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PROGRAM CCOM
—COUPLED-CHANNELS OPTICAL MODEL CALCULATION WITH AUTOMATIC PARAMETER SEARCH—

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Program CCOM
— Coupled-channels Optical Model Calculation with Automatic Parameter Search —

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A new program of coupled-channels optical model calculation has been developed for the evaluation of actinide nuclei. The code is composed of by the modules having high independency and large flexibility. The code is written by C++ language using object oriented techniques. The program has capability of fitting of the parameters even for the several nuclei at the same time. The formulae required in the calculation, details of the numerical treatments and the input parameters are described. The examples of the input file and the output are also shown.

Keywords: Nuclear Data, Evaluation, Neutron, Proton, Computer Program, Cross Sections, Optical Model, Coupled Channel Calculation

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プログラム CCOM
— 自動パラメータ検索機能付チャンネル結合光学モデル計算 —

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アクチニド原子核の核データ評価のために、新たなチャンネル結合光学モデル計算プログラムを開発した。コード独立性の高いモジュールで構成され、大きな融通性を持っている。コードはオブジェクト指向技術を用いて、C++言語で記述されている。プログラムにはパラメータのフィッティング機能があり、複数の原子核に対しても同時に行うことが可能である。計算に必要な式及び数値的取り扱い、入力パラメータについて記述してある。また入力パラメータの例及びその出力結果を示す。

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1 Introduction

Optical model is one of important methods for the evaluation of the nuclear reaction data, since it is used for the estimation of total and scattering cross sections, and of transmission coefficients for statistical model calculations. In order to make the Japanese Evaluated Nuclear Data Library(JENDL), spherical optical model codes with statistical model calculation such as ELIESE[1] and CASTHY[2] were developed at the Nuclear Data Center in JAERI. For the actinide nuclei, however, coupled-channels(CC) optical model[3, 4] can describe scattering process better than spherical optical model, because such nuclei having large deformation cause strong coupling between levels in the rotational band.

A few codes[5, 6] developed in the foreign countries were used for the coupled-channels calculations for nuclear data evaluations. Such codes are usually used as a black box and it is very difficult to add new features to the codes. It is valuable to develop a new code, whose details are known, for the further improvements of the calculation. Then a new code (CCOM) of coupled-channels optical model calculation has been developed at the Nuclear Data Center in JAERI for the evaluation of actinide nuclei. The CCOM is composed of the modules having high independency and large flexibility. The CCOM is written by C++ language using object oriented technique. The CCOM also has capability of the fitting of the parameters even for the several nuclei at the same time.

This report describes the formulae required in the calculation, details of the numerical treatments and input parameters. The examples of the input file and its output are also shown.

2 Model

2.1 Coupled-channels Equation

In this model, it is assumed that the projectile has no internal structure and the interaction with the target can be described by the one body local potential. The formulations described bellow are mainly based on the Ref. [4].

The model Hamiltonian of the system is written as

$$H = H_A + H_a + T + V, \tag{1}$$

where H_A and H_a are Hamiltonians of the target and projectile, respectively. T and V are kinetic energy operator and optical potential of relative motion of target and projectile, respectively. The V depends on the relative coordinate of particles and also the internal coordinate of the target. The wave function of the target Φ_n in the state n is the eigen

function of H_A: $H_A\Phi_n = \epsilon_n\Phi_n$. Expanding by angular momentum, the total wave function is written as

$$\Psi = \sum_{c,J,M} \psi_c^{JM} r^{-1} f_c^{JM}(r), \tag{2}$$

$$\psi_c^{JM} = \left[\left[i^l Y_l \otimes \chi_s\right]_j \otimes \Phi_{n(I)}\right]_{JM}, \tag{3}$$

where c is the channel of reaction representing $\{l, j, n\}$, $f_c(r)$ shows the radial dependence of the wave function for the channel c, I is the spin of the target in the state n, Y_l is spherical harmonics, χ_s is the wave function of the projectile having the spin s and $[\phi_{j_1} \otimes \phi_{j_2}]_{JM} = \sum_{m_1,m_2}\langle j_1 j_2 m_1 m_2|JM\rangle\phi_{j_1}\phi_{j_2}$. From Eq. (1) and Eq. (2) with integrating for the coordinates except r for the wave function, the coupled-channels Schrödinger equation is obtained,

$$\left(\frac{d^2}{dr^2} - \frac{l_c(l_c+1)}{r^2} + k_c^2\right) f_c^{JM}(r) = \sum_{c'} \langle\psi_c|V|\psi_{c'}\rangle\, f_{c'}^{JM}(r), \tag{4}$$

where k_c indicates wave number in the channel c.

The deformation of the potential is assumed to be described by the the potential radius which is the function of the polar angles (θ' and ϕ') in the body-fixed frame. The radius is written by the expansion of the spherical harmonics,

$$R(\theta', \phi') = R_o\left\{1 + \sum_\lambda \beta_{\lambda 0} Y_{\lambda 0}^*(\theta', \phi')\right\}, \quad \lambda = 2, 4, 6, \ldots \tag{5}$$

Here the potential is assumed to have an axial symmetric shape and not to be changed by the rotational excitation. The potential can be expanded by the spherical harmonics as

$$\begin{aligned} V(\mathbf{r}') &= \sum_\lambda V_\lambda(r')\left\{i^\lambda Y_{\lambda 0}(\hat{\mathbf{r}}')\right\}^* \\ &= \sum_\lambda V_\lambda(r)\left\{i^\lambda \sum_\mu D_{0\mu}^\lambda(\Omega)^* Y_{\lambda\mu}(\hat{\mathbf{r}})\right\}^* \\ &= \sum_{\lambda\mu} V_{\lambda\mu}(r)\left\{i^\lambda Y_{\lambda\mu}(\hat{\mathbf{r}})\right\}^*, \end{aligned} \tag{6}$$

$$V_\lambda(r') = \int d\hat{\mathbf{r}}' V(\mathbf{r}') i^\lambda Y_{\lambda 0}(\hat{\mathbf{r}}'), \tag{7}$$

where $r' = |\mathbf{r}'|$, $\hat{\mathbf{r}}' = (\theta', \phi')$ and $d\hat{\mathbf{r}}' = \sin\theta' d\theta' d\phi'$. The $D_{mm'}^l$ is the D function which is defined by the matrix element of the rotation operator which is a function of the Euler angle, Ω. The wave function of the target nucleus Φ_{IMK} with the spin I for the level in the rotational band is expressed as

$$\Phi_{n(I)} = \Phi_{IMK} = \frac{\hat{I}}{\sqrt{8\pi^2}} D_{KM}^I(\Omega)\phi_K(\xi), \tag{8}$$

where ϕ_K and ξ are the intrinsic wave function and its coordinate, respectively, and $\hat{I} = \sqrt{2I+1}$. The reduced matrix element is calculated as

$$\begin{aligned}(I'M'|V_{\lambda\mu}|IM) &= \int\int \mathrm{d}\xi \mathrm{d}\Omega \Phi^*_{I'M'K} V_{\lambda\mu} \Phi_{IMK} \\ &= \langle I\lambda M\mu | I'M' \rangle (I'||V_\lambda||I) \qquad (9) \\ (I'||V_\lambda||I) &= \hat{I}\hat{I'}^{-1} V_\lambda(r) \langle I\lambda K0|I'K\rangle. \qquad (10)\end{aligned}$$

Finally, from Eqs. (3), (6) and (9) the coupling matrix element $\langle \psi_c|V|\psi_{c'}\rangle$ in Eq. (4) is obtained by

$$\begin{aligned}\langle \psi_c|V|\psi_{c'}\rangle &= \frac{1}{\sqrt{4\pi}} \sum_\lambda i^{l-l'-\lambda}(-)^{J-I-s} \hat{l}\hat{l'}\hat{j}\hat{j'}\hat{I'} \langle ll'00|\lambda 0\rangle \\ &\quad \times W(jj'll';\lambda I) W(jj'II';\lambda J)(I'||V_\lambda||I), \qquad (11)\end{aligned}$$

where W shows the Racah coefficient.

2.2 Cross Section

In asymptotic region where the nuclear potential is negligible except for the Coulomb potential, the Schrödinger equation has the form

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\eta k}{r} + k^2\right) f_l(r) = 0, \qquad (12)$$

where η is the Coulomb parameter: $\eta = ZZ'e^2\mu/\hbar^2 k$. The Coulomb wave functions $F_l(\rho)$ (regular) and $G_l(\rho)$ (irregular) are the independent solutions of Eq. (12), where $\rho = kr$. For $\rho \to \infty$

$$\begin{aligned}F_l(\rho) &\sim \sin(\rho - \eta \log 2\rho - \frac{1}{2}l\pi + \sigma_l), \qquad (13) \\ G_l(\rho) &\sim \cos(\rho - \eta \log 2\rho - \frac{1}{2}l\pi + \sigma_l), \qquad (14) \\ \sigma_l &= \arg\Gamma(l+1+i\eta). \qquad (15)\end{aligned}$$

In the case for the closed channels, the Schrödinger equation is given by

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\eta k}{r} - k^2\right) f_l(r) = 0. \qquad (16)$$

The solution of Eq. (16) is given by Whittaker's function $W_{-\eta,l+1/2}(2\rho)$[7], which is decreasing exponentially. If $\eta = 0$, the solution is given by the irregular modified spherical Bessel function multiplied by ρ.

The cross sections are obtained from the asymptotic behaviour of the wave function, which is given by the solution of Eq. (4). In the present system, total angular momentum J and

parity π are conserved through the scattering process. The C-matrix element $C_{cc'}^{J^\pi}$ for J^π from the initial channel c' to the final channel c is defined by

$$\tilde{f}_{cc'}^{J^\pi} \underset{r\to\infty}{\sim} \begin{cases} F_{l_c}(k_c r)\delta_{cc'} + \sqrt{\frac{k_{c'}}{k_c}} C_{cc'}^{J^\pi} \{G_{l_c}(k_c r) + iF_{l_c}(k_c r)\} & (E > 0), \\ W_{-\eta_c, l_c+1/2}(2k_c r) & (E \le 0), \end{cases} \tag{17}$$

where $\tilde{f}_{cc'}^{J^\pi}$ is the solution of Eq. (4). The C-matrix is related to S-matrix by

$$C_{cc'}^{J^\pi} = \frac{i}{2}\left(\delta_{cc'} - S_{cc'}^{J^\pi}\right). \tag{18}$$

If N channels are coupled for J^π, Eq. (4) has N sets of the independent solutions having no singularity at $r = 0$. The i-th set of the solution is represented by a vector with the elements of N channels,

$$\mathbf{f}^i = \begin{pmatrix} f_1^i \\ \vdots \\ f_N^i \end{pmatrix}. \tag{19}$$

The wave function having the asymptotic behaviour of Eq. (17) for the initial channel c' can be expressed by a linear combination of the n independent solutions,

$$\tilde{\mathbf{f}}^{c'} = \begin{pmatrix} \tilde{f}_{1c'} \\ \vdots \\ \tilde{f}_{Nc'} \end{pmatrix} = \sum_{i=1}^{N} a_i^{c'} \mathbf{f}^i, \qquad (c' = 1 \ldots N). \tag{20}$$

From the condition of the smooth connection of Eq. (20) and Eq. (17), $2N$ linear equations of $C_{cc'}$ and $a_i^{c'}$ are obtained,

$$\begin{pmatrix} \mathrm{f}_1 & -\mathrm{H}_1 \\ \mathrm{f}_2 & -\mathrm{H}_2 \end{pmatrix} \begin{pmatrix} \mathrm{A} \\ \bar{\mathrm{C}} \end{pmatrix} = \begin{pmatrix} \mathrm{F}_1 \\ \mathrm{F}_2 \end{pmatrix}, \tag{21}$$

where

$$\mathrm{F}_i = \mathrm{diag}\left(F_{l_1}(k_1 r_i), \ldots, F_{l_c}(k_c r_i), \ldots, F_{l_N}(k_N r_i)\right), \tag{22}$$

$$\mathrm{G}_i = \mathrm{diag}\left(G_{l_1}(k_1 r_i), \ldots, G_{l_c}(k_c r_i), \ldots, G_{l_N}(k_N r_i)\right), \tag{23}$$

$$\mathrm{H}_i = \mathrm{G}_i + i\mathrm{F}_i, \tag{24}$$

$$\mathrm{diag}\left(X_1, \cdots, X_N\right) = \begin{pmatrix} X_1 & & 0 \\ & \ddots & \\ 0 & & X_N \end{pmatrix}, \tag{25}$$

$$\mathrm{f}_i = \left(\tilde{\mathrm{f}}^1(r_i), \ldots, \tilde{\mathrm{f}}^c(r_i), \ldots, \tilde{\mathrm{f}}^N(r_i)\right), \tag{26}$$

$$\mathrm{A} = \begin{pmatrix} a_1^1 & \cdots & a_N^1 \\ \vdots & \ddots & \vdots \\ a_1^N & \cdots & a_N^N \end{pmatrix}, \tag{27}$$

$$\bar{\mathrm{C}} = \begin{pmatrix} \bar{C}_{11} & \cdots & \bar{C}_{1N} \\ \vdots & \ddots & \vdots \\ \bar{C}_{N1} & \cdots & \bar{C}_{NN} \end{pmatrix}, \tag{28}$$

$$\bar{C}_{cc'} = \sqrt{\frac{k_c'}{k_c}} C_{cc'}. \tag{29}$$

Here, the matching condition is that the wave functions coincide at the two asymptotic radial points (r_1, r_2). The matrix element of H_i will be changed to the Whittaker's function $W(2k_c r_i)$ in the case for the closed channel. The final result of the C-matrix is obtained from Eqs. (21) and (29).

The cross sections of total (σ_t), scattering (σ_i) to i-th level and reaction (σ_r) are calculated from the C-matrix,

$$\sigma_t = \sum_{J^\pi} \frac{4\pi}{k_0^2} \frac{2J+1}{(2s+1)(2I_0+1)} \sum_{cc'(n_{c'}=0)} \mathrm{Im} C_{cc'}^{J^\pi}, \tag{30}$$

$$\sigma_i = \sum_{J^\pi} \frac{4\pi}{k_0^2} \frac{2J+1}{(2s+1)(2I_0+1)} \sum_{cc'(n_{c'}=0, n_c=i)} \left|C_{cc'}^{J^\pi}\right|^2, \tag{31}$$

$$\sigma_r = \sum_{J^\pi} \frac{\pi}{k_0^2} \frac{2J+1}{(2s+1)(2I_0+1)} \sum_{cc'(n_{c'}=0)} \left(1 - \left|S_{cc'}^{J^\pi}\right|^2\right), \tag{32}$$

where k_0 and I_0 indicate wave number and spin of target for initial channel, respectively. The conditions of $n_c = i$ and $= 0$ means sum over the channels in the i-th excited or initial channel levels, respectively. The S-matrix element $S_{cc'}^{J^\pi}$ in Eq. (32) is obtained from Eq. (18). The total cross section σ_t and elastic scattering cross section σ_0 are not defined for a charged projectile. The transmission coefficient T_l for the orbital angular momentum l is obtained by

$$T_l = \frac{1}{2l+1} \sum_{J^\pi} \frac{2J+1}{(2s+1)(2I_0+1)} \sum_{cc'(n_{c'}=0, l_{c'}=l)} \left(1 - \left|S_{cc'}^{J^\pi}\right|^2\right). \tag{33}$$

The scattering amplitude $A_{imM,m'M'}$ from the initial state having z-projections of the spin of the projectile (m') and target (M') to the final state (mM) at the i-th excited level is

obtained by

$$
\begin{aligned}
A_{imM,m'M'}(\theta) &= \frac{4\pi}{k_0} \sum_{cc'(n_c=i,n_{c'}=0)} \sum_{\substack{l_c l_{c'} j_c j_{c'} J \\ m_{l_c} m_{l_{c'}} m_{j_c} m_{j_{c'}} M_J}} \\
&\quad \langle l_c s_c m_{l_c} m | j_c m_{j_c} \rangle \langle j_c I_c m_{j_c} M | J M_J \rangle \\
&\quad \times \langle l_{c'} s_{c'} m_{l_{c'}} m' | j_{c'} m_{j_{c'}} \rangle \langle j_{c'} I_{c'} m_{j_{c'}} M' | J M_J \rangle \\
&\quad \times e^{i(\sigma_c + \sigma_{c'})} C_{cc'} Y_{l_c m_{l_c}}(\theta, 0) Y_{l_{c'} 0}(0,0)^*, \qquad (34)
\end{aligned}
$$

where θ is the scattering angle. The projectile is assumed to move along the z-axis at initial channel. The angular distribution of scattering cross sections to the i-th level are calculated by

$$
\frac{\mathrm{d}\sigma_i}{\mathrm{d}\Omega}(\theta) = \sum_{mMm'M'} \frac{1}{(2s+1)(2I_0+1)} \left| f_C(\theta)\delta_{mm'}\delta_{MM'} + A_{imM,m'M'}(\theta) \right|^2, \qquad (35)
$$

where f_C is Coulomb scattering amplitude given by

$$
\begin{aligned}
f_C(\theta) &= -\frac{\eta_0}{2k_0 \sin\frac{\theta}{2}} \exp\left\{ -i\eta_0 \log\left(\sin^2\frac{\theta}{2}\right) + 2i\sigma_0 \right\}, \qquad (36) \\
\sigma_0 &= \arg\Gamma(1 + i\eta_0), \qquad (37) \\
\eta_0 &= \frac{ZZ'e^2\mu}{\hbar^2 k_0} = \frac{\mu c^2 \alpha}{\hbar c k_0}, \qquad (38)
\end{aligned}
$$

where α is the fine-structure constant and c is the speed of light.

3 Details of Calculation

3.1 Expansion of Potential

The optical potentials are assumed to have the shapes of Woods-Saxon and its derivative.

$$
V(r) = V_i f_i(r) + W_j g_j(r) + V_s h_s(r) \boldsymbol{\sigma} \cdot \mathbf{l} + V_C(r), \qquad (39)
$$

where V_i, W_j and V_s are the strength of potential of complex number and V_C shows Coulomb potential which is calculated from charge distribution of target nucleus. The $f_i(r)$, $g_j(r)$ and $h_s(r)$ are the form factors given by

$$
\begin{aligned}
f_i(r) &= \left(1 + e^{\frac{r-R_i}{a_i}}\right)^{-1}, \qquad (40) \\
g_i(r) &= -4a_i \frac{d}{dr} f_i, \qquad (41) \\
h_i(r) &= \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r} \frac{d}{dr} f_i(r), \qquad (42)
\end{aligned}
$$

where $\left(\frac{\hbar}{m_\pi c}\right)^2 = 2$.

The charge distribution $\rho(\mathbf{r}')$ of target is assumed to be uniform inside of the charge radius $R(\hat{\mathbf{r}}')$, Eq. (5), and zero outside. The Coulomb potential V_C is expanded by the spherical harmonics,

$$\begin{aligned} V_C(\mathbf{r}) &= \int d\mathbf{r}' \frac{ZZ'e^2\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \\ &= \frac{ZZ'e^2}{V_0}\int d\mathbf{r}'\Theta\left(R(\hat{\mathbf{r}}')-r'\right)\sum_{lm}\frac{4\pi}{2l+1}\frac{r_>^{l+1}}{r_<^l}Y_{lm}(\hat{\mathbf{r}})Y_{lm}(\hat{\mathbf{r}}')^* \\ &= \sum_{lm}Y_{lm}(\hat{\mathbf{r}})\int d\hat{\mathbf{r}}'Y_{lm}^*(\hat{\mathbf{r}}')\tilde{V}_{Cl}(r,\hat{\mathbf{r}}')\frac{3ZZ'e^2}{(2l+1)R_0^3A}, \end{aligned} \tag{43}$$

for $R(\hat{\mathbf{r}}') \le r'$

$$\tilde{V}_{Cl}(r,\hat{\mathbf{r}}') = \frac{R(\hat{\mathbf{r}}')^{l+3}}{(l+3)r} \tag{44}$$

for $R(\hat{\mathbf{r}}') > r'$

$$\tilde{V}_{Cl}(r,\hat{\mathbf{r}}') = \frac{r^2}{l+3} + \begin{cases} \frac{r^2}{l-2}\left(1-\frac{r^{l-2}}{R(\hat{\mathbf{r}}')^{l-2}}\right) & (l\neq 2), \\ r^l\log\frac{R(\hat{\mathbf{r}}')}{r} & (l=2), \end{cases} \tag{45}$$

where $r_< = \min(r,r')$, $r_> = \max(r,r')$ and $\Theta(x)$ is the step function

$$\Theta(x) = \begin{cases} 0 & (x<0), \\ 1 & (x>0). \end{cases} \tag{46}$$

The V_0 is volume of charge distribution and A is the ratio to the volume of the sphere of radius R_0,

$$V_0 = \int d\mathbf{r}'\Theta\left(R(\hat{\mathbf{r}}')-r'\right) \tag{47}$$

$$= R_0^3\left[\frac{4\pi}{3}+\sum_l\beta_l^2+\frac{1}{6\sqrt{\pi}}\sum_{l_1l_2l_3}\hat{l_1}\hat{l_2}\hat{l_3}\begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}^2\beta_{l_1}\beta_{l_2}\beta_{l_3}\right] \tag{48}$$

$$A = \frac{3V_0}{4\pi R_0^3} \tag{49}$$

The expanded potentials, Eq. (7) and (43), are calculated by the numerical integration of optical potentials at radial grid points to solve the Schrödinger equation, Eq. (4).

3.2 Solution of Schrödinger Equation

The Schrödinger equation, Eq. (4), can be written simply as

$$\frac{d^2}{dr^2}f_i(r) = \sum_j V_{ij}(r)f_j(r), \tag{50}$$

and by vector representation,

$$f''(r) = V(r)f(r). \tag{51}$$

The modified Numerov method[8] is used to integrate Eq. (51). It is obtained from the Taylor's expansion of $f(r)$ with Eq. (51),

$$\begin{aligned}
\xi(r+h) &\equiv f(r+h) - \frac{h^2}{12}f''(r+h) \\
&= 2f(r) + \frac{5}{6}f''(r) - f(r-h) + \frac{h^2}{12}f''(r-h) + O(h^6) \\
&= 2\xi(r) - \xi(r-h) + u(r) + O(h^6), \qquad (52) \\
u(r) &= h^2 f''(r) \\
&= \frac{h^2}{1 - h^2V(r)/12}\xi(r) \\
&= h^2V(r)\left(1 + \frac{h^2}{12}V(r)\right)\xi(r) + O(h^6) \qquad (53)
\end{aligned}$$

and

$$f(r) = \xi(r) + \frac{1}{12}u(r). \tag{54}$$

The value of the i-th solution at matching radius is obtained by Eq. (52) and Eq. (54) with neglecting the terms of $O(h^6)$ using the initial value of

$$\xi^i(0) = 0, \tag{55}$$

$$\xi^i(h) = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \xi_i^i(h) \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{56}$$

$$\begin{aligned}
\xi_i^i(h) &= \frac{(kh)^{l+1}}{(2l+1)!!}, \qquad (57) \\
k &= \sqrt{\frac{2\mu\left(E - V(0)\right)}{\hbar^2}}.
\end{aligned}$$

4 Description of Code

The code is written by C++ language using the standard template library (STL) and GNU Scientific Library (GSL)[9]. The list of files with the brief description about functions and classes of the code is shown.

4.1 List of Files, Functions and Classes

- `calc.cpp`, `calc.h`: main calculation functions

  functions:

  - *cmatrix*: calculate C-matrix
  - *smatrix*: calculate S-matrix from C-matrix
  - *scat_amp*: calculate scattering amplitude from C-matrix
  - *cross_section*: calculate cross sections
  - *cross_section_da*: calculate angular distributions of scattering cross sections
  - *cross_section_integ*: calculate total, reaction and scattering cross sections
  - *calc*: main function to calculate cross sections at each incident energies

- `cblas-mat.cpp`, `cblas-mat.h`: matrix class

  classes:

  - *cblass_matrix_z*: matrix class of complex number used to call CBLAS functions used in the function *solve*.

- `ccom.cpp`: main program

  functions:

  - *main*: main function; makes a instance of *Input_param* class, reads input parameters and calls *main_fit* function
  - *main_fit*: calls the function *fit* for the fitting, and the function *calc* to get the final results

- `const.h`: define some physical constants

  $\hbar c$, fine-structure constant α, atomic mass unit ...

- `fit.cpp`, `fit.h`: fitting functions

  functions:

  - *fit*: main fitting function; iterate up to the convergence
  - *calx*: obtain cross sections for all experimental data points
  - *expb_f*: make a vector of difference between experiment and calculated values multiplied by the weights of inverse of experimental errors
  - *expb_df*: make Jacobian matrix, derivative of calculated values by parameters

- `func.cpp`, `func.h`: special functions

  spherical harmonics, coulomb wave functions, Clebsch-Gordan coefficient, Racah coefficient, ...

- `input.cpp`, `input.h`: class of input parameters

  classes:

  - *cs_data*: contain the experimental data
  - *Sys_param*: parameters to define system of scattering
  - *Cal_param*: energies and angles to calculate as final results
  - *Input_param*:contain all input parameters

- `omp.cpp`, `omp.h`: calculate the optical potential parameters from the input parameters

  functions

  - *get_omp*: select the function *get_omp_id* to calculate optical potential parameters depending on *id*
  - *get_omp_id*: calculate optical potential from the list of input parameters by the formula of *id*

- `potential.cpp`, `potential.h`: class of from factor and potential

  classes:

  - *FormFactor*: calculate form factors
  - *Potential*: calculate the optical potential and get multi-pole expansion of potential

- `solv.cpp`, `solv.h`: functions to integrate Schrödinger equation

  functions:

  - *gcouple*: calculate angular momentum dependent coupling coefficients
  - *set_vcouple*: calculate coupling matrix elements
  - *set_u*: calculate u, Eq. (53)
  - *solve*: integrate Schrödinger equation by the modified Numerov method and obtain the wave function at matching radius

- `system.cpp`, `system.h`: define system of scattering

  classes:

- *Cross_Section*: contain calculated cross sections
- *Particle*: properties of particle, mass, Z, A, levels, spin, parity
- *Quantum*: quantum number to define channel, l, l', s, s', j, j', J^π, ...
- *Channel*: contain all channel information
- *System*: contain all parameters to define system of scattering

4.2 OMP Function

The optical model parameters (OMP) are calculated from the input parameters by the function *get_omp_id*, which can be modified to get different OMP energy dependence. For a simple example, the OMP having the linear energy and asymmetry parameter dependence are shown.

```
1  void get_omp_om0(System *sys, valarray<double> &p,
2                   valarray<double> &omp, valarray<double> &beta)
3  {
4      double en=sys->energy_lab;
5
6      int z=sys->targ.z, a=sys->targ.a, n=a-z;
7      double eta=double(n-z)/double(a);
8
9      double v0, r0, a0;
10
11     omp.resize(21);
12
13     for(int i=0, i3; i<7; i++){
14         i3=i*3;
15         v0=0;
16         r0=0;
17         a0=0;
18         switch(i){
19         case 0: // V
20             v0=-(p[0]-p[1]*eta-p[2]*en);
21             r0=p[3];
22             a0=p[4];
23             break;
24         case 1: // W
25             break;
26         case 2: // Vs
27             break;
28         case 3: // Ws
29             v0=-(p[5]-p[6]*eta+p[7]*en);
30             r0=p[8];
31             a0=p[9];
32             break;
33         case 4: // Vso
34             v0=-p[10];
```

```
35              r0=p[11];
36              a0=p[12];
37              break;
38          case 5: // Wso
39              break;
40          case 6: // Vc
41              v0=sys->get_zz();
42              r0=p[13];
43              break;
44          default:
45              break;
46          }
47          omp[i3]=v0;
48          omp[i3+1]=r0;
49          omp[i3+2]=a0;
50      }
51      beta.resize(2);
52      beta[0]=p[14];
53      beta[1]=p[15];
54  }
```

The lines 1 and 2 define the arguments of the function. The arguments sys and p are the input parameters. The sys contains all parameters of the present system and the p is the array of parameters for the OMP calculation. The function will return omp and beta, which are the OMP and deformation parameters, respectively,

$$\texttt{omp[i*3]} = V_i, \tag{58}$$

$$\texttt{omp[i*3+1]} = r_i, \tag{59}$$

$$\texttt{omp[i*3+2]} = a_i, \tag{60}$$

$$\texttt{beta[j]} = \beta_{2(j+1)}, \tag{61}$$

where $i = 0, \ldots, 6$: 0; real Woods-Saxon, 1; imaginary Woods-Saxon, 2; real derivative Woods-Saxon, 3; imaginary derivative Woods-Saxon, 4; real spin-orbit, 5; imaginary spin-orbit, 6; Coulomb. The line 4-7 define E, Z_t, A_t, etc. The line 9-50 calculate OMP parameters and the line 51-53 define β.

The OMP having more complicated energy dependence is shown as the next expamle.

```
1  void get_omp_suk2003(System *sys, valarray<double> &p,
2                valarray<double> &omp, valarray<double> &beta)
3  {
4      double en0=sys->energy_lab, en, en2, ef;
5
6      int zp=sys->proj.z, z=sys->targ.z, a=sys->targ.a, n=a-z;
7      double c0, c1, c2, eta=double(n-z)/double(a), a3=pow(a, 1./3.);
8
9      double v0, r0, a0;
10
```

```
    omp.resize(21);

    if(zp == 1 && sys->efp != 0)
        ef=sys->efp;
    else if(zp == 0 && sys->efn != 0)
        ef=sys->efn;
    else
        ef=p[35];

    en=en0-ef;
    en2=en*en;

    c0= zp > 0 ? 1 : -1;
    c1=1+c0*p[28]*eta/(p[0]+p[1]*(a-232)+p[4]);
    c2=(p[5]*p[4]*exp(-p[5]*en)-p[2]-2*p[3]*en)*c1;

    for(int i=0; i<7; i++){
        v0=0;
        r0=0;
        a0=0;
        switch(i){
        case 0: // V
            v0=(p[0]+p[1]*(a-232)+p[2]*en+p[3]*en2 +p[4]*exp(-p[5]*en))*c1
                +p[27]*z*zp/a3*c2;
            v0*=-1;
            r0=p[17]*(1-p[18]*en2/(en2+p[16]*p[16]));
            a0=p[19]+p[20]*en;
            break;
        case 1: // W
            v0=-p[10]*en2/(en2+p[11]*p[11]);
            r0=p[23];
            a0=p[24];
            break;
        case 2: // Vs
            break;
        case 3: // Ws
            v0=-(p[6]+p[7]*(a-232)+c0*p[29]*eta)*exp(-p[8]*en)
                *en2/(en2+p[9]*p[9]);
            r0=p[21];
            a0=p[22];
            break;
        case 4: // Vso
            v0=-p[12]*exp(-p[13]*en);
            r0=p[30];
            a0=p[31];
            break;
        case 5: // Wso
            v0=-p[14]*en2/(en2+p[15]*p[15]);
            r0=p[30];
            a0=p[31];
            break;
        case 6: // Vc
            v0=sys->get_zz();
```

```
64              r0=p[25];
65              break;
66          default:
67              break;
68          }
69
70          int i3=i*3;
71          omp[i3]=v0;
72          omp[i3+1]=r0;
73          omp[i3+2]=a0;
74      }
75
76      if(sys->beta.size() > 0){
77          beta.resize(sys->beta.size());
78          beta=sys->beta;
79      }
80      else{
81          beta.resize(3);
82          beta[0]=p[32];
83          beta[1]=p[33];
84          beta[2]=p[34];
85      }
86  }
```

The parameters used in the code is almost same as the previous example. The additional parameters are Fermi energies in lines 13-18. The lines 76-85 shows that the deformation parameter will be used if defined in the system section of the input.

5 Input Parameters

5.1 Description of Input Parameters

The input parameters are identified by tags with free format. The tags and values should be separated by white-space characters. The parenthesis is used to define variables whose number is not fixed. The input file is constructed by the repetition of " **tag** val_1 val_2 ...".

The units used in the input and output are MeV, mb and fm for the energy, cross section and length, respectively. For the angular distributions of the cross section, $\frac{d\sigma}{d\Omega}$, mb/sr is used with the angle in degree.

- *comment*
  - #: comment out until end of line
  - /* ...*/: comment out from "/*" to "*/"
- *system*: define system

- `system`: add new system; system is identified by the number 0, 1, 2, ...
- `za` Z_p A_p m_p Z_t A_t m_t: proton number, mass number and mass of projectile and target
- `lev` I π Ex: add level of spin I, parity π(+/-), excitation energy Ex
- `efermi` ϵ_{F_p} ϵ_{F_n}: Fermi energy for proton and neutron (used for some OMP parametrisation)
- `beta` (β_2 β_4 ...): deformation parameters
- `mesh` r_m N: matching radius and number of mesh points (should be defined before the tag `system`)
- `jmax` J_m: maximum of total angular momentum to calculate (should be defined before the tag `system`)
- `vlmax` λ_m: maximum angular momentum for multi-pole expansion of potential (should be defined before the tag `system`)

- *calculation*: make final result
  - `ene` (E_1, E_2, ...): incident energies to be calculated (should be defined before the tag `calc`)
  - `angle` N_a, Δ_a: number of angles, increase of angle for angular distribution (should be defined before the tag `calc`)
  - `calc` (i j ...): make calculation for the system i, j, ...

- *experimental data*: used for fitting
  - `data`: beginning of experimental data
  - `range` E_1 E_2: experimental data used in the range from E_1 to E_2 (should be defined before the tag `ene`)
  - `system` i: define the system number
  - `ene` E: define incident energy
  - `tot` σ_t $\Delta\sigma_t$: total cross section and error
  - `reac` σ_r $\Delta\sigma_r$: reaction cross section and error
  - `s0` S_0 ΔS_0: s-wave neutron strength function and error in the unit of 10^{-4}
  - `s1` S_1 ΔS_1: p-wave neutron strength function and error in the unit of 10^{-4}
  - `r'` R' $\Delta R'$: scattering length and error

- **scat** i j **etag**

  θ_0 σ_0 $\Delta\sigma_0$

  θ_1 σ_1 $\Delta\sigma_1$

  ...

  etag:

  angular distribution of sum of the cross sections scattering to the levels between i and j. θ_i, σ_i and $\Delta\sigma_i$ are angle, cross section, and error, respectively. The "**etag**" defines the string indicating end of data of the scattering cross sections

- **dend**: end of experimental data

- *others*:

  - **param** id_{omp} (p_0 p_1 ...): parameters to calculate optical potentials; can be used for fitting. id_{omp} defines the OMP parametrisation to be used.
  - **output** *file*: file name of output. "-" means standard output. If this tag is not used, output file name is *input.out* for input file *input.in*.
  - **fit** (i j ...): parameters p_i, p_j, ... to be used for fitting
  - **end**: end of input

5.2 Example of Input File

5.2.1 Example 1: Simple Calculation

This is an example of the calculation for ^{238}U + n system coupled 5 levels using the optical optential of Ref. [10].

test1.in

```
# -------------------- system --------------------
system    # 0   92- U -238
za 0 1 1.00866  92 238 238.051
lev  0.00 +    0.00000
lev  2.00 +    0.04491
lev  4.00 +    0.14841
lev  6.00 +    0.30721
lev  8.00 +    0.51830
# -------------------- calc  --------------------
ene ( 1 2 )
angle 19 10   # 0 10 20 ... 180
calc ( 0 )
# -----------------------------------------------
param om1 ( 51.32134 24 0.57 0.20  1.256 0.62
            5.04567  12 0.40 0.001 1.26  0.58
            6.0 1.12 0.5 1.3 0.198 0.057 )
end
```

The default values of jmax = 40, vlmax = 8 and mesh = (20,100) defined in the file input.cpp will be used. The following command is used to run the program with making the output file test1.out.

```
ccom test1.in
```

test1.out

```
# param om1 ( 51.3213 24 0.57 0.2 1.256 0.62 5.04567 12 0.4 0.001 ....
#-------------------------------------------------
#   system 0 za 0 1 1.00866 92 238 238.051 nlev 5
#-------------------------------------------------
# 0: Energy: 1
# cross section: 1 6929.04 2764.52 3788.55 324.37 50.6842 0.913304 0.00253666
# En, S0, S1, R': 1 0.655753 1.35069 5.49075
# En, transmission coefficient: 1 0.411152 0.625599 0.203342 0.12236 ...
# angular distribution
0 1832.45 1811.45 11.0627 9.6828 0.255607 0.000153664
10 1736.25 1714.76 11.6258 9.61084 0.249071 0.000154146
20 1476.17 1453 13.5475 9.38442 0.230463 0.000154378
30 1125.5 1099.09 17.2303 8.9776 0.202534 0.000151723
40 772.191 741.03 22.6279 8.36426 0.169133 0.000144273
50 486.817 450.289 28.8558 7.53802 0.134356 0.000132361
60 303.227 262.203 34.3925 6.52956 0.101771 0.000118423
70 217.042 173.816 37.7385 5.41309 0.0739624 0.00010579
80 197.881 155.473 38.0591 4.29596 0.0524101 9.78078e-05
90 206.71 167.969 35.4114 3.2915 0.0376043 9.81145e-05
100 210.89 177.846 30.5302 2.48474 0.0292099 0.000111437
110 193.006 166.61 24.4631 1.90717 0.0262382 0.000143388
120 152.561 132.662 18.3376 1.53377 0.0272633 0.000198327
130 101.484 86.877 13.272 1.30371 0.0307095 0.000276061
140 55.7336 44.3337 10.2117 1.15265 0.0351412 0.000369591
150 26.5626 15.9295 9.55475 1.03845 0.0394547 0.000465788
160 15.4528 3.68044 10.7807 0.948095 0.0429239 0.000548909
170 15.2476 1.78423 12.5303 0.887338 0.0451359 0.000604938
180 16.578 2.33906 13.3267 0.865736 0.0458924 0.000624663


# 1: Energy: 2
# cross section: 2 7189.9 3124.2 3495.34 443.079 111.428 15.4311 0.422913
# En, S0, S1, R': 2 0.551698 0.938799 5.274
# En, transmission coefficient: 2 0.48919 0.707341 0.382783 0.587136 ...
# angular distribution
0 3662.72 3617.48 29.0254 12.9286 3.24841 0.0326258
10 3298.52 3254.94 27.479 12.8424 3.22817 0.0320615
20 2387.83 2346.73 25.2643 12.6549 3.15435 0.0304472
30 1346.93 1304.44 26.9131 12.5536 2.99691 0.0280002
40 553.536 504.12 33.9179 12.7424 2.7311 0.0250345
50 154.558 96.1319 42.7727 13.2714 2.35967 0.0219209
60 70.1936 6.35024 47.999 13.9034 1.92191 0.019071
70 128.4 65.9575 46.7659 14.1764 1.48347 0.0169532
80 192.825 137.277 40.763 13.658 1.11104 0.0161454
90 208.609 161.217 34.3484 12.1807 0.8455 0.0174033
```

```
100 180.359 138.465 31.2792 9.9029 0.689625 0.0216317
110 132.553 92.1998 32.4688 7.23748 0.61741 0.0296131
120 85.8746 44.9148 35.6167 4.70617 0.595372 0.0415236
130 53.6057 13.3379 36.8889 2.72362 0.59875 0.0565461
140 45.7899 9.4653 34.2125 1.42488 0.61432 0.072917
150 68.3418 37.4305 29.4917 0.696124 0.635037 0.0884175
160 114.961 87.3026 26.5551 0.346579 0.655298 0.100983
170 162.735 135.15 26.5893 0.2159 0.669952 0.109097
180 183.057 154.887 27.1944 0.18808 0.675284 0.111894
```

The line 1 shows the used parameter set and the line 3 indicates Z, A, mass and levels. The numerical values at the line 6 are the incident energy and the cross sections of total, reaction, elastic, 1st inelastic, 2nd inelastic, ... The transmission coefficients are shown at the line 8, where the values are lined in the order of incident energy, T_0, T_1, T_2, ..., T_l, ... The lines 10-28 show angular distributions of scattering cross sections. The columns show angle, sum of all scattering, elastic, inelastic to the 1st level, the 2nd level, ... The results for next energy begin from the 31st line.

To get the table of energy dependence of cross sections, following command may be useful.

```
awk -F : '/cross section/{print $2}' test1.out
```

5.2.2 Example 2: Fitting

An example of the input file for fitting of the OMP is shown. For the case of the reduced number of the coupled levels in the previous example, the energy dependence of the OMP is searched. The total cross section, the angular distributions of elastic and inelastic scattering, s- and p-wave strength functions and scattering radius are used for fitting.

test2.in

```
# -------------------- system --------------------
system    # 0   92- U -238
za 0 1 1.00866  92 238 238.051
lev  0.00 +    0.00000
lev  2.00 +    0.04491
lev  4.00 +    0.14841
# -------------------- calc  --------------------
ene ( 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
      1 1.2 1.4 1.6 1.8 2 2.5 3 3.5 4 5 6 7 8 9
      10 12 14 16 18 20 )
angle 0 2     # no angular distribution
calc ( 0 )    # energy dependence

ene ( 3.4 )
angle 91 2    # 0 2 4 6 ... 180
calc ( 0 )    # angular distribution
# ---------------------------------------------
```

```
param om1 ( 51.32134 24 0.57 0.020  1.256 0.62
            5.04567  12 0.40 0.001 1.26  0.58
            6.0 1.12 0.5 1.3 0.198 0.057 )
fit ( 0 2 6 8 )
# -------------------- data  --------------------
data
system 0
    ene 0.0001 s0 1.2 0.1 s1 1.7 0.3 r' 9.6 0.1
    ene 0.1 tot 11814.2 49.1913
    ene 0.2 tot 10696.8 27.5866
    ene 0.5 tot 8387.69 12.3136
    ene 1   tot 7065.96 6.94642
    ene 1.4 tot 6936.05 6.47929
    ene 1.8 tot 7160.01 7.76091
    ene 2   tot 7307.15 6.62315
    ene 2.5 tot 7630.9 5.56785
    ene 3   tot 7858.7 6.65072
    ene 3.5 tot 7968.68 7.88627
    ene 4   tot 7994.81 8.59415
    ene 4.5 tot 7877.03 9.00727
    ene 5   tot 7664.56 7.2575
    ene 7   tot 6674.51 4.80028
    ene 10  tot 5881.1 4.97937
    ene 14  tot 5853.65 5.75409
    ene 18  tot 6147.31 5.01827
    ene 20  tot 6213.03 5.29372

 scat 0 0 -----
   2.0100000e+01  2.8672000e+03  1.7490000e+02
   3.0100000e+01  1.5405000e+03  9.5500000e+01
   4.0200000e+01  3.1000000e+02  2.3900000e+01
   4.5200000e+01  1.4470000e+02  1.1700000e+01
   5.0200000e+01  2.7700000e+01  3.4000000e+00
   6.0200000e+01  3.7100000e+01  5.4000000e+00
   6.5200000e+01  8.4600000e+01  8.2000000e+00
   8.0200000e+01  1.1390000e+02  1.2200000e+01
   8.5200000e+01  1.0560000e+02  9.8000000e+00
   9.0200000e+01  8.7400000e+01  8.7000000e+00
   1.0020000e+02  3.3400000e+01  4.2000000e+00
   1.0520000e+02  2.7000000e+01  3.6000000e+00
   1.1020000e+02  1.0700000e+01  1.9000000e+00
   1.2020000e+02  2.5000000e+00  7.0000000e-01
   1.3020000e+02  5.8000000e+00  1.5000000e+00
   1.4020000e+02  1.4500000e+01  2.7000000e+00
   1.5010000e+02  2.4600000e+01  3.7000000e+00
   1.6010000e+02  3.3900000e+01  4.4000000e+00
  -----

 scat 1 1 -----
   4.0200000e+01  8.2200000e+01  9.7000000e+00
   4.5200000e+01  6.1900000e+01  6.6000000e+00
   5.0200000e+01  4.5900000e+01  6.2000000e+00
   6.0200000e+01  3.6500000e+01  5.9000000e+00
```

```
71    6.5200000e+01  4.3900000e+01  5.1000000e+00
72    8.0200000e+01  5.1300000e+01  7.4000000e+00
73    8.5200000e+01  5.0300000e+01  5.8000000e+00
74    9.0200000e+01  5.2900000e+01  5.8000000e+00
75    1.0020000e+02  3.0700000e+01  4.1000000e+00
76    1.0520000e+02  2.0400000e+01  3.1000000e+00
77    1.1020000e+02  1.7200000e+01  2.8000000e+00
78    1.2020000e+02  1.0400000e+01  2.1000000e+00
79    1.3020000e+02  3.4600000e+01  4.6000000e+00
80    1.4020000e+02  4.3000000e+01  5.2000000e+00
81    1.5010000e+02  2.8400000e+01  3.9000000e+00
82    1.6010000e+02  1.9900000e+01  3.1000000e+00
83   -----
84
85  scat 2 2 -----
86    4.0200000e+01  2.1900000e+01  4.5000000e+00
87    4.5200000e+01  2.2200000e+01  3.5000000e+00
88    5.0200000e+01  1.5800000e+01  3.5000000e+00
89    6.0200000e+01  1.2200000e+01  3.3000000e+00
90    6.5200000e+01  9.9000000e+00  2.1000000e+00
91    8.0200000e+01  9.0000000e+00  2.8000000e+00
92    8.5200000e+01  9.9000000e+00  2.2000000e+00
93    9.0200000e+01  1.0100000e+01  2.6000000e+00
94    1.0520000e+02  9.7000000e+00  2.2000000e+00
95    1.1020000e+02  8.4000000e+00  2.0000000e+00
96    1.2020000e+02  6.8000000e+00  1.8000000e+00
97    1.3020000e+02  6.6000000e+00  1.7000000e+00
98    1.4020000e+02  4.8000000e+00  1.5000000e+00
99    1.5010000e+02  3.9000000e+00  1.3000000e+00
100   1.6010000e+02  3.1000000e+00  1.1000000e+00
101   -----
102 dend
103 end
```

The parameters to be fitted is shown at the line 21. In the *om*1 parametrisation, p[0] and p[2] are constant and linear terms of energy dependence of real potential, respectively, and p[6] and p[8] for imaginary potential. The fitting data are shown from the line 23. The line 24 shows the system to be calculated; it is defined at lines 2-6. At the line 25 s- and p-wave strength functions and scattering radius are written. The lines 26-43 show the total cross sections. The data for angular distribution for the elastic scattering are written at the lines 45-64. The line 66-83 and line 85-101 are for the inelastic scattering to 1st and 2nd excited levels, respectively.

test2.out

```
1 # param om1 ( 51.3213 24 0.57 0.02 1.256 0.62 5.04567 12 0.4 0.001 1.26 0.58 ...
2 # fit ( 0 2 6 8 )
3 # fitting started
4 # iter:   0 x =  51.3213400    0.5700000    5.0456700    0.4000000 |f(x)| = 142.68
5 # iter:   1 x =  52.2212321    0.5886197    5.1215875    0.5132671 |f(x)| = 72.1206
6 # iter:   2 x =  52.0315561    0.5575361    5.1235479    0.4939006 |f(x)| = 66.3312
7 # iter:   3 x =  52.0803911    0.5601253    4.9158329    0.5312031 |f(x)| = 66.0273
8 # iter:   4 x =  52.0769483    0.5571478    4.8741173    0.5409622 |f(x)| = 65.9834
```

```
 9  # iter:    5 x =  52.0802561    0.5565554    4.8467365    0.5468730 |f(x)| = 65.9735
10  # iter:    6 x =  52.0810143    0.5561466    4.8358709    0.5492956 |f(x)| = 65.9715
11  # iter:    7 x =  52.0814727    0.5559865    4.8307129    0.5504341 |f(x)| = 65.9708
12  # iter:    8 x =  52.0816644    0.5559102    4.8284067    0.5509443 |f(x)| = 65.9706
13  # iter:    9 x =  52.0817541    0.5558761    4.8273536    0.5511770 |f(x)| = 65.9706
14  # iter:   10 x =  52.0817945    0.5558606    4.8268760    0.5512826 |f(x)| = 65.9705
15  # p(0) =     52.08179 +/-     0.00892 |  1.000  0.409 -0.709  0.515
16  # p(1) =      0.55586 +/-     0.00243 |  0.409  1.000 -0.049 -0.029
17  # p(2) =      4.82688 +/-     0.03573 | -0.709 -0.049  1.000 -0.836
18  # p(3) =      0.55128 +/-     0.00749 |  0.515 -0.029 -0.836  1.000
19  # status = success
20  # param om1 ( 52.0818 24 0.555861 0.02 1.256 0.62 4.82688 12 0.551283 0.001 ...
21  #-------------------------------------------------
22  #   system 0 za 0 1 1.00866 92 238 238.051 nlev 3
23  #-------------------------------------------------
24  # 0: Energy: 0.1
25  # cross section: 0.1 11975.1 3167.02 8796.25 11.865 0
26  # En, S0, S1, R': 0.1 0.639172 2.63677 8.3665
27  # En, transmission coefficient: 0.1 0.12673 0.11523 0.00191502 5.78636e-05 ...
28
29
30  # 1: Energy: 0.2
31  # cross section: 0.2 11018.1 3408.16 7563.34 46.4354 0.155721
32  # En, S0, S1, R': 0.2 0.632752 2.65966 7.75804
33  # En, transmission coefficient: 0.2 0.177423 0.269376 0.009617 0.000656405 ...
34                          .........................
```

The lines 4-14 show results for the each iterations. The last column shows $\sqrt{\sum_i (y_i - f_i)^2/\sigma_i^2}$, where y_i and σ_i are the experimental data and its error for fitting, respectively, and f_i is the calculated value. At the line 15-18, the final results with the estimation of errors and correlations of the fitted parameters are shown. The line 20 shows the new parameter set obtained by fitting. From the line 21, the final calculated cross sections are shown. The result of fitting is shown in Fig. 1.

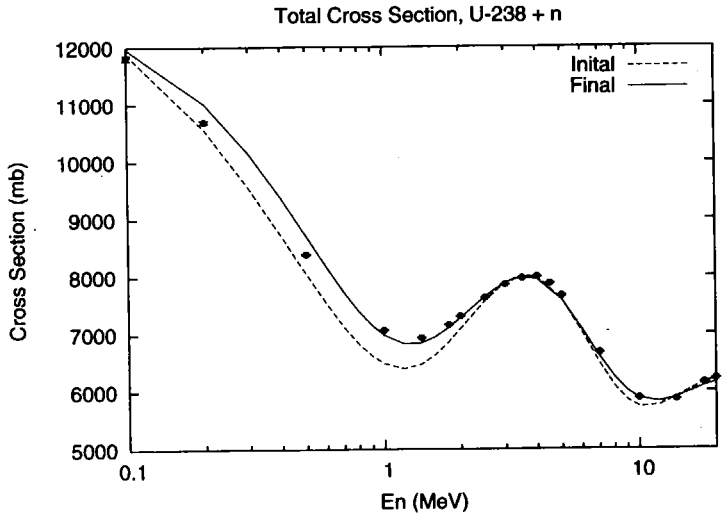

Fig. 1: Total cross sections calculated by initial and final parameters in the fitting.

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国際単位系 (SI) と換算表

表1　SI基本単位および補助単位

量	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質量	モル	mol
光度	カンデラ	cd
平面角	ラジアン	rad
立体角	ステラジアン	sr

表2　SIと併用される単位

名称	記号
分，時，日	min，h，d
度，分，秒	°，′，″
リットル	l，L
トン	t
電子ボルト	eV
原子質量単位	u

1 eV = 1.60218 × 10^{-19} J

1 u = 1.66054 × 10^{-27} kg

表3　固有の名称をもつSI組立単位

量	名称	記号	他のSI単位による表現
周波数	ヘルツ	Hz	s^{-1}
力	ニュートン	N	$m\cdot kg/s^2$
圧力，応力	パスカル	Pa	N/m^2
エネルギー，仕事，熱量	ジュール	J	N·m
工率，放射束	ワット	W	J/s
電気量，電荷	クーロン	C	A·s
電位，電圧，起電力	ボルト	V	W/A
静電容量	ファラド	F	C/V
電気抵抗	オーム	Ω	V/A
コンダクタンス	ジーメンス	S	A/V
磁束	ウェーバ	Wb	V·s
磁束密度	テスラ	T	Wb/m^2
インダクタンス	ヘンリー	H	Wb/A
セルシウス温度	セルシウス度	℃	
光束	ルーメン	lm	cd·sr
照度	ルクス	lx	lm/m^2
放射能	ベクレル	Bq	s^{-1}
吸収線量	グレイ	Gy	J/kg
線量当量	シーベルト	Sv	J/kg

表4　SIと共に暫定的に維持される単位

名称	記号
オングストローム	Å
バーン	b
バール	bar
ガル	Gal
キュリー	Ci
レントゲン	R
ラド	rad
レム	rem

1 Å = 0.1 nm = 10^{-10} m

1 b = 100 fm^2 = 10^{-28} m^2

1 bar = 0.1 MPa = 10^5 Pa

1 Gal = 1 cm/s^2 = 10^{-2} m/s^2

1 Ci = 3.7 × 10^{10} Bq

1 R = 2.58 × 10^{-4} C/kg

1 rad = 1 cGy = 10^{-2} Gy

1 rem = 1 cSv = 10^{-2} Sv

表5　SI接頭語

倍数	接頭語	記号
10^{18}	エクサ	E
10^{15}	ペタ	P
10^{12}	テラ	T
10^{9}	ギガ	G
10^{6}	メガ	M
10^{3}	キロ	k
10^{2}	ヘクト	h
10^{1}	デカ	da
10^{-1}	デシ	d
10^{-2}	センチ	c
10^{-3}	ミリ	m
10^{-6}	マイクロ	μ
10^{-9}	ナノ	n
10^{-12}	ピコ	p
10^{-15}	フェムト	f
10^{-18}	アト	a

（注）

1. 表1－5は「国際単位系」第5版，国際度量衡局 1985年刊行による。ただし，1 eVおよび1 uの値はCODATAの1986年推奨値によった。
2. 表4には海里，ノット，アール，ヘクタールも含まれているが日常の単位なのでここでは省略した。
3. barは，JISでは流体の圧力を表わす場合に限り表2のカテゴリーに分類されている。
4. EC閣僚理事会指令ではbar，barnおよび「血圧の単位」mmHgを表2のカテゴリーに入れている。

換算表

力	N(=10^5 dyn)	kgf	lbf
	1	0.101972	0.224809
	9.80665	1	2.20462
	4.44822	0.453592	1

粘度　1 Pa·s(N·s/m^2) = 10 P(ポアズ)(g/(cm·s))

動粘度　1 m^2/s = 10^4 St(ストークス)(cm^2/s)

圧力	MPa(=10 bar)	kgf/cm^2	atm	mmHg(Torr)	lbf/in^2(psi)
	1	10.1972	9.86923	7.50062 × 10^3	145.038
	0.0980665	1	0.967841	735.559	14.2233
	0.101325	1.03323	1	760	14.6959
	1.33322 × 10^{-4}	1.35951 × 10^{-3}	1.31579 × 10^{-3}	1	1.93368 × 10^{-2}
	6.89476 × 10^{-3}	7.03070 × 10^{-2}	6.80460 × 10^{-2}	51.7149	1

エネルギー・仕事・熱量	J(=10^7 erg)	kgf·m	kW·h	cal(計量法)	Btu	ft·lbf	eV
	1	0.101972	2.77778 × 10^{-7}	0.238889	9.47813 × 10^{-4}	0.737562	6.24150 × 10^{18}
	9.80665	1	2.72407 × 10^{-6}	2.34270	9.29487 × 10^{-3}	7.23301	6.12082 × 10^{19}
	3.6 × 10^6	3.67098 × 10^5	1	8.59999 × 10^5	3412.13	2.65522 × 10^6	2.24694 × 10^{25}
	4.18605	0.426858	1.16279 × 10^{-6}	1	3.96759 × 10^{-3}	3.08747	2.61272 × 10^{19}
	1055.06	107.586	2.93072 × 10^{-4}	252.042	1	778.172	6.58515 × 10^{21}
	1.35582	0.138255	3.76616 × 10^{-7}	0.323890	1.28506 × 10^{-3}	1	8.46233 × 10^{18}
	1.60218 × 10^{-19}	1.63377 × 10^{-20}	4.45050 × 10^{-26}	3.82743 × 10^{-20}	1.51857 × 10^{-22}	1.18171 × 10^{-19}	1

1 cal = 4.18605 J（計量法）

= 4.184 J （熱化学）

= 4.1855 J （15 °C）

= 4.1868 J（国際蒸気表）

仕事率　1 PS（仏馬力）

= 75 kgf·m/s

= 735.499 W

放射能	Bq	Ci
	1	2.70270 × 10^{-11}
	3.7 × 10^{10}	1

吸収線量	Gy	rad
	1	100
	0.01	1

照射線量	C/kg	R
	1	3876
	2.58 × 10^{-4}	1

線量当量	Sv	rem
	1	100
	0.01	1

（86年12月26日現在）

Program CCOM-Coupled-channels Optical Model Calculation with Automatic Parameter Search-