Capture cross section with quantum diffusion approach

V.V.Sargsyan[a,b], S.Yu.Grigoryev [a,*], G.G.Adamian,[a,**], N.V.Antonenko[a]

[a] *Joint Institute for Nuclear Research, 141980 Dubna, Russia*
[b] *Institut für Theoretische Physik der Justus–Liebig–Universität, D–35392 Giessen, Germany*

Abstract

A C++ code for calculating the capture of a projectile by target nucleus is presented. The model is based on the quantum diffusion approach developed for considering collisions of nuclei at energies below and just above the Coulomb barrier. The code provides the capture cross sections and other characteristics as functions of $E_{\rm c.m.}$. The formalism of the model is briefly described. Also the code uses the Fortran subroutine to calculate the nucleus-nucleus potential.

Keywords: sub-barrier fusion, dissipative dynamics, S-factor

PACS: 25.70.Ji, 24.10.Eq, 03.65.-w

PROGRAM SUMMARY

Title of program: NeutronPairTransferCapture

Version: 1.0

Catalogue number:

Program obtained from: `http://intel-robot.ru/external/www5/`

* *E-mail address:* grigorsu@gmail.com

** *E-mail address:* adamian@theor.jinr.ru

E-mail: grigorsu@gmail.com, sargsyan@theor.jinr.ru

License: GNU Public License

Computers: all

Operating system: tested on Linux Ubuntu 14.04, 16.04, Debian 8.0

Compilator: GNU Fortran (Debian 4.9.2-10) 4.9.2, g++ (Debian 4.9.2-10) 4.9.2, MinGW 4.9.2

Program language: C++, Fortran

Memory required to execute: depending on the complexity of the problem, at least 64 MB RAM recommended

Other programs called: GSL-2.2.1 GNU Scientific Library in C++ is required. It is available from https://www.gnu.org/software/gsl .

External files needed: none

Keywords: Neutron-pair transfer

Nature of the physical problem: ....

Method of solution: ....

Restrictions on complexity of the problem: Usually limited only by the available memory.

Typical running time: several seconds up to 10 minutes, depending on HardWare.

* Items marked with an asterisk are only required for new versions of programs previously published in the CPC Program Library.

1. Model

1.1. The capture cross

In our model the collision of nuclei is considered in terms of a single collective variable: the relative distance R between the centers of colliding nuclei. Besides the dissipation of kinetic energy of the radial motion there is dissipation of angular momentum, i.e. the approach of the sticking limit [2, 3]. Because the dissipation of angular momentum mainly occurs behind the Coulomb barrier, for simplicity, it can be disregarded to treat the passage of this barrier. The nuclear deformation effects are taken into consideration through the dependence of the nucleus-nucleus potential on the deformations and orientations of colliding nuclei. Thus, the total cross section of the capture of projectile by a target nucleus reads as the sum of partial capture cross sections

$$\begin{aligned}\sigma_{\rm cap}(E_{\rm c.m.}) &= \sum_L \sigma_{\rm cap}(E_{\rm c.m.}, L) \\ &= \pi\lambda\!\!\!^{-2} \sum_L (2L+1) \int_0^{\pi/2} d\theta_1 \sin(\theta_1) \int_0^{\pi/2} d\theta_2 \sin(\theta_2) P_{\rm cap}\left(E_{\rm c.m.}, L, \theta_1, \theta_2\right)\end{aligned} \quad (1)$$

where $\lambda\!\!\!^{-2} = \hbar^2/(2\mu E_{\rm c.m.})$ is the reduced de Broglie wavelength, $\mu = m_0 A_1 A_2/(A_1 + A_2)$ is the reduced mass (m_0 is the nucleon mass), and the summation is in possible values of angular momentum L at given bombarding energy $E_{\rm c.m.}$. Knowing the potential of the interacting nuclei for each orientation at a given L, and the influence of intrinsic excitation of nuclei on the dynamics of relative distance R, one can obtain the partial capture probability $P_{\rm cap}$, which is the probability of passing the potential barrier.

In general case the capture probability $P_{\rm cap}$ is obtained by integrating the propagator G from the initial state (R_0, P_0) at time $t = 0$ to the final state (R, P) at time t:

$$P_{\rm cap} = \lim_{t\to\infty} \int_{-\infty}^{r_{\rm in}} dR \int_{-\infty}^{\infty} dP G(R, P, t|R_0, P_0, t = 0). \tag{2}$$

Here, $r_{\rm in}$ is the internal turning point of the nucleus-nucleus potential $V(R, Z_i, A_i, \theta_i, L)$ for $E_{\rm c.m.}$ smaller than the height $V_b = V(R_b, Z_i, A_i, \theta_i, L)$ of the Coulomb barrier. To obtain analytical expressions for the capture cross-section, we use the following procedure. For each angular momentum L and given orientation angles θ_i, the realistic nucleus-nucleus potential is calculated and the classical action is found for this potential. Then the value of $P_{\rm cap}\,(E_{\rm c.m.}, L, \theta_1, \theta_2)$ is analytically calculated for the inverted oscillator potential which has the same barrier height V_b and classical action. So, the frequency Ω of this oscillator is defined from the condition of equality of the classical actions and depends on $E_{\rm c.m.}$, L, and θ_i. If the initial energy of colliding nuclei is above the potential barrier at $R = R_b$, then we set $\Omega = \sqrt{-\frac{1}{\mu}\frac{\partial^2 V(R)}{\partial R^2}\Big|_{R_b}}$.

As shown in Ref. [7], in the case of inverted oscillator the propagator G has the following form:

$$G = \pi^{-1} |\det \mathbf{\Sigma}^{-1}|^{1/2} \exp(-\mathbf{q}^T \mathbf{\Sigma}^{-1} \boldsymbol{q}) \tag{3}$$

where $q_R(t) = R - \overline{R(t)}$, $q_P(t) = P - \overline{P(t)}$, $\overline{R(t=0)} = R_0$, $\overline{P(t=0)} = P_0$, $\Sigma_{ij}(t) = 2\overline{q_i(t) q_j(t)}$, $\Sigma_{ij}(t=0) = 0$, $i, j = R, P$. Using Eqs. (2) and (3), we find a simple expression for the capture cross-section:

$$P_{\rm cap} = \lim_{t\to\infty} \frac{1}{2} {\rm erfc}\left[\frac{-r_{\rm in} + \overline{R(t)}}{\sqrt{\Sigma_{RR}(t)}}\right]. \tag{4}$$

So, the main ingredients of our calculation are the nucleus-nucleus potential and time dependencies of $\overline{R(t)}$ and $\Sigma_{RR}(t)$.

1.2. The nucleus-nucleus potential

The potential describing the interaction of two nuclei can be written in the form [1]

$$V(R, Z_i, A_i, \theta_i, L) = V_{\rm C}(R, Z_i, A_i, \theta_i) + V_{\rm N}(R, Z_i, A_i, \theta_i) + \frac{\hbar^2 L(L+1)}{2\mu R^2}, \quad (5)$$

where $V_{\rm N}$, $V_{\rm C}$, and the last summand stand for the nuclear, the Coulomb, and the centrifugal potentials, respectively. The nuclei are proposed to be spherical or deformed. The potential depends on the distance R between the center of mass of two interacting nuclei, mass A_i and charge Z_i of nuclei ($i = 1, 2$), the orientation angles θ_i of the deformed (with the quadrupole deformation parameters β_i) nuclei and the angular momentum L.

For the nuclear part of V, we use the double-folding formalism

$$V_{\rm N} = \int \rho_1(\mathbf{r_1})\rho_2(\mathbf{R} - \mathbf{r_2})F(\mathbf{r_1} - \mathbf{r_2})d\mathbf{r_1}d\mathbf{r_2}, \quad (6)$$

where $F(\mathbf{r_1} - \mathbf{r_2}) = C_0[F_{\rm in}\frac{\rho_0(\mathbf{r_1})}{\rho_{00}} + F_{\rm ex}(1 - \frac{\rho_0(\mathbf{r_1})}{\rho_{00}})]\delta(\mathbf{r_1} - \mathbf{r_2})$ is the density-depending effective nucleon-nucleon interaction and $\rho_0(\mathbf{r}) = \rho_1(\mathbf{r}) + \rho_2(\mathbf{R} - \mathbf{r})$, $F_{\rm in,ex} = f_{\rm in,ex} + f'_{\rm in,ex}\frac{(N_1-Z_1)(N_2-Z_2)}{(N_1+Z_1)(N_2+Z_2)}$, $\rho_1(\mathbf{r_1})$, N_1, Z_1 and $\rho_2(\mathbf{r_2})$, N_2, Z_2 are the nucleon densities, neutron numbers, charge numbers of, respectively, the projectile and the target nucleus. Note, that the parameters of effective nucleon-nucleon interaction are fixed and set: $C_0 = 300$ MeV fm^3, $f_{\rm in} = 0.09$, $f_{\rm ex} = -2.59$, $f'_{\rm in} = 0.42$, $f'_{\rm ex} = 0.54$ and $\rho_{00} = 0.17$ fm^{-3}. The nucleus-nucleus potential [1] used here naturally contains the repulsive part because of the density-dependent nucleon-nucleon forces in Eq. (6). Note, that as the

centrifugal part of the potential grows, the pocket depth becomes smaller and the position of the potential pocket minimum moves towards the barrier of the hight $V_b = V(R_b)$ at $R = R_b$. The value of R_b is approximately equal to $R_1 + R_2 + 2$ fm where R_1 and R_2 are the radii of colliding nuclei, $R_i = r_0 A_i^{1/3}$. The program provides us the values of V_b and R_b for spherical nuclei. Because there are some uncertainties in the calculation of the potential, the program allows us also to enter the user value of V_b for spherical nuclei. In this case the calculated nucleus-nucleus potential is correspondingly shifted.

The densities of the nuclei are taken in the two-parameter symmetrized Woods-Saxon form. The nuclear radius parameter r_0 and the diffuseness parameters a_i can depend on the charge and mass numbers of the nuclei [1].

The Coulomb interaction of two deformed nuclei with the quadrupole deformation parameters β_i is as follows

$$V_{\rm C}(R, Z_i, A_i, \theta_i) = \frac{Z_1 Z_2 e^2}{R} + \\ + \left(\frac{9}{20\pi}\right)^{1/2} \frac{Z_1 Z_2 e^2}{R^3} \sum_{i=1,2} R_i^2 \beta_i \left[1 + \frac{2}{7}\left(\frac{5}{\pi}\right)^{1/2} \beta_i\right] P_2(\cos\theta_i) \qquad (7)$$

where $P_2(\cos\theta_i)$ is the Legendre polynomial.

In the calculations of nucleus-nucleus potential the parameters of effective nucleon-nucleon interaction are fixed for all nuclei. We set the nuclear radius parameter $r_0 = 1.15$ fm and the diffuseness parameter $a = 0.48$ fm for the He, $a = 0.5$ fm for the Li, $a = 0.53$ fm for $4 \leq Z \leq 9$, $a = 0.55$ fm for $10 \leq Z \leq 88$ and $a = 0.56$ fm for $Z \geq 89$.

1.3. Quantum non-Markovian dynamics

The Hamiltonian H of two colliding nuclei explicitly depends on R, the canonically conjugate collective momentum P, and the internal degrees of

freedom [8, 9]. If the coupling between the collective subsystem and the thermostat is realized in terms of the collective coordinate R and the internal coordinates q_ν, then the total Hamiltonian of the system is written as

$$\begin{aligned} H &= H_c + H_b + H_{cb}, \\ H_c &= \frac{1}{2\mu}P^2 - \frac{\mu\omega^2}{2}R^2, \\ H_b &= \sum_\nu \hbar\omega_\nu b_\nu^+ b_\nu, \\ H_{cb} &= \frac{\kappa}{\hbar}\lambda^{1/2}R\sum_\nu \Gamma_\nu(b_\nu^+ + b_\nu) + \frac{\kappa^2}{\hbar^2}\lambda R^2\sum_\nu \frac{|\Gamma_\nu|^2}{\hbar\omega_\nu}. \end{aligned} \tag{8}$$

Here, b_ν^+ and b_ν are the phonon creation and annihilation operators describing the internal excitations at energy $\hbar\omega_\nu$. The operators H_c and H_b are the Hamiltonians of the collective and internal subsystems, respectively. The first term in H_{cb} describes the coupling between the collective motion and the internal excitations and is the source of the dissipation term in the equations for the operators of collective variables. For example, in the description of nuclear interaction at low energies, this term corresponds to the effect of the mean field of each nucleus on the one-particle motion in other nucleus. In Eq. (8), Γ_ν is the coupling constant between the collective subsystem and the internal coordinates, and λ is a parameter determining an average force of coupling to the thermostat, $\kappa = (2\mu\omega\lambda/\hbar)^{1/2}$. The additional term in H_{cb} compensates for the potential renormalization appearing because the collective and internal subsystems are coupled [8]. Our aim is to derive and analytically solve the Langevin equations for the collective operators R and P. The quadratic Hamiltonian admits an exact solution of the equations of motion for the collective coordinates.

Using Hamiltonian (8), we obtain the system of integro-differential stochastic equations (the system of generalized nonlinear Langevin equations) [5]

$$\begin{aligned}\dot{R}(t) &= \frac{P(t)}{\mu},\\ \dot{P}(t) &= -\mu\omega^2 R(t) - \kappa^2 \int\limits_0^t d\tau K(t-\tau)\dot{R}(\tau) + \kappa F(t). \end{aligned} \tag{9}$$

The integral term in these equations means that the considered system is non-Markovian and has some memory over the trajectory preceding the instant t. As seen from the equation for $P(t)$, the coupling term of the Hamiltonian results in the random momentum-related force,

$$\begin{aligned} F(t) &= F_p(t)/\kappa = -\frac{\lambda^{1/2}}{\hbar}\sum_\nu \Gamma_\nu[f_\nu^+(t) + f_\nu(t)] = \sum_\nu F^\nu(t),\\ f_\nu^+(t) &= [b_\nu^+(0) + \frac{1}{\hbar^2\omega_\nu}\kappa\lambda^{1/2}\Gamma_\nu]e^{i\omega_\nu t}, \end{aligned} \tag{10}$$

and a dissipation kernel,

$$K(t-\tau) = \frac{2\lambda}{\hbar^2}\sum_\nu \frac{\Gamma_\nu^2}{\hbar\omega_\nu}\cos(\omega_\nu[t-\tau]). \tag{11}$$

As seen from Eqs. (10) and (11), the random force and the dissipation kernel are independent of the dynamical coordinates and momenta. The temperature and fluctuations are related to the distribution of the initial coordinates and momenta in the internal subsystem (at $t = 0$). The random force operators F^ν are identified with the fluctuations because the initial conditions for the thermostat operators are ambiguous. These fluctuations have zero mean values and nonzero variances [10].

To solve Eqs. (9) analytically, we use the Laplace transform method. After finding expressions for the images, we obtain explicit expressions for

the originals,

$$R(t) = A_t R(0) + B_t P(0) + \kappa \int_0^t d\tau B_\tau F(t-\tau),$$

$$P(t) = M_t R(0) + N_t P(0) + \kappa \int_0^t d\tau N_\tau F(t-\tau), \tag{12}$$

where

$$\begin{aligned} B_t &= \frac{1}{\mu}\mathcal{L}^{-1}\left[\frac{1}{s^2 + 2\hbar\omega s K(s) + \tilde{\delta}/\mu}\right], \\ A_t &= \mathcal{L}^{-1}\left[\frac{s + 2\hbar\omega K(s)}{s^2 + 2\hbar\omega s K(s) + \tilde{\delta}/\mu}\right] = \mu\dot{B}_t + \kappa^2 \int_0^t d\tau B_\tau K(t-\tau), \\ M_t &= -\mu\tilde{\delta} B_t, \\ N_t &= \mu\dot{B}_t. \end{aligned} \tag{13}$$

Here, $\mathcal{L}^{-1}$ denotes the inverse Laplace transform, and $K(s)$ is the image of the dissipation kernel $K(t)$. The symbols t and τ indicate the temporal dependence and $\tilde{\delta} = -\mu\omega^2$.

As follows from Eq. (4), to obtain the capture cross-section one need to know the first and second moments for the collective coordinate $R(t)$: $\overline{R(t)}$ and $\Sigma_{RR}(t)$. From Eq. (12) we have for the first moments

$$\begin{aligned} \overline{R(t)} &= A_t \overline{R(0)} + B_t \overline{P(0)}, \\ \overline{P(t)} &= M_t \overline{R(0)} + N_t \overline{P(0)}, \end{aligned} \tag{14}$$

and for the second moment

$$\begin{aligned} \frac{1}{2}\Sigma_{RR}(t) &= \sigma_{RR} = \overline{R(t)^2} - \overline{R(t)}^{\,2} \\ = A_t^2 \sigma_{RR}(0) &+ A_t B_t \sigma_{RP}(0) + B_t^2 \sigma_{PP}(0) + J_{RR}(t) \end{aligned} \tag{15}$$

where

$$J_{RR}(t) = \frac{2\omega\mu\lambda}{\hbar}\sum_{\nu}|\Gamma_{\nu}|^2\coth\left[\frac{\hbar\omega_{\nu}}{2T}\right]\times$$
$$\times \int_0^t d\tau^{'}B_{\tau^{'}}\int_0^t d\tau^{''}B_{\tau^{''}}\cos[\omega_{\nu}(\tau^{'}-\tau^{''})]. \quad (16)$$

To set the initial energy of the colliding nuclei, we take $\sigma_{RR}(0) = \sigma_{RP}(0) = \sigma_{PP}(0) = 0$. To define the initial values of $\overline{R(0)}$ and $\overline{P(0)}$, we consider two regime of interactions. At large R, where the nuclei are well separated, the friction does not play a significant role. When the nuclei approach each other, the dynamics of the colliding nuclei strongly depends on friction and diffusion. So, the dependence of friction on R is taken in a simple way. The interaction parameter $R = R_{\rm int} = 1.1$ fm is introduced. If the initial energy of colliding nuclei is less than $E_{\rm c.m.} < V(R_b + R_{\rm int})$, we set $\overline{P(0)} = 0$ and find $\overline{R(0)}$ from the equality

$$-\frac{\mu\Omega^2}{2}\overline{R(0)}^2 = E_{\rm c.m.} - V_b.$$

In this case the friction plays a negligible role in the transition through the barrier. If $E_{\rm c.m.} > V(R_b + R_{\rm int})$, we set $\overline{R(0)} = R_{\rm int}$ and find $\overline{P(0)}$ from the condition

$$\frac{\overline{P(0)}^2}{2\mu} - \frac{\mu\Omega^2}{2}R_{\rm int}^2 = E_{\rm c.m.} - V_b.$$

To obtain analytical expressions, in the expressions above the sums $\sum_{\nu}...$ are replaced by the integral $\int_0^{\infty} dw g(w)...$ over the frequency with the density $g(w)$ of states for the thermostat (see [10, 5]). So,

$$\frac{g(w)|\Gamma(w)|^2}{\hbar^2 w} = \frac{\gamma^2}{\pi(\gamma^2 + w^2)},$$

and

$$K(t) = \frac{\lambda\gamma}{\hbar} e^{-\gamma|t|}$$

from Eq. (11). This choice of $g(w)$ is justified because it results in the Markovian limit at $\gamma \to \infty$. Substituting the image

$$K(s) = \frac{\lambda\gamma}{\hbar(s+\gamma)}$$

of the dissipation kernel in (13) and (16), we obtain

$$\begin{aligned} B_t &= \sum_{i=1}^{3} B_t^i = \frac{1}{\mu} \sum_{i=1}^{3} \beta_i (s_i + \gamma) e^{s_i t}, \\ A_t &= \sum_{i=1}^{3} \beta_i [s_i(s_i+\gamma) + 2\omega\lambda\gamma] e^{s_i t}, \end{aligned} \tag{17}$$

$$\begin{aligned} J_{RR}(t) &= \frac{2\omega\lambda}{\pi\mu} \int_0^\infty dw \frac{\gamma^2 w}{\gamma^2 + w^2} \coth(\hbar w/(2T)) \times \\ &\times \sum_{i,j} \beta_i \beta_j (s_i+\gamma)(s_j+\gamma) \psi(s_i, s_j, w, t), \end{aligned} \tag{18}$$

where s_i, $i = 1, 2, 3$, are the roots of the equation

$$(s+\gamma)(s^2 - \omega^2) + 2\omega\lambda\gamma s = 0, \tag{19}$$

where $\beta_1 = 1/[(s_1 - s_2)(s_1 - s_3)]$, $\beta_2 = 1/[(s_2 - s_1)(s_2 - s_3)]$, $\beta_3 = 1/[(s_3 - s_1)(s_3 - s_2)]$, and

$$\psi(s_i, s_j, w, t) = \int_0^t d\tau' e^{s_i \tau'} \int_0^t d\tau'' e^{s_j \tau''} \cos[w(\tau' - \tau'')], \tag{20}$$

can be analytically calculated. Note, that Eqs. (14) and (18) with Eq. (17) completely determine the dynamics of collective subsystem. They are used to find $\overline{R(t)}$ and $\Sigma_{RR}(t)$.

Because the relaxation time for the internal subsystem is much shorter than that for collective motion, the condition $\gamma \gg \Omega$ should be fulfilled. Note, that the non-Markovian effects appear in the calculations through the internal-excitation width γ. This parameter characterizes the density of nuclear states. We set $\hbar\gamma = 12$ MeV for the nuclei $4 \leq Z \leq 88$ and $\hbar\gamma = 24$ MeV for $Z \geq 89$.

1.4. Asymptotic expressions

In the case of inverted oscillator, Eq. (19) has three real roots, one positive ($s_1 > 0$) and two negative ($s_2, s_3 < 0$). This means that in practical calculations of the first (14) and second (18) moments one can consider only the leading term, proportional to $\sim e^{s_i t}$. In this case the integral Eq. (20) leads to $\dfrac{e^{2s_1 t}}{s_1^2 + w^2}$ and for large t we obtain

$$\begin{aligned} \Sigma_{RR}(t) &= e^{2s_1 t} \frac{4\omega\lambda\gamma^2}{\pi\mu} \beta_1^2 (s_1 + \gamma) \times \\ &\times \left[\frac{\pi T}{s_1 \gamma} + \frac{1}{s_1 - \gamma} \left[\psi^0 \left(1 + \frac{s_1}{2\pi T} \right) - \psi^0 \left(1 + \frac{\gamma}{2\pi T} \right) \right] \right], \quad (21) \end{aligned}$$

where

$$\psi^0(z) = \frac{\Gamma'(z)}{\Gamma(z)} \quad (22)$$

is the di-gamma function.

The total Hamiltonian (8) contains the coupling parameter λ and frequency ω. These values are defined through the correspondence to the realistic transport coefficients. The transport coefficients are found from Eq. (12) by differentiating in time and expressing $\overline{R(0)}$ and $\overline{P(0)}$ in terms of $\overline{R(t)}$ and

$\overline{P(t)}$:

$$\begin{aligned} \frac{d}{dt}\,\overline{R(t)} &= \frac{1}{\mu}\,\overline{P(t)}, \\ \frac{d}{dt}\,\overline{P(t)} &= -\xi(t)\,\overline{R(t)} - \lambda_P(t)\,\overline{P(t)}. \end{aligned} \tag{23}$$

From the structure of these equations one can identify the time dependent friction coefficient

$$\lambda_P(t) = \frac{A_t\dot{N}_t - B_t\dot{M}_t}{B_tM_t - A_tN_t}, \tag{24}$$

and the renormalized stiffness coefficient

$$\xi(t) = \frac{\dot{M}_tN_t - \dot{N}_tM_t}{B_tM_t - A_tN_t}. \tag{25}$$

For the asymptotic values of the friction and stiffness we obtain the expressions

$$\begin{aligned} \lambda_P(\infty) &= -(s_2 + s_1), \\ \xi(\infty) &= \tilde{\delta}\frac{(s_1+\gamma)(s_2+\gamma)}{(s_1+\gamma)(s_2+\gamma) - 2\lambda\gamma\omega} \end{aligned} \tag{26}$$

where $s_2 > s_3$. The parameters ω and λ in Eq. (8) are chosen in such a way that the asymptotic values of friction and stiffness (26) take the values $\lambda_P(\infty) = 2$ MeV and $\xi(\infty) = -\mu\Omega^2$. As known [15, 16], the realistic friction coefficients are in the range of $1 - 2$ MeV. These values are close to those obtained within the mean-field approaches [17, 18].

2. Role of neutron transfer in capture processes

The importance of the neutron transfer, if the corresponding Q_{2n}-value is positive, in nuclear capture (fusion) originates from the fact that neutrons

are insensitive to the Coulomb barrier and their transfer can start at large separations, before the projectile is captured by the target nucleus [19, 20, 21]. If the two-neutron transfer occurs before crossing the Coulomb barrier, it can lead to the population of the first 2^+ state in the recipient nucleus [22]. So, the motion to the N/Z equilibrium starts in the system before the capture. The average change of mass asymmetry is connected to the two-neutron transfer. Because after two-neutron transfer the mass numbers, the deformation parameters of the interacting nuclei, and, correspondingly, the height and shape of the Coulomb barrier are changed, one can expect an enhancement or suppression of the capture. After two-neutron transfer the residues of donor nuclei is assumed to remain in the ground state with the corresponding quadrupole deformation. For sub-barrier energies, the results of calculations are very sensitive to the quadrupole deformation parameters β_2 of the interacting nuclei. The quadrupole deformation parameters β_2 are taken from Ref. [23] for deformed even-even nuclei. In Ref. [23], the quadrupole deformation parameters β_2 are given for the first excited 2^+ states of nuclei. For the nuclei deformed in the ground state, the β_2 in 2^+ state is similar to that in the ground state and we use β_2 from Ref. [23] in the calculations. For double magic nuclei and neighboring nuclei, in the ground state we take $\beta_2 = 0$. The program takes β_i from the data file incorporated and allows us also to input the user values of β_i.

3. Design of the program

The program is located in the folder *nuclear*. It has the following structure:

bin/ - The program consist of five scripts from this folder: settings.exe, fort.exe, makeplot.exe, kinematics.exe, pcapture.exe. File fort.exe is compiled from files that are in the folder *nuclear/fort/* Another files are compiled from files with coresponding names in the folder *nuclear/source* (see below the details about how they are compiled). There is a friendly user interface on webpage Ref. [24].

conf/ - contains config files. One of them is isotopes.table.txt. This file is used to define nuclear properties (mass, quadrupole deformation parameters β, ..) by charge Z and weight A. Here is its part:

```
 Z    A        m    Element   BETA_GS   BETA_2+ E_2+(MeV)
 6   10   15698.8        C    -0.350     -0.83     3.354
 6   12       0.0        C    -0.300    -0.582     4.439
... ...       ...      ...     ...       ...       ...
 8   14    8007.46       O     0.100     0.410     6.590
 8   16    4737.00137    O     0.000     0.364     6.917
... ...       ...      ...     ...       ...       ...
```

fort/ - contains files for fort.exe: P1.FOR P2.FOR P3.FOR P4.FOR.

lib/ - contains headers: define.hh, gConf.hh, gFile.hh, gFuns.hh, gMath.hh, nuclear.function.hh, nuclear.parameters.hh, potential.hh, project_functions.hh

R/ - consist files with R-code: potentialL.R potential.R prob.R. Below There are details about how to obtain them and how to operate with them.

source/ - settings.cc makeplot.cc kinematics.cc pcapture.cc.

In the following we describe the details about main script files.

3.1. settings.exe

Compile : from the folder *nuclear/source/*:

```
g++ makeplot.cc -o ../bin/makeplot.exe
```

Run from the folder *nuclear/bin*:

```
mkdir -p R conf
./settings.exe -A1 number -A2 number -Z1 number -Z2 number  \
               [-print console|conf] [-o ../conf/conf.0.txt] \
               [-t ../conf/isotopes.table.txt] \
               [-f ../bin/INP.DAT]
./settings.exe -h
```

-print console	print to the console the details about the Elements with corresponding weights A1, A2 and charges Z1, Z2
-print conf	print all output configurations
-o conf.0.txt	print output configurations to the file conf.0.txt
-t isotopes.table.txt	file with the table of isotopes (see above)
-f INP.DAT	write the file for the potential, built by fort.exe
-h	print help
-q yes	if there is option yes for Q 2n channel

Dependencies :

project_functions.hh

isotopes.table.txt

Description : The script defines nuclear properties (mass, quadrupole deformation parameters β, ..) by charge Z and weight A. The information about this is taken from isotopes.table.txt. In our case this table has not all possible elements, so it is possible to complement changing this file.

Examples run from *nuclear/bin/* derictory:

For [A=40,Z=20]

```
./settings.exe -print console -A1 40 -Z1 20 -A2 40 -Z2 18 \
               -o ./conf/conf.0.txt  -f INP.DAT -q yes
```

Here is the output:

```
{\small}
Ca[A=40, Z=20] m: -34846.4  beta: 0     d: 0.55 beta[2+]: 0.12 E[2+]: 3.90
Ar[A=40, Z=18] m: -35039.9  beta: 0.251 d: 0.55 beta[2+]: 0.25 E[2+]: 1.46

  Q: 3.37578  MeV E[2+]:   1.525MeV
Ca[A=42, Z=20] m: -38547.2  beta: 0.247 d: 0.55 beta[2+]: 0.25 E[2+]: 1.52
Ar[A=38, Z=18] m: -34714.8  beta: 0.163 d: 0.55 beta[2+]: 0.16 E[2+]: 2.18
```

```
  Q: -13.4048  MeV  E[2+]:   1.208MeV
Ca[A=38, Z=20] m: -22058.5  beta: 0     d: 0.55 beta[2+]: 0.12 E[2+]: 2.21
Ar[A=42, Z=18] m: -34423    beta: 0.275 d: 0.55 beta[2+]: 0.27 E[2+]: 1.21

   Q2n channel found: Q: 3.37578 E[2+]: 1.525
Ca[A=42, Z=20] m: -38547.2  beta: 0.247 d: 0.55 beta[2+]: 0.25 E[2+]: 1.52
Ar[A=38, Z=18] m: -34714.8  beta: 0.163 d: 0.55 beta[2+]: 0.16 E[2+]: 2.17
```

3.2. fort.exe

./fort.exe

Compile : gfortran P1.FOR P2.FOR P3.FOR P4.FOR -o fort.exe

Run : ./fort.exe

Dependencies :

INP.DAT (see sample below)

Description :

read nuclear properties from INP.DAT **in the same directory** as where fort.exe runs and generate CaAr.DAT file in this directory.

Here is the example for 42Ca+Ar38 with weighs 42, 38; charges 20, 18; diffuseness 0.55; size charachteristics - 1.15, 0.17. INP.DAT sample:

```
42Ca+38Ar
042.00    038.00     020.00    018.00
```

```
0.5500111    0.550111
1.150     0.17        -0.10
CaAr.DAT
```

After puttins the file INP.DAT to the folder with fotr.exe script and running this script there will be the output file CaAr.DAT:

```
42Ca+38Ar
   A1  =   42.000000000000000       A2 =    38.000000000000000
   R0  =    1.1499999999999999       R□00 =   0.17000000000000001
   R1  =    3.9974254467042085       R2 =    3.8662668278928320
   A01  =   0.55001109999999998       A02 =   0.55010999999999999

   R_z        V_C         V_N          V
   7.36     70.3962    -28.0677     42.3286
   7.56     68.5376    -33.5095     35.0281
   ...        ...         ...          ...
  12.16     42.6187     -0.3737     42.2449
```

3.3. makeplot.exe

Compile : g++ makeplot.cc -o makeplot.exe

Run :

```
./makeplot.exe -i ./conf/conf.0.txt \
               -o ./conf/conf.1.txt -r ./R/potential.R
```

Dependencies :

define.hh (see folder ./lib/)

gFile.hh (see folder ./lib/)

gConf.hh (see folder ./lib/)

project_functions.hh (see folder ./lib/)

CaAr.DAT - generated by fort.exe.

./conf.0.txt - generated by settings.exe with flag -o conf.0.txt

Description : It reads potential values from CaAr.DAT, and others parameters from conf.0.txt and generates files ./conf/conf.1.txt and ./R/potential.R. The file conf.1.txt will be the copy of conf.0.txt with potential values. The R code to plot potential will be written too the file ./R/potential.R.

Examples :

conf.1.txt sample:

```
...
R          7.43         7.63         7.83          ...
En       48.5101      41.0172       36.656      34.7342   ...
...
```

3.4. kinematics.exe

Compile :

```
g++ kinematics.cc -std=c++11 -lgsl -lgslcblas -lm -o kinematics.exe
```

Run :

```
./kinematics.exe -i ./conf/conf.1.txt -o2 ./conf/conf.2.txt \
                 -o ./conf/conf.potential.txt -r ./R/potentialL.R
```

Dependencies :

gFile.hh (see folder ./lib/)

gConf.hh (see folder ./lib/)

gFuns.hh (see folder ./lib/)

potential.hh (see folder ./lib/)

./conf/conf.1.txt

Description :

It reads ./conf/conf.1.txt and find key values for potential, like L_{max}, U_{min} (see example and Figure 1) then write to ./conf/conf.2.txt and to ./conf/conf.potential.txt. The R code to plot potential for different $L = 0..L_{max}$ will be written too the file ./R/potentialL.R (see Figure 2).

Examples :

conf.2.txt

```
...
  Lmax            59
  xMin       8.14362
  xBar       10.5539
  UMin       34.4762
  UBar       50.0888
  Esp   42.252    42.752    43.252   ...
  Ed   45.6627   46.1627   46.6627   ...
...
```

conf.potential.txt

```
 L=0  xMin: 8.14 xBar: 10.5 UMin: 34.47 UBar: 50.0 UU: 48.51 41.01 ...
 L=1  xMin: 8.14 xBar: 10.5 UMin: 34.50 UBar: 50.1 UU: 48.54 41.05 ...
 L=2  xMin: 8.14 xBar: 10.5 UMin: 34.56 UBar: 50.1 UU: 48.62 41.12 ...
 ......................
 L=58 xMin: 8.68 xBar: 9.43 UMin:  84.2 UBar: 84.9 UU: 111.5 100.7 ...
 L=59 xMin: 8.72 xBar: 9.38 UMin: 85.80 UBar: 86.2 UU: 113.7 102.8 ...
  RR         7.43      7.63   ...
  U0      48.5101   41.0172   ...
  Lmax  59
```

3.5. pcapture.exe

Compile :

```
g++ pcapture.cc -lgmpxx -lgmp -lmpfr -lgsl -lgslcblas -std=c++11 \
                -o pcapture.exe
```

Run :

```
./pcapture.exe -i ./conf/conf.2.txt  -o ./conf/conf.3.txt \
               -r ./R/prob.R -e ./conf/prob.energies.txt \
               -p ./conf/conf.potential.txt
```

Dependencies :

gFile.hh (see ./lib/)

gConf.hh (see ./lib/)

gFuns.hh (see ./lib/)

gMath.hh (see ./lib/)

potential.hh (see ./lib/)

nuclear.parameters.hh (see ./lib/)

nuclear.function.hh (see ./lib/)

./conf/conf.potential.txt - generated by kinematics.exe

./conf/conf.2.txt - generated by kinematics.exe

Description : It takes all parameters from conf.2.txt, calculates and adds sigma_sp, pelss and sigma_d vectors and writes to conf.3.txt. Where sigma_sp - cross section for the spherical case, pelss - probability for L=0 and sigma_d - cross section for the deformed case.

```
     ...
sigma_sp    0.000664928  0.00122174  0.00226026    ...
pelss       9.54404e-06  1.7887e-05  3.37617e-05   ...
sigma_d     0.15987        0.54109   1.43882       ...
     ...
```


[1] G.G. Adamian *et al.*, Int. J. Mod. Phys. E **5**, 191 (1996).

[2] V.V. Volkov, Phys. Rep. **44**, 93 (1978).

[3] W.U. Schröder and J.R. Huizenga, in *Treatise on Heavy-Ion Science*, Ed. by D.A. Bromley (Plenum, New York, 1984), vol.2, p.115.

[4] H. Hofmann, Phys. Rep. **284**, 137 (1997); C. Rummel and H. Hofmann, Nucl. Phys. A **727**, 24 (2003).

[5] G.G. Adamian, N.V. Antonenko, Z. Kanokov, and V.V. Sargsyan, Teor. Mat. Fiz. **145**, 87 (2005) [Theor. Math. Phys. **145**, 1443 (2006)]; Z. Kanokov, Yu.V. Palchikov, G.G. Adamian, N.V. Antonenko, and W. Scheid, Phys. Rev. E **71**, 016121 (2005); Yu.V. Palchikov, Z. Kanokov, G.G. Adamian, N.V. Antonenko, and W. Scheid, Phys. Rev. E **71**, 016122 (2005).

[6] N. Takigawa, S. Ayik, K. Washiyama, and S. Kimura, Phys. Rev. C **69**, 054605 (2004); S. Ayik, B. Yilmaz, A. Gokalp, O. Yilmaz, and N. Takigawa, Phys. Rev. C **71**, 054611 (2005); B. Yilmaz, S. Ayik, Y. Abe, and D. Boilley, Phys. Rev. E **77**, 011121 (2008).

[7] V.V. Dodonov and V.I. Man'ko, Trudy Fiz. Inst. AN **167**, 7 (1986); H. Dekker, Phys. Rep. **80**, 1 (1981); A. Isar, A. Sandulescu, H. Scutaru, E. Stefanescu, and W. Scheid, Int. J. Mod. Phys. E **3**, 635 (1994); G.G. Adamian, N.V. Antonenko, and W. Scheid, Phys. Lett. A **244**, 482 (1998); Phys. Lett. A **260**, 39 (1999); Nucl. Phys. A **645**, 376 (1999); Yu.V. Palchikov, G.G. Adamian, N.V. Antonenko, and W. Scheid, J. Phys. A **33**, 4265 (2000); Physica A **316**, 297 (2002).

[8] A.O. Caldeira, and A.J. Leggett, Physica A. **121**, 587 (1983); Ann. Phys. **149** 374 (1983).

[9] R. V. Jolos, S. P. Ivanova, and V. V. Ivanov, Sov. J. Nucl. Phys. **40**, 74 (1984); S. P. Ivanova and R. V. Jolos, Nucl. Phys. A. **530**, 232 (1991).

[10] K. Lindenberg, and B. West. Phys. Rev. A. **30**, 568 (1984).

[11] N.G. van Kampen, *Stochastic Processes in Physics and Chemistry*, Amsterdam: North-Holland, 1981.

[12] C.W. Gardiner, *Quantum Noise*, Berlin: Springer, 1991.

[13] U. Weiss, *Quantum Dissipative Systems*. Singapore: Wold Scientific, 1999.

[14] H. Grabert, P. Schramm, G.-L. Ingold, Phys. Rep. **168**, 115 (1988); P. Talkner, Ann. Phys. **167**, 390 1986.

[15] G.G. Adamian, A.K. Nasirov, N.V. Antonenko, R.V. Jolos, Phys. Part. Nucl. **25**, 583 (1994).

[16] V.V. Sargsyan, Z. Kanokov, G.G. Adamian, N.V. Antonenko, and W. Scheid, Phys. Rev. C **80**, 034606 (2009); Phys. Rev. C **80**, 047603 (2009).

[17] K. Washiyama, D. Lacroix, S. Ayik, Phys. Rev. C **79**, 024609 (2009).

[18] S. Ayik, K. Washiyama, D. Lacroix, Phys. Rev. C **79**, 054606 (2009).

[19] P. H. Stelson, H. J. Kim, M. Beckerman, D. Shapira, and R. L. Robinson, Phys. Rev. C **41**, 1584 (1990).

[20] V. V. Sargsyan, G. G. Adamian, N. V. Antonenko, W. Scheid, and H. Q. Zhang, Phys. Rev. C **84**, 064614 (2011); **85**, 024616 (2012); **91**, 014613 (2015); V. V. Sargsyan, G. G. Adamian, N. V. Antonenko, W. Scheid, C. J. Lin, and H. Q. Zhang, ibid. 85, 017603 (2012).

[21] R. A. Broglia, C. H. Dasso, S. Landowne, and A. Winther, Phys. Rev. C 27, 2433 (1983); R. A. Broglia, C. H. Dasso, S. Landowne, and G. Pollarolo, Phys. Lett. B 133, 34 (1983).

[22] S. Szilner, *at al*, Phys. Rev. C **76**, 024604 (2007); 84, 014325 (2011); L. Corradi, *at al*, ibid. **84**, 034603 (2011).

[23] S. Raman, C.W. Nestor Jr., and P. Tikkanen, At. Data Nucl. Data Tables **78**, 1 (2001).

[24] http://intel-robot.ru/external/www5