Evaluation of the transmission coefficients in nuclear processes

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Abstract. Transmission coefficients describe the probability that a micro-particle will pass through a potential barrier. Using a quantum mechanical approach, the reflection factor is used to calculate the transmission coefficients for charged and neutral particles. There are no approximations used in the proposed method for describing incoming and outgoing wave functions of charged and neutral particles. Logarithmic derivative is calculated using a rectangular potential in the internal region. With a computer code developed by the authors, and based on Hauser-Feshbach formalism, cross-sections of fast neutron-induced reactions followed by the emission of charged particles are evaluated. When discrete states of residual nuclei are considered, the realized codes agree with experimental data well. The present quantum approach can be extended to continuum states of residual nuclei using the integral form of penetrability coefficients, including nuclear density states described by nuclear Fermi-gas model.

1. INTRODUCTION

Transmission (or penetrability) coefficients ***T***

- represents the probability of a particle to pass a potential barrier

Defined as probability

-> $T \le 1$

Importance

- nuclei decay constant
- cross section 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

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

$$W_{ab} = \left(1+\frac{2\delta_{ab}}{\nu_a}\right)\int_0^\infty \prod_c \left(1+\frac{2T_c x}{\nu_c \sum_i T_i}\right)^{-\left(\delta_{ac}+\delta_{bc}+\frac{\nu_c}{2}\right)} dx \qquad \nu_a = 1.78 + \left(T_a^{1.212} - 0.78\right)\cdot e^{-0.228\sum_c T_c}$$

Width 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

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

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

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

THEORY. QUANTUM MECHANICAL APPROACH

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

Reflection Factor

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

Logarithmic Derivative

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

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

$W_l^-(r), \quad W_l^+(r) =$

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

Regular and Irregular Coulomb Functions (F_l, G_l)

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

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

Γ, η = Gamma Function and Coulomb parameter

3. CODES

1. **TRANSMISSION COEFFICIENTS – SEMICLASSICAL METHOD**

- EVALUATION OF GAMOW FACTOR

2. **TRANSMISSION COEFFICIENTS – QUANTUM MECHANICAL APPROACH**

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

3. **HAUSER – FESHBACH APPROACH**

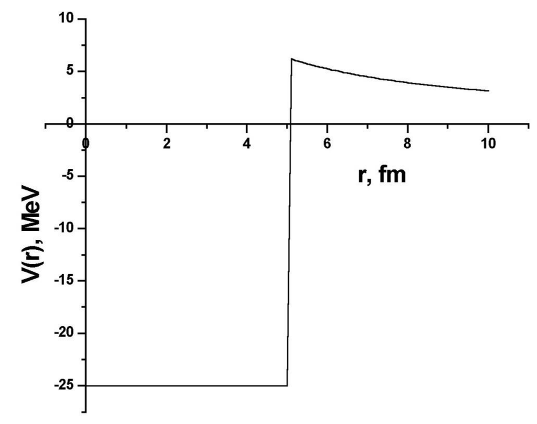
- USING BOTH APPROACHES FOR TRANSMISSION COEFFICIENTS
- ANGULAR CORRELATIONS
- EXPERIMENTAL DATA PROCESSING

CODES. COULOMB AND NUCLEAR POTENTIAL

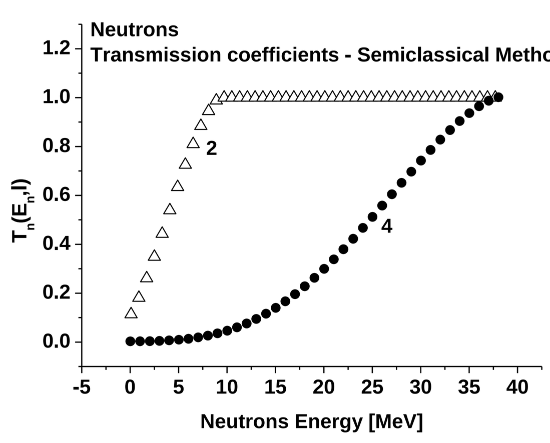
Potential - sum of Nuclear (V_0), Coulomb (V_{Coul}) and Centrifugal potential V_{cf}

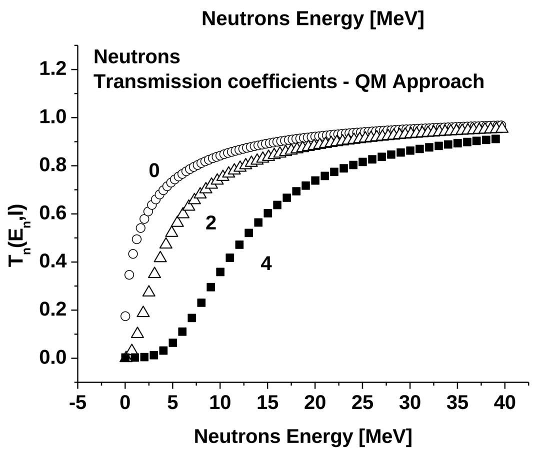
$$V(r) = \begin{cases} -V_0, r \le R \\ 0, r > R, (neutrons) \\ \frac{zZe^2}{r}, r > R, (protons, \alpha, ...) \end{cases} \qquad , V_{cf}(r,l) = \frac{h^2 l(l+1)}{2mr^2}$$

Potential – Graphical Representation



4. RESULTS AND DISCUSSION
NEUTRON TRANSMISSION COEFFICIENTS

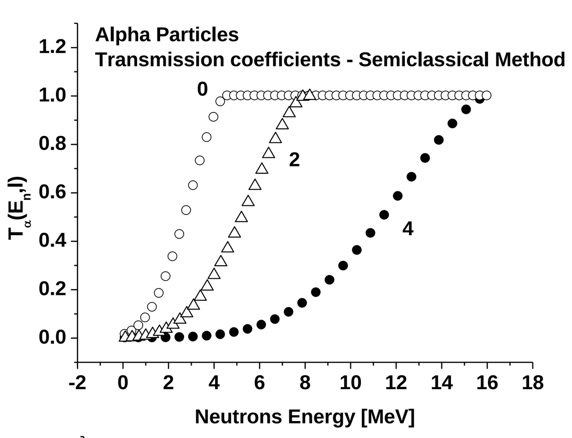


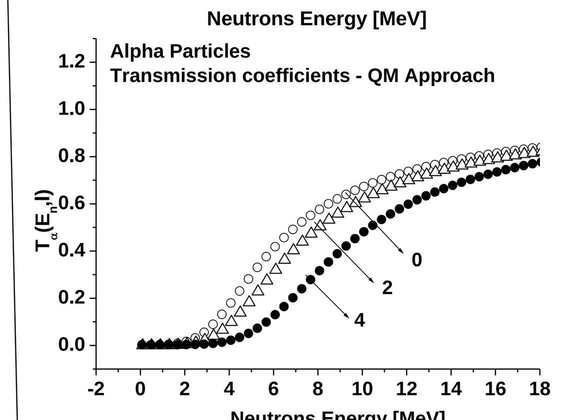


Calculated for $^{27}Al(n,\alpha)^{24}Na$ with fast neutrons

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

RESULTS. ALPHA TRANSMISSION COEFFICIENTS

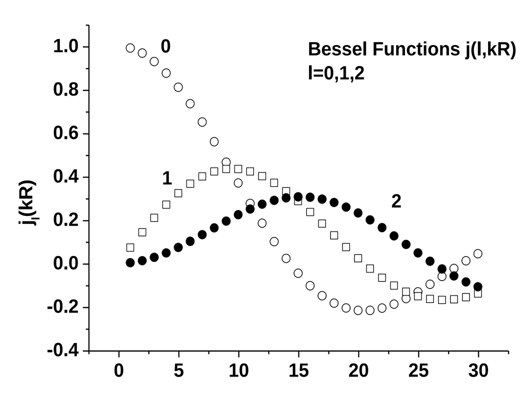




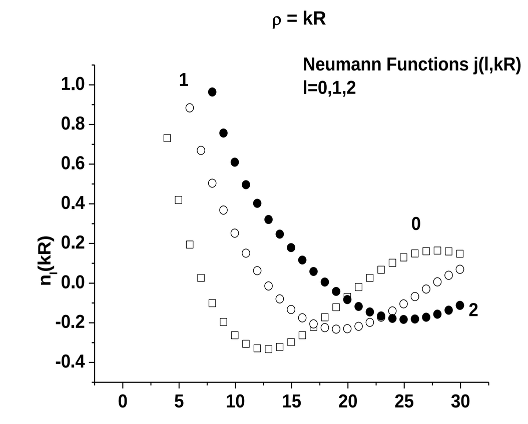
Calculated for $^{27}Al(n,\alpha)^{24}Na$ with fast neutrons

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

RESULTS. NEUTRAL PARTICLES. TRANSMISSION COEFFICIENTS



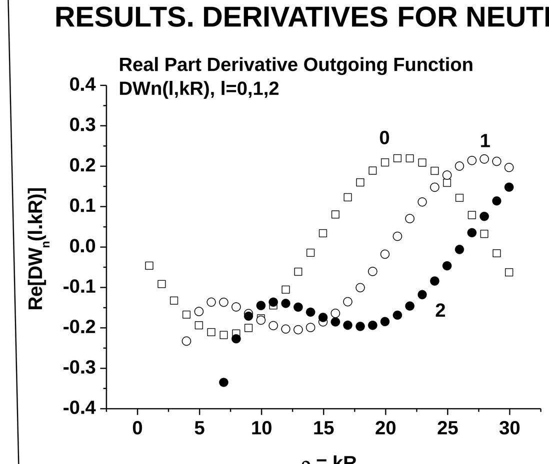
Ingoing and Outgoing Functions calculated in Quantum Mechanical Approach



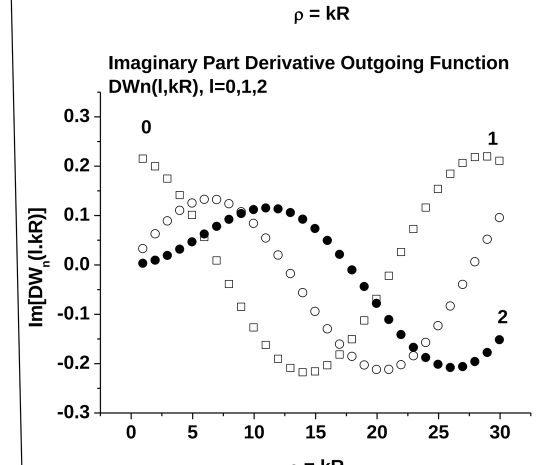
$W_l^{\pm}(r) = kr[n_l(kr) \pm ij_l(kr)]$

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

RESULTS. DERIVATIVES FOR NEUTRAL PARTICLES



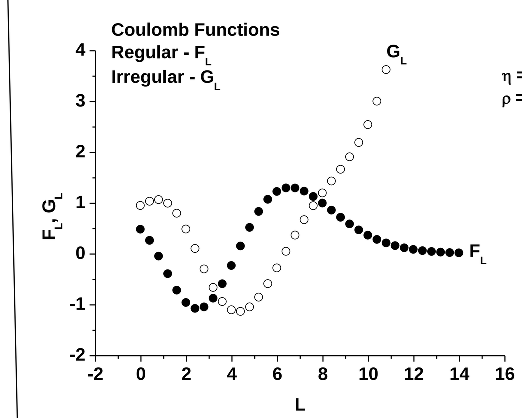
$W_l^{\pm}(r) = kr[n_l(kr) \pm ij_l(kr)]$

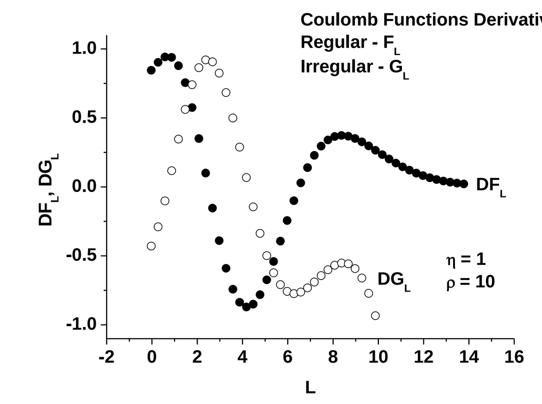


Derivative of Neutral Particle Wave Functions calculated in Quantum Mechanical approach

- Functions with Real and Imaginary part
- Importance for the calculation of Logarithmic Derivative Function

RESULTS. COULOMB FUNCTIONS FOR CHARGED PARTICLES



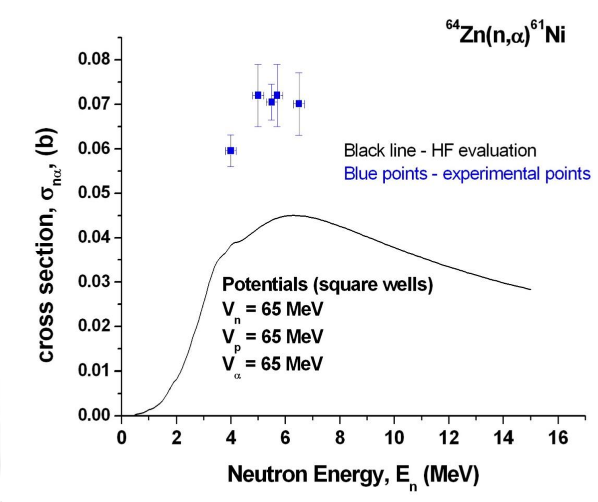


$$F_l - iG_l = \frac{e^{-\pi\rho}\rho^{l+1}}{(2l+1)!c_l(\eta)}\int_{-1}^{-i\infty} e^{-i\rho t}(1-t)^{l-i\eta}(1+t)^{l+i\eta}dt \qquad c_l(\eta) = \frac{2^l e^{-\frac{\pi\eta}{2}}\Gamma(l+1+i\eta)}{\Gamma(2l+2)}$$

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

Charged particle Regular and Irregular / Coulomb Functions (F_l, G_l) 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)

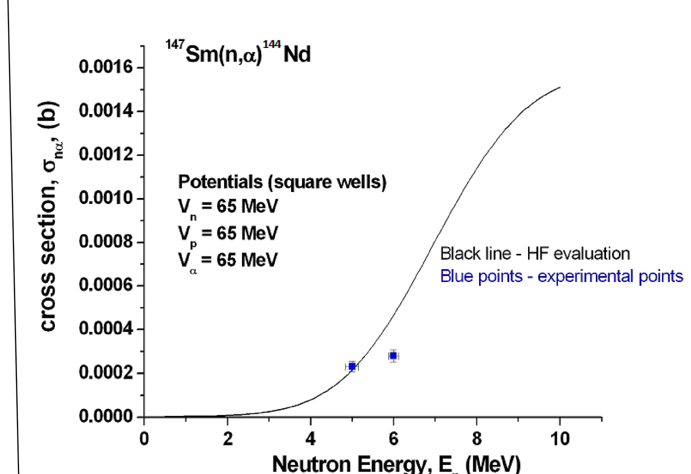
E_n, MeV	σ_1 (mb)	σ_2 (mb)
1	0.029	0.033
3	6.3	25
5	160	43

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

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



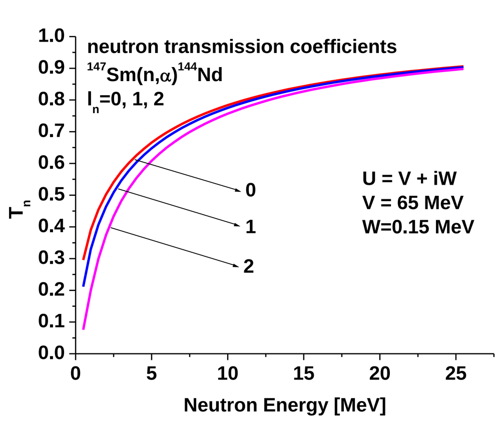
XS calculated with QM approach (2)

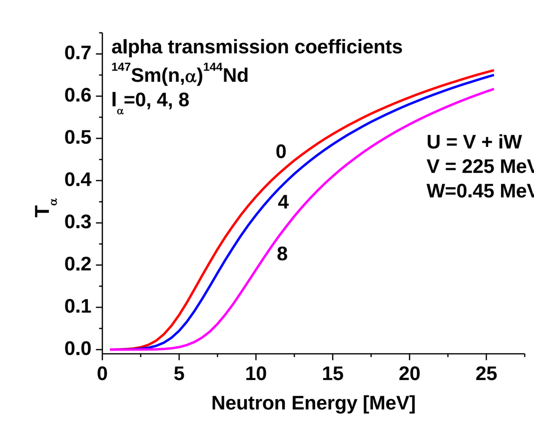
- good description for discrete states of residual nucleus
- with increasing of neutron energy other channels are open and should be considered
- Necessary to include continuum states of residual nucleus
- Realized by authors with Talys

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

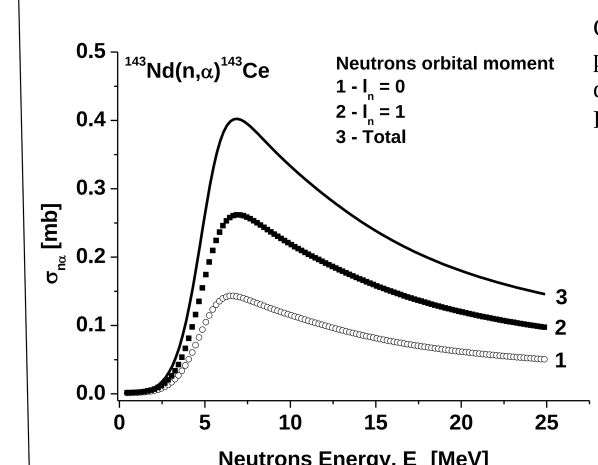




Orbital momentum: neutrons – l_n=0,1,2; alphas – l_α=0,4,8

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 + ix0.

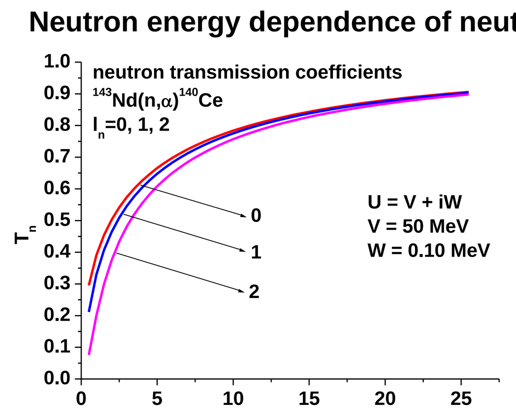
E_n [MeV]	Exp [mb]	Eval /2/ [mb]
4 ± 0.23	0.12 ± 0.01	0.14
5 ± 0.16	0.21 ± 0.01	0.26
6 ± 0.12	0.31 ± 0.03	0.37

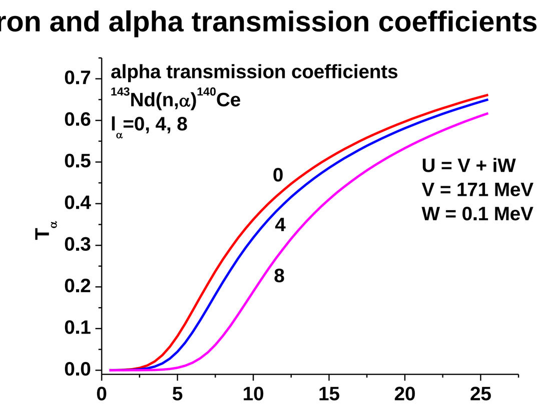
RESULTS. $^{143}Nd(n,\alpha)^{140}Ce$ Transmission coefficients – Quantum Mechanical Approach

$^{143}Nd(n,\alpha)^{140}Ce$ ($Q_{n\alpha}$ = 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





5. 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 coefficient 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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