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—COUPLED CHANNELS OPTICAL MODEL AND COLLECTIVE NUCLEAR STRUCTURE CALCULATION—

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– Coupled Channels Optical Model and Collective Nuclear Structure Calculation –

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Program OPTMAN has been developed to be a tool for optical model calculations and employed in nuclear data evaluation at Radiation Physics and Chemistry Problems Institute. The code had been continuously improved to incorporate a number of options for more than twenty years. For the last three years it was successfully applied for evaluation of minor actinides nuclear data for a contract with International Science and Technology Center with Japan as the financing party. This code is now installed on the PC and UNIX work station by the authors at Nuclear Data Center of JAERI as well as program SHEMMAN which is used for the determination of nuclear Hamiltonian parameters. This report is intended as a brief manual of these codes for the users at JAERI.

Keywords: Nuclear Data, Optical Model, Coupled Channel Calculation, Soft-rotator Model,
Collective Band Structure, Neutron and Proton Scattering Cross Sections

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プログラムOPTMAN & SHEMMAN Version 5 (1998)

— チャンネル結合光学模型と集団原子核構造の計算 —

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プログラムOPTMANはベラルーシの放射線物理化学研究所において光学模型計算のツールとして開発され、核データ評価に使用されてきた。このコードは20年以上にわたり改良され続け、多くのオプションが追加された。この3年間では国際科学技術センタープロジェクトのもと、日本の財政支援によりマイナーアクチナイトの核データ評価に使用され成功を収めている。このコードは原子核ハミルトニアンのパラメータを推定するプログラムSHEMMANと共に、著者らによって原研核データセンターのパソコンおよびUNIXワークステーションにインストールされた。このレポートでは原研でのこの2つのコードのユーザのために簡単な使い方を述べる。

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1 Introduction

First attempts to write a coupled channels optical model code at Radiation Physics and Chemistry Problems Institute were made at early seventy's. At that time the authors of the code tried to follow the algorithm of JUPITOR [1] code for rotational nuclei, as it was intended to use in evaluation of neutron cross sections of deformed heavy fissioning nuclei. Then iteration method ECIS [2] for coupled equations integration was realized as an option. Later, coupling schemes based on nuclear Hamiltonian of even-even rigid non-axial rotator (Davydov-Phillipov model)[3], non-axial β -soft rotator (Davydov-Chaban model)[4] were included in the code. Not long ago the code was extended by the options allowing account of γ -softness in zero approximation[5, 6]. Then rigid hexadecapole deformations had been taken into account[7] and as the last option octupole soft symmetric deformation of nuclei now was taken into account[8]. This model is now incorporated in programs SHEMMAN and OPTMAN, that are used for the determination of nuclear Hamiltonian parameters and optical model calculations, respectively. This report is intended as a brief manual of these programs.

We are not going to explain all the derivation of the formulae of the model in this manual. Instead, we will present only some equation which will help the readers to understand the concept of the model and the underlying parameters [9]. It must be emphasized that the optical model calculations by OPTMAN for even-even nuclei with coupling schemes built on wave functions of non-axial soft-rotator are self-consistent, as parameters of the nuclear Hamiltonian are determined by adjusting the energies of collective levels to experimental values with SHEMMAN prior to the optical model calculation. For example for ^{238}U or ^{232}Th all the levels of positive parity up to 3 MeV excitation energy can be predicted (four rotational bands), together with one negative parity band with $K \cong 0$ [8]. On the other hand in the absence of experimental level schemes, such Hamiltonian parameters for minor actinides can be taken from systematics [10]. Then, adopted Hamiltonian parameters determine coupling strength and optical coupled channels calculations become possible. At the end it is possible to compare E2 and E3 γ -transition probabilities, predicted by the model, with the experimental ones if any. Usually they coincide to a good accuracy. So experimental scattering, nuclear structure and spectroscopic data for even-even nuclei is described in a uniform approach based on the soft-rotator model.

Program SHEMMAN allowing adjustment of soft non-axial nuclear Hamiltonian parameters over experimental collective levels of even-even nuclei is also described in this report.

2 Description of the Model

Here we describe nuclear shape and nuclear optical potential. Both are described here to clear the description of model parameters that will be used below. For more details one must address to Refs. [1, 2, 8, 9, 11].

It is assumed that for rigid axial rotational model the nuclear shape in a body fixed system can be presented [1] as

$$R(\theta', \phi') = R_0 \left\{ 1 + \sum_{\lambda} \beta_{\lambda 0} Y_{\lambda 0} \right\} \quad (1)$$

On the other hand, we assume that excited states observed in even-even non-spherical nuclei can be described as a combination of rotation, β -quadrupole and octupole vibrations, and γ -quadrupole vibration. Instant nuclear shapes that correspond to such excitations can be presented [12, 13] in a body fixed system.

$$\begin{aligned} R(\theta', \varphi') &= R_0 \left\{ 1 + \sum_{\lambda \mu} \beta_{\lambda \mu} Y_{\lambda \mu} \right\} \\ &= R_0 \left\{ 1 + \beta_2 \left[\cos \gamma Y_{20}(\theta', \varphi') + \frac{1}{\sqrt{2}} \sin \gamma (Y_{22}(\theta', \varphi') + Y_{2-2}(\theta', \varphi')) \right] \right. \\ &\quad + \beta_3 \left[\cos \eta Y_{30}(\theta', \varphi') + \frac{1}{\sqrt{2}} \sin \eta (Y_{32}(\theta', \varphi') + Y_{3-2}(\theta', \varphi')) \right] \\ &\quad \left. + b_{40} Y_{40}(\theta', \varphi') + \sum_{\mu=2,4} b_{4\mu} (Y_{4\mu}(\theta', \varphi') + Y_{4-\mu}(\theta', \varphi')) \right\}. \end{aligned} \quad (2)$$

To simplify the calculations, we assume that internal octupole variables satisfy additional conditions

$$\beta_{3\pm 1} = \beta_{3\pm 3} = 0, \beta_{32} = \beta_{3-2}, \quad (3)$$

which are admissible in case for first excited states[14].

The Hamiltonian \hat{H} of the soft-rotator model consists of the kinetic energy terms for the rotation of the non-axial nuclei with quadrupole, hexadecapole and octupole deformations, the β_2 -, γ -quadrupole and octupole vibrations, and the vibrational potentials ignoring a coupling between the 3 vibration modes[5];

$$\hat{H} = \frac{\hbar^2}{2B_2} \left\{ \hat{T}_{\beta_2} + \frac{1}{\beta_2^2} \hat{T}_\gamma \right\} + \frac{\hbar^2}{2} \hat{T}_r + \frac{\hbar^2}{2B_3} \hat{T}_{\beta_3} + \frac{\beta_{20}^4}{\beta_2^2} V(\gamma) + V(\beta_2) + V(\beta_3), \quad (4)$$

where

$$\hat{T}_{\beta_2} = - \frac{1}{\beta_2^4} \frac{\partial}{\partial \beta_2} \left(\beta_2^4 \frac{\partial}{\partial \beta_2} \right), \quad (5a)$$

$$\hat{T}_\gamma = - \frac{1}{\sin 3\gamma} \frac{\partial}{\partial \gamma} \left(\sin 3\gamma \frac{\partial}{\partial \gamma} \right), \quad (5b)$$

$$\hat{T}_{\beta_3} = - \frac{1}{\beta_3^3} \frac{\partial}{\partial \beta_3} \left(\beta_3^3 \frac{\partial}{\partial \beta_3} \right). \quad (5c)$$

The symbol \hat{T}_r denotes the operator of deformed nuclear rotational energy expressed in terms of the angular momentum operator \hat{I}_i and principal moments of inertia,

$$\hat{T}_r = \sum_{i=1}^3 \frac{\hat{I}_i^2}{J_i} = \sum_{i=1}^3 \frac{\hat{I}_i^2}{J_i^{(2)} + J_i^{(3)} + J_i^{(4)}}. \quad (6)$$

Here $J_i^{(\lambda)}$ stands for the principal moments of inertia in the direction of i -th axis in the body-fixed system due to quadrupole, octupole and hexadecapole deformations depending on $\lambda=2, 3$ and 4 , respectively. The symbol \hat{I}_i denotes the projection of the angular-momentum operator on the i -th axis of the body-fixed coordinate, β_{20} denotes the quadrupole equilibrium deformation parameter at the ground state

(G.S.), and B_λ the mass parameter for multipolarity of λ . The eigenfunctions Ψ of operator (4) are defined in the space of six dynamical variables: $0 \leq \beta_2 < \infty$, $-\infty < \beta_3 < \infty$, $\frac{n\pi}{3} \leq \gamma \leq \frac{(n+1)\pi}{3}$, $0 \leq \theta_1 \leq 2\pi$, $0 \leq \theta_2 \leq \pi$ and $0 \leq \theta_3 < 2\pi$, with the volume element $d\tau = \beta_2^4 \beta_3^3 |\sin 3\gamma| d\beta_2 d\beta_3 d\gamma d\theta_1 \sin \theta_2 d\theta_2 d\theta_3$. Here $\beta_\lambda^2 = \sum \beta_{\lambda\mu} \beta_{\lambda\mu}^*$ is the measure of nucleus deformation with multipolarity λ . Below we consider nuclei that are hard with respect to octupole transverse vibrations.

For nuclei of shape determined by Eq. (2), $J_i^{(\lambda)}$ are given by

$$J_i^{(2)} = 4B_2 \beta_2^2 \sin(\gamma - 2/3\pi i) \quad (7a)$$

$$J_1^{(3)} = 4B_3 \beta_3^2 \left(\frac{1}{2} \cos^2 \eta + \frac{\sqrt{15}}{4} \sin 2\eta + 1 \right), \quad (7b)$$

$$J_2^{(3)} = 4B_3 \beta_3^2 \left(\frac{1}{2} \cos^2 \eta - \frac{\sqrt{15}}{4} \sin 2\eta + 1 \right), \quad (7c)$$

$$J_3^{(3)} = 4B_3 \beta_3^2 \sin^2 \eta, \quad (7d)$$

$$J_1^{(4)} = 4B_4 \left(\frac{5}{2} b_{40}^2 + 4b_{42}^2 + b_{44}^2 + \frac{3}{2} \sqrt{10} b_{40} b_{42} + \sqrt{7} b_{42} b_{44} \right), \quad (7e)$$

$$J_2^{(4)} = 4B_4 \left(\frac{5}{2} b_{40}^2 + 4b_{42}^2 + b_{44}^2 - \frac{3}{2} \sqrt{10} b_{40} b_{42} - \sqrt{7} b_{42} b_{44} \right), \quad (7f)$$

$$J_3^{(4)} = 4B_4 (2b_{42}^2 + 8b_{44}^2), \quad (7g)$$

with $b_{4\mu}$ that can be presented [15]

$$b_{40} = \beta_4 \left(\sqrt{7/12} \cos \delta_4 + \sqrt{5/12} \sin \delta_4 \cos \gamma_4 \right), \quad (8a)$$

$$b_{42} = \beta_4 \sqrt{1/2} \sin \delta_4 \sin \gamma_4, \quad (8b)$$

$$b_{44} = \beta_4 \sqrt{1/2} \left(\sqrt{5/12} \cos \delta_4 - \sqrt{7/12} \sin \delta_4 \cos \gamma_4 \right), \quad (8c)$$

with η , δ_4 and γ_4 -parameters determining non-axiality of octupole and hexadecapole deformations.

For the sake of convenience let's rewrite \hat{T}_r :

$$\hat{T}_r = \frac{1}{4B_2 \beta_2^2} \sum_{i=1}^3 \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}}, \quad (9)$$

where $j_i^{(\lambda)} = J_i^{(\lambda)} / 4B_\lambda \beta_\lambda^2$, $a_{\lambda 2} = (B_\lambda / B_2)(\beta_\lambda / \beta_2)^2$. To solve the Schrödinger equation we expand Eq. (9) around the minima of the potential energy of quadrupole and octupole vibrations, i.e., β_{20} , γ_0 and β_{30} :

$$\begin{aligned} \hat{T}_r = & \frac{1}{4B_2 \beta_2^2} \sum_{i=1}^3 \left\{ \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}} \Bigg|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} \right. \\ & + \frac{\partial}{\partial \gamma} \left[\frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}} \right] \Bigg|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} (\gamma - \gamma_0) \\ & + \frac{\partial}{\partial a_{32}} \left[\frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}} \right] \Bigg|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} 2a_{320} \left[\frac{\beta_3 - \beta_{30}}{\pm \beta_{30}} - \frac{\beta_2 - \beta_{20}}{\beta_{20}} \right] + \dots \end{aligned}$$

$$\left. -\frac{\partial}{\partial a_{42}} \left[\frac{\hat{I}_i^2}{j_i^{(2)} + a_{32}j_i^{(3)} + a_{42}j_i^{(4)}} \right] \right|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} 2a_{420} \left[\frac{\beta_2 - \beta_{20}}{\beta_{20}} \right] + \dots \right\}, \quad (10)$$

where $a_{\lambda 20} = (B_\lambda/B_2)(\beta_{\lambda 0}/\beta_{20})^2$ and \pm at β_{30} denotes that we bear in mind that even-even octupole deformed nuclei must have two minima at $\pm\beta_{30}$ of the potential energy that correspond to two symmetric octupole shapes. These nuclei are characterized by the double degeneration of levels, which is washed out as a result of tunneling transition through the barrier separating those nuclear shapes with opposite values of octupole deformation [16, 17].

In the zero-order approximation the operator of nuclear rotation energy is identical to that \hat{T}_r of a nucleus having quadrupole deformation, provided that the principal moments of inertia are redefined reflecting account of octupole and hexadecapole deformation. Let us change variable $\beta_3 = \beta_2\epsilon$ and assume that in the new variables, the potential energy of octupole vibrations has the form

$$V(\beta_3) + \frac{3\hbar^2}{8B_3\beta_3^2} = \frac{\hbar^2}{2B_3\mu_\epsilon^4\beta_{20}} (\epsilon \mp \epsilon_0)^2. \quad (11)$$

Owing to centrifugal forces caused by nuclear rotation, equilibrium octupole deformations are transformed due to the $\beta_3 = \beta_2\epsilon$ in direct proportion with the increase of β_2 . It is shown in Ref. [18] that, along with the choice of potential in the form of Eq. (11), this enables us to reproduce various patterns of level-energy intervals observed experimentally for positive and negative parity bands of even-even nuclei. If nevertheless scaling of β_3 by β_2 is ignored, β_3 can be taken equal to ϵ .

Let us solve the Schrödinger equation in the zero-order approximation for the expansion of the rotational-energy operator \hat{T}_r . Assuming that $\Psi = (\beta_2^{-2}\beta_3^{-3/2})/\sqrt{\sin 3\gamma}u$, we arrive at

$$\begin{aligned} & -\frac{\hbar^2}{2B_2} \frac{\partial^2 u}{\partial \beta_2^2} - \frac{\hbar^2}{2B_3\beta_2^2} \frac{\partial^2 u}{\partial \epsilon^2} - \frac{\hbar^2}{2B_2\beta_2^2} \frac{\partial^2 u}{\partial \gamma^2} + \frac{\hbar^2}{2B_2\beta_2^2} \frac{1}{4} \sum_{i=1}^3 \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32}j_i^{(3)} + a_{42}j_i^{(4)}} \Big|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} u \\ & + \left[V(\beta_2) + \frac{\hbar^2}{2B_3\mu_\epsilon^4\beta_2^2} (\epsilon \mp \epsilon_0)^2 + \frac{\beta_0^4}{\beta_2^2} V(\gamma) - \frac{\hbar^2}{2B_2\beta_2^2} \frac{9}{4} \frac{1 + \sin^2 3\gamma}{\sin^2 3\gamma} \right] u = Eu. \end{aligned} \quad (12)$$

The quadrupole and octupole variables in (12) are now separated, and the function u can be factorized. Thus we have

$$u = \psi^\pm(\beta_2, \gamma, \Theta)\varphi_{n_{\beta_3}}^\pm(\epsilon), \quad (13)$$

where

$$\varphi_{n_{\beta_3}}^\pm(\epsilon) = \frac{c_{n_{\beta_3}}}{\sqrt{2}} [\chi_{n_{\beta_3}}(\tau_\epsilon^+) \pm \chi_{n_{\beta_3}}(\tau_\epsilon^-)], \quad (14)$$

$$\tau_\epsilon^\pm = \epsilon \mp \epsilon_0. \quad (15)$$

Here, $\chi_{n_{\beta_3}}(\tau_\epsilon^\pm)$ are oscillator functions that satisfy the equation

$$\left[-\frac{\hbar^2}{2B_3} \frac{\partial^2}{\partial \epsilon^2} + \frac{\hbar^2}{2B_3\mu_\epsilon^4} (\epsilon \mp \epsilon_0)^2 \right] \chi_{n_{\beta_3}}(\tau_\epsilon^\pm) = \hbar\omega_\epsilon(n + 1/2) \chi_{n_{\beta_3}}(\tau_\epsilon^\pm), \quad (16)$$

where the frequency is given by $\omega_\epsilon = \hbar/(B_3\mu_\epsilon^2)$, $n_{\beta_3} = 0, 1, 2, \dots$ and $c_{n_{\beta_3}}$ is the normalization constant. The superscript \pm on the eigenfunctions specifies their symmetry under the transformation $\epsilon_0 \rightarrow -\epsilon_0$.

Nuclear states of positive parity are described by symmetric combinations of the oscillator functions, while states of negative parity are represented by antisymmetric combinations.

The function $\psi^\pm(\beta_2, \gamma, \Theta)$ satisfies the equation

$$\frac{\hbar^2 \beta^2}{2B_2} \frac{\partial^2 \psi^\pm}{\partial \beta_2^2} + \frac{\hbar^2}{2B_2} \frac{\partial^2 \psi^\pm}{\partial \gamma^2} - \frac{\hbar^2}{2B_2} \frac{1}{4} \sum_{i=1}^3 \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}} \Bigg|_{\substack{\beta_2 = \beta_{20} \\ \gamma = \gamma_0 \\ \beta_3 = \beta_{30}}} \psi^\pm - \left[\beta_2^2 V(\beta_2) + \beta_0^4 V_0(\gamma) - \frac{\hbar^2}{2B_2} \frac{9}{4} \frac{1 + \sin^2 3\gamma}{\sin^2 3\gamma} + E_{n_{\beta_3}}^\pm - E^\pm \beta_2^2 \right] \psi^\pm = 0, \quad (17)$$

where $E_{n_{\beta_3}}^\pm = \hbar\omega_\epsilon(n_{\beta_3} + 1/2) \mp \delta_n$ is the energy of octupole longitudinal surface vibrations, and $2\delta_n$ is the energy splitting of a doubly degenerate level due to the tunneling effect.

The only difference between equation (17) and the analogous equation (considered in detail in Ref. [5]) for vibrational and rotational state of positive parity in non-axial deformed even-even nuclei is due to the necessity of taking into account the dependence of the eigenfunctions of the rotation operator \hat{T}_r on the parity of the states under consideration. If K is even (as in our case), these functions have the form

$$\Phi_{IM\tau}^\pm(\Theta) = \sum_{K \geq 0} |IMK, \pm\rangle A_{IK}^\tau, \quad (18)$$

where

$$|IMK, \pm\rangle = ((2I+1)/(16\pi^2(1+\delta_{K0})))^{1/2} [D_{MK}^I(\Theta) \pm (-1)^I D_{M-K}^I(\Theta)], \quad (19)$$

the symbol $D_{M\pm K}^I(\Theta)$ being the rotation function. In even-even nuclei, rotational bands formed by positive parity levels are described by the wave functions $|IMK, +\rangle$ of a rigid-rotator, which transform according to the irreducible representation A of the D_2 group. Bands formed by negative-parity levels with even K are described by the functions $|IMK, -\rangle$ that realize the irreducible representation B_1 of the same group [18].

Using the results from Ref. [5], we can obtain the eigenvalues of the nuclear Hamiltonian predicting the energies of rotational-vibrational states (with allowance for the quadrupole and octupole deformability of an even-even nucleus in the zero-order approximation of \hat{T}_r expansion) in the form

$$\begin{aligned} E_{I\tau n_{\gamma} n_{\beta_3} n_{\beta_2}}^\pm &= \hbar\omega_0 \left\{ \left(\nu_{I\tau n_{\gamma} n_{\beta_3} n_{\beta_2}}^\pm + 1/2 \right) \times \left(4 - 3/P_{I\tau n_{\gamma} n_{\beta_3}}^\pm \right)^{1/2} \right. \\ &\quad + \frac{1}{2} \frac{\mu_{\beta_{20}}^2}{P_{I\tau n_{\gamma} n_{\beta_3}}^{\pm 2}} \left[\frac{2}{\mu_{\gamma_0}^2} (\nu_{n_{\gamma}} - \nu_{0_{\gamma}}) + \varepsilon_{I\tau}^\pm + \epsilon_{n_{\beta_3}}^\pm - \epsilon_{0_{\beta_3}}^+ \right] \\ &\quad \left. + \frac{1}{2} \frac{\mu_{\beta_{20}}^6}{P_{I\tau n_{\gamma} n_{\beta_3}}^{\pm 6}} \left[\frac{2}{\mu_{\gamma_0}^2} (\nu_{n_{\gamma}} - \nu_{0_{\gamma}}) + \varepsilon_{I\tau}^\pm + \epsilon_{n_{\beta_3}}^\pm - \epsilon_{0_{\beta_3}}^+ \right]^2 \right\}, \end{aligned} \quad (20)$$

where $\epsilon_{n_{\beta_3}}^\pm = \frac{2B_2}{\hbar^2} E_{n_{\beta_3}}^\pm$, and $P_{I\tau n_{\gamma} n_{\beta_3}}^\pm$ is a root of the equation

$$(P_{I\tau n_{\gamma} n_{\beta_3}}^\pm - 1) P_{I\tau n_{\gamma} n_{\beta_3}}^{\pm 3} = \mu_{\beta_{20}}^{\pm 4} \left[\frac{2}{\mu_{\gamma_0}^2} (\nu_{n_{\gamma}} - \nu_{0_{\gamma}}) + \varepsilon_{I\tau}^\pm + \epsilon_{n_{\beta_3}}^\pm - \epsilon_{0_{\beta_3}}^+ \right], \quad (21)$$

where $\hbar\omega_0$, $\mu_{\beta_{20}}$, μ_{γ_0} and γ_0 are the model parameters to be adjusted to reproduce experimentally-known band structures. The $\hbar\omega_0$ parameter denotes an overall scale factor of the level energies, $\mu_{\beta_{20}}$, μ_{γ_0} and μ_ϵ are related with the elasticity constants of β_2- , $\gamma-$ and octupole vibrations, respectively,

and γ_0 is the equilibrium point of the γ -vibration. Other quantities in the above equation are to be determined in the following way.

The quantity ν_{n_γ} denotes the eigenvalue of the γ -vibration corresponding to the quantum number of n_γ and so on. The quantity $\epsilon_{I\tau}^\pm$ is the eigenvalues of the asymmetric-rotator Hamiltonian[19, 20] with redefined principal moments of inertia (10).

$$\hat{T}_r \Phi_{IM\tau}^\pm = \epsilon_{I\tau}^\pm \Phi_{IM\tau}^\pm. \quad (22)$$

The symbol ν_{n_γ} is determined by a system of two equations corresponding to the boundary conditions for γ -vibrations, and n_γ is the number of the solution as ν_{n_γ} is growing.

$$\begin{cases} v_{\nu_{n_\gamma}} \left[-\frac{\sqrt{2}}{\mu_{\gamma_0}} \left(\frac{\pi}{3} n - \gamma_0 \right) \right] = 0 \\ v_{\nu_{n_\gamma}} \left[-\frac{\sqrt{2}}{\mu_{\gamma_0}} \left(\frac{\pi}{3} (n+1) - \gamma_0 \right) \right] = 0 \end{cases}, \quad (23)$$

where $v_{\nu_{n_\gamma}}$ denotes a solution of an oscillator equation

$$\left[\frac{d^2}{dy^2} + \nu_{n_\gamma} + \frac{1}{2} - \frac{y^2}{4} \right] v_{n_\gamma} = 0 \quad (24)$$

being a linear combination of two standard non-linear solutions

$$v_{n_\gamma}(y) = c_{n_\gamma} [D_{\nu_{n_\gamma}}(y) + a_{n_\gamma} V_{\nu_{n_\gamma}}(y)], \quad (25)$$

with $D_{\nu_{n_\gamma}}$ -well known Weber function (see [21]). $\nu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm$ is determined by boundary conditions (23), but in this case, one of the boundaries is at infinity, and this reduces the possible solution of equation (24)

$$v_\nu(y) = c_\nu D_\nu(y), \quad (26)$$

so that $\nu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm$ is determined by equation

$$D_{\nu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}}^\pm \left[-\frac{\sqrt{2} P_{I\tau n_\gamma n_{\beta_3}}^\pm}{\mu_{\beta_{20}}} \left(4 - \frac{3}{P_{I\tau n_\gamma n_{\beta_3}}^\pm} \right) \right] = 0. \quad (27)$$

At last we can write the nuclear wave function

$$\begin{aligned} \Psi_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm &= C_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm \frac{C_{n_{\beta_3}} \beta_2^{-2} \beta_3^{-3/2}}{\sqrt{2} \sqrt{\sin 3\gamma}} \sum_{K \geq 0} |IMK, \pm\rangle A_{IK}^\tau \\ &\times D_{\nu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}}^\pm \left[\frac{\sqrt{2}}{\beta_{20} P_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm} (\beta_2 - \beta_{2I\tau n_\gamma n_{\beta_3}}^\pm) \right] \\ &\times v_{n_\gamma} \left[\frac{\sqrt{2}}{\mu_{\gamma_0}} (\gamma - \gamma_0) \right] [\chi_{n_{\beta_3}}(\tau_\epsilon^+) \pm \chi_{n_{\beta_3}}(\tau_\epsilon^-)], \end{aligned} \quad (28)$$

with

$$\beta_{2I\tau n_\gamma n_{\beta_3}}^\pm = \beta_{20} P_{I\tau n_\gamma n_{\beta_3}}^\pm, \quad (29)$$

which denotes the equilibrium deformation of the stretched rotating nucleus for state $I\tau n_\gamma n_{\beta_3}$ and

$$\frac{1}{\mu_{\beta_{2I\tau n_\gamma n_{\beta_3}}}^4} = \frac{1}{\mu_{\beta_{20}}^4} + \frac{3 \left[\frac{2}{\mu_{\gamma_0}^2} (\nu_{n_\gamma} - \nu_{0_\gamma}) + \epsilon_{I\tau}^\pm + \epsilon_{n_{\beta_3}}^\pm - \epsilon_{0_{\beta_3}}^+ \right]}{P_{I\tau n_\gamma n_{\beta_3}}^\pm}, \quad (30)$$

with $\mu_{\beta_2, \tau n_\gamma n_{\beta_3}}$ being the nucleus softness for this state. The correction $\Delta E_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm$ to the energy of rotational-vibrational states due to linear terms of expansion (10) can be easily calculated by perturbation theory. If we consider $n_{\beta_3} = 0$ (as states with $n_{\beta_3} \geq 1$ lie above the experimentally resolved) this correction is given by

$$\begin{aligned} \Delta E_{I\tau n_\gamma n_{\beta_3}(=0) n_{\beta_2}}^\pm &= \hbar\omega_0 \frac{\mu_{\beta_2}^2}{\beta_{20}^2} \left\{ \frac{B_3}{B_2} \epsilon_0^2 \langle \Phi_{IM\tau}^\pm(\theta) | \sum_{i=1}^3 \frac{\partial}{\partial a_{32}} \left[\frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}} \right] \right|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} | \Phi_{IM\tau}^\pm(\theta) \rangle \right. \\ &\quad \times \left\{ \left[\frac{e^{-\epsilon_0^2/\mu_\epsilon^2}}{1 \pm e^{-\epsilon_0^2/\mu_\epsilon^2}} \left(\frac{\mu_\epsilon}{\epsilon_0 \sqrt{\pi}} \pm \frac{\mu_\epsilon}{\epsilon_0 \sqrt{\pi}} \mp 1 \right) - \frac{\text{erfc}(\epsilon_0/\mu_\epsilon)}{1 \pm e^{-\epsilon_0^2/\mu_\epsilon^2}} \right] J_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm(1/y^2) - J_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm(1/y^2) \right\} \\ &\quad \left. - \frac{B_4}{B_2} \beta_4^2 \langle \Phi_{IM\tau}^\pm(\theta) | \sum_{i=1}^3 \frac{\partial}{\partial a_{42}} \left[\frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}} \right] \right|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} | \Phi_{IM\tau}^\pm(\theta) \rangle \times J_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm((y-1)/y^2) \right\}, \quad (31) \end{aligned}$$

where

$$\begin{aligned} J_{I'\tau' n'_\gamma n'_{\beta_3} n'_{\beta_2}}^\pm [f(y)] &= \int_0^\infty f(y) D_{\nu_{I'\tau' n'_\gamma n'_{\beta_3} n'_{\beta_2}}^\pm} \left[-\frac{\sqrt{2}}{\mu_{I\tau n_\gamma n_{\beta_3}}^\pm} (y - P_{I\tau n_\gamma n_{\beta_3}}^\pm) \right] \\ &\quad \times D_{\nu_{I'\tau' n'_\gamma n'_{\beta_3} n'_{\beta_2}}^\pm} \left[-\frac{\sqrt{2}}{\mu_{I'\tau' n'_\gamma n'_{\beta_3}}^\pm} (y - P_{I'\tau' n'_\gamma n'_{\beta_3}}^\pm) \right] dy \\ &\quad \times \left\{ \int_0^\infty D_{\nu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm}^2 \left[-\frac{\sqrt{2}}{\mu_{I\tau n_\gamma n_{\beta_3}}^\pm} (y - P_{I\tau n_\gamma n_{\beta_3}}^\pm) \right] dy \right\}^{-1/2} \\ &\quad \times \left\{ \int_0^\infty D_{\nu_{I'\tau' n'_\gamma n'_{\beta_3} n'_{\beta_2}}^\pm}^2 \left[-\frac{\sqrt{2}}{\mu_{I'\tau' n'_\gamma n'_{\beta_3}}^\pm} (y' - P_{I'\tau' n'_\gamma n'_{\beta_3}}^\pm) \right] dy' \right\}^{-1/2}. \quad (32) \end{aligned}$$

The non-spherical optical potential is taken in a standard form

$$\begin{aligned} V(r) &= -V_R f_R(r) + i \left\{ 4W_D a_D \frac{d}{dr} f_D(r) - W_V [\alpha f_V(r) + (1-\alpha) f_W] \right\} \\ &\quad + \left(\frac{\hbar}{\mu_\pi c} \right)^2 V_{SO} \frac{1}{r} \frac{d}{dr} f_{so}(r) \hat{\sigma} \cdot \hat{L} + V_{Coul}(r), \quad (33) \end{aligned}$$

with the form factors

$$f_i = [1 + \exp(r - R_i)/a_i]^{-1}, \quad i = R, V, D \text{ and } SO, \quad (34a)$$

$$f_W = \exp\{-(r - R_W)/a_W)^2\} \quad (34b)$$

whose radii are given by the expression (2). The symbols $i = R, V, D, W$ and SO denote the real volume, imaginary volume, imaginary surface, imaginary Gaussian and real spin-orbit potential, respectively, with

$$V_R = V_R^0 + \frac{ZZ'}{A^{1/3}} C_{Coul} + V_R^1 E_p + V_R^2 E_p^2, \quad (35a)$$

$$W_i = \begin{cases} W_i^0 + W_i^1 E_p & (E_p \leq E_{change}) \\ W_i^0 + W_i^1 E_{change} + (E_p - E_{change}) W_i^n & (E_p > E_{change}) \end{cases} \quad i = V, D \quad (35b)$$

$$a_i = a_i^0 + a_i^1 E_p \quad i = R, V, D, SO \text{ and } W \quad (35c)$$

where E_p is energy of the incident particle. V_{Coul} is specified, following Satchler [22], up to the second order of $\sum \beta_{\lambda\mu} Y_{\lambda\mu}$,

$$\begin{aligned} V_{Coul} = & \frac{ZZ'e^2}{2R_c} \left[3 - \frac{r^2}{R_c^2} \right] \theta(R_C - r) + \frac{ZZ'e^2}{r} \theta(r - R_C) \\ & + \sum_{\lambda\mu} \frac{3ZZ'e^2}{\hat{\lambda}^2} \left[r^\lambda R_C^{-(\lambda+1)} \theta(R_C - r) + R_C^\lambda r^{-(\lambda+1)} \theta(r - R_C) \right] (\beta_{\lambda\mu} Y_{\lambda\mu}) \\ & + \sum_{\lambda\mu} \frac{3ZZ'e^2}{\hat{\lambda}^2} \left[(1-\lambda)r^\lambda R_C^{-(\lambda+1)} \theta(R_C - r) + (\lambda+2)R_C^\lambda r^{-(\lambda+1)} \theta(r - R_C) \right] \\ & \cdot \sum_{\lambda'\lambda''} \frac{\hat{\lambda}'\hat{\lambda}''}{\sqrt{4\pi}\hat{\lambda}} (\lambda'\lambda''|00|\lambda0) \sum_\mu (\beta_{\lambda'} \otimes \beta_{\lambda''})_{\lambda\mu} Y_{\lambda\mu} \end{aligned} \quad (36)$$

where $\hat{\lambda} = (2\lambda + 1)^{1/2}$, while the symbol \otimes means the vector addition, i.e.,

$$(\beta_{\lambda'} \otimes \beta_{\lambda''})_{\lambda\mu} = \sum_{\mu'\mu''} (\lambda'\lambda''\mu'\mu'' | \lambda\mu) \beta_{\lambda'\mu'} \beta_{\lambda''\mu''}. \quad (37)$$

and $\theta(r) = 1$ if $r > 0$ and $\theta(r) = 0$ if $r < 0$.

Each of the nuclear potential is expanded in a Taylor series considering β_L to be a small parameter following the recipes of Tamura[1] for vibrational nuclei, and taking account of the nuclear shape determined by Eq. (2). More specifically, writing Eq. (2) as $R = R_0 + \delta R$, where $\delta R = R_0 \sum \beta_{\lambda\mu} Y_{\lambda\mu}$, the potential can be expanded in a straight-forward manner as

$$V(R) = V(R_0) + \sum_{t=1}^{\max} \frac{\partial^t V}{\partial R^t} \Big|_{R=R_0} \frac{\delta R^t}{t!}. \quad (38)$$

The coupling potential V_{couple} is the matrix element of the second term of this expansion between 2 soft-rotator model states, and is written in the form

$$V_{couple} = \sum_{t=1}^{\max} \sum_{n=0}^t \beta_L^{t-n} \beta_{L'}^n v^{(t)}(r) \sum_{\lambda\mu} Q_{\lambda\mu}^{*LL'(t)} Y_{\lambda\mu}(\theta', \varphi'). \quad (39)$$

Here, $v^{(t)}(r)$ are the optical potential derivatives, and the $Q_{\lambda\mu}^{*LL'(t)}$ -operator reflects the non-axiality of the nucleus and the transformation to the space fixed system. We have ignored terms like $\beta_2\beta_3\beta_4$ because usually contribution from such a cross term is not significant.

Deformed potential leads to a system of coupled equations for radial wave functions determining particle scattering.

$$\left\{ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 - \frac{2\eta k}{r} \right\} f_i = \frac{2\mu}{\hbar^2} \sum_j V_{ij} f_j \quad (40)$$

Energy dependences of the potential in different channels due to energy loss for level excitation is accounted like

$$V_{ij} = V \left(E_p - \frac{1}{2}(E_i + E_j) \right), \quad (41)$$

where E_p denotes the projectile energy and E_i , E_j excitation energy for level i and j , respectively. The radial solutions beyond the range of nuclear potential can be written using regular F_l and irregular G_l Coulomb functions, with ingoing plane and outgoing waves in initial channels and pure outgoing waves in all other,

$$f_j^i = F_i \delta_{ij} + C_j^i (G_{lj} + i F_{lj}) \quad (42)$$

where index i marks ingoing waves and C_j^i is a scattering matrix that determines all optical values. Coulomb potential deformation results in arising of coupling potential multipoles decreasing as $r^{-\lambda-1}$, so that induced error for matching at radius R must be of order of $R^{-\lambda}$ and matching radius must be significantly increased or Coulomb correction procedure must be applied[24]. As potential multipole λ determines angular momentum transfer, it is important for $J^\pi = 2^+$ level excitation (for ground state with $J^\pi = 0^+$) and much less for levels with higher spins.

One can get the solution with such asymptotic behavior if a set of linearly independent solutions of homogeneous coupled system is available at matching radius - standard solution, as a result of integrating solutions linearly independent in the vicinity of origin up to the matching radius, which is set beyond the range of nuclear potential. In this case the number of integrations of coupled channels for linearly independent systems is equal to the number of coupled equations for each J^π state. Solution can be found much quicker by iterations[2] starting from non-deformed optical solution, or standard solution with a smaller number of coupled equations, as zero approximation. This procedure requires integration of single inhomogeneous equations, in which inhomogeneous term determines coupling. Of course iterations must converge, but if not for some J^π states, standard solution can be applied.

3 Program OPTMAN

3.1 Program Description

The present code consists of the main program **ROTAT**, 42 subroutines, 2 functions and a block-data. Brief description of the subroutines, functions, block-data and the main program is given in this Chapter, ordered in a natural sequence that follows their calls while code is executing.

- **ROTAT** - is the main program. It starts opening files that will be used, and then switches determining program options, such as the nuclear model, method of coupled equation solution, potential expansion and so on. In **ROTAT** one can choose from the two main options: 1 - optical model calculations without optical potential parameters adjustment; 2 - potential parameters adjustment using experimental optical data. If the first option is chosen **ROTAT** calls subroutine **ABCT**, if the second option is activated subroutine **DATET** is called.
- **ABCT** - is the subroutine, in which all the input data for optical model calculations without the parameter adjustment is organized. Subroutines **PREQU**, **RIPAT**, **ASFUT**, **KNCOE** and **QUANT** are called from **ABCT**. Subroutine **PREQU** with all its sequences is called if non-axiality of nuclei is taken into account. If angular distributions of scattered particles are to be calculated, subroutines **PLEGA** and **DISCA** are also called and results are written into an output file. This is repeated for all incident energies specified by the input data.

- PREQU- is a subroutine, that prepares averages over dynamic variables: quadrupole deformation β_2 , non-axiality γ , and octupole deformation β_3 , which determine enhancement of coupling strength between channels as comparing with rigid non-axial model [8]. If we use nuclear model with rigid β_2 , γ or β_3 the averages are equal to rigid values. PREQU calls subroutines SHEM, OVLAO, OVLAB, OVLEGE.
- SHEM - is a subroutine, that determines energies of collective excited states, indices of rotational and vibrational wave functions. The last are needed to average β_2 , γ or β_3 over initial $|i\rangle$ and final $|f\rangle$ wave functions. SHEM calls ANUDF, ANDETO, OVLAG, INERMO, MATAM, EIT12 and function ERFC(X).
- ERFC(X) - is a function that calculates the error function.
- ANUDF and ANDETO - are the subroutines that find indexes of β_2 , γ and β_3 oscillator functions satisfying boundary conditions (it is equal to quantizing energies). ANUDF uses function DGAMMA(X) and rational approximation with coefficients stored in BLOCK DATA, common /SENU/. ANDETO calls subroutine DEX12.
- DGAMMA(X) - is a gamma function of real argument $\Gamma(x)$
- DET12 - is a function that calculates the determinant of a matrix built on independent oscillator functions with two boundary conditions.
- OVLAG - is a subroutine making some necessary averages over γ oscillation functions. It calls subroutine FUDNU.
- FUDNU - is a subroutine that calculates Weber and linearly independent functions. FUDNU uses function DGAMM(X), and is called by all the subroutines averaging dynamical variables.
- OVLAB, OVLEGE, OVLAO - are subroutine making some necessary averages over β_2 , γ and β_3 oscillation functions. They all call subroutine FUDNU.
- INERMO - is a subroutine giving principal moment of inertia for a non-axial rigid nucleus.
- MATAM - is a subroutine that creates matrix determining coupling of rotational functions with different K for one J and calls VECNO.
- VECNO - is a subroutine that diagonalizes the coupling matrix, thus solving the problem of rotational energies for a rigid non-axial rotator. Necessary weights for rotational functions are prepared in this program too.
- RIPAT - is a subroutine preparing matching radius, mesh for integrating systems of coupled equations, potential expansion in all mesh points, and wave numbers of scattered particles in different channels. In accordance with previously chosen option, potential expansion appears as a result of integration of deformed optical potential with spherical functions $Y_{l0}(\theta, \phi)$ (rotational model,

deformed axial nuclei) or expanding deformed optical potential by derivatives (rigid and soft non-axial nuclei). Potential expansion is calculated in mesh points necessary for both exact and iteration solutions of coupled equation systems. If optical potential expansion appears as a result of integration of deformed optical potential with spherical functions $Y_{l0}(\theta, \phi)$ subroutine POTET is called.

- POTET - is a subroutine giving optical potential as a function of $R(\theta, \phi)$ so that integration with $Y_{l0}(\theta, \phi)$ in RIPAT can be done.
- ASFUT - is a subroutine that determines the maximum value of scattered particle angular momentum l_{max} used in calculations and the Coulomb parameter. It calls COPHA for calculation of Coulomb phases, if calculations are carried out for charged particle scattering. Then it calls subroutine BENEC and BESIM for opened and closed channels, respectively.
- COPHA - calculates Coulomb phases.
- BENEC and BESIM - evaluates regular and irregular solutions at matching radius for opened and closed channels, respectively. In case of charged particle scattering it calls subroutine RCWFN.
- RCWFN - is a subroutine that calculates Coulomb functions at matching radius. This subroutine originates from SCAT2 code.
- KNCOE - is a subroutine that calculates coefficients $Q_{\lambda\mu}^{*LL'(t)}$ in Eq. (39). When deformed non-axial optical potential is expanded to derivatives, it calls KLEGO subroutine.
- KLEGO - is a subroutine that calculates Clebsch-Gordan coefficients, uses data from BLOCK DATA.
- BLOCK DATA - data stored in common /SENU/ are coefficients of rational approximation used by subroutine ANUDF; data stored in common /LOFAK/ are logarithms of factorials used for calculations of Clebsch-Gordan and Racah coefficients.
- QUANT - is a subroutine that generates coupled channels systems for certain spin and parity J^π , and determines all the necessary quantum numbers of scattered particles by calling LOGMO. This subroutine calls CMATC and the C-matrix elements given by CMATC for growing J^π are checked to add no less than 1.0×10^{-4} barns to cross sections. When two systems with the same J and different parities obey this limit, systems with higher J are ignored. Subroutine QUANT prepares cross sections, transmission coefficients and strength functions S_0 , S_1 and S_2 .
- LOGMO - is a subroutine that generates possible angular momenta of outgoing waves with chosen J^π of compound nucleus and residual excited state.
- CMATC - is a subroutine that allows different options for coupled channels solution. Four options can be chosen: 1 - standard exact solution, 2 - standard exact solution for small systems and iterations for large systems; 3 - iterations for all systems, with non-coupled scheme as zero approximation; 4 - iterations with zero approximation taken from exact solution with few equations coupled. Number

of such coupled equations solutions used as zero approximation must not exceed 20. CMATC calls subroutines **KNDIT**, **SOSIM**, **SOSIT**, **MASCT** or **ECICC**.

- **KNDIT** - is a subroutine that determines coupling strength of different equations in a system of coupled channels, and calls **KLEGO** and **RACAH** subroutines.
- **RACAH** - is a subroutine calculating Racah coefficients.
- **SOSIM** and **SOSIT** - are subroutines integrating system of coupled equations and giving independent solutions at matching radius . The only difference is that **SOSIM** prepares solution for small coupled systems to be used as zero approximation, so it gives, in contrast with **SOSIT**, independent wave functions in all mesh points necessary for iteration method, but not only at matching radius. The method described in Ref. [25] is used for integration of coupled equations in both programs.
- **MASCT** - matches the solutions with desired asymptotic behavior and gives C-matrix elements. It calls subroutines **INMAT** and **INVER**
- **INMAT** - is a subroutine inverting complex matrix C, presented as $C=A+iB$ with A and B real.
- **INVER** - is a subroutine inverting a real matrix.
- **ECISS** - is a program, that integrates a coupled system using iterations. The method described in Ref. [26] is used here to integrate separate equations. Two options for iterations are possible: 1- spherical optical solution is used as zero approximation; 2 - standard solution for a small number of coupled equations is used as zero approximation. **ECISS** calls subroutine **MATCH** and **PADE**. Iterations are finished when all C-matrix elements in n and n+1 iterations coincide with accuracy better than 10^{-4} . Maximum number of iterations is 20. If iterations do not converge or number of iterations exceeds 20, standard solution method is activated.
- **MATCH** - is a program matching solution in a chosen channel, and giving C-matrix element.
- **PADE** - is a program applying Pade approximation[27] for C-matrix elements determinations, this highly improves the iteration convergence.
- **PLEGA** - calculates Legendre polynomials at given angles
- **DISCA** - calculates angular distributions for particles with $s = 1/2$, using analytical formulas and C-matrix elements, calls **KLEGO** and **RACAH** subroutines.
- **DATET** - is a subroutine in which all the input data for optical model calculations with optical potential parameters adjustment is organized. First, starting optical model parameters are read, then experimental optical data base is inputted. Switches are also read determining which of the optical parameter must be adjusted and its desired accuracies. **DATET** calls subroutine **PREQU** (see **ABCT** for details) for non-axial nuclear model and subroutine **SEART**.
- **SEART** - is a subroutine that minimizes χ^2 -function. It utilizes gradient method and calls **XISQT** and **DEFGT**.

- **XISQT** - is a subroutine calculating χ^2 built in a standard manner, being the average of the sum of squares of the differences between results of optical calculations and experimental ones divided by square of the appropriate experimental errors. It calls subroutines **RIPAT**, **ASFUT**, **KNCOE**, **QUANT**, **PLEGA** and **DISCA** for each energy point used to evaluate χ^2 . This sequence of subroutine calls leads to optical cross sections and is the same as in **ABCT** and is not described there.
- **DEFGT** - is a subroutine, that calculates gradient of χ^2 as a function of adjusted optical parameters.

3.2 Input Data

Input data of OPTMAN is described in this section. Data has the card image form. Units of the data are MeV, fm, barn and amu (Carbon units).

- Card 1 - FORMAT(20A4)

Any text information that identifies current calculation.

- Card 2 - FORMAT(20I2)

MEJOB, MEPOT, MEHAM, MECHA, MEPRI, MESOL, MESHA, MESH0, MEHA0, MEAPP

Switches options describing the model.

- **MEJOB** = 1 - optical calculations, = 2 adjustment of optical potential parameters;
- **MEPOT** = 1 -rotational model potential, =2 - potential expanded by derivatives;
- **MEHAM** = 1 - nuclear Hamiltonian of rotational model, = 2 - not in use yet, = 3 - Davydov-Chaban model, = 4 - Davydov-Philipov model, = 5 - nuclear Hamiltonian with account of γ softness [5, 6], =6,7 - not in use yet;
- **MECHA** = incident particle charge in unit of electron charge;
- **MEPRI** = 0 - short output, additional output as **MEPRI** is growing ;
- **MESOL** = 1 - code will choose which method of coupled channels system solution for a certain J^π should be used to reduce time of calculations, = 2 - exact solution, =3 - solution using iterations, with spherical solutions as zero approximation, >3 - solution using iterations, with exact couple channels solution with number of coupled states = **MESOL** as zero approximation, **MESOL** must be less than or equal to 20;
- **MESHA** = 1 - rigid hexadecapole deformations are not taken into account, = 2 - with account of axial rigid hexadecapole deformations, = 3 - rigid hexadecapole deformations depending on γ [7], = 4 - rigid hexadecapole deformations in the most general case [7];
- **MESH0** = 0 - nuclear shape without octupole deformations, = 1 -nuclear shape with axial octupole deformations, = 2 - nuclear shape with non-axial octupole deformations;
- **MEHA0** = 0 - nucleus is rigid to octupole deformations, = 1 - nucleus is soft to non symmetric octupole, = 2 - nucleus is soft to symmetric octupole deformations scaled by β_2 [8], = 3 - nucleus is soft to symmetric octupole deformations deformations not scaled by β_2 ;

- **MEAPP** = 0 - solution with the potential dependency on level energy losses in the channel,
=1 - quick solution without potential dependency on level energy losses, can be used when
energies of levels are much less than particle incident energy.
- Cards - 3,4,5 FORMAT(6E12.7)

Parameters of non-axial nuclear Hamiltonian. These cards are read if **MEHAM**> 1. In details this parameters are described elsewhere[7, 8, 10, 11].

HW, AMBO, AMGO, GAMO, BETO, BET4 - Card 3

- **HW** - energy scale factor $\hbar\omega_0$;
- **AMBO** - nuclear softness μ_{β_2} ;
- **AMGO** - nuclear softness μ_{γ_0} ,
- **GAMO** - equilibrium non-axiality $\gamma_0 < \pi/3$ in radians;
- **BETO** - equilibrium deformation β_{20} , for non-axial Hamiltonian;
- **BET4** - rigid deformation β_4 , for non-axial Hamiltonian.

BB42, GAMG, DELG, BET3, ETO, AMUO - Card 4

- **BB42** - $a_{42} = B_4/B_2(\beta_4/\beta_{20})^2$, where B_λ - are mass parameters;
- **GAMG** - parameters of β_4 non-axiality, γ_4 ;
- **DELG** - parameters of β_4 non-axiality, δ_4 ;
- **BET3** - if **MEHAO** = 2, **BET3**= ϵ_0 and $\beta_{30} = \beta_{20}\epsilon_0 = \text{BET3} * \text{BETO}$, if **MEHAO** = 3, **BET3**= equilibrium deformation $\beta_{30} = \epsilon_0 = \text{BET3}$;
- **ETO** - non-axiality of octupole β_3 deformation η ;
- **AMUO** - nuclear softness μ_ϵ .

HWO, BB32, GAMDE, DPAR, GHAPE - Card 5

- **HWO** - energy scale for octupole oscillations $\hbar\omega_\epsilon$, used if **MEHAO** = 1;
- **BB32** - $a_{32} = B_3/B_2(\beta_{30}/\beta_{20})^2$;
- **GAMDE** - yet not in use;
- **DPAR** - splitting of energy for the states with different parity in symmetric potential well for octupole oscillations = δ_n ;
- **GHAPE**- parameter allowing negative β_2 deformations so that $\gamma_0 = \text{GAMO} + \text{GHAPE}$.

- Card 6 - FORMAT(20I2)

Switches for details of calculations

NUR, NST, NPD, LAS, MTET, LLMA, NCMA, NSMA, KODMA Card 6 - in case **MEJOB** = 1

NUR, NST, NPD, LAS, LLMA, NCMA, NSMA, KODMA Card 6 - in case **MEJOB** = 2

- **NUR** - number of coupled levels in optical model calculations (**NUR** \leq 20)
- **NST** - number of energy points for which optical model calculations will be carried out if **MEJOB**=1; if **MEJOB** = 2, number of energy points with experimental data that will be used for optical parameters adjustment; (**NST** \leq 20)
- **NPD** - the highest multipole Y_{l0} in deformed radii expansion, $l_{max} = NPD$ for rotational model (**MEPOT** = **MEHAM** = 1), **NPD** \leq 8. For non-axial nuclear Hamiltonian models (**MEPOT** =2, **MEHAM** > 2), not in use,
- **LAS** - the highest multipole Y_{l0} in deformed potential expansion, $l_{max}=LAS$ for rotational model (**MEPOT** = **MEHAM** = 1), **LAS** \leq 8. For non-axial nuclear Hamiltonian models (**MEPOT** =2, **MEHAM** > 2), number of potential derivatives for deformed potential expansion, must be no more than 4;
- **MTET** - number of angles (in c.m.) for which angular distributions of scattered neutrons will be calculated (only for **MEJOB** = 1), in **MTET** = 0 angular distributions are not calculated. **MTET** must be no more than 40;
- **LLMA** = maximum angular momentum of scattered neutrons that is taken into account; higher are rejected. **LLMA** < 40;
- **NCMA** - maximum number of coupled equation for certain J^π ; **NCMA** \leq 60
- **NSMA** - maximum number of J^π states for which coupled channels systems are solved; **NSMA** \leq 60
- **KODMA** - = 0 coupled equations are ordered one by one, first for the first level, then for the second ,etc., - = 1, coupled equations are ordered by growing angular momentum of scattered neutrons, the total number of coupled equations \leq **NCMA**.

- Cards 7a, 7b, ... - FORMAT(6E12.7)

MEJOB = 1 - energies in which optical model cross sections are calculated, **MEJOB** = 2 - energies for experimental points which will be used for potential adjustment; **NST** \leq 20

(**EE(I)**, **I**=1,**NST**) - Cards 7a, 7b, ...

- Card 8 - FORMAT(34I2)

Flags determining charge of the incident particles Z' for which calculations for energy **EE(I)** will be carried out.

(**MCHAE(I)**, **I**=1,**NST**) Card 8

- Cards 9a, 9b,...- FORMAT(6E12.7)

Angles at which angular distributions will be calculated. IF **MTET** = 0 or **MEJOB** = 2 these cards are not read, **MTET** must be no more than 40;

(**TET(I)**, **I**=1,**MTET**) - Cards 9a, 9b,

- Cards 10a, 10b, ... FORMAT(E12.7,3I2) for **MEHAM** = 1, FORMAT(E12.7,6I2) for **MEHAM** > 1

Characteristics of nuclear levels

(**EL(I)**, **J0(I)**, **NPO(I)**, **K0(I)**, **I=1,NUR**) - Cards 10a, 10b, .. for **MEHAM** = 1

(**EL(I)**, **J0(I)**, **NPO(I)**, **NTU(I)**, **NNB(I)**, **NNG(I)**, **NNO(I)**, **I=1,NUR**) - Cards 10a, 10b, .. for **MEHAM** > 1

- **EL(I)** -energy of the I^{th} level;
- **J0(I)** - spin of the level multiplied by two;
- **NPO(I)** - parity of the level = +1 - for positive, = -1 - for negative;
- **K0(I)** - K of the levels band multiplied by two;
- **NTU(I)** - the number of rotational energy solution τ ;
- **NNB(I)** - the number of β_2 oscillation function solution n_{β_2} ;
- **NNG(I)** - the number or γ oscillation function solution n_{γ} ;
- **NNO(I)** - the number of β_3 oscillation function solution n_{β_3} .

- Cards 11a, 11b, 11c, 11d, 11e, 11f -FORMAT(6E12.7)

Optical potential parameters, for details see Chapter 2.

VR0, **VR1**, **VR2**, **RR**, **AR0**, **AR1** - Card 11a

- **VR0** - real optical potential V_R constant term V_R^0 ;
- **VR1** - real optical potential V_R linear term V_R^1 ;
- **VR2** - real optical potential V_R square term V_R^2 ;
- **RR** - real potential radius R_R ;
- **AR0** - real potential diffuseness a_R constant term a_R^0 ;
- **AR1** - real potential diffuseness a_R linear term a_R^1 ;

WD0, **WD1**, **RD**, **AD0**, **AD1**, **WC0** - Card 11b

- **WD0** - imaginary surface potential W_D constant term W_D^0 ;
- **WD1** - imaginary surface potential W_D linear term W_D^1 ;
- **RD** - imaginary surface potential radius R_D ;
- **AD0** -imaginary surface potential diffuseness a_D constant term a_D^0 ;
- **AD1** - imaginary surface potential diffuseness a_D linear term a_D^1 ;
- **WC0** - imaginary volume potential W_V constant term W_V^0 ;

WC1, **RC**, **AC0**, **AC1**, **RW**, **AW0** - Card 11c

- WC1 - imaginary volume potential W_V linear term W_V^1 ;
- RC - imaginary volume potential radius R_V ;
- ACO - imaginary volume potential diffuseness a_V constant term a_V^0 ;
- AC1 - imaginary volume potential diffuseness a_V linear term a_V^1 ;
- RW - imaginary Gaussian potential radius R_W ;
- AW0 - imaginary Gaussian potential diffuseness a_W constant term a_W^0 ;

AW1, VS, RS, AS0, AS1, ALF - Card 11d

- AW1 - imaginary Gaussian potential diffuseness a_W linear term a_W^1 ;
- VS - spin orbit potential V_{SO} ;
- RS - spin orbit potential radius R_{SO} ;
- AS0 - spin orbit potential diffuseness a_{SO} constant term a_{SO}^0 ;
- AS1 - spin orbit potential diffuseness a_{SO} linear term a_{SO}^1 ;
- ALF - mixture coefficient for imaginary volume and Gaussian potentials α ;

AT, ANEU, RZ, ZNUC, ASP, BNDC - Card 11e

- AT - nuclear mass;
- ANEU - incident particle mass;
- RZ - equivalent charged ellipsoid radius R_C ;
- ZNUC - target nuclear charge Z ,
- ASP - particle spin,
- BNDC -energy point at which linear slopes of volume and surface potential are broken (E_{change});

WDA1, WCA1, CCOUL -Card 11f

- WDA1 - imaginary surface potential W_D linear term for the projectile energies above BNDC W_D^n ;
- WCA1 - imaginary volume potential W_V linear term for the projectile energies above BNDC W_V^n ;
- CCOUL - Coulomb correction constant C_{Coul}

• Card 12 - FORMAT(6e12.7)

Input of even axial coefficients of radii deformations $\beta_{\lambda 0}$ from β_{20} to $\beta_{\lambda 0}$, $\lambda=NPD$. This card is read only for axial rotator model (**MEHAM** = 1). Note that λ is even and no more than 8.

- (**BET(I), I=2,NPD,2**) - Card 12

It is the last card of input for optical model calculations (**MEJOB** = 1), the following cards are used when potential parameters adjustment is desired.

- Card 13 - FORMAT(35I2)

Input of flags that determine which parameters will be adjusted; if **NPJ(I) = 1** the chosen parameter will be adjusted. Number of parameters to be adjusted must not exceed 20.

(**NPJ(I)**, I=1,35) Card 13

- **NPJ(1)** - flag for real optical potential V_R constant term adjustment **VRO**;
- **NPJ(2)** - flag for real optical potential V_R linear term adjustment **VR1**;
- **NPJ(3)** - flag for imaginary volume potential W_V constant term adjustment **WC0**;
- **NPJ(4)** - flag for imaginary volume potential W_V linear term adjustment **WC1**;
- **NPJ(5)** - flag for imaginary surface potential W_D constant term adjustment **WD0**;
- **NPJ(6)** - flag for imaginary surface potential W_D linear term adjustment **WD1**;
- **NPJ(7)** - flag for spin-orbit potential V_{SO} adjustment **VS**;
- **NPJ(8)** - flag for real potential diffuseness a_R constant term adjustment **AR0**;
- **NPJ(9)** - flag for imaginary volume potential diffuseness a_V constant term adjustment **AC0**;
- **NPJ(10)** - flag for imaginary Gaussian potential diffuseness a_W constant term adjustment **AW0**;
- **NPJ(11)** - flag for imaginary surface potential diffuseness a_D constant term adjustment **AD0**;
- **NPJ(12)** - flag for real potential radius R_R adjustment **RR**;
- **NPJ(13)** - flag for imaginary volume potential radius R_V adjustment **RC**;
- **NPJ(14)** - flag for imaginary Gaussian potential radius R_W adjustment **RW**;
- **NPJ(15)** - flag for imaginary surface potential radius R_D adjustment **RD**;
- **NPJ(16)** - flag for mixture coefficient α for imaginary volume and Gaussian potentials adjustment **ALF**;
- **NPJ(17)** - flag for rotational model axial rigid deformation β_{20} adjustment **BET(2)**;
- **NPJ(18)** - flag for rotational model axial rigid deformation β_{40} adjustment **BET(4)**;
- **NPJ(19)** - flag for real potential diffuseness a_R linear term adjustment **AR1**;
- **NPJ(20)** - flag for imaginary volume potential diffuseness a_V linear term adjustment **AC1**;
- **NPJ(21)** - flag for imaginary Gaussian potential diffuseness a_W linear term adjustment **AW1**;
- **NPJ(22)** - flag for imaginary surface potential diffuseness a_D linear term adjustment **AD1**;
- **NPJ(23)** - flag for equilibrium deformation β_{20} for non-axial Hamiltonian model adjustment **BETO**;

- NPJ(24) - flag for spin orbit potential radius R_{SO} adjustment RS;
- NPJ(25) - flag for spin orbit potential diffuseness a_{SO} constant term adjustment AS0;
- NPJ(26) - flag for spin orbit potential diffuseness a_{SO} linear term adjustment AS1;
- NPJ(27) - flag for rigid deformation β_4 for non-axial Hamiltonian model adjustment BET4;
- NPJ(28) - flag for equilibrium deformation β_{30} for non-axial Hamiltonian adjustment BET3;
- NPJ(29) - flag for nuclear softness $\mu_{\beta_3} = \mu_\epsilon$ adjustment AMU0;
- NPJ(30) - flag for energy point E_{change} , at which linear slopes of volume and surface potential are broken, adjustment BNDC;
- NPJ(31) - flag for imaginary surface potential W_D^n linear term for neutron incident energies above $BNDC=E_{change}$ adjustment WDA1;
- NPJ(32) - flag for imaginary volume potential W_V^n linear term for neutron incident energies above $BNDC=E_{change}$ adjustment WCA1;
- NPJ(33) - flag for nuclear softness μ_{γ_0} adjustment AMG0;
- NPJ(34) - flag for equivalent charged ellipsoid radius R_C adjustment RZ;
- NPJ(35) - flag for Coulomb correction constant adjustment CCOUL;

Next block of cards will be read for each energy point EE(I), that means NST blocks.

- Card - 14 FORMAT(6I2)

Input of flags determining which experimental data will be used in parameters adjustment (flag = 1 means used in adjustment) for the current energy EE(I).

NT(I), NR(I), NGN(I), NGD(I), NSF1(I), NSF2(I) Card 14

- NT(I) - flag of total cross section;
- NR(I) - flag of reaction cross section;
- NGN(I) - flag of integral excitation cross section of a group of levels, number of such groups, NGN(I) must be no more than 4;
- NGD(I) - flag of angular distributions of scattered neutrons with excitation of a group of levels, number of such groups, NGD(I) must be no more than 4;
- NSF1(I) - flag of S_0 strength function;
- NSF2(I) - flag of S_1 strength function;

- Card 15 FORMAT(4E12.7)

Experimental data for total and reaction cross sections for current energy, if flag = 0 may be blank.

STE(I), DST(I), SRE(I), DSR(I) Card 15

- STE(I) - experimental total cross section;
 - DST(I) - experimental total cross section error;
 - SRE(I) - experimental reaction cross section;
 - DSR(I) - experimental reaction cross section error;
- Card 16 FORMAT(4E12.7)

Experimental data for strength functions, if NSF1(I) = 0 this card is not read.

SE1(I), DS1(I), SE2(I), DS2(I) Card 16

- SE1(I) - experimental S_0 strength function;
- DS1(I) - experimental S_0 strength function error;
- SE2(I) - experimental S_1 strength function;
- DS2(I) - experimental S_1 strength function error.

- Cards 17a, 17b, FORMAT(2E12.7,2I2)

Experimental data for integral excitation of groups of levels for current energy, this card is read for each group of excited levels, that means NGN(I) times, if NGN(I) = 0, these cards are not read. Number of groups must not exceed 4.

(SNE(I,K), DSNE(I,K), NIN(I,K), NFN(I,K), K=1,NGN(I)) Cards 17a, 17b, ...

- SNE(I,K) - experimental integral cross section of a group of levels;
- DSNE(I,K) - experimental integral cross section error of a group of levels;
- NIN(I,K) - the number of the first excited level in a group as specified in Cards 10;
- NFN(I,K) - the number of the last excited level in a group as specified in Cards 10.

- Card 18 FORMAT(20I2)

Description of experimental data for angular distributions of scattered neutron with excitation of a group of levels.

(NID(I,K), NFD(I,K), MTD(I,K), K =1,NGD(I)) Card 18

- NID(I,K) - the number of the first excited level in a group as specified in Cards 10;
- NFD(I,K) - the number of the last excited level in a group as specified in Cards 10;
- MTD(I,K) - number of angles in which experimental angular distributions with excitation of a group of levels exist.

- Cards 19a, 19b, ... FORMAT(6E12.7)

Experimental angular distribution with excitation of a group of levels, this block of cards is read NGD(I) times, if NGD(I)=0, these cards are not read.

(TED(I,K,L), SNGD(I,K,L), DSD(I,K,L), L=1,MTD(I,K)) Cards 19a, 19b,...

- **TED(I,K,L)** - center-of-mass angles for angular distribution in degrees;
- **SNGD(I,K,L)** - experimental differential cross section in b/sr;
- **DSD(I,K,L)** - experimental differential cross section error in b/sr;
- Cards 20a, 20b,... **FORMAT(6E12.7)**
Estimated accuracy of parameter adjustment
(EP(I), I= 1,NV) Cards 20a, 20b,...
 - **EP(I)** - absolute accuracy for a parameter with i^{th} flag=1, NV is equal to a number of flags=1.
Number of flags =1 must not exceed 20.
- Card 21 **FORMAT(E12.7)**
0.000000E+00

This is the last card in input.

3.3 Examples

Here we are going to present two inputs. Both inputs are for optical model parameters adjustment calculations. The first one deals with the rigid-rotator model, and the second one activates the non-axial soft-rotator model. As it is described in previous chapters one who needs to get the input data set for optical model calculations without parameter adjustment must do the following simple changes in input:

1. change value of variable **MEJOB** from 2 to 1 in the 2^{nd} card of input;
2. add variable **MTET** after variable **LAS** in the 6^{th} card in input;
3. if **MTET > 0** is chosen, add cards describing angles after card 8, with flags **MCHAE(I)** determining charge of incident particle for chosen energy **E(I)**.

3.3.1 Input for the rigid-rotator model

Below one can find actual input file, that was used for adjustment of ^{238}U optical model parameters

- Card 1 - some text information
- Card 2 - defines that a run with adjustment of optical potential parameters (**MEJOB=2**) for rotational CC-model (**MEPOT=1**) will be organized; rotational model nuclear Hamiltonian will be used to determine coupling (**MEHAM=1**); output will be the shortest (**MEPRI=0**); exact method for coupled equations system solution will be used (**MESOL=2**); energy dependency of optical potential in different channels caused by energy losses due to levels excitation is ignored in this run (**MEAPP=1**). Other switches will be ignored as **MEPOT=1**.

- Card 3 - defines that three levels are coupled (**NUR=3**); potential will be adjusted using experimental data at nine energy points simultaneously (**NST=9**); the highest order L for radius deformation expansion is chosen to be equal 4 (**NPD=4**); resulting optical potential will be expanded up to Y_{80} spherical harmonic (**LAS=8**); waves with angular momentum greater than 20 will be ignored (**LLMA=20**); coupling of no more than 40 equations will be taken into account, other ignored (**NCMA=40**); no more than 40 J^π states ordered by increasing J will be taken into consideration (**NSMA=40**); coupled equations will be ordered one by one, starting with the first level, then the second and so on (**KODMA=0**).
- Cards 4,5 - nine energies, as it was stated in Card 3, in which adjustment of optical potential to experimental data will be organized in the code.
- Card 6 - nine **MCHAE(I)** flags, in our case all equal 0, that means that experimental data for incident neutrons in all energy points will be used for adjustment.
- Cards 7-9 - energies and quantum numbers of the three levels that should be coupled.
- Cards 10-15 - starting set of optical potential parameters, even in case some parts of the potential are equal to zero one must avoid setting their radii and diffusenesses to zero.
- Card 16 - β_2 and β_4 as defined by **NPD=4**.
- Card 17 - **NPJ(I)** values in our case only **NPJ(1)** and **NPJ(5)** are equal 1, constant terms of real and surface potentials will be adjusted in this run.
- Card 18 - information about experimental data at first experimental energy point ($E_n=1.5$ keV), that will be used in optical parameters adjustment. Total cross section is not used in adjustment at this energy point (**NT(1)=0**); reaction cross section is not used in adjustment at this energy (**NR(1)=0**); one experimental integral scattering cross section with excitation of a group of levels will be used for adjustment (**NGN(1)=1**); S_0 strength function will be adjusted at this energy (**NSF1(1)=1**); S_1 strength function will be adjusted at this energy (**NSF2(1)=1**).
- Card 19 - total and reaction cross sections and their errors at first energy; as **NT(1)** and **NR(1)** are equal to zero this card is blank.
- Card 20 - experimental S_0 and S_1 values with their errors.
- Card 21 - experimental scattering cross section and its error for excitation of a group of levels and **NIN(1,1)**, **NFM(1,1)** numbers of the first and last excited level in a group, in our case both equal to 1, that means experimental elastic scattering cross section is inputted for adjustment.
- Card 22 -information about experimental data at second energy point used for adjustment. Only total cross section will be adjusted at this energy point (**NT(2)=1**), other switches are equal to zero.


```

24 010000000000
25 .6940000+01 .1400000-00 .0000000-00 .0000000-00
26 010000030000
27 .8040000+01 .1610000-00 .0000000-00 .0000000-00
28 010118020216030315
29 .2010000+02 .2866800+01 .1749000-00 .3010000+02 .1540100+01 .9580000-01
30 .4020000+02 .3096000-00 .2390000-01 .4520000+02 .1443000-00 .1170000-01
31 .5020000+02 .2730000-01 .3400000-02 .6020000+02 .3670000-01 .5400000-02
32 .6520000+02 .8420000-01 .8200000-02 .8020000+02 .1135000-00 .1220000-01
33 .8520000+02 .1052000-00 .9800000-02 .9020000+02 .8700000-01 .8700000-02
34 .1002000+03 .3300000-01 .4200000-02 .1052000+03 .2660000-01 .3600000-02
35 .1102000+03 .1030000-01 .1900000-02 .1202000+03 .2100000-02 .7000000-03
36 .1302000+03 .5400000-02 .1500000-02 .1402000+03 .1410000-01 .2700000-02
37 .1501000+03 .2420000-01 .3700000-02 .1601000+03 .3350000-01 .4400000-02
38 .4020000+02 .8160000-01 .9700000-02 .4520000+02 .6130000-01 .6600000-02
39 .5020000+02 .4530000-01 .6200000-02 .6020000+02 .3590000-01 .5900000-02
40 .6520000+02 .4330000-01 .5100000-02 .8020000+02 .5070000-01 .7400000-02
41 .8520000+02 .4970000-01 .5800000-02 .9020000+02 .5230000-01 .5800000-02
42 .1002000+03 .3010000-01 .4100000-02 .1052000+03 .1980000-01 .3100000-02
43 .1102000+03 .1660000-01 .2800000-02 .1202000+03 .9800000-02 .2100000-02
44 .1302000+03 .3400000-01 .4600000-02 .1402000+03 .4240000-01 .5200000-02
45 .1501000+03 .2780000-01 .3900000-02 .1601000+03 .1930000-01 .3100000-02
46 .4020000+02 .2190000-01 .4500000-02 .4520000+02 .2220000-01 .3500000-02
47 .5020000+02 .1580000-01 .3500000-02 .6020000+02 .1220000-01 .3300000-02
48 .6520000+02 .9900000-02 .2100000-02 .8020000+02 .9000000-02 .2800000-02
49 .8520000+02 .9900000-02 .2200000-02 .9020000+02 .1010000-01 .2600000-02
50 .1052000+03 .9700000-02 .2200000-02 .1102000+03 .8400000-02 .2000000-02
51 .1202000+03 .6800000-02 .1800000-02 .1302000+03 .6600000-02 .1700000-02
52 .1402000+03 .4800000-02 .1500000-02 .1501000+03 .3900000-02 .1300000-02
53 .1601000+03 .3100000-02 .1100000-02
54 010000010000
55 .5960000+01 .1000000-00 .0000000-00 .0000000-00
56 010333
57 .2400000+02 .1200000+00 .1200000-01 .3000000+02 .3200000+00 .3200000-01
58 .3450000+02 .4050000-00 .4050000-01 .4000000+02 .3000000-00 .3000000-01
59 .4450000+02 .1380000-00 .1380000-01 .5000000+02 .5700000-01 .5700000-02
60 .5500000+02 .5800000-01 .5800000-02 .6000000+02 .7200000-01 .7200000-02
61 .6500000+02 .8000000-01 .1200000-01 .7000000+02 .5000000-01 .7500000-02
62 .7500000+02 .2700000-01 .4000000-02 .8000000+02 .1250000-01 .2000000-02
63 .8500000+02 .1180000-01 .1500000-02 .9500000+02 .2000000-01 .3000000-03
64 .1050000+03 .1520000-01 .3000000-02 .1150000+03 .8000000-02 .2000000-02
65 .1250000+03 .9000000-02 .2000000-02 .1350000+03 .6000000-02 .1500000-02
66 .9240000+01 .8856000+01 .8860000-00 .3245000+02 .4330000-00 .3000000-01
67 .3887000+02 .4490000-00 .3200000-01 .4650000+02 .1290000-00 .9000000-02
68 .1678000+02 .2081000+01 .1460000-00 .2391000+02 .1710000-00 .1200000-01
69 .5392000+02 .5300000-01 .4000000-02 .6164000+02 .8500000-01 .6000000-02
70 .6896000+02 .6800000-01 .5000000-02 .8367000+02 .1500000-01 .2000000-02
71 .9897000+02 .2100000-01 .3000000-02 .1134500+03 .5800000-02 .2000000-02
72 .1289100+03 .1200000-01 .3000000-02 .1440600+03 .4600000-02 .2100000-02
73 .1591000+03 .7300000-02 .2500000-02 .
74 010000000000
75 .6250000+01 .1500000-00 .0000000-00 .0000000-00

```

```

76 010000010000
77 .5940000+01 .1000000-00 .0000000-00 .0000000-00
78 010340
79 .1786000E+02.2061000E+01.8244000E-01.2181000E+02.8312000E+00.3324800E-01
80 .2578000E+02.3177000E+00.1270800E-01.2776000E+02.2454000E+00.9816000E-02
81 .2865000E+02.1943000E+00.7772000E-02.3194000E+02.2153000E+00.8611999E-02
82 .3592000E+02.2857000E+00.1142800E-01.3871000E+02.3030000E+00.1212000E-01
83 .4369000E+02.2352000E+00.9408000E-02.4718000E+02.1562000E+00.6248000E-02
84 .5117000E+02.9487000E-01.3794800E-02.5416000E+02.5911000E-01.2364400E-02
85 .5915000E+02.6205000E-01.2482000E-02.6264000E+02.8345000E-01.3338000E-02
86 .6664000E+02.1043000E+00.4172000E-02.6963000E+02.1132000E+00.4528000E-02
87 .7562000E+02.9620000E-01.3848000E-02.7862000E+02.7150000E-01.2860000E-02
88 .8261000E+02.4671000E-01.1868400E-02.8561000E+02.3355000E-01.1500021E-02
89 .9110000E+02.2740000E-01.1499876E-02.9409000E+02.2678000E-01.1499948E-02
90 .9809000E+02.3055000E-01.1500005E-02.1011000E+03.3392000E-01.1499942E-02
91 .1066000E+03.3063000E-01.1499951E-02.1096000E+03.2543000E-01.1500116E-02
92 .1136000E+03.2277000E-01.1500088E-02.1166000E+03.1894000E-01.1500048E-02
93 .1225000E+03.1651000E-01.1499934E-02.1255000E+03.1301000E-01.1500053E-02
94 .1290000E+03.9657000E-02.1499732E-02.1320000E+03.9843000E-02.1500073E-02
95 .1385000E+03.9784000E-02.1499887E-02.1415000E+03.1301000E-01.1500053E-02
96 .1445000E+03.1380000E-01.1500060E-02.1475000E+03.1735000E-01.1500081E-02
97 .1485000E+03.1414000E-01.1500254E-02.1514000E+03.1517000E-01.1500009E-02
98 .1544000E+03.1167000E-01.1499595E-02.1574000E+03.1087000E-01.1500060E-02
99 010000010000
100 .7230000+01 .1400000-00 .0000000-00 .0000000-00
101 010340
102 .1790000E+02.4519000E+01.1355700E+00.2080000E+02.3339000E+01.1001700E+00
103 .2580000E+02.1776000E+01.5328000E-01.2770000E+02.1429000E+01.4287000E-01
104 .2870000E+02.1127000E+01.3381000E-01.3070000E+02.9064000E+00.2719200E-01
105 .3570000E+02.3473000E+00.1041900E-01.3860000E+02.1886000E+00.5658000E-02
106 .4360000E+02.9908000E-01.2972400E-02.4660000E+02.7204000E-01.2161200E-02
107 .5160000E+02.6900000E-01.2070000E-02.5460000E+02.5854000E-01.1999726E-02
108 .5910000E+02.5952000E-01.1999872E-02.6210000E+02.6173000E-01.2000052E-02
109 .6700000E+02.7399000E-01.2219700E-02.7000000E+02.8620000E-01.2586000E-02
110 .7460000E+02.1088000E+00.3264000E-02.7750000E+02.1138000E+00.3414000E-02
111 .8270000E+02.1090000E+00.3270000E-02.8550000E+02.9458000E-01.2837400E-02
112 .9000000E+02.7417000E-01.2225100E-02.9300000E+02.5475000E-01.2000018E-02
113 .9800000E+02.3134000E-01.2000119E-02.1010000E+03.2495000E-01.1999992E-02
114 .1055000E+03.2159000E-01.2000098E-02.1085000E+03.2423000E-01.1999944E-02
115 .1134000E+03.3247000E-01.2000152E-02.1164000E+03.4041000E-01.1999891E-02
116 .1209000E+03.4188000E-01.2000189E-02.1239000E+03.4475000E-01.1999877E-02
117 .1289000E+03.4449000E-01.1999825E-02.1319000E+03.4192000E-01.2000003E-02
118 .1364000E+03.3739000E-01.1999991E-02.1394000E+03.3843000E-01.1999897E-02
119 .1443000E+03.2995000E-01.2000061E-02.1463000E+03.2530000E-01.1999965E-02
120 .1473000E+03.2545000E-01.2000116E-02.1493000E+03.2457000E-01.1999998E-02
121 .1542000E+03.1755000E-01.2000700E-02.1572000E+03.1532000E-01.1999260E-02
122 010000000000
123 .5800000+01 .1500000-00 .0000000-00 .0000000-00
124 .1000000-01 .1000000-01
125 0.000000000000

```

3.3.2 Input for the soft-rotator model

Input for the soft-rotator model is similar to that for the rigid-rotator model. So we have no need to repeat all the details that can be found by reading the input description for the rigid-rotator model. All the changes are found in the first 21 cards of the input shown below. So we decided to describe them, yet most of them have the same meanings for both models.

- Card 1 - some text information
- Card 2 - defines that a run with adjustment of optical potential parameters (**MEJOB=2**) for soft-rotator CC-model (**MEPOT=2**) will be organized, nuclear non-axial Hamiltonian with account of β and γ softness will be used to determine coupling (**MEHAM=5**); output will be the shortest (**MEPRI=0**); iteration method with wave functions from spherical calculations as zero approximation for coupled equations system solution will be used (**MESOL=3**); rigid hexadecapole deformations will be taken into account in the most common way (**MESHA=4**), with non-axial octupole deformations (**MESH0=2**) which are soft, symmetric and scaled by β_2 (**MEHA0=2**); energy dependence of optical potential in different channels caused by energy losses due to levels excitation will be taken into account in this run (**MEAPP=0**).
- Cards 3-5 -(Attention! these Cards do not present in input for rigid-rotator) parameters of nuclear Hamiltonian as described in Chapter IV
- Card 6 - defines that five levels (**NUR=5**) will be coupled; potential will be adjusted using experimental data at ten energy points simultaneously (**NST=10**); deformed optical potential will be expanded by derivatives up to the fourth power (**LAS=4**); waves with angular momentum greater than 30 will be ignored (**LLMA=30**); coupling of no more than 40 equations will be taken into account, other ignored (**NCMA=40**); no more than 40 J^π states ordered by increasing J will be taken into consideration (**NSMA=40**); coupled equations will be ordered one by one, by increasing angular momentum, total number no more than **NCMA=40** (**KODMA=0**).
- Cards 7,8 - ten energy points, as it was stated in Card 6, in which adjustment of optical potential to experimental data will be organized in the code.
- Card 9 -ten **MCHAE(I)** flags, in our case eight flags equal to 0, two flags - to 1 that means experimental data for incident neutrons in first eight energy points and for protons in the last two will be used for adjustment.
- Cards 10-14 - energies and quantum numbers of the five levels that should be coupled.
- Cards 15-20 - starting set of optical potential parameters, even in case where some parts of the potential strengths are equal to zero one must avoid setting radii and diffusenesses to zero.

Attention

As comparing with rigid-rotator input, the card related with radius deformations are not needed in this input (deformations are already determined in nuclear Hamiltonian parameter part of input).

- Cards 21... - NPJ(I) input and other are the same as explained in rigid-rotator input.

```
1 C-12 OCTUPOLE CALCULATION bet3=ksi*bet2
2 02020500000304020200 --> ME: JOB POT HAM CHA PRI SOL SHA SHO HAO (20I2)
3 0.42825E+01 0.27943E+01 0.11930E+00 0.32107E+00 0.16700E+00 0.11600E+00
4 0.14694E+00 0.21419E-03 0.52045E+00 0.25600E+00 0.21005E-01 0.88079E+00
5 0.35000E+00 0.22130E+00 0.00000E+00 0.17221E+01 0.00000E+00
6 0510040430404001 --> NUR NST NPD LAS LLMA NCMA NSMA KODMA
7 .2090000+02 .2080000+02 .2200000+02 .2200000+02 .2400000+02 .2600000+02
8 .2820000+02 .4030000+02 .4000000+02 .4948000+02
9 0000000000000000000101
10 .0000000-0000+101000000
11 .4440000+0104+101000000
12 .9640000+0106-101000001
13 .7650000+0100+101010000
14 .1780000+0204+102000000
15 .5078000+02-.3510000-00 .0000000+00 .1177700+01 .5380000-00 .3520000-02
16 .6940000+01-.1460000-00 .1130100+01 .3840000-00 .3630000-02 .4050000+01
17 -.4150000-01 .1143800+01 .3570000+00 .1840000-02 .1000000+01 .1000000+01
18 .0000000-00 .7300000+01 .1194200+01 .5820000-00 .0000000-02 .1000000+01
19 .1200000+021.00866520 .1240000+01 .6000000+01 .5000000-00 .2712000+02
20 -.047000 .124 .46
21 00010000001000000000000000000000000000000000000000000000000000000000000000000
22 010000030000
23 .1450000+01 .5000000-01 .0000000-00 .0000000-00
24 010134040432030332
25 0.10827E+02 0.10147E+01 0.87000E-02 0.13542E+02 0.90149E+00 0.70600E-02 ols020.9
26 0.16240E+02 0.80964E+00 0.65300E-02 0.18933E+02 0.71743E+00 0.60400E-02
27 0.21627E+02 0.62305E+00 0.55300E-02 0.27013E+02 0.44466E+00 0.40300E-02
28 0.32382E+02 0.29082E+00 0.31600E-02 0.37740E+02 0.17096E+00 0.23500E-02
29 0.43072E+02 0.96560E-01 0.15800E-02 0.48371E+02 0.50840E-01 0.95000E-03
30 0.53658E+02 0.28660E-01 0.85000E-03 0.58909E+02 0.19560E-01 0.70000E-03
31 0.64132E+02 0.20350E-01 0.67000E-03 0.69329E+02 0.20790E-01 0.66000E-03
32 0.74484E+02 0.23150E-01 0.67000E-03 0.79613E+02 0.23510E-01 0.66000E-03
33 0.84704E+02 0.21420E-01 0.64000E-03 0.89759E+02 0.18060E-01 0.49000E-03
34 0.94778E+02 0.13980E-01 0.44000E-03 0.99759E+02 0.11060E-01 0.42000E-03
35 0.10470E+03 0.83900E-02 0.37000E-03 0.10962E+03 0.65800E-02 0.24000E-03
36 0.11449E+03 0.50900E-02 0.23000E-03 0.11933E+03 0.40400E-02 0.19000E-03
37 0.12413E+03 0.30700E-02 0.19000E-03 0.12891E+03 0.25000E-02 0.17000E-03
38 0.13365E+03 0.20000E-02 0.18000E-03 0.13837E+03 0.21400E-02 0.18000E-03
39 0.14306E+03 0.15000E-02 0.20000E-03 0.14774E+03 0.10900E-02 0.19000E-03
40 0.15239E+03 0.95000E-03 0.26000E-03 0.15701E+03 0.61000E-03 0.31000E-03
41 0.16164E+03 0.39000E-03 0.25000E-03 0.16164E+03 0.39000E-03 0.25000E-03
42 0.13842E+02 0.29590E-02 0.47900E-03 0.16605E+02 0.23700E-02 0.42900E-03 ols720.9
43 0.19365E+02 0.14010E-02 0.41100E-03 0.22121E+02 0.15670E-02 0.30700E-03
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44 0.27621E+02 0.12020E-02 0.22400E-03 0.33102E+02 0.64200E-03 0.27400E-03
 45 0.38559E+02 0.63200E-03 0.22500E-03 0.43989E+02 0.70800E-03 0.21300E-03
 46 0.49388E+02 0.60200E-03 0.15300E-03 0.54755E+02 0.10990E-02 0.20400E-03
 47 0.60086E+02 0.80300E-03 0.18700E-03 0.65377E+02 0.46700E-03 0.18000E-03
 48 0.70628E+02 0.45100E-03 0.17000E-03 0.75836E+02 0.38700E-03 0.17800E-03
 49 0.81000E+02 0.31000E-03 0.15200E-03 0.86118E+02 0.12600E-03 0.15700E-03
 50 0.91189E+02 0.25700E-03 0.11400E-03 0.96212E+02 0.20400E-03 0.12500E-03
 51 0.10119E+03 0.12100E-03 0.11300E-03 0.10612E+03 0.18600E-03 0.12900E-03
 52 0.11100E+03 0.23100E-03 0.92000E-04 0.11584E+03 0.31000E-03 0.10500E-03
 53 0.12063E+03 0.17800E-03 0.75000E-04 0.12538E+03 0.27600E-03 0.82000E-04
 54 0.13009E+03 0.34700E-03 0.72000E-04 0.13475E+03 0.13900E-03 0.75000E-04
 55 0.13939E+03 0.13800E-03 0.73000E-04 0.14399E+03 0.21900E-03 0.78000E-04
 56 0.14856E+03 0.15000E-03 0.65000E-04 0.15310E+03 0.65000E-04 0.65000E-04
 57 0.15762E+03 0.12600E-03 0.86000E-04 0.16212E+03 0.71000E-04 0.82000E-04
 58 0.13974E+02 0.36200E-02 0.48200E-03 0.16762E+02 0.30630E-02 0.44900E-03 ols920.9
 59 0.19548E+02 0.27490E-02 0.43600E-03 0.22329E+02 0.29090E-02 0.31600E-03
 60 0.27879E+02 0.28430E-02 0.26000E-03 0.33406E+02 0.28360E-02 0.32000E-03
 61 0.38908E+02 0.29460E-02 0.28800E-03 0.44381E+02 0.30690E-02 0.26800E-03
 62 0.49820E+02 0.28310E-02 0.20000E-03 0.55223E+02 0.29870E-02 0.25400E-03
 63 0.60586E+02 0.29870E-02 0.24000E-03 0.65907E+02 0.28150E-02 0.24700E-03
 64 0.71182E+02 0.27230E-02 0.24100E-03 0.76411E+02 0.25810E-02 0.24700E-03
 65 0.81591E+02 0.31060E-02 0.23100E-03 0.86720E+02 0.27670E-02 0.23700E-03
 66 0.91798E+02 0.30100E-02 0.18700E-03 0.96825E+02 0.30220E-02 0.19600E-03
 67 0.10180E+03 0.27050E-02 0.18500E-03 0.10672E+03 0.22630E-02 0.18800E-03
 68 0.11159E+03 0.21140E-02 0.13100E-03 0.11641E+03 0.21620E-02 0.13600E-03
 69 0.12118E+03 0.17140E-02 0.11200E-03 0.12591E+03 0.17950E-02 0.11800E-03
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 75 .1450000+01 .5000000-01 .0000000-00 .0000000-00
 76 010130040425030326
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 78 .21431E+02 .63506E+00 .24767E-01 .25642E+02 .48591E+00 .99612E-02
 79 .34056E+02 .24781E+00 .53155E-02 .42462E+02 .10403E+00 .21108E-02
 80 .50991E+02 .38214E-01 .19203E-02 .55374E+02 .26647E-01 .15519E-02
 81 .59780E+02 .23198E-01 .14056E-02 .64097E+02 .20466E-01 .61357E-03
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 84 .92551E+02 .18764E-01 .14191E-02 .10042E+03 .14512E-01 .10182E-02
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 86 .12392E+03 .24200E-02 .43313E-03 .12771E+03 .24390E-02 .41402E-03
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 89 .15022E+03 .46400E-03 .15769E-03 .15221E+03 .86300E-03 .46975E-03
 90 .15421E+03 .52500E-03 .14702E-03 .15647E+03 .71300E-03 .51066E-03
 91 .15810E+03 .97000E-03 .42988E-03 .16187E+03 .85400E-03 .57722E-03
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 93 0.22200E+02 0.22930E-02 0.74700E-03 0.26400E+02 0.18480E-02 0.26400E-03
 94 0.34700E+02 0.85300E-03 0.22300E-03 0.43900E+02 0.17000E-03 0.94000E-04
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98  0.77300E+02 0.38500E-03 0.23600E-03 0.86100E+02 0.18100E-03 0.14100E-03
99  0.94400E+02 0.28600E-03 0.27800E-03 0.10210E+03 0.42000E-03 0.29800E-03
100 0.10970E+03 0.23600E-03 0.16600E-03 0.11780E+03 0.17400E-03 0.13700E-03
101 0.12550E+03 0.27500E-03 0.18000E-03 0.12910E+03 0.45100E-03 0.30000E-03
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105 0.14100E+02 0.32760E-02 0.17260E-02 0.18400E+02 0.27130E-02 0.50600E-03 men920.8
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108 0.53100E+02 0.27740E-02 0.33000E-03 0.57400E+02 0.29490E-02 0.40400E-03
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116 0.14000E+03 0.10040E-02 0.13400E-03 0.14780E+03 0.84700E-03 0.18700E-03
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119  .1450000+01 .5000000-01 .0000000-00 .0000000-00
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123 0.21627E+02 0.65454E+00 0.49500E-02 0.27013E+02 0.46760E+00 0.38500E-02
124 0.32382E+02 0.30358E+00 0.35600E-02 0.37740E+02 0.17945E+00 0.26300E-02
125 0.43072E+02 0.10025E+00 0.17200E-02 0.48371E+02 0.54440E-01 0.10900E-02
126 0.53658E+02 0.33320E-01 0.10700E-02 0.58909E+02 0.22580E-01 0.95000E-03
127 0.64132E+02 0.20900E-01 0.87000E-03 0.69329E+02 0.19100E-01 0.81000E-03
128 0.74484E+02 0.20420E-01 0.82000E-03 0.79613E+02 0.19540E-01 0.80000E-03
129 0.84704E+02 0.18790E-01 0.81000E-03 0.89759E+02 0.16610E-01 0.53000E-03
130 0.94778E+02 0.13730E-01 0.50000E-03 0.99759E+02 0.11710E-01 0.37000E-03
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132 0.11449E+03 0.42900E-02 0.25000E-03 0.11933E+03 0.31500E-02 0.17000E-03
133 0.12413E+03 0.24300E-02 0.17000E-03 0.12891E+03 0.15500E-02 0.16000E-03
134 0.13365E+03 0.15500E-02 0.17000E-03 0.13837E+03 0.14800E-02 0.17000E-03
135 0.14306E+03 0.17300E-02 0.18000E-03 0.14774E+03 0.16700E-02 0.21000E-03
136 0.15239E+03 0.15600E-02 0.16000E-03 0.15701E+03 0.14200E-02 0.18000E-03
137 0.16164E+03 0.12300E-02 0.15000E-03
138 0.13679E+02 0.28610E-01 0.90900E-03 0.16410E+02 0.27947E-01 0.87100E-03 ols422.0
139 0.19138E+02 0.25594E-01 0.82300E-03 0.21864E+02 0.25135E-01 0.58500E-03
140 0.27303E+02 0.22449E-01 0.53400E-03 0.32725E+02 0.19509E-01 0.70500E-03
141 0.38126E+02 0.16585E-01 0.62900E-03 0.43504E+02 0.14790E-01 0.49200E-03
142 0.48855E+02 0.12705E-01 0.39000E-03 0.54177E+02 0.10311E-01 0.49500E-03
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145 0.80269E+02 0.41650E-02 0.32900E-03 0.85373E+02 0.27250E-02 0.28500E-03
146 0.90435E+02 0.25900E-02 0.19000E-03 0.95456E+02 0.29830E-02 0.20300E-03
147 0.10044E+03 0.27680E-02 0.15700E-03 0.10537E+03 0.24710E-02 0.15000E-03

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 150 0.12947E+03 0.18790E-02 0.96000E-04 0.13418E+03 0.18280E-02 0.10100E-03
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 154 0.13821E+02 0.21610E-02 0.51700E-03 0.16579E+02 0.23790E-02 0.46400E-03 ols722.0
 155 0.19335E+02 0.13280E-02 0.42200E-03 0.22087E+02 0.17110E-02 0.30900E-03
 156 0.27579E+02 0.92100E-03 0.25600E-03 0.33052E+02 0.56400E-03 0.33700E-03
 157 0.38501E+02 0.39400E-03 0.29200E-03 0.43924E+02 0.61100E-03 0.23100E-03
 158 0.49318E+02 0.68100E-03 0.18300E-03 0.54678E+02 0.17600E-03 0.26700E-03
 159 0.60004E+02 0.74500E-03 0.22000E-03 0.65291E+02 0.25400E-03 0.25300E-03
 160 0.70538E+02-0.42000E-04 0.21000E-03 0.75742E+02 0.38900E-03 0.23900E-03
 161 0.80903E+02-0.23300E-03 0.18400E-03 0.86019E+02 0.31200E-03 0.23500E-03
 162 0.91089E+02 0.18000E-03 0.13500E-03 0.96112E+02 0.16100E-03 0.14000E-03
 163 0.10109E+03 0.17500E-03 0.91000E-04 0.10602E+03 0.10700E-03 0.97000E-04
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 165 0.12054E+03 0.28900E-03 0.69000E-04 0.12529E+03 0.13400E-03 0.76000E-04
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 167 0.13932E+03 0.18700E-03 0.79000E-04 0.14392E+03 0.19900E-03 0.85000E-04
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 172 0.27809E+02 0.23740E-02 0.28700E-03 0.33324E+02 0.25270E-02 0.39900E-03
 173 0.38814E+02 0.26760E-02 0.36800E-03 0.44275E+02 0.28330E-02 0.29700E-03
 174 0.49703E+02 0.31410E-02 0.24400E-03 0.55097E+02 0.27270E-02 0.35800E-03
 175 0.60451E+02 0.33480E-02 0.31500E-03 0.65764E+02 0.30300E-02 0.35400E-03
 176 0.71033E+02 0.29040E-02 0.31500E-03 0.76256E+02 0.33770E-02 0.34000E-03
 177 0.81431E+02 0.30670E-02 0.32100E-03 0.86558E+02 0.29080E-02 0.32800E-03
 178 0.91634E+02 0.30220E-02 0.21600E-03 0.96659E+02 0.29620E-02 0.22200E-03
 179 0.10163E+03 0.26610E-02 0.16300E-03 0.10656E+03 0.27250E-02 0.16400E-03
 180 0.11143E+03 0.25440E-02 0.15900E-03 0.11626E+03 0.22450E-02 0.16100E-03
 181 0.12103E+03 0.23600E-02 0.11600E-03 0.12576E+03 0.20130E-02 0.11500E-03
 182 0.13045E+03 0.19830E-02 0.12300E-03 0.13510E+03 0.16590E-02 0.12300E-03
 183 0.13970E+03 0.16430E-02 0.11500E-03 0.14427E+03 0.14870E-02 0.11000E-03
 184 0.14881E+03 0.14790E-02 0.10500E-03 0.15332E+03 0.12840E-02 0.10800E-03
 185 0.15781E+03 0.13140E-02 0.10300E-03 0.16227E+03 0.12230E-02 0.10200E-03
 186 010000040000
 187 .1450000+01 .5000000-01 .0000000-00 .0000000-00
 188 010140020238040439030339
 189 .13061E+02 .86476E+00 .21801E-01 .15115E+02 .81428E+00 .18044E-01 men0022.
 190 .17181E+02 .74606E+00 .16533E-01 .21330E+02 .62469E+00 .16536E-01
 191 .21336E+02 .60410E+00 .14674E-01 .25503E+02 .46699E+00 .11320E-01
 192 .29673E+02 .35089E+00 .80599E-02 .33843E+02 .24545E+00 .70518E-02
 193 .34240E+02 .24791E+00 .75290E-02 .38017E+02 .16345E+00 .48136E-02
 194 .42207E+02 .10366E+00 .30911E-02 .46268E+02 .67951E-01 .20976E-02
 195 .46444E+02 .63069E-01 .19949E-02 .50772E+02 .39783E-01 .11792E-02
 196 .55200E+02 .26802E-01 .92923E-03 .59591E+02 .22504E-01 .71585E-03
 197 .59646E+02 .22047E-01 .80516E-03 .63991E+02 .20314E-01 .78493E-03
 198 .70272E+02 .20348E-01 .79154E-03 .72317E+02 .20621E-01 .66606E-03
 199 .76394E+02 .20472E-01 .74088E-03 .84384E+02 .18677E-01 .60121E-03

200	.84436E+02	.18998E-01	.59958E-03	.92372E+02	.14307E-01	.55568E-03
201	.96210E+02	.12406E-01	.41573E-03	.10024E+03	.96070E-02	.50081E-03
202	.10807E+03	.59080E-02	.39383E-03	.10821E+03	.59880E-02	.21563E-03
203	.11586E+03	.31370E-02	.33183E-03	.11967E+03	.27050E-02	.12062E-03
204	.12375E+03	.20910E-02	.28304E-03	.13162E+03	.16290E-02	.83226E-04
205	.13212E+03	.16290E-02	.28980E-03	.13905E+03	.18000E-02	.21501E-03
206	.14252E+03	.16500E-02	.96657E-04	.14611E+03	.12710E-02	.21152E-03
207	.15435E+03	.47800E-03	.15745E-03	.15456E+03	.65200E-03	.49982E-04
208	.15877E+03	.14520E-02	.35427E-03	.16206E+03	.22250E-02	.62215E-03
209	0.13300E+02	0.32296E-01	0.17630E-02	0.15400E+02	0.32620E-01	0.13180E-02 men422.0
210	0.17600E+02	0.32090E-01	0.12600E-02	0.21800E+02	0.29980E-01	0.16900E-02
211	0.21900E+02	0.27528E-01	0.86200E-03	0.26100E+02	0.25181E-01	0.14190E-02
212	0.30400E+02	0.22323E-01	0.84100E-03	0.34600E+02	0.19100E-01	0.80000E-03
213	0.35200E+02	0.20383E-01	0.64700E-03	0.38900E+02	0.16974E-01	0.72500E-03
214	0.43200E+02	0.14420E-01	0.61100E-03	0.47400E+02	0.12353E-01	0.56000E-03
215	0.47400E+02	0.13659E-01	0.44300E-03	0.51700E+02	0.11003E-01	0.39600E-03
216	0.55900E+02	0.90850E-02	0.41300E-03	0.60000E+02	0.78010E-02	0.26600E-03
217	0.60100E+02	0.82240E-02	0.41400E-03	0.64300E+02	0.62560E-02	0.37700E-03
218	0.70500E+02	0.50720E-02	0.30900E-03	0.72500E+02	0.44210E-02	0.16600E-03
219	0.76700E+02	0.36040E-02	0.23200E-03	0.85000E+02	0.27000E-02	0.11100E-03
220	0.85100E+02	0.29990E-02	0.16600E-03	0.93300E+02	0.23350E-02	0.18800E-03
221	0.97200E+02	0.22410E-02	0.99000E-04	0.10120E+03	0.25840E-02	0.24800E-03
222	0.10900E+03	0.21800E-02	0.26100E-03	0.10930E+03	0.20460E-02	0.90000E-04
223	0.11680E+03	0.17230E-02	0.14600E-03	0.12060E+03	0.18820E-02	0.93000E-04
224	0.12450E+03	0.16000E-02	0.16100E-03	0.13210E+03	0.14920E-02	0.82000E-04
225	0.13260E+03	0.15750E-02	0.28900E-03	0.13960E+03	0.18570E-02	0.21800E-03
226	0.14330E+03	0.15480E-02	0.92000E-04	0.14690E+03	0.14880E-02	0.18500E-03
227	0.15430E+03	0.10910E-02	0.13300E-03	0.15440E+03	0.15890E-02	0.45200E-03
228	0.14100E+02	0.20190E-02	0.48500E-03	0.16100E+02	0.23590E-02	0.30000E-03 men722.0
229	0.18100E+02	0.16770E-02	0.22500E-03	0.21400E+02	0.13100E-02	0.17300E-03
230	0.22300E+02	0.95100E-03	0.26100E-03	0.26500E+02	0.10400E-02	0.27600E-03
231	0.30800E+02	0.11120E-02	0.29400E-03	0.34200E+02	0.34900E-03	0.98000E-04
232	0.34800E+02	0.36800E-03	0.94000E-04	0.35300E+02	0.69700E-03	0.13800E-03
233	0.39800E+02	0.48300E-03	0.13300E-03	0.44200E+02	0.69200E-03	0.11700E-03
234	0.46900E+02	0.38400E-03	0.86000E-04	0.48500E+02	0.68000E-03	0.11300E-03
235	0.52800E+02	0.77600E-03	0.99000E-04	0.56900E+02	0.59000E-03	0.99000E-04
236	0.59500E+02	0.60300E-03	0.97000E-04	0.61100E+02	0.59000E-03	0.99000E-04
237	0.65200E+02	0.74000E-03	0.98000E-04	0.71300E+02	0.70400E-03	0.10000E-03
238	0.71900E+02	0.52800E-03	0.92000E-04	0.77400E+02	0.44300E-03	0.75000E-04
239	0.84100E+02	0.21800E-03	0.66000E-04	0.85600E+02	0.29800E-03	0.55000E-04
240	0.93900E+02	0.22500E-03	0.55000E-04	0.96200E+02	0.75000E-04	0.59000E-04
241	0.10210E+03	0.27200E-03	0.68000E-04	0.10840E+03	0.22900E-03	0.71000E-04
242	0.11000E+03	0.21600E-03	0.66000E-04	0.11770E+03	0.35600E-03	0.77000E-04
243	0.11980E+03	0.43500E-03	0.76000E-04	0.11980E+03	0.20800E-03	0.72000E-04
244	0.13130E+03	0.33200E-03	0.86000E-04	0.13300E+03	0.33000E-03	0.76000E-04
245	0.13990E+03	0.27000E-03	0.65000E-04	0.14270E+03	0.32900E-03	0.89000E-04
246	0.14730E+03	0.32900E-03	0.65000E-04	0.15410E+03	0.18400E-03	0.66000E-04
247	0.15440E+03	0.26700E-03	0.74000E-04			
248	0.14500E+02	0.34740E-02	0.85600E-03	0.16600E+02	0.30880E-02	0.41700E-03 men9.22.0
249	0.18700E+02	0.29020E-02	0.55100E-03	0.21400E+02	0.23270E-02	0.12300E-03
250	0.22900E+02	0.27620E-02	0.41500E-03	0.27200E+02	0.23620E-02	0.37200E-03
251	0.31600E+02	0.26970E-02	0.26800E-03	0.34700E+02	0.23680E-02	0.11000E-03

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254 0.48800E+02 0.28400E-02 0.27600E-03 0.53100E+02 0.29350E-02 0.20400E-03
255 0.57300E+02 0.32890E-02 0.30700E-03 0.59400E+02 0.32070E-02 0.11700E-03
256 0.61600E+02 0.36610E-02 0.31200E-03 0.65800E+02 0.31140E-02 0.26800E-03
257 0.71800E+02 0.33430E-02 0.12200E-03 0.72100E+02 0.30340E-02 0.23500E-03
258 0.78300E+02 0.31700E-02 0.19800E-03 0.84000E+02 0.31410E-02 0.11300E-03
259 0.86500E+02 0.28370E-02 0.13400E-03 0.94500E+02 0.26370E-02 0.16800E-03
260 0.96100E+02 0.27980E-02 0.10900E-03 0.10250E+03 0.24070E-02 0.19400E-03
261 0.10830E+03 0.24020E-02 0.10200E-03 0.11030E+03 0.25160E-02 0.16600E-03
262 0.11800E+03 0.23790E-02 0.16200E-03 0.11970E+03 0.20390E-02 0.88000E-04
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266 0.15450E+03 0.98700E-03 0.14200E-03 0.15810E+03 0.81800E-03 0.16900E-03
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268 010000040000
269 .1450000+01 .5000000-01 .0000000-00 .0000000-00
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271 .13048E+02 .10126E+01 .25244E-01 .15103E+02 .92414E+00 .22512E-01 men24.0
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292 0.59800E+02 0.76340E-02 0.27000E-03 0.72400E+02 0.33280E-02 0.14100E-03
293 0.85000E+02 0.22030E-02 0.10000E-03 0.97100E+02 0.23380E-02 0.10200E-03
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298 0.21500E+02 0.71500E-03 0.12300E-03 0.22000E+02 0.16590E-02 0.67100E-03
299 0.26200E+02 0.17110E-02 0.61600E-03 0.30500E+02 0.11230E-02 0.31200E-03
300 0.34300E+02 0.19500E-03 0.82000E-04 0.34900E+02 0.51200E-03 0.32400E-03
301 0.39400E+02 0.34900E-03 0.25200E-03 0.43900E+02 0.81800E-03 0.24400E-03
302 0.46100E+02 0.32800E-03 0.21300E-03 0.47000E+02 0.28500E-03 0.77000E-04
303 0.52600E+02 0.46500E-03 0.12800E-03 0.58800E+02 0.51900E-03 0.21100E-03

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304 0.59200E+02 0.23300E-03 0.71000E-04 0.59500E+02 0.32100E-03 0.77000E-04
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 307 0.84200E+02 0.34000E-03 0.76000E-04 0.85800E+02 0.58600E-03 0.13300E-03
 308 0.93700E+02 0.38900E-03 0.12000E-03 0.96300E+02 0.18600E-03 0.54000E-04
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 366 0.13640E+03 0.79000E-04 0.85000E-04 0.14200E+03 0.14100E-03 0.98000E-04
 367 0.14740E+03 0.19600E-03 0.97000E-04 0.15280E+03 0.35800E-03 0.16800E-03
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 370 .31200E+02 .22060E-02 .36100E-03 .35600E+02 .25750E-02 .21800E-03
 371 .39900E+02 .27800E-02 .32400E-03 .44200E+02 .28290E-02 .34100E-03
 372 .50600E+02 .29530E-02 .43000E-03 .56900E+02 .30990E-02 .22700E-03
 373 .63200E+02 .25380E-02 .28100E-03 .69600E+02 .19990E-02 .23800E-03
 374 .75800E+02 .22750E-02 .17100E-03 .82000E+02 .18880E-02 .22300E-03
 375 .88000E+02 .17410E-02 .21900E-03 .94100E+02 .17080E-02 .24300E-03
 376 .10000E+03 .15650E-02 .14700E-03 .10600E+03 .15020E-02 .14000E-03
 377 .11180E+03 .11200E-02 .17300E-03 .11800E+03 .13300E-02 .19200E-03
 378 .12520E+03 .11910E-02 .14600E-03 .13070E+03 .10220E-02 .12800E-03
 379 .13630E+03 .67900E-03 .14400E-03 .14180E+03 .54200E-03 .11400E-03
 380 .14750E+03 .61300E-03 .12100E-03 .15300E+03 .56900E-03 .13500E-03
 381 .15830E+03 .69000E-03 .20600E-03
 382 010000030000
 383 .1350000+01 .5000000-01 .0000000-00 .0000000-00
 384 010113020213030313
 385 .2160000+02 .6750800+00 .8097600-01 .3240000+02 .3338900+00 .3997500-01
 386 .4310000+02 .6779000-01 .8276800-02 .5370000+02 .2986800-01 .3634700-02
 387 .6420000+02 .2494200-01 .3611400-02 .7450000+02 .1926700-01 .2369000-02
 388 .8480000+02 .1157400-01 .1473100-02 .9480000+02 .6296700-02 .7773100-03
 389 .1048000+03 .3745600-02 .4590300-03 .1145000+03 .2338500-02 .2974100-03
 390 .1242000+03 .1447200-02 .2074400-03 .1337000+03 .1181400-02 .2118100-03
 391 .1431000+03 .1034700-02 .1556600-03
 392 .2180000+02 .1976400-01 .4631500-02 .3270000+02 .1876900-01 .2898100-02
 393 .4340000+02 .1422500-01 .1998300-02 .5410000+02 .7314500-02 .1336600-02
 394 .6460000+02 .5535300-02 .7948000-03 .7500000+02 .2728400-02 .5170200-03
 395 .8520000+02 .2514500-02 .3073400-03 .9530000+02 .2233600-02 .4401100-03
 396 .1052000+03 .2250900-02 .2910900-03 .1150000+03 .1448300-02 .2057500-03
 397 .1246000+03 .1191000-02 .1800100-03 .1341000+03 .1064800-02 .1782800-03
 398 .1434000+03 .1073300-02 .1532000-03
 399 .2210000+02 .2857600-02 .1222000-02 .3300000+02 .4597900-02 .2176600-02
 400 .4390000+02 .3057300-02 .1442700-02 .5470000+02 .4606800-02 .2142600-02
 401 .6530000+02 .3703500-02 .1325700-02 .7570000+02 .1964200-02 .7158500-03
 402 .8600000+02 .1850700-02 .6716400-03 .9610000+02 .1094500-02 .3962500-03
 403 .1060000+03 .9346600-03 .3214700-03 .1157000+03 .6892500-03 .3333100-03
 404 .1253000+03 .9684100-03 .3443500-03 .1347000+03 .9070600-03 .4168800-03
 405 .1439000+03 .6470300-03 .2916300-03
 406 010000010000
 407 .1160000+01 .3000000-01 .0000000-00 .0000000-00

408 010116
 409 1.6300E+01 9.2830E-01 1.9300E-02 2.1710E+01 5.9330E-01 1.0200E-02 FIN040.3 0
 410 2.7110E+01 3.0170E-01 5.2800E-03 3.2500E+01 1.5490E-01 3.2100E-03
 411 3.7870E+01 6.2740E-02 2.0500E-03 4.3220E+01 2.4300E-02 1.3400E-03
 412 4.8540E+01 1.7520E-02 8.0900E-04 5.3830E+01 1.4680E-02 5.8700E-04
 413 5.9100E+01 8.8580E-03 3.6800E-04 6.4330E+01 9.0510E-03 3.3400E-04
 414 6.9530E+01 6.1060E-03 1.9100E-04 7.4700E+01 4.9520E-03 1.4500E-04
 415 7.9830E+01 2.8570E-03 1.1200E-04 8.4920E+01 1.7330E-03 8.0300E-05
 416 8.9980E+01 1.0280E-03 6.5800E-05 9.5000E+01 6.6210E-04 6.2700E-05
 417 000000040000
 418 .1060000+01 .3000000-00 .0000000-00 .0000000-00
 419 010139020239030338040439
 420 .1087000E+02.8570001E+00.1714000E-01.1358000E+02.8420001E+00.1684000E-01 blum 0+
 421 .2171000E+02.5330001E+00.1066000E-01.2441000E+02.4730000E+00.9460000E-02
 422 .3250000E+02.1770000E+00.3540000E-02.3519000E+02.1280000E+00.2560000E-02
 423 .4321000E+02.3440000E-01.1376000E-02.4588000E+02.2440000E-01.4880000E-03
 424 .5383000E+02.1180000E-01.3540000E-03.5647000E+02.1100000E-01.6600000E-03
 425 .6433000E+02.1010000E-01.2020000E-03.6693000E+02.9400000E-02.3760000E-03
 426 .7469000E+02.6910000E-02.2073000E-03.7726000E+02.5800000E-02.4060000E-03
 427 .8492000E+02.2890000E-02.8670001E-04.8745000E+02.2360000E-02.4720000E-04
 428 .9499000E+02.1270000E-02.5080000E-04.9749000E+02.1080000E-02.3240000E-04
 429 .1049100E+03.7300000E-03.2190000E-04.1073700E+03.7500000E-03.5250000E-04
 430 .1146800E+03.5400000E-03.2160000E-04.1195200E+03.4000000E-03.3200000E-04
 431 .1267000E+03.3300000E-03.2310000E-04.1290800E+03.3200000E-03.1280000E-04
 432 .1361700E+03.2200000E-03.1320000E-04.1385200E+03.2300000E-03.1380000E-04
 433 .1408600E+03.2300000E-03.2990000E-04.1432000E+03.2100000E-03.2100000E-04
 434 .1455300E+03.2100000E-03.5880000E-04.1478500E+03.2300000E-03.3220000E-04
 435 .1501700E+03.1800000E-03.1440000E-04.1524900E+03.2000000E-03.2600000E-04
 436 .1548000E+03.1400000E-03.2380000E-04.1571000E+03.2200000E-03.5280000E-04
 437 .1594000E+03.1700000E-03.6460000E-04.1617000E+03.1600000E-03.2400000E-04
 438 .1640000E+03.5000000E-04.2500000E-04.1662900E+03.8000001E-04.2800000E-04
 439 .1685800E+03.7000000E-04.2240000E-04
 440 .1092000E+02.1790000E-01.1611000E-02.1365000E+02.1580000E-01.1106000E-02 blum 2+
 441 .2182000E+02.1530000E-01.6120000E-03.2453000E+02.1620000E-01.6480001E-03
 442 .3266000E+02.1530000E-01.3060000E-03.3536000E+02.1430000E-01.2860000E-03
 443 .4342000E+02.1130000E-01.3390000E-03.4609000E+02.9900000E-02.2970000E-03
 444 .5407000E+02.6000000E-02.1800000E-03.5671000E+02.4600000E-02.4140000E-03
 445 .6460000E+02.2600000E-02.1040000E-03.6721000E+02.2100000E-02.1050000E-03
 446 .7499000E+02.1570000E-02.4710000E-04.7756000E+02.1350000E-02.4050000E-04
 447 .8523000E+02.1050000E-02.6300000E-04.8776000E+02.1270000E-02.7620000E-04
 448 .9531000E+02.8000000E-03.4800000E-04.9780000E+02.7600000E-03.6080000E-04
 449 .1002800E+03.6000000E-03.3000000E-04.1027600E+03.6100000E-03.4880000E-04
 450 .1052200E+03.4500000E-03.2250000E-04.1076800E+03.4100000E-03.4100000E-04
 451 .1101200E+03.3400000E-03.4080000E-04.1125600E+03.2800000E-03.6160000E-04
 452 .1149800E+03.2700000E-03.3240000E-04.1222000E+03.2300000E-03.2070000E-04
 453 .1245900E+03.2500000E-03.3250000E-04.1269700E+03.3300000E-03.5280001E-04
 454 .1293400E+03.3600000E-03.3240000E-04.1317000E+03.3600000E-03.3240000E-04
 455 .1340600E+03.4700000E-03.7990000E-04.1364000E+03.4700000E-03.7990000E-04
 456 .1387400E+03.5700000E-03.5130000E-04.1410700E+03.5600000E-03.1512000E-03
 457 .1434000E+03.6900000E-03.1518000E-03.1457200E+03.6800001E-03.2040000E-03
 458 .1480300E+03.9000000E-03.2520000E-03.1526400E+03.5800000E-03.5220000E-04
 459 .1572300E+03.5300000E-03.9010000E-04

```

460 .1375000E+02.1470000E-02.5145000E-03.1650000E+02.2310000E-02.6930000E-03 blum 3-
461 .1924000E+02.2090000E-02.2090000E-03.2198000E+02.1750000E-02.5075000E-03
462 .2471000E+02.1830000E-02.4392000E-03.2744000E+02.1880000E-02.4700000E-03
463 .3017000E+02.3070000E-02.4298000E-03.3289000E+02.2890000E-02.2023000E-03
464 .3560000E+02.3180000E-02.3180000E-03.3831000E+02.3620000E-02.3620000E-03
465 .4102000E+02.4000000E-02.8000000E-03.4371000E+02.3540000E-02.1416000E-03
466 .4640000E+02.3200000E-02.4800000E-03.4908000E+02.3380000E-02.3380000E-03
467 .5176000E+02.3910000E-02.7820001E-03.5442000E+02.3260000E-02.1630000E-03
468 .5708000E+02.2930000E-02.5860000E-03.5973000E+02.2790000E-02.2790000E-03
469 .6237000E+02.2970000E-02.5940000E-03.6500000E+02.2290000E-02.1603000E-03
470 .6762000E+02.2000000E-02.2000000E-03.7023000E+02.1830000E-02.2745000E-03
471 .7283000E+02.1880000E-02.4700000E-03.7543000E+02.1420000E-02.1420000E-03
472 .7801000E+02.1340000E-02.1340000E-03.8058000E+02.1270000E-02.1270000E-03
473 .8314000E+02.1450000E-02.1450000E-03.8568000E+02.1010000E-02.1010000E-03
474 .8822000E+02.9700001E-03.8730000E-04.9075000E+02.7200001E-03.1728000E-03
475 .9327000E+02.9900001E-03.9900000E-04.9577000E+02.6900000E-03.4140000E-04
476 .9826000E+02.6700000E-03.4020000E-04.1007500E+03.5800000E-03.6380000E-04
477 .1032200E+03.6900000E-03.4140000E-04.1056800E+03.6200000E-03.4960000E-04
478 .1081300E+03.5800000E-03.4060000E-04.1105700E+03.5000000E-03.4000000E-04 blum 02+
479 .1097000E+02.5970000E-02.2686500E-02.1371000E+02.1530000E-02.6120000E-03
480 .1645000E+02.2420000E-02.6050001E-03.1918000E+02.6100000E-03.2013000E-03
481 .2191000E+02.4300000E-03.2064000E-03.2464000E+02.3600000E-03.2052000E-03
482 .2736000E+02.3800000E-03.7220000E-04.3008000E+02.3400000E-03.6120000E-04
483 .3279000E+02.6800001E-03.1360000E-03.3550000E+02.6900000E-03.2070000E-03
484 .3820000E+02.6000000E-03.6000000E-04.4090000E+02.8500001E-03.3400000E-03
485 .4359000E+02.6700000E-03.7370000E-04.4627000E+02.5400000E-03.8100001E-04
486 .4895000E+02.5200000E-03.8320000E-04.5162000E+02.5400000E-03.1350000E-03
487 .5428000E+02.4300000E-03.5160000E-04.5693000E+02.3500000E-03.4200000E-04
488 .5957000E+02.3500000E-03.4200000E-04.6221000E+02.2900000E-03.7250000E-04
489 .6484000E+02.2900000E-03.3190000E-04.6745000E+02.2600000E-03.3120000E-04
490 .7006000E+02.3000000E-03.5100000E-04.7266000E+02.4300000E-03.6020000E-04
491 .7525000E+02.2500000E-03.7250000E-04.7782000E+02.2900000E-03.3190000E-04
492 .8039000E+02.2600000E-03.3120000E-04.8295000E+02.3300000E-03.4290000E-04
493 .8550000E+02.2400000E-03.3120000E-04.8803000E+02.2000000E-03.3000000E-04
494 .9056000E+02.2100000E-03.7980000E-04.9307000E+02.1400000E-03.7000000E-04
495 .9558000E+02.1400000E-03.1960000E-04.9807000E+02.1000000E-03.2000000E-04
496 .1005600E+03.1100000E-03.4950000E-04.1030300E+03.1300000E-03.1950000E-04
497 .1054900E+03.1000000E-03.2000000E-04.1079400E+03.6000000E-04.1980000E-04
498 .1103800E+03.6000000E-04.1980000E-04
499 000000030000
500 .9060000+00 .3000000-00 .0000000-00 .0000000-00
501 010140020240040426
502 .1088000E+02.7610000E+00.1065400E-01.1305000E+02.7590001E+00.1138500E-01 fan 0+ el
503 .1956000E+02.5360000E+00.8040000E-02.2172000E+02.4440000E+00.6660000E-02
504 .2821000E+02.2130000E+00.3195000E-02.3037000E+02.1570000E+00.2355000E-02
505 .3682000E+02.5370000E-01.9129001E-03.3896000E+02.3680000E-01.5520000E-03
506 .4537000E+02.1260000E-01.1890000E-03.4750000E+02.1020000E-01.1632000E-03
507 .5386000E+02.7560000E-02.1058400E-03.5597000E+02.7390000E-02.1404100E-03
508 .6227000E+02.5760001E-02.1094400E-03.6436000E+02.5200000E-02.9880000E-04
509 .7060000E+02.3230000E-02.6137000E-04.7267000E+02.2690000E-02.5111000E-04
510 .7473000E+02.2260000E-02.4294000E-04.7679000E+02.1820000E-02.3458000E-04
511 .7884000E+02.1510000E-02.2869000E-04.8088000E+02.1240000E-02.2108000E-04

```

512 .8292000E+02.1020000E-02.1938000E-04.8496000E+02.8870001E-03.1685300E-04
 513 .8698000E+02.7500000E-03.1425000E-04.8900000E+02.6540000E-03.1308000E-04
 514 .9102000E+02.5790000E-03.1100100E-04.9303000E+02.5100000E-03.1020000E-04
 515 .9702000E+02.4250000E-03.9350001E-05.1010000E+03.3530000E-03.6707000E-05
 516 .1049500E+03.2940000E-03.6174000E-05.1088800E+03.2470000E-03.5434000E-05
 517 .1127800E+03.1890000E-03.3969000E-05.1166600E+03.1570000E-03.3768000E-05
 518 .1205100E+03.1160000E-03.2552000E-05.1243500E+03.1010000E-03.3333000E-05
 519 .1281600E+03.7380000E-04.2583000E-05.1319500E+03.6790001E-04.2444400E-05
 520 .1357300E+03.6080000E-04.2249600E-05.1394800E+03.5060000E-04.1669800E-05
 521 .1432200E+03.4110000E-04.1315200E-05.1469400E+03.3630000E-04.1560900E-05
 522 .1092000E+02.1230000E-01.1968000E-03.1528000E+02.1120000E-01.2016000E-03 fan 2+
 523 .1746000E+02.1130000E-01.2034000E-03.2181000E+02.1140000E-01.2052000E-03
 524 .2398000E+02.1180000E-01.2124000E-03.2832000E+02.1210000E-01.2178000E-03
 525 .3264000E+02.1170000E-01.2106000E-03.3696000E+02.1050000E-01.1785000E-03
 526 .4126000E+02.8820000E-02.1499400E-03.4340000E+02.7690000E-02.1461100E-03
 527 .4767000E+02.5750000E-02.9775001E-04.5193000E+02.3000000E-02.5400000E-04
 528 .5405000E+02.3320000E-02.6640000E-04.5828000E+02.2280000E-02.4104000E-04
 529 .6248000E+02.1630000E-02.3097000E-04.6358000E+02.1440000E-02.2736000E-04
 530 .6875000E+02.1170000E-02.2223000E-04.7290000E+02.9970000E-03.2093700E-04
 531 .7496000E+02.9080000E-03.1997600E-04.7908000E+02.7110001E-03.1493100E-04
 532 .8316000E+02.6180000E-03.1297800E-04.8520000E+02.5650001E-03.1186500E-04
 533 .8925000E+02.4300000E-03.9890000E-05.9328000E+02.3280000E-03.7872000E-05
 534 .9528000E+02.3750000E-03.9000000E-05.9926000E+02.1980000E-03.4158000E-05
 535 .1032200E+03.1470000E-03.3528000E-05.1051900E+03.1240000E-03.2852000E-05
 536 .1091200E+03.9320000E-04.2050400E-05.1130100E+03.7820000E-04.1876800E-05
 537 .1149500E+03.7470000E-04.1942200E-05.1188100E+03.7400000E-04.1702000E-05
 538 .1245600E+03.7600000E-04.2660000E-05.1283600E+03.8150000E-04.2771000E-05
 539 .1321500E+03.1080000E-03.3672000E-05.1340300E+03.1290000E-03.4128000E-05
 540 .1377800E+03.1390000E-03.4448000E-05.1415200E+03.2030000E-03.6699000E-05
 541 .1433800E+03.1610000E-03.5152000E-05.1470900E+03.1530000E-03.5049000E-05
 542 .1094000E+02.2250000E-02.4500000E-04.1533000E+02.8780000E-03.1843800E-04 fan 02+
 543 .1970000E+02.4910000E-03.1031100E-04.2406000E+02.3460000E-03.8995999E-05
 544 .2841000E+02.5070001E-03.1318200E-04.3275000E+02.6470000E-03.1358700E-04
 545 .3707000E+02.7450000E-03.1564500E-04.4138000E+02.6960000E-03.1461600E-04
 546 .4568000E+02.5620000E-03.1011600E-04.4995000E+02.4350000E-03.1000500E-04
 547 .5421000E+02.2920000E-03.7592000E-05.5844000E+02.2480000E-03.5207999E-05
 548 .6266000E+02.2120000E-03.4876000E-05.6685000E+02.1940000E-03.4268000E-05
 549 .7102000E+02.1650000E-03.3795000E-05.7516000E+02.1460000E-03.3504000E-05
 550 .7928000E+02.1110000E-03.2886000E-05.8337000E+02.8440000E-04.2025600E-05
 551 .8743000E+02.6050000E-04.1875500E-05.9147000E+02.4190000E-04.1508400E-05
 552 .9548000E+02.2900000E-04.1334000E-05.9947000E+02.2570000E-04.9252000E-06
 553 .1034300E+03.2290000E-04.1167900E-05.1073600E+03.2110000E-04.8651000E-06
 554 .1112700E+03.1800000E-04.7200000E-06.1190000E+03.2000000E-04.8800001E-06
 555 .100000-02 .100000-02 .100000-02 .100000-02 .100000-02
 556 0.00000+00

3.4 Running the Code OPTMAN and Description of Output Files

As one runs the code it will first ask the name of the input file and, after it will be read, the code asks to give the name for the output file, in which all the calculated information will be stored. While running, two more files are created by the code: CR-SECT and TRANSME. File CR-SECT contains one line for each calculated energy. Line starts with a value of energy, and then follow total, reaction cross sections and level excitation cross sections ordered by their excitation energies. File TRANSME contains nucleon transmission coefficients for each calculated energy. For each energy, the first line indicates the energy and number of nucleon transmission coefficients, and then lines with transmissions follow ordered by growing angular momentum starting with $T_{l=0}$ by six in a line. As the calculated transmission coefficients are intended to be used for the code STAPRE [28] they are averaged over J dependence and depend only on angular momentum l . When one runs optical parameter adjustment files CR-SECT and TRANSME are organized but are blank. Below we present these files for a run in which optical calculations of ^{238}U cross sections are organized, as well as the appropriate input file

Input

```

1 U-238 TEST RIGID ROTATOR WC AT THE END
2 01010100000201000001 --> ME: JOB POT HAM CHA PRI SOL SHA SHO HAO APP (20I2)
3 030404081420404000 --> NUR NST NPD LAS MTET LLMA NCMA NSMA KODMA
4 .1500000-02 .1300000+01 .3400000+01 .1410000+02
5 00000000
6 .0000000+02 .5000000+01 .1000000+02 .2000000+01 .3000000+02 .4000000+02
7 .5000000+02 .6000000+02 .8000000+02 .1000000+03 .1200000+03 .1400000+03
8 .1600000+03 .1800000+03
9 .0000000-0000+100 --->EL(I) JO(I) NPO(I) KO(I), I=1,NUR
10 .4490000-0104+100
11 .1484000-0008+100
12 .4578000+02-.2690000-00 .0000000+001.2540000 .6430000-00 .1860000-02
13 .2700000+01 .4900000-001.238000000 .5750000-00 .7800000-03 .0000000+01
14 .0000000-00 .1238000+01 .5750000+00 .0000000-02 .1000000+01 .1000000+01
15 .0000000-00 .4650000+011.120000000 .6650000-00 .1000000-02 .1000000+01
16 .2380000+031.00866520 .1000000+01 .9200000+02 .5000000-00 .1000000+02
17 -.059 .211 .46
18 .2240000+00 .6000000-01

```

Output

```

1 U-238 TEST RIGID ROTATOR WC AT THE END
2 INTERACTION OF PARTICLE HAVING CHARGE = 0 AND SPIN = .50
3 WITH NUCLEI A= 238.0000000
4 COUPLED CHANNELS METHOD
5
6 HAMILTONN-A RV POTENTIAL EXPANDED BY YLO
7
8 NUMBER OF COUPLED LEVELS 3 NPD = 4
9 NUMBER OF TERMS IN POTENTIAL EXPANSION 8
10
11
12 ENERGY LEVEL'S SPIN PARITY BAND
13
14 1 .0000000E+00 0 1 0
15 2 .4490000E-01 4 1 0
16 3 .1484000E+00 8 1 0
17

```

```

18          POTENTIAL  PARAMETERS   V(R)
19
20  VR0=45.7800    VR1= -.2690    VR2= .0000    RR= 1.2540    AR0= .6430    AR1= .0019
21  WD0= 2.7000    WD1= .4900     RD= 1.2380    AD0= .5750    AD1= .0008
22  WC0= .0000    WC1= .0000     RC= 1.2380    AC0= .5750    AC1= .0000
23                           RW= 1.0000    AW0= 1.0000    AW1= .0000
24  VS0= 4.6500     RS= 1.1200    AS0= .6650    AS1= .0010
25  ALF= 1.0000    ANEU= 1.0087    RZ= 1.0000
26  BNDC=10.0000    WDA1= -.0590    WCA1= .2110    CCOUL= .4600
27
28          NUCLEUS CHARGE 92.0000
29
30          NPD      DEFORMATION PARAMETER VALUES
31          2           .2240
32          4           .0600
33
34
35  ORB. MOMENT      TRANSITIONS        SR          SI
36
37          0           .0274944277    .9728834643    -.1612555029
38          1           .0002312476    .9998843674    -.0000631930
39          2           .0000000525    .3999999738    -.0000000514
40          3           .0000000000    .0000000000    .0000000000
41          4           .0000000000    .0000000000    .0000000000
42          5           .0000000000    .0000000000    .0000000000
43          6           .0000000000    .0000000000    .0000000000
44          ANGULAR DISTRIBUTIONS OF SCATTERED PARTICLES
45
46          .000E+00    .934E+00
47          .500E+01    .934E+00
48          .100E+02    .934E+00
49          .200E+01    .934E+00
50          .300E+02    .934E+00
51          .400E+02    .933E+00
52          .500E+02    .933E+00
53          .600E+02    .933E+00
54          .800E+02    .932E+00
55          .100E+03    .931E+00
56          .120E+03    .930E+00
57          .140E+03    .929E+00
58          .160E+03    .929E+00
59          .180E+03    .929E+00
60
61          LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS
62          ANGULAR DISTRIBUTIONS
63          .9313077E+00    .9282733E-03    .1345119E-05    .5650901E-09
64
65  NEUTRON ENERGY = .001500
66  TOTAL CR-SECT.=24.040847
67  REACTION CR-SECT. =12.337688
68
69          NMAX      CR-SECT. OF LEVEL EXCITATION
70          1           11.703159
71
72          STRENGTH FUNCTIONS
73  SF0= .1129846E-03    SF1= .1875807E-03    SF2= .7497614E-04
74
75
76  ORB. MOMENT      TRANSITIONS        SR          SI
77
78          0           .5407706876    -.0548264359    .5867665579
79          1           .7776263691    .1427060007    -.3224574828
80          2           .3579688613    .5832699114    -.4852868006
81          3           .2657438486    .8426269898    .0247077607
82          4           .0197175826    .9889082058    .0015455535
83          5           .0023559842    .9987392524    .0005148431
84          6           .0000614104    .9999686311    .0000448413
85          7           .0000006613    .4666663337    .0000005022
86          8           .0000000000    .0000000000    .0000000000
87          9           .0000000000    .0000000000    .0000000000
88          ANGULAR DISTRIBUTIONS OF SCATTERED PARTICLES
89

```

```

90   .000E+00   .220E+01   .102E-01   .178E-01
91   .500E+01   .216E+01   .104E-01   .178E-01
92   .100E+02   .204E+01   .111E-01   .179E-01
93   .200E+01   .220E+01   .103E-01   .178E-01
94   .300E+02   .110E+01   .201E-01   .181E-01
95   .400E+02   .614E+00   .284E-01   .181E-01
96   .500E+02   .274E+00   .363E-01   .179E-01
97   .600E+02   .104E+00   .404E-01   .171E-01
98   .800E+02   .930E-01   .332E-01   .132E-01
99   .100E+03   .146E+00   .201E-01   .735E-02
100  .120E+03   .847E-01   .182E-01   .299E-02
101  .140E+03   .778E-02   .232E-01   .157E-02
102  .160E+03   .198E-01   .299E-01   .141E-02
103  .180E+03   .513E-01   .341E-01   .140E-02
104
105      LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS
106          ANGULAR DISTRIBUTIONS
107  .2496442E+00   .1535664E+00   .9749604E-01   .7489508E-01   .3993361E-01   .7844980E-02   .2282470E-02   .2850742E-03
108  .3832869E-04   .3158323E-05   .2126454E-06   .1104856E-07   .3680770E-09   .5395040E-11
109
110      LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS
111          ANGULAR DISTRIBUTIONS
112  .2663852E-01   .1513261E-02   -.6723583E-03   -.2797437E-02   -.4782439E-03   .2914185E-03   .2302848E-03   -.5597154E-05
113  .1039405E-04   -.1614099E-06   .6844667E-07   .4501489E-09   .1029445E-09   .8716127E-12
114
115      LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS
116          ANGULAR DISTRIBUTIONS
117  .1003045E-01   .3676970E-02   -.8963797E-04   -.4822031E-03   .1120421E-04   .5374686E-04   -.6612278E-05   -.2404662E-05
118  .6380974E-06   -.7758602E-07   .5645249E-08   -.2312791E-09   .7529014E-11   -.5106472E-13
119
120  NEUTRON ENERGY = 1.300000
121  TOTAL CR-SECT.= 6.995650
122  REACTION CR-SECT. = 3.397733
123
124  NMAX          CR-SECT. OF LEVEL EXCITATION
125    1             3.137122
126    2             .334750
127    3             .126046
128
129          STRENGTH FUNCTIONS
130  SF0=  .7548515E-04   SF1=  .1331453E-03   SF2=  .1070318E-03
131
132
133  ORB. MOMENT     TRANSITIONS          SR          SI
134
135    0             .5577102229   .3311094193   -.4525202453
136    1             .7180265763   -.1349644986   -.1783473512
137    2             .5177070869   -.4358932210   -.4223075069
138    3             .8383433458   .1160479471   -.0994900230
139    4             .3255665839   .7696604477   -.0991316374
140    5             .1765134409   .8999672901   -.0156440174
141    6             .0181542416   .9895029843   .0061002693
142    7             .0008527476   .9995689311   .0006949676
143    8             .0000563058   .4705590569   .0000296323
144    9             .0000000000   .0000000000   .0000000000
145   10             .0000000000   .0000000000   .0000000000
146   11             .0000000000   .0000000000   .0000000000
147   12             .0000000000   .0000000000   .0000000000
148   13             .0000000000   .0000000000   .0000000000
149          ANGULAR DISTRIBUTIONS OF SCATTERED PARTICLES
150
151  .000E+00   .697E+01   .942E-01   .249E-01
152  .500E+01   .671E+01   .919E-01   .248E-01
153  .100E+02   .600E+01   .854E-01   .245E-01
154  .200E+01   .693E+01   .938E-01   .249E-01
155  .300E+02   .159E+01   .517E-01   .215E-01
156  .400E+02   .366E+00   .430E-01   .194E-01
157  .500E+02   .109E-01   .384E-01   .176E-01
158  .600E+02   .443E-01   .378E-01   .163E-01
159  .800E+02   .115E+00   .421E-01   .143E-01
160  .100E+03   .336E-01   .259E-01   .137E-01
161  .120E+03   .176E-02   .200E-01   .982E-02

```

162 .140E+03 .168E-01 .358E-01 .374E-02
 163 .160E+03 .414E-01 .126E-01 .112E-02
 164 .180E+03 .668E-01 .120E-02 .647E-03
 165
 166 LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS
 167 ANGULAR DISTRIBUTIONS
 168 .3401660E+00 .2815885E+00 .2297020E+00 .1794673E+00 .1404215E+00 .9132186E-01 .4828161E-01 .2043379E-01
 169 .7614475E-02 .2018063E-02 .4245268E-03 .6579814E-04 .7361614E-05 .6818135E-06 .5877842E-07 .2563544E-08
 170
 171 LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS
 172 ANGULAR DISTRIBUTIONS
 173 .3450456E-01 .5984823E-02 .1397793E-02 .7913153E-03 .5772249E-03 .2126130E-02 -.6813597E-03 .2144054E-04
 174 .3925361E-03 -.3310421E-04 .8804384E-04 -.2451962E-05 .2564283E-05 .1035521E-06 .2038266E-07 .1274667E-08
 175
 176 LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS
 177 ANGULAR DISTRIBUTIONS
 178 .1294502E-01 .3230753E-02 -.3510258E-03 .5134243E-03 .1399794E-03 -.1253763E-03 .5809133E-04 .2133412E-04
 179 -.3288489E-04 -.4978319E-05 .5146703E-05 -.8319955E-06 .2781706E-06 .2626972E-08 .1908389E-08 .8538932E-10
 180
 181 NEUTRON ENERGY = 3.400000
 182 TOTAL CR-SECT.= 8.016514
 183 REACTION CR-SECT. = 3.145592
 184
 185 NMAX CR-SECT. OF LEVEL EXCITATION
 186 1 4.274653
 187 2 .433697
 188 3 .162672
 189
 190 STRENGTH FUNCTIONS
 191 SF0= .4813813E-04 SF1= .6734553E-04 SF2= .5931979E-04
 192
 193
 194 ORB. MOMENT TRANSITIONS SR SI
 195
 196 0 .7949535915 .3364793649 .0796669607
 197 1 .8377749013 .3019397626 .1073973854
 198 2 .8059901123 .3120428342 -.0822787726
 199 3 .8276205489 .3213141085 -.1252040668
 200 4 .8627073763 .0426292809 -.2240325128
 201 5 .7766346757 -.2092960992 -.3356698981
 202 6 .8934161712 -.1162993629 -.1963532015
 203 7 .7776847532 .3680435927 .0267996061
 204 8 .4542675005 .7279876681 .0247170121
 205 9 .2055163621 .8851603870 .0382070450
 206 10 .0447868491 .9758354205 .0266085430
 207 11 .0061470419 .9967785663 .0062938933
 208 12 .0009670287 .9995013417 .0013325396
 209 13 .0000675948 .4814471772 .0001107500
 210 14 .0000000000 .0000000000 .0000000000
 211 15 .0000000000 .0000000000 .0000000000
 212 16 .0000000000 .0000000000 .0000000000
 213 17 .0000000000 .0000000000 .0000000000
 214 18 .0000000000 .0000000000 .0000000000
 215 19 .0000000000 .0000000000 .0000000000
 216 ANGULAR DISTRIBUTIONS OF SCATTERED PARTICLES
 217
 218 .000E+00 .155E+02 .870E-01 .129E-01
 219 .500E+01 .134E+02 .758E-01 .124E-01
 220 .100E+02 .857E+01 .579E-01 .112E-01
 221 .200E+01 .151E+02 .850E-01 .128E-01
 222 .300E+02 .238E+00 .513E-01 .801E-02
 223 .400E+02 .359E+00 .286E-01 .656E-02
 224 .500E+02 .280E-01 .215E-01 .384E-02
 225 .600E+02 .548E-01 .161E-01 .338E-02
 226 .800E+02 .478E-02 .885E-02 .202E-02
 227 .100E+03 .955E-02 .662E-02 .140E-02
 228 .120E+03 .173E-02 .352E-02 .106E-02
 229 .140E+03 .157E-02 .216E-02 .178E-02
 230 .160E+03 .136E-02 .445E-02 .657E-03
 231 .180E+03 .401E-02 .370E-03 .186E-04
 232
 233 LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS

```

234          ANGULAR DISTRIBUTIONS
235 .2169721E+00 .1993133E+00 .1763675E+00 .1544290E+00 .1356657E+00 .1198747E+00 .1065129E+00 .9442640E-01
236 .8322722E-01 .7232104E-01 .6139694E-01 .4893149E-01 .3501097E-01 .2210825E-01 .1229202E-01 .5999121E-02
237 .2580793E-02 .9841503E-03 .3348526E-03 .1044880E-03 .2939878E-04 .7601317E-05 .1647692E-05 .2952810E-06
238 .4040170E-07 .3856037E-08

239          LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS
240          ANGULAR DISTRIBUTIONS
241 .1391306E-01 .7157487E-02 .3416861E-02 .1530038E-02 .8179860E-03 .3074620E-03 -.4655379E-05 -.1938243E-03
242 -.3159855E-03 -.2323154E-03 -.1376489E-03 .7628150E-04 .4508407E-05 .4777175E-04 .1574431E-03 .1986169E-03
243 .1900428E-03 .1336121E-03 .6119289E-04 .2684775E-04 .9372812E-05 .2862068E-05 .7188029E-06 .1491447E-06
244 .2339039E-07 .2453030E-08

245          LEGANDR. COEFFICIENTS FOR SCATTERED NEUTRONS
246          ANGULAR DISTRIBUTIONS
247 .2788973E-02 .1099205E-02 .5225680E-03 .2324250E-03 .4406615E-04 .5158041E-04 -.3723558E-04 .1358247E-04
248 -.8883187E-05 .1031904E-04 .4726963E-04 .2091378E-04 .2793833E-04 .1379010E-04 -.1118524E-04 -.1287525E-04
249 -.3910168E-05 .7840165E-06 .5420030E-06 .1134484E-05 .5378902E-06 .2108293E-06 .6091845E-07 .1397836E-07
250 .2664912E-08 .3048388E-09

251          NEUTRON ENERGY =14.10000
252          TOTAL CR-SECT.= 5.984123
253          REACTION CR-SECT. = 3.047687

254          NMAX          CR-SECT. OF LEVEL EXCITATION
255          1              2.726552
256          2              .174837
257          3              .035047

258          STRENGTH FUNCTIONS
259          SF0= .3369398E-04      SF1= .3625086E-04      SF2= .3643721E-04

```

CR-SECT

```

1 1.50000E-03 2.40408E+01 1.23377E+01 1.17032E+01
2 1.30000E+00 6.99565E+00 3.39773E+00 3.13712E+00 3.34750E-01 1.26046E-01
3 3.40000E+00 8.01651E+00 3.14559E+00 4.27465E+00 4.33597E-01 1.62672E-01
4 1.41000E+01 5.98412E+00 3.04769E+00 2.72655E+00 1.74837E-01 3.50473E-02

```

TRANSME

```

1 .150000E-02 7
2 .02749443 .00023125 .00000005 .00000000 .00000000 .00000000
3 .00000000
4 .130000E+01 10
5 .54077069 .77762637 .35796886 .26574385 .01971758 .00235598
6 .00006141 .00000066 .00000000 .00000000
7 .340000E+01 14
8 .55771022 .71802658 .51770709 .83834335 .32556658 .17651344
9 .01815424 .00085275 .00005631 .00000000 .00000000 .00000000
10 .00000000 .00000000
11 .141000E+02 20
12 .79495359 .83777490 .80599011 .82762055 .86270738 .77663468
13 .89341617 .77768475 .45426750 .20551636 .04478685 .00614704
14 .00096703 .00006759 .00000000 .00000000 .00000000 .00000000
15 .00000000 .00000000

```

4 Program SHEMMAN

As was mentioned before, the CC-calculations with coupling built on the soft-rotator model are self-consistent, as parameters of non-axial soft nuclear Hamiltonian, which determine coupling, are first tested to predict collective levels of the nucleus. A code SHEMMAN adjusts such parameters comparing experimental and calculated levels. It uses the same search procedure as OPTMAN, but the χ^2 function is now the sum of squares of the calculated and experimental level energy differences divided by the squares of experimental energies. Here we describe input for nuclear Hamiltonian parameters adjustment using SHEMMAN code.

4.1 Input Data

Input data of SHEMMAN is described here. Data has the card image form. Units of the data are MeV.

- Card 1 - Any text information that identifies current calculations
- Card 2 - FORMAT(25I2)

NPRI, NUR, MEHAM, MESHA, MESH0, MEHA0

Switches describing adjustment and form of nuclear Hamiltonian

- NPRI - detailed output including a comparison of the experimental and calculated level energies; nuclear Hamiltonian parameters and the χ^2 value are written at each NPRI iteration during the search;
- NUR - number of experimental levels adjusted ($NUR \leq 20$);
- MEHAM, MESHA, MESH0, MEHA0 - switches determining nuclear Hamiltonian model, with the meaning described in OPTMAN code input

- Cards 3-5 FORMAT(6E12.7)

Parameters of non-axial nuclear Hamiltonian

HW, AMBO, AMGO, GAMO, BET0, BET4 - Card 3

BB42, GAMG, DELG, BET3, ETO, AMU0 - Card 4

HWO, BB32, GAMDE, DPAR, GHAPE - Card 5

The input format, sequence and meaning of the parameters are the same as in OPTMAN code - see description of OPTMAN input for details.

- Cards 6a,6b, ...FORMAT(E10.4,6I2)

Characteristics of nuclear levels

(ES(I), JU(I), NPI(I), NTU(I), NNB(I), NNG(I), NNO(I), I=1,NUR)

- ES(I) - energy of experimental level;
- JU(I) - spin of level (not multiplied by 2);

- **NPI(I)** - parity of level =+1 -for positive,=-1 -for negative;
- **NTU(I)** - the number of rotational energy solution τ ;
- **NNB(I)** - the number of β_2 oscillation function solution n_{β_2} ;
- **NNG(I)** - the number of γ oscillation function solution n_{γ} ;
- **NNO(I)** - the number of β_3 oscillation function solution n_{β_3} ;

meaning of these parameters are also described in OPTMAN input

- Card 7 - **FORMAT(25I2)**

Input of flags that determine which parameters of nuclear Hamiltonian will be adjusted, if **NPJ(I)=1**
the chosen parameter will be adjusted

(**NPJ(I),I=1,16**) Card 7

- **NPJ(1)** - flag for energy scale factor $\hbar\omega_0$ HW;
- **NPJ(2)** - flag for nuclear softness $\mu_{\beta_{20}}$ AMBO;
- **NPJ(3)** - flag for nuclear softness μ_{γ_0} AMGO;
- **NPJ(4)** - flag for equilibrium non-axiality γ_0 GAMO;
- **NPJ(5)** - flag for a_{42} BB42;
- **NPJ(6)** - flag for non-axiality γ_4 GAMG;
- **NPJ(7)** - flag for non-axiality δ_4 DELG;
- **NPJ(8)** - flag for β_3 deformation ϵ_0 if HEHAO=2, β_{30} if HEHAO=3 BET3;
- **NPJ(9)** - flag for β_3 non-axiality η ETO;
- **NPJ(10)** - flag for β_3 softness μ_ϵ AMUO;
- **NPJ(11)** - flag for $\hbar\omega_0$ energy scale factor of octupole oscillations $\hbar\omega_\epsilon$, used if MEHAO=1 HWO;
- **NPJ(12)** - flag for a_{32} BB32;
- **NPJ(13)** - flag not in use;
- **NPJ(14)** - flag for energy splitting parameter δ_n DPAR;
- **NPJ(15)** - flag no in use;
- **NPJ(16)** - flag awaking γ transition calculations between levels (if this flag =1, other flags are ignored);

- Cards 8a,8b **FORMAT(8D10.4)**

(**EP(I), I=1,NV**)

- **EP(I)** - absolute accuracy for parameter with I^{th} flag=1, NV is equal to the number of flags=1;

This is the last card in input.

4.2 Examples

Here we present input for ^{62}Ni nuclear Hamiltonian adjustment

```

1 GAMBET=> NI-62    BET3=BETO*KSI
2 200705010202
3 0.13346E+01 0.16260E+01 0.62668E+00 0.30681E+00 0.10280E+00 0.14883E-01
4 0.11933E-01 0.11365E+00 0.69740E+00 0.57435E+00 0.94804E-01 0.25984E+00
5 0.35000E+00 0.10000E-03 0.00000E+00 0.64753E+01 0.00000E+00
6 0.00000-0000+101000000 iLEVELS OF Ni-62
7 1.17280-0002+101000000 ES(I),JU(I),NPI(I),NTU(I),NNB(I),NNG(I),NNO(I)
8 2.04840-0000+101010000
9 2.33610+0004+101000000
10 3.55270+0003+101000000
11 3.15770-0002+102000000
12 3.51850-0002+101010000
13 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14 1.0000-05

```

Here we present output file for ^{62}Ni nuclear Hamiltonian adjustment

```

1 GAMBET=> NI-62    BET3=BETO*KSI
2 .11728D+01 .11301D+01 .36419D-01 2 1 0 0 0 .24D+01 .31D+00 .00D+00 .23D+01 .83D-02 .00D+00
3 .20484D+01 .22176D+01 -.82599D-01 0 1 1 0 0 .00D+00 .31D+00 .00D+00 .10D+01 .83D-02 .00D+00
4 .23361D+01 .24250D+01 -.38045D-01 4 1 0 0 0 .77D+01 .31D+00 .00D+00 .30D+01 .83D-02 .00D+00
5 .35527D+01 .35381D+01 .41157D-02 3 1 0 0 0 .14D+02 .31D+00 .00D+00 .34D+01 .83D-02 .00D+00
6 .31577D+01 .31577D+01 .47452D-05 2 2 0 0 0 .12D+02 .31D+00 .00D+00 .33D+01 .83D-02 .00D+00
7 .35185D+01 .36217D+01 -.29320D-01 2 1 1 0 0 .24D+01 .31D+00 .00D+00 .23D+01 .83D-02 .00D+00
8 0 .174547962452915D-02
9 .1334600D+01
10 .11728D+01 .11301D+01 .36412D-01 2 1 0 0 0 .24D+01 .31D+00 .00D+00 .23D+01 .83D-02 .00D+00
11 .20484D+01 .22176D+01 -.82607D-01 0 1 1 0 0 .00D+00 .31D+00 .00D+00 .10D+01 .83D-02 .00D+00
12 .23361D+01 .24250D+01 -.38052D-01 4 1 0 0 0 .77D+01 .31D+00 .00D+00 .30D+01 .83D-02 .00D+00
13 .35527D+01 .35381D+01 .41083D-02 3 1 0 0 0 .14D+02 .31D+00 .00D+00 .34D+01 .83D-02 .00D+00
14 .31577D+01 .31577D+01 -.27476D-05 2 2 0 0 0 .12D+02 .31D+00 .00D+00 .33D+01 .83D-02 .00D+00
15 .35185D+01 .36217D+01 -.29328D-01 2 1 1 0 0 .24D+01 .31D+00 .00D+00 .23D+01 .83D-02 .00D+00
16 .11728D+01 .10807D+01 .78494D-01 2 1 0 0 0 .24D+01 .31D+00 .00D+00 .23D+01 .83D-02 .00D+00
17 .20484D+01 .21208D+01 -.35326D-01 0 1 1 0 0 .00D+00 .31D+00 .00D+00 .10D+01 .83D-02 .00D+00
18 .23361D+01 .23191D+01 .72825D-02 4 1 0 0 0 .77D+01 .31D+00 .00D+00 .30D+01 .83D-02 .00D+00
19 .35527D+01 .33836D+01 .47602D-01 3 1 0 0 0 .14D+02 .31D+00 .00D+00 .34D+01 .83D-02 .00D+00
20 .31577D+01 .30198D+01 .43670D-01 2 2 0 0 0 .12D+02 .31D+00 .00D+00 .33D+01 .83D-02 .00D+00
21 .35185D+01 .34635D+01 .15626D-01 2 1 1 0 0 .24D+01 .31D+00 .00D+00 .23D+01 .83D-02 .00D+00
22 .11728D+01 .11202D+01 .44834D-01 2 1 0 0 0 .24D+01 .31D+00 .00D+00 .23D+01 .83D-02 .00D+00
23 .20484D+01 .21982D+01 -.73144D-01 0 1 1 0 0 .00D+00 .31D+00 .00D+00 .10D+01 .83D-02 .00D+00
24 .23361D+01 .24038D+01 -.28979D-01 4 1 0 0 0 .77D+01 .31D+00 .00D+00 .30D+01 .83D-02 .00D+00
25 .35527D+01 .35072D+01 .12813D-01 3 1 0 0 0 .14D+02 .31D+00 .00D+00 .34D+01 .83D-02 .00D+00
26 .31577D+01 .31301D+01 .87379D-02 2 2 0 0 0 .12D+02 .31D+00 .00D+00 .33D+01 .83D-02 .00D+00
27 .35185D+01 .35900D+01 -.20331D-01 2 1 1 0 0 .24D+01 .31D+00 .00D+00 .23D+01 .83D-02 .00D+00
28 1 .147563509171138D-02
29 .1322945D+01
30 .13229E+01 .16260E+01 .62668E+00 .30681E+00 .10280E+00 .14883E-01
31 .11933E-01 .11365E+00 .69740E+00 .57435E+00 .94804E-01 .25984E+00
32 .35000E+00 .10000E-03 .00000E+00 .64753E+01 .00000E+00
33 1 .136415746767726D-02
34 .1311289D+01
35 .13113E+01 .16260E+01 .62668E+00 .30681E+00 .10280E+00 .14883E-01
36 .11933E-01 .11365E+00 .69740E+00 .57435E+00 .94804E-01 .25984E+00
37 .35000E+00 .10000E-03 .00000E+00 .64753E+01 .00000E+00
38 1 .136086597192448D-02
39 .1308958D+01
40 .13090E+01 .16260E+01 .62668E+00 .30681E+00 .10280E+00 .14883E-01
41 .11933E-01 .11365E+00 .69740E+00 .57435E+00 .94804E-01 .25984E+00
42 .35000E+00 .10000E-03 .00000E+00 .64753E+01 .00000E+00

```

4.3 Running the SHEMMAN code

The code will first ask the name of input file, then code will suggest to give the name of the output file. While running, after each adjustment, χ^2 value, best Hamiltonian parameters and Hamiltonian parameters organized in the format necessary for OPTMAN code, will be given. After each NPRI adjustments detailed information about current search is outputted. In case where all NPJ(I)=0, initial information including χ^2 and level energies is printed and the code stops.

5 Conclusions

Programs OPTMAN and SHEMMAN are now installed on computers (PC and UNIX Work Station) at JAERI Nuclear Data Center and is opened for JAERI users. This manual is written by the authors of the code (E. Sh. Soukhovitskii, Y. V. Porodzinskii) and users at JAERI (O. Iwamoto, S. Chiba, K. Shibata). The contribution of the latter can guarantee that the manual is complete enough so that new users, not acquainted with the code, will use it without problems. The L^AT_EX file of the manual can be retrieved from the home page of JAERI nuclear data center (<http://cracker.tokai.jaeri.go.jp/>).

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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·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
功率、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	ファラード	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	°C	
光束度	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
線量等量	シーベルト	Sv	J/kg

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=1.60218×10⁻¹⁹J

1 u=1.66054×10⁻²⁷kg

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)

- 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、1eVおよび1uの値はCODATAの1986年推奨値によった。
- 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。
- barは、JISでは液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。
- EC関係理事会指令では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/m²)=10 P(ボアズ)(g/(cm·s))

動粘度 1 m²/s=10⁴St(ストークス)(cm²/s)

圧力	MPa(=10bar)	kgf/cm ²	atm	mmHg(Torr)	lbf/in ² (psi)
	1	10.1972	9.86923	7.50062×10 ³	145.038
力	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 cal = 4.18605J (計量法)
	1	0.101972	2.77778×10 ⁻⁷	0.238889	9.47813×10 ⁻⁴	0.737562	6.24150×10 ¹⁸	= 4.184J (熱化学)
9.80665	1	2.72407×10 ⁻⁶	2.34270	9.29487×10 ⁻³	7.23301	6.12082×10 ¹⁹		= 4.1855J (15°C)
3.6×10 ⁶	3.67098×10 ⁵	1	8.59999×10 ⁵	3412.13	2.65522×10 ⁶	2.24694×10 ²⁵		= 4.1868J (国際蒸気表)
4.18605	0.426858	1.16279×10 ⁻⁶	1	3.96759×10 ⁻³	3.08747	2.61272×10 ¹⁹		仕事率 1 PS(仏馬力)
1055.06	107.586	2.93072×10 ⁻⁴	252.042	1	778.172	6.58515×10 ²¹		= 75 kgf·m/s
1.35582	0.138255	3.76616×10 ⁻⁷	0.323890	1.28506×10 ⁻³	1	8.46233×10 ¹⁸		= 735.499W
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		

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)

