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Program ELIESE-1
FORTRAN-II Program for Analyses of Elastic and Inelastic Scattering Cross Sections

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Preface

One day, Mr. Researcher visited Miss Eliese Janudac and had a conversation with her about recent research works in science.

Mr. Researcher; "Almost all researchers today are using the electronic computer. This is, seems to me, quite nonsense."

Eliese; "Why ?"

Mr. Researcher; "Because, the electronic computer does work very fast in numerical computation, but it's incompetent and it's also unkind. So then every researcher should spend much time and much money to computing work, not to his own research work."

Eliese, with a puzzled look; "I don't understand what you're going to say ! What's the reason for incompetence of electronic computer ?"

"Well," Mr. Researcher explained, "Suppose Mr. A has written a source program with several mistakes which are quite trivial, for example, a comma was missed or a period was used instead of a comma, so on. The electronic computer points out the program error for the first mistake and stops to work, so that Mr. A can correct it but not the others. In other words, the computer points out every program error in every run of compiling process. Similar problems happen in also writing the input data. So I would say that the only a few percent of all machine running time is actually used for real computing work."

Eliese; "Oh my goodness ! Your saying is based on your own way ! You are not saying that the researcher's mistake should be corrected by himself, but that the electronic computer should correct the researcher's error. I don't think it's fair !"

Mr. Researcher; "You're probably right ! But ..... "

Eliese; "Wait ! I would emphasize that every people should read carefully the computer manual or the program manual in order to avoid the mistakes. Now, here is a manual for the Program ELIESE-1. I would like to recommend it to all who are going to use ELIESE-1."

Contents

目　次

1. Introduction

This is the manual of IBM-7090 code named as ELIESE-1, which can be used for calculations of any kinds of cross sections for elastic and inelastic scattering of neutrons, protons and alpha particles by means of optical model and of HAUSER-FESHBACH's method in compound nuclear process. The Program ELIESE-1 has been prepared by a working group on fast neutron cross sections, as one of the 1963 projects of Japanese Nuclear Data Committee which is an ad-hoc committee of the Atomic Energy Society of Japan. The members of the working group, contributors to ELIESE-1, are composed of people from several laboratories, universities and companies in Japan, so that it should be emphasized that the completion of ELIESE-1 is due to an excellent collaboration of such people.

Although the similar programs are available by request at the present time, ELIESE-1 has some advantages in working with the cross section evaluation. These advantages may be seen in the detailed description of ELIESE-1 on succeeding sections. It, however, does not imply that the Program ELIESE-1 is the best one, but that many improvements have been included taking account of user's convenience. The policy in making the code was that every user could use it with more results but with less pains. This is reflected in ELIESE-1 as the fact, for example, that it is quite easy to prepare the input data by means of relative address. In order to find the unexpected errors if any in ELIESE-1, the calculated results were compared carefully with those by other programs, ABACUS-2, etc., for typical examples. The comparison of the results by ELIESE-1 with those by other codes will be given in a later section where the running time and the stability against mesh size are also illustrated. It is expected, however, that further improvements might be required in the next step of code development. Some of the modifications are already under planning, and more refined program will be available in near future as Program ELIESE-2.

As mentioned in the first paragraph, the Program ELIESE-1 is used in calculating the cross sections of elastic scattering and of inelastic scattering leaving a few of the low-lying excited states because of the characteristics of optical model and HAUSER-FESHBACH's method. Originally, however, it has been required to calculate the cross sections of inelastic scattering exciting also the higher excited levels. In these cases, the effects of competing processes play an important role. With the Program ELIESE-1, it is possible to take account of the competition between nucleon emitting processes. For example, (n, p) reaction can be included as the only competing process in calculating the cross sections of (n, n'). As the competing processes in above example, the inclusion of (n, γ) and (n, α) reactions seems to be one of the important subjects in preparing the Program ELIESE-2.

In sections 2 and 3 of this manual, the mathematical descriptions of optical model and of HAUSER-FESHBACH's method are given. It is not our objective to mention the physical view point but to explain the formulas used in ELIESE-1. The methods of numerical evaluation of formulas described in sections 2 and 3 are explained in section 4. Following sections, 5 to 8, are devoted to describing the Program ELIESE-1 itself. Brief explanations about sub-routines and symbols used in ELIESE-1 are given in sections 5 and 7, respectively. Section 6 is used in explaining the method of preparing the input data for initial case and for succeeding cases. The list of the Program ELIESE-1 appears in section 8. Typical examples of calculated results using ELIESE-1 are shown in section 9 with a few remarks.

Although all the members of the working group on fast neutron cross sections should be responsible for Program ELIESE-1, the present manual has been prepared by not all but a few members listed below:

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2. Mathematical Description of Shape Elastic Scattering Process

This section is devoted to describing the analysis of the elastic scattering process in terms of the optical potential model[1], so we are not concerned with the physical problems but with the mathematical description of the optical model. The optical potential is a very useful tool not only in analysing the scattering phenomena but in understanding the nuclear reactions by means of distorted wave approximation or of compound nucleus model.

In ELIESE-1, the calculations are restricted to only neutrons, protons and alpha particles since the masses of these particles are already set in the Program. Cross sections, energies and lengths are expressed in units of milli-barns, MeV and fermis, respectively.

2. 1 Schroedinger equations

Basic radial Schroedinger equations of this program, in center of mass system, are written as

$$\left\{\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+k^2+\mathfrak{V}_C(r)+l\mathfrak{V}_{so}(r)-\mathfrak{V}_{Coul}(r)\right\}\varphi_l^{(+)}(r)=0, \tag{2.1}$$

$$\left\{\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+k^2+\mathfrak{V}_C(r)-(l+1)\mathfrak{V}_{so}(r)-\mathfrak{V}_{Coul}(r)\right\}\varphi_l^{(-)}(r)=0, \tag{2.2}$$

where $\mathfrak{V}_C(r)$, $\mathfrak{V}_{so}(r)$ and $\mathfrak{V}_{Coul}(r)$ are the central, spin-orbit and Coulomb potentials, respectively. The wave functions $\varphi_l^{(+)}(r)$ and $\varphi_l^{(-)}(r)$ are the radial wave functions corresponding to spin up and spin down. For alpha particles, spin-orbit force is zero, then eq. (2. 2) is identical to eq. (2. 1). Wave number k in eqs. (2. 1) and (2. 2) is defined by

$$k=(2\mu E/\hbar^2)^{1/2}, \tag{2.3}$$

where μ and E are reduced mass and relative energy between an incident particle and a target nucleus, respectively, and are given as follows;

$$\mu=\frac{mM}{m+M}, \tag{2.4}$$

$$E=\frac{M}{m+M}E_0, \tag{2.5}$$

where m and M are masses of incident particle and target nucleus and E_0 is the energy in laboratory system.

2. 2 Potential form and parameters

2. 2. 1 Central nuclear potential

In the optical model, we can write the central nuclear potential as

$$\mathfrak{V}_C(r)=\mathfrak{V}_{CR}(r)+i\mathfrak{V}_{CI}(r), \tag{2.6}$$

where $\mathfrak{V}_{CR}(r)$ is the real part and $\mathfrak{V}_{CI}(r)$ is the imaginary part, respectively.

i) Real part $\mathfrak{V}_{CR}(r)$

We assume Woods-Saxon form for $\mathfrak{V}_{CR}(r)$ and represent as

$$\mathfrak{V}_{CR}(r)=\frac{2\mu}{\hbar^2}V_C\mathfrak{F}_{CR}(r), \tag{2.7}$$

where $\mathfrak{F}_{CR}(r)$ is the shape function written as

$$\mathfrak{F}_{CR}(r)=\frac{1}{1+\exp\{(r-R_0)/a_0\}}, \tag{2.8}$$

and V_C is the well depth parameter expressed by

$$V_C=V_{C,0}+V_{C,1}(E-1.2ZZ'e^2/R_C)+(V_{asym,0}+V_{asym,1}\cdot E)(N-Z)/A. \tag{2.9}$$

This well depth parameter V_C is asssumed to be linear form in the energy including the symmetric term for charged particles. The parameter R_0 in eq. (2.8) is the nuclear radius at which potential depth becomes half value of the maximum. With the conventional nuclear radius parameter r_0 and mass number A, we have

$$R_0=r_0A^{1/3}. \tag{2.10}$$

The parameter a_0 in eq. (2.8) is the diffuseness parameter of nuclear surface.

ii) Imaginary part $\mathfrak{V}_{CI}(r)$

Imaginary part of the central nuclear potential $\mathfrak{V}_{CI}(r)$ is represented as

$$\mathfrak{V}_{CI}(r)=\frac{2\mu}{\hbar^2}(W_1\mathfrak{F}_{CI}(r)+W_S\mathfrak{F}_{CS}(r)). \tag{2.11}$$

The first term in parentheses stands for the volume absorption of the incident particle and the second term for the surface absorption. Shape functions $\mathfrak{F}_{CI}(r)$ and $\mathfrak{F}_{CS}(r)$ are respectively written as

$$\mathfrak{F}_{CI}(r)=\begin{cases}1 & ; \text{ Uniform} \quad (2.12)\\ \dfrac{1}{1+\exp\{(r-R_I)/a_I\}} & ; \text{ Woods-Saxon} \quad (2.12')\end{cases}$$

$$\mathfrak{F}_{CS}(r)=\begin{cases}\exp\{-[(r-R_S)/b]^2\} & ; \text{ Gaussian} \quad (2.13)\\ \dfrac{4\cdot\exp\{(r-R_S)/b\}}{[1+\exp\{(r-R_S)/b\}]^2} & ; \text{ Derivative Woods-Saxon} \quad (2.13')\end{cases}$$

Radial parameter R_I is defined in the same way as R_0 with parameter r_I instead of r_0

$$R_I=r_IA^{1/3}. \tag{2.14}$$

Parameter R_S is defined by

$$R_S=R_0+C_R, \tag{2.14'}$$

where C_R is any constant value which determines the position of the center of surface potential.

Well depth parameters W_I and W_S in eq. (2.11) are assumed to be linear form with respect to the energy,

$$W_I=W_{I,0}+W_{I,1}\cdot E, \tag{2.15}$$

and

$$W_S=W_{S,0}+W_{S,1}\cdot E. \tag{2.16}$$

A remark is necessary with regard to uniform volume absorption potential. In adding this volume absorption potential to any surface absorption potential, joining point of these two potentials is defined by

$$r_{IC}=R_S-b\sqrt{\ln(W_S/W_I)} \quad \text{for Gaussian} \tag{2.17}$$

and

$$r_{IC}=R_S+b\ln\alpha \quad \text{for Derivative Woods-Saxon} \tag{2.18}$$

where α is

$$\alpha=\{2W_S-W_I-2\sqrt{W_S^2-W_S\cdot W_I}\}/W_I. \tag{2.19}$$

Therefore, in the case of uniform volume absorption plus any surface absorption, we must represent the imaginary part of the nuclear central potential as

$$\mathfrak{V}_{CI}(r)=\frac{2\mu}{\hbar^2}W_I\mathfrak{F}_{CI}(r) \quad ; \quad r\leq r_{IC} \tag{2.20}$$

$$=\frac{2\mu}{\hbar^2}W_S\mathfrak{F}_{CS}(r) \quad ; \quad r>r_{IC} \tag{2.21}$$

2.2.2 Spin-orbit potential

Spin-orbit force is written in the Thomas form,

$$\mathfrak{V}_{SO}(r)=\frac{2\mu}{\hbar^2}C_{SO}\frac{V_{SO}+iW_{SO}}{r}\frac{1}{a_0}\frac{\exp\{(r-R_0)/a_0\}}{[1+\exp\{(r-R_0)/a_0\}]^2}, \tag{2.22}$$

where C_{SO} is defined with π-meson mass

$$C_{SO}=(\hbar/m_\pi c)^2. \tag{2.23}$$

Here c is the light velocity and m_π is defined by

$$m_\pi=\frac{1}{3}(m_{\pi^+}+m_{\pi^-}+m_{\pi^0}). \tag{2.24}$$

Well depth parameters are the same form as (2.9), (2.15) and (2 16), and are written as

$$V_{SO}=V_{SO,0}+V_{SO,1}E, \tag{2.25}$$

$$W_{SO}=W_{SO,0}+W_{SO,1}E. \tag{2.26}$$

2.2.3 Coulomb potential

Coulomb potential in the interior region is defined with the assumption of uniform charge distribution, and therefore represented as

$$\mathfrak{V}_{Coul}(r)=\frac{2\mu}{\hbar^2}\frac{ZZ'e^2}{2R_C}\left(3-\frac{r^2}{R_C^2}\right) \quad ; \quad r\leq R_C, \tag{2.27}$$

$$=\frac{2\mu}{\hbar^2}\frac{ZZ'e^2}{r} \quad ; \quad r>R_C, \tag{2.28}$$

where R_C is written with parameter r_C as

$$R_C=r_C A^{1/3}. \tag{2.29}$$

In the Program ELIESE-1, sign is used for the parameter r_C in order to discriminate the kind of the incident particles.

We now integrate the eqs. (2.1) and (2.2) numerically, as explained in section 4. They are connected smoothly to their asymptotic solutions at the matching point.

2.3 Matching radius

In this sub-section, we intend to explain the definition of the matching radius r_M. At this point, we may consider the wave functions to have their symptotic forms, that is, the value of each potential must be negligible order of magnitude in comparison with incident energy. Thus, the matching radius r_M is defined as the maximum value of the solutions of the following equations,

$$\frac{1}{k^2}\mathfrak{V}_{CR}(r_M)\leq 10^{-4}, \tag{2.30}$$

$$\frac{1}{k^2}\mathfrak{V}_{CI}(r_M)\leq 10^{-4}, \tag{2.31}$$

and the condition $r_M\geq R_C$.

2. 4 Asymptotic form of wave function

Asymtotic expression for wave function consists of the incoming and outgoing parts. Well known expression is

$$\varphi_l^{(+)}(r) \longrightarrow u_l^{(-)}(\rho) - \eta_l^{(+)} u_l^{(+)}(\rho), \tag{2.32}$$

where $u_l^{(\pm)}(\rho)$ is defined with the spherical Neumann and Bessel functions (or Whittaker functions) multiplied by their argument, $\rho = kr$. The wave functions $u_l^{(+)}(\rho)$ and $u_l^{(-)}(\rho)$ stand for the outgoing and incoming waves, respectively.

$$u_l^{(\pm)}(\rho) = G_l(\rho) \mp i F_l(\rho). \tag{2.33}$$

In eq. (2.32), $\eta_l^{(+)}$ is called the scattering amplitude and is related with the scattering phase shift $\delta_l^{(+)}$ as

$$\eta_l^{(+)} = \exp(2i\delta_l^{(+)}). \tag{2.34}$$

This amplitude is the most important quantity and can be obtained by joining the interior wave function to its asymptotic wave function smoothly at $\rho_M = kr_M$.

The maximum angular momentum l_{max} is defined by the following condition,

$$[G_l(\rho_M)/G_0(\rho_M)]^2 > 10^6. \tag{2.35}$$

In the case of neutron, the condition (2.35) means that the penetrabilities of the partial waves effective to the process are larger than 10^{-6}.

Next, we describe the method of obtaining the irregular solutions of asymptotic wave equations, $G_l(\rho)$'s. They are derived by the recurrence formula[2]

$$G_{l+1}(\rho_M) = \frac{l+1}{\sqrt{\eta^2 + (l+1)^2}} \left\{ (2l+1) \left(\frac{\eta}{l(l+1)} + \frac{1}{\rho_M} \right) G_l(\rho_M) - \frac{1}{l} (\eta^2 + l^2)^{1/2} G_{l-1}(\rho_M) \right\}, \tag{2.36}$$

where η is Coulomb parameter defined by

$$\eta = \frac{\mu Z Z' e^2}{\hbar^2 k}. \tag{2.37}$$

For the neutron, η is, of course, zero, and

$$G_0(\rho_M) = \cos \rho_M, \tag{2.38}$$

$$G_1(\rho_M) = \frac{1}{\rho_M} \cos \rho_M + \sin \rho_M. \tag{2.39}$$

If an incident particle is proton or alpha particle, we must find $G_0(\rho)$ and $G_0'(\rho)$ at the asymptotic radius ρ_A (see section 4). Asymptotic radius ρ_A is defined by[2]

$$\rho_A = 2\eta \quad ; \quad \text{for} \quad \eta \geq 4, \tag{2.40}$$

$$= 2\eta + 9 \quad ; \quad \text{for} \quad \eta < 4. \tag{2.41}$$

The Coulomb wave equation for s-wave

$$\frac{d^2 G_0}{d\rho^2} + \left(1 - \frac{2\eta}{\rho} \right) G_0 = 0 \tag{2.42}$$

is integrated from ρ_A to ρ_M. Using $G_0(\rho_M)$ and $G_0'(\rho_M)$, we obtain $G_1(\rho_M)$ from

$$G_1(\rho_M) = \frac{1}{\sqrt{\eta^2 + 1}} \left\{ \left(\eta + \frac{1}{\rho_M} \right) G_0(\rho_M) - G_0'(\rho_M) \right\}. \tag{2.43}$$

Now we have had $G_0(\rho_M)$ and $G_1(\rho_M)$. Thus any $G_l(\rho_M)$ is obtained by the eq. (2.36).

Regular wave functions $F_l(\rho_M)$'s are obtained by means of well known STEGUN and ABRAMOWITZ's downward recurrence method[3]. In section 4, we shall explain this method in detail.

Derivatives of $G_l(\rho_M)$ and $F_l(\rho_M)$ may be obtained from the formula

$$X_l'(\rho_M)=\frac{1}{l-1}\left\{\left(\frac{(l+1)^2}{\rho_M}+\eta\right)X_l(\rho_M)-((l+1)^2+\eta^2)^{1/2}X_{l+1}(\rho_M)\right\}, \tag{2.44}$$

where $X_l(\rho_M)$ stands for either $G_l(\rho_M)$ or $F_l(\rho_M)$.

2.5 Scattering amplitude

Scattering amplitude $\gamma_l^{(\pm)}$ is given by the formula

$$\gamma_l^{(\pm)}=-\frac{f_l^{(\pm)}-(\Delta_l-is_l)}{f_l^{(\pm)}-(\Delta_l+is_l)}\frac{u_l^{(-)}(\rho_M)}{u_l^{(+)}(\rho_M)}, \tag{2.45}$$

where $f_l^{(\pm)}$ is the logarithmic derivative of the interior wave function defined at $r=r_M$,

$$f_l^{(\pm)}=r_M\left[\frac{d\varphi_l^{(\pm)}}{dr}\Big/\varphi_l^{(\pm)}\right]_{r_M} \tag{2.46}$$

Corresponding quantity for the incoming and outgoing wave functions in the asymptotic region is

$$\Delta_l\pm is_l=\rho_M\left[\frac{du_l^{(\pm)}}{d\rho}\Big/u_l^{(\pm)}\right]_{\rho_M} \tag{2.47}$$

2.6 Cross sections

We have defined l_{max} by the formula (2.35). This l_{max} is somewhat larger than the largest value of the angular momenta which contribute effectively to the cross sections. This latter value of the angular momentum is indicated by a notation $l_{max\,C}$, and defined by the condition

$$\sigma_C^{(l_{max\,C})}\Big/\sum_{l=0}^{l_{max\,C}-1}\sigma_C^{(l)}\leq 10^{-4}, \tag{2.48}$$

where $\sigma_C^{(l)}$ is the partial cross section of the formation of compound nucleus. This cross section is obtained by using the transmission coefficient

$$T_l^{(\pm)}(E)=1-|\gamma_l^{(\pm)}|^2, \tag{2.49}$$

and is written as

$$\sigma_C^{(l)}=\frac{\pi}{k^2}\{(l+1)T_l^{(+)}+lT_l^{(-)}\}\times 10. \tag{2.50}$$

Cross section of the formation of compound nucleus is then

$$\sigma_C=\sum_{l=0}^{l_{max\,C}}\sigma_C^{(l)}. \tag{2.51}$$

Elastic scattering and total cross sections for neutrons are calculated by the formulas

$$\sigma_e=\frac{\pi}{k^2}\sum_{l=0}^{l_{max\,C}}\{(l+1)|1-\gamma_l^{(+)}|^2+l|1-\gamma_l^{(-)}|^2\}\times 10, \tag{2.52}$$

and

$$\sigma_t=\sigma_e+\sigma_C. \tag{2.53}$$

Formulas (2.52) and (2.53) cannot be used for the charged particles, because of the Coulomb scattering.

Differential elastic scattering cross section for neutrons is calculated as follows,

$$\frac{d\sigma_e}{d\Omega}=\{|A(\theta)|^2+|B(\theta)|^2\}\times 10, \tag{2.54}$$

where

$$A(\theta)=\frac{i}{2k}\sum_{l=0}^{l_{max\,C}}\{(l+1)(1-\gamma_l^{(+)})+l(1-\gamma_l^{(-)})\}P_l(\cos\theta), \tag{2.55}$$

and

$$B(\theta)=\frac{1}{2k}\sum_{l=0}^{l_{max}C}\{\eta_l^{(-)}-\eta_l^{(+)}\}P_l^1(\cos\theta). \tag{2.56}$$

Coefficient of the Legendre expansion of the formula (2.54) is necessary for the reactor calculations, and is expressed by the formula

$$B_L=\frac{1}{8k^2}\sum_{l_1=0}^{l_{max}C}\sum_{l_2=|l_1-L|}^{l_1+L}\sum_{j_1=|l_1-1/2|}^{l_1+1/2}\sum_{j_2=|l_2-1/2|}^{l_2+1/2}[Z(l_1j_1l_2j_2;\ \frac{1}{2}L)]^2 \times\mathfrak{Re}[(1-\eta_{l_1}^{j_1})(1-\eta_{l_2}^{j_2})^*]\times 10, \tag{2.57}$$

where Z is the Z-coefficient given by BLATT and BIEDENHARN[4], and is expressed in a general form

$$Z(l_1j_1l_2j_2;\ sL)=(-i)^{-l_1+l_2+L}(2l_1+1)^{1/2}(2l_2+1)^{1/2} \times(2j_1+1)^{1/2}(2j_2+1)^{1/2}(l_1l_200|L0)W(l_1j_1l_2j_2;\ sL). \tag{2.57-1}$$

The Z-coefficient above does not vanish if the following conditions are satisfied:

Conditions

1. l_1+l_2+L=even
2. $|l-s|\leq j\leq l+s$
3. $|l_1-L|\leq l_2\leq l_1+L$
4. $|j_1-L|\leq j_2\leq j_1+L$

(2.57-2)

In eq. (2.57-1), $W(l_1j_1l_2j_2;\ sL)$ is so-called Racah coefficient[5] and is given as

$$\begin{aligned}W(abcd;\ ef)=&[(a+b-e)!(a+e-b)!(b+e-a)!(c+d-e)!(c+e-d)!\\&\times(d+e-c)!(a+c-f)!(a+f-c)!(c+f-a)!(b+d-f)!(b+f-d)!\\&\times(d+f-b)!/\{(a+b+e+1)!(c+d+e+1)!(a+c+f+1)!(b+d+f+1)!\}]^2\\&\times\sum_z(-)^z(a+b+c+d+1-z)!/\{(a+b-e-z)!(c+d-e-z)!(a+c-f-z)!\\&\times(b+d-f-z)!z!(e+f-a-d+z)!(e+f-b-c+z)!\}.\end{aligned} \tag{2.57-3}$$

In eq. (2.57), $\eta_l^{(\pm)}$ is expressed by η_l^j, corresponding to $j=l\pm 1/2$.

For elastically scattered protons, differential cross section is also given by the formula (2.54), but $A(\theta)$ and $B(\theta)$ are somewhat different from (2.55) and (2.56). The corresponding expressions are

$$A(\theta)=f_C(\theta)+\frac{i}{2k}\sum_{l=0}^{l_{max}C}e^{2i\sigma_l}\{(l+1)(1-\eta_l^{(+)})+l(1-\eta_l^{(-)})\}P_l(\cos\theta), \tag{2.58}$$

and

$$B(\theta)=\frac{1}{2k}\sum_{l=0}^{l_{max}C}e^{2i\sigma_l}[\eta_l^{(-)}-\eta_l^{(+)}]\cdot P_l^1(\cos\theta). \tag{2.59}$$

Coulomb scattering amplitude $f_C(\theta)$ is given by

$$f_C(\theta)=\frac{-\eta}{2k\sin^2(\theta/2)}\exp[-i\eta\ln(\sin^2(\theta/2))+2i\sigma_0]. \tag{2.60}$$

Phase shift of the Coulomb scattering σ_l is given by the recurrence relation

$$e^{2i\sigma_l}=\frac{(l+i\eta)(l-1+i\eta)\cdots\cdots(1+i\eta)}{(l-i\eta)(l-1-i\eta)\cdots\cdots(1-i\eta)}e^{2i\sigma_0}, \tag{2.61}$$

where

$$\begin{aligned}\sigma_0=&-\eta+\frac{\eta}{2}\ln(16+\eta^2)+\frac{7}{2}\tan^{-1}\left(\frac{\eta}{4}\right)-\left[\tan^{-1}\eta+\tan^{-1}\left(\frac{\eta}{2}\right)+\tan^{-1}\left(\frac{\eta}{3}\right)\right]\\&-\frac{\eta}{12(16+\eta^2)}\left\{1+\frac{\eta^2-48}{30(16+\eta^2)^2}+\frac{\eta^4-160\eta^2+1280}{105(16+\eta^2)^4}\right\}.\end{aligned} \tag{2.62}$$

Sometimes we are interested in the Rutherford ratio of the elastically scattered protons. Cross section of the Rutherford scattering is

$$\left(\frac{d\sigma_e}{d\Omega}\right)_R = |f_c(\theta)|^2 \times 10, \tag{2.63}$$

and then Rutherford ra[illegible] of the cross section is defined by the formula

$$\left(\frac{d\sigma_e}{d\Omega}\right)_{R\text{-}[illegible]} = \frac{d\sigma_e}{d\Omega} \Big/ \left(\frac{d\sigma_e}{d\Omega}\right)_R \tag{2.64}$$

When alpha particle is an incident particle, we can write the scattering amplitude

$$\eta_l^{(+)} = \eta_l^{(-)} = \eta_l, \tag{2.65}$$

and therefore

$$A(\theta) = f_c(\theta) + \frac{i}{2k} \sum_{l=0}^{l=l_c} e^{2i\sigma_l}(2l+1)(1-\eta_l)P_l(\cos\theta), \tag{2.66}$$

$$B(\theta) = 0. \tag{2.67}$$

2. 7 Chi square deviation

Experimental and calculated angular distributions of scattered particles may be compared by means of the chi square deviation,

$$\chi_e^2 = \sum_\theta \left[\frac{\sigma^{th}(\theta) - a\sigma^{ex}(\theta)}{\Delta\sigma^{ex}(\theta)}\right]^2, \tag{2.68}$$

where a is a normalization factor which is a measure of the discrepancy of the absolute values between experimental and calculated cross sections, and is given by

$$a = \frac{\sum\left[\frac{\sigma^{ex}(\theta)\cdot\sigma^{th}(\theta)}{(\Delta\sigma^{ex}(\theta))^2}\right]}{\sum[\sigma^{ex}(\theta)/\Delta\sigma^{ex}(\theta)]^2}, \tag{2.69}$$

where $\sigma^{ex}(\theta)$ and $\sigma^{th}(\theta)$ are experimental and calculated differential cross sections, and $\Delta\sigma^{ex}(\theta)$ is the experimental error in differential cross section. In our program, it is also possible to calculate the chi square deviation setting a to unity.

2. 8 Legendre polynomials

Legendre polynomials are computed by the following relations,

$$P_0(\cos\theta) = 1, \tag{2.70}$$

$$P_1(\cos\theta) = \cos\theta, \tag{2.71}$$

$$P_{l+1}(\cos\theta) = \frac{1}{l+1}\{(2l+1)\cos\theta \cdot P_l(\cos\theta) - lP_{l-1}(\cos\theta)\}, \tag{2.72}$$

$$P_l^1(\cos\theta) = \frac{l+1}{\sin\theta}\{\cos\theta \cdot P_l(\cos\theta) - P_{l+1}(\cos\theta)\}. \tag{2.73}$$

2. 9 Transformation of the cross sections from center of mass system (CMS) to laboratory system (LAB)

i) Angles

Let us define the parameter γ as follows,

$$\gamma = \left(\frac{mm'}{MM'}\right)^{1/2}\left(\frac{E}{E'}\right)^{1/2}, \tag{2.74}$$

where primed quantities are referred to those of final stage and the energies are in center of mass system. Relations between the scattering angles in CMS and LAB are

$$\cos\theta_L=\frac{\gamma+\cos\theta_c}{(1+2\gamma\cos\theta_c+\gamma^2)^{1/2}}, \tag{2.75}$$

or

$$\tan\theta_L=\frac{\sin\theta_c}{\gamma+\cos\theta_c}. \tag{2.76}$$

ii) Cross sections

Relation between angular distributions in CMS and LAB is

$$\left(\frac{d\sigma}{d\Omega}\right)_L=\frac{(1+2\gamma\cos\theta_c+\gamma^2)^{3/2}}{|1+\gamma\cos\theta_c|}\left(\frac{d\sigma}{d\Omega}\right)_c \tag{2.77}$$

2. 10 Recurrence formula for Coulomb phase factor $\exp(2i\sigma_l)$

Relation given by the formula (2. 61) can be separated into real and imaginary parts;

$$\mathfrak{Re}\,(e^{2i\sigma_{l+1}})=\left[\frac{(l+1)^2-\eta^2}{(l+1)^2+\eta^2}\mathfrak{Re}\,(e^{2i\sigma_l})\right]-\left[\frac{2\eta(l+1)}{(l+1)^2+\eta^2}\mathfrak{Im}(e^{2i\sigma_l})\right], \tag{2.78}$$

$$\mathfrak{Im}(e^{2i\sigma_{l+1}})=\left[\frac{(l+1)^2-\eta^2}{(l+1)^2+\eta^2}\mathfrak{Im}(e^{2i\sigma_l})\right]+\left[\frac{2\eta(l+1)}{(l+1)^2+\eta^2}\mathfrak{Re}\,(e^{2i\sigma_l})\right]. \tag{2.79}$$

For the s-wave phase shift, σ_0 has been given by the formula (2. 62) and then one can obtain the Coulomb phase shift associated with any l-value, using the above recurrence relations.

3. Mathematical Description of Compound Nuclear Process —Hauser-Feshbach's Method[6]—

In this section, we consider the nuclear process via the compound nucleus formation, in the case of the incident and outgoing particles being neutrons. Target and residual nuclei are specified by their spin I, parity π and excitation energy $\varepsilon(=E-E')$. Now we consider the case of the inelastic scattering of neutrons which will be expressed as $(EI\pi \to E'I'\pi')$.

3. 1 Angular distribution of the inelastic scattering process

Angular distribution of the inelastically scattered neutrons is calculated by the following formula

$$\frac{d\sigma(EI\pi\to E'I'\pi')}{d\Omega}=\sum_{L=0}^{2l_{max}C} B_L(EI\pi\to E'I'\pi')P_L(\cos\theta), \tag{3.1}$$

where

$$B_L(EI\pi\to E'I'\pi')=\frac{1}{8k^2}\frac{(-)^{I-I'}}{(2I+1)}\sum_{J\Pi}\frac{(2J+1)^2}{\sigma_{J\Pi}}\sum_{jl}\omega_{\Pi}(\pi l)\tau_{l\pi}{}^{j}(EIJL) \times\sum_{j'l'}\omega_{\Pi}(\pi' l')\tau_{l'\pi'}{}^{j'}(E'I'JL)\times 10. \tag{3.2}$$

Here J and Π are spin and parity of the compound system, and $\omega_{\Pi}(\pi l)$ is introduced by taking account of parity conservation,

$$\omega_{\Pi}(\pi l)=\frac{1}{2}|\Pi+(-)^{l}\pi|. \tag{3.3}$$

In eq. (3.2), $\tau_{l\pi}{}^{j}(EIJL)$ is

$$\tau_{l\pi}{}^{j}(EIJL)=T_l{}^{j}(EI\pi)Z(ljlj;\tfrac{1}{2}L)W(jJjJ;IL), \tag{3.4}$$

where $T_l{}^{j}(EI\pi)$ is the same quantity given by the formula (2.49), and Z-coefficient and Racah coefficient are mentioned in eqs. (2.57-1) to (2.57-3). In the final state, as the reciprocal process, $T_{l'}{}^{j'}(E'I'\pi')$ is calculated with emitted neutron energy and angular momentum. In the denominator of the formula (3.2), $\sigma_{J\Pi}$ is the sum of $T_l{}^{j}$ corresponding to all possible nuclear states;

$$\sigma_{J\Pi}=\sum_{EI\pi}\sum_{j=|J-I|}^{J+I}\sum_{l=|j-1/2|}^{j+1/2}\omega_{\Pi}(\pi l)T_l{}^{j}(EI\pi). \tag{3.5}$$

In general, we should take all possible nuclear reactions into account, such as (n, p), (n, α), (n, γ) and so on, but in our program (n, p) process can only be considered as a competing process. Besides, the contributions from highly excited levels which are in continuum region, are not included in this program. We intend to improve these points in future.

3. 2 Excitation function

By integrating the eq. (3.1) over the angles, the excitation function is obtained as

$$\sigma(EI\pi\to E'I'\pi')=4\pi B_0(EI\pi\to E'I'\pi'), \tag{3.6}$$

where $B_0(EI\pi\to E'I'\pi')$ is

$$B_0(EI\pi\to E'I'\pi')=\frac{1}{8k^2}\frac{1}{(2I+1)}\sum_{J\Pi}\frac{2J+1}{\sigma_{J\Pi}}\sum_{jl}\omega_{\Pi}(\pi l)T_l{}^{j}(EI\pi) \times\sum_{j'l'}\omega_{\Pi}(\pi' l')T_{l'}{}^{j'}(E'I'\pi')\times 10. \tag{3.7}$$

Total inelastic scattering cross section is then

$$\sigma_{in}(EI\pi)=\sum_{E'I'\pi'}\sigma(EI\pi\to E'I'\pi'). \tag{3.8}$$

3. 3 Compound elastic scattering cross section

Compound elastic scattering cross section is defined by setting $(E'I'\pi')$ equal to $(EI\pi)$. Then, angular distribution of the compound elastic process is

$$\frac{d\sigma_{ce}(EI\pi)}{d\Omega}=\sum_{L=0}^{2l'_{max}C}B_L(EI\pi)P_L(\cos\theta), \tag{3.9}$$

where

$$B_L(EI\pi)=\frac{10}{8k^2(2I+1)}\sum_{J\Pi}\frac{1}{\sigma_{J\Pi}}[(2J+1)\sum_{jl}\omega_{\Pi}(\pi l)T_{lj}^{J}(EIJL)]^2. \tag{3.10}$$

Integrating this over the angles, we obtain the compound elastic scattering cross section,

$$\sigma_{ce}(EI\pi)=4\pi B_0(EI\pi), \tag{3.11}$$

where

$$B_0(EI\pi)=\frac{10}{8k^2(2I+1)}\sum_{J\Pi}\frac{2J+1}{\sigma_{J\Pi}}[\sum_{jl}\omega_{\Pi}(\pi l)T_{lj}^{J}(EI\pi)]^2. \tag{3.12}$$

In these calculations, we must take care of the relations between angular momenta. The selection rules on the angular momenta are as follows:

i) L=even and $0\le L\le \mathrm{Min}(2l_{maxC}, 2l'_{maxC})$.

ii) $J_{min}=0$, if I is half odd integer.
$=1/2$, if I is integer.

iii) $J_{min}\le J\le \mathrm{Min}\left(l_{maxC}+I+\frac{1}{2},\ l'_{maxC}+I'+\frac{1}{2}\right)$

iv) $|J-I|\le j\le J+I\le l_{maxC}+\frac{1}{2}$.

$|J-I'|\le j'\le J+I'\le l'_{maxC}+\frac{1}{2}$.

v) $|j-\frac{1}{2}|\le l\le j+\frac{1}{2}\le l_{maxC}$.

$|j'-\frac{1}{2}|\le l'\le j'+\frac{1}{2}\le l'_{maxC}$.

4. Methods of Numerical Calculations

4. 1 Basic constants

Some basic constants set in the program are

$$\left.\begin{aligned} m_n &= 1.008982 \\ m_p &= 1.007593 \\ m_\alpha &= 4.003870 \\ C_{so} &= (1.42926)^2 \end{aligned}\right\} \tag{4.0}$$

$$\left(\frac{2\mu_0}{\hbar^2}\right)^{1/2} = 0.2157135, \tag{4.1}$$

$$\frac{2\mu_0 e^2}{\hbar^2} = 0.0688747, \tag{4.2}$$

$$\frac{2\mu_0}{\hbar^2} C_{so} = 0.0977178, \tag{4.3}$$

$$\eta = \frac{\mu Z Z' e^2}{\hbar^2 k} = \frac{Z Z' e^2}{\sqrt{2}\hbar}\left(\frac{\mu}{E}\right)^{1/2} = 0.157452 Z Z' \left(\frac{\mu}{E}\right)^{1/2}. \tag{4.4}$$

4. 2 Initial values of wave functions

In numerical integration of Schroedinger equations, we must have the values of the wave functions at first two mesh points as the starting values of the functions. We can obtain these values by power series expansion of the functions;

$$\varphi_l^{(\pm)}(r) = \sum_{n=0}^{\infty} a_{n,l}^{(\pm)} r^{n+l+1}. \tag{4.5}$$

Relations between expansion coefficients are

$$a_{n,l}^{(\pm)} = \frac{-1}{n(2l+n+1)}\left\{\left(k^2 + \mathfrak{V}_c(r) - \frac{3k\eta}{R_c}\right) a_{n-2,l}^{(\pm)} + \frac{k\eta}{R_c^3} a_{n-4,l}^{(\pm)} - b_l^{(\pm)} \mathfrak{V}_{so}(r) a_{n-1,l}^{(\pm)}\right\}. \tag{4.6}$$

where

$$b_l^{(+)} = l, \tag{4.7}$$

$$b_l^{(-)} = -(l+1), \tag{4.8}$$

and

$$\mathfrak{V}_{so}(r) = \frac{2\mu}{\hbar^2} C_{so} \frac{1}{a_0} (V_{so} + iW_{so}) \frac{\exp\{(r-R_0)/a_0\}}{[1+\exp\{(r-R_0)/a_0\}]^2} \tag{4.9}$$

In eq. (4. 6), we assume that the potential values at these mesh points are nearly constant. In particular, Gaussian and derivative Woods-Saxon potential values at these mesh points are reset to the constant values in the program. First four values of the expansion coefficients are

$$a_{1,l}^{(\pm)} = \frac{-1}{2(l+1)} b_l^{(\pm)} \mathfrak{V}_{so}(r) a_{0,l}^{(\pm)}, \tag{4.10}$$

$$a_{2,l}^{(\pm)} = \frac{-1}{2(2l+3)}\left\{\left(k^2 + \mathfrak{V}_c(r) - \frac{3k\eta}{R_c}\right) a_{0,l}^{(\pm)} + b_l^{(\pm)} \mathfrak{V}_{so}(r) a_{1,l}^{(\pm)}\right\}, \tag{4.11}$$

$$a_{3,l}^{(\pm)} = \frac{-1}{3(2l+4)}\left\{\left(k^2 + \mathfrak{V}_c(r) - \frac{3k\eta}{R_c}\right) a_{1,l}^{(\pm)} + b_l^{(\pm)} \mathfrak{V}_{so}(r) a_{2,l}^{(\pm)}\right\}. \tag{4.12}$$

and

$$a_{4,l}{}^{(\pm)}=\frac{-1}{4(2l+5)}\left\{\left(k^2+\mathfrak{V}_C(r)-\frac{3k\eta}{R_C}\right)a_{2,l}{}^{(\pm)}+b_l{}^{(\pm)}\mathfrak{V}_{SO}(r)a_{3,l}{}^{(\pm)}\right.$$
$$\left.+\frac{k\eta}{R_C{}^3}a_{0,l}{}^{(\pm)}\right\}, \qquad (4.13)$$

where $a_{0,l}{}^{(\pm)}$ is a normalization constant and can be set to unity.

4. 3 Numerical integration of wave functions

The method used for numerical integration is the Fox-Goodwin's two points method. Eqs. (2.1) and (2.2) are rewritten as

$$\frac{d^2\varphi_l{}^{(\pm)}}{dr^2}=Q_l{}^{(\pm)}(r)\cdot\varphi_l{}^{(\pm)}. \qquad (4.14)$$

With Fox-Goodwin's method, we can write this equation as follows;

$$\varphi_l{}^{(\pm)}(n+1)=\frac{(2+\frac{5}{6}h^2Q_l{}^{(\pm)}(n))\cdot\varphi_l{}^{(\pm)}(n)-(1-\frac{1}{12}h^2Q_l{}^{(\pm)}(n-1))\cdot\varphi_l{}^{(\pm)}(n-1)}{1-\frac{1}{12}h^2Q_l{}^{(\pm)}(n+1)}, \qquad (4.15)$$

where h is the step length in this numerical integration, and n indicates the mesh point. Derivative of the function is calculated by Lagrange's six points method;

$$\frac{d}{dr}\varphi_l{}^{(\pm)}(n)=\frac{1}{h}\left\{\frac{1}{60}(\varphi_l{}^{(\pm)}(n+3)-\varphi_l{}^{(\pm)}(n-3))+\frac{3}{20}(\varphi_l{}^{(\pm)}(n-2)\right.$$
$$\left.-\varphi_l{}^{(\pm)}(n+2))+\frac{3}{4}(\varphi_l{}^{(\pm)}(n+1)-\varphi_l{}^{(\pm)}(n-1))\right\}. \qquad (4.16)$$

4. 4 External wave function $F_l(\rho_M)$

In section II, we have shown the method by which the function $G_l(\rho_M)$ and the maximum angular momentum l_{max} are defined. Using l_{max} and $G_l(\rho_M)$ for $l\leq l_{max}$, we will explain the method[3] of the calculation of $F_l(\rho_M)$ in this section.

Let

$$l^{(1)}=l_{max}+10, \qquad (4.17)$$

$$F_{l^{(1)}+1}^{(1)}=0, \qquad (4.18)$$

and

$$F_{l^{(1)}}{}^{(1)}=10^{-36}. \qquad (4.19)$$

With these starting values, we can obtain $F_l(\rho_M)$ corresponding to lower l-values by the following recurrence formula;

$$F_{l-1}{}^{(1)}=\frac{l}{\sqrt{\eta^2+l^2}}\left\{(2l+1)\left(\frac{\eta}{l(l+1)}+\frac{1}{\rho_M}\right)F_l{}^{(1)}-\frac{1}{l+1}(\eta^2+(l+1)^2)^{1/2}F_{l+1}{}^{(1)}\right\}. \qquad (4.20)$$

For $l=0$, we obtain the normalization factor by means of Wronskian's rule,

$$\alpha=(1+\eta^2)^{1/2}(F_0{}^{(1)}G_1-G_0F_1{}^{(1)}), \qquad (4.21)$$

and

$$F_l(\rho_M)=F_l{}^{(1)}(\rho_M)/\alpha. \qquad (4.22)$$

If $F_l(\rho_M)$ has the correct value, Wronskian's rule must be satisfied for $l\leq l_{max}$;

$$F_l'(\rho_M)G_l(\rho_M)-F_l(\rho_M)G_l'(\rho_M)=1, \qquad (4.23)$$

if it has not, above method is repeated by resetting $l^{(1)}$ as $l^{(1)}+5$.

4. 5 Coulomb wave function for s-wave

At $\rho=\rho_M$, we can calculate G_0 and G_0' by means of the following formulas.[2)]

i) $\eta\geq 4$

In this case, we set $\rho_A=2\eta$ and

$$G_0(\rho_A)=1.223404016\eta^{1/6}\{1+0.04959570165\eta^{-4/3}-0.008888888889\eta^{-2}+0.002455199181\eta^{-10/3}-0.0009108958061\eta^{-4}+0.0002534684115\eta^{-16/3}\}, \tag{4.24}$$

and

$$G_0'(\rho_A)=-0.7078817734\eta^{-1/6}\{1-0.1728260369\eta^{-2/3}+0.0003174603174\eta^{-2}-0.003581214850\eta^{-8/3}+0.0003117824680\eta^{-4}-0.0009073966427\eta^{-14/3}\}. \tag{4.25}$$

ii) $\eta<4$

Let $\rho_A=9+2\eta$ and $\varphi=\rho_A-\eta\cdot\ln(2\rho_A)+\sigma_0$, then G_0 and G_0' are given by

$$G_0(\rho_A)=s\cdot\cos\varphi-t\cdot\sin\varphi, \tag{4.26}$$

and

$$G_0'(\rho_A)=S\cdot\cos\varphi-T\cdot\sin\varphi, \tag{4.27}$$

where

$$s=\sum s_n, \tag{4.28}$$
$$t=\sum t_n, \tag{4.29}$$
$$S=\sum S_n, \tag{4.30}$$

and

$$T=\sum T_n. \tag{4.31}$$

They are calculated by means of the relations;

$$s_{n+1}=A_n s_n-B_n t_n, \tag{4.32}$$
$$t_{n+1}=A_n t_n+B_n s_n, \tag{4.33}$$
$$S_{n+1}=A_n S_n-B_n T_n-\frac{s_{n+1}}{\rho_A}, \tag{4.34}$$

and

$$T_{n+1}=A_n T_n+B_n S_n-\frac{t_{n+1}}{\rho_A}, \tag{4.35}$$

Coefficients A_n and B_n are respectively given by

$$A_n=\frac{2n+1}{2(n+1)\rho_A}\eta, \tag{4.36}$$

and

$$B_n=\frac{\eta^2-n(n+1)}{2(n+1)\rho_A}. \tag{4.37}$$

The initial values are

$$s_0=1, \tag{4.38}$$
$$t_0=0, \tag{4.39}$$
$$S_0=0, \tag{4.40}$$
$$T_0=1-(\eta/\rho_A). \tag{4.41}$$

iii) Numerical integration of G_0 and G_0' from ρ_A to ρ_M

Wave equation for G_0 is rewritten as

$$\frac{d^2G_0}{d\rho^2}=\left(\frac{2\eta}{\rho}-1\right)G_0=f(\rho)\cdot G_0. \tag{4.42}$$

This equation is integrated from ρ_A to ρ_M by means of Fox-Goodwin's method. Therefore, we must find the initial values at two mesh points. In our program, these initial values are calcu-

lated by means of Picard's five points method;

$$G_0(1)=G_0(0)-h_cG_0'(0)+\frac{1}{1440}\{367f(0)G_0(0)+540f(1)G_0(1)-282f(2)G_0(2)+116f(3)G_0(3)-21f(4)G_0(4)\}, \quad (4.43)$$

$$G_0(2)=G_0(0)-2h_cG_0'(0)+\frac{1}{1440}h_c^2\{848f(0)G_0(0)+2304f(1)G_0(1)-480f(2)G_0(2)+256f(3)G_0(3)-48f(4)G_0(4)\}, \quad (4.44)$$

$$G_0(3)=G_0(0)-3h_cG_0'(0)+\frac{1}{1440}h_c^2\{1323f(0)G_0(0)+4212f(1)G_0(1)+486f(2)G_0(2)+540f(3)G_0(3)-81f(4)G_0(4)\}, \quad (4.45)$$

$$G_0(4)=G_0(0)-4h_cG_0'(0)+\frac{1}{1440}h_c^2\{1792f(0)G_0(0)+6144f(1)G_0(1)+1536f(2)G_0(2)+2048f(3)G_0(3)+0\}. \quad (4.46)$$

These are simple algebraic equations and easily solved. Arguments of $G_0(n)$ and $f(n)$ mean the n^{th} mesh point and h_c is step length of this numerical method. $G_0(3)$ and $G_0(4)$ are used as initial values of Fox-Goodwin's method. Derivative at $\rho=\rho_M$ is given by means of the same method as the formula (4.16).

5. Program Description

5. 1 Machine specifications

The Program ELIESE-1 has been written for an IBM 7090 FORTRAN-II with a 32,768 words memory and at least two tape units.

5. 2 General description of the program

The Program ELIESE-1 is composed of the main-program and 31 sub-programs. CHART 1 shows the flow-chart of ELIESE-1 main-program. The ELIESE-1 sub-programs may be divided into four classes listed below:

1. Input Routine reads the input data required for the actual computation.
   SUBROUTINE INPUT
2. Computation Routine computes cross sections and chi-square deviations for a given set of input data.

SUBROUTINE PREP	SUBROUTINE ANGLE
SUBROUTINE WELL	SUBROUTINE SPHBES
SUBROUTINE GZERO	SUBROUTINE PICARD
SUBROUTINE GOASMA	SUBROUTINE GFLMAX
SUBROUTINE RUTH	SUBROUTINE POTEN
SUBROUTINE INIT (L)	SUBROUTINE INTEG (I,)
SUBROUTINE ETASIG (L)	SUBROUTINE LEGEND
SUBROUTINE AMPAB	SUBROUTINE BLL
SUBROUTINE LABRAT	SUBROUTINE CHISOS
SUBROUTINE COMPND	SUBROUTINE COMJP (L, A)
SUBROUTINE CLBGD (A)*	SUBROUTINE ZETC (A)*
SUBROUTINE WRACA (A)*	SUBROUTINE ZFACT (A)*

   * Function type sub-program

3. Output Routine generates the calculated results.

SUBROUTINE OUTPUT	SUBROUTINE INLIST
SUBROUTINE OUTIN	SUBROUTINE ALOCK

   SUBROUTINE BLOCK (FAP language)

4. Check Routine finds out an overflow and/or a divide check condition.
   SUBROUTINE OFLOW (L, A)

The program assumes the presence of the following FORTRAN elementary function subroutines:

LOGF (natural logarithm)	SINF (sine)
COSF (cosine)	EXPF (exponential)
SQRTF (square root)	ATANF (arc-tangent)

5. 3 Detailed descriptions of the specific routines of the program

1. SUBROUTINE PREP sets up a reduced mass, a wave number, potential well depth parameters, a matching radius, Coulomb parameters and other basic quantities used in the computation.
2. SUBROUTINE ANGLES sets up angle points and angular variables.

3. SUBROUTINE WELL computes the potential shape functions at each mesh point.
4. SUBROUTINE SPHBES generates the functions $G_l(\rho)$, $F_l(\rho)$, $G_l'(\rho)$ and $F_l'(\rho)$ for neutron, and determines the maximum angular momentum l_{max}.
5. SUBROUTINE GZERO computes the functions $G_0(\rho)$ and $G_0'(\rho)$ at $\rho=\rho_A$ for charged particle.
6. SUBROUTINE PICARD computes the functions $G_0(\rho+h)$, $G_0(\rho+2h)$, $G_0(\rho+3h)$ and $G_0(\rho+4h)$ for charged particle.
7. SUBROUTINE GOASMA integrates the Coulomb wave equation for $G_0(\rho)$ from ρ_A to ρ_M, and generates the derivative $G_0'(\rho_M)$.
8. SUBROUTINE GFLMAX generates the functions $G_l(\rho)$, $F_l(\rho)$, $G_l'(\rho)$ and $F_l'(\rho)$ for charged particle, and determines the maximum angular momentum l_{max}.
9. SUBROUTINE RUTH computes the Rutherford scattering amplitudes and the cross sections.
10. SUBROUTINE POTEN computes the potential values at each mesh point.
11. SUBROUTINE INIT (L) sets up the starting values for the numerical integration of the internal wave equations.
12. SUBROUTINE INTEG (L) integrates the internal wave equations up to ρ_M, and generates the derivatives.
13. SUBROUTINE ETASIG (L) computes the scattering amplitudes $\eta_l^{(+)}$, the penetrabilities T_l^J and the reaction cross section, and determines $l_{max,C}$.
14. SUBROUTINE LEGEND generates the Legendre polynomials.
15. SUBROUTINE AMPAB computes $A(\theta)$, $B(\theta)$ and the differential cross section.
16. SUBROUTINE BLL computes the coefficients of the Legendre expansion of the differential cross section for neutron scattering.
17. SUBROUTINE LABRAT transforms the differential cross sections from center of mass system to laboratory system.
18. SUBROUTINE CHISOS computes the chi-square deviation of the differential cross sections in the center of mass system.
19. SUBROUTINE COMPND computes the cross section of the compound nuclear process by means of HAUSER-FESHBACH's method.
20. SUBROUTINE COMJP (L, A) computes σ_{JII} expressed by (3.5).