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PHYSICS AND NUMERICAL METHODS OF OPTMAN :  
A COUPLED-CHANNELS METHOD BASED ON  
SOFT-ROTATOR MODEL FOR A DESCRIPTION OF  
COLLECTIVE NUCLEAR STRUCTURE AND EXCITATIONS

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## Physics and Numerical Methods of OPTMAN : A Coupled-channels Method Based on Soft-rotator Model for a Description of Collective Nuclear Structure and Excitations

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This report gives a detailed description of the theory and computational algorithms of modernized coupled-channels optical model code OPTMAN based on the soft-rotator model for the collective nuclear structure and excitations. This work was performed under the Project Agreement B-521 with the International Science and Technology Center (Moscow), financing party of which is Japan. As a result of this work, the computational method of OPTMAN was totally updated, and an user-friendly interface was attached.

**Keywords:** OPTMAN, Soft-rotator Model, Coupled-channels Method, ISTC B-521, Theory, Numerical Algorithms, Interface

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## OPTMANにおける物理と数値計算手法：軟回転体模型に基づくチャンネル結合法による原子核の集団準位構造とその励起の記述

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軟回転体模型ハミルトニアンに基づくチャンネル結合光学模型によって原子核の集団励起構造と反応断面積を記述する計算コード OPTMAN における最新の理論と数値計算アルゴリズムの解説を行う。本研究は、国際科学技術センター (ISTC モスクワ) のプロジェクト B-521 として、日本のサポートの下で行われている。本プロジェクトにより OPTMAN における数値計算アルゴリズムは完全に改訂され、またユーザーフレンドリーなインターフェースが設けられた。

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## 1. INTRODUCTION

For more than twenty years, an original coupled-channels optical model code OPTMAN has been developed at Joint Institute of Energy and Nuclear Research to investigate nucleon-nucleus interaction mechanisms and as a basic tool for nuclear data evaluation for reactor design and other applications. Results of such activities for, e.g.,  $^{235}\text{U}$ ,  $^{239}\text{Pu}$ ,  $^{236}\text{U}$ ,  $^{233}\text{U}$ ,  $^{238}\text{Pu}$  etc., were included in evaluated Nuclear Data Library BROND [1] of former Soviet Union. Except for the standard rigid rotator and harmonic vibrator coupling scheme encoded in widely-used JUPITER [2] and ECIS [3] codes, level-coupling schemes based on a non-axial soft-rotator model are included for the even-even nuclei in OPTMAN. This allows account of stretching of soft nuclei by rotations, which results in change of equilibrium deformations for excited collective states compared with that of the ground state. This is a critical point for reliable predictions [4–6] based on the coupled-channels method.

Over many years, OPTMAN was developed and used for evaluation of reactor oriented nuclear data. So it was written originally considering only neutrons as the projectile with possible upper incident energy of about 20MeV. In 1995-1998, this code was successfully used as a theoretical base for nuclear data evaluation for minor actinides carried out in the framework of ISTC Project CIS-03-95, financial party of which was Japan. In 1997 OPTMAN code was installed at Nuclear Data Center of Japan Atomic Energy Research Institute and an active collaboration started. After that time, many new options were added to the code following demands from a broad range of applications: power reactors, shielding design, radiotherapy, transmutations of nuclear wastes and nucleosynthesis.

Calculations with OPTMAN are now possible both for neutrons and protons as the projectile, and the upper incident nucleon energy is extended to at least 200 MeV [7]. Current version of soft-rotator model of OPTMAN takes into account the non-axial quadrupole, octupole and hexadecapole deformations, and  $\beta_2$ ,  $\beta_3$  and  $\gamma$ -vibrations with account of nuclear volume conservation. With these options, OPTMAN is able to analyze the collective level structure, E2, E3, E4  $\gamma$ -transition probabilities and reaction data in a self-consistent manner, which makes results of such analyses more reliable. We have found that this model was flexible enough so that OPTMAN can be applied not only to heavy rotational nuclei

[8,9], but can be applied very successfully even to a very light nucleus, namely  $^{12}\text{C}$  [10,11] and light one  $^{28}\text{Si}$  [12], and also to vibrational nuclei such as  $^{52}\text{Cr}$  [13],  $^{56}\text{Fe}$  [14,15] and  $^{58}\text{Ni}$  [16]. In the mean time, energy dependence of the optical potential has been continuously improved guided by physical principles. Now, such features as the high-energy saturation behaviour consistent with Dirac phenomenology, relativistic generalization of Elton and Madland, and properties stemming from the nuclear matter theory are taken into consideration.

Therefore, OPTMAN has capabilities applicable for analyses of nucleon interaction with light, medium and heavy nuclei for a wide energy range, which will be crucially important to fulfill many nuclear-data demands. Nevertheless, the code, especially the mathematical algorithms are not described in detail before, so it may be still a “black box” for most of the users. On the other hand, large computational resources available today made a complete modernization of the code possible. Furthermore, currently available theoretical approaches were included with some new, more accurate advanced mathematical solutions and algorithms. They have made the code a user-friendly program complex for coupled-channels optical model calculations.

This report gives a description of the physics and computation algorithms developed and incorporated into modernized OPTMAN code according to the ISTC B-521 Project's Working Plan, financing party of which is Japan.

## 2. DESCRIPTION OF THE SOFT-ROTATOR MODEL

We assume that the low-lying excited states observed in even-even non-spherical nuclei can be described as a combination of rotation,  $\beta$ -quadrupole and octupole vibrations, and  $\gamma$ -quadrupole vibration. Instant nuclear shapes that correspond to such excitations can be presented [17,18] in a body fixed system:

$$\begin{aligned} R(\theta', \varphi') &= R_0 r_\beta(\theta', \varphi') \\ &= R_0 \left\{ 1 + \sum_{\lambda\mu} \beta_{\lambda\mu} Y_{\lambda\mu}(\theta', \varphi') \right\} \\ &= R_0 \left\{ 1 + \beta_2 \left[ \cos \gamma Y_{20}(\theta', \varphi') + \frac{1}{\sqrt{2}} \sin \gamma (Y_{22}(\theta', \varphi') + Y_{2-2}(\theta', \varphi')) \right] \right\} \end{aligned}$$



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

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

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

which are admissible in the case for the first excited states [19].

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  $\beta_2$ -,  $\gamma$ -quadrupole and octupole vibrations, and the vibrational potentials ignoring a coupling between the three vibration modes [5]:

$$\hat{H} = \frac{\hbar^2}{2B_2} \left\{ \hat{T}_{\beta_2} + \frac{1}{\beta_2^2} \hat{T}_\gamma \right\} + \frac{\hbar^2}{2} \hat{T}_r + \frac{\hbar^2}{2B_3} \hat{T}_{\beta_3} + \frac{\beta_{20}^4}{\beta_2^2} V(\gamma) + V(\beta_2) + V(\beta_3), \quad (3)$$

where

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

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

$$\hat{T}_{\beta_3} = -\frac{1}{\beta_3^3} \frac{\partial}{\partial \beta_3} \left( \beta_3^3 \frac{\partial}{\partial \beta_3} \right). \quad (6)$$

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

$$\hat{T}_r = \sum_{i=1}^3 \frac{\hat{I}_i^2}{J_i} = \sum_{i=1}^3 \frac{\hat{I}_i^2}{J_i^{(2)} + J_i^{(3)} + J_i^{(4)}}. \quad (7)$$

Here,  $J_i^{(\lambda)}$  stands for the principal moments of inertia in the direction of the  $i$ -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,  $\beta_{20}$  -the quadrupole equilibrium

deformation parameter at the ground state (G.S.) and  $B_\lambda$  -the mass parameter for multipolarity of  $\lambda$ . The eigenfunctions  $\Omega$  of operator (3) 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  $\lambda$ . Below we consider nuclei that are hard with respect to octupole transverse and hexadecapole vibrations.

For nuclei of shapes determined by Eq. (1),  $J_i^{(\lambda)}$  is given by [20]

$$J_i^{(2)} = 4B_2\beta_2^2 \sin(\gamma - 2/3\pi i), \quad (i = 1..3) \quad (8)$$

$$J_1^{(3)} = 4B_3\beta_3^2 \left( \frac{1}{2} \cos^2 \eta + \frac{\sqrt{15}}{4} \sin 2\eta + 1 \right), \quad (9)$$

$$J_2^{(3)} = 4B_3\beta_3^2 \left( \frac{1}{2} \cos^2 \eta - \frac{\sqrt{15}}{4} \sin 2\eta + 1 \right), \quad (10)$$

$$J_3^{(3)} = 4B_3\beta_3^2 \sin^2 \eta, \quad (11)$$

$$J_1^{(4)} = 4B_4 \left( \frac{5}{2} b_{40}^2 + 4b_{42}^2 + b_{44}^2 + \frac{3}{2} \sqrt{10} b_{40} b_{42} + \sqrt{7} b_{42} b_{44} \right), \quad (12)$$

$$J_2^{(4)} = 4B_4 \left( \frac{5}{2} b_{40}^2 + 4b_{42}^2 + b_{44}^2 - \frac{3}{2} \sqrt{10} b_{40} b_{42} - \sqrt{7} b_{42} b_{44} \right), \quad (13)$$

$$J_3^{(4)} = 4B_4 (2b_{42}^2 + 8b_{44}^2) \quad (14)$$

with  $b_{4\mu}$  that can be presented as [21]:

$$b_{40} = \beta_4 \left( \sqrt{7/12} \cos \delta_4 + \sqrt{5/12} \sin \delta_4 \cos \gamma_4 \right), \quad (15)$$

$$b_{42} = \beta_4 \sqrt{1/2} \sin \delta_4 \sin \gamma_4, \quad (16)$$

$$b_{44} = \beta_4 \sqrt{1/2} \left( \sqrt{5/12} \cos \delta_4 - \sqrt{7/12} \sin \delta_4 \cos \gamma_4 \right) \quad (17)$$

with parameters  $\eta$ ,  $\delta_4$ , and  $\gamma_4$  determining the non-axiality of octupole and hexadecapole deformations.

For convenience, let us rewrite the operator  $\hat{T}_r$  as

$$\hat{T}_r = \frac{1}{4B_2\beta_2^2} \sum_{i=1}^3 \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32}j_i^{(3)} + a_{42}j_i^{(4)}}, \quad (18)$$

where  $j_i^{(\lambda)} = J_i^{(\lambda)}/4B_\lambda\beta_\lambda^2$  and  $a_{\lambda 2} = (B_\lambda/B_2)(\beta_\lambda/\beta_2)^2$ . To solve the Schrödinger equation in a perturbative way, we expand Eq. (18) around the minima of the potential energy of the quadrupole and octupole vibrations, *i.e.*  $\beta_{20}$ ,  $\gamma_0$  and  $\beta_{30}$ :

$$\begin{aligned}
\hat{T}_r = & \frac{1}{4B_2\beta_2^2} \sum_{i=1}^3 \left\{ \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32}j_i^{(3)} + a_{42}j_i^{(4)}} \right\} \bigg|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} \\
& + \frac{\partial}{\partial \gamma} \left[ \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32}j_i^{(3)} + a_{42}j_i^{(4)}} \right] \bigg|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} (\gamma - \gamma_0) \\
& + \frac{\partial}{\partial a_{32}} \left[ \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32}j_i^{(3)} + a_{42}j_i^{(4)}} \right] \bigg|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} 2a_{320} \left[ \frac{\beta_3 \mp \beta_{30}}{\pm \beta_{30}} - \frac{\beta_2 - \beta_{20}}{\beta_{20}} \right] + \dots \\
& - \frac{\partial}{\partial a_{42}} \left[ \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32}j_i^{(3)} + a_{42}j_i^{(4)}} \right] \bigg|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} 2a_{420} \left[ \frac{\beta_2 - \beta_{20}}{\beta_{20}} \right] + \dots \Bigg\}, \quad (19)
\end{aligned}$$

where  $a_{\lambda 20} = (B_\lambda/B_2)(\beta_{\lambda 0}/\beta_{20})^2$  and sign  $\pm$  in front of  $\beta_{30}$  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 a barrier separating those nuclear shapes with opposite values of octupole deformation which is expressed as [22,23]:

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

Owing to centrifugal forces caused by nuclear rotation, equilibrium octupole deformation changes as  $\beta_3 = \beta_2\epsilon$  in direct proportion to  $\beta_2$ . It is shown in [24] that, along with the choice of potential in the form of Eq. (20), this enables us to reproduce various patterns of level-energy intervals observed experimentally for positive and negative parity bands of even-even nuclei

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

$$\begin{aligned}
& -\frac{\hbar^2}{2B_2} \frac{\partial^2 u}{\partial \beta_2^2} - \frac{\hbar^2}{2B_3\beta_2^2} \frac{\partial^2 u}{\partial \epsilon^2} - \frac{\hbar^2}{2B_2\beta_2^2} \frac{\partial^2 u}{\partial \gamma^2} + \frac{\hbar^2}{2B_2\beta_2^2} \frac{1}{4} \sum_{i=1}^3 \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32}j_i^{(3)} + a_{42}j_i^{(4)}} \bigg|_{\substack{\beta_2=\beta_{20} \\ \gamma=\gamma_0 \\ \beta_3=\beta_{30}}} u \\
& + \left[ V(\beta_2) + \frac{\hbar^2}{2B_3\mu_\epsilon^4\beta_2^2} (\epsilon \mp \epsilon_0)^2 + \frac{\beta_0^4}{\beta_2^2} V(\gamma) - \frac{\hbar^2}{2B_2\beta_2^2} \frac{9}{4} \frac{1 + \sin^2 3\gamma}{\sin^2 3\gamma} \right] u = Eu. \quad (21)
\end{aligned}$$

The quadrupole and octupole variables in (21) are separated now. Therefore, the function  $u$  can be factorized into these variables. Thus we can write as

$$u = \psi^\pm(\beta_2, \gamma, \Theta) \varphi_{n_{\beta_3}}^\pm(\epsilon), \quad (22)$$

where

$$\varphi_{n_{\beta_3}}^\pm(\epsilon) = \frac{C_{n_{\beta_3}}}{\sqrt{2}} [\chi_{n_{\beta_3}}(\tau_\epsilon^+) \pm \chi_{n_{\beta_3}}(\tau_\epsilon^-)], \quad (23)$$

$$\tau_\epsilon^\pm = \epsilon \mp \epsilon_0. \quad (24)$$

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

$$\left[ -\frac{\hbar^2}{2B_3} \frac{\partial^2}{\partial \epsilon^2} + \frac{\hbar^2}{2B_3 \mu_\epsilon^4} (\epsilon \mp \epsilon_0)^2 \right] \chi_{n_{\beta_3}}(\tau_\epsilon^\pm) = \hbar \omega_\epsilon (n + 1/2) \chi_{n_{\beta_3}}(\tau_\epsilon^\pm), \quad (25)$$

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 of Eq. (23) 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

$$\begin{aligned} & \frac{\hbar^2 \beta^2}{2B_2} \frac{\partial^2 \psi^\pm}{\partial \beta_2^2} + \frac{\hbar^2}{2B_2} \frac{\partial^2 \psi^\pm}{\partial \gamma^2} - \frac{\hbar^2}{2B_2} \frac{1}{4} \sum_{i=1}^3 \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}} \bigg|_{\substack{\beta_2 = \beta_{20} \\ \gamma = \gamma_0 \\ \beta_3 = \beta_{30}}} \psi^\pm \\ & - \left[ \beta_2^2 V(\beta_2) + \beta_0^4 V_0(\gamma) - \frac{\hbar^2}{2B_2} \frac{9}{4} \frac{1 + \sin^2 3\gamma}{\sin^2 3\gamma} + E_{n_{\beta_3}}^\pm - E^\pm \beta_2^2 \right] \psi^\pm = 0, \end{aligned} \quad (26)$$

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 (26) and the analogous equation (considered in detail in [5]) for vibrational and rotational state of positive parity in non-axial deformed even-even nuclei is due to the necessity of taking account of 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

$$\Phi_{IM\tau}^\pm(\Theta) = \sum_{K \geq 0} |IMK, \pm\rangle A_{IK}^\tau, \quad (27)$$

where

$$|IMK, \pm\rangle = ((2I+1)/(16\pi^2(1+\delta_{K0})))^{1/2} [D_{MK}^I(\Theta) \pm (-1)^I D_{M-K}^I(\Theta)], \quad (28)$$

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 [24].

Using the results from [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 zeroth order approximation of  $\hat{T}_r$  expansion) in the form

$$\begin{aligned} E_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm &= \hbar\omega_0 \left\{ \left( \nu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm + 1/2 \right) \times \left( 4 - 3/P_{I\tau n_\gamma n_{\beta_3}}^\pm \right)^{1/2} \right. \\ &\quad + \frac{1}{2} \frac{\mu_{\beta_{20}}^2}{P_{I\tau n_\gamma n_{\beta_3}}^{\pm 2}} \left[ \frac{2}{\mu_{\gamma_0}^2} (\nu_{n_\gamma} - \nu_{0_\gamma}) + \varepsilon_{I\tau}^\pm + \epsilon_{n_{\beta_3}}^\pm - \epsilon_{0_{\beta_3}}^+ \right] \\ &\quad \left. + \frac{1}{2} \frac{\mu_{\beta_{20}}^6}{P_{I\tau n_\gamma n_{\beta_3}}^{\pm 6}} \left[ \frac{2}{\mu_{\gamma_0}^2} (\nu_{n_\gamma} - \nu_{0_\gamma}) + \varepsilon_{I\tau}^\pm + \epsilon_{n_{\beta_3}}^\pm - \epsilon_{0_{\beta_3}}^+ \right]^2 \right\}, \quad (29) \end{aligned}$$

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

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

where  $\hbar\omega_0$ ,  $\mu_{\beta_{20}}$ ,  $\mu_{\gamma_0}$  and  $\gamma_0$  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,  $\mu_{\beta_{20}}$ ,  $\mu_{\gamma_0}$  and  $\mu_\epsilon$  are related to the elasticity constants of  $\beta_2$ -,  $\gamma$ - and octupole vibrations, respectively and  $\gamma_0$  is the equilibrium point of the  $\gamma$ -vibration.

Other quantities in the above equation are to be determined in the following way. The quantity  $\nu_{n_\gamma}$  denotes the eigenvalue of the  $\gamma$ -vibration corresponding to the quantum number of  $n_\gamma$ . The quantity  $\varepsilon_{I\tau}^\pm$  is the eigenvalues of the asymmetric-rotator Hamiltonian [25,26] corresponding to the first term of the r.h.s. of Eq. (19),

$$\hat{T}_r^0 \Phi_{IM\tau}^\pm = \varepsilon_{I\tau}^\pm \Phi_{IM\tau}^\pm. \quad (31)$$

The symbol  $\nu_{n_\gamma}$  is determined by a system of two equations corresponding to the boundary conditions for  $\gamma$ -vibrations, and  $n_\gamma$  is the number of the solutions:

$$\begin{cases} v_{\nu_{n_\gamma}} \left[ -\frac{\sqrt{2}}{\mu_{\gamma_0}} \left( \frac{\pi}{3} n - \gamma_0 \right) \right] = 0 \\ v_{\nu_{n_\gamma}} \left[ -\frac{\sqrt{2}}{\mu_{\gamma_0}} \left( \frac{\pi}{3} (n+1) - \gamma_0 \right) \right] = 0 \end{cases}, \quad (32)$$

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

$$\left[ \frac{d^2}{dy^2} + \nu_{n_\gamma} + \frac{1}{2} - \frac{y^2}{4} \right] v_{n_\gamma} = 0, \quad (33)$$

which is a linear combination of two independent solutions:

$$v_{n_\gamma}(y) = c_{n_\gamma} [D_{\nu_{n_\gamma}}(y) + a_{n_\gamma} V_{\nu_{n_\gamma}}(y)], \quad (34)$$

where  $D_{\nu_{n_\gamma}}$  denotes the well-known Weber function (see [27]). The symbol  $\nu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm$  is determined also by the boundary conditions (32). For the  $\beta_2$  variable, however, one of the boundaries is at infinity where the function  $V$  in the above equation diverges. Therefore, this reduces the possible solution of equation (33) to be

$$v_\nu(y) = c_\nu D_\nu(y), \quad (35)$$

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

$$D_{\nu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm} \left[ -\frac{\sqrt{2} P_{I\tau n_\gamma n_{\beta_3}}^\pm}{\mu_{\beta_{20}}} \left( 4 - \frac{3}{P_{I\tau n_\gamma n_{\beta_3}}^\pm} \right) \right] = 0. \quad (36)$$

Finally, we can write the full wave function for the soft-rotator Hamiltonian as

$$\begin{aligned} \Omega_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm &= C_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm \frac{C_{n_{\beta_3}} \beta_2^{-2} \beta_3^{-3/2}}{\sqrt{2} \sqrt{\sin 3\gamma}} \sum_{K \geq 0} |IMK, \pm\rangle A_{IK}^\tau \\ &\times D_{\nu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm} \left[ \frac{\sqrt{2}}{\beta_{20} \mu_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm} \left( \beta_2 - \beta_{2I\tau n_\gamma n_{\beta_3}}^\pm \right) \right] \\ &\times v_{n_\gamma} \left[ \frac{\sqrt{2}}{\mu_{\gamma_0}} (\gamma - \gamma_0) \right] [\chi_{n_{\beta_3}}(\tau_\epsilon^+) \pm \chi_{n_{\beta_3}}(\tau_\epsilon^-)], \end{aligned} \quad (37)$$

with

$$\beta_{2I\tau n_\gamma n_{\beta_3}}^\pm = \beta_{20} P_{I\tau n_\gamma n_{\beta_3}}^\pm, \quad (38)$$

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

$$\frac{1}{\mu_{\beta_2 I_{\tau n_{\gamma} n_{\beta_3}}}^{\pm 4}} = \frac{1}{\mu_{\beta_2 0}^4} + \frac{3 \left[ \frac{2}{\mu_{\beta_2 0}^2} (\nu_{n_{\gamma}} - \nu_{0_{\gamma}}) + \epsilon_{I\tau}^{\pm} + \epsilon_{n_{\beta_3}}^{\pm} - \epsilon_{0_{\beta_3}}^{\pm} \right]}{P_{I_{\tau n_{\gamma} n_{\beta_3}}}^{\pm}}, \quad (39)$$

with  $\mu_{\beta_2 I_{\tau n_{\gamma} n_{\beta_3}}}$  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 (19) can be easily calculated by a perturbative way. If we consider  $n_{\beta_3} = 0$  (as states with  $n_{\beta_3} \geq 1$  lie above the experimentally resolved ones), this correction is given by

$$\begin{aligned} \Delta E_{I_{\tau n_{\gamma} n_{\beta_3} (=0) n_{\beta_2}}}^{\pm} &= h\omega_0 \frac{\mu_{\beta_2}^2}{\beta_{20}^2} \left\{ \frac{B_3}{B_2} \epsilon_0^2 \langle \Phi_{IM\tau}^{\pm}(\theta) | \sum_{i=1}^3 \frac{\partial}{\partial a_{32}} \left[ \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}} \right] \right|_{\substack{\beta_2 = \beta_{20} \\ \gamma = \gamma_0 \\ \beta_3 = \beta_{30}}} | \Phi_{IM\tau}^{\pm}(\theta) \rangle \right. \\ &\quad \times \left\{ \left[ \frac{e^{-\epsilon_0^2/\mu_{\epsilon}^2}}{1 \pm e^{-\epsilon_0^2/\mu_{\epsilon}^2}} \left( \frac{\mu_{\epsilon}}{\epsilon_0 \sqrt{\pi}} \pm \frac{\mu_{\epsilon}}{\epsilon_0 \sqrt{\pi}} \mp 1 \right) - \frac{\text{erfc}(\epsilon_0/\mu_{\epsilon})}{1 \pm e^{-\epsilon_0^2/\mu_{\epsilon}^2}} \right] J_{I_{\tau n_{\gamma} n_{\beta_3} n_{\beta_2}}}^{\pm}(1/y^2) - J_{I_{\tau n_{\gamma} n_{\beta_3} n_{\beta_2}}}^{\pm}(1/y^2) \right\} \\ &\quad \left. - \frac{B_4}{B_2} \beta_4^2 \langle \Phi_{IM\tau}^{\pm}(\theta) | \sum_{i=1}^3 \frac{\partial}{\partial a_{42}} \left[ \frac{\hat{I}_i^2}{j_i^{(2)} + a_{32} j_i^{(3)} + a_{42} j_i^{(4)}} \right] \right|_{\substack{\beta_2 = \beta_{20} \\ \gamma = \gamma_0 \\ \beta_3 = \beta_{30}}} | \Phi_{IM\tau}^{\pm}(\theta) \rangle \times J_{I_{\tau n_{\gamma} n_{\beta_3} n_{\beta_2}}}^{\pm}[(y-1)/y^2] \right\} \quad (40) \end{aligned}$$

where

$$\begin{aligned} J_{I_{\tau n_{\gamma} n_{\beta_3} n_{\beta_2}} I' \tau' n'_{\gamma} n'_{\beta_3} n'_{\beta_2}}^{\pm} [f(y)] &= \int_0^{\infty} f(y) D_{\nu_{I_{\tau n_{\gamma} n_{\beta_3} n_{\beta_2}}}}^{\pm} \left[ -\frac{\sqrt{2}}{\mu_{I_{\tau n_{\gamma} n_{\beta_3}}}^{\pm}} (y - P_{I_{\tau n_{\gamma} n_{\beta_3}}}^{\pm}) \right] \\ &\quad \times D_{\nu_{I' \tau' n'_{\gamma} n'_{\beta_3} n'_{\beta_2}}}^{\pm} \left[ -\frac{\sqrt{2}}{\mu_{I' \tau' n'_{\gamma} n'_{\beta_3}}^{\pm}} (y - P_{I' \tau' n'_{\gamma} n'_{\beta_3}}^{\pm}) \right] dy \\ &\quad \times \left\{ \int_0^{\infty} D_{\nu_{I_{\tau n_{\gamma} n_{\beta_3} n_{\beta_2}}}}^2 \left[ -\frac{\sqrt{2}}{\mu_{I_{\tau n_{\gamma} n_{\beta_3}}}^{\pm}} (y - P_{I_{\tau n_{\gamma} n_{\beta_3}}}^{\pm}) \right] dy \right\}^{-1/2} \\ &\quad \times \left\{ \int_0^{\infty} D_{\nu_{I' \tau' n'_{\gamma} n'_{\beta_3} n'_{\beta_2}}}^2 \left[ -\frac{\sqrt{2}}{\mu_{I' \tau' n'_{\gamma} n'_{\beta_3}}^{\pm}} (y' - P_{I' \tau' n'_{\gamma} n'_{\beta_3}}^{\pm}) \right] dy' \right\}^{-1/2}. \quad (41) \end{aligned}$$

### 3. OPTICAL POTENTIAL AND CHANNEL COUPLING

Multipoles of the deformed nuclear potential arising from deformed nuclear shape are determined by expanding it in a Taylor series, considering  $(\sum_{\lambda\mu} \beta_{\lambda\mu} Y_{\lambda\mu}(\theta', \varphi'))$  in Eq.(1) to be small:

$$V(r, R(\theta', \varphi')) = V(r, R_0) + \sum_{t=1}^{max} \frac{\partial^t V(r, R)}{\partial R^t} \Big|_{R(\theta', \varphi')=R_0} \frac{R_0^t}{t!} \left( \sum_{\lambda\mu} \beta_{\lambda\mu} Y_{\lambda\mu}(\theta', \varphi') \right)^t, \quad (42)$$

in which body fixed coordinates  $(\theta', \varphi')$  can be easily converted to the Laboratory ones by using the rotation function  $D$ :

$$Y_{\lambda\mu}(\theta', \varphi') = \sum_{\nu} D_{\mu\nu}^{\lambda*} Y_{\lambda\mu}(\theta, \varphi), \quad (43)$$

so that coupling potential can be written in a form:

$$V_{coupl}(r, \theta, \varphi, \gamma, \beta_{\lambda}) = \sum_{t-m \dots -n \geq 0} v^t(r) \beta_{\lambda}^{t-m \dots -n} \beta_{\lambda'}^m \cdot \beta_{\lambda''}^n \cdot \sum_{\nu\mu} Q_{\nu\mu}^{(tm \dots n \lambda' \lambda'' \dots \lambda''')}^* Y_{\nu\mu}(\theta, \varphi). \quad (44)$$

Here,  $v^t(r) = \frac{\partial^t V(r, R)}{\partial R^t} \Big|_{R(\theta', \varphi')=R_0}$  with the deformed optical nuclear potential taken to be a standard spherical form, but now with the account of deformed instant nuclear shapes:

$$\begin{aligned} V(r, R(\theta', \varphi')) = & -V_R f_R(r, R(\theta', \varphi')) \\ & + i \left\{ 4W_D a_D \frac{d}{dr} f_D(r, R(\theta', \varphi')) - W_V [\alpha f_V(r, R(\theta', \varphi')) + (1 - \alpha) f_W(r, R(\theta', \varphi'))] \right\} \\ & + \left( \frac{\hbar}{\mu\pi c} \right)^2 (V_{SO} + iW_{SO}) \frac{1}{r} \frac{d}{dr} f_{SO}(r, R(\theta', \varphi')) \boldsymbol{\sigma} \cdot \mathbf{L} + V_{Coul}(r, R(\theta', \varphi')), \end{aligned} \quad (45)$$

where the form factors are given as

$$f_i = [1 + \exp(r - R_i(\theta', \varphi'))/a_i]^{-1}, \quad R_i(\theta', \varphi') = R_i^0 r_{\beta}(\theta', \varphi') = r_i A^{1/3} r_{\beta}(\theta', \varphi'), \quad (46)$$

$$f_W = \exp\{-((r - R_W(\theta', \varphi'))/a_W)^2\}, \quad R_W(\theta', \varphi') = R_W^0 r_{\beta}(\theta', \varphi') = r_W A^{1/3} r_{\beta}(\theta', \varphi'), \quad (47)$$

with  $r_{\beta}(\theta', \varphi')$  as defined by Eq. (1). The subscripts  $i = R, V, D$  and  $so$  denote the real volume, imaginary volume, imaginary surface and real spin-orbit potentials.

For the reasons mentioned above, we need the potential expansion expressed with an evident dependence on deformation. For Coulomb potential  $V_{Coul}(r, R(\theta', \varphi'))$ , such expansion with an evident dependence on the deformations becomes possible as we follow the suggestion of Satchler *et al.* [28], using a multipole expansion of the Coulomb potential  $V_{Coul}$  for a charged ellipsoid with a uniform charge density within the Coulomb radius  $R_C$  and zero outside. Up to the second order of  $\sum \beta_{\lambda\mu} Y_{\lambda\mu}$ , it reads:

$$V_{Coul}(r, R(\theta', \varphi')) = \frac{ZZ'e^2}{2R_c} \left[ 3 - \frac{r^2}{R_c^2} \right] \theta(R_C - r) + \frac{ZZ'e^2}{r} \theta(r - R_C)$$



$$\begin{aligned}
& + \sum_{\lambda\mu} \frac{3ZZ'e^2}{2\lambda+1} \left[ r^\lambda R_C^{-(\lambda+1)} \theta(R_C - r) + R_C^\lambda r^{-(\lambda+1)} \theta(r - R_C) \right] (\beta_{\lambda\mu} Y_{\lambda\mu}) \\
& + \sum_{\lambda\mu} \frac{3ZZ'e^2}{2\lambda+1} \left[ (1-\lambda) r^\lambda R_C^{-(\lambda+1)} \theta(R_C - r) + (\lambda+2) R_C^\lambda r^{-(\lambda+1)} \theta(r - R_C) \right] \\
& \times \sum_{\lambda'\lambda''} \frac{\hat{\lambda}'\hat{\lambda}''}{(4\pi)^{1/2}\hat{\lambda}} (\lambda'\lambda''00 | \lambda 0) \sum_{\mu} (\beta_{\lambda'} \otimes \beta_{\lambda'')_{\lambda\mu}} Y_{\lambda\mu}, \tag{48}
\end{aligned}$$

where  $Z', Z$  are charges of incident particle and nucleus,  $\hat{\lambda} = (2\lambda + 1)^{1/2}$ , while the symbol  $\otimes$  means the vector addition, *i.e.*

$$(\beta_{\lambda'} \otimes \beta_{\lambda'')_{\lambda\mu}} = \sum_{\mu'\mu''} (\lambda'\lambda''\mu'\mu'' | \lambda\mu) \beta_{\lambda'\mu'} \beta_{\lambda''\mu''} \tag{49}$$

and  $\theta(r) = 1$ , if  $r > 0$  and  $\theta(r) = 0$ , if  $r < 0$ . This form of expansion gives contributions to  $v^i(r)$  for  $t = 1$  and 2 in addition to the couplings coming from the nuclear potential.

Coulomb potential deformation results in a dependence on  $r$  of the coupling potential multipoles as  $r^{-\lambda-1}$  so that induced error for matching at radius  $R$  must be of order of  $R^{-\lambda}$ , and hence the matching radius must be significantly increased or Coulomb correction procedure must be applied [29]. As potential multipole  $\lambda$  determines angular momentum transfer, it is important for excitation of the  $J^\pi = 2^+$  level (for ground state with  $J^\pi = 0^+$ ) but much less for levels with higher spins.

The Coulomb potential used in the present work included some modifications to formula (48). Instead of the spherical term, which is  $\frac{ZZ'e^2}{2R_C} \left[ 3 - \frac{r^2}{R_C^2} \right] \theta(R_C - r) + \frac{ZZ'e^2}{r} \theta(r - R_C)$  for uniform charge density within the Coulomb radius  $R_C$  and zero outside, one can use Coulomb potential spherical term calculated taking into account the diffuseness of the charge distribution with charge density form factor equal to  $f_C = [1 + \exp(r - R_C)/a_C]^{-1}$ . Our model involves quadrupole, octupole and hexadecapole instant nuclear deformations, *i.e.* the Coulomb expansion of the potential can in principle give additional coupling strength between collective states with an angular momentum transfer of 0 to 8. However, in the Coulomb expansion used in this model, we truncate the dynamic square terms which lead to zero angular momentum transfer. This is equivalent to introducing a dynamic negative deformation  $\beta_{00}$  in the radial expansion given in Eq. (1):

$$\beta_{00} = - \sum_{\lambda} (-1)^\lambda \frac{\hat{\lambda}}{(4\pi)^{1/2}} (\beta_{\lambda} \otimes \beta_{\lambda})_{00}, \tag{50}$$

which is required as a condition to conserve the nuclear volume, *i.e.* the nuclear charge [25]. This correction is necessary to have the correct asymptotic behavior for the spherical term of the Coulomb potential which must be equal to  $ZZ'e^2/r$ . The additional coupling due to the Coulomb potential was obtained in the same manner as for the nuclear one [30] with deformed radii as described above.

As we consider  $\beta_{\lambda\mu}$  to be dynamic in the soft-rotator nuclear model, nuclear shape described in Eq. (1) will violate nuclear mass conservation. To conserve nuclear mass for uniform nuclear density case, one must add a dynamic negative deformation  $\beta_{00}$  to the radial expansion given in Eq. (1). This is required as the condition to conserve the nuclear volume [25] which is equivalent to mass and nuclear charge conservation for uniform nuclear and nuclear charge density case adopted in [25]. So the radius describing shape of nuclei with constant volume becomes

$$R(\theta', \varphi') = R_0 \left\{ 1 + \beta_{00}Y_{00} + \sum_{\lambda\mu} \beta_{\lambda\mu}Y_{\lambda\mu}(\theta', \varphi') \right\} \quad (51)$$

Additional  $\beta_{00}$  deformation leads to additional zero nuclear potential multipole that couples levels with equal spin and parity  $I^\pi$ .

In case of nuclear density with diffuseness, one must use the following zero multipole deformation  $\beta'_{00}$  to conserve nuclear mass [31].

$$\beta'_{00} = -\left(\frac{R_0}{2a}\right)\beta_{00} \frac{\int \frac{\partial^2 f(r, R, a)}{\partial x^2} \Big|_{x_0} r^2 dr}{\int \frac{\partial f(r, R, a)}{\partial x} \Big|_{x_0} r^2 dr} \quad (52)$$

Here  $f(r, R, a) = f(x)$  denotes the nuclear density form factor,  $x = \frac{r-R}{a}$ , and  $x_0 = \frac{r-R_0}{a}$ . We can write the above equation as follows since integrals in it are just constants,

$$\beta'_{00} = C_\beta \beta_{00}. \quad (53)$$

In our code we use nuclear real potential form factor  $f_R(r, R, a)$  instead of nuclear density form factor. As  $C_\beta$  appears to be close to unity, we take substitution of nuclear density form factor by real potential one as an acceptable approximation. Such an approximation leads to simultaneous conservation of nuclear volume and real potential volume integral in nuclear

shape oscillations, so there is an additional reason to use it. Thus considering nuclear mass and nuclear charge conservation, the multipoles of the deformed nuclear potential arising from deformed nuclear shape are determined by expanding nuclear potential in a Taylor series, now considering  $(\beta'_{00}Y_{00} + \sum \beta_{\lambda\mu}Y_{\lambda\mu}(\theta', \varphi'))$  in Eq.(1) to be small:

$$V(r, R(\theta', \varphi')) = V(r, R_0) + \sum_{t=1}^{\max} \frac{\partial^t V(r, R)}{\partial R^t} \bigg|_{R(\theta', \varphi')=R_0} \frac{R_0^t}{t!} (\beta'_{00}Y_{00} + \sum_{\lambda\mu} \beta_{\lambda\mu}Y_{\lambda\mu}(\theta', \varphi'))^t, \quad (54)$$

One can see that account of nuclear volume conservation leads to additional zero multipole term starting with the first nuclear potential derivative, which will additionally couple states with equal spins and parity  $I^\pi$  and themselves. This term is proportional to  $(\beta_{\lambda\mu})^2$  and must be taken into account, as account of terms up to  $(\beta_{\lambda\mu})^4$  is necessary to describe experimental data consistently [32].

Starting with full wave function which is defined by wave functions of nucleon +nuclei system [2]

$$\begin{aligned} \Psi^\pm &= r^{-1} \sum_{Jnl_n j_n} R_{Jnl_n j_n}(r) |(l_n s) j_n; I_n \tau n_{\beta_2} n_\gamma n_{\beta_3}; JM\rangle \\ &\equiv r^{-1} \sum_{Jnl_n j_n} R_{Jnl_n j_n}(r) \sum_{m_{j_n}, M_{I_n}} (j_n I_n m_{j_n} M_n | JM) \mathcal{Y}_{l_n j_n m_{j_n}} \Omega_{I_n M_n \tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm \end{aligned} \quad (55)$$

and inserting it in the Schrödinger equation we are coming to the equation for radial wave functions:

$$\left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k_n^2 - \frac{2\mu V_{centr}(r)}{\hbar^2} \right) R_{nlj}(r) = \frac{2\mu}{\hbar^2} \sum_{n'l'j'} V_{nlj, n'l'j'}(r) R_{n'l'j'}(r) \quad (56)$$

with a coupling potential  $V_{nlj, n'l'j'}(r)$  for coupling built on soft-rotator nuclear Hamiltonian wave functions:

$$\begin{aligned} V(r)_{nlj, n'l'j'} &= \langle (ls)j; I\tau n_{\beta_2} n_\gamma n_{\beta_3}; JM | \sum_{t-m...-n \geq 0} v^t(r) \beta_\lambda^{t-m...-n} \beta_{\lambda'}^m \cdot \beta_{\lambda''}^n \\ &\quad \times \sum_{\nu\mu} Q_{\nu\mu}^{(tm...n\lambda'\lambda''\lambda''')*} Y_{\nu\mu}(\theta, \varphi) | (l's)j'; I'\tau' n'_{\beta_2} n'_\gamma n'_{\beta_3}; JM \rangle \\ &= (-1)^{J-I'-s+l+l'+(l'-l)/2} \frac{1}{\sqrt{4\pi}} l'l'j'j' \\ &\quad \times \sum_t v^t(r) \sum_{t-m...-n \geq 0} \langle f | \beta_\lambda^{t-m...-n} \beta_{\lambda'}^m \cdot \beta_{\lambda''}^n | i \rangle \\ &\quad \times \sum_\nu (ll'00|\nu 0) W(jIj'I; \nu J) W(ljl'j'; s\nu) \\ &\quad \times \langle I\tau n_\gamma | | Q_{\nu\mu}^{(tm...n\lambda'\lambda''\lambda''')*} | | I'\tau' n'_\gamma \rangle. \end{aligned} \quad (57)$$

Here  $|i\rangle$  and  $|f\rangle$  parts of initial and final states nuclear wave functions depending on different modes of variables  $\beta_\lambda$ , while  $|I\tau n_\gamma\rangle$  is the rest part of the full nuclear wave function, holding dependence of nuclear level rotational quantum numbers  $I$ ,  $\tau$  and non-axiality  $\gamma$ -oscillations.

In rigid rotator or harmonic oscillator case, system of coupled equations has the same form as Eq. (56), but coupling potential  $V(r)_{nlj,n'l'j'}$  differs and can be found in [2].

### 3.1 The Main Essence of the CC built on Soft-rotator Nuclear Model

As our wave functions are factorized to different oscillation modes, the matrix element in the fourth line of Eq. (57) can be also factorized:

$$\langle f | \beta_\lambda^{t-m\dots-n} \beta_{\lambda'}^m \cdot \beta_{\lambda''}^n | i \rangle = \langle f_\lambda | \beta_\lambda^{t-m\dots-n} | i_\lambda \rangle \langle f_{\lambda'} | \beta_{\lambda'}^m | i_{\lambda'} \rangle \cdot \langle f_{\lambda''} | \beta_{\lambda''}^n | i_{\lambda''} \rangle. \quad (58)$$

Here  $|i_\lambda\rangle$  and  $|f_\lambda\rangle$  stand for factorized parts of initial and final states nuclear wave functions, describing  $\lambda$ -multipole oscillations.

In Rigid Case:

$$\langle f_\lambda | \beta_\lambda^t | i_\lambda \rangle = \langle G.S. | \beta_\lambda^t | G.S. \rangle = (\langle f_\lambda | \beta_\lambda | i_\lambda \rangle)^t = \beta_\lambda^t = \beta_{\lambda G.S.}^t.$$

In Case of Soft-Rotator wave functions:

$$\langle f_\lambda | \beta_\lambda^t | i_\lambda \rangle \neq \langle f'_\lambda | \beta_\lambda^t | i'_\lambda \rangle \neq \langle G.S. | \beta_\lambda^t | G.S. \rangle \neq (\langle f_\lambda | \beta_\lambda | i_\lambda \rangle)^t \neq \beta_{\lambda G.S.}^t.$$

Usually for initial and final states from one band :

$$\langle f_\lambda | \beta_\lambda^t | i_\lambda \rangle / \langle G.S. | \beta_\lambda^t | G.S. \rangle > 1$$

and can be less than unity for interband case.

For quadrupole oscillations  $\langle f_{\lambda=2} | \beta_2^t | i_{\lambda=2} \rangle = \beta_{20}^t J_{I\tau n_\gamma n_{\beta_3} n_{\beta_2}}^\pm [y^t]$ , with  $J_{I'\tau' n'_\gamma n'_{\beta_3} n'_{\beta_2}}^\pm [f(y)]$  determined by Eq.(41). So it is easy to understand that enhancement of the coupling strength compared with the rigid-rotator model [2] arises because the dynamic variables in deformed nuclear optical potential expansion are averaged over the wave functions of the

appropriate collective nuclear shape motions given by the solutions of the soft-rotator model Hamiltonian solutions. Such enhancement is equal to  $\langle i_\lambda | \beta_\lambda^t | f_\lambda \rangle / \beta_{\lambda G.S.}^t$  and this ratio is usually greater than unity, as a soft-rotating nucleus is rotating with increasing velocity for collective states with higher spins  $I$  and thus is increasingly stretched due to the centrifugal force, so that equilibrium deformations  $\beta_{\lambda I\tau}$  for states with higher spins  $I$  are greater than equilibrium G.S. deformation  $\beta_{\lambda G.S.}$ . As the deformation potential energy  $V(\beta_\lambda)$  of the soft rotator model in terms of nuclear softness  $\mu_\lambda$  is considered to be  $\sim \frac{1}{\mu_\lambda} (\beta_\lambda - \beta_{\lambda G.S.})^2$ , the coupling enhancement is larger for nuclei with larger softness  $\mu_\lambda$  and vanishes for nuclei with small  $\mu_\lambda$ . Of course this also concerns the functions  $\cos \gamma$  and  $\sin \gamma$  appearing in matrix element  $\langle I\tau n_\gamma || Q_{\nu\mu}^{(tm \dots n\lambda' \lambda'' \dots \lambda''')} || I'\tau' n'_\gamma \rangle$  of Eq.(57), which are in turn averaged over non-axiality  $\gamma$ -vibrations eigenfunctions. Such enhancements are different for different combinations of initial and final states, and also depend on the powers of potential expansion  $t$ . In this way, the soft-rotator model predicts the redistribution of coupling strength, *i.e.* the particle current between the channels, which in turn changes the estimates of direct level excitation cross sections without introducing additional assumptions and/or parameters.

#### 4. SOLUTIONS OF SCATTERING PROBLEMS

Let us rewrite system of equations (56) in more convenient form:

$$\frac{d^2 f_j(r)}{dr^2} = \sum_k V_{jk}(r) f_k(r). \quad (59)$$

To solve the scattering problem, we need to find the normalized solutions  $f n_j^i(r)$  which, in asymptotic region where nuclear forces become absent, must become an incoming plane wave with a unit current plus an outgoing wave in initial ( $i$ ) channel and pure outgoing waves in all other final ( $j$ ) channels

$$f n_j^i(r) = \delta_{ij} F_{ij}(\eta, r) + \sqrt{\frac{k_i}{k_j}} C_{ij} (F_{ij}(\eta, r) + G_{ij}(\eta, r)), \quad (60)$$

where  $F_l(\eta, r)$  and  $G_l(\eta, r)$  are Coulomb functions, that are already normalized to a unit current, and  $C_{ij}$ -matrix describes scattering. The symbol  $\eta$  denotes the Sommerfeld parameter

$$\eta = \frac{ZZ'e^2\mu}{\hbar^2 k}. \quad (61)$$

#### 4.1 Accurate Solution of Coupled-channels System for Radial Functions and Matching

Solutions, determining  $C_{ij}$ -matrix, can be found if we have a system of independent solutions  $f_j^m(r)$  of Eq. (59), each vanishing at the origin, number of which is equal to the number of coupled equations  $N$ :  $m = 1, N$ . In the vicinity of the origin, the central potential may be considered to be constant and is equal to its value at the origin  $V_{centr}(0)$ , while coupling terms  $V_{nlj,n'l'j'}(r)$  and Coulomb potential vanish. Therefore, Eq. (56) reduces to:

$$\left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k_n^2 - \frac{2\mu V_{centr}(0)}{\hbar^2} \right) R_{nlj}(r) = 0 \quad (62)$$

It is easy to see that solutions of the above equation will be independent if they depend on  $r$  at the origin as:

$$f_j^m(r) = \delta_{mj} r^{(l_j+1)}, \quad (63)$$

This dependence can be used as boundary conditions for integrating Eq. (59) to get its necessary independent solutions.

OPTMAN code uses Störmer [33] algorithm for step by step integration from the origin to the matching radius:

$$\begin{aligned} f_j^m(r+h) = & 2f_j^m(r) - f_j^m(r-h) + h^2 \left[ 229 \sum_k V_{jk}(r) f_k^m(r) \right. \\ & - 176 \sum_k V_{jk}(r-h) f_k^m(r-h) + 194 \sum_k V_{jk}(r-2h) f_k^m(r-2h) \\ & \left. - 96 \sum_k V_{jk}(r-3h) f_k^m(r-3h) + 19 \sum_k V_{jk}(r-4h) f_k^m(r-4h) \right]. \end{aligned} \quad (64)$$

Please note that above we are integrating system of homogeneously coupled equations and use that  $f''(r) = \sum_k V_{jk}(r) f_k(r)$ .

In case of  $N$  coupled equations, number of arithmetic operations for one step integration of one system line is proportional to  $N \times (M + L)$ , where  $M$  is the number of operations

necessary to calculate coupling potential  $V_{jk}$ , and  $L$  ( $\sim 10$ ) denotes number of arithmetic operations necessary to make summations and multiplications for each  $k$  for one step integrations using Eq. (64) with all components preliminary prepared. Then number of arithmetic operations for one step integration for all system lines is proportional to  $N \times N \times (M + L)$ . If  $K$  is the number of integration steps, number of arithmetic operations necessary to get one independent solution of coupled equation system is proportional to  $N^2 \times (M + L) \times K$ . And to get  $N$  independent solutions, necessary for matching, we need  $N^3 \times (M + L) \times K$ . So number of arithmetic operations in suggested algorithm and thus computational time grows as the number of coupled equations in the power of three. In case for three levels with spins  $0^+$ ,  $2^+$ ,  $4^+$ ,  $N = \sum_I (2I + 1)$  is equal to 15. If we include  $6^+$  level in coupling scheme,  $N$  becomes 28, almost twice so that  $N^3$  and thus necessary computational time becomes  $\sim 8$  times longer. Soft-rotator model describes at least collective levels from 3-4 low lying bands, including negative parity one. It is shown that coupling of the first levels from this bands cannot be ignored in reliable optical calculations. For such calculations  $N$  may be 50 and more. One can evaluate typical number of arithmetic operations, thus computational time, considering that typical number of integration steps from origin to the matching radius is about 100-200 and number of operations necessary to calculate coupling potential  $V_{jk}$ , Eq. (57) due to its complicity is about 60 for neutrons and 180 for protons, yet most potential elements  $V_{jk}$  are calculated in advance and can be used repeatedly. Such algorithm requests about  $\sim 10^9$  arithmetic operations to solve typical coupled-channels system of equations. Please note that running scattering problem we need solutions for a number of coupled-channels systems for each spin and parity  $J^\pi$ , giving significant contribution to calculated cross-sections (about 100 for 200 MeV incident energies). It can be concluded that suggested algorithm is rather time consuming. Looking at Eq. (64) one can see that for one step integration for any of integrated solutions  $f_j^m(r)$  potential  $V_{jk}(r)$  is the same, so once it is organized we can perform one step integration for all solutions  $f_j^m(r)$  simultaneously. In this case number of arithmetic operations necessary for integration for all independent solutions reduces to  $N^2 \times (M + L) \times K + N^2 \times (N - 1) \times L \times K = N^2 \times K \times (M + L + (N - 1) \times L)$ . One can see that for large  $N$  suggested algorithm of simultaneous  $f_j^m(r)$  functions integration is about

$M/L \approx 6 - 20$  times quicker. This quicker algorithm is now realized in subroutine SOSIT.

After independent solutions  $f_j^m(r)$  are found, one can easily get  $C_{ij}$ -matrix, matching the solutions to have the desired asymptotic wave functions behavior. Matching approach used in our code is suggested by [3].

We consider, that numerical solution  $f_j^m(r)$  is a linear combination of the normalized solutions  $fn_j^i(r)$ , each having an incoming wave with a unit current only for channel  $i$ , so that for asymptotic radius  $R$  region we can write:

$$f_j^m(R \pm h) = \sum_i a_{mi} \left\{ F_j(R \pm h) \delta_{ij} + \sqrt{\frac{k_i}{k_j}} C_{ij} [F_j(R \pm h) + i G_j(R \pm h)] \right\}. \quad (65)$$

Then, we can determine matrices

$$\begin{aligned} A_{mj} &\equiv \frac{f_j^m(R+h)G_j(R-h) - f_j^m(R-h)G_j(R+h)}{F_j(R+h)G_j(R-h) - F_j(R-h)G_j(R+h)} = \sum_i a_{mi} \left\{ \delta_{ij} + i \sqrt{\frac{k_i}{k_j}} C_{ij} \right\} \\ B_{mj} &\equiv \frac{f_j^m(R+h)F_j(R-h) - f_j^m(R-h)G_j(R-h)}{F_j(R+h)G_j(R-h) - F_j(R-h)G_j(R+h)} = - \sum_i a_{mi} \sqrt{\frac{k_i}{k_j}} C_{ij}, \end{aligned} \quad (66)$$

giving matching equations:

$$B_{mj} = - \sum_i (A_{mi} + i B_{mi}) \sqrt{\frac{k_i}{k_j}} C_{ij}. \quad (67)$$

One can see that it is necessary to invert  $(A_{mi} + i B_{mi})$  matrix with complex elements determined by Eq. (66) to get  $C_{ij}$  elements.

The normalized solutions  $fn_j^i(r)$  can be easily determined as:

$$fn_j^i(r) = - \sum_{k,m} \sqrt{\frac{k_i}{k_k}} C_{ik} B_{km}^{-1} f_j^m(r). \quad (68)$$

## 4.2 Iterative Approach to Solve a System of Coupled Equations

The algorithm described above for accurate solution of coupled-channels system is quick, but is still rather time consuming, as to get one solution with necessary asymptotic behavior we need to get  $N$  independent solutions first. "Sequential iteration method for coupled equations" - ECIS, developed by J. Raynal [34] is also realized in OPTMAN code. It is



more quicker, but faces iteration convergence problem for some specific scattering cases. We modernized this algorithm improving its convergence.

Let us rewrite Eq. (59), presenting coupling in line  $j$  of system of coupled equations as inhomogeneous term of homogeneous uncoupled equation:

$$\frac{d^2 f_j(r)}{dr^2} = V_{jj}(r)f_j(r) + \sum_{k \neq j} V_{jk}(r)f_k(r). \quad (69)$$

If we have some  $n$ -order iteration solution  $f_j^n(r)$  of Eq. (69) we can find next iteration  $f_j^{n+1}(r)$  solution by integrating step-by-step by radius the following inhomogeneous equations:

$$\frac{d^2 f_j^{n+1}(r)}{dr^2} = V_{jj}(r)f_j^{n+1}(r) + W_j(r) \quad (70)$$

with  $W_j(r) = \sum_{k \neq j} V_{jk}(r)f_k^n(r)$ . To solve the scattering problem, derived solution  $f_j^{n+1}(r)$  must have the right asymptotic physical behavior at the infinity - a plane incoming wave with a unit current for initial channels, otherwise no incoming plane wave plus a spherical outgoing wave.

First we match non-normalized derived solution  $f_j^{n+1}(r)$ , that gives:

$$f_j^{n+1}(r) = AF_{l_j}(r) + B(F_{l_j}(r) + G_{l_j}(r)). \quad (71)$$

To get the normalized  $f_j^{n+1}(r)$  with the right asymptotic form Eq. (60), let us recollect that we can add any homogeneous solution to inhomogeneous ones, and it will be still the solution of inhomogeneous one. If normalized homogeneous solution  $f_j^H(r)$  has the following asymptotic form:

$$f_j^H(r) = F_{l_j}(r) + C(F_{l_j}(r) + G_{l_j}(r)), \quad (72)$$

normalized function should be

$$f_j^{n+1} = f_j^{n+1}(r) - (A - \delta_{ij})f_j^H(r), \quad (73)$$

where  $i$  mean wave functions with scattering through ground state. It is easy to see that normalizing Eq. (73) determines  $C_{ij}$ -matrix to be:  $C_{ij} = B - C(A - \delta_{ij})$ .

Modified Numerov method [35] is applied to integrate inhomogeneous equation (70). For inhomogeneous equation:

$$f''(r) = V(r)f(r) + W(r), \quad (74)$$

the integration algorithms is:

$$\xi(r+h) = 2\xi(r) - \xi(r-h) + u(r) + [W(r+h) + 10W(r) + W(r-h)]/12$$

with  $u(r) = (h^2V(r) + h^4V^2(r)/12)\xi(r)$  and  $f(r) = \xi(r) + u(r)/12$ .

Original ECIS code [34] uses homogeneous solutions of Eq. (70) as zeroth order iteration approximation  $f_j^0(r)\delta_{ij}$ . To improve iterations convergence imaginary part of the diagonal potential  $V_{jj}(r)$  for such zeroth order iteration approximation solutions must be enlarged by a factor  $(1 + \beta_2)$ . This can be easily understood if one recollects that predictions of inelastic scattering by spherical optical model need such enlargement of the central imaginary potential to give results similar to coupled-channels predictions. Number of arithmetic operations necessary for such coupled-channels solution is  $N^2 \times M \times K \times I$ ; here  $N$ ,  $M$  and  $K$  are defined before, while  $I$  is the number of iterations necessary to convergence, it is usually not high ( $\sim 10$ ) and decreases as the incident energy increases or coupling decreases (conditions determining reliable DWBA approach, which as one can see is the first iteration results). Number of arithmetic operations necessary to solve a system of coupled equations for fixed spin  $J^\pi$  using this algorithm is almost the same as the accurate solution algorithm described before with simultaneous independent solutions integration, if number of iterations  $L \sim 10$ . But for the systems with high spin  $J^\pi$  one iteration is usually enough for solution, as absolute contribution of such states is small, so that high relative solution errors for states with such  $J^\pi$  are acceptable, that makes iteration algorithm much more effective. Nevertheless there are many special cases in which iteration procedure using homogeneous solutions of Eq. (70) as zeroth order iteration approximation do not converge. In this case we suggest to use wave functions from accurate coupled-channels solutions Eq. (68) for coupled system with truncated rank to be used as zeroth order approximations. For such functions, found with coupling of only several levels that are mostly strong coupled, number of coupled equations is small, allowing a quick solution. These solutions describe ground

and first excited states wave functions much more accurately than simple homogeneous solutions, as now ground state wave functions used as zeroth order approximation already account existence of coupling with the most strongly coupled excited levels and thus can be used as starting approximations, allowing converging the problems that do not converge in simple approach.

### 4.3 Asymptotic wave functions used to be matched with numerical solutions

Numerical solutions should be matched with Coulomb wave functions  $F_l(kr)$  and  $G_l(kr)$ , that are solutions of Eq. (56) in the outer region where nuclear potential vanishes and system becomes uncoupled. Coulomb functions are the solutions of the following equation:

$$u_l''(\rho) - \left[ l(l+1)/\rho^2 + 2\eta/\rho \mp 1 \right] u_l(\rho) = 0, \quad (75)$$

sign  $\mp$  is for the channels with positive and negative (opened and closed) channels,  $\rho = k_n r$  and  $\eta = \frac{ZZ'e^2\mu}{\hbar^2 k_n}$ . For positive energies  $F_l(kr)$  and  $G_l(kr)$  are two Coulomb functions [27] regular and irregular at  $\rho = 0$ . In case of  $\eta = 0$  they are reduced to spherical Bessel and Neuman functions multiplied by  $\rho$ :

$$\begin{aligned} F_l(\rho) &= \left(\frac{\pi\rho}{2}\right)^{1/2} J_{l+1/2}(\rho) = \rho j_l(\rho) \\ G_l(\rho) &= (-1)^l \left(\frac{\pi\rho}{2}\right)^{1/2} J_{-(l+1/2)}(\rho) = (-1)^l \rho j_{-l}(\rho) = -\rho \eta_l(\rho), \end{aligned} \quad (76)$$

that can be easily calculated by recurrence [36].

For closed channels and  $\eta > 0$  the only solution allowed from physical point of view is the Whittaker function, which is exponentially decreasing:

$$u_l(\rho) = W(-\eta, l+1/2, 2\rho). \quad (77)$$

But for matching procedures of accurate solutions of Eq. (65) and iteration ones of Eq. (71), we need also linear independent exponentially increasing solution. Both these functions are not easily calculated with high accuracy for the set of appearing  $l$ ,  $\rho$  and  $\eta$  values. On the other hand, values of decreasing and increasing functions may differ by too many orders of magnitude, that can make numerical matching inaccurate. To get the Coulomb functions

for closed channels with necessary accuracy it was decided to consider them to be unity at  $R - h$  matching point and get their values at  $R + h$  point by several step numerical integration of Eqs. (75). Such integration gives correct relative function values with very high accuracy, as integration is done on a very short variable interval of  $2h$ . The accuracy of the calculated functions is checked using Wronskian relationship:

$$F_l(\rho)G'_l(\rho) - G_l(\rho)F'_l(\rho) = \text{const}, \quad (78)$$

so that Wronskian for calculated  $F_l(\rho)$  and  $G_l(\rho)$  functions is checked to be the same at  $k(R - h)$  and  $k(R + h)$  matching points

It is quite clear that such a definition gives functions with arbitrary normalization, but for closed channels we are not interested in absolute value of appropriate  $C$ -matrix element of Eq. (60) as there is no current of scattered particles through these channels.

## 5. C-MATRIX AND COUPLED CHANNELS OPTICAL MODEL PREDICTIONS

Using the  $C$ -matrix, all optical model cross-sections can be calculated.

Differential nucleon scattering cross-section with excitation of  $n$ -th level averaged over incoming particle spin  $s$  and nuclear target spin  $I_1$  projection  $M$  (scattering of unpolarized nucleon with unpolarized target) can be calculated as:

$$\begin{aligned} \frac{d\sigma_n}{d\Omega} = & \frac{(-1)^{I_1 - I_n}}{2k_1^2(2I_1 + 1)} \sum_{\substack{j_1 j_2 j_1' j_2' l_1 l_2 \\ j_1' j_2' l_1' l_2'}} \exp[i(\sigma_{l_1'} - \sigma_{l_2'})] C_{1l_1 j_1, n l_1' j_1'}^{J_1} C_{1l_2 j_2, n l_2' j_2'}^{*J_2} \hat{J}_1^2 \hat{J}_2^2 \hat{j}_1 \hat{j}_2 \hat{j}_1' \hat{j}_2' \\ & \times \sum_{L=|l_2' - l_1'|}^{l_2' + l_1'} P_L(\cos \theta) \frac{1}{4} [1 + (-1)^{l_1 + l_2 - L}] [1 + (-1)^{l_1' + l_2' - L}] \\ & \times (j_1 j_2 1/2 - 1/2 | L 0) (j_1' j_2' 1/2 - 1/2 | L 0) W(J_1 j_1 J_2 j_2; I_1 L) W(J_1 j_1' J_2 j_2'; I_1 L) \\ & + \delta_{1n} \left\{ \frac{1}{k_1(2I_1 + 1)} \sum_{J_1 l_1} (2J_1 + 1) \text{Re} [\exp(i\sigma_{l_1}) f_c^*(\theta) C_{1l_1 j_1, n l_1 j_1}^{J_1}] P_{l_1}(\cos \theta) + |f_c(\theta)|^2 \right\}, \quad (79) \end{aligned}$$

where  $\sigma_{l_n}$  and  $\eta_n = \mu Z Z' e^2 / \hbar^2 k_n$  are the corresponding Coulomb phase shift and Sommerfeld parameter accordingly.  $f_c(\theta) = -\frac{\eta_1}{2k_1 \sin^2 \theta/2} \exp 2i[\sigma_{l_1} - \eta_1 \ln \sin \theta/2]$  is the Coulomb amplitude, which vanishes in case of neutron scattering.

Integrated scattering cross-sections  $\sigma_n$  can be derived from Eq. (79). Please note, that due to Coulomb discontinuity at zero angle, such integration is impossible for elastic proton scattering:

$$\sigma_n = \frac{2\pi}{k_1^2(2I_1 + 1)} \sum_{Jl_j l'_{j'}} (2J + 1) |C_{1l_j n l'_{j'}}^J|^2. \quad (80)$$

Total neutron cross section  $\sigma_{nT}$  is determined by optical theorem [36]:

$$\sigma_{nT} = \frac{2\pi}{k_1^2(2I_1 + 1)} \sum_{Jl_j} (2J + 1) \text{Im } C_{1l_j 1l_j}^J, \quad (81)$$

and compound formation cross section is:

$$\sigma_c = \sigma_{nT} - \sum_n \sigma_n = \frac{2\pi}{k_1^2(2I_1 + 1)} \sum_{Jl_j} (2J + 1) \left( \text{Im } C_{1l_j 1l_j}^J - \sum_{n l'_{j'}} |C_{1l_j n l'_{j'}}^J|^2 \right). \quad (82)$$

Generalized transmission coefficients are determined by Eq. (82):

$$T_{l_j}^J = 4 \left( \text{Im } C_{1l_j 1l_j}^J - \sum_{n l'_{j'}} |C_{1l_j n l'_{j'}}^J|^2 \right). \quad (83)$$

### 5.1 Legendre Polynomial Expansion of Angular Distributions of Scattered Particles

Formula (79) allows to calculate angular distributions of scattered nucleons to be compared with experimentally measured. On the other hand, OPTMAN code intends to present such angular distributions as Legendre polynomial expansion giving coefficients of such expansion to be used in evaluated nuclear data files.

According to ENDF-6 Formats Manual [37], angular distributions for neutrons (File 4, LTT=1), which is also applicable to inelastically scattered protons (File 6, LAW=2), may be presented as :

$$\frac{d\sigma_n}{d\Omega} = \frac{\sigma_n}{2\pi} \sum_{L=0}^{NL} \frac{2L+1}{2} a_L(E) P_L(\cos \theta). \quad (84)$$

One can see from formula (79) that  $a_L(E)$  are real numbers and can be presented (please note, that term with Coulomb amplitude vanishes for neutrons and inelastic proton scattering) as:

$$\begin{aligned}
a_L(E) = & \frac{2\pi(-1)^{I_1-I_n}}{\sigma_n k_1^2 (2L+1)(2I_1+1)} \sum_{\substack{J_1 J_2 j_1 j_2 l_1 l_2 \\ j'_1 j'_2 l'_1 l'_2}} \exp \left[ i(\sigma_{l'_1} - \sigma_{l'_2}) \right] C_{1l_1 j_1, n l'_1 j'_1}^{J_1} C_{1l_2 j_2, n l'_2 j'_2}^{*J_2} \widehat{J}_1^2 \widehat{J}_2^2 \widehat{j}_1 \widehat{j}_2 \widehat{j}'_1 \widehat{j}'_2 \\
& \times \frac{1}{4} \left[ 1 + (-1)^{l_1+l_2-L} \right] \left[ 1 + (-1)^{l'_1+l'_2-L} \right] \\
& \times (j_1 j_2 1/2 - 1/2 | L0) (j'_1 j'_2 1/2 - 1/2 | L0) W(J_1 j_1 J_2 j_2; I_1 L) W(J_1 j'_1 J_2 j'_2; I_1 L), \quad (85)
\end{aligned}$$

with maximum  $L$  number  $NL = \max(l'_2 + l'_1)$ .

In case of elastically scattered protons presence of Coulomb amplitude must be taken into account. According to ENDF-6 Formats Manual [37] angular distributions for protons (File 6, LAW=5) may be presented as:

$$\begin{aligned}
\frac{d\sigma_n}{d\Omega} = & \frac{\eta_1^2}{4k_1^2 \sin^4 \theta/2} - \frac{\eta_1}{\sin^2 \theta/2} \operatorname{Re} \left\{ \exp \left[ i\eta \ln (\sin^2 \theta/2) \right] \sum_{L=0}^{ML} \frac{2L+1}{2} a_L(E) P_L(\cos \theta) \right\} \\
& + \sum_{L=0}^{NL} \frac{2L+1}{2} b_L(E) P_L(\cos \theta). \quad (86)
\end{aligned}$$

Comparing ENDF-6 format formula with (79) gives  $a_L(E)$  :

$$a_L(E) = \frac{1}{k_1^2 (2L+1)(2I_1+1)} \sum_{J_1 j_1} (2J_1+1) C_{1l_1 j_1, L j_1}^{J_1}, \quad (87)$$

with maximum  $L$  number  $ML = \max(l_1)$ . These  $a_L(E)$  have complex values, while  $b_L(E)$  are real and similar to  $a_L(E)$  for neutrons:

$$\begin{aligned}
b_L(E) = & \frac{(-1)^{I_1-I_n}}{k_1^2 (2L+1)(2I_1+1)} \sum_{\substack{J_1 J_2 j_1 j_2 l_1 l_2 \\ j'_1 j'_2 l'_1 l'_2}} \exp \left[ i(\sigma_{l'_1} - \sigma_{l'_2}) \right] C_{1l_1 j_1, n l'_1 j'_1}^{J_1} C_{1l_2 j_2, n l'_2 j'_2}^{*J_2} \widehat{J}_1^2 \widehat{J}_2^2 \widehat{j}_1 \widehat{j}_2 \widehat{j}'_1 \widehat{j}'_2 \\
& \times \frac{1}{4} \left[ 1 + (-1)^{l_1+l_2-L} \right] \left[ 1 + (-1)^{l'_1+l'_2-L} \right] \\
& \times (j_1 j_2 1/2 - 1/2 | L0) (j'_1 j'_2 1/2 - 1/2 | L0) W(J_1 j_1 J_2 j_2; I_1 L) W(J_1 j'_1 J_2 j'_2; I_1 L), \quad (88)
\end{aligned}$$

with the only difference that  $b_L(E)$  coefficients are not scaled by  $\sigma_n/2\pi$  value.

## 6. ENERGY DEPENDENCE OF OPTICAL POTENTIAL PARAMETERS

Options of OPTMAN code on the energy dependence of optical potential parameters allow different possibilities. The reason is that there is significant difference for optical potentials used in spherical and CC calculations. In spherical case, optical model calculations

for a certain incident energy request the knowledge of the potential only for a specified incident energy, while CC calculations request inherent optical potential energy dependence due to account of energy losses for different coupled channels. As we intend to allow OPT-MAN CC code to analyze data in a wide energy region (at least up to 200 MeV incident energies) both for neutrons and protons simultaneously, we keep a global form of optical potential which incorporates the energy dependence of potential, that is derived by considering the dispersion relationship as proposed by Delaroche *et al.* [38], and the high-energy saturation behavior consistent with the Dirac phenomenology. The imaginary components of this potential form vanish at Fermi energy (property stemming from nuclear matter theory). Such an energy dependence allows data analysis without unphysical discontinuities in the whole energy range of interest both for neutrons and protons (constant potential terms, allowing simple potential linear dependencies, shown by bold characters below for imaginary surface, volume and spin-orbit potentials, can be also used, but please note that being non-zero, they do not vanish at Fermi energies):

$$V_R = (V_R^0 + V_R^1 E^* + V_R^2 E^{*2} + V_R^3 E^{*3} + V_R^{DISP} e^{-\lambda_R E^*}) \left[ 1 + \frac{1}{V_R^0 + V_R^{DISP}} (-1)^{Z'+1} C_{viso} \frac{A - 2Z}{A} \right] + C_{coul} \frac{ZZ'}{A^{1/3}} \varphi_{coul}(E^*), \quad (89)$$

$$W_D = \left[ W_D^{DISP} + (-1)^{Z'+1} C_{viso} \frac{A - 2Z}{A} \right] e^{-\lambda_D E^*} \frac{E^{*S}}{E^{*S} + WID_D^S} + \mathbf{W}_D^0 + \mathbf{W}_D^1 E^*, \quad (90)$$

$$W_V = W_V^{DISP} \frac{E^{*S}}{E^{*S} + WID_V^S} + \mathbf{W}_V^0 + \mathbf{W}_V^1 E^*, \quad (91)$$

$$V_{SO} = V_{SO}^0 e^{-\lambda_{so} E^*}, \quad (92)$$

$$W_{SO} = W_{SO}^{DISP} \frac{E^{*S}}{E^{*S} + WID_{SO}^S} + \mathbf{W}_{SO}^0 + \mathbf{W}_{SO}^1 E^*. \quad (93)$$

Here,  $E^* = (E_p - E_{fm})$ , with  $E_p$  - energy of the projectile and  $E_{fm}$  - the Fermi energy, determined as  $E_{fm}(Z, A) = -\frac{1}{2} [S_n(Z, A) + S_n(Z, A + 1)]$  for neutrons and  $E_{fm}(Z, A) = -\frac{1}{2} [S_p(Z, A) + S_p(Z + 1, A + 1)]$  for protons, where  $S_i(Z, A)$  denotes the separation energy of nucleon  $i$  from a nucleus labeled by  $Z$  and  $A$ , while  $Z'$ ,  $Z$  and  $A$  are charges of incident particle, nucleus and nucleus mass number, respectively. As we intend to analyze neutron and proton scattering data simultaneously, we want to have unique optical potential for nucleons with form suggested by Ref. [38] plus a term  $C_{coul} ZZ'/A^{1/3} \varphi_{coul}(E^*)$  describing the Coulomb

correction to the real optical potential and isospin terms  $(-1)^{Z'+1}C_{viso}(A-2Z)/A\varphi_{viso}(E^*)$  and  $(-1)^{Z'+1}C_{wiso}(A-2Z)/A\cdot\varphi_{wiso}(E^*)$ . We assumed that energy dependences of  $\varphi_{viso}(E^*)$  and  $\varphi_{wiso}(E^*)$  are the same as those of real and imaginary surface potentials (see Eq. (89,90)), while  $\varphi_{coul}(E^*)$  can be constant (just unity) or considered to be the minus derivative of Eq. (89) , so that

$$\varphi_{coul}(E_p) = (\lambda_R V_R^{DISP} e^{-\lambda_R E^*} - V_R^1 - 2V_R^2 E^* + 3V_R^3 E^*) \left[ 1 + \frac{1}{V_R^0 + V_R^{DISP}} (-1)^{Z'+1} C_{viso} \frac{A-2Z}{A} \right]. \quad (94)$$

The parameters  $WID_D$ ,  $WID_V$ ,  $W_D^{DISP}$ ,  $W_V^{DISP}$ ,  $W_{SO}^{DISP}$ ,  $\lambda_D$  and  $\lambda_R$  were taken to be equal for neutrons and protons. We consider, that Lane model [39] works, therefore the neutron-proton optical potential difference of the suggested potential stems from the isospin terms, the Coulomb correction terms and difference of the neutron-proton Fermi energies.

Real  $r_R$  and Coulomb  $r_C$  potential radii can be considered to be energy dependent as experimental data analyses [8,38] indicate dispersion-like energy dependence:

$$r_R(E^*) = r_R^0 \left[ 1 - \frac{C_R E^{*S}}{E^{*S} + WID_R^S} \right] \quad (95)$$

$$r_C(E^*) = r_C^0 \left[ 1 - \frac{C_C E^{*S}}{E^{*S} + WID_C^S} \right] \quad (96)$$

Potential diffusenesses  $a_i$  can be energy dependent, reflecting that they may grow or decrease with nuclear excitation energy:

$$a_i = a_i^0 + a_i^1 E^* \quad (97)$$

with  $a_D^1$  assumed to be zero above an energy  $E_{bound}$ .

If energy losses due to collective levels excitation as compared to the nucleon incident energies involved in the analysis are noticeable, the dependence of the local optical potential for different channels can be taken into account as:

$$V_{if} = V \left( E_p - \frac{E_i + E_f}{2} \right),$$

where  $i$  and  $f$  denote initial and final channels, while  $E_i$  and  $E_f$  the corresponding level energies.



## 7. RELATIVISTIC GENERALIZATION OF NON-RELATIVISTIC SCHRÖDINGER EQUATION

Upper boundary of incident energy of the OPTMAN code is supposed to be about 200 MeV, so our non-relativistic Schrödinger formalism involved relativistic generalization suggested by Elton [40]. The nucleon wave number  $k$  was taken in the relativistic form:

$$(\hbar k)^2 = [E^2 - (M_p c^2)^2]/c^2 \quad (98)$$

where  $E$  denotes the total energy of projectile,  $M_p$  the projectile rest mass, and  $c$  the light velocity. To allow non-relativistic motion of the target with rest mass  $M_T$ , incident particle mass  $M_p$  was replaced with the relativistic projectile energy  $E$  in reduced mass formulae, so that the quantity  $k$  and optical potential values were multiplied by a coefficient:

$$\frac{1}{1 + E/(M_T c^2)} \quad (99)$$

Following Elton's [40] suggestions, we multiply optical potential strengths except for the spin-orbit and Coulomb terms by a factor  $K(E)$ , as a relativistic optical potential generalization. Elton [40] suggests it to be  $E/(M_p c^2)$ . Therefore, the factor grows without limit as the projectile energy  $E$  grows. We use this factor as suggested by Madland [41],  $K(E) = 2E/(E + M_p c^2)$ , which saturates at 2 as incident energy grows, as it looks more physical and allows easier fitting of experimental data. Of course, optical potential can be in any case fitted to the experimental data without such multiplier, so that such relativistic correction can be included while fitting. However, we agree with Elton [40] that "it is advantageous to separate out known relativistic factor in the central potential", as this may allow successful extrapolation of optical potential from low incident projectile energy region to higher and *vice versa*. One can see that for low energies all these relativistic generalization factors have non-relativistic kinematic limit.

## 8. POTENTIAL ADJUSTMENT

Such best fit optical potential parameters can be found by automatic minimization of  $\chi^2$  value:

$$\chi^2 = \frac{1}{N + M + L + 3} \left[ \sum_{i=1}^N \frac{1}{K_i} \sum_{j=1}^{K_i} \left( \frac{d\sigma_{ij}/d\Omega_{calc} - d\sigma_{ij}/d\Omega_{exp}}{\Delta\sigma_{ij}/d\Omega_{exp}} \right)^2 + \sum_{i=1}^M \left( \frac{\sigma_{tot_{calc_i}} - \sigma_{tot_{eval_i}}}{\Delta\sigma_{tot_{eval_i}}} \right)^2 \right] \\ + \sum_{i=1}^L \left( \frac{\sigma_{reac_{calc_i}} - \sigma_{reac_{eval_i}}}{\Delta\sigma_{reac_{eval_i}}} \right)^2 + \left( \frac{S_{cal}^0 - S_{eval}^0}{\Delta S_{eval}^0} \right)^2 + \left( \frac{S_{cal}^1 - S_{eval}^1}{\Delta S_{eval}^1} \right)^2 + \left( \frac{R'_{cal} - R'_{eval}}{\Delta R'_{eval}} \right)^2, \quad (100)$$

here  $K_i$  is the number of angles for which angular distribution is measured for incident energy  $i$ , and the number of such energies is  $N$ , while numbers of total and reaction cross-section data are  $M$  and  $L$ , respectively. The symbols  $S^0$ ,  $S^1$  and  $R'$  denote s-, p-wave strength functions and scattering radius, respectively. All the other optical observable, if any, can be also included in  $\chi^2$  search criteria.

## 9. ANALYSIS OF B(E2) DATA

The  $\gamma$ -transition probability  $B(E\lambda)$  of soft rotator model can also be calculated. For instance  $B(E2)$  calculated in homogeneously charged deformed ellipsoid approximation accounting linear terms of inner  $b_{2\mu}$  dynamic variables (higher terms can be taken into consideration, see ([25]) is

$$B(E2; I\tau n_\gamma n_{\beta_3} n_{\beta_2} \rightarrow I'\tau' n'_\gamma n'_{\beta_3} n'_{\beta_2}) = \frac{5Q_0^2}{16\pi} \left\{ \sum_{K,K' \geq 0} \frac{A_{IK}^\tau A_{I'K'}^{\tau'}}{[(1 + \delta_{0K})(1 + \delta_{0K'})]^{1/2}} \right. \\ \times [\langle n_\gamma | \cos \gamma | n'_\gamma \rangle [(I'2K'0|IK) + (-1)^{I'}(I'2 - K'0|IK)\delta_{K0}] \delta_{KK'} \\ + \sqrt{1/2} \langle n_\gamma | \sin \gamma | n'_\gamma \rangle [(I'2K'2|IK)\delta_{K,K'+2} + (I'2K' - 2|IK)\delta_{K,K'-2} \\ \left. + (-1)^{I'}(I'2 - K'2|IK)\delta_{K,2-K'}] \right\}^2 \left[ J_{\substack{I\tau n_\gamma n_{\beta_3} n_{\beta_2} \\ I'\tau' n'_\gamma n'_{\beta_3} n'_{\beta_2}}} [y] \right]^2, \quad (101)$$

here  $J_{\substack{I\tau n_\gamma n_{\beta_3} n_{\beta_2} \\ I'\tau' n'_\gamma n'_{\beta_3} n'_{\beta_2}}} [y]$  is enhancement factor due to nuclei softness determined by Eq.(41).

## 10. CONCLUSION

According to the ISTC B-521 Project's Working Plan we finalized modernizing OPT-MAN code's computational approaches and new, more accurate numerical algorithms became possible now due to available large computational resources. We developed two modernized algorithms for solution of coupled channels equations in scattering problem. First is

the accurate system solution, which is 6-20 times faster than previously used. Second quick solution algorithm is the iteration one with the improved convergence. We also improved the accuracy of matching procedure in case of charged scattered particles. More grounded optical potential parameters dependences guided by physical principles made it possible a global optical potential search. All the algorithms are already included in the currently modernized code OPTMAN. Users of the code can choose one of these algorithms when running optical calculations. Instead, OPTMAN code has a capability to select the optimal option, depending on the number of couple equations, on the coupling strength, incident particle energy, and system spin. Current version of modernized OPTMAN code was used to find best fit nuclear optical parameters for  $^{12}\text{C}$  [11],  $^{24,26}\text{Mg}$  [42],  $^{28-30}\text{Si}$  [12] and  $^{52}\text{Cr}$  [13]. They are already used for predictions of cross sections for  $^{12}\text{C}$ , natural Si and Mg for Japanese high energy nuclear data evaluation.

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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 <sup>-1</sup>
力	ニュートン	N	m·kg/s <sup>2</sup>
圧 力 , 応 力	パスカル	Pa	N/m <sup>2</sup>
エネルギー, 仕事, 熱量	ジュール	J	N·m
工 率 , 放 射 束	ワ ッ ト	W	J/s
電 気 量 , 電 荷	クーロン	C	A·s
電位, 電圧, 起電力	ボ ル ト	V	W/A
静 電 容 量	ファラド	F	C/V
電 気 抵 抗	オ ー ム	Ω	V/A
コンダクタンス	ジーメンズ	S	A/V
磁 束	ウェーバ	Wb	V·s
磁 束 密 度	テ ス ラ	T	Wb/m <sup>2</sup>
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 <sup>2</sup>
放 射 能	ベクレル	Bq	s <sup>-1</sup>
吸 収 線 量	グレイ	Gy	J/kg
線 量 当 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

$$1 \text{ eV} = 1.60218 \times 10^{-19} \text{ J}$$

$$1 \text{ u} = 1.66054 \times 10^{-27} \text{ kg}$$

表 4 SI と共に暫定的に維持される単位

名 称	記 号
オングストローム	Å
バ ー ン	b
バ ー ル	bar
ガ ル	Gal
キ ュ リ ー	Ci
レ ント ゲ ン	R
ラ ヌ ー	rad
レ ム	rem

$$1 \text{ Å} = 0.1 \text{ nm} = 10^{-10} \text{ m}$$

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

$$1 \text{ bar} = 0.1 \text{ MPa} = 10^5 \text{ Pa}$$

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

$$1 \text{ Ci} = 3.7 \times 10^{10} \text{ Bq}$$

$$1 \text{ R} = 2.58 \times 10^{-4} \text{ C/kg}$$

$$1 \text{ rad} = 1 \text{ cGy} = 10^{-2} \text{ Gy}$$

$$1 \text{ rem} = 1 \text{ cSv} = 10^{-2} \text{ Sv}$$

表 5 SI 接頭語

倍数	接頭語	記 号
10 <sup>18</sup>	エクサ	E
10 <sup>15</sup>	ペタ	P
10 <sup>12</sup>	テラ	T
10 <sup>9</sup>	ギガ	G
10 <sup>6</sup>	メガ	M
10 <sup>3</sup>	キロ	k
10 <sup>2</sup>	ヘクト	h
10 <sup>1</sup>	デカ	da
10 <sup>-1</sup>	デシ	d
10 <sup>-2</sup>	センチ	c
10 <sup>-3</sup>	ミリ	m
10 <sup>-6</sup>	マイクロ	μ
10 <sup>-9</sup>	ナノ	n
10 <sup>-12</sup>	ピコ	p
10 <sup>-15</sup>	フェムト	f
10 <sup>-18</sup>	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, 1 eV および 1 u 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 では流体の圧力を表わす場合に限り表 2 のカテゴリーに分類されている。
- EC 閣僚理事会指令では bar, barn および「血圧の単位」mmHg を表 2 のカテゴリーに入れている。

換 算 表

力	N (=10 <sup>5</sup> dyn)	kgf	lbf
	1	0.101972	0.224809
	9.80665	1	2.20462
	4.44822	0.453592	1

$$\text{粘 度 } 1 \text{ Pa} \cdot \text{s} (\text{N} \cdot \text{s/m}^2) = 10 \text{ P (ポアズ)} (\text{g}/(\text{cm} \cdot \text{s}))$$

$$\text{動粘度 } 1 \text{ m}^2/\text{s} = 10^4 \text{ St (ストークス)} (\text{cm}^2/\text{s})$$

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

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

$$1 \text{ cal} = 4.18605 \text{ J (計量法)}$$

$$= 4.184 \text{ J (熱化学)}$$

$$= 4.1855 \text{ J (15 °C)}$$

$$= 4.1868 \text{ J (国際蒸気表)}$$

$$\text{仕事率 } 1 \text{ PS (仏馬力)}$$

$$= 75 \text{ kgf} \cdot \text{m/s}$$

$$= 735.499 \text{ W}$$

放射能	Bq	Ci
	1	2.70270 × 10 <sup>-11</sup>
	3.7 × 10 <sup>10</sup>	1

吸収線量	Gy	rad
	1	100
	0.01	1

照射線量	C/kg	R
	1	3876
	2.58 × 10 <sup>-4</sup>	1

線量当量	Sv	rem
	1	100
	0.01	1

