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Evaluation of transmission coefficients in nuclear processes

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Abstract. Transmission coefficients for charged and neutral particles, without approximations for incoming and outgoing wave functions, were assessed using a quantum mechanical method based on reflection factor. Further, logarithmic derivative, using a rectangular potential in the internal region was computed. With a computer code developed by the authors, based on Hauser-Feshbach formalism, cross-sections of fast neutron-induced reactions followed by the emission of charged particles were calculated. The code results show good agreement with experimental data when discrete states of residual nuclei are taken into account. By using integral form of penetrability coefficients, the current quantum-mechanical technique should be extended to continuous states of residual nuclei, including matching density levels represented by the Fermi-gas model.

1 Introduction

In quantum physics, transmission coefficients, also known as penetration coefficients, are the probability that a microparticle would cross a potential barrier. In terms of quantum mechanics, this probability has the following general form [1,2]:

$$T = \left|J_{trans}\right| \cdot \left|J_{inc}\right|^{-1} \quad (1)$$

where J_{trans}, J_{inc} are the current densities for particles passing the barrier and for incident particles ones, respectively.

2 Elements of theory

Transmission coefficients, defined as probabilities, have positive values lower than 1. They represent a pure quantum effect, the tunnel effect, when a micro-particle with energy lower than the height of the potential can overpass the barrier. It is an important effect, not only for fundamental researches but also for many technical and engineering applications. Emission of alpha particles by atomic nuclei was explained for the first time with the help of tunnel effect, and quantitative description of decay time of nuclei was done using Gamow factor [3,4].

In the (n,α) reactions induced by fast neutrons on medium and heavy nuclei, usually, nuclear process is going through compound mechanisms described by statistical model of nuclear reactions where cross section is given by Hauser – Feshbach relation [5]:

$$\sigma_{n\alpha} = \pi \lambda_n^2 T_n T_\alpha \left(\sum_c T_c \right) W_{n\alpha}{}^{-1} \quad (2)$$

where T are the transmission coefficients for incident neutrons and emergent alpha channels, respectively; $W_{n\alpha}$ is widths fluctuation correction factor.

Transmission coefficients can be computed in a number of ways and they represent the main parameters of cross section expressions. One of the most common ways to calculate transmission coefficients is to use Gamow factor expressed by the integral [1]:

$$T(l,E) = \exp\left\{ -\sqrt{\frac{8m}{\hbar^2}} \int_D \left[V(r) + \frac{zZe^2}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} - E \right]^{1/2} dr \right\} \quad (3)$$

where the terms under the integral are nuclear, Coulomb, centrifugal potentials, respectively, and E is the energy of alpha particles.

There are few ways to calculate the width fluctuation correction factor. In the present work, the method described in [6] was applied. According to this method, transmissions are:

$$T(l,E) = 1 - \left|U_l(E)\right|^2 \quad (4)$$

where U is the reflection factor depending on E and l, the energy and orbital momentum of emitted particle.

Reflection factor contains the logarithmic derivative D_l and a series of functions, as solutions of the radial Schrodinger equation for different states, and initial conditions. General form of reflection factor is [1]:

$$U_l = \left\{ \frac{D_l - R\left[\frac{1}{W_l^-}\frac{dW_l^-}{dr}\right]}{D_l - R\left[\frac{1}{W_l^+}\frac{dW_l^+}{dr}\right]} \frac{W_l^-}{W_l^+} \right\}_R \quad D_l = R\left[\frac{1}{W_l}\frac{dW_l}{dr}\right]_R \quad (5)$$

$$W_l(r) \sim W_l^-(r) - U_l W_l^+(r) \quad (5.1)$$

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where W_l is the inner wave function expressed by a linear combination of ongoing and outgoing functions $W^{\pm}$. Logarithmic derivative is calculated at $r=R$, the radius of nuclear potential.

Ingoing and outgoing functions for neutral and charged particles have the expressions:

$$W_l^{\pm}(r) = kr\left[n_l(kr) \pm ij_l(kr)\right] \qquad (6.1)$$

$$W_l^{\pm}(r) = kr\left[F_l(kr) \pm iG_l(kr)\right] \qquad (6.2)$$

where n_l, j_l are Neumann and Bessel functions and F_l, G_l are the regular and irregular Coulomb functions.

Neumann, Bessel and Coulomb functions are solutions of reduced Schrodinger equations for neutral and charged particles, respectively:

$$\frac{d^2 w_l}{d\rho^2} + \left[1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2}\right] w_l = 0 \qquad (7)$$

with $\rho = kR > 0, -\infty < \eta < +\infty, l = 0,1,2,...$ where ρ is the reduced radius; k is the wave number and η is the Coulomb factor ($\eta = 0$ for neutral particles).

If the solutions for neutral particles (6.1) are relatively easy to calculate numerically, for charged particles the solution of the equation (6.2) is more complicated and has an integral form in complex plane. The regular and irregular Coulomb functions are:

$$F_l - iG_l = \frac{e^{-\pi\rho}\rho^{l+1}}{(2l+1)!c_l(\eta)} \int_{-1}^{-i\infty} e^{-i\rho t}(1-t)^{l-i\eta}(1+t)^{l+i\eta}\,dt, \qquad (8)$$

$$c_l(\eta) = \frac{2^l e^{-\frac{\pi\eta}{2}} \left|\Gamma(l+1+i\eta)\right|}{\Gamma(2l+2)}$$

3 Results and discussions

Computer codes consist in relations for transmission coefficients and Hauser–Feshbach approach. Subsequent expressions of the reflection factor, inner wave functions, functions for neutral and charged particles with no approximations were calculated. Real and imaginary parts of regular and irregular Coulomb functions (6) were also obtained. Regular and irregular Coulomb functions and their derivative are represented in Figure 1. Programs were applied for the following nuclear reactions: ^{26}Al(n,α)^{23}Na and ^{143}Nd(n,α)^{140}Ce.

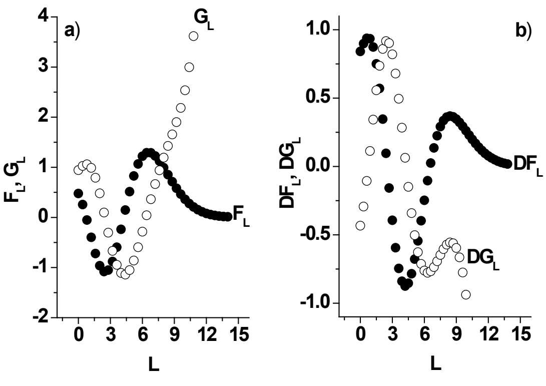

Figure 1. Dependence by orbital momentum L of a) Regular and irregular Coulomb functions (F_l, G_l) b) Derivatives of regular and irregular Coulomb functions (DF_l, DG_l)

In Figure 2, neutron transmission coefficients were calculated in ^{26}Al(n,α)^{23}Na *(Q=2.96* MeV) reaction with fast neutrons. In Figure 2a, transmission coefficients were evaluated using the semi-classical approach based on the Gamow integral (3). In Figure 2b, for the same nuclear reaction, transmission coefficients were evaluated in the frame of the quantum–mechanical formalism (4-8). For incident neutrons with momentum *l=0*, transmission coefficients are equal to *1* in the semi-classical approach (case *l=0* not shown in Figure 2a).

The coefficients are smoothly increasing with the neutron energy and slowly are tending to *1* applying quantum method (Figure 2b). Differences are given by the presence of centrifugal potential and evaluation method. In both cases, transmission coefficients are reaching the maximum value *1* but in quantum approach, coefficients are increasing slower than in the semi-classical way. Nuclear potential is rectangular and has a finite range *R*. Outside of nuclear range, Coulomb potential is acting.

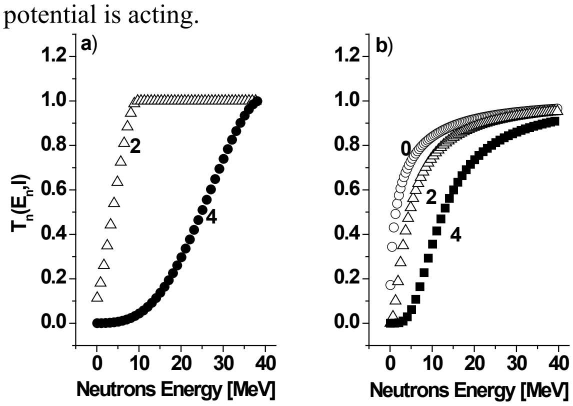

Figure 2. Neutron transmission coefficients in ^{26}Al(n,α)^{23}Na, for different orbital momentum in the following approaches a) Semi-classical (*l=2, 4*) b) Quantum–mechanical (*l=0,2,4*)

In Figure 3 alpha transmission coefficients for the same fast neutron reaction on ^{26}Al are shown. The influence of centrifugal potential (due to orbital momentum) and of Coulomb one is easy to observe. Also, if in the semi-classical calculations, alpha transmission coefficients, even in the presence of orbital momentum relative fast are equal to *1*, in quantum mechanical approach, alpha transmission coefficients slowly are increasing to *1*.

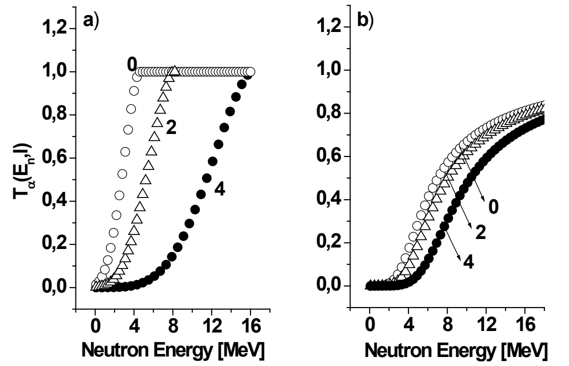

Figure 3. Alpha transmission coefficients in ^{26}Al(n,α)^{23}Na, for different orbital momentum (*l = 0,2 4*), in the following approaches a) Semi-classical b) Quantum– mechanical

The main question is to choose the appropriate method. In the author's opinions, the answer to this issue is a matter of the precision of calculation of the cross sections and other parameters. Previous author's calculations of the time of life of alpha emitter nuclei showed improved results applying quantum approach.

Using quantum mechanical method, cross sections for many (n,α) reactions with fast neutrons were calculated. One of the best descriptions of the cross sections is in the case of ^{143}Nd(n,α)^{140}Ce ($Q=9.72$ MeV) for fast neutrons with energies up to *6* MeV considering in the calculations *10* discrete states of residual nucleus ^{140}Ce. Nuclear potentials in the incident and emergent channels are rectangular with real and imaginary part ($V=U+iW$). Incident neutrons have orbital momentum $l=0,1$. Nuclear process is described by the compound nucleus reaction mechanism.

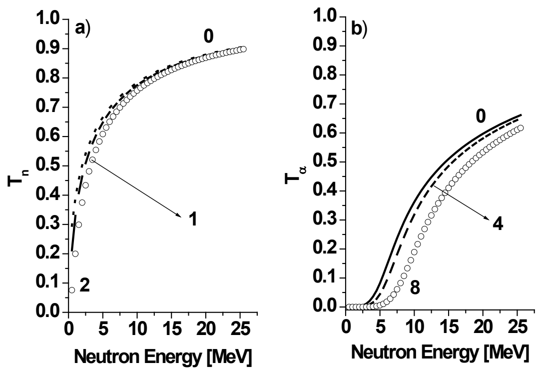

Figure 4. Transmission coefficients in ^{143}Nd(n,α)^{140}Ce. Orbital momentum: a) Neutrons, $l_n = 0,1,2$; Alphas, $l_\alpha = 0,4,8$

Experimental cross section data in the case of discrete states are well described by theoretical calculations using the quantum mechanical approach. With the increasing of the neutron incident energy, it is necessary to include more discrete states or to use the approximation of continuum states proposed in Talys as the authors did in [7] for the investigations of other (n,α) reactions with fast neutrons.

In Table 1 theoretical and experimental cross section data for Ce are shown. Theoretical approach describes very well experimental data [8].

Table 1. ^{143}Nd(n,α)^{140}Ce.Teoretical and experimental cross sections (XS) for $E_n=4,5,6$ MeV

En [MeV]	XS^{exp} [mb]	XS^{theor} [mb]
4±0.23	0.12±0.01	0.14
5±0.16	0.21±0.01	0.26
6±0.12	0.31±0.03	0.37

In the incident neutron channel nuclear potential is $V=U+iW=(50+i0.1)$ MeV and in alpha emergent channel, $V=U+iW=(171+i0.1)$ MeV.

4 Conclusions

Transmission coefficients were evaluated by two methods: the semi-classical one using Gamow integral and quantum-mechanical approach based on reflection factor. In quantum approach, ingoing and outgoing wave functions were calculated without approximations. Differences in the shape of transmission coefficients were evidenced. In the quantum-mechanical approach, transmission coefficients are smoothly increasing with incident energy. Also, with the increasing of alpha particle orbital momentum, transmissions are decreasing.

Transmissions were used for (n,α) cross sections for neutrons with some MeV. Codes were realized by implementing Hauser-Feshbach formalism and quantum-mechanical approach for transmission coefficients. Rectangular optical potential, with real and imaginary parts, in incident and emergent channels was considered. A good agreement between cross section experimental and theoretical data were obtained, considering 10 discrete states of residual nuclei for neutron, gamma and proton emergent channels, respectively.

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