New Quantum Approach for Evaluation of Transmission Coefficients in Nuclear Processes

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Abstract. Transmission coefficients (or penetrabilities) are defined as the probability of a micro-particle crossing a potential barrier and they are important in the investigation of nuclear reaction mechanisms and the structure of atomic nuclei. These coefficients are of interest in the evaluation of the decay constant of excited nuclear states and of the cross-sections. Applying a quantum mechanical approach, starting from the reflection factor, transmission coefficients for charged and neutral particles are obtained. In the proposed method, for regular and irregular functions of charged and neutral particles no approximations are used in the description of ingoing and outgoing wave functions. A logarithmic derivative is calculated using a rectangular potential in the internal region. Transmission coefficients obtained by authors were used in the evaluation of the decay constant of some alpha emitters nuclei. Cross-section of fast neutrons induced reactions followed by emission of charged particles are evaluated with a computer code realized by authors where Hauser – Feshbach formalism is implemented. The realized codes give a good agreement between experimental and theoretical data in the case of discrete states of residual nucleus. The present method can be extended in the case of continuum states of residual nucleus applying the integral form of penetrabilities coefficients including nuclear density states described by Fermi-gas model of the atomic nucleus.

1. Introduction

Transmission (or penetrability) coefficients *T*
- represents the probability of a particle to pass a potential barrier

Defined as probability
-> T ≤ 1

Importance
- nuclei decay constant
- cross sections evaluations

Few approaches in the evaluations of Transmission coefficients
- semiclassic ("so-called") – using the Gamov Factor
- quantum – mechanical approach – using the reflection factor

2. Theory/ Hauser-Feshbach Formalism. Cross Sections

$$\sigma_{\alpha\beta} = \pi\lambda_\alpha^2 \frac{T_\alpha T_\beta}{\sum_c T_c} \qquad \sigma_{\alpha\beta} = \pi\lambda_\alpha^2 \frac{T_\alpha T_\beta}{\sum_c T_c} W_{\alpha\beta}$$

$W_{\alpha\beta}$ = Widths Fluctuation Correction Factor **(WFC)**

Historically first Hauser-Feshbach expression

WFC. Indicates a correlation between the ingoing channel (incident) and outgoing channels

At low energies (<1 MeV) WFC=1 - no correlation between *in* and *out* channels

For neutron induced reactions with emission of charged particles this factor is slowly decreasing with energy for fast neutrons

It is calculated by complicate procedures (ex Moldauer expression)

THEORY. WIDTH FLUCTUATION CORRECTION FACTOR

$$W_{ab} = \left(1+\frac{2\delta_{ab}}{\nu_a}\right)\int_0^\infty \prod_c \left(1+\frac{2T_c x}{\nu_c \sum_i T_i}\right)^{-\left(\delta_{ac}+\delta_{bc}+\frac{\nu_c}{2}\right)} dx$$

$$\nu_a = 1.78 + \left(T_a^{1.212} - 0.78\right)\cdot e^{-0.228\sum_c T_c}$$

Widths Fluctuation Correction Factor (WFC)
- Represents a correlation between incident and emergent channels
- At low energies WFC = 1
- Then slowly decreasing with energy
- Mainly three ways of evaluation
- Moldauer expression chosen

THEORY. T – Semi-classical Method

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

The integral represents the Gamow factor

m= reduced mass

V(r) = nuclear potential (rectangular, Wood – Saxon etc)

h_bar = reduced Planck constant

$\frac{zZe^2}{r}$ = Coulomb potential
z = Charge of incident particles
Z = charge of residual nucleus

$\frac{\hbar^2 l(l+1)}{2mr^2}$ = centrifugal potential

THEORY. QUANTUM MECHANICAL APPROACH

$T(l,E) = 1 - |U_l(E)|^2$ TC as a function of reflection factor

Reflection Factor

$$U_l = \left\{\frac{D_l - R\left[\frac{1}{W_l^-}\frac{dW_l^-}{dr}\right]W_l^-}{D_l - R\left[\frac{1}{W_l^+}\frac{dW_l^+}{dr}\right]W_l^+}\right\}_{r=R}$$

Logarithmic Derivative

$$D_l = R\left[\frac{1}{W_l}\frac{dW_l}{dr}\right]_{r=R}$$

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

$W_l^-(r),\ W_l^+(r) =$ Inner Wave Function as Linear Combination of Ingoing (+) and Outgoing (-) Functions

$$\frac{d^2W_l(r)}{dr^2} + \frac{2m}{\hbar^2}\left[E_l - V(r) - \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]W_l(r) = 0$$ Radial Schrodinger Equation

THEORY. REGULAR AND IRREGULAR FUNCTIONS

$W_l^+(r) = kr[n_l(kr) + ij_l(kr)]$

$W_l^-(r) = kr[n_l(kr) - ij_l(kr)]$

Neutral Particles: Wave Function (WF) – Linear Combination of Neumann (n_l) and Bassel Functions (j_l)

$W_l^+(r) = kr[F_l(kr) + iG_l(kr)]$

$W_l^-(r) = kr[F_l(kr) - iG_l(kr)]$

Charged Particles: WF – Linear Combination of Regular (F_l) and Irregular (G_l) Coulomb Functions

THEORY. NEUTRAL & CHARGED PARTICLES WF

$$\frac{d^2w_l}{d\rho^2} + \left[1 - \frac{l(l+1)}{\rho^2}\right]w_l = 0$$
$\rho = kR > 0, l = 0,1,2,....$

Neutral Particles WF – as solutions of the differential Schrodinger Equation

$$\frac{d^2w_l}{d\rho^2} + \left[1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2}\right]w_l = 0$$
$\rho = kR > 0, -\infty < \eta < +\infty, l = 0,1,2,....$

Charged Particles WF – as solutions of the differential Schrodinger Equation with Coulomb Term ~1/ρ

THEORY. CHARGED PARTICLES. INTEGRAL FUNCTION

Regular and Irregular Coulomb Functions (F_l, G_l)

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

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

$\Gamma,\ \eta =$ Gamma Function and Coulomb parameter

COMPUTER CODES

1. TRANSMISSION COEFFCIENTS – SEMICLASSICAL METHOD

- EVALUATION OF GAMOW FACTOR

2. TRANSMISSION COEFFICIENTS – QUANTUM MECHANICAL APPROACH

- TRANSMISSION COEFFCIENTS – STARTING WITH REFLECTION FACTOR
- FUNCTIONS FOR NEUTRAL AND CHARGED PARTICLES – FULL CALCULATED WITHOUT APPROXIMATIONS
- FOR CHARGED PARTICLES – USED INTEGRAL REPRESENTATION OF REGULAR AND IRREGULAR FUNCTIONS
- IN THE INNER REGION – WAVE FUNCTION -> PLANE WAVE

3. HAUSER – FESHBACH APPROACH

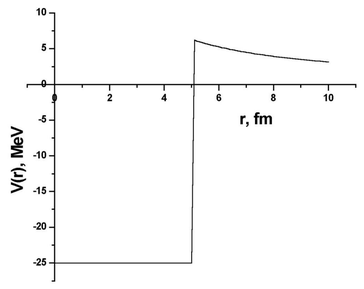
- USING BOTH APPROACHES FOR TRANSMISSION COEFFICIENTS
- ANGULAR CORRELATIONS
- EXPERIMENTAL DATA PROCESSING

COMPUTER CODES. COULOMB AND NUCLEAR POTENTIAL

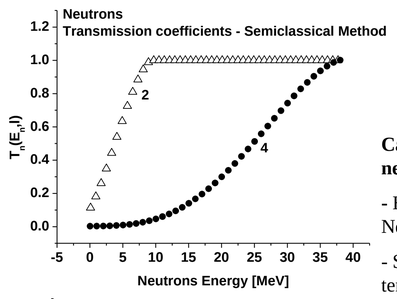
Potential - sum of Nuclear (V_0), Coulomb (V_{Coul}) and Centrifugal potential V_{cf}

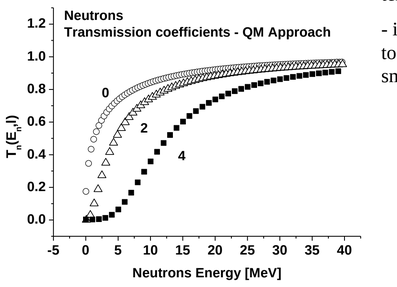
$$V(r) = \begin{cases} -V_0, r \le R \\ 0, r > R, (neutrons) \\ \frac{zZe^2}{r}, r > R, (protons, \alpha, ...) \end{cases} \qquad V_{cf}(r,l) = \frac{\hbar^2 l(l+1)}{2mr^2}$$

Potential – Graphical Representation



RESULTS. NEUTRON TRANSMISSION COEFFICIENTS

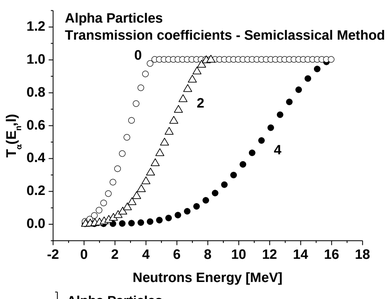


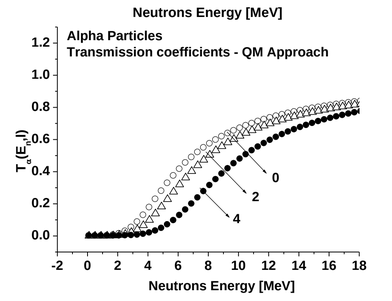


Calculated for $^{27}Al(n,\alpha)^{24}Na$ with fast neutrons

- Heat of reaction – Q = 2.95 MeV; Neutrons orbital momentum, l_n = 0, 2, 4
- Shape of energy dependences – same tendency but not the same shape
- in semiclassical method–faster is going to 1, in Quantum Mechanical approach – smoothly increasing to 1

RESULTS. ALPHA TRANSMISSION COEFFICIENTS

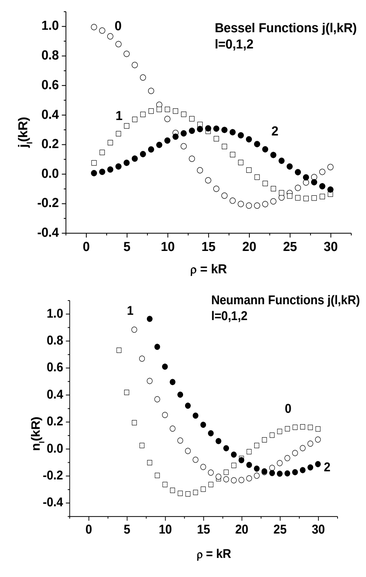




Calculated for $^{27}Al(n,\alpha)^{24}Na$ with fast neutrons

- Heat of reaction – Q = 2.95 MeV; Alphas orbital momentum, l_α = 0, 2, 4
- Semiclassical method–faster is going to 1, in QM approach – smooth increasing to 1
- In the same way that neutrons behave
- Important for cross sections and angular correlations

RESULTS. NEUTRAL PARTICLES. TRANSMISSION COEFFICIENTS

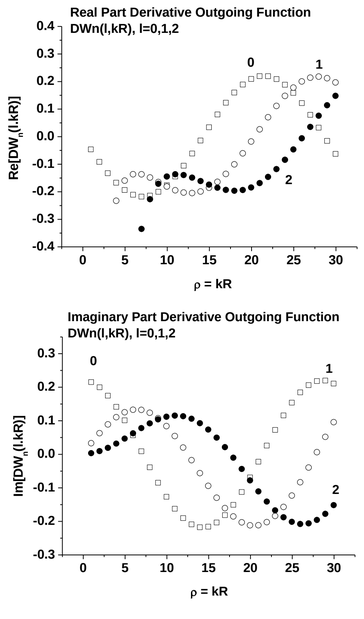


Ingoing and Outgoing Functions calculated in Quantum Mechanical approach

$W_l^\pm(r) = kr[n_l(kr) \pm ij_l(kr)]$

$$\frac{d^2w_l}{d\rho^2} + \left[1 - \frac{l(l+1)}{\rho^2}\right]w_l = 0$$
$\rho = kR > 0, l = 0,1,2,....$

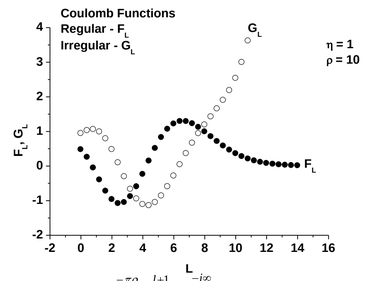
RESULTS. DERIVATIVES FOR NEUTRAL PARTICLES

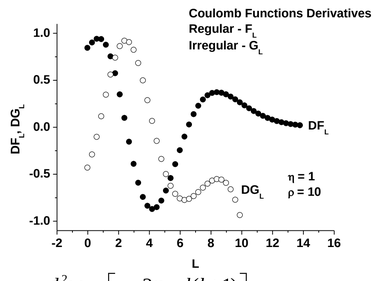


$W_l^\pm(r) = kr[n_l(kr) \pm ij_l(kr)]$

Derivative of Neutral Particles Wave Functions calculated in Quantum Mechanical approach
- Functions with Real and Imaginary part
- Important for the calculation of Logarithmic Derivative Function

RESULTS. COULOMB FUNCTIONS FOR CHARGED PARTICLES





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

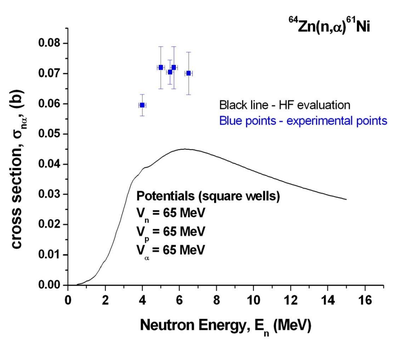
$$\frac{d^2w_l}{d\rho^2} + \left[1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2}\right]w_l = 0$$

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

$\rho = kR > 0, -\infty < \eta < +\infty, l = 0,1,2,....$

Charged particles Regular and Irregular / Coulomb Functions (Fl, Gl) for Alpha particles in $^{27}Al(n,\alpha)^{24}Na$ Process with Fast Neutrons / Functions with Real and Imaginary part / Necessary for Logarithmic Derivative

CROSS-SECTION EVALUATIONS FOR $^{64}Zn(n,\alpha)^{61}Ni$ REACTION



Theoretical Evaluations / Gamow Factor(1) / QM Approach (2)

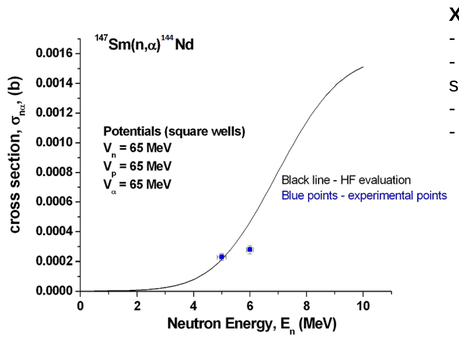
E_n, MeV	σ_1 (mb)	σ_2 (mb)
1	0.029	0.033
3	6.3	25
5	160	43

$$\sigma_{\alpha\beta} = \pi\lambda_\alpha^2 \frac{T_\alpha T_\beta}{\sum_c T_c} W_{\alpha\beta}$$

Experimental Data

E_n (MeV)	σ (mb)
5.0 ± 0.26	72.5 ± 7
5.7 ± 0.15	72.0 ± 7
6.5 ± 0.2	70.8 ± 7

CROSS-SECTION EVALUATIONS FOR $^{147}Sm(n,\alpha)^{144}Nd$ REACTION

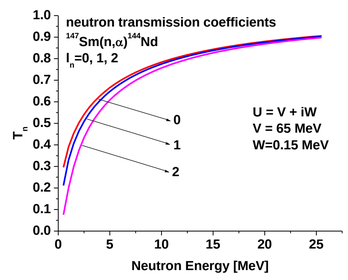


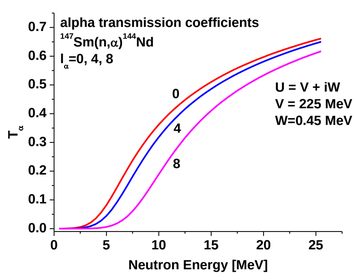
XS calculated with QM approach (2)
- good description for discrete states of residual nucleus
- with increasing of neutron energy other channels are open and should be considered
- Necessary to include continuum states of residual nucleus
- Realized by authors with Talys

E_n, MeV	σ_2 (mb)	E_n, MeV	σ_{exp}(mb)
2	0.11	2⌖0.10	0.197 ⌖0.035
3	0.23	5⌖0.16	0.23 ⌖0.023
6	0.94	6⌖0.12	0.28 ⌖0.023

RESULTS. - $^{147}Sm(n,\alpha)^{144}Nd$ – Transmission coefficients

Energy dependence of neutron and alpha transmission coefficients

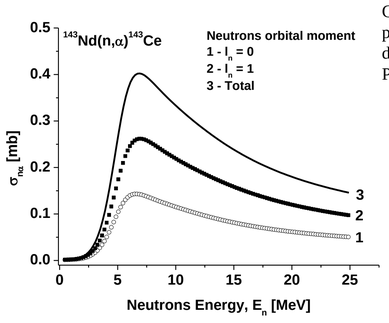




Orbital momentum: neutrons – l_n=0,1,2; alphas – l_α=0,4,8

Calculated with our soft based on the considered quantum mechanical approach

RESULTS. $^{143}Nd(n,\alpha)^{140}Ce$ Compound Nucleus mechanism and Hauser-Feshbach approach



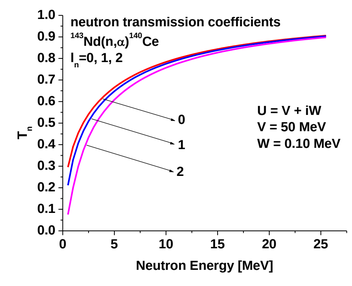
Cross Sections are very low / Difficult to obtain experimental data / Only compound processes and discrete states of residual nucleus are involved / Shape of energy dependences as expected / Neutrons with orbital momentum l_n = 0,1 / Type of Optical Potential U = V + iW = 172 + I x 0.

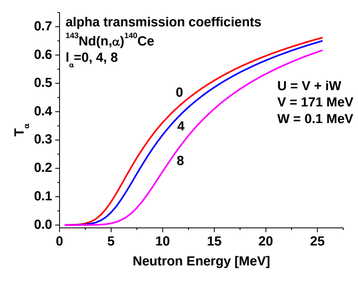
E_n [MeV]	Exp [mb]	Eval /2/ [mb]
4⌖0.23	0.12 ⌖0.01	0.14
5⌖0.16	0.21 ⌖0.01	0.26
6⌖0.12	0.31 ⌖0.03	0.37

RESULTS. $^{143}Nd(n,\alpha)^{140}Ce$ Transmission coefficients – Quantum Mechanical Approach

$^{143}Nd(n,\alpha)^{140}Ce$ ($Q_{n\alpha}$ = 9.72 MeV) neutrons 0.5 to 25 MeV - orbital momentum l_n = 0,1,2; l_α = 0,4,8
- Spin and parity of ^{143}Nd and ^{140}Ce nuclei, J^Π = (7/2)$^-$ and 0$^+$, respectively
- considered γ, p, n, n', α channels;

Neutron energy dependence of neutron and alpha transmission coefficients





CONCLUSIONS

Transmission coefficients were evaluated by two methods
- Semiclassical Method using Gamow Factor
- Quantum Mechanical Approach using Reflection Factor

QM Approach – Ingoing and Outgoing Wave Functions were calculated without approximations
- Differences in the shape of Transmission Coefficients were evidenced
- In the considered Quantum Mechanical Approach Transmission Coefficients are smoothly increasing with energy and slowly tend to 1

Transmission Coefficients were used in the (n,α) processes with fast neutrons with energies of few MeV

Codes were realized by implementing Hauser-Feshbach formalism and considered Quantum Mechanical Approach for transmission coefficients calculations
- Rectangular optical potential were used
- Good description of cross-section for few MeV neutron energy, of interest in the investigations of nuclear reaction mechanisms and astrophysics

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