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WORKSHOP ON NUCLEAR MODEL COMPUTER CODES

16 January - 3 February 1984

STRONG CHANNEL COUPLING METHOD FOR CROSS-SECTION CALCULATIONS

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The code ECIS[1] has been developed to study polarization effects in inelastic proton scattering[2] around 20 MeV. It takes into account spin-orbit deformation which has large effects on the inelastic analyzing powers. Such experimental data have been measured recently for neutrons but are less precise and more difficult to get than those for charged particles. This code is also used for heavy ions scattering and includes a special method to deal with long range contributions of the Coulomb interaction[3]. It has been extended to deal with many kinds of coupled channel problems and its last version is ECIS 79.

The code uses an iteration procedure which will be described in details because it is not secure. The convergence of results can be obtained with Pade approximants but there is some numerical limit which must be understood. This iteration procedure is necessary with spin-orbit deformation. We shall give some informations on the integration methods in order to show how to check the precision of the results and on automatic search methods on the parameters.

There are two versions of the code : a single precision one for CDC-like computers and a mixed single-double precision for IBM. This last version can be used on a VAX computer after some modifications of constants. The code uses a working array where all quantities are stored. The size of this array varies widely from problem to problem. When possible, it uses dynamic allocation of this array (CDC, CRAY, UNIVAC). On an IBM the size of the working array can be controled by the job card.

1. THE PHYSICAL PROBLEM

There are standard nuclear models as rotational and vibrational models for which the code computes reduced matrix elements and form factors. The models can be generalized if the user provides himself these reduced matrix elements and form-factors.

1.1. The optical model

The elastic scattering of a particle by a medium or heavy nucleus of mass A and charge Z for an energy E is described by the solution of

$$(T-E+V_{opt})\psi = 0 \qquad (1)$$

where T is the kinetic energy. The usual optical model is :

$$V_{opt} = -V_1 f(r,a_1,R_1) - iV_2 f(r,a_2,R_2) + 4ia_3 V_3 \frac{d}{dr} f(r,a_3,R_3) + \left(\frac{\hbar}{2M\pi}\right)^2 2\vec{s}.\vec{\nabla}\{V_4 f(r,a_4,R_4) + iV_5 f(r,a_5,R_5)\}\wedge\vec{\nabla} + V_{coul} \qquad (2)$$

where f is the Saxon-Woods form factor :

$$V(r,a,R) = (1+\exp((r-R')/a))^{-1} \quad \text{with} \quad R' = R\,A^{1/3}$$

The first form factor in (1) is the real potential ; the second and the third are the volume and the surface imaginary potential (the surface imaginary potential is used for nucleon and deuterons at low energy, the volume imaginary potential is used above 50 MeV or for heavier particles). The fourth and the fifth form factors are the real and imaginary spin-orbit potentials : $M\pi$ is the pion rest mass, and $\vec{s}$ the spin of the incident particle. The factor 2 is introduced because the Pauli matrix σ is used for spin 1/2 particles instead of $\vec{s}$. This factor 2 is generalized to any spin for coupled channel calculations, but not in the spherical optical model. As a consequence, the strength of the spin-orbit interaction used in coupled channel calculations is the half of the one published in the literature for a particle of spin larger or equal to unity. The expression written in (2) is the spin-orbit which has to be taken into account in coupled channel calculations. For the elastic scattering, it reduces to the usual expression 1/r d/dr f(r,a,R). For an incident particle of charge z, the coulomb potential V_{coul} is usually calculated from a uniformly charged sphere of radius $R'_c = R_c\,A^{1/3}$:

$$V_{coul} = \frac{z\,Ze^2}{R'_c}\left(\frac{3}{2} - \frac{r^2}{2R'^2_c}\right) \quad \text{for} \quad r < R'_c$$

$$= \frac{z\,Ze^2}{r} \quad \text{for} \quad r > R'_c \qquad (3)$$

There is also a coulomb spin orbit term, due to the interaction of the magnetic moment of the incident particle and the electric field of the target. This term is very important for the description of the polarization at small angles of the elastic scattering of neutrons. It is not included in the code ECIS 79.

The solution of Eq. (1) must be a plane wave plus an outgoing wave.

Its asymptotic form must be given by

$$\psi_\sigma = \exp(i\vec{k}.\vec{r}+i\eta\,\ell n(kr-\vec{k}.\vec{r}))\,|\sigma> + \Sigma_{\sigma'}\,\frac{1}{r}\,f_{\sigma\sigma'}(\theta)$$
$$\exp(ikr-\eta\,\ell n(2kr))\,|\sigma'> \qquad (4)$$

where σ is the component of the spin at the infinity, k the momentum and η the Coulomb parameter. The solution can be expanded on spin-angular functions

$$Y_{\ell sjm} = i^\ell \Sigma <\ell s\mu\sigma|jm>Y_\ell^\mu(\hat{r})|s\sigma> \qquad (5)$$

with

$$\psi_\sigma = 4\pi\,\frac{1}{kr}\,\Sigma\ \exp(i\sigma_\ell)f_{\ell j}(r) <\ell s\mu\sigma|jm>Y_{\ell sjm}Y_\ell^{\mu*}(\hat{k}) \qquad (6)$$

where σ_ℓ is the Coulomb phase shift. Introducing this expansion in (1) and projecting on the various spin angular functions, we obtain

$$\left\{\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2 - \frac{2\mu}{\hbar^2}\left(V^{opt}_{central} + \gamma\, V^{opt}_{sp.or}\right)\right\} f_{\ell j}(r) = 0 \qquad (7)$$

where μ is the reduced mass and γ the eigenvalue of $(2\vec{\ell}.\vec{s})$. We obtain single equations for any spin if there are only central and spin-orbit potential. However, for a spin larger or equal to 1, a tensor potential leads to coupled equations. The solution of Eq. (7) must vanish at the origin ; beyond the range of nuclear potentials, it can be expressed by the two standard solutions of the equations : the regular Coulomb function, $F_\ell(\eta,kr)$ and the irregular one, $G_\ell(\eta,kr)$:

$$f_{\ell j}(r) = F_\ell(\eta,kr) + C_\ell^j(G_\ell(\eta,kr)+i\,F_\ell(\eta,kr)) \qquad (8)$$

Introducing this asymptotic form into Eq. (6) and identifying it with Eq. (4), we obtain

$$f_{\sigma\sigma'}(\theta) = \delta_{\sigma\sigma'}f_\ell(\theta) + \frac{4\pi}{k}\sum_{\ell,j}\exp(2i\sigma_\ell)C_\ell^j<\ell s\mu\sigma|jm><\ell s\mu'\sigma'|jm>$$
$$Y_\ell^{\mu*}(\hat{k})Y_\ell^{\mu'}(\hat{r}) \qquad (9)$$

where $f_\ell(\theta)$ is the Coulomb amplitude :

$$f_\ell(\theta) = -\frac{\eta}{2k\,\sin^2\frac{1}{2}\theta}\exp\left(-i\eta\,\ell n\left(\sin^2\frac{1}{2}\theta\right) + 2i\sigma_o\right) \qquad (10)$$

Cross-section and polarizations are computed from these amplitudes.

1.2. The rotational and the vibrational model

The optical model can be extended to describe the target nucleus in its excited states. In the rotational model, the radii R are replaced in the optical potential by

$$R = R_o(1 + \Sigma_\lambda\,\beta_\lambda\,Y_{\lambda 0}(\theta')) \qquad (11)$$

where the β_λ describe a static deformation of the nucleus (with axial symmetry). In the vibrational model, the target is spherically symmetric but

$$R = R_o(1+\sum_{\lambda\mu}\alpha_{\lambda\mu}\,Y_{\lambda\mu}(\theta'))$$
$$= R_o\left(1 + \Sigma_\lambda\,\frac{\beta_\lambda}{\sqrt{2\lambda+1}}\,\Sigma_\mu(b^+_{\lambda\mu}+(-)^\mu b_{\lambda-\mu})Y_{\lambda\mu}(\theta')\right) \qquad (12)$$

where $b^+_{\lambda\mu}$ and $b_{\lambda,\mu}$ are the creation and annihilation operators of nuclear phonons.

In the rotational model, the potential is a function of the intrinsic axis of symmetry of the target. It can be expanded into multipoles :

$$V(r,\hat{r}') = 4\pi\sum_{\lambda\mu}V_\lambda(r)Y_\lambda^\mu(\hat{r})Y_\lambda^{\mu*}(\hat{r}') \qquad (13)$$

usually by a numerical Gauss Legendre integration on the angle between $\hat{r}$ and $\hat{r}'$. In the vibrational model, one uses a Taylor series expansion

$$V = V_o + \frac{\partial V}{dR}R_o\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_\nu^\mu + \frac{1}{2}\frac{\partial^2 V}{dR^2}R_o^2\left(\sum_{\lambda,\mu}\alpha_{\lambda\mu}Y_\nu^\mu\right)^2 \qquad (14)$$

limited to the first or to the second derivative.

The procedure to obtain coupled equations is the same as the one of optical model. Instead of the spin-angular functions (5), we use the target-spin-angular functions :

$$Y_{\ell sjIJM} = i^\ell\,\Sigma\,Y_{\ell sjm}\,\Phi_I^{m'}<j\ Imm'|JM> \qquad (15)$$

where $\Phi_I^{m'}$ is the wave function of the target. In the rotational model, a member of a rotational spectrum starting with 0^+ is

$$\Phi_I^{m'} = \sqrt{\frac{2I+1}{8\pi^2}}\,R^{(I)*}_{m'0}(\hat{r}')\chi(r') \qquad (16)$$

where $\chi(r')$ is the intrinsic function. In the vibrational model Φ_I^m is simply a one phonon or a two-phonons state. These equations are :

$$\left\{\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2\right\} f_{\ell jIJ}(r) - \frac{\hbar^2}{2\mu} \sum_{\ell' j' I'} V_{\ell jI,\ell' j' I',J}\, f_{\ell' j' I' J}(r) = 0 \tag{17}$$

The interaction (13) and (14) appears as a sum of scalar form factors $f_\lambda(r)(V_\lambda(r)$ for the rotational model, optical potential and its derivatives for the vibrational model) multiplied by a scalar product of $Y_\ell(\hat{r})$ with an operator Q_λ in the space of the target (another Y_ℓ for the rotational model, phonon creation and annihilation operators in the vibrational model). So, the Wigner-Eckart theorem gives :

$$V_{\ell jI,\ell',j',I',J} = \sum_\lambda f_\lambda(r)(-)^{J+I-s-\lambda}\, i^{\ell'-\ell}$$
$$\sqrt{\frac{(2j+1)(2j'+1)(2\ell+1)(2\ell'+1)(2\lambda+1)}{4\pi}} \begin{pmatrix} \ell & \lambda & \ell' \\ o & o & o \end{pmatrix}$$
$$\begin{Bmatrix} \ell & \lambda & \ell' \\ j' & s & j \end{Bmatrix} \begin{Bmatrix} j' & \lambda & j \\ I & J & I' \end{Bmatrix} \langle I \| Q_\lambda \| I' \rangle \tag{18}$$

for the central terms of the potential. This coefficient is real when $i^\lambda Y_\lambda$ is used systematically instead of Y_λ. For s = 0 and s = 1/2 the first 6j coefficient can be eliminated.

The product $f_\lambda(r)\langle I \| Q_\lambda \| I' \rangle$ is the aim of coupled channel calculations. It is the link between nuclear structure and scattering mechanism. If I and I' are both the 2^+ state, it is strong in the rotational model and vanishes at the first order in vibrational model. The existence of such a "reorientation term" shows up in the results of coupled channel calculations.

The number of coupled equations is larger than the number of channels taken into account. With n channels, s_i the spin of the particle, I_i the spin of the target, ε_i the product of intrinsic parities in the i-th channel for J sufficiently large and a parity π, this number is

$$N = \sum_i \frac{1}{2}\left[(2I_i+1)(2s_i+1)+\eta_i\right] \tag{19}$$

with $\eta_i = 0$ if I_i or s_i is half integer and $\eta_i = \varepsilon_i(-)^{I_i+s_i+J\pi}$, if I_i and s_i are integers. For example, the scattering of spin 1/2 particles on a $0^+-2^+-4^+-6^+$ rotational band involves 28 equations. The number of coupled equations decreases when the total J is smaller than the largest value of I_i+s_i because some quantum numbers are forbidden.

The solution of Eq. (17) must have the asymptotic form of Eq. (8) as long as the initial channel is concerned and pure outgoing waves for all the other equations. The asymptotic form of the radial solution is

$$f_i^j = F_{\ell_j}\,\delta_{ji} + C_j^i(G_{\ell_j} + iF_{\ell_j}) \tag{20}$$

The scattering amplitudes can be written in the helicity formalism (5) in which the spins of the particle are projected on their momentum. This transformation is obtained by choosing an axis of quantification along k_i for the initial state and along k_f in the final state : the helicity of the target is opposite of the projection of its spin. An amplitude is

$$f_{\mu_f\sigma_f\mu_i\sigma_i}(\theta) = \sum_J f^{(J)}_{\mu_f\sigma_f\mu_i\sigma_i} R^{(J)}_{\sigma_f-\mu_f,\sigma_i-\mu_i}(\theta) \tag{21}$$

with

$$f^{(J)}_{\mu_f\sigma_f,\mu_i\sigma_i} = \frac{1}{k_i}\sum \exp(i\,\sigma_{\ell_i}+i\sigma_{\ell_f})C_f^i \tag{22}$$
$$\langle \ell_i s 0\sigma_i | j_i\sigma_i\rangle\langle j_i I_i \sigma_i-\mu_i | JM_i\rangle\langle \ell_j s 0\sigma_f | j_f\sigma_f\rangle\langle j_f I_f\sigma_f-\mu_f | JM_f\rangle$$

where C_f^i is taken from Eq. (20). The cross-section is

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{1}{(2s_i+1)(2I_i+1)}\frac{k_f}{k_i}\sum |f_{\mu_f\sigma_f,\mu_i\sigma_i}(\theta)|^2 \tag{23}$$

A factor $\sqrt{k_f/k_i}$ can be included in $f^{(J)}$ as given by Eq. (22).

1.3. Spin orbit interaction

There are two effects which do not change merely the problem to solve coupled equations instead of a single one when going from optical model to coupled channel equations. One of them is the Coulomb interaction : the form factor for the excitation of a 2^+ states decreases as $1/r^3$ and the error introduced by integration from 0 to R is of order $1/R^2$. This difficulty can be overcomed by long range integration or some special calculation[3]. In optical model, the same problem arises from the Coulomb spin-orbit which decreases also as $1/r^3$.

The cross section is

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{e_1}{(2s_i+1)(2I_i+1)} A^{oooo}_{oooo} \qquad (38)$$

which is equivalent to (23). An observable P is defined by

$$P\, A^{oooo}_{oooo} = \sum_{\lambda_i\mu_i} x^{\lambda_3\mu_3\lambda_4\mu_4}_{\lambda_1\mu_1\lambda_2\mu_2} A^{\lambda_3\mu_3\lambda_4\mu_4}_{\lambda_1\mu_1\lambda_2\mu_2} \qquad (39)$$

For an analyzing power, $\lambda_3 = \lambda_4 = 0$ and the result do not depend on the axis of quantification of the final state. For a polarization experiment, the use of the helicity formalism leads to an axis of quantification along the direction of the outgoing particle, but in the center of mass system : we obtain Wolfenstein parameters only for a very heavy target. A rotation must be performed on the scattering matrix if $\lambda_3 \neq 0$ to project the spin of the outgoing particle on its direction in the laboratory system ; another rotation must be performed for the target if $\lambda_4 \neq 0$.

Furthermore, some theoretical considerations deal with a description of the outgoing polarizations with respect to the incident beam : for the scattering of spin 1/2 on spin 0, it is the case of Q, whereas the Wolfenstein parameters A,A',R and R' are defined with respect to the directions in the laboratory system. Between Q and the Wolfenstein parameters there is a relation involving the angle θ. We cannot define an angular distribution with such a dependence on the scattering angle.

So, the observable (39) is defined in the scattering plane and can be

- defined in the center of mass system
- defined in the laboratory system
- defined with respect to the incident beam.

Parity requirement implies that the A are real if the sum of λ is even and pure imaginary number if this sum is odd. Furthermore :

$$A^{\lambda_3\mu_3\lambda_4\mu_4}_{\lambda_1\mu_1\lambda_2\mu_2} = (-)^{\Sigma\lambda+\Sigma\mu} A^{\lambda_3-\mu_3,\lambda_4-\mu_4}_{\lambda_1-\mu_1,\lambda_2-\mu_2} \qquad (40)$$

can be used to reduce the sum in (39). For example, the spin-flip observable SF is

$$SF\, A^{oooo}_{oooo} = \frac{1}{2}\left\{A^{oooo}_{oooo} + A^{1100}_{1100} + A^{1100}_{1-100}\right\} \qquad (41)$$

but is easier to define by the identification number 7. The coefficients x in (39) and real or pure imaginary if the sum on λ is even or odd : one value only is entered for each of them. However, vector polarization and analysing power, tensor analysing powers and spin-flip do not need a detailed input.

It is also possible to give the coefficients x for a description with respect to the axis perpendicular to the reaction plane. In this case, the sum on μ must be even and the x are complex numbers. It is also possible to give a Cartesian description instead of a tensorial one : for example, one can ask for the population of the substate m in the final target to compute γ correlations. The code ECIS 79 transforms these data to a description in the scattering plane.

2. INTEGRATION METHODS

There are very efficient integration methods to solve a second order linear differential equation without first derivative. These methods are more efficient than those needed to solve first order linear differential equations.

The integration methods can be separated into self starting methods which need only two values at some points to compute the function at the next point and the other methods which need more informations on the function at the preceding points. With the first group, we can use equal steps ; with the second one, we needs a less elaborated method to generate the starting values. Numerical methods for the optical model have been studied in Ref [8] and for coupled channels in Ref [1]. We repeat what is needed to understand the code ECIS 79.

Let us consider a system of N inhomogeneous differential equations

$$f_i''(r) = \Sigma_j V_{ij}(r) f_j(r) + W_i(r) \qquad (1)$$

In fact, we use coupled homogeneous equations or single inhomogeneous equations.

2.1. Integration

The Euler method is the simplest : the second difference of the function is identified with its second derivative. The function at r+h

is given by

$$f_i(r+h) = 2f_i(r)-f_i(r-h)+h^2W_i(r)+h^2\,\Sigma_j V_{ij}(r)f_j(r) \qquad (2)$$

when the truncation error $\Delta = h^4 f_i^{IV}(r)/12$ is neglected. The final error is of the order h^2. This method has been often used to solve coupled equations.

The Cowell method[9] is based on a simple relation between a function and its second derivative at three equidistant points :

$$f_i(r+h)-h^2f_i''(r+h)/12 = 2f_i(r)+5h^2f_i''(r)\,16-f_i(r-h)+h^2f_i''(r+h)/12 \qquad (3)$$

with a truncation error $\Delta = h^6 f_i^{(VI)}(r)/240$. The function at point r and r-h completely defines the solution ; for a single equation, the algorithm gives $\xi(r+h)$, from which

$$f(r+h) = \left(\xi(r+h) + \frac{h^2}{12}\,W(r+h)\right)/\left(1 - \frac{h^2}{12}\,V(r+h)\right) \qquad (4)$$

can be obtained easily. With a system of coupled differential equations, one has to solve a system of linear equations.

The Numerov method[10] uses exactly the same relation but does not evaluate the function f at any point and considers only the expression ξ.

For a single equation, the algorithm is :

$$\xi(r+h) = 2\xi(r)-\xi(r-h)+u(r)$$

$$u(r) = h^2f''(r) = \frac{h^2V(r)}{1-h^2V(r)/12}\left(\xi(r) + \frac{h^2W(r)}{12}\right) + h^2W(r) \qquad (5)$$

The modified Numerov method[8] replaces the division in the last algorithm by an expansion to the order of accuracy of the truncation error :

$$\xi(r+h) = 2\xi(r)-\xi(r-h)+u(r)$$

$$u(r) = h^2V(r)(1+h^2V(r)/12)(\xi(r)-h^2W(r)/12)+h^2W(r) \qquad (6)$$

The truncation error is now $\Delta = h^6V^2(r)f(r)/144-h^6f^{(VI)}(r)/240$.

If V(r) is constant, the truncation error is smaller than for the Numerov method and of opposite sign. For these two methods, the function f(r)

can be obtained by

$$f(r) = \xi(r)+u(r)/12 \qquad (7)$$

or by

$$f(r) = (\xi(r+h)+10\xi(r)+\xi(r-h)/12 \qquad (8)$$

The application of these methods to coupled channels is straightforward. The matrix of the N solutions at the point r+h can be obtained from the matrix of the solutions at the points r and r-h by

$$\xi_i^k(r+h) = 2\xi_i^k(r)-\xi_i^k(r-h)+u_i^k(r) \qquad (9)$$

$$u_i^k(r) = \Sigma_i V_{ij}(r)\xi_j^k(r)$$

With the modified Numerov method :

$$V_{ij}(r) = h^2V_{ij}(r) + \frac{h^4}{12}\,\Sigma_k\, V_{ik}(r)V_{ki}(r) \qquad (10)$$

but for the Numerov method, one has to solve :

$$\Sigma_k\left(\delta_{ik} - \frac{h^2}{12}\,V_{ik}(r)\right)V_{kj}(r) = h^2V_{ij}(r) \qquad (11)$$

At the limit of a large number of equations, the numbers of operations needed to multiply two matrices as in (10) or to solve the linear equations as in (11) are the same. However, the Numerov method is more tedious to use than the Modified Numerov Method. The computation of V can be reduced by a factor 2, taking into account the symmetry of V. The second part of the algorithm (9) is also a multiplication of matrices and the number of operations of the first part can be neglected. So, the number of operations by step is one and half multiplication of matrices, at most $3N^3/2$ operations. The Störmer method[11] uses only one matrix multiplication and the de Vogelaere method uses two of them and needs the potential at the middle of the step ; these two methods are not self starting.

4 - Asymptotic values of the solutions

The solutions must vanish at the origin. To obtain N independent

solutions of an homogeneous system with

$$\xi_i^j(0) = 0 \qquad \xi_i^j(h) = \varepsilon\delta_{ij} \tag{12}$$

However, with $\ell=1$, the solution behaves as r^2 around the origin and the limit of ξ when r goes to the origin is not zero. A better starting value is

$$\xi_i^j(0) = -\xi_i^j(h)/5 \qquad \ell = 1 \tag{13}$$

but this point can be neglected because it introduces a correction of order h^5, smaller than the total error.

A set of inhomogeneous equations cannot be solved without the knowledge of the solutions of the homogeneous system. A special solution of the inhomogeneous system can be obtained with the starting values

$$\xi_j^i(0) = 0 \qquad \xi_j^i(h) = 0 \tag{14}$$

A finite value at the point h comes from the admixture of the solution of the homogeneous system which has to be added.

To compute fusion cross-section, one can use a strong imaginary potential which make the wave function very small inside the nucleus, or one can start the integration from the radius of the nucleus. The starting values are similar to (12). Some modifications allow such a calculation with the code ECIS 79.

The starting conditions define theoretically N independent solutions. Numerically, it can happen, chiefly when large angular momenta are involved, that two or more than two solutions become identical and the matching cannot be done. To avoid this difficulty, one can do a Schmidt's orthogonalization between the solutions from time to time.

The integration is performed up to some point for which the potentials vanish. There, one has to compute the coefficients C_j^i of Eq. (1.20) of the asymptotic form. The matching is usually done with the functions and their first derivative, but it can also be done with the functions at the points R-h and R+h, or even with $\xi(R-h)$ and $\xi(R+h)$.

There are subroutines for Coulomb functions $F_\ell(\eta,kr)$, $G_\ell(\eta,kr)$ and their first derivative From these value, four steps of Numerov integration with half stepsize and an interpolation formula for the first derivative gives us $F_\ell(\eta;k(R\pm h))$ and $G_\ell(\eta,k(R\pm h))$; where

$$F_\ell(\eta,kr) = F_\ell(\eta,kr) - h^2F''_\ell(\eta,kr)/12 \tag{14}$$

The numerical solution k is a linear combination with coefficients α_j^k of the solutions which have ingoing waves only for the equation j :

$$\xi_i^k(R\pm h) = \Sigma_j\, \alpha_j^k\{F_i(R\pm h)\delta_{ij}+C_i^j[G_i(R\pm h)+i\,F_i(R\pm h)]\} \tag{15}$$

With the matrices

$$A_i^k = \frac{\xi_i^k(R+h)G_i(R-h)-\xi_i^k(R-h)G_i(R+h)}{F_i(R+h)G_i(R-h)-F_i(R-h)G_i(R+h)} = \Sigma_j\alpha_j^k\{\delta_{ij}+C_i^j\}$$

$$B_i^k = \frac{\xi_i^k(R+h)F_i(R-h)-\xi_i^k(R-h)G_i(R+h)}{F_i(R+h)G_i(R-h)-F_i(R-h)G_i(R+h)} = -\Sigma_j\alpha_j^kC_i^j \tag{16}$$

the matching equations are :

$$B_i^k = -\Sigma_j(A_j^k+iB_j^k)C_i^j \tag{17}$$

This is a linear system of equations. When solved for a single second member (i fixed) the C_i^j are obtained for a fixed value of i, all value of j. Wronskian relations allows the transposition of the matrix C.

Coulomb corrections forbid the use of (14) in the code ECIS 79 because these corrections need the value of the Coulomb functions and their derivative at the matching point. Therefore, matching with functions and derivatives are used in this case : denominators of A and B reduce to the Wronskian of regular and irregular Coulomb function which is k. Derivatives are computed with :

$$f(R) = \frac{1}{24h}\{14[\xi(R+h)-\xi(R-h)]+\xi(R+2h)-\xi(R-2h)\} \tag{18}$$

and the error, $-\frac{h^4}{60}f^{(IV)}(R)$, is of the same order as the total error accumulated in the integration.

2.3. Wronskian relations

The solutions of coupled equations satisfy relations similar to the Wronskian for a single equation. With these relations, the symmetry properties of the matrix C can be deduced from the symmetry of the potential. The errors due to the integration (truncation, round-off and matching errors) can be evaluated.

Let us consider two of the most general systems of coupled inhomogeneous differential equations :

$$-\frac{\hbar^2}{2m_i}\frac{d^2}{dr^2}f_i(r) + \sum_j V_{ij}(r)f_j(r)+W_i(r) = 0$$
$$-\frac{\hbar^2}{2m_i}\frac{d^2}{dr^2}g_i(r) + \sum_j \bar{V}_{ij}(r)f_j(r)+\bar{W}_i(r) = 0 \qquad (19)$$

and compute the expression :

$$W = \int_0^k \Sigma_i -\frac{\hbar^2}{2m_i}\{f_i(r)g_i'(r)-g_i(r)f_i'(r)\}dr$$
$$= \sum_{i,j}\int_0^R (V_{ij}(r)-\bar{V}_{ji}(r))f_i(r)g_j(r)dr+\Sigma_i\int_0^R W_i(r)g_i(r)dr-\Sigma_i\int_0^R \bar{W}_i(r)f_i(r)dr \qquad (20)$$

If g(r) and f(r) vanish at the origin and have an ingoing wave for the equations j and k respectively, we obtain

$$W = \hbar^2\left[\frac{k_k}{2m_k}C(f)^i_k - \frac{k_j}{2m_j}C(g)^k_i\right] \qquad (21)$$

When the sets of equations (19) are identical and there is no inhomogeneous term, the second member of (20) vanishes because the coupling $V_{ij}(r)$ is symmetric :

$$\frac{k_j}{m_j}C^i_j = \frac{k_i}{m_i}C^j_i \qquad (22)$$

To apply Wronskians to integration errors, let us consider a set of equations :

$$f_i''(r) = -\Sigma_j V_{ij}(r)f_j(r) \qquad (23)$$

If the integration method does not use first derivatives, the numerical solution is given by

$$\bar{f}_i(r+h) = 2\bar{f}_i(r)-\bar{f}_i(r-h)-h^2[\bar{f}_i''(r)] \qquad (24)$$

while the true solution is

$$f_i(r+h) = 2f_i(r)-f_i(r-h)-h^2[f''(r)]+\Delta_i \qquad (25)$$

The bracket $[f''(r)]$ is the second derivative only to the order h^2. The numerical function is a solution of

$$\bar{C}_j''(r) = -\Sigma_j V_{ij}\bar{f}_j(r) + \frac{\Delta_i}{h^2} \qquad (26)$$

and the error is

$$\Delta C^k_j = \bar{C}^k_j - C^k_j = -\frac{2m_j}{h^2\hbar^2 k_j}\Sigma_i\int f^k_i(r)\Delta^k_i dr \qquad (27)$$

So, a truncation error of the order h^6 leads to a total error of order h^4. If the round-off error is due to chopping, the error in each step is $N\varepsilon f(r)$ where ε is the precision of the computer and N a constant which depends on the program. The same method as above yields the total error which is the same as adding a constant term $N\varepsilon/h^2$ to all the diagonal potentials (which is equivalent to an error on the energy). On an IBM computer, we use single precision for the potentials and double precision in the integration algorithm to avoid round-off errors. When the integration method uses first derivatives, the total truncation error is different[8] and there is no round off error.

The error coming from a matching point too close to the origin is given by

$$\Delta C^k_n = \frac{2m}{\hbar^2 k}\sum_{ij}\int_R^\infty f^n_i(r)V_{ij}(r)f^k_j(r)dr \qquad (28)$$

Any kind of error is coherent and corresponds to a change of the hamiltonian.

2.4. Stability and step-size

Near the matching point, the potentials vanish. The equations reduce

to $y'' = iy$. The integration method is then a recurrence relation with constant coefficients. Using $f(nh) = x^n$ we get a characteristic equation which is

$$\left(1 \pm \frac{h^2}{12}\right)(1+x^2)-(2\pm 5h^2/6)\,x = 0$$

for the Numerov method and

$$(1+x^2)-(2\pm h^2+h^4/12)\,x = 0$$

for the Modified Numerov Method. The study of these equation gives some hints of the behaviour of the solution when a large step size is used[1].

In the assumption of constant potential, a correction term can be introduced in the algorithm to cancel the truncation error with the Numerov method and the Modified Numerous method. No improvement has to be expected for the inelastic scattering.

Default option for a matching radius is the real radius plus 10 times the diffuseness. Such a value do not take into account the spreading of the rotational model. Default option for the step size is the minimum of half a diffuseness and 1/2k. It does not take into account the spreading in the rotational model which allows a larger step size. It does not take into account the smallness of k at low energy, but the limitation with respect to the diffuseness is usually enough. In all cases, a decrease by 19% of the step size divides the errors by 2.

3. E.C.I.S.

The ECIS method is an iteration procedure which allows us to find the solution (1-20) of the system of coupled equations, written as

$$y_i''+V_{ii}y_i = -\mu \sum_{j\neq i} V_{ij}y_j-\mu \sum_{j\neq i} V'_{ij}y'_j \qquad (1)$$

with $\mu = 1$. The coupling potential V_{ij} is symmetric. The derivative coupling V'_{ij} comes from the spin-orbit deformation ; it is non diagonal and antisymmetric. The equations (1) are ordered : ground state and excited state in decreasing order of coupling. The principle is to write down an expansion of the solution in power of μ but to use all the informations available to get the solutions. Three convergence parameters control the computation : a convergence criterium for the S matrix ε_1 = EITER, a minimum value for the functions ε_2 = ACONV and a convergences criterium ε_3 = CONJ. Default values are 10^{-4}.

3.2. Differential method

The optical solutions y_i^{opt} must be obtained for each equation. They are the solutions for $\mu = 0$. As the asymptotic value is of order of unity, we compute the point above which the solution is larger than ε_2 ; below this point, the function is neglected. This point is further and further when the angular momentum increases. Let us use the index o for the ground state and i = 1,2,...n-1 for the other equations.

The zeroth order solution is

$$y_o^{(0)} = y_o^{opt} \to F_{\ell_o}+C_o^{(0)}(G_{\ell_o}+sF_{\ell_o}) \qquad (2)$$

$$y_i^{(0)} = 0$$

In the first iteration, Eq. (1) is considered with only $y_o^{(0)}$ in the second member. First derivatives are obtained numerically with a seven points interpolation formula. The solution $y_1^{(1)}$ is the linear combination $\bar{y}_1+\alpha y_1^{opt}$ of an arbitrary solution $\bar{y}_1$ of the inhomogeneous equation and the optical solution with α such as the solution is purely outgoing. The coefficient of the outgoing wave is

$$C_1^{(1)} = \bar{C}_1+\alpha C_o^{(0)} \qquad (3)$$

For the next equation, it is possible to compute $y_2^{(1)}$ with $y_o^{(0)}$ and $y_1^{(1)}$ in the second member. This sequential procedure leads to a result which is not the first order result in μ and depends upon the sequence along which the equations are iterated. The first iteration ends by solving the equation for $y_o^{(1)}$ with all the $y_i^{(1)}$ in the second member.

In the other iterations, all the last solutions are used in the second member. They are replaced by 0 up to the point where there are larger than ε_2. If $|C_i^{(n)}-C_i^{(n-1)}|$ is less than ε_1 for all i, the set of equations is regarded as solved. From the fourth iteration, a symmetric Pade approximant can be constructed with the $C_i^{(n)}$ for a given i.

This method fails for a large excitation. In Eq. (3) the value of α

is such that a large cancellation occurs and the result is not reliable. For a large excitation, it is better to use the integral method.

3.2. Integral method

For each homogeneous single differential equation, there is an "irregular" solution of which the asymptotic form is

$$y^{in}(r) \underset{r\to\infty}{\to} G_\ell(\eta,kr)+iF_\ell(\eta,kr)$$

which can be obtained by backwards integration. This function increases strongly near the origin, chiefly for large angular momenta ; however, it is neglected up to the point where the regular solution is larger than ε_2. With these two solution, one can build the Green's function and write the solution

$$y_i^{(n)}(r) = y_i^{opt}(r)\delta_{io} + \frac{1}{k_i}\, y_i^{opt}(r)\int_r^\infty y_i^{irr}(r')W(r')dr' + \frac{1}{k_i}\, y_i^{irr}(r)\int_0^r y_i^{opt}(r')W(r')dr' \qquad (4)$$

where W(r') stands for the second member of (1). The result is

$$C_i^{(n)} = \frac{1}{k_i}\int_0^\infty y_i^{opt}(r')W(r')dr' \qquad (5)$$

Near the origin, the irregular solution is large but the product in or with the integrals is of the order of the regular solution, which is very small. For any doubt on the possibility to neglect these functions near the origin, the constant ε_2 can be decreased.

Storage requirements are the same in the two methods. In the second [illegible]

[illegible] not straightforwards. A method with an error of order h^4 is described in Ref. 1.

3.3. Pade approximants

When the second iterations leads to results identical to those of the first one (difference less than ε_1), only one iteration is performed for higher angular momenta. However, for heavy ion scattering, the two first iterations can be identical because there is no inelastic scattering at very low angular momentum : the limitation to one iteration has to be postponed to a minimum angular momentum corresponding to the grazing angle. The computation is stopped when all the C matrix elements are less than ε_3.

At the fourth iteration, if convergences is not obtained for this equation but was obtained for all the other equations solved in this iteration, a Padé subroutine is called. The principle is to consider $C_i^{(n)}$ as the sum of the n first terms of the Taylor expansion of some function for the value unity of the variable λ. For a 0^+-2^+ calculation with the first order vibrational model, there is no reorientation terms and the elastic scattering is an even function of μ, the inelastic scattering is an odd function of μ : the variable λ appears to be μ^2. In any other calculation, the variable is an unknown function of μ.

From

$$C_i^{(n)} = \sum_{p=1}^{n} \lambda^p a_p \quad , \quad \lambda = 1 \qquad (6)$$

the coefficients a_p are computed. The Padé approximant replaces this Taylor expansion by the ratio of two polynomials with the same number of coefficients. An accurate result can be obtained further than the poles of the function which limit the circle of convergence of the Taylor expansion. In practice, we obtain good results up to 5 times the radius of convergence. This limitation comes from the lack of precision of the com- [illegible]

When the Taylor expansion diverges or converges slowly, the Padé approximant generates a polynomial denominator for each equation. The smallest or the few smallest zeroes of the denominator are the same for all the equations. There are complex values. If μ is replaced by one of

these zeroes λ_j in Eq. (1) the coefficient of the outgoing wave of all the equations blows up. For this value of μ, the set of equations (1) has a solution which is purely outgoing in all channels. This is the definition of a Weinberg state.

If λ_j are the Weinberg eigenvalues and x_i^j the amplitudes of the outgoing waves with a proper normalization

$$C_i(\lambda) = \Sigma_j \, x_i^j \frac{1}{\lambda_j - \lambda}$$

$$C_i^{(n)} = \Sigma_j \frac{x_i^j}{\lambda_j} \sum_{m=1}^{n} \left(\frac{1}{\lambda_j}\right)^n \qquad (7)$$

If λ_j is small, each iteration gives the result of the last one multiplied by the large number $1/\lambda_j$.

Padé approximants are computed for a fixed value of i. The expression written above shows that this is a loss of information because the denominator is independent of i. This has no importance if the divergence is weak. In case of strong divergence, no method has been found to get better results taking into account this property : the lack of precision of intermediate results cannot be overcome.

In the code ECIS 79, there is a maximum number of iterations (default value 20). However, if a C-matrix element becomes too large (of the order of 10^{10}), the iterations are stopped because it becomes hopeless to extract the result (smaller than unity) by differences between so large numbers. The Padé approximant at the n^{th}-iteration is evaluated with n,n-1 to 3 coefficients. The two nearest successive results are searched. If they differ by less than ε_2, their mean value is assumed to be the result. When convergence is not obtained, there is the possibility to use the mean value of the two nearest results or to do again the computation for this angular momentum and parity with the usual method of coupled equations.

With a deformed spin-orbit the iterations are compulsory. The usual method of coupled equations cannot deal with first derivatives and the system of equations is not symmetric, although symmetry is assumed by the code.

4. AUTOMATIC SEARCH

The aim of the automatic search methods is to find as quickly as possible the parameters of the model which insure the best fit to the data.

4.1. Definition of a χ^2

The experimental data are composed of n angular distributions which consist of n_i experimental values at a given angle. Each angular distribution is characterized by the level to which it is related and some identification number which is :

0 for a cross-section

1 for a cross-section divided by Rutherford's cross-section (usual presentation of elastic scattering for charged particle).

2 for a vector analysing power

3 for a vector polarization

4,5,6 for a tensor analysing power

7 for a spin-flip

8 is reserved to a set of reaction cross-sections (the level will be given instead of the angle)

a negative number for any other kind of polarization defined by the user.

An angular distribution is also characterized by a weight ω_i, a positive number which is the weight in the total χ^2 of the partial χ^2 related to this angular distribution (default value 1), an experimental normalization λ_i^o by which data must be divided (default value 1) and its error $\Delta\lambda_i$. The experimental normalization λ_i^o can be positive or negative (-1 is a change of sign of a polarization without having to change data) ; it is fixed if $\Delta\lambda_i = 0$, otherwise it is included in the χ^2 as another data.

Each of the n_i experimental data of an angular distribution consists in :

- the angle θ_j
- the experimental value $Q_i(\theta_j)$
- the experimental error $\Delta Q_i(\theta_j)$ which can be given as a percentage for a cross-section but not for a polarization

- a width of detector $\Delta\theta_j$
- an angular error $\delta\theta_j$

The total χ^2 is defined as a sum on the partial χ^2 :

$$\chi^2 = \Sigma_i \omega_i \chi_i^2 \qquad (1)$$

and the partial χ_i^2 is

$$\chi_i^2 = \min_{\lambda_i} \left[\Sigma_j \left\{ \frac{\lambda_i \bar{R}_i(\theta_j) - Q(\theta_j)}{\Delta R_i(\theta_j)} \right\}^2 + \left(\frac{\lambda_i - \lambda_i^o}{\Delta\lambda_i} \right)^2 \right] \qquad (2)$$

The last term is included only if $\Delta\lambda_i \neq 0$, otherwise $\lambda_i = \lambda_i^o$. Note that, even if it is seldom used, $\Delta\lambda_i$ proceeds from the best analysis of the experimental situation : the error at each point is the sum of its own statistical error and a normalization error which is the same for all the points of the angular distribution. The calculated mean values are :

$$\bar{R}_i(\theta_j) = \frac{1}{3} \{ R_i(\theta_j - \Delta\theta_j) + R_i(\theta_j) + R_i(\theta_j + \Delta\theta_j) \} \qquad (3)$$

which reduces to $R_i(\theta_j)$ if $\Delta\theta_j = 0$. It is a crude integration corresponding to a half width of detector $\sqrt{2}\Delta\theta_j$. The "calculated experimental error" is such that

$$\Delta R_i(\theta_j)^2 = \Delta Q_i(\theta_j)^2 + \{ \delta\theta_i R_i'(\theta_j) Q_i(\theta_j) / R(\theta_j) \}^2 \qquad (4)$$

where the derivative

$$R_i'(\theta_j) = \frac{1}{2\Delta\theta_i} [R_i(\theta_j + \Delta\theta_j) - R_i(\theta_j - \Delta\theta_j)] \qquad (5)$$

The "calculated experimental error" reduces to the experimental error when $\delta\theta_i = 0$ and can be used only with $\Delta\theta_i \neq 0$. It reduces the χ^2 when the slope of the theoretical curve is large. The ratio $Q_i(\theta_j)/R(\theta_j)$ is introduced to allow a minimization with respect to the normalization.

There is an alternate definition of the χ^2 which can be used only for cross-section and which is called the symmetrized χ^2. It is

$$\chi_i^{2\ sym} = \Sigma_j \left\{ \frac{\bar{R}_i(\theta_j) - Q_i(\theta_j)}{\Delta R_i(\theta_j)} \right\}^2 \frac{Q(\theta_j)}{\bar{R}(\theta_j)} \qquad (6)$$

If $\bar{R}_i(\theta_j) = Q_i(\theta_j)$ and $\bar{R}_i(\theta_j) = 2Q_i(\theta_j)$, the normal χ^2 is 1 and the symmetrized χ^2 is 1/2 ; for the same error and $Q_i(\theta_j) = 2\bar{R}_i(\theta_j)$, the usual χ^2 is 1/4 and the symmetrized χ^2 is still 1/2.

An angular distribution can deal with p unresolved levels. It appears only once in the χ^2 but p times in the number of angular distribution, the p-1 first times with no data. These p angular distributions must have the same identification number.

4.2. Principle of the search

The results $\bar{R}_i(\theta_j; x_1 \ldots x_m)$ are functions of some parameters x_i of the model which one wants to vary. The χ^2 criterium is a sum of squares

$$\chi^2 = \sum_{i=1}^{n} \sum_{j=1}^{n_i} f_{ij}^2(x_1 \ldots x_m) \qquad (7)$$

with the functions

$$f_{ij}(x_1 \ldots x_m) = \omega_i^{1/2} \frac{\lambda_i R_i(\theta_j; x_1 \ldots x_m) - Q(\theta_j)}{\Delta R_i(\theta_j)} \qquad (8)$$

where λ_i is the value at the minimum. Strictly speaking, there are also functions coming from the renormalization but we have to recognize that they are forgotten in the search. To find its minimum, it is necessary to know its behaviour around the point where the first calculation is done

$$\chi^2(x_i + \delta x_i) = \chi^2(x_i) + \Sigma_i \frac{\partial \chi^2}{\partial x_i} \delta x_i + \frac{1}{2} \sum_{i,j} \frac{\partial^2 \chi^2}{\partial x_i \partial x_j} \delta x_i \delta x_j \qquad (9)$$

If the number m of variables in search is large, the number of terms in the right side of this equation, 1+m(m+3)/2, is very large. As the χ^2 is a sum of squares, it is better to require only the approximation :

$$\chi^2(x_k + \delta x_k) = \sum_{i,j} \left[f_{ij}(x_k) + \Sigma_\ell \frac{\partial f_{ij}(x_k)}{\partial x_\ell} \delta x_\ell \right]^2 \qquad (10)$$

for which we need the functions for m+1 sets of parameters if differences are used instead of derivatives.

The derivatives $\frac{\partial f_{ij}}{\partial x_k}$ can be obtained from the derivatives of the