ. (IV.17) becomes :

$$x_1\epsilon M(H,K,\overline{k}R)^{-\lambda-1}_{l_i,l_f+1} + x_2\epsilon^{-1}M(H,K,\overline{k}R)^{-\lambda-1}_{l_i-1,l_f} - x_3\epsilon^{-1}M(H,K,\overline{k}R)^{-\lambda-1}_{l_i+1,l_f}$$
$$-x_4\epsilon M(H,K,\overline{k}R)^{-\lambda-1}_{l_i,l_f-1} - \big[x_1(l_f-1) + x_2l_i - x_3(l_i+1) - x_4(l_f+\lambda+1)\big]M(H,K,\overline{k}R)^{-\lambda-2}_{l_i,l_f}$$
$$= (x_1+x_4)\frac{1}{(\overline{k}R)^{\lambda+1}}H_{l_i}(0,\epsilon\overline{k}R)\ K_{l_f}(0,\epsilon^{-1}\overline{k}R)$$
$$+(x_1+x_2+x_3+x_4)\int_{\overline{k}R}^{\infty}\frac{1}{\rho^{\lambda+1}}\big[\frac{d}{d\rho}H_{l_i}(0,\epsilon\rho)\big]K_{l_f}(0,\epsilon^{-1}\rho)d\rho \tag{IV.40}$$

The integrals needed are all of natural parity. Therefore, it is no more possible to compute them from stored integrals with $l_i = l_f$ and $\lambda = 1$. They have to be computed from stored integrals with $l_i = l_f$ and $\lambda = 2$. The recurrence relation is then :

$$2(l-1)M(H,K,\overline{k}R)^{-3}_{l-1,l-1} - (2l+1)(\epsilon^2+\epsilon^{-2})M(H,K,\overline{k}R)^{-3}_{l,l} + 2(l+2)M(H,K,\overline{k}R)^{-3}_{l+1,l+1}$$
$$= \frac{1}{(\overline{k}R)^2}\Big[H_{l-1}(k_iR)K_{l-1}(k_fR) - H_{l+1}(k_iR)K_{l-1}(k_fR)\Big] \tag{IV.41}$$

The integral from 0 to ∞, when $k_i > k_f$, is given by :

$$M(H,K,\overline{k}R)^{-\lambda-1}_{l_i,l_f} = \frac{\pi}{2^{\lambda+1}}\frac{k_f^{l_f}}{k_i^{l_f-\lambda+2}}\frac{\Gamma(\frac{1}{2}[l_i+l_f-\lambda+2])\Gamma(\lambda)}{\Gamma(\frac{1}{2}[l_i+l_f-\lambda+1])\Gamma(\frac{1}{2}[l_i-l_f+\lambda+1])\Gamma(\frac{1}{2}[l_i+l_f+\lambda+1])}$$
$$\times{}_2F_1\big[\frac{1}{2}(l_i+l_f-\lambda+2), \frac{1}{2}(l_i-l_f-\lambda+1); 1-\lambda; 1-\big(\frac{k_f}{k_i}\big)^2\big] \tag{IV.42}$$

This expression has to be used with $\lambda = 2$ and $l_i = l_f = 1$ to start the recurrence; a second value is not needed because the recurrence can be started by assuming the product of the angular momentum with the integral to be $\frac{1}{3}$ for $l_i = l_f = 0$. When $k_i = k_f$, the integrals are simply :

$$M(H,K,\overline{k}R) = \frac{1}{2l_i(l_i+1)}. \tag{IV.43}$$

.

To express any integral with the stored integrals, the coefficients described above in the general case are such that $\alpha_1 = \alpha_4 = 0$. The dipole integral cannot be expressed if $k_i = k_f$, but these integrals are used only for the Coulomb spin-orbit and it is the quadrupole integral which is needed for a dipole excitation. All the coefficients up to $\lambda = 6$ have been obtained, but only those up to $\lambda = 4$ are in `ECIS88` and all are on `COMMENT` cards in `ECIS94`.

C Coulomb excitations

The Coulomb potential as given by Equ. (III.21) is proportional to the product of charges of the particle and the target. In fact, it is the monopole folding of a charge distribution with the interaction $1/|r_1 - r_2|$. This charge distribution can be :

- a sphere with constant density,
- a plain Woods-Saxon distribution,
- a Woods-Saxon distribution multiplies by $1 + cr^2$,

of which the volume integral is the product of charges.

C.1 Coulomb deformation and heavy-ion option

This excitation is defined by the reduced electric transition probability $B(E\lambda)$ which is related to the Coulomb deformation β_c by :

$$B(E\lambda) = \Big(\frac{3}{4\pi} Ze\beta_c R_c'^{\lambda+1}\Big)^2 \tag{IV.44}$$

where Z is the charge of the excited nucleus (see for example in : [69] HODGSON, P., E., *"Nucleon Heavy-Ion Reactions"*, Clarendon Press Oxford (1978) page 268 or in : [70] SATCHLER, G., R., *"Direct Nuclear Reactions"*, *"International series of monographs on physics 68"*, Clarendon Press Oxford, Oxford University Press New-York (1983) page 629. This relation do not give the sign of the deformation. A transition distribution is obtained with the deformation length $\beta_c R_c'$ and the transition form factor is the result of multipolarity λ obtained in the folding with $1/|r_1 - r_2|$.

In the usual notations, $R_c' = R_c A^{1/3}$ where R_c is the "reduced Coulomb radius" and A is the mass of the target. In the "heavy-ion option", for a target of mass A and a particle of mass a, the radius R' is given in terms of the reduced radius R by :

$$R' = R\big(A^{1/3} + a^{1/3}\big) \tag{IV.45}$$

and, as it is the deformation length which matters, the deformations are replaced by :

$$\beta' = \frac{A^{1/3}}{A^{1/3} + a^{1/3}}\beta, \tag{IV.46}$$

except for the Coulomb deformations (central and spin-orbit) which are replaced by :

$$\beta_c' = \Big(\frac{A^{1/3}}{A^{1/3} + a^{1/3}}\Big)^{\lambda}\beta_c, \tag{IV.47}$$

for a multipole λ. However, if `LO(6)=.TRUE.`, which means that deformations lengths are read instead of deformations, only Coulomb deformations are changed with a power $\lambda - 1$ instead of λ in Equ. (IV.47).

The introduction of magnetic multipole Coulomb excitation followed a question of Mme I. LINK from Strasbourg and was subject of discussions with Dr M. MERMAZ at Saclay and J. KIENER at Orsay. For relations between electric and magnetic excitation, we follow Ref. [65].

C.2 Electric multipole excitation

An electric multipole transition $B(E\lambda)$ is defined as an angular momentum transfer $\Delta L = \lambda$, a spin transfer $2\Delta S = 0$ and J transfer $2\Delta J = 2\lambda$ but can as well being defined with the same angular transfer, a spin transfer $2\Delta S = 2\lambda$ and a J transfer $2\Delta J = 0$. In Ref. [65], formulae (II B.32) and (II B.34) gives for an electric excitation :

$$d\sigma_{E\lambda} = \Big(\frac{Z_1 e}{\hbar v_i}\Big)^2 \frac{4k_i k_f}{(2\lambda+1)^3}\, B(E\lambda) \sum_\mu \mid < \vec{k}_f \,|\, r_p^{-\lambda-1} Y_{\lambda\mu}(\theta_p,\phi_p)) \,|\, \vec{k}_i > \mid^2 d\Omega, \tag{IV.48}$$

in the exterior region. This interaction needs geometrical factors given by Equ. (III.45) and (III.44).

C.3 Magnetic multipole excitation

A magnetic multipole transition $B(M\lambda)$ is defined as an angular momentum transfer $\Delta L = \lambda + 1$, a spin transfer $2\Delta S = 0$ and J transfer $2\Delta J = 2\lambda$. It is defined in the code by $2\Delta S = -2$ but $2\Delta S = -1$ in the input. The use of $\Delta L = \lambda + 1$ is necessary to go through the parity verifications.

In Ref. [65], formulae (II B.33) and (II B.35) gives for a magnetic excitation :

$$d\sigma_{M\lambda} = \Big(\frac{Z_1 e}{\hbar c}\Big)^2 \frac{v_f}{v_i} \frac{4}{\lambda^2(2\lambda+1)^3}\, B(M\lambda) \sum_\mu \mid < \vec{k}_f \,|\, \vec{l}_p.\vec{\nabla}_p[r_p^{-\lambda-1} Y_{\lambda\mu}(\theta_p,\phi_p)] \,|\, \vec{k}_i > \mid^2 d\Omega. \tag{IV.49}$$

in the exterior region. The ratio of a magnetic excitation $\lambda - 1$ to an electric excitation λ given by Equ. (IV.47) is :

$$\frac{d\sigma_{M\lambda-1}}{d\sigma_{E\lambda}} = \frac{v_i v_f}{k_i k_f c^2} \frac{(2\lambda+1)^3}{(\lambda-1)^2(2\lambda-1)^3} \frac{B(M\lambda-1)}{B(E\lambda)} \frac{\sum_\mu \mid < \vec{k}_f \,|\, \vec{l}_p.\vec{\nabla}_p(r_p^{-\lambda} Y_{\lambda-1\mu}(\theta_p,\phi_p)) \,|\, \vec{k}_i > \mid^2 d\Omega}{\sum_\mu \mid < \vec{k}_f \,|\, r_p^{-\lambda-1} Y_{\lambda\mu}(\theta_p,\phi_p)) \,|\, \vec{k}_i > \mid^2 d\Omega}, \tag{IV.50}$$

that is the product of a coefficient of the potentials R_p^2 such that :

$$R_p = \frac{\hbar}{mc} \Big(\frac{(2\lambda+1)^3}{(\lambda-1)^2(2\lambda-1)^3}\Big)^{\frac{1}{2}} \Big(\frac{B(M\lambda-1)}{B(E\lambda)}\Big)^{\frac{1}{2}} \tag{IV.51}$$

obtained using :

$$\frac{v_i}{k_i} = \frac{v_f}{k_f} = \frac{\hbar}{m} \tag{IV.52}$$

and a ratio R_g^2 such that :

$$R_g^2 = \frac{\sum_\mu \mid < \vec{k}_f \,|\, \vec{l}_p.\vec{\nabla}_p(r_p^{-\lambda} Y_{\lambda-1\mu}(\theta_p,\phi_p)) \,|\, \vec{k}_p > \mid^2 d\Omega}{\sum_\mu \mid < \vec{k}_f \,|\, r_p^{-\lambda-1} Y_{\lambda\mu}(\theta_p,\phi_p)) \,|\, \vec{k}_p > \mid^2 d\Omega} \tag{IV.53}$$

The coefficient R_p is the product of three terms :

$$R_p = R_{p_1} R_{p_2} R_{p_3}, \qquad R_{p_1} = \Big(\frac{B(M\lambda-1)}{B(E\lambda)}\Big)^{\frac{1}{2}}, \qquad R_{p_2} = \frac{\hbar}{mc}, \qquad R_{p_3} = \Big(\frac{(2\lambda+1)^3}{(\lambda-1)^2(2\lambda-1)^3}\Big)^{\frac{1}{2}} \tag{IV.54}$$

In practice :

- the factor R_{p_1} will be taken into account in the reduced nuclear matrix element multiplying by it the reduced nuclear matrix element of the electric transition to obtain the reduced nuclear matrix element of the magnetic transition,
- the factor R_{p_2} will be taken into account by multiplying by it a normalised Coulomb transition form factor of an electric excitation to obtain the magnetic transition form factor,

- the factor R_{p_3} will be factorised with R_g for convenience.

For the coefficient R_g, the gradient acting on $r^{-\lambda}Y_{\lambda\mu}(\hat{r})$ generates only terms in $r^{-\lambda-1}Y_{\lambda+1,\mu}(\hat{r})$. So, in the exterior region, the form factors of a magnetic excitation $B(M\lambda-1)$ is the same as the form factor of an electric excitation $B(E\lambda)$. As the interior region has no importance in this case, we can use for the magnetic transition form factor a Coulomb electric transition form factor multiplied by the ratio R_{p_2} given in Equ. (IV.54). Between partial waves $|l_i>$ and $|l_f>$, the ratio of a magnetic multipole excitation $B(M\lambda-1)$ to an electric multipole excitation $B(E\lambda)$ is :

$$\begin{aligned}
&\frac{< i^{l_f}Y_{l_fm_f}(\theta,\phi)\,|\,i^{\lambda}\vec{l}.\vec{\nabla}(r^{-\lambda}Y_{\lambda-1\mu}(\theta,\phi))\,|\,i^{l_i}Y_{l_im_i}(\theta,\phi)>}{< i^{l_f}Y_{l_fm_f}(\theta,\phi)\,|\,i^{\lambda}r^{-\lambda-1}Y_{\lambda\mu}(\theta,\phi)\,|\,i^{l_i}Y_{l_im_i}(\theta,\phi)>}\\
&= -(2\lambda-1)[\lambda l_i(2l_i+1)(l_i+1)]^{\frac{1}{2}}\sum_q(-)^{\lambda+l_i-\mu-m_i+q}\begin{pmatrix}\lambda & 1 & \lambda-1\\ -\mu-q & q & \mu\end{pmatrix}\\
&\begin{pmatrix}l_i & 1 & l_i\\ -m_i+q & -q & m_i\end{pmatrix}\begin{pmatrix}l_i & \lambda & l_f\\ m_i-q & \mu+q & -m_f\end{pmatrix}\begin{pmatrix}l_i & \lambda & l_f\\ m_i & \mu & -m_f\end{pmatrix}^{-1}\\
&= (2\lambda-1)[\lambda l_i(2l_i+1)(l_i+1)]^{\frac{1}{2}}\begin{Bmatrix}l_f & l_i & \lambda-1\\ 1 & \lambda & l_i\end{Bmatrix}\begin{pmatrix}l_i & \lambda-1 & l_f\\ m_i & \mu & -m_f\end{pmatrix}\begin{pmatrix}l_i & \lambda & l_f\\ m_i & \mu & -m_f\end{pmatrix}^{-1}\\
&= \frac{1}{2}\Big[\frac{2\lambda-1}{2\lambda+1}\Big]^{\frac{1}{2}}[(l_f+l_i+\lambda+1)(l_f+l_i-\lambda+1)(l_f-l_i+\lambda)(l_i-l_f+\lambda)]^{\frac{1}{2}}\\
&\begin{pmatrix}l_i & \lambda-1 & l_f\\ m_i & \mu & -m_f\end{pmatrix}\begin{pmatrix}l_i & \lambda & l_f\\ m_i & \mu & -m_f\end{pmatrix}^{-1}
\end{aligned}\tag{IV.55}$$

using :

$$\begin{Bmatrix}l_f & l_i & \lambda-1\\ 1 & \lambda & l_i\end{Bmatrix} = (-)^{l_i+l_f+\lambda}\frac{1}{2}\Big[\frac{(l_f+l_i+\lambda+1)(l_f+l_i-\lambda+1)(l_f-l_i+\lambda)(l_i-l_f+\lambda)}{l_i(2l_i+1)(l_i+1)(2\lambda-1)\lambda(2\lambda+1)}\Big]^{\frac{1}{2}}\tag{IV.56}$$

and taking into account that $l_i+l_f+\lambda$ is even. This formula agrees with (II B.48) of Ref. [65] if $2l_i$ is replaced by $(2l_i+1)$ in it.

The ratio of the couplings between a state $|(l_is)j_iI_iJ>$ and a state $|(l_fs)j_fI_fJ>$ is :

$$\begin{aligned}
&-\frac{1}{2}\Big[\frac{2\lambda-1)}{2\lambda+1}\Big]^{\frac{1}{2}}\Big[(l_f+l_i+\lambda+1)(l_f+l_i-\lambda+1)(l_f-l_i+\lambda)(l_i-l_f+\lambda)\Big]^{\frac{1}{2}}\\
&\begin{Bmatrix}j_f & \lambda-1 & j_i\\ I_i & J & I_f\end{Bmatrix}\begin{Bmatrix}j_f & \lambda-1 & j_i\\ l_i & s & l_f\end{Bmatrix}\begin{Bmatrix}j_f & \lambda & j_i\\ I_i & J & I_f\end{Bmatrix}^{-1}\begin{Bmatrix}j_f & \lambda & j_i\\ l_i & s & l_f\end{Bmatrix}^{-1}
\end{aligned}\tag{IV.57}$$

that is Equ. (III.44) written with $S=0$, $I^t=L=\lambda$ but with $L=\lambda-1$ instead of $L=\lambda$ in the $6j$ and the $9j$ coefficients, multiplied by the factor written in the first line of Equ. (IV.57).

For an excitation $1^+\to 2^+$, the relative values of the coefficient el of the electric transition and ma of the magnetic one are :

$$\begin{array}{lll}
J=l_i=l_f & el=1/J & ma=J\\
J=l_i=l_f\pm 1 & el=1 & ma=0\\
J=l_i\pm 1, l_f=l_i & el=1 & ma=J\\
J=l_i\pm 1, l_f=l_i\mp 2 & el=0 & ma=0
\end{array}\tag{IV.58}$$

C.4 Magnetic reduced matrix elements

The reduced matrix element of the magnetic excitation $B(M\lambda-1)$ is the one of the electric excitation $B(E\lambda)$ multiplied by the ratio R_{p_1} reduced transition probabilities given in Equ. (IV.54). To do so, they should be expressed in compatible units (see [71] SKORKA, S., J¿, HERTEL, J. and RETZ-SCHMIDT, T., W., *"Compilation of electromagnetic transition rates in light nuclei ($A\leq 40$)"*, Nuclear Data Sheet **A2** (1967) page 347). Usually, the reduced electric probabilities $B(El)$ are given in units $e^2\mathrm{fm}^{2l}$ and the reduced magnetic probabilities $B(Ml)$ in units $\mu_0^2\mathrm{fm}^{2l-2}$: the value of $B(Ml)$ must be multiplied by .01106 to obtain it in units $e^2\mathrm{fm}^2$.

Chapter V

Excitation of particle and target

We consider the scattering of ^8Be on ^{64}Ni to have integer values of the masses at the power one third. We use the rotational model with a positive deformation for ^{64}Ni and a negative deformation for ^8Be. The following test case :

```
|BE8 + NI64   EXCITATION OF NI64    - 1 -  (ECIS94)
|TFFFFFFFFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFF
|    2    3
|.25       10.
|          10.                 8.        64.       0.
|2.        1.
|    2    4
|.45
|20.       1.        .5
|10.       1.        .5
|          1.        .5
|          1.        .5
|          1.        .5
|          1.        .5
|1.
|          1.        .5
|2.        2.        178.
|FIN
```

describes the excitation of a 2^+ state in ^{64}Ni at 1 MeV. The computation is limited to 3 J-values because the output is very detailed: the coefficients of each form-factor for all sets of equations are printed (`LO(58).TRUE.`) to compare one test with the others. The coulomb potential has been suppressed to get significant results. The usual coupled equations (`LO(21)=.TRUE.`) with Schmidt's orthogonalisation (`LO(42)=.TRUE.`) are used for more precision.

This Chapter is the transcription of the similar study in "Notes on ECIS79" which was starting with :

```
|BE8 + NI64   EXCITATION OF NI64    - 1 -  (ECIS79)
|TFFFFFFFFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFTFF
|TTTTTTTTFFFFFFFFFFFFFFFFFFFFFFFFFFFFFFFFFFFTFFTFFFFFF
|    2
|.25       10.       2.
|          10.                 8.        64.       0.
|2.        1.
|    2    4          .45
```

```
|20.       1.        .5
|10.       1.        .5
|
|
|
|1.
|2.        2.        178.
|FIN
```

The second cards 3, 4 and 5 are changed; the input of deformations is, different and there are two more potentials. The new input is the same for `ECIS88`, but there will be differences between `ECIS88` and `ECIS94` from the 5th example.

A Excitation of the particle

A.1 Interchange particle-target

The excitation of a 2^+ state at Mev in ^8Be can be described by interchanging particle and target and choosing a Laboratory energy such that the Center of Mass energy is the same as in the previous case :

```
|BE8 + NI64   EXCITATION OF BE8     - 2 -
|TFFFFFFFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFF
|    2    3
|.25       10.
|          80.                64.       8.        0.
|2.        1.
|    2    4
|-.9
|20.       1.        .5
|10.       1.        .5
|          1.        .5
|          1.        .5
|          1.        .5
|          1.        .5
|1.
|          1.        .5
|2.        2.        178.
|FIN
```

In this case, the result would be the same as in the test case "– 1 –", if $\beta_2 = .9$ had been used instead of $\beta_2 = -.9$.

A.2 Use of external potentials

However, the test case "– 1 –" can be done with external potentials, using `LO(7)=.TRUE.` :

```
|BE8 + NI64   EXCITATION OF NI64 . EXTERNAL POTENTIALS  - 3 -
|TFFFFFTFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFF
|    2    3
|.25       10.
```

```
|          10.                8.        64.       0.
|2.         1.
|2.         2.        178.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    2    2    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    1    1         1         2        -5
|20.        6.        .5
|           .3
|    1    1         2         2        -5
|10.        6.        .5
|           .3
|    1    1         3                  -1
|
|    1    1         4                  -1
|
|    1    1         7                  -1
|0.         6.
|    2    2    1    1         2        -5
|20.        6.        .5
|           .3
|    2    2    1    2         2        -5
|10.        6.        .5
|           .3
|    2    2    1    3                  -2
|
|    2    2    1    4                  -2
|
|    2    2    2    1         2        -5
|20.        6.        .5
|           .3
|    2    2    2    2         2        -5
|10.        6.        .5
|           .3
|    2    2    2    3                  -2
|
|    2    2    2    4                  -2
|
|FIN
```

and the test case “– 2 –” can be done by changing only the energy in the laboratory system and the sign of the deformation and exchanging the masses :

```
|BE8 + NI64   EXCITATION OF BE8. EXTERNAL POTENTIALS  - 4 -
|TFFFFFTFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    2    3
|.25        10.
|           10.                8.        64.       0.
|2.         1.
|2.         2.        178.
|    1    1    0
|    1    2    1
```

```
|    1    2    0    0     -1.000000000000
|    2    2    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    1    1         1         2        -5
|20.       6.        .5
|           -.3
|    1    1         2         2        -5
|10.       6.        .5
|           -.3
|    1    1         3                  -1
|
|    1    1         4                  -1
|
|    1    1         7                  -1
|0.        6.
|    2    2    1    1         2        -5
|20.       6.        .5
|           -.3
|    2    2    1    2         2        -5
|10.       6.        .5
|           -.3
|    2    2    1    3                  -2
|
|    2    2    1    4                  -2
|
|    2    2    2    1         2        -5
|20.       6.        .5
|           -.3
|    2    2    2    2         2        -5
|10.       6.        .5
|           -.3
|    2    2    2    3                  -2
|
|    2    2    2    4                  -2
|
|FIN
```

A.3 Change of spin for the particle

The excited state of the particle can be described as the scattering of a spin 2 particle on a target of spin 0 :

```
|BE8 + NI64 EXCITATION OF PARTICLE.EXTERNAL POTENTIALS  - 5 -
|TFFFFFTFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFF
|    2    3
|.25       10.
|           10.                 8.        64.       0.
|           1.        2.        8.        64.       0.
|2.         2.        178.
|    1    1    0
|    1    2    1
|    1    2    4    0     -1.000000000000     (1)
|    2    2    2
```

```
|    1    2    4    0      1.195228338242     (1)
|    2    4    8    0      1.195228338242     (1)
|    1    1         1         2        -5
|20.       6.        .5
|           -.3
|    1    1         2         2        -5
|10.       6.        .5
|           -.3
|    1    1         3                  -1
|
|    1    1         4                  -1
|
|    1    1         5                  -1
|
|    1    1         6                  -1
|
|    1    1         7                  -1
|0.        6.
|    1    1         8                  -1
|
|    2    2    1    1         2        -5
|20.       6.        .5
|           -.3
|    2    2    1    2         2        -5
|10.       6.        .5
|           -.3
|    2    2    1    3                  -2
|
|    2    2    1    4                  -2
|
|    2    2    2    1         2        -5
|20.       6.        .5
|           -.3
|    2    2    2    2         2        -5
|10.       6.        .5
|           -.3
|    2    2    2    3                  -2
|
|    2    2    2    4                  -2
|
|FIN
```

The interaction which was $L = 2$, $S = 0$, $J = 2$ in the previous test cases is now $L = 2$, $S = 2$, $J = 0$ and the one which was $L = 4$, $S = 0$, $J = 4$ is now $L = 4$, $S = 4$, $J = 0$. The nuclear reduced matrix elements (1) are the same as the previous one, but were multiplied by the reduced "spin" matrix element which is $\sqrt{2S+1}$ in `ECIS79` and `ECIS88`.

As the particle of one of the levels does not have a spin zero, a complex spin-orbit potential and a coulomb spin orbit potential must be read. As this last one is 0, use `LO(46)=.TRUE.` to avoid long range "Coulomb corrections" for this calculation.

B Excitation of the target and of the particle

We assume that there is no interaction between the level for which the target is excited and the one for which the particle is excited. In the rotational model, such an interaction could be only of second order

and it is smaller than the reorientation terms. In the second order vibrational model, such an interaction exists and is identical to the reorientation terms.

This is obtained by adding the test case "– 3 –" to the test case "– 4 –"or the test case "– 5 –". However, the deformation of the optical potential of test case "– 3 –" is positive and the one of the other test cases is negative. We shall use an optical potential without deformation.

B.1 Excitation of the two nuclei

The three levels involved are the scattering of a spin zero particle on a spin zero target, of the spin zero particle on a 2^+ state as in test case "– 3 –", and of a spin two particle on a spin zero target as in test case "– 5 –" :

```
|BE8 + NI64   EXCITATION OF PARTICLE AND TARGET  - 6 -
|TFFFFFTFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    3    3
|.25       10.
|           10.                 8.        64.       0.
|2.         1.
|           1.        2.        8.        64.       0.
|2.         2.        178.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    1    3    1
|    2    2    4    0     -1.000000000000     (1)
|    2    2    2
|    1    2    0    0      1.195228338242
|    3    4    0    0      1.195228338242
|    2    3    0
|    3    3    2
|    2    2    4    0      1.195228338242     (1)
|    4    4    8    0      1.195228338242     (1)
|    1    1         1         2        -1
|20.       6.        .5
|    1    1         2         2        -1
|10.       6.        .5
|    1    1         3                  -1
|
|    1    1         4                  -1
|
|    1    1         5                  -1
|
|    1    1         6                  -1
|
|    1    1         7                  -1
|0.        6.
|    1    1         8                  -1
|
|    2    2    1    1         2        -5
|20.       6.        .5
|           .3
|    2    2    1    2         2        -5
|10.       6.        .5
```

```
|          .3
|    2    2    1    3                   -2
|
|    2    2    1    4                   -2
|
|    2    2    2    1         2         -5
|20.       6.        .5
|          .3
|    2    2    2    2         2         -5
|10.       6.        .5
|          .3
|    2    2    2    3                   -2
|
|    2    2    2    4                   -2
|
|    3    3    1    1         2         -5
|20.       6.        .5
|          -.3
|    3    3    1    2         2         -5
|10.       6.        .5
|          -.3
|    3    3    1    3                   -2
|
|    3    3    1    4                   -2
|
|    3    3    2    1         2         -5
|20.       6.        .5
|          -.3
|    3    3    2    2         2         -5
|10.       6.        .5
|          -.3
|    3    3    2    3                   -2
|
|    3    3    2    4                   -2
|
|FIN
```

The reduced nuclear matrix elements are the ones of test cases "– 2 –" and "– 5 –". The form factors "1" and "3" are the ones of test case "– 2 –" (positive deformation) and the form factors "2" and "4"are the ones of the test case "– 5 –" (negative deformation). The nuclear matrix elements (1) have no more to be multiplied by $\sqrt{2S+1}$ in `ECIS94`.

B.2 Two excitations of the target

In this test case, the three levels are the scattering of a spin zero particle on a spin zero target and two 2^+ states of the target :

```
|BE8 + NI64   TWO EXCITATIONS OF TARGET  - 7 -
|TFFFFFTFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    3    3
|.25       10.
|          10.                 8.        64.       0.
|2.        1.
|2.        1.
```

```
|2.        2.        178.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    1    3    1
|    2    2    0    0     -1.000000000000
|    2    2    2
|    1    2    0    0      1.195228338242
|    3    4    0    0      1.195228338242
|    2    3    0
|    3    3    2
|    2    2    0    0      1.195228338242
|    4    4    0    0      1.195228338242
|    1    1         1         2        -1
|20.       6.        .5
|    1    1         2         2        -1
|10.       6.        .5
|    1    1         3                  -1
|
|    1    1         4                  -1
|
|    1    1         7                  -1
|0.        6.
|    2    2    1    1         2        -5
|20.       6.        .5
|          .3
|......... SAME CARDS AS IN - 6 - ............
```

The reduced nuclear matrix elements are the ones of the pure rotational model and there is no complex spin-orbit to be read with the optical potential because the particle has spin zero for all the levels.

C Double excitation

The double excitation can be described as the scattering of a particle with spin 2 on a target with spin 2, or as the sum of levels with spin 0 to 4 which are the channel spins.

C.1 One level description

The four channels are the scattering of a particle of spin zero and of spin two on a target with a spin zero and two. The coupling between the levels where the particle has a fixed spin and the target the spins zero and two is the same as in the rotational model for the excitation of a 2^+ state by a particle of spin zero or two. The coupling between the channels where the target has a given spin is the same as in test case "– 5 –" . The reorientation terms of the double excitation level are the sum of the reorientation terms of the 2^+ of ^8Be and the 2^+ state state of ^{64}Ni :

```
|BE8 + NI64   DOUBLE EXCITATION DESCRIPTION ONE LEVEL  - 8 -
|TFFFFFTFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    4    3
|.25       10.
|          10.                 8.        64.       0.
|2.        1.
|          2.        2.        8.        64.       0.
```

```
|2.        3.
|2.        2.        178.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    1    3    1
|    2    2    4    0     -1.000000000000     (1)
|    1    4    0
|    2    2    2
|    1    2    0    0      1.195228338242
|    3    4    0    0      1.195228338242
|    2    3    0
|    2    4    1
|    2    2    4    0     -2.2360680         (2)
|    3    3    2
|    2    2    4    0      1.195228338242     (1)
|    4    4    8    0      1.195228338242     (1)
|    3    4    1
|    1    2    0    0     -1.000000000000
|    4    4    4
|    1    2    0    0      1.195228338242
|    3    4    0    0      1.195228338242
|    2    2    4    0      2.672612419       (2)
|    4    4    8    0      2.672612419       (2)
|......... SAME CARDS AS IN - 6 - ............
```

The reduced nuclear matrix (2) are the usual nuclear matrix elements multiplied by the reduced matrix element in the spin space of the target $\sqrt{2I+1}$. This remains in `ECIS94`, whereas the reduced matrix elements (1) and (2) had to be multiplied by $\sqrt{2S+1}$ in `ECIS79` and `ECIS88`.

C.2 Many levels description

The level where the particle and the target are in a 2^+ state can be replaced by five levels with spin 0^+, 1^+, 2^+, 3^+ and 4^+, resulting from the coupling of the spins of the particle and of the target (channel spin). The cross-section will be the sum of the five cross-sections. The data set is :

```
|BE8 + NI64  DOUBLE EXCITATION DESCRIPTION FIVE LEVELS  - 9 -
|TFFFFFTFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFF
|    8    3
|.25       10.
|          10.                8.        64.       0.
|2.        1.
|          2.        2.       8.        64.       0.
|          3.                 8.        64.       0.
|1.        3.
|2.        3.
|3.        3.
|4.        3.
|2.        2.        178.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    1    3    1
|    2    2    4    0     -1.000000000000     (1)
```

```
|    1    4    0
|    1    5    0
|    1    6    0
|    1    7    0
|    1    8    0
|    2    2    2
|    1    2    0    0      1.195228338242
|    3    4    0    0      1.195228338242
|    2    3    0
|    2    4    1
|    2    2    0    0      -.4472135955      (3)
|    2    5    1
|    2    2    0    0      .7745966692       (3)
|    2    6    1
|    2    2    0    0      -1.               (3)
|    2    7    1
|    2    2    0    0      1.183215957       (3)
|    2    8    1
|    2    2    0    0      -1.341640786      (3)
|    3    3    2
|    2    2    4    0      1.195228338242     (1)
|    4    4    8    0      1.195228338242     (1)
|    3    4    1
|    1    2    4    0     -0.447213596000    (4)
|    3    5    1
|    1    2    4    2     0.774596669        (4)
|    3    6    1
|    1    2    4    4     -1.0000000000      (4)
|    3    7    1
|    1    2    4    6     1.183215957        (4)
|    3    8    1
|    1    2    4    8     -1.341640786000    (4)
|    4    4    0
|    4    5    0
|    4    6    2
|    1    2    0    0     .534522483825      (5)
|    2    2    0    0     .534522483825      (5)
|    4    7    0
|    4    8    2
|    3    4    0    0     .534522483825      (5)
|    4    4    0    0     .534522483825      (5)
|    5    5    2
|    1    2    0    0     -.547722555751     (5)
|    2    2    0    0     -.547722555751     (5)
|    5    6    2
|    1    2    0    0     -.462910049886     (5)
|    2    2    0    0      .462910049886     (5)
|    5    7    4
|    1    2    0    0     .585540043769      (5)
|    2    2    0    0     .585540043769      (5)
|    3    4    0    0     -.377964473009     (5)
|    4    4    0    0     -.377964473009     (5)
|    5    8    2
|    3    4    0    0     -.845154254729     (5)
|    4    4    0    0      .845154254729     (5)
```

```
|    6    6    4
|    1    2    0    0     -.256120416286     (5)
|    2    2    0    0     -.256120416286     (5)
|    3    4    0    0     .341493888381      (5)
|    4    4    0    0     .341493888381      (5)
|    6    7    4
|    1    2    0    0     -.808122035642     (5)
|    2    2    0    0      .808122035642     (5)
|    3    4    0    0      .714285714286     (5)
|    4    4    0    0     -.714285714286     (5)
|    6    8    4
|    1    2    0    0     .458162128993      (5)
|    2    2    0    0     .458162128993      (5)
|    3    4    0    0     .895404529326      (5)
|    4    4    0    0     .895404529326      (5)
|    7    7    4
|    1    2    0    0     .292770021885      (5)
|    2    2    0    0     .292770021885      (5)
|    3    4    0    0     -.886405260428     (5)
|    4    4    0    0     -.886405260428     (5)
|    7    8    4
|    1    2    0    0     -.958314847500     (5)
|    2    2    0    0      .958314847500     (5)
|    3    4    0    0     -.749149177244     (5)
|    4    4    0    0      .749149177244     (5)
|    8    8    4
|    1    2    0    0     1.20131123696      (5)
|    2    2    0    0     1.20131123696      (5)
|    3    4    0    0     .456568516759      (5)
|    4    4    0    0     .456568516759      (5)
|......... SAME CARDS AS IN - 6 - ............
```

The reduced nuclear matrix element in the spins spaces between a target of spin I_1 and a particle of spin s_1, coupled to J_1 and a target of spin I_2 and a particle of spin s_2, coupled to J_2 is :

$$\sqrt{(2I+1)(2S+1)(2L+1)(2J_1+1)(2J_2+1)} \left\{ \begin{array}{ccc} I_1 & I_2 & I \\ s_1 & s_2 & S \\ J_1 & J_2 & L \end{array} \right\} \tag{V.1}$$

where $S = 0$ for the form factors 1 and 3, $I = 0$ for the form factors 2 and 4.

- For the reduced nuclear matrix elements (3) above, $s_1 = I = 0$ and the $9j$ coefficient reduces to $0.04(-)^{J_2}$.
- For the reduced nuclear matrix elements (4) above, $I_1 = S = 0$ and the $9j$ coefficient reduces to 0.04. They are multiplied by a reduced matrix element in the spin space which is $\sqrt{5}$. However, they must be multiplied by $(-)^{J_2}$ (?) .
- For the reduced nuclear matrix elements (5) above, $I_1 = I_2 = s_1 = s_2 = 2$ and $I = 0$ or $S = 0$. In this reduced nuclear matrix element, the $9j$ coefficient becomes a 6-j coefficient and the result is :

$$\sqrt{(2L+1)(2J_1+1)(2J_2+1)/5} \left\{ \begin{array}{ccc} J_1 & J_2 & L \\ 2 & 2 & 2 \end{array} \right\} \tag{V.2}$$

  with a phase $(-)^{J_2}$ if $S = 0$ and $(-)^{J_1}$ if $I = 0$.

In fact, the explanation given above is what was given in the "Notes on ECIS79" and do not seem accurate. Perhaps, the result is due to the occurence of 0 for S or I. Nevertheless, using the vibrational model with two different phonons 2^+ and with $0^+, 1^+, 2^+, 3^+, 4^+$ 2-phonons states :

- the reduced nuclear matrix elements (3) and (4) are the same if the second phonon is coupled to the first one (with the other order, the sign of the matrix elements between the 1-phonon 2^+ states and the 1^+ and 3^+ 2-phonons states is changed),
- the second order vibrational nuclear matrix elements :

  $L = 0$ does not exist here,
  $L = 2$ are multiplied here by $\sqrt{5}/2$,
  $L = 4$ are multiplied here by $5/6$.

The excitation of the particle can be replaced by the excitation of a second 2^+ in the target. The data set is:

```
|BE8 + NI64 DOUBLE EXCITATION DESCRIPTION FIVE LEVELS  - 10 -
|TFFFFFTFFFFTFFFTFFFFTFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    8    3
|.25       10.
|          10.                 8.        64.       0.
|2.        1.
|2.        2.
|          3.
|1.        3.
|2.        3.
|3.        3.
|4.        3.
|2.        2.        178.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    1    3    1
|    2    2    0    0     -1.000000000000
|    1    4    0
|    1    5    0
|    1    6    0
|    1    7    0
|    1    8    0
|    2    2    2
|    1    2    0    0      1.195228338242
|    3    4    0    0      1.195228338242
|    2    3    0
|    2    4    1
|    2    2    0    0      -.4472135955      (3)
|    2    5    1
|    2    2    0    0      .7745966692       (3)
|    2    6    1
|    2    2    0    0      -1.               (3)
|    2    7    1
|    2    2    0    0      1.183215957       (3)
|    2    8    1
|    2    2    0    0      -1.341640786      (3)
|    3    3    2
|    2    2    0    0      1.195228338242
|    4    4    0    0      1.195228338242
|    3    4    1
|    1    2    0    0     -0.447213596000    (3)
```

```
|    3    5    1
|    1    2    0    0     -0.774596669       (3)
|    3    6    1
|    1    2    0    0     -1.0000000000      (3)
|    3    7    1
|    1    2    0    0      -1.183215957      (3)
|    3    8    1
|    1    2    0    0      -1.341640786      (3)
|    4    4    0
|    4    5    0
|    4    6    2
|    1    2    0    0     .534522483825      (5)
|    2    2    0    0     .534522483825      (5)
|    4    7    0
|    4    8    2
|    3    4    0    0     .534522483825      (5)
|    4    4    0    0     .534522483825      (5)
|    5    5    2
|    1    2    0    0     -.547722555751     (5)
|    2    2    0    0     -.547722555751     (5)
|    5    6    2
|    1    2    0    0     -.462910049886     (5)
|    2    2    0    0      .462910049886     (5)
|    5    7    4
|    1    2    0    0     .585540043769      (5)
|    2    2    0    0     .585540043769      (5)
|    3    4    0    0     -.377964473009     (5)
|    4    4    0    0     -.377964473009     (5)
|    5    8    2
|    3    4    0    0     -.845154254729     (5)
|    4    4    0    0      .845154254729     (5)
|    6    6    4
|    1    2    0    0     -.256120416286     (5)
|    2    2    0    0     -.256120416286     (5)
|    3    4    0    0     .341493888381      (5)
|    4    4    0    0     .341493888381      (5)
|    6    7    4
|    1    2    0    0     -.808122035642     (5)
|    2    2    0    0      .808122035642     (5)
|    3    4    0    0      .714285714286     (5)
|    4    4    0    0     -.714285714286     (5)
|    6    8    4
|    1    2    0    0     .458162128993      (5)
|    2    2    0    0     .458162128993      (5)
|    3    4    0    0     .895404529326      (5)
|    4    4    0    0     .895404529326      (5)
|    7    7    4
|    1    2    0    0     .292770021885      (5)
|    2    2    0    0     .292770021885      (5)
|    3    4    0    0     -.886405260428     (5)
|    4    4    0    0     -.886405260428     (5)
|    7    8    4
|    1    2    0    0     -.958314847500     (5)
|    2    2    0    0      .958314847500     (5)
|    3    4    0    0     -.749149177244     (5)
```

```
|    4    4    0    0      .749149177244     (5)
|    8    8    4
|    1    2    0    0     1.20131123696      (5)
|    2    2    0    0     1.20131123696      (5)
|    3    4    0    0     .456568516759      (5)
|    4    4    0    0     .456568516759      (5)
|.... SAME CARDS AS IN - 9 - WITHOUT SPIN-ORBIT ...
```

There is a change of sign for the reduced nuclear matrix elements of the second and the third level with the double excitation states with spins 1^+ and 3^+,due to the reversal of the coupling of the two 2^+.

D Identical projectile and target

In the description of Input for ECIS94, there is :

```
|      18- LO(18) PROJECTILE-TARGET ANTISYMMETRISATION, VALID ONLY FOR   ECIS-068
|                 SAME SPIN OF THE PARTICLE AND THE TARGET. FOR SPIN 0,  ECIS-069
|                 THE S-MATRIX IS COMPUTED ONLY FOR EVEN TOTAL SPINS.    ECIS-070
|                 FOR SPIN NON 0., THE AMPLITUDES ARE SYMMETRISED BUT    ECIS-071
|                 THIS DO NOT CORRECT THE LACK OF SYMMETRY OF THE        ECIS-072
|                 INTERACTION BETWEEN PARTICLE AND TARGET.               ECIS-073
```

which means that the cross-sections are computed correctly, but the reaction cross-sections printed at the beginning of each angular distribution must be multiplied by two. The elastic cross-section includes a symmetrised Coulomb amplitude, but is divided by the Rutherford's cross-section which is not symmetrised. With usual parameters, the calculation is not correct because it takes into account only the excitation of the target. To discuss and explain how to do such a calculation, we consider the dummy test case of ^8Be on ^8Be in the rotational model. The test cases are limited to $J = 4$ and use a reduced radius of 1.5 with the heavy ions convention. The data set for the usual rotational model is :

```
|BE8 + BE8   EXCITATION OF BE8 TARGET  - 11 -
|TFFFFFFFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFF
|    2    5
|.25       10.
|          10.                 8.        8.        0.
|2.        1.
|    2    4
|-.6
|20.       1.5       .5
|10.       1.5       .5
|          1.5       .5
|          1.5       .5
|          1.5       .5
|          1.5       .5
|1.5
|          1.5       .5
|2.        2.        90.
|FIN
```

We shall repeat the indications given above for non identical particle and target and we shall give the simplifications which appear when particle and target are identical.

D.1 Excitation of the particle

The same test case can be run with matrix elements and potentials read from cards with `LO(7)=.TRUE.` :

```
|BE8 + BE8   EXCITATION OF BE8 . EXTERNAL POTENTIALS  - 12 -
|TFFFFFTFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    2    5
|.25       10.
|          10.                 8.        8.        0.
|2.        1.
|2.        2.        90.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    2    2    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    1    1         1         2        -5
|20.       6.        .5
|          -.3
|    1    1         2         2        -5
|10.       6.        .5
|          -.3
|    1    1         3                  -1
|
|    1    1         4                  -1
|
|    1    1         7                  -1
|0.        6.
|    2    2    1    1         2        -5
|20.       6.        .5
|          -.3
|    2    2    1    2         2        -5
|10.       6.        .5
|          -.3
|    2    2    1    3                  -2
|
|    2    2    1    4                  -2
|
|    2    2    2    1         2        -5
|20.       6.        .5
|          -.3
|    2    2    2    2         2        -5
|10.       6.        .5
|          -.3
|    2    2    2    3                  -2
|
|    2    2    2    4                  -2
|
|FIN
```

The same result is obtained if the particle has a spin 2 in the final state and the target a spin 0 as in the test case "– 5 –" above. The interaction $L = 2$, $S = 0$, $J = 2$ between the ground state and the excited state is changed into an interaction $L = 2$, $S = 2$, $J = 0$. It is the same for the reorientation interaction $L = 2$. The reorientation interaction $L = 4$, $S = 0$, $J = 4$ becomes an interaction $L = 4$, $S = 4$, $J = 0$.

The nuclear nuclear matrix were multiplied by $\sqrt{2S+1}$ for `ECIS79` and `ECIS88` but not for `ECIS94`. As the excited state has a non-zero spin, a complex spin-orbit potential and a coulomb spin-orbit potential must be given anf `LO(46)` set `.TRUE.`.

```
|BE8 + BE8 EXCITATION OF BE8.EXCHANGE PARTICLE-TARGET  - 13 -
|TFFFFFTFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    2    5
|.25       10.
|          10.                 8.        8.        0.
|          1.        2.        8.        8.        0.
|2.        2.        90.
|    1    1    0
|    1    2    1
|    1    2    4    0     -1.000000000000     (1)
|    2    2    2
|    1    2    4    0      1.195228338242     (1)
|    2    4    8    0      1.195228338242     (1)
|    1    1         1         2        -5
|20.       6.        .5
|          -.3
|    1    1         2         2        -5
|10.       6.        .5
|          -.3
|    1    1         3                  -1
|
|    1    1         4                  -1
|
|    1    1         5                  -1
|
|    1    1         6                  -1
|
|    1    1         7                  -1
|0.        6.
|    1    1         8                  -1
|
|    2    2    1    1         2        -5
|20.       6.        .5
|          -.3
|    2    2    1    2         2        -5
|10.       6.        .5
|          -.3
|    2    2    1    3                  -2
|
|    2    2    1    4                  -2
|
|    2    2    2    1         2        -5
|20.       6.        .5
|          -.3
|    2    2    2    2         2        -5
|10.       6.        .5
|          -.3
|    2    2    2    3                  -2
|
|    2    2    2    4                  -2
|
```

```
|FIN
```

D.2 Excitation of the particle and the target

The two channels of excitation of the particle and of the target can be taken into account with the following data :

```
|BE8 + BE8   EXCITATION OF PARTICLE AND TARGET  - 14 -
|TFFFFFTFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    3    5
|.25       10.
|          10.                 8.        8.        0.
|2.        1.
|          1.        2.        8.        8.        0.
|2.        2.        90.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    1    3    1
|    1    2    4    0     -1.000000000000     (1)
|    2    2    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    2    3    0
|    3    3    2
|    1    2    4    0      1.195228338242     (1)
|    2    4    8    0      1.195228338242     (1)
|.............. SAME CARDS AS IN - 13 - ...........
```

This data set is similar to the test case “– 6 –” when particle and target are not identical, but there is only one kind of deformation and the central potential is kept deformed. The interaction between the excited state of the target and the excited state of the particle have been neglected. The result of this test case is not the same as the one of test cases “– 11 –” to “– 12 –”.

As above, in test case “– 7 –”, the two excited states can be attributed to the target. As they are degenerated, the waves functions for the two excited states are identical and can be replaced by only one wave function in the equations after some modifications of the nuclear matrix elements. Data are the following :

```
|BE8 + BE8   SIMPLIFIED EXCIT. OF PARTICLE AND TARGET  - 15 -
|TFFFFFTFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    2    5
|.25       10.
|          10.                 8.        8.        0.
|2.        1.
|2.        2.        90.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.414213562       (6)
|    2    2    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|.............. SAME CARDS AS IN - 12 - ........
```

The interaction between the ground state and the excited state has been multiplied by $\sqrt{2}$ and the reorientation terms are the sum of the reorientation terms and of the coupling terms between the two excited states, but we did not consider the interaction between the two excited states in this example.

As there is only one kind of deformations involved, this calculation can be done in the framework of standard rotational model by giving the nuclear matrix elements on card (`LO(15)=.TRUE.`, `LO(7)=.FALSE.`). The data set is :

```
|BE8 + BE8   SIMPLIFIED EXCIT. OF PARTICLE AND TARGET  - 16 -
|TFFFFFFFFFFTFFTTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    2    5
|.25        10.
|           10.                 8.        8.        0.
|2.         1.
|    2    4
|-.6
|20.        1.5       .5
|10.        1.5       .5
|           1.5       .5
|           1.5       .5
|           1.5       .5
|           1.5       .5
|1.5
|           1.5       .5
|2.         2.        90.
|    1    1    0
|    1    2    1
| 3000    2    0    0     -1.414213562       (6)
|    2    2    2
| 3000    2    0    0      1.195228338242
| 5000    4    0    0      1.195228338242
|FIN
```

which almost as simple as the data set "– 11 –".

D.3 Double excitation

The data set for the excitation of the target, the excitation of the particle and the simultaneous excitation of the target and the particle is obtained from the cases "– 12 –" and "– 13 –" when there is no interaction between the excited states. The nuclear matrix elements for the excitation of the target are independent of the excitation of particle and the one of the particle are independent of the the excitation of the target :

```
|BE8 + BE8   DOUBLE EXCITATION DESCRIPTION ONE LEVEL  - 17 -
|TFFFFFTFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    4    5
|.25        10.
|           10.                 8.        8.        0.
|2.         1.
|           1.         2.       8.        8.        0.
|2.         2.
|2.         2.        90.
|    1    1    0
|    1    2    1
```

```
|    1    2    0    0     -1.000000000000
|    1    3    1
|    1    2    4    0     -1.000000000000     (1)
|    1    4    0
|    2    2    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    2    3    0
|    2    4    1
|    1    2    4    0     -2.236067977       (2)
|    3    3    2
|    1    2    4    0      1.195228338242     (1)
|    2    4    8    0      1.195228338242     (1)
|    3    4    1
|    1    2    0    0     -1.000000000000
|    4    4    4
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    1    2    4    0      2.672612419       (2)
|    2    4    8    0      2.672612419       (2)
|.............. SAME CARDS AS IN - 13 - ..........
```

where the interaction of the two single excitation channels with the double excitation were not the same with `ECIS79` and `ECIS88` but are the same for `ECIS94`.

One can use the channel spin description of the double excitation as for the test case "– 9 –" or "– 10 –". One can see on the test case "– 10 –" that the 1^+ and the 3^+ states are not coupled to the other states, so they must not be taken into account. The equivalent to the test case "– 9 –" is :

```
|BE8 + BE8   DOUBLE EXCIT. DESCRIPTION THREE LEVELS  - 18 -
|TFFFFFTFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    6    5
|.25       10.
|          10.                 8.        8.        0.
|2.         1.
|          1.        2.        8.        8.        0.
|          2.                  8.        8.        0.
|2.         2.
|4.         2.
|2.         2.        90.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    1    3    1
|    1    2    4    0     -1.000000000000     (1)
|    1    4    0
|    1    5    0
|    1    6    0
|    2    2    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    2    3    0
|    2    4    1
|    1    2    0    0      -.4472135955      (3)
|    2    5    1
```

```
|    1    2    0    0      -1.              (3)
|    2    6    1
|    1    2    0    0      -1.341640786     (3)
|    3    3    2
|    1    2    4    0      1.195228338242    (1)
|    2    4    8    0      1.195228338242    (1)
|    3    4    1
|    1    2    4    0     -0.447213596000   (4)
|    3    5    1
|    1    2    4    4     -1.0000000000     (4)
|    3    6    1
|    1    2    4    8     -1.341640786000   (4)
|    4    4    0
|    4    5    1
|    1    2    0    0     1.06904496765     (5)
|    4    6    1
|    2    4    0    0     1.06904496765     (5)
|    5    5    2
|    1    2    0    0     -.512240832572    (5)
|    2    4    0    0     .682987776762     (5)
|    5    6    2
|    1    2    0    0     .916324257986     (5)
|    2    4    0    0     1.79080905865     (5)
|    6    6    2
|    1    2    0    0     2.40262247392     (5)
|    2    4    0    0     .913137033518     (5)
|.............. SAME CARDS AS IN - 13 - ..........
```

and the equivalent of test case “– 10 –” is :

```
|BE8 + BE8   DOUBLE EXCIT. DESCRIPTION THREE LEVELS  - 19 -
|TFFFFFTFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    6    5
|.25       10.
|          10.                8.        8.        0.
|2.        1.
|2.        1.
|          2.
|2.        2.
|4.        2.
|2.        2.        90.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.000000000000
|    1    3    1
|    1    2    0    0     -1.000000000000
|    1    4    0
|    1    5    0
|    1    6    0
|    2    2    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    2    3    0
|    2    4    1
|    1    2    0    0      -.4472135955     (3)
```

```
|    2    5    1
|    1    2    0    0      -1.               (3)
|    2    6    1
|    1    2    0    0      -1.341640786      (3)
|    3    3    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    3    4    1
|    1    2    0    0     -0.447213596000    (3)
|    3    5    1
|    1    2    0    0     -1.0000000000      (3)
|    3    6    1
|    1    2    0    0     -1.341640786000    (3)
|    4    4    0
|    4    5    1
|    1    2    0    0     1.06904496765      (5)
|    4    6    1
|    2    4    0    0     1.06904496765      (5)
|    5    5    2
|    1    2    0    0     -.512240832572     (5)
|    2    4    0    0     .682987776762      (5)
|    5    6    2
|    1    2    0    0     .916324257986      (5)
|    2    4    0    0     1.79080905865      (5)
|    6    6    2
|    1    2    0    0     2.40262247392      (5)
|    2    4    0    0     .913137033518      (5)
|.............. SAME CARDS AS IN - 12 - ..........
```

The absence of the double excitation channels 1^+ and 3^+ reduces the number of equations from 20 to 17. Furthermore, as the two single excitation levels are degenerated and have the same coupling to the other states, they can be replaced by a single level with reduced matrix elements multiplied by $\sqrt{2}$ as for the test case "– 16 –". The number of coupled equations decreases to 13. The data are :

```
|BE8 + BE8   DOUBLE EXCIT. DESCRIPTION THREE LEVELS  - 20 -
|TFFFFFTFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFTFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    5    5
|.25       10.
|          10.                 8.        8.        0.
|2.        1.
|          2.
|2.        2.
|4.        2.
|2.        2.        90.
|    1    1    0
|    1    2    1
|    1    2    0    0     -1.414213562       (6)
|    1    3    0
|    1    4    0
|    1    5    0
|    2    2    2
|    1    2    0    0      1.195228338242
|    2    4    0    0      1.195228338242
|    2    3    1
|    1    2    0    0     -.632455532034     (6)
```

```
|    2    4    1
|    1    2    0    0     -1.414213562       (6)
|    2    5    1
|    1    2    0    0      -1.8973665961     (6)
|    3    3    0
|    3    4    1
|    1    2    0    0     1.06904496765      (5)
|    3    5    1
|    2    4    0    0     1.06904496765      (5)
|    4    4    2
|    1    2    0    0     -.512240832572     (5)
|    2    4    0    0     .682987776762      (5)
|    4    5    2
|    1    2    0    0     .916324257986      (5)
|    2    4    0    0     1.79080905865      (5)
|    5    5    2
|    1    2    0    0     2.40262247392      (5)
|    2    4    0    0     .913137033518      (5)
|.............. SAME CARDS AS IN - 12 - ..........
```

This calculation can be done with the usual rotational model by giving the nuclear reduced matrix elements on cards (`LO(15)=.TRUE.`) as in the test case "– 15 - " with respect to the "– 14 - ". This was already possible for the test case test case "– 19 –", but not for the test case "– 18 –" which involves transfers of spin. The data set is :

```
|BE8 + BE8   DOUBLE EXCIT. DESCRIPTION THREE LEVELS  - 21 -
|TFFFFFFFFFFFTFFTTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFTFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFF
|    5    5
|.25       10.
|          10.                 8.        8.        0.
|2.        1.
|          2.
|2.        2.
|4.        2.
|    2    4
|-.6
|20.       1.5       .5
|10.       1.5       .5
|          1.5       .5
|          1.5       .5
|          1.5       .5
|          1.5       .5
|1.5
|          1.5       .5
|2.        2.       90.
|    1    1    0
|    1    2    1
| 3000    2    0    0     -1.414213562       (6)
|    1    3    0
|    1    4    0
|    1    5    0
|    2    2    2
| 3000    2    0    0      1.195228338242
| 5000    4    0    0      1.195228338242
|    2    3    1
```

```
| 3000    2    0    0     -.632455532034     (3)
|    2    4    1
| 3000    2    0    0     -1.414213562       (6)
|    2    5    1
| 3000    2    0    0      -1.8973665961     (3)
|    3    3    0
|    3    4    1
| 3000    2    0    0     1.06904496765      (5)
|    3    5    1
| 5000    4    0    0     1.06904496765      (5)
|    4    4    2
| 3000    2    0    0     -.512240832572     (5)
| 5000    4    0    0     .682987776762      (5)
|    4    5    2
| 3000    2    0    0     .916324257986      (5)
| 5000    4    0    0     1.79080905865      (5)
|    5    5    2
| 3000    2    0    0     2.40262247392      (5)
| 5000    4    0    0     .913137033518      (5)
|FIN
```

This is the simplest data set involving the minimum number of coupled equations in the rotational model.

The drawback of the use of channel spin is that the programme does not give the cross-section for double excitation but the five or three cross-sections must be summed to get the result.

E Miscellaneous

Until here, we have considered only the rotational model. In this case, there are no description of the interaction between the excited states available in the programme. We shall give some indications for the vibrational model and derive the modifications of the couplings due to the elimination of identical levels.

E.1 Vibrational model

Between heavy ions, the vibrational model can be derived, assuming two distinct phonons, one for each nuclei. Assuming two different nuclei of mass 8 with a 2^+ state at 1 Mev for one and 2 Mev for the other, the test case is :

```
|BE8 + BE8   VIBRATIONAL TWO DIFFERENT LEVELS    - 22 -
|FTFFFFFFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFFF
|TTTTTTTTFFFFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    8    5
|.25       10.
|          10.                8.        8.        0.
|
|2.        1.
|    1    1
|2.        2.
|    1    2
|          3.
|    2    1    2
|1.        3.
|    2    1    2
|2.        3.
```

```
|    2    1    2
|3.        3.
|    2    1    2
|4.        3.
|    2    1    2
|    2     .6
|    2     .6
|20.       1.5       .5
|10.       1.5       .5
|
|
|
|
|1.5
|
|2.        2.        90.
|FIN
```

Here, the channel spin is used naturally because the double excitation state appears as five degenerated two-phonons states with spins 0^+, 1^+, 2^+, 3^+ and 4^+.

If the two 2^+ are degenerated, the 1^+ and the 3^+ two-phonons states are no more coupled to the ground-state. We can skip them and the data set is :

```
|BE8 + BE8   VIBRATIONAL TWO IDENTICAL LEVELS    - 23 -
|FTFFFFFFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFFF
|TTTTTTTTFFTFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    6    5
|.25       10.
|          10.                 8.        8.        0.
|
|2.        1.5
|    1    1
|2.        1.5
|    1    2
|          3.
|    2    1    2
|2.        3.
|    2    1    2
|4.        3.
|    2    1    2
|    2     .6
|    2     .6
|20.       1.5       .5
|10.       1.5       .5
|
|
|
|
|1.5
|
|2.        2.        90.
|FIN
```

One of the 2^+ levels can be eliminated if the nuclear matrix elements with the ground state and with the double excitation states are multiplied by $\sqrt{2}$ and the interaction between these two levels added

to the reorientation terms. By adding the nuclear matrix elements related to the same form factor as printed in the output of test case "– 23 –", one get the test case :

```
|BE8 + BE8   VIBRATIONAL SYMMETRISED LEVELS    - 24 -
|FTFFFFFFFFFFTFFTTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFFF
|TTTTTTTTFFTFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    5    5
|.25       10.
|           10.                 8.        8.        0.
|
|2.         1.5
|    1    1
|           3.
|    2    1    1
|2.         3.
|    2    1    1
|4.         3.
|    2    1    1
|    2     .6
|20.        1.5       .5
|10.        1.5       .5
|
|
|
|
|1.5
|
|2.         2.        90.
|    1    1    1
|    3    0    0    0      2.000000000000        (7)
|    1    2    1
|    1    2    0    0     -1.414213562373        (8)
|    1    3    1
|    3    0    0    0      0.894427191000
|    1    4    1
|    3    2    0    0      1.069044967650
|    1    5    1
|    3    4    0    0      1.434274331201
|    2    2    3
|    3    0    0    0      6.260990336000        (7)
|    3    2    0    0      2.138089935300        (7)
|    3    4    0    0      2.868548662402        (7)
|    2    3    1
|    1    2    0    0     -0.632455532034        (8)
|    2    4    1
|    1    2    0    0     -1.414213562373        (8)
|    2    5    1
|    1    2    0    0     -1.897366596101        (8)
|    3    3    1
|    3    0    0    0      2.800000000000        (7)
|    3    4    1
|    3    2    0    0      0.956182887468        (7)
|    3    5    1
|    3    4    0    0      1.282853961180        (7)
|    4    4    3
|    3    0    0    0      6.260990337000        (7)
```

```
|    3    2    0    0     -0.458162128992        (7)
|    3    4    0    0      0.819585332306        (7)
|    4    5    2
|    3    2    0    0      0.819585332306        (7)
|    3    4    0    0      2.148970870382        (7)
|    5    5    3
|    3    0    0    0      8.400000000000        (7)
|    3    2    0    0      2.148970870382        (7)
|    3    4    0    0      1.095764440222        (7)
|FIN
```

As all the nuclear matrix elements of first order have been multiplied by $\sqrt{2}$: there are noted by (6). The nuclear matrix elements noted by (7) are sums on the two phonons and those noted by (8) are sums of couplings and reorientation terms.

In the first order vibrational model it is not needed to give the nuclear matrix elements on cards : the deformation can be multiplied by $\sqrt{2}$ and the double excitation states defined with two different phonons to avoid some symmetrisation factor. A dummy second phonon can be introduced by defining the double excitation 2^+ state as a two-phonon state with different phonons. The test case "– 22 –" with `LO(2)=.FALSE.` instead of `.TRUE.` can be replaced by :

```
|BE8 + BE8 FIRST ORDER VIBRATIONAL ONE LEVEL    - 25 -
|FFFFFFFFFFFFTFFFTFTFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFFF
|TTTTTTTTFFTFFFFFFFFFFTFFTFFFFFFFFFFFFFFFFFFFFFFFFF
|    5    3
|.25        10.
|           10.                  8.        8.        0.
|
|2.         1.5
|    1    1
|           3.
|    2    1    2
|2.         3.
|    2    1    2
|4.         3.
|    2    1    2
|    2     .848528
|    2    1.848528
|20.        1.5       .5
|10.        1.5       .5
|
|
|
|
|1.5
|
|2.         2.        90.
|FIN
```

If double excitation is not taken into account, it is enought to multiply the deformation by $\sqrt{2}$ to generate the couplings in the first order as well as the second order vibrational model.

E.2 Justification of the elimination of one level

Let us note by y_1, y_2 ,y_3 and y_4 the four functions of the ground state, the excited state of the target, the excited state of the particle and double excitation level, for a given J-value and parity. In fact there

are more than one function y_2, y_3 or y_4, but the result is the same. The system of equations is :

$$\begin{aligned}
0 &= \frac{d^2}{dr^2}\, y_1 + V_1 y_1 + V_{11} y_1 + V_{12} y_2 + V_{12} y_3 + V_{14} y_4 \\
0 &= \frac{d^2}{dr^2}\, y_2 + V_2 y_2 + V_{12} y_1 + V_{22} y_2 + W_{22} y_3 + V_{24} y_4 \\
0 &= \frac{d^2}{dr^2}\, y_3 + V_2 y_3 + V_{12} y_1 + W_{22} y_2 + V_{22} y_3 + V_{34} y_4 \\
0 &= \frac{d^2}{dr^2}\, y_4 + V_4 y_4 + V_{14} y_1 + V_{24} y_2 + V_{24} y_3 + V_{44} y_4
\end{aligned} \tag{V.3}$$

where V_1, V_2, V_4 are the potentials, V_{11}, V_{22}, V_{44} the reorientation terms, V_{12}, V_{14}, W_{22}, V_{24} the couplings between different channels. Using :

$$y_2 = \frac{1}{\sqrt{2}}(u_2 + u_3), \qquad y_3 = \frac{1}{\sqrt{2}}(u_2 - u_3), \tag{V.4}$$

this system of equations can be written :

$$\begin{aligned}
0 &= \frac{d^2}{dr^2}\, y_1 + V_1 y_1 + V_{11} y_1 + \sqrt{2} V_{12} u_2 + V_{14} y_4 \\
0 &= \frac{d^2}{dr^2}\, u_2 + V_2 u_2 + \sqrt{2} V_{12} y_1 + (V_{22} + W_{22}) u_2 + \sqrt{2} V_{24} y_4 \\
0 &= \frac{d^2}{dr^2}\, y_4 + V_4 y_1 + V_{14} y_1 + \sqrt{2} V_{24} u_2 + V_{44} y_4 \\
0 &= \frac{d^2}{dr^2}\, u_3 + V_2 u_3 + (V_{22} - W_{22}) u_3
\end{aligned} \tag{V.5}$$

The last equation is not coupled to the others. As it is not the ground state, its solution is zero and $y_2 = y_3 = u_2/\sqrt{2}$. The C-matrix elements of y_2 or y_3 are those of u_2 divided by $\sqrt{2}$, so the cross-sections related to y_2 and y_3 are the half of the one computed with u_2. The cross-section obtained with u_2 is the sum of the excitation of the target and of the particle. The symmetrisation, skipping odd J-values and doubling even J-values is independent of the problem of excitation of the target and of the particle.

In the three first equations above, the coupling between u_2 and y_1 or y_4 is the coupling of y_2 or y_3 with y_1 or y_4 multiplied by $\sqrt{2}$. The reorientation terms for u_2 is $V_{22} + W_{22}$, that is the sum of the reorientation terms of y_2 or y_3 and the coupling terms between y_2 and y_3.

In the rotational model, the coupling between the two excited states must be smaller and of the order of the reorientation terms in second order vibrational model. They should be obtained by an angular integration on a multipole. We have neglected them here. The use of the multipole of order zero for the central potential can also be discussed to know if the deformation should be increased (multiplied by $\sqrt{2}$). With such an increase, it is not necessary to give the nuclear reduced matrix elements on cards as far as double excitation is not included. In the rotational model, it is not equivalent to increase the deformation or the nuclear matrix element.

In the vibrational model, after the correction introduced in January 1981 to the second order coupling between two one boson states, which makes it equal to the reorientation terms, the particle and target excitation can be taken into account by multiplying the deformation by $\sqrt{2}$ as well in the second order as in the first order if double excitation is not taken into account.

E.3 Summary of test cases

The output of these test cases varies from one to another. The total output is very large because the main value is 1200 lines by test.

The following test cases must give identical results:

1. "– 1 –" and "– 3 –" excitation of ^{64}Ni.

2. "– 2 –" , "– 4 –" and "– 5 –" excitation of ^8Be.
3. "– 6 –" and "– 7 –" excitation of ^{64}Ni and ^8Be.
4. "– 8 –" , "– 9 –" and "– 10 –" in summing the last five levels of the two last tests to obtain the last cross-section of the first one.
5. "– 11 –" , "– 12 –" and "– 13 –" excitation of one ^8Be.
6. "– 14 –" , "– 15 –" and "– 16 –" excitation of the two ^8Be.
7. "– 17 –" , "– 18 –" , "– 19 –" , "– 20 –" and "– 21 –" double excitation, but, in some cases, some cross-sections are the sum of cross-sections obtained in another tests.
8. "– 22 –" second order vibrational model for two 2^+ in ^8Be.
9. "– 23 –" and "– 24 –" double excitation of ^8Be in second order vibrational model (only these two examples deal with mutual excitation).
10. "– 25 –" first order vibrational model for double excitation in 2^+ of ^8Be.

The nuclear reduced matrix elements are -1. between the ground state and the excited state and the two reorientation ones are $\sqrt{10/7}$ in the rotational model. The others couplings in the vibrational model are too various to be listed here. The signification of the indications between parenthesis is :

(1) were multiplied by $\sqrt{2S+1}$ with $2S$ in column 15 in `ECIS79` and `ECIS88`, without change for `ECIS94`.

(2) multiplied by $\sqrt{(2S+1)(2I+1)}$ where I is the spin of the target in `ECIS79` and `ECIS88`, by $\sqrt{2I+1}$ in `ECIS94`.

(3) multiplied by a $9j$ coefficient as discussed after test case "– 9 –".

(4) multiplied by a $9j$ coefficient as discussed after test case "– 9 –".

(5) multiplied by a $9j$ coefficient as discussed after test case "– 9 –".

(6) multiplied by $\sqrt{2}$ to eliminate one level.

(7) summed on equivalent form factors.

(8) summation of coupling and reorientation terms.

Chapter VI

Transfer reactions

We consider the most general case of transfer reaction. We define the approximations which allows to use the codes ECIS and indicate the input of these codes. We shall follow : [72] OHMURA, T., IMANISHI, B., ICHIMURA, M., KAWAI, M., *"Study of Deuteron Stripping Reaction by Coupled Channel Theory. I – Variational Formulation and Discussion on Basic Equation –"*, Progress of Theor. Phys., **41** (1969) 391; *... II – Properties of Interaction Kernel and Method of Numerical Solution –"*, Progress of Theor. Phys., **43** (1970) 347; *" ... III – Numerical Results without Non Orthogonality –"*, Progress of Theor. Phys.,**44** (1970) 1242 with slightly generalised notations.

Results of ECIS79 have been compared with results of CHUCK and results of ECIS94 with DWUCK.

A Notations

Let us consider a target of mass M_a at the point $\vec{R}_a$ and a particle of mass M_d which is a bound state of a "neutron" of mass M_n at the point $\vec{R}_n$ and of a "proton" of mass M_p at the point $\vec{R}_p$. In an other channel, the "neutron" can be bound to the nucleus of mass M_a: the target is then a nucleus of mass $M_b = M_a + M_n$ at the point $\vec{R}_b$ and the particle is the proton.

A.1 Systems of coordinates

There are two systems of Jacobi coordinates after elimination of the centre of mass. The first, suitable for the first level is :

$$\begin{aligned} \vec{R}_{ad} &= \frac{M_n\vec{R}_n + M_p\vec{R}_p}{M_n + M_p} - \vec{R}_a = \vec{R}, \\ \vec{R}_{np} &= \vec{R}_p - \vec{R}_n, \end{aligned} \tag{VI.1}$$

The second one is more suitable for the second level :

$$\begin{aligned} \vec{R}_{bp} &= \vec{R}_p - \frac{M_n\vec{R}_n + M_a\vec{R}_a}{M_a + M_n} = \vec{r}. \\ \vec{R}_{an} &= \vec{R}_n - \vec{R}_a. \end{aligned} \tag{VI.2}$$

Any of these vectors can be expressed in terms of two others. These relations will be useful. They are :

$$\vec{R}_{ad} = -\frac{M_n(M_a + M_n + M_p)}{M_a(M_n + M_p)}\vec{R}_{np} + \frac{M_a + M_n}{M_a}\vec{R}_{bp}$$

$$
\begin{aligned}
&= \frac{M_p}{M_n+M_p}\vec{R}_{bp} + \frac{M_n(M_a+M_n+M_p)}{(M_a+M_n)(M_n+M_p)}\vec{R}_{an} \\
&= \vec{R}_{an} + \frac{M_p}{M_n+M_p}\vec{R}_{np}, \\
\vec{R}_{np} &= -\frac{M_a(M_n+M_p)}{M_n(M_a+M_n+M_p)}\vec{R}_{ad} + \frac{(M_a+M_n)(M_n+M_p)}{M_n(M_a+M_n+M_p)}\vec{R}_{bp} \\
&= \vec{R}_{bp} - M\_aover M_a + M_n\vec{R}_{an} \\
&= \frac{M_n+M_p}{M_p}(\vec{R}_{ad} - \vec{R}_{an}),
\end{aligned} \tag{VI.3}
$$

and :

$$
\begin{aligned}
\vec{R}_{bp} &= \frac{M_a}{M_a+M_n}\vec{R}_{ad} + \frac{M_n(M_a+M_n+M_p}{(M_a+M_n)(M_n+M_p)}\vec{R}_{np} \\
&= \vec{R}_{np} + \frac{M_a}{M_a+M_n}\vec{R}_{an} \\
&= \frac{M_n+M_p}{M_p}\vec{R}_{ad} - \frac{M_n(M_a+M_n+M_p)}{M_p(M_a+M_n)}\vec{R}_{ap}, \\
\vec{R}_{an} &= \vec{R}_{ad} - \frac{M_p}{M_n+M_p}\vec{R}_{np} \\
&= \frac{M_a+M_n}{M_a}(\vec{R}_{bp} - \vec{R}_{np}) \\
&= \frac{(M_a+M_n)(M_n+M_p)}{M_n(M_a+M_n+M_p)}\vec{R}_{ad} - \frac{M_p(M_a+M_n)}{M_n(M_a+M_n+M_p)}\vec{R}_{bp}.
\end{aligned} \tag{VI.4}
$$

A.2 Hamiltonian and wave function

The total Hamiltonian can be written in two alternative forms. For the deuteron channel :

$$H = H_a - a_{np}\Delta_{R_{np}}|_R + V_{np}(\vec{R}_{np}) - a_d\Delta_R|_{R_{np}} + V_{an}(\vec{R}_{an}) + V_{ap}(\vec{R}_{ap}) \tag{VI.5}$$

For the proton channel :

$$H = H_b - a_p\Delta_r|_{R_{np}} + V_{ap}(\vec{R}_{ap}) + V_{np}(\vec{R}_{np}) \tag{VI.6}$$

with :

$$H_b = H_a - a_n\Delta_{R_{np}}|_r + V_{an}(\vec{R}_{an}) \tag{VI.7}$$

Here the a's are related to the reduced masses (or the reduced energies in the relativistic option). They are:

$$
\begin{aligned}
a_d &= \frac{M_a+M_n+M_p}{2M_a(M_n+M_p)}\hbar^2, & a_{np} &= \frac{M_n+M_p}{2M_nM_p}\hbar^2, \\
a_p &= \frac{M_a+M_n+M_p}{2M_p(M_a+M_n)}\hbar^2, & a_n &= \frac{M_a+M_n}{2M_aM_n}\hbar^2.
\end{aligned} \tag{VI.8}
$$

The intrinsic wave functions of the target A, the target B and the particle in the initial channel are respectively $F_a(\vec{x})$, $F_b(\vec{x},\vec{R}_{an})$, $F_d(\vec{R}_{np})$ where $\vec{x}$ are internal coordinates. They satisfy the equations :

$$
\begin{aligned}
H_aF_a(\vec{x}) &= E_aF_a(\vec{x}), \\
H_bF_b(\vec{x},\vec{R}_{an} &= E_bF_b(\vec{x},\vec{R}_{an}), \\
\Big[-a_{np}\Delta_{R_{np}} + V_{np}(\vec{R}_{np})\Big]F_d(R_{np}) &= E_dF_d(R_{np}).
\end{aligned} \tag{VI.9}
$$

Furthermore, we assume that :

$$
\begin{aligned}
F_a(\vec{x},\vec{R}_{an}) &= F_a(\vec{x})F_n(\vec{R}_{an}), \\
\Big[-a_n\Delta_{R_{an}} + V_{an}(\vec{R}_{an})\Big]F_n(\vec{R}_{an})) &= E_nF_n(\vec{R}_{an}).
\end{aligned} \tag{VI.10}
$$

The total wave function is :

$$F(\vec{x},\vec{R}_{an},\vec{R}_{bp}) = F_a(\vec{x})F_d(\vec{R}_{np})F_1(\vec{R}) + F_b(\vec{x},\vec{R}_{an})F_2(\vec{r}) \tag{VI.11}$$

B System of coupled equations

The system of coupled equations is obtained from :

$$[H-E]\ F(\vec{x},\vec{R}_{an},\vec{R}_{bp}) = 0 \tag{VI.12}$$

by projection on $F_a(\vec{x})F_d(\vec{R}_{np})$ and on $F_b(\vec{x},\vec{R}_{an})$. In the first case, the total expression is integrated on the variables $\vec{x}$ and $\vec{R}_{np}$ and the result is a function of $\vec{R}_{ad} = \vec{R}$. In the second case, the total expression is integrated on $\vec{x}$ and $\vec{R}_{an}$ and the result is a function of $\vec{R}_{bp} = \vec{r}$.

B.1 Tri-dimensional equations

The first equation obtained is :

$$\begin{aligned} &-a_d\big(\Delta_R + k_d^2\big)F_1(\vec{R}) + U_{ad}(\vec{R})F_1(\vec{R}) \\ &+ \int F_d(\vec{R}_{np})\Big[- a_p\big(\Delta_r|_{R_{an}} + k_p^2\big) + V_{ap}(\vec{R}_{ap}) + V_{np}(\vec{R}_{np})\Big]F_n(\vec{R}_{an})F_2(\vec{r})d\vec{R}_{np} = 0 \end{aligned} \tag{VI.13}$$

with :

$$U_{ad}(\vec{R}) = \int F_d(\vec{R}_{np})\Big[V_{an}(\vec{R}_{an}) + V_{ap}(\vec{R}_{ap})\Big]F_d(\vec{R}_{np})d\vec{R}_{np} \tag{VI.14}$$

The second equation is :

$$\begin{aligned} &-a_p\big(\Delta_r + k_p^2\big)F_2(\vec{r}) + U_{bp}(\vec{r})F_2(\vec{r}) \\ &+ \int F_n(\vec{R}_{an})\Big[- a_p\big(\Delta_r|_{R_{an}} + k_p^2\big) + V_{ap}(\vec{R}_{ap}) + V_{np}(\vec{R}_{np})\Big]F_d(\vec{R}_{np})F_1(\vec{R})d\vec{R}_{an} = 0 \end{aligned} \tag{VI.15}$$

with :

$$U_{bp}(\vec{R}) = \int F_n(\vec{R}_{an})\Big[V_{np}(\vec{R}_{np}) + V_{ap}(\vec{R}_{ap})\Big]F_n(\vec{R}_{an})d\vec{R}_{an} \tag{VI.16}$$

In these integro-differential equations, all the variables can be expressed in terms of $\vec{R}$ and $\vec{r}$: this introduces the Jacobian of the transformation from $\vec{R}_{ad},\vec{R}_{np}$ or $\vec{R}_{bp},\vec{R}_{an}$ to $\vec{R}_{ad},\vec{R}_{bp}$ in front of these integrals. These two Jacobians are :

$$J = \Big[\frac{(M_n+M_p)(M_a+M_n)}{M_n(M_a+M_n+M_p)}\Big]^3 \tag{VI.17}$$

We obtain:

$$\begin{aligned} - a_d\big(\Delta_R + k_d^2\big)F_1(\vec{R}) + U_{ad}(\vec{R})F_1(\vec{R}) + \int K(\vec{R},\vec{r})F_2(\vec{r})d\vec{r} &= 0, \\ -a_p\big(\Delta_r + k_p^2\big)F_2(\vec{r}) + U_{bp}(\vec{r})F_2(\vec{r}) + \int K(\vec{R},\vec{r})F_1(\vec{R})d\vec{R} &= 0 \end{aligned} \tag{VI.18}$$

with :

$$K(\vec{R},\vec{r}) = J\ F_d(\vec{R}_{np})\Big[- a_p\big(\Delta_r|_{R_{an}} + k_p^2\big) + V_{ap}(\vec{R}_{ap}) + V_{np}(\vec{R}_{np})\Big]F_n(\vec{R}_{an}) \tag{VI.19}$$

The derivative term can be replaced by derivation of the bound functions $F_d(\vec{R}_{np})$ and $F_n(\vec{R}_{an})$ (see Ref. [72]). The result is :

$$K(\vec{R},\vec{r}) = J\ \Big[- a_p\big(\Delta_r|_R + k_p^2\big) + V_{ap}(\vec{R}_{ap}) + V_{np}(\vec{R}_{np})\Big]F_n(\vec{R}_{an})F_d(\vec{R}_{np}) \tag{VI.20}$$

and can be divided into a non-orthogonality term :

$$K_N(\vec{R},\vec{r}) = J\ \Big[- a_p\big(\Delta_r|_R + k_p^2\big) + U_{bp}(\vec{R}_{bp})\Big] F_n(\vec{R}_{an}) F_d(\vec{R}_{np}) \tag{VI.21}$$

which do not exist in inelastic scattering and :

$$K_V(\vec{R},\vec{r}) = J\ \Big[V_{ap}(\vec{R}_{ap}) + V_{np}(\vec{R}_{np}) - U_{bp}(\vec{R}_{bp})\Big] F_n(\vec{R}_{an}) F_d(\vec{R}_{np}) \tag{VI.22}$$

which is the only term which remains in `DWBA` because $K_N(\vec{R},\vec{r})$ is identical to the homogeneous part of the equation for $F_2(\vec{r})$, multiplied by some function.

B.2 Radial equations

If the waves functions $F_1(\vec{R})$ and $F_2(\vec{r})$ are expanded into partial waves, a set of radial equations are obtained. The transition potential $K(\vec{R},\vec{r})$ is characterised by :

- the transfer of an angular momentum $\vec{L}$ which is the angular momentum $\vec{L}_n$ of the "neutron" in $F_n(\vec{R}_{an})$,
- the transfer of a spin to the particle, which is the one of the "neutron",
- the transfer of a total spin J to the nucleus, which is the total momentum of the "neutron" wave function $F_n(\vec{R}_{an})$.

The geometrical coefficients are the one implied by these three transfers. Note, in `ECIS`, the phase i^{L_n} and the extra phase i for odd values of L_n.

Without taking into account the spins, the wave functions F_1 and F_2 can be written :

$$\begin{aligned} F_1(\vec{R}) &= \sum_L i^L Y_L^M(\hat{R})\ \frac{1}{R}\ F_1(L,R), \\ F_2(\vec{r}) &= \sum_l i^l Y_l^m(\hat{r})\ \frac{1}{r}\ F_1(l,r). \end{aligned} \tag{VI.23}$$

The system of coupled equations is :

$$\begin{aligned} &-a_d\Big[\frac{d^2}{dR^2} + k_d^2 - \frac{L_i(L_i+1)}{R^2}\Big] F_1(L_i,R) + \sum_{L_j} U_{ad}(L_i,L_j,R) F_1(L_j,R) \\ &+ \sum_{l_j} \int G_{L_i,l_j} RrK(R,r) F_2(l_j,r) dr = 0 \\ &-a_p\Big[\frac{d^2}{dr^2} + k_p^2 - \frac{l_i(l_i+1)}{r^2}\Big] F_2(l_i,r) + \sum_{l_j} U_{bp}(l_i,l_j,r) F_2(l_j,r) \\ &+ \sum_{L_j} \int G_{l_i,L_j} RrK(R,r) F_1(L_j,R) dR = 0 \end{aligned} \tag{VI.24}$$

where $G_{L,l}$ is some geometrical coefficient.

C Zero-range approximation

We neglect the non-orthogonality term $K_N(\vec{R},\vec{r})$ and we assume $V_{ap}(\vec{R}_{ap}) = U_{bp}(\vec{R}_{bp})$ in $K_V(\vec{R},\vec{r})$. The zero-range approximation is obtained if we replace the product $V_{np}(\vec{R}_{np}) F_d(\vec{R}_{np})$ by a δ-function of $\vec{R}_{np}$.

C.1 Coupled differential equations

In the interaction :

$$K(\vec{R},\vec{r}) = J\ V_{np}(\vec{R}_{np})F_d(\vec{R}_{np})F_n(\vec{R}_{an}) \tag{VI.25}$$

the product $V_{np}(\vec{R}_{np})F_d(\vec{R}_{np})$ is replaced by a δ-function of :

$$\vec{R}_{np} = -\frac{M_a(M_n+M_p)}{M_n(M_a+M_n+M_p)}\vec{R}_{ad} + \frac{(M_a+M_n)(M_n+M_p)}{M_n(M_a+M_n+M_p)}\vec{R}_{bp} \tag{VI.26}$$

multiplied by some strength C_0 which is usually -122.5 mev (124.7 MeV in Ref. [72]). The δ-function can be replaced by a δ-function on the lengths divided by :

$$\frac{M_a(M_n+M_a)(M_n+M_p)^2Rr}{[M_n(M_a+M_n+M_p)]^2} \tag{VI.27}$$

with a δ-function on directions of R and r. So :

$$K(\vec{R},\vec{r}) = C_0\frac{(M_n+M_p)(M_a+M_n)^2}{M_aM_n(M_a+M_n+M_p)}F_n(\vec{R}_{an})\frac{\delta(R_{np})}{Rr} \tag{VI.28}$$

and after integration the system of coupled equations becomes :

$$\begin{aligned}
&-a_d\Big[\frac{d^2}{dR^2}+k_d^2-\frac{L_i(L_i+1)}{R^2}\Big]F_1(L_i,R)+\sum_{L_j}U_{ad}(L_i,L_j,R)F_1(L_j,R)\\
&+\sum_{l_j}C_0G_{L_i,l_j}\frac{M_a+M_n}{M_a}F_n(R)F_2(l_j,\frac{M_a}{M_a+M_n}R)=0,\\
&-a_p\Big[\frac{d^2}{dr^2}+k_p^2-\frac{l_i(l_i+1)}{r^2}\Big]F_2(l_i,r)+\sum_{l_j}U_{bp}(l_i,l_j,r)F_2(l_j,r)\\
&+\sum_{L_j}C_0G_{l_i,L_j}(\frac{M_a+M_n}{M_a})^2F_n(\frac{M_a+M_n}{M_a}r)F_1(L_j,\frac{M_a+M_n}{M_a}r)=0.
\end{aligned} \tag{VI.29}$$

These equations are not symmetric. Note that M_a and M_a+M_p are the masses of the target for the two levels. From now on, we shall use:

$$M_1 = M_a \qquad M_2 = M_a+M_n \tag{VI.30}$$

C.2 Symmetric equations

To obtain more symmetric equations, we shall use different units of lengths in each channel: in channel i, we use $s = M_iR_i/M_0$, that is the step size $h_i = hM_0/M_i$, where M_0 is the mass of the target in some first channel labelled by 0. The equations are :

$$\begin{aligned}
&-a_d\Big(\frac{M_1}{M_0}\Big)^2\Big[\frac{d^2}{ds^2}+\Big(\frac{M_0}{M_1}\Big)^2k_d^2-\frac{L_i(L_i+1)}{s^2}\Big]F_1(L_i,s)+\sum_{L_j}U_{ad}(L_i,L_j,s)F_1(L_j,s)\\
&+\sum_{l_j}C_0G_{L_i,l_j}\frac{M_2}{M_1}F_n(s)F_2(l_j,s)=0,\\
&-a_p\Big(\frac{M_2}{M_0}\Big)^2\Big[\frac{d^2}{ds^2}+\Big(\frac{M_0}{M_2}\Big)^2k_p^2-\frac{l_i(l_i+1)}{s^2}\Big]F_2(l_i,s)+\sum_{l_j}U_{bp}(l_i,l_j,s)F_2(l_j,s)\\
&+\sum_{L_j}C_0G_{l_i,L_j}(\frac{M_2}{M_1})^2F_n(s)F_1(L_j,s)=0.
\end{aligned} \tag{VI.31}$$

With the following notations :

$$V_{11} = U_{ad}(s), \qquad V_{12} = GC_0\Big[\frac{M_2}{M_1}\Big]^{\frac{3}{2}} F_n(s), \qquad V_{22} = U_{bp}(s), \tag{VI.32}$$

and using the coefficients :

$$A_1 = \Big[\frac{M_0}{M_1 a_d}\Big]^{\frac{1}{2}} \qquad A_2 = \Big[\frac{M_0}{M_2 a_p}\Big]^{\frac{1}{2}} \qquad B_1 = \frac{M_0}{M_1 a_d^{\frac{1}{2}}} \qquad B_2 = \frac{M_0}{M_1 a_p^{\frac{1}{2}}} \tag{VI.33}$$

wave functions and potentials can be redefined with :

$$F_i(s) = A_i G_i(s) \qquad U_{ij}(s) = B_i B_j V_{ij}(s) \tag{VI.34}$$

to get the symmetric set of equations :

$$\begin{aligned} -\Big[\frac{d^2}{ds^2} + \big(\frac{M_0}{M_1}\big)^2 k_d^2 - \frac{L(L+1)}{s^2}\Big] G_1(s) \quad &+U_{11}(s)G_1(s) + U_{12}(s)G_2(s) = 0 \\ -\Big[\frac{d^2}{ds^2} + \big(\frac{M_0}{M_2}\big)^2 k_p^2 - \frac{l(l+1)}{s^2}\Big] G_2(s) \quad &+U_{22}(s)G_2(s) + U_{12}(s)G_1(s) = 0 \end{aligned} \tag{VI.35}$$

in which $[M_0/M_1]k_d$ and $[M_0/M_2]k_p$ appear instead of the wave numbers. In `ECIS`, the mass of the target in the first channel is chosen as M_0. In the subroutine `COLF` the wave number is multiplied by M_0/M_I, because this product plays the same role in all parts of the code.

D Use of ECIS94

D.1 Possibilities of the code

The code `ECIS94` as well as `ECIS79` allows zero-range calculations without the non-orthogonality term using external nuclear matrix elements and form factors (`LO(7)=.TRUE.`). The step sizes for each levels are related with respect to the difference of masses, unless tt LO(93)=.TRUE. (`LO(48)=.TRUE.` in `ECIS79`): this control can be used to interchange particle and target in some level, in which case there is no recoil correction. For the transfer of a neutron with angular momentum L_n and total spin J_n, the data needed for the reduced matrix elements are :

- `columns 1- 5` Sequence number or blank.
- `columns 6-10` angular momentum L_n.
- `columns 11-15` 1 (twice the spin of the neutron).
- `columns 16-20` $2J_n$ twice the total spin.
- `columns 21-40` the nuclear matrix element which depends upon the form factor, but includes :
  - a reduced nuclear matrix element in the spin space which is not the same in `ECIS79` and `ECIS94`,
  - a reduced nuclear matrix element in the target space,
  - a recoil factor $[(a+1)/a]^{3/2}$ if `LO(48)=.FALSE.`.

The form factor can be given by points. However, they are two "standard" possibilities:

-7 Laguerre polynomial,

-8 solution in a real Woods-Saxon potential of which the depth is searched for a given binding energy.

In these two cases, there is a discrepancy in the code between these form factors and the macroscopic ones such that the reduced nuclear matrix element has to be divided by $\sqrt{4\pi}$.

D.2 Example

The following example has been chosen to compare ECIS79 with the code CHUCK. The original test case was intended for Zr but the mass of the target has been decreased to enforce the recoil effects.

For ECIS94, this test case is :

```
|COMPARAISON AVEC CHUCK POUR BE8
|FFFFFFTFFFFFFFFFFFFFFFFFFFFFFTFFFFFFFFFFFFFFFFFTFFFF
|TTTTTFFFFFFFFFFFFFFFFTFFFFFFFFFFFFFFFFFFFFFFFFFFFFF
|    2         1    2         3    3
|.12       18.
|           15.       1.        2.        8.        4.
|3.5     2 -5.        .5        1.        9.        4.
|0.         2.5       137.5
|    1    1
|    1    2    1
|    1    4    1    7    142.84024                        (1)
|    2    2
|    1    1    0    1    0    0    0   -1
|104.3     2.14      .78
|    1    1    0    2    0    0    0   -1
|
|    1    1    0    3    0    0    0   -1
|
|    1    1    0    4    0    0    0   -1
|13.9      2.52      .8
|    1    1    0    5    0    0    0   -1
|3.5       2.14      .78
|    1    1    0    6    0    0    0   -1
|
|    1    1    0    7    0    0    0   -1
|4.         2.5
|    1    1    0    8    0    0    0   -1
|
|    2    2    0    1    0    0    0   -1
|54.9      2.3713    .7
|    2    2   0    2    0    0    0    -1
|.41       2.7249    .63
|    2    2    0    3    0    0    0   -1
|
|    2    2    0    4    0    0    0   -1
|8.7875    2.7249    .63
|    2    2    0    5    0    0    0   -1
|8.3825    2.609     .53
|    2    2    0    6    0    0    0   -1
|
|    2    2    0    7    0    0    0   -1
|4.         2.6001
|    2    2    0    8    0    0    0   -1
|
|    1    2    1    1    0    0    0   -8
|7.2        9.        1.        0.        0.        1.25      .65
|0.         1.        1.        1.
|FIN
```

There is no spin-orbit for the bound wave-functions because CHUCK takes is proportional to the central

potential and ECIS keeps it constant. As the first channel is the deuteron channel, there is no need to indicate to the code to use the deuteron step size : for the inverse reaction, a "2" should be in column 45 of the third card before FIN. The "deformation" in the test with the code CHUCK was 122.5 . The value (1) used here is the same

- divided by $\sqrt{4\pi}$, due to the normalisation of bound-states in ECIS,
- multiplied by the reduced matrix element in the spin space which is $\sqrt{3}/2$ in ECIS94 but was $\sqrt{3}$ for ECIS79,
- multiplied by the reduced matrix element in the target space, which is $\sqrt{8}$,
- multiplied by the recoil factor which is $(9./8.)^{3/2}$.

Chapter VII

Miscellaneous

A Relativistic cinematics

This section is to explain some expressions which are used in the programme when relativistic cinematics are used (`LO(8)=.TRUE.`) and compare then to the non-relativistic ones (`LO(8)=.FALSE.`). The code includes in subroutine `CALC` the following values :

```
|       CM=931.5017646D0                                                CALC-085
|       CHB=197.328604D0                                                CALC-086
|       CZ=137.0360411D0                                                CALC-087
```

in the `IBM` version (single precision in the `CDC` version). They are the values of the Atomic Mass Unit M_u in MeV fm/c^2 and of $\hbar c$ in MeV fm respectively where c is the speed of light in vacuum. In these explanations, we supposes the masses multiplied by `CM` and the wave numbers by `CHB`.

A.1 Notations

Let us consider a particle of mass m_i and energy E_{lab} in the Laboratory system and a target of mass M_i; in the final state with an excitation energy Q, an outgoing particle of mass m_f and a residual nucleus of mass M_f:

- in non-relativistic cinematics, the mass M_f is unaltered;
- in relativistic cinematics :
$$M_f = m_i + M_i - m_f + Q/M_u \tag{VII.1}$$
in such a way that the total energy in the center of mass system is a constant. However, this correction is dropped in the Schrödinger formalism if they are Coulomb corrections.

A.2 Energy in the center of mass system

The relativistic energy of the incoming particle in the Laboratory System is given by $e_i = m_i + E_{lab}$, as a pure extension of the non-relativistic case. Its momentum p_i is such that $e_i^2 = m_i^2 + p_i^2$. A change of frame along the quantification axis is obtained by :

$$P = p\cosh x + e\sinh x, \qquad E = p\sinh x + e\cosh x \tag{VII.2}$$

The change to the Center of mass system is obtained with :

$$P_{cm} = p_i\cosh x + e_i\sinh x + M_i\sinh x = 0, \qquad E_{cm} = p_i\sinh x + e_i\cosh x + M_i\cosh x \tag{VII.3}$$

from which $\sinh x$ and $\cosh x$ can be eliminated to obtain :

$$E_{cm_i} = E_{cm} - m_i - M_i = [(m_i + M_i)^2 + 2E_{lab}M_i]^{\frac{1}{2}}, \qquad E_{cm_f} = E_{cm_i} - Q/M_u \tag{VII.4}$$

for each channel.

A.3 Wave numbers - Momenta

From :

$$E_{cm} = (m_f^2 + p_f^2)^{\frac{1}{2}} + (M_f^2 + p_f^2)^{\frac{1}{2}} \tag{VII.5}$$

we get :

$$\begin{aligned} p_f^2 &= \frac{[(E_{cm} - m_f - M_f)(E_{cm} + m_f + M_f)(E_{cm} + m_f - M_f)(E_{cm} - m_f + M_f)}{4E_{cm}^2} \\ &= \frac{(E_{cm_f}(E_{cm_f} + 2m_f + 2M_f)(E_{cm_f} + 2m_f)(E_{cm_f} + 2M_f)}{4(E_{cm_i} + m_i + M_i)^2} \end{aligned} \tag{VII.6}$$

With relativistic cinematics without Dirac formalism, the reduced mass μ_{nr} is replaced by the reduced energy μ_r :

$$\mu_{nr} = \frac{m_f M_f}{m_f + M_f}, \qquad \mu_r = \frac{(m_f^2 + p_f^2)^{\frac{1}{2}}(M_f^2 + p_f^2)^{\frac{1}{2}}}{E_{cm}} = \frac{E_{cm}^4 - (m_f^2 - M_f^2)^2}{4E_{cm}^3}, \tag{VII.7}$$

but, with Coulomb corrections, M_i is used instead of M_f in order to have the same reduced mass for all the levels : until their generalisation, the Coulomb corrections are valid only with a product of the wave number by the Coulomb parameter constant in all the channels.

Without relativistic cinematics, the residual target mass M_f is not corrected by the excitation energy. The center of mass energy of each levels are given by :

$$E_{cm_i} = \frac{E_{lab}M_i}{m_i + M_i}, \qquad E_{cm_f} = E_{cm_i} - Q, \qquad p_f^2 = \frac{2M_u}{\hbar^2}\frac{E_{cm_f} m_f M_f}{m_f + M_f}. \tag{VII.8}$$

A.4 Observables in the laboratory system

We shall note the incoming particle, the initial target, the outgoing particle and the residual target as particles 1, 2, 3 and 4 respectively. In order to compute the rotation to be applied to the S matrix to obtain a description of polarisation phenomena in the Laboratory system, we have to consider the following frames :

1. the center of mass with Oz in incoming direction;
2. the center of mass with Oz in outgoing direction of particle 3;
3. the system in which particle 3 is at rest and Oz opposite to outgoing direction of particle 4; the description of polarisations is invariant in this change of frame;
4. the system in which particle 3 is at rest and Oz opposite to incoming particle 2; the description of polarisations has to be rotated for this change of frame;
5. the system where particle 2 is at rest and Oz along the outgoing particle 3; the polarisations are invariant;
6. the system where particle 2 is at rest and Oz along the incoming particle m_i; the description in this frame can be obtained easily from the description in frame (1).

We note by p_n the momentum of the particle n in the center of mass frame; by e_n their relativistic energy and by m_n their mass. In fact, $p_1 = p_2$ and $p_3 = p_4$. We shall give z, x and time components of the quadri-vector $(\vec{p}, e)$ for each particle in each frame.

A.4.a Center of mass system - Oz incoming direction

For an outgoing particle 3 at the angle α in the center of mass system, the 4 quadri-vectors are:

$$(1)\left|\begin{array}{l} p_1 \\ 0 \\ e_1 \end{array}\right. \quad (2)\left|\begin{array}{l} -p_1 \\ 0 \\ e_2 \end{array}\right. \quad (3)\left|\begin{array}{l} p_3\cos\alpha \\ p_3\sin\alpha \\ e_3 \end{array}\right. \quad (4)\left|\begin{array}{l} -p_3\cos\alpha \\ -p_3\sin\alpha \\ e_4 \end{array}\right. \tag{VII.9}$$

A.4.b Center of mass system - Oz outgoing direction

This new frame is obtained by a rotation in the ordinary space :

$$(1)\left|\begin{array}{l} p_1\cos\alpha \\ -p_1\sin\alpha \\ e_1 \end{array}\right. \quad (2)\left|\begin{array}{l} -p_1\cos\alpha \\ p_1\cos\alpha \\ e_2 \end{array}\right. \quad (3)\left|\begin{array}{l} p_3 \\ 0 \\ e_3 \end{array}\right. \quad (4)\left|\begin{array}{l} -p_3 \\ 0 \\ e_4 \end{array}\right. \tag{VII.10}$$

A.4.c Particle 3 rest system - Oz outgoing direction

This new frame is obtained by a special Lorentz transformation with $\cosh x = e_3/m_3$ and $\sinh x = -p_3/m_3$:

$$(1)\left|\begin{array}{l} (p_1e_3\cos\alpha - e_1p_3)/m_3 \\ -p_1\sin\alpha \\ (e_1e_3 - p_1p_3\cos\alpha)/m_3 \end{array}\right. \quad (2)\left|\begin{array}{l} -(p_1e_3\cos\alpha + e_2p_3)/m_3 \\ p_1\sin\alpha \\ (e_2e_3 + p_1p_3\cos\alpha)/m_3 \end{array}\right. \quad (3)\left|\begin{array}{l} 0 \\ 0 \\ m_3 \end{array}\right. \quad (4)\left|\begin{array}{l} -p_3(e_3+e_4)/m_3 \\ 0 \\ (e_3e_4 + p_3^2)/m_3 \end{array}\right. \tag{VII.11}$$

A.4.d Particle 3 rest system - Oz opposite to particle 2

The axis Oz must be opposite to the momentum of particle 2. This rotation β is such that :

$$\sin\beta = -\frac{\sin\alpha}{y} \qquad \cos\beta = \frac{e_3p_1\cos\alpha + e_2p_3}{p_1m_3y}$$
$$y^2 = \frac{m_3^2p_1^2 + p_3^2p_1^2\cos^2\alpha + 2p_1p_3e_2e_3\cos\alpha + p_3^2e_2^2}{p_1^2m_3^2} \tag{VII.12}$$

The expressions obtained are :

$$(1)\left|\begin{array}{l} z_{14} \\ -(e_1+e_2)p_1\sin\alpha/(m_3y) \\ (e_1e_3 - p_1p_3\cos\alpha)/m_3 \end{array}\right. \quad (2)\left|\begin{array}{l} -p_1y \\ 0 \\ (e_2e_3 + p_1p_3\cos\alpha)/m_3 \end{array}\right. \quad (3)\left|\begin{array}{l} 0 \\ 0 \\ m_3 \end{array}\right. \quad (4)\left|\begin{array}{l} z_{44} \\ -(e_3+e_4)p_3\sin\alpha/(m_3y) \\ (e_3e_4 + p_3^2)/m_3 \end{array}\right. \tag{VII.13}$$

where :

$$z_{14} = yp1 - \frac{(e_1+e_2)p_3(e_3p_1\cos\alpha + e_2p_3)}{m_3^2p_1y}, \qquad z_{44} = -\frac{(e_3+e_4)p_3(e_3p_1\cos\alpha + e_2p_3)}{m_3^2p_1y}. \tag{VII.14}$$

The angle β is the angle of transformation of the scattering matrix in the helicity formalism. In the non-relativistic case, $e_3 = m_3$ and $e_2 = m_2$; the angle β is then the angle in the Laboratory system minus the angle in the Center of mass system. For the target, the quantification axis is opposite to the momentum is the Center of mass system: in the formulae above, p_3 must be changed into $-p_3$, e_3 and m_3 in e_4 and m_4 respectively.

A.5 Angles in the laboratory system

The transformations can be continued :

A.5.a Laboratory system - Oz outgoing direction

This frame is obtained by a special Lorentz transformation with :

$$\cosh x = \frac{e_2e_3 + p_1p_3\cos\alpha}{m_2m_3}, \qquad \sinh x = \frac{yp_1}{m_2} \tag{VII.15}$$

The expressions obtained are :

$$(1)\left|\begin{array}{l} z_{15} \\ -(e_1+e_2)p_3\sin\alpha/(m_3y) \\ (e_1e_2+p_1^2)/m_2 \end{array}\right. \quad (2)\left|\begin{array}{l} 0 \\ 0 \\ m_2 \end{array}\right. \quad (3)\left|\begin{array}{l} m_3p_1y/m_2 \\ 0 \\ (e_2e_3+p_1p_3\cos\alpha)/m_2 \end{array}\right. \quad (4)\left|\begin{array}{l} z_{45} \\ -(e_3+e_4)p_3\sin\alpha/(m_3y) \\ (e_2e_4-p_1p_3\cos\alpha)/m_2 \end{array}\right. \tag{VII.16}$$

where :

$$z_{15} = \frac{(e_1+e_2)(e_2p_3\cos\alpha + e_3p_1)}{m_2m_3y}, \qquad z_{45} = \frac{p_1p_3e_2(e_4-e_3)\cos\alpha + p_1^2e_3e_4 - p_3^2e_2^2 + p_1^2p_3^2\sin^2\alpha}{m_2m_3p_1y}. \tag{VII.17}$$

The scattering angle in the Laboratory system γ corresponding to the scattering angle α in the center of mass system is such that :

$$\begin{aligned} \sin\gamma &= \frac{\sin\alpha}{z}, \qquad \cos\gamma = \frac{e_2p_3\cos\alpha + e_3p_1}{p_1m_2z} \\ z^2 &= \frac{p_1^2p_3^2\cos^2\alpha + 2p_1p_3e_2e_3\cos\alpha + p_3^2m_2^2 + e_3^2p_1^2}{p_3^2m_2^2} \end{aligned} \tag{VII.18}$$

A.5.b Laboratory system - Oz incoming direction

This frame is obtained by a rotation of angle γ in the tri-dimensional space or from the first frame by a special Lorentz transformation with $\cosh x = e_2/m_2$ and $\sinh x = p_1/m_2$:

$$(1)\left|\begin{array}{l} p_1(e_1+e_2)/m_2 \\ 0 \\ (e_1e_2+p_1^2)/m_2 \end{array}\right. \quad (2)\left|\begin{array}{l} 0 \\ 0 \\ m_2 \end{array}\right. \quad (3)\left|\begin{array}{l} (p_3e_2\cos\alpha + p_1e_3)/m_2 \\ p_3\sin\alpha \\ (e_2e_3+p_1p_3\cos\alpha)/m_2 \end{array}\right. \quad (4)\left|\begin{array}{l} (p_1e_4 - p_3e_2\cos\alpha)/m_2 \\ -p_3\sin\alpha \\ (e_2e_4-p_1p_3\cos\alpha)/m_2 \end{array}\right. \tag{VII.19}$$

The angle γ in the laboratory system is given in function of the angle α in the center of mass system by :

$$\sin\gamma = x\sin\alpha, \qquad \cos\gamma = x\frac{e_2p_3\cos\alpha + e_3p_1}{m_2p_3} \tag{VII.20}$$

Using :

$$A = \frac{e_2}{m_2}, \qquad B = \frac{e_3p_1}{m_2p_3}, \tag{VII.21}$$

we have :

$$\tan\gamma = \frac{\sin\alpha}{A\cos\alpha + B} \tag{VII.22}$$

This relation can be inverted by :

$$\tan\alpha = \sin\gamma\frac{B\cos\gamma + AC}{C\cos\gamma - AB\sin^2\gamma}, \qquad C^2 = (A^2-B^2)\sin^2\gamma + \cos^2\gamma \tag{VII.23}$$

The factor multiplying the cross-section in the center of mass system to obtain the cross-section in the Laboratory system is:

$$\frac{d(\cos\alpha)}{d(\cos\gamma)} = \frac{\left[(A\cos\alpha+B)^2 + \sin^2\alpha\right]^{\frac{3}{2}}}{A + B\cos\alpha} \tag{VII.24}$$

In the non relativistic case, these formulae are simplified only by the fact that $A = 1$ because $e_2 = m = 2$. .

A.6 Conclusions

If the observables are not defined in the center of mass system, the scattering matrix has to be rotated. For a scattering angle α in the center of mass system, the rotation needed to describe the polarisation of the outgoing particle is given by Equ. (VII.12), that is :

$$\tan\beta = -\frac{p_1 m_3 \sin\alpha}{e_3 p_1 \cos\alpha + e_2 p_3} \tag{VII.25}$$

and the rotation needed to describe the polarisation of the target nucleus is :

$$\tan\beta = -\frac{p_1 m_4 \sin\alpha}{e_4 p_1 \cos\alpha - e_2 p_4} \tag{VII.26}$$

with relativistic kinematics. In the non relativistic approximation, the energies e are replaced by the masses m in Equ. (VII.24) and (VII.26).

If the observables are defined with only one axis of quantification along the incoming direction, the collision matrix must be rotated with the angle $-\alpha$.

If an angular distribution is requested in the Laboratory system, the angle α in the center of mass system is given by Equ. (VII.23) for the angle γ in the Laboratory system. Cross-sections only must be multiplyed by the factor given by Equ. (VII.24). Here also, the non relativistic approximation is obtained by replacing the energies e by the masses m.

B Coefficients $3j$, $6j$ and $9j$

Clebsch-Gordan coefficients are used only in the computation of reduced nuclear matrix elements, with the function `DJCG`. These reduced matrix elements need also some $6j$ computed by the function `DJ6J`. Clebsch-Gordan coefficients with magnetic quantum numbers zero or $(1/2, 0, -1/2)$ are given by the function `DCGS`. The subroutine `QUAN`, which computes the couplings of Equ. (III.44) needs the $9j$ coefficients given by the function `DJ9J` only for transitions with $\Delta S \neq 0$ and functions `DCGS` and `DJ6J` for all transitions.

On the contrary, the Clebsch-Gordan needed in subroutine `SCHE` to transform the results into the helicity formalism by Equ. (III.64) are obtained by recurrence.

An array of logarithms of factorials is used by the functions `DJCG`, `DJ6J` and `DCGS`.

B.1 The functions for geometric coefficients

All the arguments of these four functions are integer double values of the quantum numbers.

B.1.a Clebsch-Gordan coefficients

If one of the angular momenta is zero, the simple result is returned. If one of the magnetic quantum numbers is zero and the others 0 and $\pm\frac{1}{2}$, the simpler formula of function `DCGS` is used.

In the general case, the subroutine use the formula (21) of Appendix C in : [73] MESSIAH, A., *"Mécanique quantique"*, Dunod, Paris (1960) page 910. The last term of the sum is computed. The sum is then obtained by the `DO LOOP` :

```
|C K2,K3,K4,N1,N2,N3 ARE THE ARGUMENTS OF THE FACTORIALS IN THE LAST TERMDJCG-061
|      DO 2 I=1,K                                                       DJCG-062
|      A1=(K2-I)*(K3-I)*(K4-I)                                          DJCG-063
|      A2=(N1+I)*(N2+I)*(N3+I)                                          DJCG-064
|    2 DJCG=A4-DJCG*A2/A1                                               DJCG-065
```

Exponential is used only for the first term.

B.1.b 6j coefficients

If one of the angular momenta is zero, a simple result is returned.

In the general case, the subroutine use the formula (36) of Appendix C in Ref. [73] page 915. As for Clebsch-Gordan coefficients, the last term of the sum is computed. The sum is then obtained by a similar `DO LOOP`.

B.1.c Simple 3j coefficients

Due to the relation :

$$\begin{pmatrix} j' & J & j \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} = -\sqrt{(2l+1)(2j+1)} \begin{pmatrix} l & l' & J \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l & l' & J \\ j' & j & \frac{1}{2} \end{Bmatrix}, \tag{VII.27}$$

such a $3j$ coefficient can be used to compute Equ. (III.44) when $S = 0$ and the spins are $\frac{1}{2}$. This relation shows up in the helicity formalism for multipole expansion of an interaction (see Ref. [62]).

The function `DCGS` computes :

$$CGS = (-)^{j'+\frac{1}{2}} \sqrt{(2j+1)(2j'+1)} \begin{pmatrix} j & L & j' \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \tag{VII.28}$$

if j and j' are half integers and :

$$CGS = (-)^{j'+1} \begin{pmatrix} j & L & j' \\ 0 & 0 & 0 \end{pmatrix} \tag{VII.29}$$

if j and j' are integers.

Using :

$$g(n) = \frac{m!}{\sqrt{(n!)}} = \frac{1}{2^m} \begin{cases} \sqrt{\frac{2.4.6...n}{3.5.7...(n-1)}} & \text{if} \quad n \text{ is even} \\ \sqrt{\frac{2.4.6...(n-1)}{3.5.7...n}} & \text{if} \quad n \text{ is odd} \end{cases} \tag{VII.30}$$

where m is the integer part of $n/2$, these coefficients are :

$$CGS = (-)^{\text{Int}\{(L+j-j'+2)/2\}} \frac{g(L+j+j'+1)}{g(L+j-j')g(L-j+j')g(j+j'-L)} \tag{VII.31}$$

If j and j' are integer, this result must be :

- multiplyed by 2 if $L+j+j'$ is even,
- 0 if $L+j+j'$ is odd.

These two conditions are $\text{Int}\{(L+j+j'+1)/2\} - \text{Int}\{(L+j-j')/2\} - \text{Int}\{(L-j+j')/2\} - \text{Int}\{(j+j'-L)/2\}$ positive or zero respectively. If this quantity is negative, j and j' are half integers.

B.1.d 9j coefficients

The subroutine use the formula (41) of Appendix C in Ref. [73] page 917, which is :

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \\ j_7 & j_8 & j_9 \end{Bmatrix} = \sum_x (-)2x \begin{Bmatrix} j_1 & j_2 & j_3 \\ j_6 & j_9 & x \end{Bmatrix} \begin{Bmatrix} j_4 & j_5 & j_6 \\ j_2 & x & j_8 \end{Bmatrix} \begin{Bmatrix} j_7 & j_8 & j_9 \\ x & j_1 & j_4 \end{Bmatrix} \tag{VII.32}$$

A cyclic permutation of the lines is done to get the shortest sum on x in Equ. (VII.32). Then, the three series of $6j$ coefficients are computed by recurrence. For the first of them :

$$(x+1)A(x)\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_6 & j_9 & x-1 \end{Bmatrix} + B(x)\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_6 & j_9 & x \end{Bmatrix} + xA(x+1)\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_6 & j_9 & x+1 \end{Bmatrix} = 0 \quad \text{(VII.33)}$$

with :

$$\begin{aligned} A(x) &= \Big\{(j_1-j_9-x)(j_1-j_9+x)(j_1+j_9-x+1)(j_1+j_9+x+1)(j_2-j_6-x)(j_2-j_6+x) \\ &\quad (j_2+j_6-x+1)(j_2+j_6+x+1)\Big\}^{\frac{1}{2}} \\ B(x) &= (2x+1)\Big\{(j_1-j_9)(j_1+j_9+1)(j_6-j_2)(j_2+j_6+1) + \big[j_1(j_1+1)+j_2(j_2+1) \\ &\quad +j_6(j_6+1)+j_9(j_9+1)-2j_3(j_3+1)-x(x+1)\big]x(x+1)\Big\} \end{aligned} \quad \text{(VII.34)}$$

This is not a relation between "contiguous" $6j$ coefficients as defined in : [74] RAYNAL, J.,*On the definition and properties of generalized 6-j symbols"*, J. Math. Phys. **20** (1979) page 2398, but can be obtained by writing three such relations and eliminating two $6j$ coefficients between them. This relation is used to compute the $6j$ coefficients for $x_m \le x \le x_M$ with $x_m = \max\{|j_1-j_2|, |j_6-j_9|\}$ and $x_M = \min\{j_1+j_2, j_6+j_9\}$ starting from $x = x_M$ with the value 1. The first recurrence reduces to a two terms relations because the coefficient of the $6j$ coefficient for $x = x_M+1$, which does not exist, vanishes. The sum N_1 of the values obtained multiplied by $(2x+1)$ is computed; if it is larger than 10^{15}, all the values obtained before are divided by 10^{15} and N_1 is divided by 10^{30}. This method needs a working array to store all these unnormalised $6j$ coefficients and no table of logarithm. As used in `ECIS`, the series of $6j$ coefficients are short because two of the three quantum numbers L, S or I^t are in each of them.

The result of Equ. (VII.32) must be normalised by dividing by the square root of the product $N_1N_2N_3$. As the sign of the $6j$ coefficient with $x = x_M$ is $(-)^{2x_M}$ as can be seen in formula (36) in Ref. [73] when the sum reduces to only one term and as all the three x_M and x are integer or half integer at the same time, the product of all these signs is plus. The result has the correct sign.

B.2 Recurrence for $3j$ coefficients

Two different recurrence relations are used in the code `ECIS94` for two very different purposes.

B.2.a Transformation to helicity formalism

To use conveniently Equ. (III.64), for a given total angular momentum J and parity π, one needs a tri-dimensional array of which the dimensions correspond to :

1. all sets of quantum numbers (l_i, s_i, j_i, I_i) or (l_f, s_f, f_f, I_f) involved for this value of J and π,
2. all the $(2s+1)$ Clebsch-Gordan $< l, s, 0, \sigma | j, \sigma >$ for these values of (l, s, j),
3. all the $(2I+1)$ Clebsch-Gordan $jI\sigma{-}\mu JM$ for these values of (j, σ, I).

In practice, this array is built with the dimensions in the order (2),(3),(1).

The Clebsch-Gordan coefficients are ordered by increasing helicity. They can be obtained by elementary recurrence relations between "contiguous" coefficients as defined in : [75] RAYNAL, J., *"On the definition and properties of generalized 3-j symbols"*, J. Math. Phys. **19** (1978) page 467. More explicitly, a part of the Equ. (A7) in Ref. [74] is :

$$C^{te} = \Big\{-\frac{1}{2}\big[a(a+1)+b(b+1)-c(c+1)\big]-\alpha\beta-\frac{1}{3}(\alpha-\beta)\Big\}\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}$$

$$
\begin{aligned}
& -\Big\{(a+\alpha)(a-\alpha+1)(b-\beta)(b+\beta+1)\Big\}^{\frac{1}{2}} \begin{pmatrix} a & b & c \\ \alpha-1 & \beta+1 & \gamma \end{pmatrix} \\
= & \Big\{\frac{1}{2}\big[a(a+1)+b(b+1)-c(c+1)\big]+\alpha\beta-\frac{1}{3}(\alpha-\beta)\Big\} \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \\
& +\Big\{(a-\alpha)(a+\alpha+1)(b+\beta)(b-\beta+1)\Big\}^{\frac{1}{2}} \begin{pmatrix} a & b & c \\ \alpha+1 & \beta-1 & \gamma \end{pmatrix}
\end{aligned} \tag{VII.35}
$$

which can be simplified in this simple case into :

$$
\begin{aligned}
0 = & \Big\{(a+\alpha)(a-\alpha+1)(b-\beta)(b+\beta+1)\Big\}^{\frac{1}{2}} \begin{pmatrix} a & b & c \\ \alpha-1 & \beta+1 & \gamma \end{pmatrix} \\
& +\Big\{\big[a(a+1)+b(b+1)-c(c+1)\big]+2\alpha\beta\Big\} \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \\
& +\Big\{(a-\alpha)(a+\alpha+1)(b+\beta)(b-\beta+1)\Big\}^{\frac{1}{2}} \begin{pmatrix} a & b & c \\ \alpha+1 & \beta-1 & \gamma \end{pmatrix}
\end{aligned} \tag{VII.36}
$$

and give for the $< j, I, \sigma, -\mu | J, \sigma-\mu >$ the following recurrence relation :

$$
\begin{aligned}
0 = & \Big\{(I-\mu)(I+\mu+1)(J-\mu+\sigma)(J+\mu-\sigma+1)\Big\}^{\frac{1}{2}} < j, I, \sigma, -\mu-1 | J, \sigma-\mu-1 > \\
& -\Big\{\big[I(I+1)+J(J+1)-j(j+1)\big]+2\mu(\sigma-\mu)\Big\} < j, I, \sigma, -\mu | J, \sigma-\mu > \\
& +\Big\{(I+\mu)(I-\mu+1)(J+\mu-\sigma)(J-\mu+\sigma+1)\Big\}^{\frac{1}{2}} < j, I, \sigma, -\mu+1 | J, \sigma-\mu+1 >
\end{aligned} \tag{VII.37}
$$

and a simpler recurrence relation for $< l, s, 0, \sigma | j, \sigma >$. The sign of $< l, s, 0, -s | j, -s >$ is positive and if this coefficient does not exist, the sign of $< l, s, 0, -j | j, -j >$ is $(-)^{s-j}$. Similarly, the sign of $< j, I, \sigma, -I | J, -I >$ is also positive and if this coefficient does not exist the sign of $< j, I, \sigma, -J-\sigma | J, -J >$ is $(-)^{I-J-\sigma}$. Consequently, starting the recurrences from the most negative values, the sign is given by the number of coefficients which do not verify the usual relations on quantum numbers. Normalised values are easily obtained, summing the squares of the unnormalised coefficients for each recurrence.

B.2.b Cross-section expansion in Legendre polynomials

Two similar recurrence computations of Clebsch-Gordan coefficients are needed to obtain the coefficients of Legendre polynomials describing cross-sections.

The first of them is to obtain the product of the two reduced rotation matrix elements in the helicity Coulomb amplitude as given by Equ. (III.65). As given by Equ. (69) of Appendix C in Ref. [73] page 920, their product is :

$$
r^{(s)}_{\sigma_f,\sigma_i}(\theta) r^{(I)}_{-\mu_f,-\mu_i}(\theta) = \sum_{j=|I-s|}^{I+s} < s, I, \sigma_i, -\mu_i | j, \sigma_i-\mu_i >< s, I, \sigma_f, -\mu_f | j, \sigma_f-\mu_f > r^{(j)}_{\sigma_f-\mu_f,\sigma_i-\mu_i}(\theta) \tag{VII.38}
$$

The recurrence relation needed here is not between "contiguous" coefficients, but similar to the one used for $6j$ coefficients when computing $9j$ coefficients as shown in section (B.1.d) by Equ. (VII.33) and (VII.34). The recurrence relation can be found of Appendix C in Ref. [73], formula (20) page 910, which is :

$$
\begin{aligned}
& A(J) < j_1, j_2, m_1, m_2 | J-1, M > + B(J) < j_1, j_2, m_1, m_2 | J, M > \\
& + A(J+1) < j_1, j_2, m_1, m_2 | J+1, M >= 0 \\
& A(J) = \frac{1}{J} \sqrt{\frac{[J^2-M^2][(j_1+j_2+1)^2-J^2][J^2-(j_1-j_2)^2]}{(2J-1)(2J+1)}}, \\
& B(J) = m_1 - m_2 + M \, \frac{j_2(j_2+1)-j_1(j_1+1)}{J(J+1)}
\end{aligned} \tag{VII.39}
$$

This recurrence relation is used for increasing values of j. The normalisation is obtained by dividing by the square root of the sum of unnormalised values. The sign is such that the product of Clebsch-Gordan coefficients is positive for the highest value of j in Equ. (VII.38).

The second occurence is for the angular distribution of compound nucleus, which is given by :

$$\Big(\frac{d\sigma(\theta)}{d\Omega}\Big)_{c.n.} = \frac{1}{(2s_i+1)(2I_i+1)} \sum_{\sigma_i\sigma_f\mu_i\mu_f} \sum_J f^{(J)\ hel\ c.n.}_{\mu_f\sigma_f\mu_i\sigma_i} |r^{(J)}_{\sigma_f-\mu_f,\sigma_i-\mu_i}(\theta)|^2, \tag{VII.40}$$

which can be expressed in terms of Legendre polynonials with the relation :

$$|r^{(J)}_{m,m'}(\theta)|^2 = (-)^{m-m'} \sum_{\lambda=0}^{2J} < J,J,m,-m|\lambda,0 >< J,J,m',-m'|\lambda,0 > P_\lambda(\cos\theta) \tag{VII.41}$$

The recurrence relation needed here is the same. After simplification for this application, Equ. (VII.39) is :

$$\begin{aligned} &A(J) < j,j,m,-m|J-1,0 > + B(J) < j,j,m,-m|J,0 > \\ &+A(J+1) < j,j,m,-m|J+1,0 >= 0 \\ &A(J) = J\sqrt{\frac{(2j+1)^2-J^2}{(2J-1)(2J+1)}}, \qquad B(J) = 2m \end{aligned} \tag{VII.42}$$

Recurrences start from values 1 for $\lambda = 0$ because :

$$(-)^{m-m'} < J,J,m,-m|0,0 >< J,J,m',-m'|0,0 >= \frac{1}{2J+1} \tag{VII.43}$$

Contributions of odd values of J disappear in the sum on helicities.

C Reduced rotation matrix elements

The subroutine `EMRO` computes an array of reduced rotation matrix elements $r^{(J)}_{m,m'}(\theta)$ for $J_m \le J \le J_M$ where $J_m = \max\{m,m'\}$ and J_M is the maximum value involved. But reduced matrix elements are also computed by recurrence to rotate the scattering matrix, to factorise $(1 - x\cos\theta)$ in the amplitudes and to express the cross-sections with Legendre polynomials. For reduced rotation matrix elements, see Ref. [73] and in : [76] VARSHALOVICH, D., A., MOSKALIEV, A., N. and KHERSONSKII, V., K., *"Kvantovaya Teoriya Uglovogo Momenta"*, (*"Quantum Theory of Angular Momenta"*), Nauka, Leningrad (1975) Chapter 4.

C.1 Recurrence with respect to J

This recurrence is a simplification of Equ. (1) of section (4.8) of Ref. [76], page 79. It can be rewritten as :

$$\begin{aligned} &(J+1)\sqrt{(J+m)(J-m)(J+m')(J-m')}\ r^{(J-1)}_{m,m'}(\theta) + (2J+1)\big[mm' - J(J+1)\cos\theta\big]\ r^{(J)}_{m,m'}(\theta) \\ &+J\sqrt{(J+1+m)(J+1-m)(J+1+m')(J+1-m')}\ r^{(J+1)}_{m,m'}(\theta) = 0 \end{aligned} \tag{VII.44}$$

which allows the computation of $r^{(J_m+1)}_{m,m'}(\theta)$ for $J_m = \max\{m,m'\}$ if $r^{(J_m)}_{m,m'}(\theta)$ is known because the coefficient of $r^{(J_m-1)}_{m,m'}(\theta)$ vanishes. This starting value is given by Equ. (73) of Appendix C in Ref. [73] page 922 :

$$r^{(j)}_{m,j}(\theta) = (-)^{j-m} r^{(j)}_{j,m}(\theta) = \sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}\ \xi^{j+m}\eta^{j-m}, \qquad \xi = \cos\frac{1}{2}\theta, \qquad \eta = \sin\frac{1}{2}\theta \tag{VII.45}$$

which is obtained easily because the arguments of the subroutine EMRO, which computes the reduced rotation matrix elements include ξ, η, $\cos\theta$ and an array of square roots of integers. The recurrence given by Equ. (VII.44) used upwards seems to be stable without limitation.

If $m' = 0$, the recurrence of Equ. (VII.44) can be simplified to give :

$$\sqrt{(J+m)(J-m)}\; r^{(J-1)}_{m,0}(\theta) - (2J+1)\cos\theta\; r^{(J)}_{m,0}(\theta) + \sqrt{(J+1+m)(J+1-m)}\; r^{(J+1)}_{m,0}(\theta) = 0 \quad \text{(VII.46)}$$

If $m = 0$, we obtain the same equation with m' instead of m. The starting value are :

$$r^{(j)}_{0,j}(\theta) = (-)^j r^{(j)}_{j,0}(\theta) = \sqrt{\frac{(2j)!}{j!j!}}\; (\xi\eta)^j \quad \text{(VII.47)}$$

If $m = m' = 0$, the subroutine uses :

$$J\; r^{(J-1)}_{0,0}(\theta) - (2J+1)\cos\theta\; r^{(J)}_{0,0}(\theta) + (J+1)\; r^{(J+1)}_{0,0}(\theta) = 0 \quad \text{(VII.48)}$$

starting with $r^{(0)}_{0,0}(\theta) = 1$.

For the angular distribution of a level, this calculation is done only once for all the amplitudes involving the same values of m and m', but also for $-m$ and $-m'$, using the relation :

$$r^{(J)}_{m,m'}(\theta) = (-)^{m-m'} r^{(J)}_{-m,-m'}(\theta) \quad \text{(VII.49)}$$

C.2 Recurrence with respect to m

It can be necessary to multiply the scattering matrix by the reduced rotation matrix $r^{(j)}(\alpha)$ where j is the spin of the outgoing particle or of the recoil nucleus and α the angle given by Equ. (VII.25) or (VII.26) respectively or $\alpha = -\theta$ for observables described with only one axis of quantification. The recurrence relation is Equ. (16) or (17) of section (4.8) in [76], page 81. It is :

$$\sqrt{(j+m')(j-m'+1)}\; r^{(j)}_{m,m'-1}(\alpha) + 2\frac{m - m'\cos\alpha}{\sin\alpha}\; r^{(j)}_{m,m'}(\alpha) + \sqrt{(j-m')(j+m'+1)}\; r^{(j)}_{m,m'+1}(\alpha) = 0 \quad \text{(VII.50)}$$

which can start with $r^{(j)}_{m,j}(\alpha)$ given by :

$$\sqrt{(j+m)(j-m+1)}\; r^{(j)}_{m-1,j}(\alpha) - 2\frac{j - m\cos\alpha}{\sin\alpha}\; r^{(j)}_{m,j}(\alpha) + \sqrt{(j-m)(j+m+1)}\; r^{(j)}_{m+1,j}(\alpha) = 0 \quad \text{(VII.51)}$$

This relation is used to compute $r^{(j)}_{m,j}(\alpha)$ for m varying from $-j$ to j, starting with :

$$r^{(j)}_{-j,j} = (-\sin\frac{1}{2}\alpha)^{2j} \quad \text{(VII.52)}$$

and Equ. (VII.50) is used to compute $r^{(j)}_{m,m'}$ for m' varying from j to m. The other reduced rotation matrix elements are obtained from Equ. (VII.49).

C.3 Factorisation of $(1 - x\cos\theta)$

To accelerate convergence with respect to the total spin J, it is convenient to replace the amplitude f by an amplitude f' such that :

$$\sum_J f^{(J)}_{\mu_f\sigma_f,\mu_i\sigma_i} r^{(J)}_{m,m'}(\theta) = \frac{1}{1 - x\cos\theta} \sum_J f'^{(J)}_{\mu_f\sigma_f,\mu_i\sigma_i} r^{(J)}_{m,m'}(\theta) \quad \text{(VII.53)}$$

with $m = \sigma_f - \mu_f$ and $m' = \sigma_i - \mu_i$. Multiplying the two sides by $(1 - x\cos\theta)$ and using the Equ. (VII.44) to express the product of a reduced rotation matrix element by $\cos\theta$, we can identify the coefficients of the same $r^{(j)}_{m,m'}(\theta)$ to get :

$$\begin{aligned} f'^{(j)}_{\mu_f\sigma_f,\mu_i\sigma_i} &= -x\frac{\sqrt{(j-m)(j+m)(j-m')(j+m')}}{j(2j+1)} f^{(j-1)}_{\mu_f\sigma_f,\mu_i\sigma_i} + \Big[1 - x\frac{mm'}{J(J+1)}\Big] f^{(j)}_{\mu_f\sigma_f,\mu_i\sigma_i} \\ &\quad -x\frac{\sqrt{(j+1-m)(j+1+m)(j+1-m')(j+1+m')}}{(j+1)(2j+1)} f^{(j+1)}_{\mu_f\sigma_f,\mu_i\sigma_i} \end{aligned} \tag{VII.54}$$

which allows to obtain $f'^{(j)}$ up to $j = J_M - 1$ if the values of $f^{(j)}$ are known up to $j = J_m$. Writting this new amplitude $f'^{(j)} = f^{(j)} - xf''^{(j)}$, the value of x is obtained by :

$$D1 = \frac{1}{2}\sum_{j=J_M-5}^{j=J_M-1}(2j+1)^2\big[f^{(j)}f''^{(j)*} + f^{(j)*}f''^{(j)}\big], \qquad D2 = \sum_{j=J_M-5}^{j=J_M-1}(2j+1)^2\big[f''^{(j)}f''^{(j)*}\big], \qquad x = \frac{D1}{D2} \tag{VII.55}$$

but with the restriction $|x| < 1$. The value of x is stored instead of the real part of $f^{(J_M)}$. This process can be done again several times.

C.4 Expression of cross-sections in Legendre polynomials

If the inelastic scattering amplitudes or the elastic scattering amplitude of a chargeless particle is known up to J_M, the cross-section can be expressed as a sum of Legendre polynomials $P_l(\cos\theta)$ with l from $l = 0$ to $l = 2J_M$. For the elastic cross-section of a charged particle, the Coulomb cross-section must be subtracted; the remaining cross-section cannot be expanded into Legendre polynomials because it involves an interference term with the Coulomb amplitude and the Legendre expansion of the Coulomb amplitude does not converge. So, the difference between elastic and pure Coulomb cross-section must be multiplied by some power of $(1 - \cos\theta)$ before being expanded in Legendre polynomials.

C.4.a Legendre expansion without Coulomb amplitude

The contribution to the cross-section of an helicity amplitude being :

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{1}{(2s_i+1)(2I_i+1)}\left|\sum_J f^{(J)\ hel.}_{\mu_f\sigma_f\mu_i\sigma_i} r^{(J)}_{\sigma_f-\mu_f,\sigma_i-\mu_i}(\theta)\right|^2 \tag{VII.56}$$

its expression as an expansion on Legendre polynomials and the coefficients are :

$$\frac{d\sigma(\theta)}{d\Omega} = \sum_L (2L+1)A_L P_L(\cos\theta), \qquad A_L = \frac{1}{2}\int \frac{d\sigma(\theta)}{d\Omega} P_L(\cos\theta) d\cos\theta \tag{VII.57}$$

The coefficient of $P_0(\cos\theta)$ is quite trivial :

$$A_0 = \frac{1}{(2s_i+1)(2I_i+1)}\sum_J \frac{1}{2J+1}\left|f^{(J)\ hel.}_{\mu_f\sigma_f\mu_i\sigma_i}\right|^2 \tag{VII.58}$$

and can be generalised to any $P_L(\cos\theta)$ if one defines :

$$F_L = P_L(\cos\theta) f^{hel.}_{\mu_f\sigma_f\mu_i\sigma_i} = \sum_J F^{(J)}_L r^{(J)}_{\sigma_f-\mu_f,\sigma_i-\mu_i}(\theta) \tag{VII.59}$$

and use :

$$A_L = \frac{1}{(2s_i+1)(2I_i+1)}\sum_J \frac{1}{2J+1} f^{(J)\ hel.}_{\mu_f\sigma_f\mu_i\sigma_i} F^{(J)\ *}_L. \tag{VII.60}$$

The F_L can be obtained with the same recurrence relations as the $P_L(\cos\theta)$. This give for their coefficients, using again $m = \sigma_f - \mu_f$ and $m' = \sigma_i - \mu_i$:

$$\begin{aligned} F_L^{(J)} &= -\frac{L-1}{L}F_{L-2}^{(J)} - \frac{2L-1}{L}\Big\{\frac{\sqrt{(J-m)(J+m)(J-m')(J+m')}}{J(2J-1)}F_{L-1}^{(J-1)} + \frac{mm'}{J(J+1)}F_{L-1}^{(J)} \\ &\quad + \frac{\sqrt{(J+1-m)(J+1+m)(J+1-m')(J+1+m')}}{(J+1)(2J+3)}F_{L-1}^{(J+1)}\Big\} \end{aligned} \tag{VII.61}$$

easy to use because the dependence on L is very simple and the dependence in J is the same for every L and can be stored. In this process, the number of J values increases with L.

C.4.b Legendre expansion of Coulomb amplitude

To generalise this calculation to the elastic scattering of charged particle, the helicity amplitude in Equ. (VII.59) does not include the coulomb amplitude. To obtain F_0 :

1. the helicity amplitude without Coulomb amplitude is multiplied by $(1-\cos\theta)^2$, using recurrence relations on the reduced rotation matrix elements and also by $(1+\cos\theta)$ for identical particles, giving $h(\theta)$,
2. the two reduced matrix elements in the spin space are multiplied as shown by Equ. (VII.38), giving some function $g(\theta)$,
3. the Legendre expansion of the Coulomb amplitude multiplied by $(1-\cos\theta)^n$ or $(1-\cos^2\theta)^n$ is generated as :
$$c(\theta) = \sum_L (2L+1)C_L^{(n)}\ P_L(\cos\theta) \tag{VII.62}$$
4. $g(\theta)$ is multiplied by $c(\theta)$ and added to $h(\theta)$ to get the function F_0 used in Equ. (VII.60) to compute A_0 :
$$F_0 = h(\theta) + g(\theta)\ c(\theta) = h(\theta) + \sum_L (2L+1)C_L^{(n)}G_L \tag{VII.63}$$
where the G_L are defined with respect to $g(\theta)$ as F_L was defined with the helicity amplitude in Equ. (VII.59).

Then, the computation of the coefficients A_L can be done as in the absence of Coulomb amplitude. This expansion must be done up to $J_M + L_M$ where L_M is the maximum L value for the A_L requested and J_M the maximum J value of the amplitudes.

The Legendre expansion of the coulomb amplitude multiplied by any power of $(1-\cos\theta)$ is :

$$(1-\cos\theta)^n f_c(\theta) = \sum_l (2l+1)C_l^{(n)}P_l(\cos\theta) \tag{VII.64}$$

For a symmetrised amplitude, we can use the relation :

$$(1-\cos^2\theta)^n = \sum_{m=0}^{m=n} \frac{n!}{m!(n-m)!}(-)^m 2^{n-m}(1-\cos\theta)^{n+m} \tag{VII.65}$$

The coefficients $C_l^{(n)}$ have quite simple recurrence relations. For a given value of n, all the coefficients needed are given by :

$$C_{l+1}^{(n)} = \frac{l+1-n+i\eta}{l+1+n-i\eta}C_l^{(n)} \tag{VII.66}$$

starting with :

$$C_0^{(n)} = -2^n\frac{i\eta}{n-i\eta}C_0^{(0)} \tag{VII.67}$$

With the convention $\sigma_0 = 0$ used in `ECIS`, $C_0^{(0)} = 1/(2ik)$.

Chapter VIII

Description of the subroutines

We shall describe the subroutines in the order of their appearance in the code ECIS94. The Table of Contents of these paragraph will reproduce a flow chart of the programme.*Italic characters shifted to the right side indicates comments related to a calling subroutine.*

All the steps of the calculation are managed by 240 logicals from LO(1) to LO(250). They are :

(a) from LO(1) to LO(100), the values read in the second and the third cards of the input; the meaning of those which are used can be found in the "DESCRIPTION OF INPUT".

(b) from LO(101) to LO(200), the opposite values of the preceding one.

(c) from LO(201) to LO(250), internal controls of the code; the meaning of those which are used is given as comment cards in subroutine CALC reproduced below.

```
|C LO(201) IS TRUE IF THERE IS NO REAL SPIN-ORBIT POTENTIAL              CALC-038
|C LO(202) IS TRUE IF THERE IS NO IMAGINARY SPIN-ORBIT POTENTIAL         CALC-039
|C LO(203) IS TRUE IF THERE IS NO COULOMB SPIN-ORBIT POTENTIAL           CALC-040
|C LO(204) IS TRUE IF CONVERGENCE IS OBTAINED IN THE ITERATION           CALC-041
|C LO(205) IS TRUE IF CONVERGENCE IS OBTAINED FOR THIS EQUATION          CALC-042
|C LO(206) IS TRUE WHEN THE ITERATION IS NOT THE LAST ONE PERMITTED      CALC-043
|C LO(207) IS TRUE IF ALL THE COUPLINGS HAVE TO BE CALCULATED BEFOREHAND CALC-044
|C LO(208) IS TRUE IF THE DIAGONAL COULOMB CORRECTIONS ARE NEEDED        CALC-045
|C LO(209) IS TRUE FOR DIRAC POTENTIALS                                  CALC-046
|C LO(210) IS TRUE IF DERIVATIVES ARE NEEDED                            CALC-047
|C LO(211) IS TRUE IF DEFORMATIONS ARE CHANGED IN SEARCH                CALC-048
|C LO(212) IS TRUE IF NUCLEAR PARAMETERS ARE CHANGED IN SEARCH          CALC-049
|C LO(213) IS TRUE IF NUCLEAR MATRIX ELEMENTS ARE CHANGED IN SEARCH     CALC-050
|C LO(214) IS TRUE IF SPIN-ORBIT PARAMETRISATION IS CHANGED IN SEARCH   CALC-051
|C LO(215) IS TRUE FOR NO OUTPUT                                         CALC-052
|C LO(216) IS TRUE FOR A STOP, FOR EXAMPLE THE WORKING FIELD IS TOO SMALLCALC-053
|C LO(217) IS TRUE FOR ALL THE CALCULATIONS EXCEPT THE FIRST             CALC-054
|C LO(218) IS TRUE FOR LAST RESULTS                                      CALC-055
|C LO(219) IS TRUE FOR RESULTS WITHOUT DOING THE CALCULATION AGAIN       CALC-056
|C LO(220) IS TRUE FOR OUTPUT AND LAST CALCULATION IS THE BEST ONE       CALC-057
|C LO(221) IS TRUE FOR OPTICAL MODEL WITHOUT COUPLING                    CALC-058
|C LO(222) IS TRUE IF IT IS THE FIRST COMPUTATION FOR THIS ENERGY        CALC-059
|C LO(223) IS TRUE IF LO(18) IS .TRUE. AND NO SPIN IN THE INITIAL STATE  CALC-060
|C LO(224) IS TRUE FOR COMPOUND NUCLEUS OR PUNCH OF TRANSMISSION COEFF.  CALC-061
|C LO(225) IS TRUE IN CAL1 FOR A CALL TO USUAL COUPLED EQUATIONS SUBR.   CALC-062
|C LO(226) IS TRUE IF THERE ARE OBSERVABLES IN THE LABORATORY SYSTEM     CALC-063
|C LO(227) IS TRUE FOR COULOMB CORRECTIONS WITH PURE REGULAR FUNCTIONS   CALC-064
|C LO(228) IS TRUE FOR NO COPY OF UNCOUPLED FUNCTIONS AND PHASE-SHIFT    CALC-065
```

A Subroutines ECIS/CALS, HORA, STIM and MEMO

For the MAIN, the subroutines ECIS/CALS, HORA, STIM and MEMO, see Chapter II, *"Use on various Computers".*

1. The MAIN defines only the working array and calls CALC, directly or via the Assembler subroutine ECIS on IBM, or via CALS on CDC 7600.

2. 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.

3. The subroutine STIM should give the time remaining for the JOB. This subroutine is very machine dependent. It is called directly by CALC to obtain the time needed by a single calculation to stop an automatic search when LO(34)=.TRUE. and to save results or a search before being stopped by time limitation. STIM allows to the subroutine HORA to print the elapsed time.

4. The subroutine MEMO is called from anywhere to increase the size of the working array. On computers other than CDC or UNIVAC this subroutine stops the calculation if the request is absolute. This subroutine is also very machine dependent.

We shall not quote the calls to HORA or MEMO in the description of the subroutines.

B Subroutine CALC

The main subroutine is CALC, from which the calculation never returns. Its arguments are the working array and its length. The same working array is floating values and integers in the CDC version, also double precision in the IBM version. This subroutine calls the subroutines CALX, COLF, REDM, EXTP, CAL1, VARI, FITE, REST, EVAL which we describe below. Meaning of addresses stored in the common /DECOU/ and defined in CALC after the return from CALX are given on COMMENT cards.

The computation is normally stopped by a control word read in subroutine CALX, so there is usually a warning at the compilation "subprogram exit cannot be reached from entry".

The calculation never returns to the first instructions which are values of the Atomic Mass Unit M_u, $\hbar c$ and fine structure constant, as shown in section (VII.A) and the calculation of $M/(\hbar c)$, $2M/(\hbar c)^2$ and $\hbar c\alpha$. Then CALC calls CALX.

C Subroutine CALX

At the beginning of this subroutine is given on comment cards the meaning of the arrays SP, IPI, WV which store all the informations relative to the levels. They are followed by the meaning of data and addresses stored in the common /DECOU/ and some informations on other commons. The subroutine calls INPA, INPB, INPC, LECL, LECT, DEPH, LECD and OBSE.

This subroutine reads all the input except for nuclear matrix elements and external form factors and new parameters if LO(37)=.TRUE.. This input starts by a title card :

- if this title is "FIN ", the calculation is stopped,
- if this title is "DESCRIPTION ", the description of the input is printed.

C.1 Subroutines INPA, INPB, INPC

These three 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 programme. Output can be listed as FORTRAN or by "enscript -2Bhr -L58" after suppression of the first column. It is 27 pages long.

After the printing, a new title card is read in CALX. *If the title card is neither "*FIN *" or "*DESCRIPTION *", the subroutine* CALX *reads the first card of logical control (card 2) : if* LO(36)=.TRUE. *(restart of a computation from file 8), the subroutine returns to* CALC *which calls to the subroutine* REST. *If* LO(36)=.FALSE.*, the second card of logical control (card 3) and card 4 (integers) are read. Some logical controls can be changed (for example, the real spin-orbit must be deformed if the imaginary spin-orbit is deformed) before being printed. Then the card 5 (floating values) is read and default values for card 4 and 5 are set and the values printed. The logicals from* LO(211) *to* LO(220) *are set .FALSE. and* LO(222) *is set .TRUE..*

Then, informations needed when some logicals are .TRUE. are read :

- *limitation on angular momenta for coulomb corrections if* LO(45)=.TRUE.*,*
- *compound nucleus data or indication to calculate the Legendre Polynomial expression of cross-sections if* LO(84)*,* LO(85)*,* LO(86) *or* LO(65) *is .TRUE.,*
- *interpolation on total spin if* LO(43)=.TRUE.*.*

Some default options are set. The subroutine computes storage requirements as soon as it can be done and calls LECL*,* LECT *and* DEPH *with only some storage calculations between them.*

C.2 Subroutine LECL

This subroutine reads energies, masses, spins and product of charges for all the levels. Informations relevant of the nuclear model are read for coupled states but not for uncoupled states introduced in a compound nucleus calculation. For the level I, the informations are stored in SP(3,I), IPI(3,I) and WV(11,I) in the following order :

SP(1,I) s_I spin of incident particle,

SP(2,I) I_I spin of the target,

SP(3,I) Z_I product of the charges of the particle and the target,

IPI(1,I) π_I parity (0 for "+" and 1 for "–"),

IPI(2,I) $n_I = 2s_I + 1$ multiplicity of the incident particle,

IPI(3,I) $N_I = 2I_I + 1$ multiplicity of the target,

IPI(4,I) position of the potential used,

IPI(5-6,I) beginning and end in the description of amplitudes (defined in DEPH),

IPI(7-8,I) beginning and end in the description of observables (defined in DEPH),

IPI(9,I) cross-reference to potentials (if there are more potentials than levels, this table is extended to the number of potentials),

WV(1,I) m_I mass of the incident particle,

WV(2,I) M_I mass of the target (for relativistic kinematics, LO(8)=.TRUE., the target mass is corrected by addition of Q/M_u but this correction is dropped if LO(44)=.TRUE. to compute the wave number in the Schrödinger formalism),

`WV(3,I)` E_I energy in the center of mass system; for the incident channel, this energy is given by Equ. (VII.8) if `LO(8)=.FALSE.` (non relativistic kinematics) or by Equ. (VII.4) if `LO(8)=.TRUE.` (relativistic kinematics); for the other channels $E_I = E_1 - Q$.

For the other entries of `WV`, see description of `COLF`.

The wave number of the ground state is computed only to obtain the default options of matching radius and step size in `LECT`. The same computation will be done in `COLF` for all the levels.

C.3 Subroutine LECT

This subroutine reads the description of the phonons if there are some in the nuclear model, the deformations for the rotational model and the optical potentials if `LO(7)=.FALSE.` (no external potential). The default value of the matching radius is so that the largest potential is less than the data `ACONV` of card 5 and the default value of the step size to the smaller of half diffuseness and $1/(2k)$ where k is the wave number of the ground state. The step size is modified to be the matching radius divided by an integer. The logical asking for deformation of the real spin-orbit, the imaginary spin-orbit, the coulomb or the spin-orbit coulomb potentials is set `.FALSE.` if these interactions vanish.

If `LO(7)=.TRUE.`, the default value of the matching radius is 20fm and the default value of the step size is given only by the wave number. The logicals for deformation of spin-orbit potentials can be changed if there is no spins in the levels. However, without spin-orbit coulomb potential and no coulomb corrections, one must use `LO(46)=.TRUE.`. This subroutine returns also in the `COMMON TITLE` the factor `XZ` equal to 10 divided by the multiplicity of the initial channel (`IPI(2,1)` and `IPI(3,1)` defined in `LECL`), used by the subroutine `SCAT` to express the cross-sections in millibarns.

Then the subroutine reads :

- angles for equidistant angular distributions if `LO(66)=.FALSE.`,
- spin-orbit parametrisation if `LO(4)=.TRUE.`,
- Hauser-Feshbach parameters if `LO(82)=.TRUE.`,
- Fission penetrabilities if `LO(85)=.TRUE.`,
- Gamma penetrabilities if `LO(86)=.TRUE.`.

C.4 Subroutine DEPH

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.

In the first one, 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. The number of solutions and of equation for each parity is obtained in NCT. For each level, beginning and end addresses are stored in `IPI(5,I)` and `IPI(6,I)` respectively.

In the second part, the default output is generated unless `LO(94)=.TRUE.`, in which case the instructions are read. For each level, beginning and end addresses of instructions are stored in `IPI(7,I)` and `IPI(8,I)` respectively. This subroutine reads also instructions for restricted coulomb corrections if `LO(44)` and `LO(46)=.TRUE.`. Addresses of coulomb corrections are stored after the array of beginning and end of coupling `NIV` (see `REDM`) in `NIV(I,J,3)`.

If `LO(31)=.TRUE.`*, the subroutine* `CALX` *reads number of angular distributions and of parameters in search.*

C.5 Subroutine LECD

This subroutine reads the angular distributions.

The subroutine CALX *reads identifications and step sizes of the parameters in search if* LO(32)=.TRUE. *and if their number and the number of angular distributions are non zero.*

C.6 Subroutine OBSE

This subroutine computes for all the observables the indications (described on COMMENT cards) for the do-loops and the geometrical coefficients which will be needed in SCAT to obtain the observables requested. A first part reads indications for non standard observables and transform them into tensor notations. 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.

After return from OBSE*, the subroutine* CALX *computes some storage requirement and a table of logarithms of factorial as long as needed.*

After return to CALC *from* CALX*, the subroutine* REST *is called with* KF=1 *if* LO(36)=.TRUE. *(restart of a search). If* LO(36)=.FALSE. *the subroutine* COLF *is called.*

D Subroutine COLF

This subroutine and the other subroutines called in it compute the matching values and the stored integrals for coulomb corrections. The array WV(11,I) is completed for all the levels, coupled or uncoupled. Using the recoil ratio R_{ec} to take into account recoil corrections for a zero-range interaction when the masses are not the same in all the channels ($R_{ec} = 1$ for the incident channel, but for the excited channels $R_{ec} = M_1/M_i$ if the mass of the particle is not the same and if LO(93)=.FALSE.), the content of this array is :

WV(4,I) k_I wave number; if LO(8)=.FALSE. : it is given by Equ. (VII.8) and if LO(8)=.TRUE. by Equ. (VII.6),

WV(5,I) η_I coulomb parameter,

WV(6,I) $\sqrt{R_{ec}k_I/k_1}$, square root of ratio of wave numbers,

WV(7,I) E_{Irel} relativistic energy in the center of mass system in Dirac formalism in Mev,

WV(8,I) square root of $2m/\hbar^2$,

WV(9,I) k_iR_{ec}, wave number multiplied by ratio of step sizes,

WV(10,I) $h_i^2k_i^2$ where h_i is the last item,

WV(11,I) $h_i = h_1R_{ec}$ step size of this channel.

The subroutine COCL is called for closed channels and the subroutine FCOU for open channels.

D.1 Subroutine COCL

This subroutine computes matching values for closed channels. For $L = 0$, it uses asymptotic expansion with/without backwards integration. For the other values of L, it uses upwards recurrence. This subroutine comes from the Buck and Hill's code INCH.

D.2 Subroutine FCOU

This subroutine and the subroutines called by it are described in Ref. [18] and Ref. [19]. 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 for VAX computers to handle squares of Coulomb functions.

The subroutine FCOU calls FCZ0 to obtain coulomb functions and their derivatives for $L = 0$ and computes the other ones by recurrence. It uses upwards recurrence for irregular to the end and for regular functions as long as $\rho > \eta + [\eta^2 + L(L+1)]^{\frac{1}{2}}$, downwards recurrence for the regular function starting from the maximum L requested plus $25 + 5|\eta|$ normalised with the last value obtained from upwards recurrence.

D.2.a Subroutines FCZ0

The subroutine FCZ0 computes the coulomb functions for $L = 0$. It calls the function SIGM to obtain the phase-shift. For some values of the coulomb parameter and the radius, it calls the subroutines YFRI or YFAS. For some other values near the origin, it computes the regular function by expansion into Chebyschev polynomial (Clenshaw expansion) or series expansion and calls YFIR for the irregular one.

D.2.b Subroutine YFRI

For some values of the matching radius and of the coulomb parameter, it calls YFCL. For other values, it uses Riccati methods, "Riccati at the origin" or "asymptotic Riccati".

D.2.c Subroutine YFAS

Computes coulomb functions with the asymptotic expansions.

D.2.d Subroutine YFIR

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.

D.2.e Subroutine YFCL

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.

D.2.f Functions SIGM, PSI

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.

The subroutine COLF *checks if some coulomb functions are too large. If the power of* $10.^{15}$ *returned by* FCOU *is not zero, it limits the number of Coulomb functions to avoid them (with a ratio* 10^{30} *between regular and irregular functions, the phase-shift obtained by the code cannot be significative). If coulomb corrections have to be used, it calls subroutine* CORI *to compute the stored integrals with all the previous channel up this one, if the pair of channels are both open and the corrections requested.*

D.3 Subroutine CORI

If $\eta_i > 2.2\eta_f$, the code is unable to do the calculation and stops. If $\eta_i = 0$, η_f must be also zero : the subroutine CORZ is called and CORI returns.

In any other case, the subroutine CORI calls the subroutine CORO to obtain the integrals from R_m to ∞ of product of regular and irregular Coulomb functions with $L = 0$ and $L = 1$, divided by r and r^2. Then, if $\eta_i = \eta_f$ and $k_i = k_f$, the integrals from 0 to infinity of the product of two regular Coulomb functions divided by r^2 are obtained by Equ IV.23. Details are given in section (IV.B).

D.3.a Subroutine CORO

This subroutine computes the integrals from R_m to ∞ of the product of two different regular or irregular coulomb functions with the same angular momentum $L = 0$ and $L = 1$ divided by r and r^2 (16 values). With $3R_s = \max[(5|\eta_i| + 22.5)\sqrt{k_f/k_i}, (5|\eta_f| + 22.5)\sqrt{k_i/k_f}, .18\sqrt{\eta = i\eta_f})$, these integrals are computed from $\max(R_m, R_s)$ to ∞ by a generalisation of the method described in Ref. [66]. If $R_s > R_m$, the integral between R_m and R_s is computed by 40 points Gauss integrations, each Gauss integration being for $\Delta r < 20$.

D.3.b Subroutine CORZ

This subroutine computes integrals from R_m to ∞ of products of regular and irregular functions of the same L divided by r^3 and integrals from 0 to ∞ of regular functions od the same L divided by r^3.

Then the coulomb phase-shift minus the one for $L = 0$ are computed in COLF.
After return from COLF*, the subroutine* CALC *calls* REDM.

E Subroutine REDM

This subroutine generates or reads the reduced nuclear matrix elements between the coupled levels. If LO(7)=.FALSE. (standard nuclear model) and LO(15)=.FALSE. (reduced nuclear matrix elements not read), REDM calls the subroutines VIBM, ROTM or ROAM. If LO(7)=.TRUE. or LO(15)=.TRUE., this subroutine reads the reduced matrix elements. Then, the informations are stored in IQ(4,I) and T(4,I) which are in equivalence, for I=1 to IT.

IQ(1,I) Form factor identification (see DESCRIPTION OF INPUT),

IQ(2,I) L transferred angular momentum,

IQ(3,I) $10000(2\Delta S) + 10(2\Delta J) + 10a + b$, where $a = b = 0$ usually, but $a = 1$ for existence of spin-orbit deformation and $b = 1$ for a magnetic Coulomb excitation with $\lambda = L - 1$,

T(4,I) Reduced nuclear matrix element multiplied by $(-1)^{\mathrm{Int}(L/2)}$.

The address of the first and the last reduced nuclear matrix element between level I and level J are in NIV(1,I,J) and NIV(2,I,J) respectively. The table NIV is completed if there are uncoupled states for which an angular distribution is requested and the reduced nuclear matrix elements written on file 7 as they should be read if LO(61)=.TRUE. .

Then, the table of IM multipoles, IVQ(3,I) is generated :

IVQ(1,I) L transferred angular momentum,

IVQ(2,I) $2\Delta S$ twice the transferred spin to the particle,

`IVQ(3,I)` $2\Delta J$ twice the transferred spin to the target or 0 if $\Delta S = 0$.

followed by a table of form factors `IVZ(7,I)` including correction terms (with external potentials and monopole or dipole corrections to vibrations in the rotational model) :

`IVZ(1,I)` Form factor control number,

`IVZ(2,I)` Address in the table of multipoles,

`IVZ(3,I)` 0 or address of the first spin-orbit form factor,

`IVZ(4,I)` 0 or address of the temporary Coulomb form factor,

`IVZ(5,I)` 0 or address of the temporary Coulomb spin-orbit form factor,

`IVZ(6,I)` 0 or address of correction term (positive for corrected term, negative for correction term),

`IVZ(7,I)` L transferred angular momentum.

The array `IQ` has been changed to be :

`IQ(1,I)` Address in the table of form factors IVZ

`IQ(2,I)` Address in the table of multipoles IVQ

`IQ(3,I)` 0 or address of the spin-orbit form factor

but `T(4,I)` is unchanged. A table `ITX` of the 8 starting addresses of potentials and 8 starting addresses of transition form-factors is built with :

`NV` Number of real form factors (`INVT+2 INLS`),

`MV` Number of imaginary form factors,

`INVT` Number of transitions, without correction terms,

`INLS` Number of spin-orbit form factors not taking into account multiplication by 2,

`INVC` Number of coulomb transition form factors,

`INVD` Idem for coulomb spin-orbit,

`INTC` Same as INVT but including correction terms.

These numbers include dummy central form factors for magnetic coulomb excitations.

The reduced nuclear matrix elements are written and/or punch on file 7 on request.

In a search, this subroutine is called again if some nuclear parameter is changed (there is no nuclear parameter if `LO(7)=.TRUE.`). At the end of a search is called again if reduced nuclear matrix elements have to be printed or punched.

E.1 Subroutine `VIBM`

Computes the reduced nuclear matrix elements of the vibrational model, taking into account that the phonons amplitudes and a factor $(n!\sqrt{4\pi})^{-1}$ is shifted to the radial form factors. This subroutine is limited to two-phonons states and second order vibrations and uses the functions `DJCG` and `DJ6J`. There is a transposition relation :

E.2 Subroutine ROTM

Computes the reduced nuclear matrix elements of the symmetric rotational model. This subroutine calls the function DJCG.

E.3 Subroutine ROAM

Computes the reduced nuclear matrix elements of the asymmetric rotational model. This subroutine calls the function DJCG. If LO(2)=.TRUE. the mixing parameter of the second level is used as the asymmetry gamma angle and the mixing parameter of the first levels are computed from it.

E.4 Function DJCG

Computes Clebsh-Gordan coefficients. The subroutine verifies triangular relations. For more details see section (VII.B.1.a).

E.5 Function DJ6J

Computes $6j$ coefficients. The function tests if some angular momentum is zero to use simpler expression. For more details see section (VII.B.1.b).

After the call to REDM*, at the first calculation (*LO(225)=.TRUE.*), if* LO(7)=.TRUE. *(external potentials), the subroutine* EXTP *is called. After return from it, informations from* REDM *are copied after those of* EXTP *and the whole is shifted down (to prevent against variation of the size of informations from* REDM *in a search).*

F Subroutine EXTP

The subroutine EXTP calls only the function DCGS to obtain the geometrical coefficient of a particle-hole excitation. The form factors are read in any order. In case of error, the subroutine prints the list of form factors not yet read under the form (I,J) where $\hat{I}$ varies from 1 to 8 and $\hat{J}$ is the potential if less or equal to the number n_p of potentials and J$-n_p$ is the form factor in the order printed by REDM if $j > n_p$; the subroutine stops after this output.

The subroutine CALC *computes storage requirements for potentials, calls the subroutine* STIM *to obtain remaining time before calculation. Then,* CALC *calls* CAL1.

G Subroutine CAL1

This subroutine computes from form factors to final results. It calls the subroutines POTE, CONU, QUAN, MTCH, INTI, INTR, INCH, SCAM, SCHE and RESU. If the computation is the last one of a search :

- if no printing is requested, LO(219)=.TRUE.,
- if the printing related to LO(53) or LO(55) to LO(58) and the punching related to LO(62), LO(64) or LO(65) (this last one if LO(41)=.TRUE.) are not requested, and if the last χ^2 is the best one, LO(220)=.TRUE.,
- if LO(220)=.FALSE., all the calculation has to be done again.

If LO(220)=.TRUE. and the printing of potentials is requested, CAL1 calls the subroutine POTE and the subroutine SCHE after return. If LO(219)=.TRUE., CAL1 calls the subroutine SCHE.

First, CAL1 set to 0 all the memories needed for the computation of potentials and calls POTE.

G.1 Subroutine POTE

This subroutine computes the form factors.

It calls the subroutines ROTP, FOLD and STDP.

If LO(220)=.TRUE. and LO(51)=.TRUE., this subroutine prints only the form factors.

For standard models, there is a do-loop on the potentials, of which only the first is deformed. For each potential, POTE calls the subroutine ROTP and, if LO(17)=.TRUE. (folding), the subroutine FOLD. Instead of that, if LO(7)=.TRUE. (external potentials), POTE calls the subroutine STDP. If LO(61)=.TRUE., the potentials are punched on file 7 with the format needed by subroutine EXTP. In the Schrödinger formalism, volume and surface potentials are added together.

If there are some, corrections are done. Separately for central , spin-orbit, coulomb and spin-orbit coulomb transition form factor in the Schrödinger formalism, the scalar, vector, tensor, coulomb transition form factors in the Dirac formalism, the correction form factor is added to the form factor to be corrected in such a way that the integral with r^{L+2} vanishes. For spin-orbit transition form factors in the Schrödinger formalism, it is the form factor V_λ/r^2 which is used with a factor r^{L+4}.

From there, the subroutine proceeds quite differently for the two formalism :

- **Schrödinger formalism** including equivalent for a Dirac formalism.

  The coulomb potentials are added to the central ones, keeping their strengths in VCO for the potentials (correction to r^{-1} behaviour) and in VDO for the transitions. The coulomb magnetic form factors are multiplied by $\hbar c/m_r M_u$. The potentials are printed on request.

- **Dirac formalism**

  The Schrödinger potential for each level j is computed separately and stored in the array V(*,I,J) with I=1 to I=14, real part for odd I and imaginary part for even I :

V(*, 1,J)	Central potential,
V(*, 3,J)	Spin-orbit potential,
V(*, 5,J)	$D = E + m - V_v + V_s$ divided by $\hbar c$,
V(*, 7,J)	$D' = E - m - V_v - V_s$ divided by $\hbar c$,
V(*, 9,J)	$(E + m - V_v + V_s)^{\frac{1}{2}}$ more precisely square root of V(*, 5,J),
V(*,11,J)	$(E + m - V_v + V_s)^{-1}$ multiplied by $\hbar c$,
V(*,13,J)	Tensor potential multiplied by $\hbar c$.

  The transitions are stored after that beginning by the scalar and vector ones :

V(*, 1,J)	$V_v^\lambda + V_s^\lambda$ to use between large components,
V(*, 3,J)	$V_v^\lambda - V_s^\lambda$ to use between small components.

  followed by the tensor ones :

V(*, 1,J)	derivative of the tensor potential $\frac{d}{dr}V_T^\lambda$,
V(*, 3,J)	tensor potential V_T^λ divided by r.

The strengths of the coulomb potentials are kept in VCO and those of coulomb transitions in VDO. The coulomb magnetic form factors are multiplied by $\hbar c/m_r M_u$. The potentials are printed on request.

G.1.a Subroutine ROTP

This subroutine computes the potentials and the transition form factors for all the standard models. It calls the subroutines ROTD, ROTZ, COPO and DERI.

If a diffuseness, except for the coulomb potentials, is less than .02 times the step size, it is changed into the maximum of its opposite and .02*step size; if a radius is less than the step size and symmetrised Woods-Saxon potentials are not used, it is changed into the maximum of its opposite and the step size (this can be useful in a search).

For the asymmetric rotational model, this subroutine uses a large array of weights and rotation matrix elements which are DATA in ROTD. The symmetric rotational model uses one half of a 20 points Gauss-Legendre integration of which abscissae and weights are DATA in POTE. A table of deformation is built for all the transition for factors and the subroutine ROTD is called to get the number of points of angular integration, starting values, increments and so on.

For each value of r and for each angle (see ROTD), up to the fourth derivative can be needed (spin-orbit transition for the third order of the anharmonic vibrational model). They are stored in VR(6,10) (10 for the 8 components of the potential plus 2 Schrödinger spin-orbit, 6 for up to the second derivative and third order vibration in the Dirac formalism). In the Dirac formalism using Schrödinger equivalent (LO(99)=.TRUE.), the subroutine ROTZ is called. In other formalisms, the coulomb potentials and transitions for a non diffuse charge are computed; the charge distributions of diffuse charges are obtained as the other components of the potential. The angular integrated values are stored differently in the two formalism.

If there is a charge diffuseness, ROTP calls COPO to obtain the coulomb potential or transition form factor from the charge distribution or transition. For spin-orbit coulomb potentials, ROTP has also to call the subroutine DERI.

G.1.a.i Subroutine ROTD

This subroutine returns the number of angular integration points, the weight, the radii and its two first derivatives at each point of each form factor.

- In the symmetric rotational model, 20 points Gauss-Legendre integration method is used, reduced to 10 points by symmetry. For a vibration, the angular dependence of the boson is included in the weight.
- In the asymmetric rotational model, 36 values of (θ, ϕ) have been chosen : the values od θ are $N\pi/14$ and for each value of N, there are $N+1$ values of ϕ equidistant from 0 to $\pi/2$. The matrix of which the elements are the rotation matrix elements for these angles and $L \leq 14$ with L and K even has been inverted. The coefficients of the 15 lowest (L, K) are stored as integration weights.
- In the vibrational model, the angular integration reduces to one point.

G.1.a.ii Subroutine ROTZ

The Schrödinger equivalent equation to the Dirac equation is supposed to describe also the inelastic scattering. For the vibrational model, the result of elastic scattering should be the same than the fure Dirac formalism; inelastic scattering is described by derivatives of these potential. In the rotational model, result should be different because gradient and Laplacian are computed on potentials depending on θ instead of its monopole part.

G.1.a.iii Subroutine COPO

Computes the coulomb potential and the coulomb interactions from the density distribution of charge and the form factors of charge transition.

G.1.a.iv Subroutine DERI

Tis subroutine returns the derivative $x(r) = -\frac{d}{dr}y(r)$ of a function $y(r)$ known by n equidistant points by steps h or this result divided by r. The formulae used are given by Equ. (III.95) to Equ. (III.97). The subroutine stops if there are less than 7 points.

G.1.b Subroutine FOLD

When called directly from POTE, this subroutine folds separately the real potential, the imaginary potential and the coulomb potential with a particle density which can be a Woods-Saxon distribution or a Gaussian one. This subroutine can be called from the subroutine STDP to perform the same operations on each components of the potentials and of the transition form factors independently. To obtain spin-orbit form factors, and derivatives in Dirac formalism, the subroutine DERI is used.

G.1.c Subroutine STDP

This subroutine computes the external form factors of which the parameters are read in EXTP and calls the subroutines INTP, STBF, COPO, DERI and FOLD. The form factors can be :

- Copy of another form factor,
- Interpolated from values read on cards by subroutine INTP, eventually derived with subroutine DERI for spin-orbit form factors or Dirac formalism,
- Woods-Saxon volume and surface form factors at some power and their derivatives which can be deformed with even or odd deformation,
- Single or product of two Laguerre polynomials or solutions in a Woods-Saxon potential computed ib subroutine STBF,
- Sums of Bessel functions or their derivatives. For $L = 0$, the zeros are $z_n = n\pi$; for $L = 1$ to $L = 11$, the $L + 1$ first zeros are stored as data; all the others are given by Mc Mahon formula which can be written here :

$$\begin{aligned} z_n &= (n + \frac{1}{2}L)\pi - \frac{L(L+1)}{(2n+L)\pi}\big[1 + \frac{7L(L+1)-6}{3(2n+L)^2\pi^2} + \frac{166L^2(L+1)^2 - 408L(L+1) + 360}{15(2n+L)^4\pi^4} \\ &\quad + \frac{6949L^3(L+1)^3 - 3352L^2(L+1)^2 + 81180L(L+1) - 75600}{105(2n+L)^6\pi^6}\big] \end{aligned} \tag{VIII.1}$$

(see Ref. [67], page 371).

If folding is requested for some form-factors, STDP calls FOLD.

G.1.c.i Subroutine INTP

Interpolates the form factors between the points given multiplied by a normalisation factor g. It is :

$$V(r) = g\sum_{i=1}^{i=4} V(r_i)\prod_{j\neq i}\frac{r - r_j}{r_i 0 r_j} \tag{VIII.2}$$

with, as long as possible, $x_1 < x_2 < x < x_3 < x_4$.

G.1.c.ii Subroutine STBF

This subroutine computes a Laguerre polynomials or search on the depth of a real Woods-Saxon potential for a bound state with a given binding energy. With negative binding energy, this subroutine returns a real scattering state normalised to $sinkr + \delta$ at infinity.

For the last calculation, after return from POTE, CAL1 *calls* SCHE *if* LO(220)=.TRUE.. *In all other cases, the memories needed for the S-matrix, the compound nucleus results and the integrated cross-sections are set to 0. If there is compound nucleus (*LO(81)=.TRUE.*), the subroutine* CONU *is called.*

G.2 Subroutine CONU

This subroutine does the preliminary calculations for compound nucleus, as introduced in ANLECIS by [77] MOLDAUER, P., A., *"ANLECIS"*, presented at the Workshop on Nuclear Model Computer Codes, Trieste (1984). If there are uncoupled states, CONU computes their transmission coefficients, using the subroutines MTCH and INSH or INRH in the Schrödinger and the Dirac formalism respectively.

There is a pseudo-loop on parities (first, same parity for the levels and the angular momentum and, last, opposite parities) and inside it, another do-loop on the total angular momentum. Inside these two pseudo-loops, CAL1 *calls the subroutine* QUAN.

G.3 Subroutine QUAN

This subroutine find the quantum numbers of all the equations coupled for a given total angular momentum J and a given parity. If there are none for the first level, it returns to CAL1. The subroutine computes all the coupling between equations and scans if some coefficients are zeros or can be summed up. The coefficients between levels I1 and I2 are multiplied by WV(8,I1)*WV(8,I2). Results less than 10^{-10} are eliminated. The address of the first coefficient is stored in NVI(1,I1,I2), the address of the last one in NVI(2,I1,I2) and the address of the last derivative one in NVI(3,I1,I2). The subroutine counts the number of couplings coupling between the equations and tests if there will be derivatives of the functions. This subroutine calls the functions DCGS, DJ6J and DJ9J.

G.3.a Function DCGS

This subroutine computes special Clebsch-Gordan coefficients for which the formula involves no summation. For more details, see section (VII.B.1.c).

G.3.b Function DJ9J

Computes 9-j coefficients. The subroutine verifies triangular relations. For more details see section (VII.B.1.d).

After the return from QUAN, *if there is no equation for the first level, the pseudo-loop is ended; otherwise,* CAL1 *calls the subroutine* MTCH. *Up to the call to subroutine* SCAM, *all the levels are considered as incoming if compound nucleus or output of transmission coefficients are requested.*

G.4 Subroutine MTCH

If LO(227)=.FALSE., as in the beginning of the do-loop on angular momenta of the subroutine CAL1, this subroutine computes matching values for each equation and corrections to the S-matrix by integrals from the matching radius to infinity of regular and irregular Coulomb functions divided by some power of r if Coulomb corrections are requested. At the end of the do-loop, it can be called with LO(227)=.TRUE. and computes only integrals from 0 to infinity of products of regular Coulomb functions to obtain the reactance K-matrix. MTCH calls the subroutines CORA to get the coefficients α and β of Equ IV.23 and LINS to obtain the S-matrix from a K-matrix. For more details, see section (IV.A).

G.4.a Subroutine CORA

For given angular momenta, this subroutine returns the four coefficients α needed in the asymptotic region in Equ IV.23, if its last argument is .TRUE. (this argument is LO(227). When this last argument is .FALSE., it returns also the four other coefficients β needed for finite integrals. For limitations, see INPUT DESCRIPTION.

G.4.b Subroutine LINS

This subroutine solves a complex linear system of equations with real and imaginary parts in different array. This subroutine is also called by INCH.

After return from MTCH *and after some storage evaluations :*

- *If* LO(227)=.TRUE.*, the subroutine* CAL1 *skips the numerical integration and calls* SCAM *at the end of the loop on total angular momentum,*
- *If* LO(100)=.TRUE. *(Dirac formalism), the subroutine* CAL1 *calls first* INTR *and then* SCAM*,*
- *If* LO(21)=.TRUE. *or* LO(225)=.TRUE. *(Schrödinger formalism with usual coupled equations), the subroutine* CAL1 *calls first* INCH *and then* SCAM*.*
- *In other cases, the subroutine* CAL1 *calls* INTI *and then :*
  - *If convergence is not obtained (*LO(204)=.FALSE.*) and if* LO(23)=.TRUE. *to allow that,* LO(225) *is set* .TRUE. *and the subroutine* QUAN *is called again with the same quantum numbers.*
  - *In any other case, the subroutine* CAL1 *calls* SCAM*.*

G.5 Subroutine INTI

This subroutine solves the set of coupled equations by iterations. First, it calls the subroutine INSH to solve the diagonal homogeneous equations, unless there is indications from QUAN that this solution has been conserved. If all the coupling have to be computed (LO(207)=.TRUE.), their are computed and the address of the real and the imaginary coupling between equation I1 and I2 are stored in NVI(1,I1,I2) and NVI(2,I1,I2), those of the derivative coupling in NVI(3,I1,I2) and NVI(4,I1,I2). The system is solved for each equations related to the first level :

- This uncoupled solution and its phase-shift is transferred as the corresponding function of the complete solution, eventually with a preliminary call to the subroutine INSI to derive the uncoupled function,
- The iteration procedure is started :
  - If there are Coulomb corrections, the matching conditions are computed, using the phase-shifts known at that stage,

- The subroutine INSI is called,
- The equations of which the coupling is too small are counted,
- The maximum phase-shift is computed to be compared to 10^{10} to decide that it is the last iteration.

G.5.a Subroutine INSH

This subroutine solves a single homogeneous equation. It computes the potential and solve the equation with the Numerov or the Modified Numerov method, with a correction term if LO(26)=.TRUE.. The matching is with two points. If there is only elastic scattering, computation of transmission coefficients for uncoupled state, the subroutine returns. Otherwise, the solution is normalised, the point from which the solution is larger than a minimum value obtained. For DWBA (LO(92)=.TRUE.), the subroutine returns at this point; otherwise, the irregular solution computed by backward integration down to this point.

G.5.b Subroutine INSI

This subroutine solves the inhomogeneous equation. The second members are obtained by multiplication of the coupled solution with the potentials and the geometrical coefficient or with the coupling if LO(207)=.TRUE. (usually quicker). The contribution of the derivative of coupled solution is added. the subroutine compute from which point the inhomogeneous term is not too small. Unless there is no inhomogeneous term :

- the integral of the regular uncoupled function with the inhomogeneous term is computed,
- the phase-shift is obtained,
- if LO(92)=.FALSE. (not pure DWBA) the backward integral with the irregular uncoupled function and the solution taking into account correction for the Green's function are obtained in the same loop,
- the subroutine computes the point from which the solution is not too small.

If the difference with last iteration is too large, that the iteration is at least the fourth one, that convergence was obtained for all the other equations in this iteration, INSI calls the subroutine PADE. If needed, it computes the derivative multiplied by r with formulae analogous to those of DERI. This subroutine can be used to do only this last derivation.

G.5.c Subroutine PADE

This subroutine is called by INSI and INRI. It computes Pade approximants with the results of all the iterations. It evaluates them with all the partial series and returns the mean value of the two nearest successive results if convergence is obtained.

G.5.d Subroutine INCH

This subroutine is called by CAL1 as an alternative to the call to subroutine INTI to use usual coupled equations instead of iterations. It solves the system of coupled equations with the Modified Numerov method. It computes the matrices of coupling in as many points as possible, leaving free the place of a first matrix. Then it computes $V'_{i,j} = V_{i,j} - h^2 \sum_k V_{i,k} V_{k,j}/12$, shifting the result downwards. These values are used in the integration procedure. If LO(42)=.TRUE., there is a Schmidt's orthogonalisation procedure between the solutions every ITERM points. The matching uses the values at two points. The C-matrix is obtained by a call to the subroutine LINS. Lines of the C-matrix are computed instead of columns. However, if coulomb corrections, Hauser-Feshbach corrections or punch of penetrabilities are requested, the complete matrix is computed. For Coulomb corrections, another system of linear equations is built and solved with the subroutine LINS (see Ref. [7], Equ (35) and explanations above it).

G.6 Subroutine INTR

This subroutine is similar to INTI. It calls the subroutines INRH and INRI instead of INSH and INSI. The mean difference is the storage of tensor form factors.

G.6.a Subroutine INRH

This subroutine solves a single homogeneous equation with the Schrödinger equivalent potential obtained in POTE. It computes the potential and solve the equation with the Numerov or the Modified Numerov method, with a correction term if LO(26)=.TRUE.. The matching is with two points. If there is only elastic scattering, computation of transmission coefficients for uncoupled state, the subroutine returns. Otherwise, the large component is computed and the point from which it is larger than a minimum value obtained, the two solutions are derived and the small components obtained with the Dirac equation.

G.6.b Subroutine INRI

This subroutine solves the inhomogeneous equation in the Dirac formalism. With tensor interaction instead of deformed spin-orbit, the operations are very similar to those of subroutine INSI. The subroutine INRI calls the subroutine PADE in the same circumstances as subroutine INSI. Corrections for finite step size are given by Equ. (III.106) and (III.107).

G.7 Subroutine SCAM

This subroutine computes the transmission coefficients if they are requested. For compound nucleus, SCAM computes gamma, fission and find transmission coefficients of uncoupled states related to this total angular momentum. This subroutine stores the results of coupled equations in a two dimensional array in such a way that one index is the total angular momentum and, for a fixed values of the other, the quantum numbers are increased by the difference of total angular momentum. This disposition will make interpolation easier. If iterations are used, the crude results are multiplied by WV(6,I) where I is the level, to avoid any further factor in the computation of cross-sections. If usual coupled equations are used, they are divided by this quantities to take into account that a line of the matrix has been obtained instead of a column. If compound nucleus is used, results related to this total angular momentum are computed and stored. SCAM calls the subroutine DIAG to diagonalise the S-matrix if LO(83)=.FALSE..

G.7.a Subroutine DIAG

This subroutine diagonalises a hermitian complex matrix with an extension of Jacobi's method. Real and imaginary values are in different array.

> *In subroutine* CAL1*, there are the tests of convergence to end the pseudo-loop on total angular momentum or to shift from nuclear to asymptotic region when there are coulomb corrections.*
>
> *If the pseudo-loops are ended,* CAL1 *calls the subroutine* SCHE, RESU, *set* LO(217)=.TRUE., LO(222)=.FALSE. *and returns.*

G.8 Subroutine SCHE

This subroutine computes an array of square roots of integer. If LO(219)=.TRUE., the subroutine returns; if LO(220)=.TRUE., it calls LCSP if requested and returns. In other cases, this subroutine replaces the values stored by the subroutine SCAM by the scattering coefficients in the helicity formalism. First, the subroutine computes a table of quantum numbers. Then, the interpolations are done if they are needed (on the complex values or on their polar expression, by the method used in subroutine INTP).

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 and computes the Hauser-Feshbach corrections if they are requested. The scattering coefficients are symmetrised for identical particle and target with non zero spins. Then, the reactions cross-sections are computed. If `LO(65)=.TRUE.` (Legendre expansions printed and punched), the subroutine `LCSP` is called. If `LO(220)=.FALSE.` and `LO(41)=.TRUE.` (factorisation of $1 - x\cos\theta$), new amplitudes f'^J are computed as described in section (VII.C.3).

G.8.a Subroutine LCSP

This subroutine computes the coefficients of the expansion of the cross-sections in terms of Legendre polynomials. For charges particles elastic scattering, the cross-section is multiplied by $(1-\cos\theta)^n$ where n is given (default option $n = 2$) for different particle and target, by $(1-\cos^2\theta)^n$ for identical particle and target. Only even coefficients are given for compound nucleus contribution. See section (VII.C.4).

G.9 Subroutine RESU

This subroutine prints comparison of computed values and experimental values, computes experimental normalisations and χ^2, prints results at equidistant angles. In a search, if the computation is ended, the subroutine copies the scattering matrices related to the best χ^2. Then, for each angular distribution, `RESU` calls the subroutine `SCAT` for each data and computes the partial χ^2. If the χ^2 is the best obtained up here, the scattering matrices are copied in another array. If complete output is requested, results are printed and a graph can be drawn by a call to the subroutine `GRAL`; cross-sections and polarisations are computed at equidistant angles by the subroutine `SCAT` and a graph can be drawn by the subroutine `GRAL`. If results are requested in the Laboratory system, the angles are transformed by Equ. (VII.23) before the call to subroutine `SCAT` and the cross-sections multiplyed by the factor given in Equ. (VII.24).

G.9.a Subroutine SCAT

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 `EMRO`. A simple loop gives the cross-section in all cases (they are the sum of the squares of the amplitudes multiplied by `XZ` computed in subroutine `LECT`) 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 `OBSE` 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 by Equ. (VII.25), (VII.26) or the angle $-\theta$.

G.9.b Subroutine EMRO

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. Square roots are avoided by a table of square roots of integer as argument. In fact, there are three independent computations: one if none of the two magnetic quantum numbers are zeros, the second if one of them is zero and the third if both of them are zeros.

G.9.c Subroutine GRAL

This subroutine prints graphs of cross-sections or polarisations. For different values of its last argument, it can print or not experimental data on the same graph.

After the return from `CAL1`, *in the subroutine* `CALC` *:*

- *if there is no automatic search of if it is to its end,*
  - *if* LO(37)=.TRUE. *the subroutine* EVAL *is called,*
  - *if* LO(37)=.FALSE. *the working array is given back and the subroutine* CAL1 *is called; the computation can be stopped by a card "FIN ".*
- *if there is an automatic search which is not finished,*
  - *the subroutine* STIM *is called to get the time needed in* CAL1*,*
  - *the subroutine* VARI *is called with* KF=1*,*
  - *if* LO(35)=.TRUE. *and it is the last run allowed for the job, the subroutine* REST *is called with* KF=0*,*
  - *then the subroutine* FITE *is called,*
  - *the subroutine* VARI *is called with* KF=0*.*

H Subroutine VARI

This subroutine is called before FITE with its first argument KF=1 and after the return from FITE with KF=. Its second argument is the control KE of FITE. At the first call (KF=1 and KE=0), the subroutine defines the variables in search. For all the calls with KF=1, the χ^2 value are only printed. When called after FITE, the parameters are set to their values for the next evaluation and if the calculation has to be stopped for any reason, the final parameters are printed.

I Subroutine REST

The first argument of this subroutine, KF can be 0 or 1. If KF=0, the commons and the beginning of the working array which is needed to restart the calculation are written on tape 8. If KF=1, these commons and the working array are read from the tape to restart the search.

J Subroutine FITE

This is the χ^2 minimising subroutine FITEX written by G. SCHWEIMER, slightly modified. It calls the subroutines FIT1 and FIT2.

J.1 Subroutine FIT1

Minimisation of the χ^2 for one variable. It is used if there is only one variable in search but also if the subroutine FITE find a linear dependency of the χ^2 on the variables.

J.2 Subroutine FIT2

This subroutine replaces the subroutines LILESQ and INVATA of G. SCHWEIMER. If the last argument LLO=.TRUE. , it solves a linear least square problem $||B - A * D|| = Min.$ If LLO=.FALSE., it inverses the product matrix $A^{\dagger}A$. The same Householder transformation is used in the two cases.

After return from the second call to VARI*,* CALC *calls* REDM *if a nuclear parameter has been changed or at the end of a search if the nuclear matrix elements have to be printed or punched. Then,* CALC *calls again* CAL1*.*

If LO(36)=.TRUE. *after return from* CALX*,* CAL1 *calls* REST *with* KF=1 *to restart a search. Then* CAL1 *calls* FITE *if the search is not ended or goes to the second call of* VARI *if the search was ended.*

At the end of a search, CALC *calls* REST *with* KF=0 *if* LO(35)=.TRUE. *and calls* EVAL *if* LO(37)=.TRUE.*. Otherwise,* CALC *calls again* CALX*.*

K Subroutine EVAL

This subroutine is called if LO(37)=.TRUE. . All the parameters on which there can be automatic search can be changed for a new calculation. The total energy can also be changed in this subroutine, to simplify the input for the calculation of an excitation function.

> *After the call to* EVAL*, the subroutine* CALC *calls again the subroutine* COLF *if the total energy has been changed, the subroutine* REDM *if some nuclear parameters or nuclear matrix elements are modified, the subroutine* CAL1 *in the other cases.*

L Summary

Without the calls to MEMO, HORA and STIM, the structure of the code is given by the following table :

```
| CALC  CALX (INPA, INPB, INPC, LECL, LECT, DEPH, LECD, OBSE)
|  ''   COLF  FCOU  FCZO......
|  ''    ''   COCL
|  ''    ''   CORI  CORO  FCOU  FCZO.....
|  ''    ''    ''   CORZ
|  ''   REDM  VIBM (DJCG, DJ6J)
|  ''    ''   ROTM  DJCG
|  ''    ''   ROAM  DJCG
|  ''   EXTP  DJCG
|  ''   CAL1  POTE  ROTP (ROTD, ROTZ, COPO, DERI)
|  ''    ''    ''   STDP  STBF  FCOU  FCZO......
|  ''    ''    ''    ''   FOLD  DERI
|  ''    ''    ''    ''  (INTP, COPO, DERI)
|  ''    ''    ''   FOLD  DERI
|  ''    ''   CONU  MTCh (CORA, LINS)
|  ''    ''    ''  (INSH, INRH)
|  ''    ''   QUAN (DCGS, FJ6J, DJ9J)
|  ''    ''   MTCH (CORA, LINS)
|  ''    ''   INTI  INSH
|  ''    ''    ''   INSI  PADE
|  ''    ''   INCH (INSH, LINS)
|  ''    ''   INTR  INRH
|  ''    ''    ''   INRI  PADE
|  ''    ''   SCAM  DIAG
|  ''    ''   SCHE (DJ6J, LCSP)
|  ''    ''   RESU  SCAT  EMRO
|  ''    ''    ''   GRAL
|  ''   VARI
|  ''   REST
|  ''   FITE (FIT1, FIT2)
|  ''   EVAL
```

where (PRO1,PRO2,PRO3) means that these 3 subroutine are called by the subroutine written on the left and call nothing by themselves. For Coulomb functions, this Table must be complete by :

```
| FCOU  FCZO  YFAS
|  ''    ''   YFIR (YFAS,PSI)
|  ''    ''   YFRI  YFCL  PSI
|  ''    ''   SIGM
```

which occurs in 3 places.

Chapter IX

Conclusion

A Test cases

Nine test cases have been chosen to help to use ECIS94. There are quite arbitrary. There are identifyed by TSTx in columns 73-80.

The first of them, with the titles :

```
ESSAI DU NOYAU COMPOSE - USUAL COUPLED EQUATIONS                          TST1-000
ESSAI DU NOYAU COMPOSE - USUAL ITERATIONS                                TST1-024
ESSAI DU NOYAU COMPOSE - ITERATIONS WITH DEFORMED SPIN-ORBIT POTENTIAL   TST1-048
```

is compound nucleus at low energy. The same calculation with 3 levels and 2 uncoupled levels is done :

- without spin-orbit deformation, without iterations and without angular distribution of uncoupled states,
- without spin-orbit deformation, with iterations and with angular distribution of the first uncoupled states,
- with spin-orbit deformation, with iterations and with angular distribution of the two uncoupled states,

Results show that the spin-orbit deformation does not matter in this case.

The second test case, with the title :

```
28 SI + 104 MEV ALPHAS, SYMMETRIC ROTATOR, NON STANDARD OBSERVABLES      TST2-000
```

shows different ways to define observables.

The third test case, with the title :

```
CA40 A 497 MEV  RELATIVISTE SAME AS ECIS88                               TST3-000
```

shows the use of Dirac formalism.

The fourth test case, with the title :

```
 12N+208PB 780 MEV ELECTIC AND MAGNETIC COULOM INTERACTION               TST4-000
```

use a magnetic $M1$ and electric $E2$ Coulomb interactions.

The fifth test case, with the title :

```
COMPARAISON AVEC CHUCK POUR BE8  DWBA                                  TST5-000
COMPARAISON AVEC CHUCK POUR BE8  COUPLED EQUATIONS                     TST5-047
```

is the example of section (VI.D.2) and shows that the result with coupled equations is quite different of the result of `DWBA`.

The sixth test case, with the title :

```
TEST EXTERNAL POTENTIALS  INPUT AS ECIS88                              TST6-000
TEST EXTERNAL POTENTIALS  NEW INPUT                                    TST6-106
```

compare an input with external potentials as needed by `ECIS88` with one of the new possibilities of `ECIS94`. The last calculation is done again to show the use of the subroutine `EVAL`.

The seventh test case, with the title :

```
ESSAI PARTICULES IDENTIQUES ET POLYNOMES DE LEGENDRE                   TST7-000
```

is a calculation with identical particle of spin one half. The expansion in Legendre polynomials of the cross-sections are written on file 7.

The eighth test case, with the title :

```
 28SI + 16O  56.MEV  G.S. , 1.78 MEV.   HEAVY IONS OPTION              TST8-000
 28SI + 16O  56.MEV  G.S. , 1.78 MEV.   RESTART                        TST8-110
```

is an automatic search on 3 parameters which needs about 24 calculations. After 12 calculations, the job is saved on file 8 and restarted to the end.

The ninth test case, with the title :

```
NEUTRON DE 14. MEV SUR GADOLINIUM  COUL. SPIN-ORBITE DEFORME           TST9-000
NEUTRON DE 14. MEV SUR GADOLINIUM  COUL. SPIN-ORBITE NON DEFORME       TST9-019
```

is a calculation for neutron with spin-orbit Coulomb potential. The two calculations, with and without deformation of this interaction gives almost the same results.

B Missing topics

Many points quite important are not in this report :

- a detailed description of the reduced matrix elements used in the macroscopic models,
- relation between form factors of `ECIS94` and of `DWBA91`
- more details on identical particle and target,
- more details on the use of form factors expanded with Bessel functions,
- details on the manipulation of symmetrised Woods-Saxon form factors,
- explanations on the interpolations,
- and so on.

The most important point missing here is **Compound Nucleus**.

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