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 likelihood that a microparticle would cross a potential barrier. This probability has the following general form in terms of quantification [1,2]:

 (1)

where *Jtrans*, *Jinc* are the current densities for particles passing the barrier and for incident particles ones, respectively.

1. 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,) reactions induced by fast neutrons on Al and Nd nuclei, nuclear process is going through compound mechanisms described by statistical model of nuclear reactions where cross sections are given by Hauser – Feshbach relation [5]:

 (2)

where *T* are the transmission coefficients for incident neutrons and emergent alpha channels, respectively; *Wn* is widths fluctuation correction factor.

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

 (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 widths fluctuation correction factor. In the present work the method described in [6] was applied. ccording to this method [1], transmissions are:

 (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 *Dl* and a series of wave functions, as solutions of radial Schrodinger equation for different states, and initial conditions. General form of reflection factor is [1]:

, (5)  (5.1)

where *Wl* is the inner wave function expressed by a linear combination of ongoing and outgoing functions *W*. Logarithmic derivative is calculated at *r = R*, the radius of nuclear potential.

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

 (6.1)  (6.2)

where *nl*, *jl* are Neumann and Bessel functions and *Fl*, *Gl* are the regular and irregular Coulomb functions.

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

 (7)

whithwhere **is the reduced radius; *k* is the wave number and **is the Coulomb factor (*= 0* for neutral particles).

If the solutions for the first equation from (7) are relatively easy to calculate numerically, for charged particles, the solution of the second equation is more complicated and has an integral form in complex plane. The regular and irregular Coulomb functions are:

 (8)

1. Results and discussions

Computer codes consist in relations for transmission coefficients and Hauser–Feeshbach approach. Subsequent expressions of reflection factor, inner wave functions, functions for neutral and charged particles were calculated with no approximations. Real and imaginary part for regular and irregular Coulomb functions (6) were also obtained. Programs were applied for the following nuclear reactions: 27Al(n,)24Na and 143Nd(n,)140Ce. Regular and irregular Coulomb functions and their derivative are represented in Fig. 1.



Fig. 1. Dependence by orbital momentum *L* of a) Regular and irregular Coulomb functions (*Fl, Gl*) b) Derivatives of regular and irregular Coulomb functions (*DFl, DGl*)

In Fig. 2, neutron transmission coefficients were calculated in 27Al(n,)24Na *(Q = 2.95* MeV) reaction with fast neutrons. In Figure 2a, transmission coefficients were evaluated using semi-classical approach based on 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 orbital momentum *l=0*, transmission coefficients are equal with 1 in the semi-classical approach (Figure 2a) and, lower than *1*, smoothly increasing with the neutron energy in Figure 2b. Differences are given by the presence of centrifugal potential and the method of evaluations. 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 acting in a finite range *R*, outside of nuclear range, Coulomb potential is acting.



Fig. 2. Neutron transmission coefficients in 27Al(n,)24Na, for different orbital momentum (*l = 0, 1, 2)*, in the following approaches a) Semi-classical b) Quantum–mechanical

In Fig. 3 alpha transmission coefficients for the same fast neutrons reaction on 27Al are shown.

The influence of centrifugal potential (due to orbital momentum) and of Coulomb one it 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 with *1*, in quantum mechanical approach, alpha transmission very slow are increasing to the maximal *1* value.



Fig. 3. Alphas transmission coefficients in 27Al(n,)24Na, 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 more correct approach. In the author’s opinions, the answer to this issue it 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,) reactions with fast neutrons were calculated. One of the best description of the cross sections is in the case of 143Nd(n,)140Ce for fast neutrons with energies up to *6* MeV considering in the calculations *10* discrete states of residual nucleus 140Ce. 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 compound nucleus reaction mechanism.



Fig. 4. Transmission coefficients in 143Nd(n,)140Ce. Orbital momentum: a) Neutrons, *ln = 0,1,2*; Alphas, *l=0,4,8*

Experimental cross sections data in the case of discrete states are well described by theoretical calculations using 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 propesd in Talys as the authors did in [7] for the investigations of other (n,) 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.**  143Nd(n,)140Ce.Teoretical and experimental cross sections (XS) for *En = 4, 5, 6* MeV

|  |  |  |
| --- | --- | --- |
| En [MeV] | XSexp [mb] | XStheor [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 *V = U + iW = (50 + i 0.1)* MeV and in alpha emergent channel *V = U + iW = (171 + i 0.1)* MeV.

1. Conclusions

Transmission coefficients were evaluated by two methods: semi-classical method 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 particles orbital momentum transmissions are decreasing. Transmissions were used for (n,) 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 part, in incident and emergent channels were considered. A good agreement between cross section experimental and theoretical data were obtained, considering 10 discrete states of residual nuclei with neutron, gamma and proton emergent channels, respectively.

References

1. A. Foderaro, The Neutron Interaction Theory, The MIT Press, Cambridge, Massachusetts and London, England (1971)
2. David. J. Griffiths, Introduction in Quantum Mechanics (Second Edition), Cambridge University Press, New York (2016)
3. G.A. Gamow, Zur Quantentheorie des Atomkernes. Z. Phys. **51**, 204 (1928). <https://doi.org/10.1007/BF01343196>
4. E.U. Condon, R.W. Guerney, Wave Mechanism and Radioactive Disintegration. Nature. **122**, 439 (1928). <https://doi.org/10.1038/122439a0>
5. V. Hauser, W. Feshbach, , The Inelastic Scattering of Neutrons. Phys. Rev., **87**, 2, 366 (1952). <https://doi.org/10.1103/PhysRev.87.366>
6. P. A. Moldauer, Average Compound-Nucleus Cross Sections. Rev. Mod. Phys., **36**, 1079 (1964). <https://doi.org/10.1103/RevModPhys.36.1079>
7. C. Oprea, A, Mihul, A.I. Oprea, Neutron capture cross sections and strength functions on 147Sm. CERN-Proceedings-2019-001, 125 (2019) <https://doi.org/10.23727/CERN-Proceedings-2019-001>
8. C. Oprea, A.I. Oprea, Alpha Particles Emission in Fast Neutrons Processes on 143Nd Nucleus. Bulletin of the Russian Academy of Sciences: Physics, 85, 11, 1410 (2022). [https://link.springer.com/article/10.3103/S1062873822110193](https://link.springer.com/article/10.3103/S1062873822110193%22%20%5Ct%20%22_blank)