DE LA RECHERCHE À L'INDUSTRIE

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ON THE USE OF THE GENERALIZED SPRT METHOD IN THE EQUIVALENT HARD SPHERE APPROXIMATION FOR NUCLEAR DATA EVALUATION

G. Noguere, P. Archier, O. Bouland, R. Capote, C. De Saint Jean,
S. Kopecky, P. Schillebeeckx, I. Sirakov, P. Tamagno

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Context

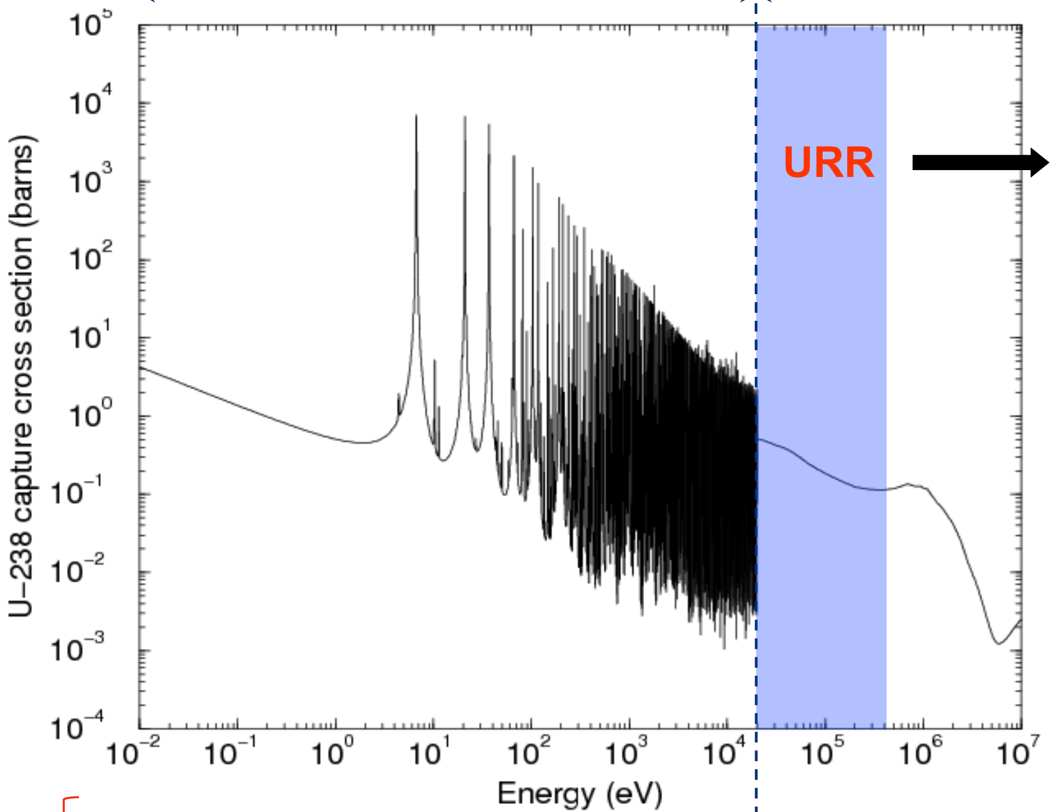
The analysis of the Unresolved Resonance Range of the neutron cross sections can be decomposed in three main steps:

- Statistical analysis of the resonance parameters ? ESTMA method
- **Optimization of the optical model parameters with constraints on the neutron strenght functions ? SPRT method implemented in the ECIS and OPTMAN code**
- Conversion of the average parameters in ENDF-6 format ? URR option of the TALYS code

Context

RRR

« Continuum »



URR parameters calculated with the TALYS code

Probability Tables for neutron transport calculations

R-Matrix formalism

Optical model (ECIS, OPTMAN)

Statistical model (TALYS)

Conrad

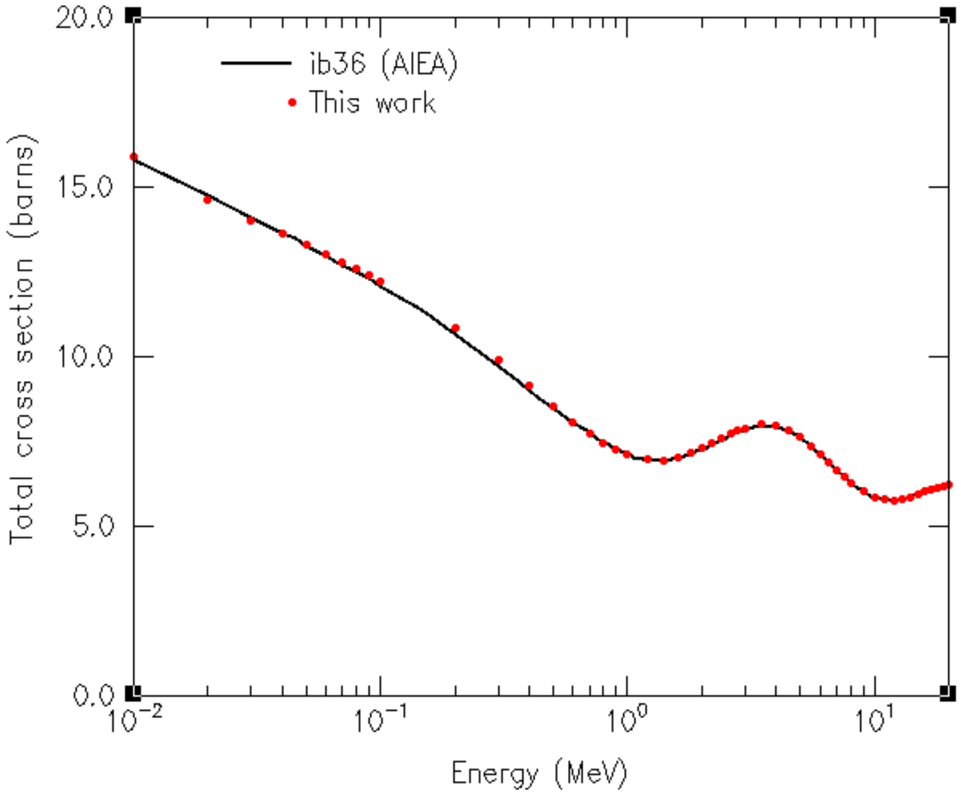
ESTIMA method

SPRT method
ECIS, OPTMAN codes

Partial wave breakdown analysis

The **SPRT method** is used to determine the scattering radii and the neutron strenght functions S_L (L= 0,1,2…) from optical model calculations

[?] Tests with Optical Model Parameters of Soukhovitski et al., J. Phys. G 30, 905 (2004)



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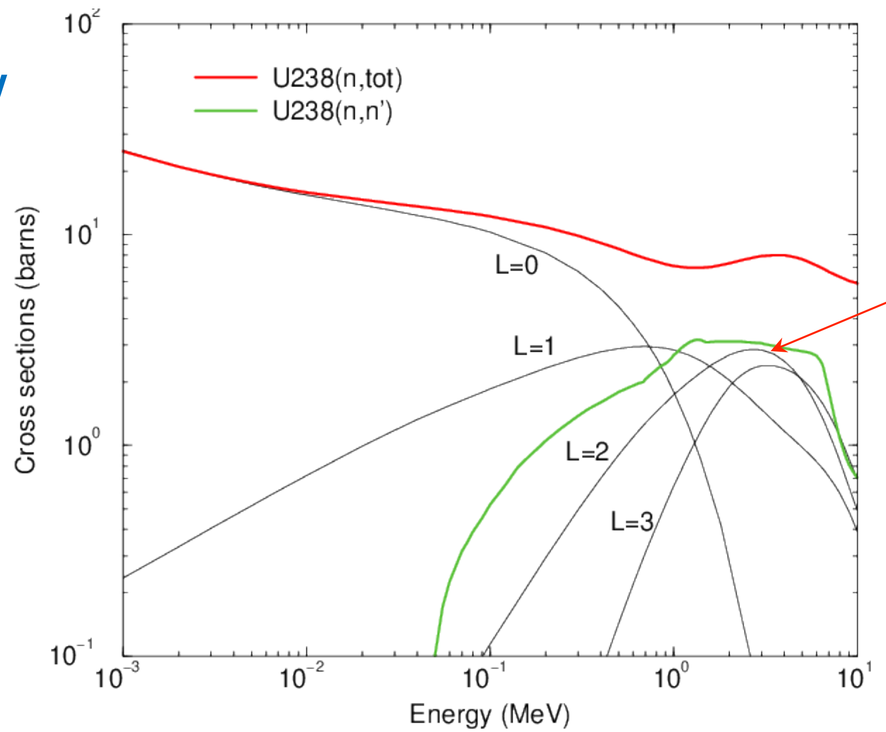
s-waves (L=0) is the dominant contribution at low neutron energy

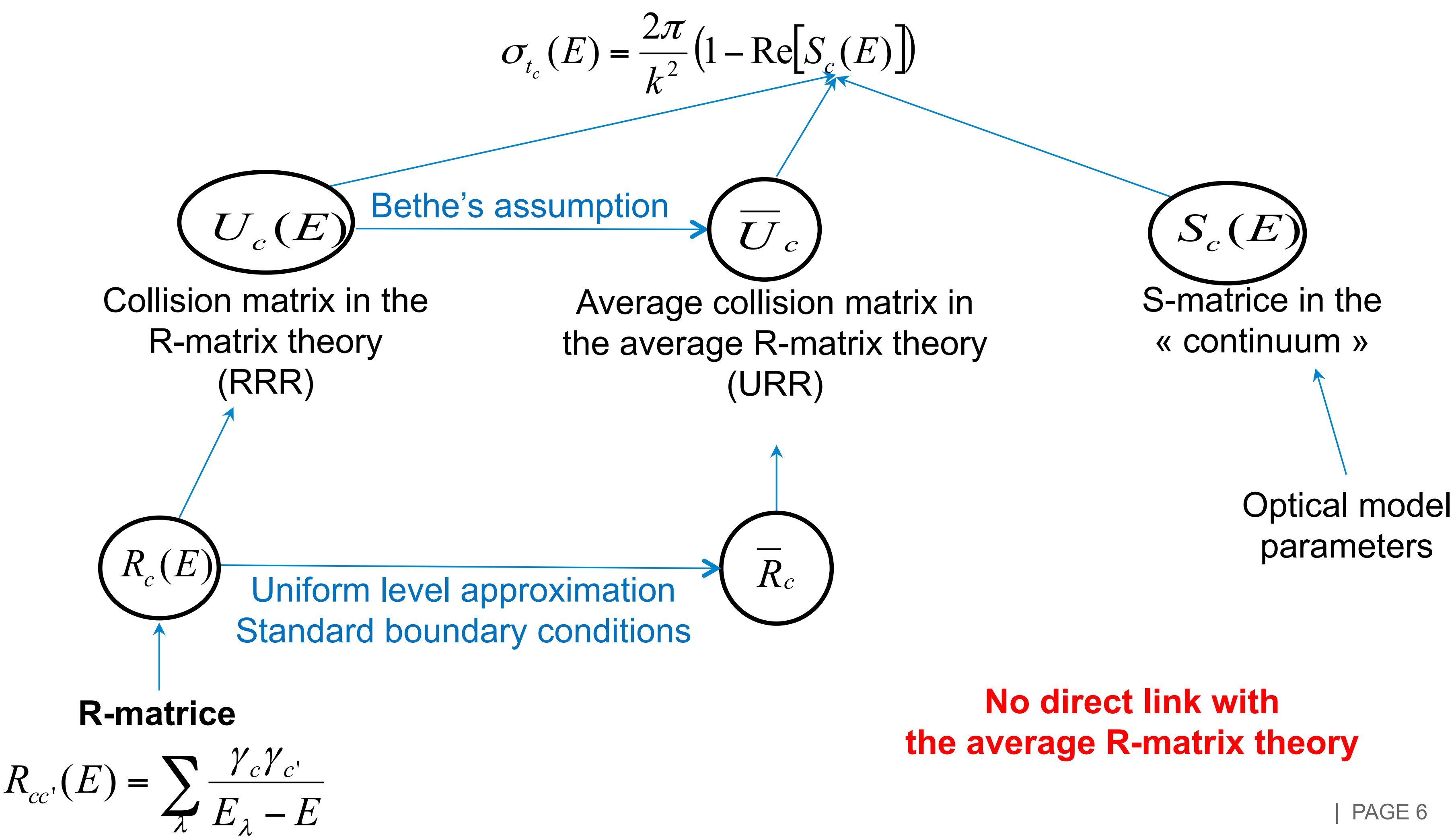


d-waves (L=2) becomes the dominant contribution arround 3 MeV

[?] Relationship between S_0 and S_2 ?

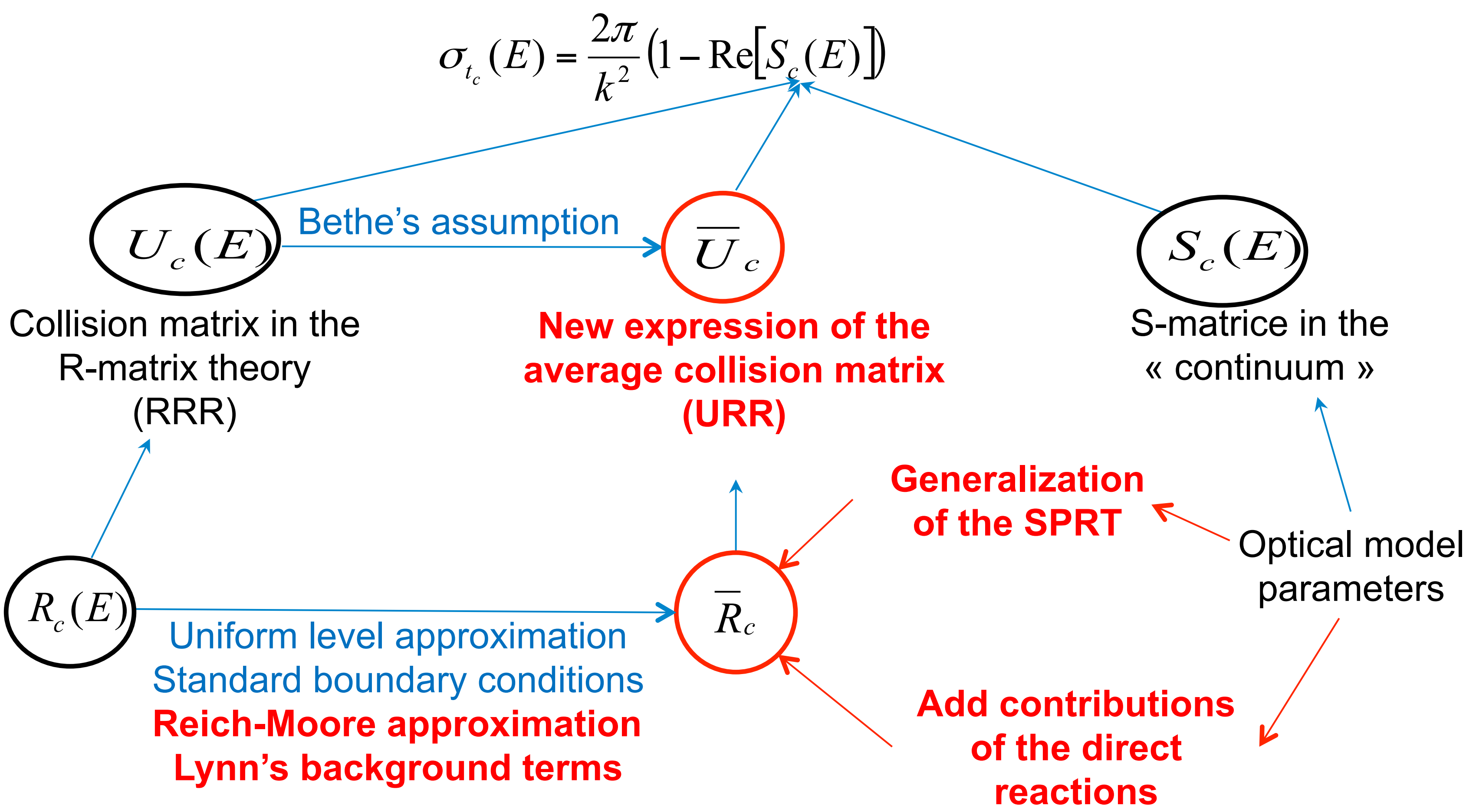
Theory of average cross section

Generic expression valid in the **RRR**, **URR** and **« continuum »**



Theory of average cross section

Generic expression valid in the **RRR**, **URR** and **« continuum »**



Average collision matrix

Neutron strength function

$$S_c = \frac{\left\langle \Gamma_{n_c}^{L} \right\rangle}{D_c}$$

Phase shift

$$\overline{U}_c = e^{2i\phi_c} \frac{1 + iP_L \overline{R}_c^{\infty} - \dfrac{\pi S_c \sqrt{E} P_L}{2P_0} - \pi P_L s_c^{loc}}{1 - iP_L \overline{R}_c^{\infty} + \dfrac{\pi S_c \sqrt{E} P_L}{2P_0} + \pi P_L s_c^{loc}}$$

Penetration factor

Distant level parameters (diffusion)

Contribution of the direct reactions

Average collision matrix with contributions of the direct reactions

Free parameters ? S_c $R^{?}$ P_L $?_L$ et s^{loc}

Average collision matrix

Phase shift

$$\overline{U}_c = e^{2i\phi_c} \frac{1 + iP_L \overline{R}_c^{\infty} - \frac{\pi S_c \sqrt{E} P_L}{2P_0} - \pi P_L s_c^{loc}}{1 - iP_L \overline{R}_c^{\infty} + \frac{\pi S_c \sqrt{E} P_L}{2P_0} + \pi P_L s_c^{loc}}$$

Penetration factor

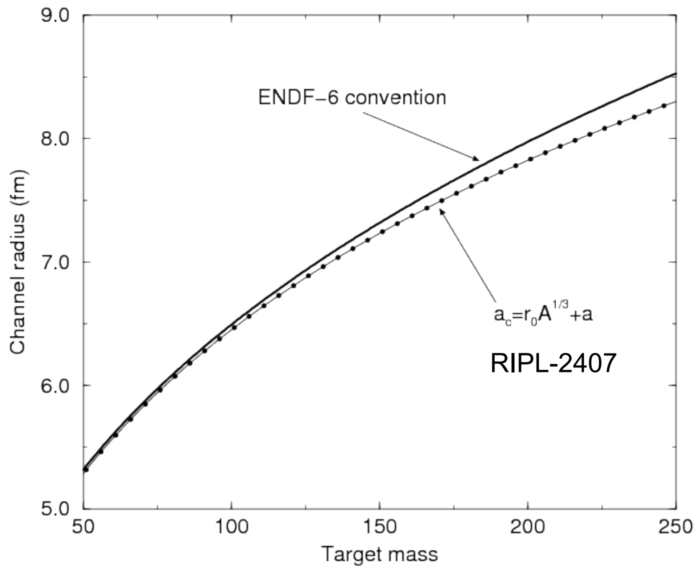
The phase shift and the penetration factor depend on the channel radius a_c

Definition of the channel radius a_c

The channel radius a_c (or matching radius when it explicitly refers to boundary condition parameter) satisfies the following condition (neutral indicent particle)

$$\begin{cases} V(r) = V_v(r) + V_s(r) + V_{so}(r) & r \le a_c \\ V(r) \approx 0 & r > a_c \end{cases}$$

① The channel radii are more or less chosen arbitrarily. Mostly the channel radius is defined as a simple function of the mass of the target nucleus plus a constant term (**ENDF convention**)



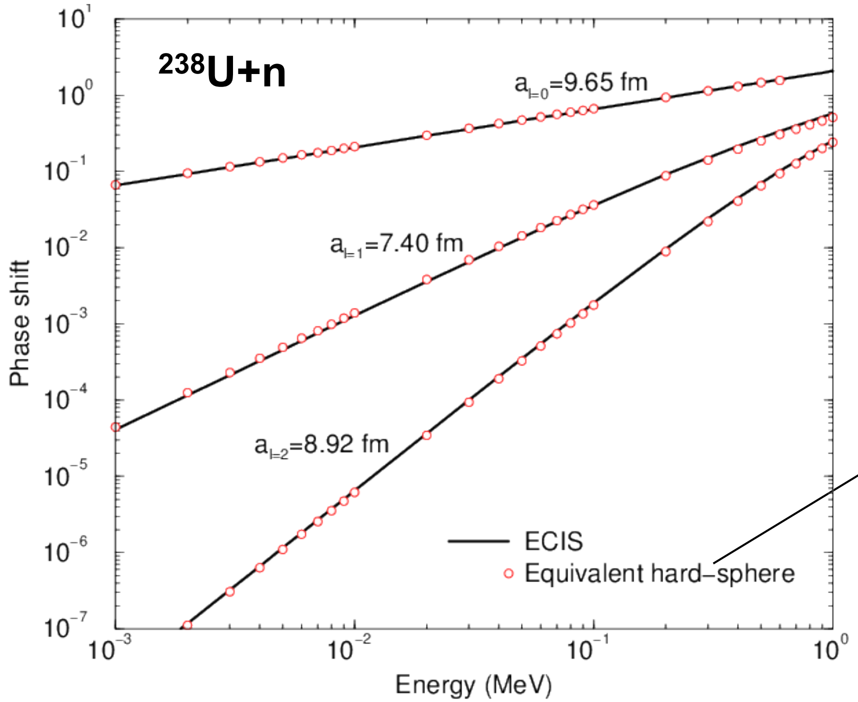
$$\left. \begin{aligned} a_c &= r_0 A^{1/3} + a \\ r_0 &= 1.23 \\ a &= 0.8 \end{aligned} \right\}$$

For ^{238}U a_c=8.42 fm

② a_c can be deduced from the phase shift $?_c$ calculated by Optical Model

Definition of the channel radius a_c

Link between a_c and the phase shift ?$_c$ calculated by Optical Model



For V(r)=0 and small angular momentum L

the usual presentation of ?$_c$ in terms of Bessel and Neumann functions becomes:

$$\begin{cases} \phi_0(\rho) = \rho \\ \phi_1(\rho) = \rho - \tan^{-1}(\rho) \\ \phi_2(\rho) = \rho - \tan^{-1}\left(\frac{3\rho}{3-\rho^2}\right) \end{cases}$$

$$\rho = ka_c$$

? Good agreement between ECIS calculations and equivalent hard-sphere approximation

Definition of the channel radius a_c

Verification of a_c via the relationship between the penetration factor P_c and the neutron transmission coefficient T_c

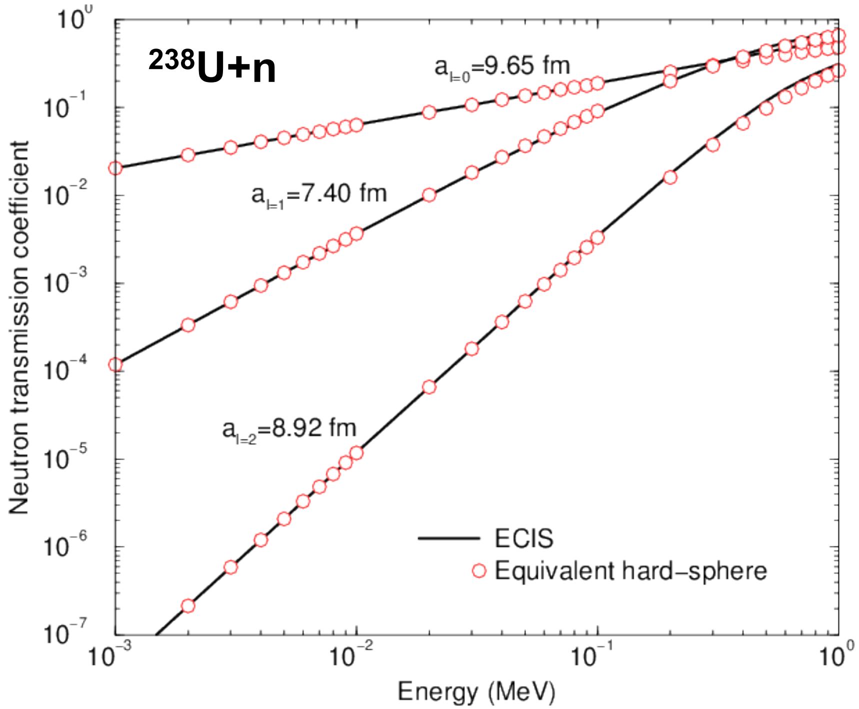
$$T_c = 1 - \left|\overline{U}_c\right|^2$$

For V(r)=0 and small angular momentum L

$$\begin{cases} P_0(\rho) = \rho \\ P_1(\rho) = \dfrac{\rho^3}{1+\rho^2} \\ P_2(\rho) = \dfrac{\rho^5}{9+3\rho^2+\rho^4} \end{cases}$$

$$\rho = k a_c$$

With a_c being the channel radius determined from the phase shift



Good agreement up to 300 keV

Average collision matrix

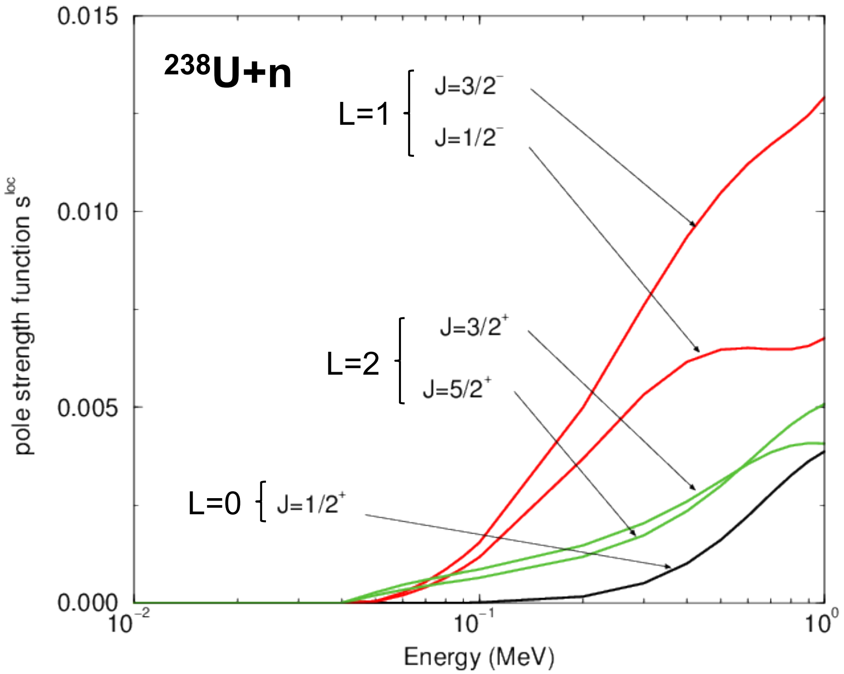
$$\overline{U}_c = e^{2i\phi_c} \frac{1 + iP_L \overline{R}_c^{\infty} - \dfrac{\pi S_c \sqrt{E} P_L}{2P_0} - \pi P_L s_c^{loc}}{1 - iP_L \overline{R}_c^{\infty} + \dfrac{\pi S_c \sqrt{E} P_L}{2P_0} + \pi P_L s_c^{loc}}$$

Contribution of the direct reactions (absorption)

Direct contributions s^{loc} are estimated with Optical Model Calculations

Pole strength function s^{loc}

The pole strength function s^{loc} is directly estimated from Optical Model Calculations



$$T_c = 1 - \left|\overline{U}_c\right|^2$$

$$T_c \approx \underbrace{\frac{4\pi P_l s_c}{\left[1 + \pi P_l s_c\right]^2 + P_l^2 \overline{R}_c^{\infty 2}}}_{\text{compound}} + \underbrace{\frac{4\pi P_l s_c^{loc}}{\left[1 + \pi P_l s_c\right]^2 + P_l^2 \overline{R}_c^{\infty 2}}}_{\text{direct}}$$

[?] Contribution s^{loc} (direct reactions) for L=0 and L=2 are nearly similar (?)

For spherical or weakly deformed nuclei [?] s^{loc}=0

Average collision matrix

Neutron strength function

$$S_c = \frac{\left\langle \Gamma_{n_c}^L \right\rangle}{D_c}$$

$$\overline{U}_c = e^{2i\phi_c} \frac{1 + iP_L \overline{R}_c^{\infty} - \dfrac{\pi S_c \sqrt{E} P_L}{2P_0} - \pi P_L s_c^{loc}}{1 - iP_L \overline{R}_c^{\infty} + \dfrac{\pi S_c \sqrt{E} P_L}{2P_0} + \pi P_L s_c^{loc}}$$

Distant level parameters (diffusion)

Simultaneous determination of the neutron strength functions and distant level parameters

SPRT method

Generalisation of the SPRT method (E. Rich, NSE, 2009)

The generalisation of the method aims to provide a partial-wave description of the nuclear scattering by solving the equations :

$$\begin{cases} \sigma_{t_c}(S_c, \overline{R}_c^{\infty}, E) = \sigma_{t_c}(C_c) \\ \sigma_{e_c}(S_c, \overline{R}_c^{\infty}, E) = \sigma_{e_c}(C_c) \end{cases}$$

The neutron strength function S_c and the distant level parameter R? are free parameters, and C_c is the collision matrix calculated with Optical Model codes (ECIS, OPTMAN)

$$P_L \overline{R}_c^{\infty} = \frac{2\alpha_c \cos[2\phi_L] + (1-2\beta_c)\sin[2\phi_L]}{1+2\gamma_c^2 - 2\beta_c + (1-2\beta_c)\cos[2\phi_L] - 2\alpha_c \sin[2\phi_L]}$$

$$\frac{\pi S_c \sqrt{E} P_L}{2P_0} = \frac{2(\beta_c - \gamma_c^2)}{1+2\gamma_c^2 - 2\beta_c + (1-2\beta_c)\cos[2\phi_L] - 2\alpha_c \sin[2\phi_L]} - \pi P_L s_c^{loc}$$

For U238 (ground state spin I=0) ?

$$\begin{cases} \alpha_c = \mathrm{Re}[C_c] \\ \beta_c = \mathrm{Im}[C_c] \\ \gamma_c = |C_c| \end{cases}$$

SPRT method

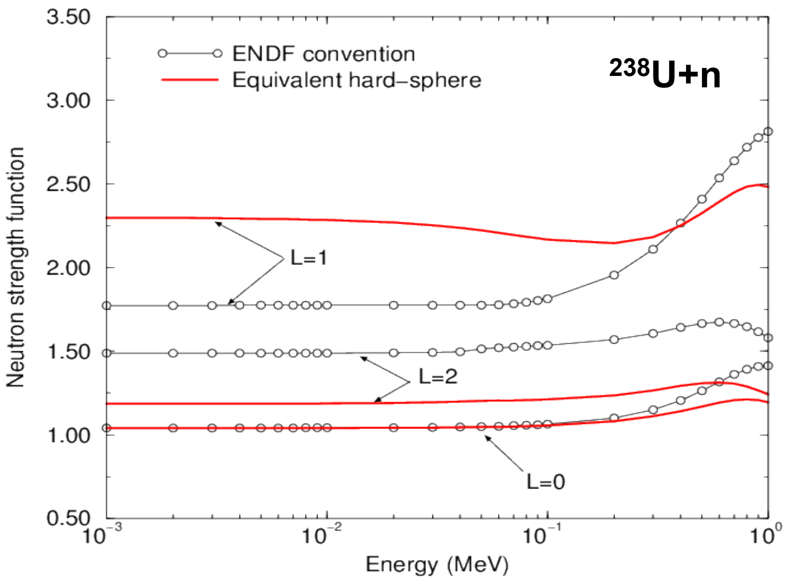
Distant level parameters and neutron strength functions

a_0=9.65 fm
a_1=7.40 fm
a_2=8.92 fm

Equivalent hard-sphere radius
Channel radius determined via the phase shift

a_0=8.42 fm
a_1=8.42 fm
a_2=8.42 fm

Channel radius in the **ENDF convention**



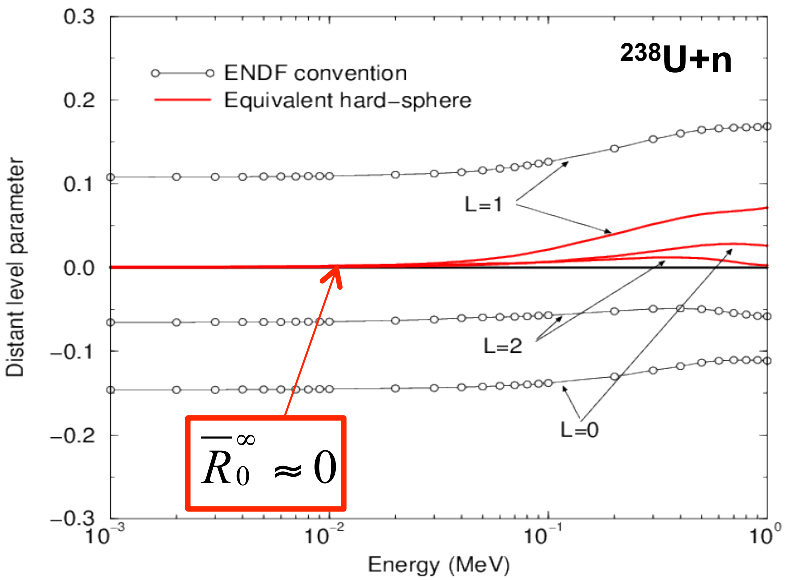
The channel radii determined via the phase shift calculated by Optical Model improved the agreement between S_0 and S_2 and seem to confirm the empirical rule (F. Frohner, O. Bouland, NSE, 2001)

S_0 ? S_2 ?cst

SPRT method

Distant level parameters and neutron strength functions

a_0=9.65 fm a_1=7.40 fm a_2=8.92 fm	**Equivalent hard-sphere radius** Channel radius determined via the phase shift
a_0=8.42 fm a_1=8.42 fm a_2=8.42 fm	Channel radius in the **ENDF convention**



? link with the effective radius R'

At low energy, the elastic cross section becomes the potential scattering cross section (hard sphere)

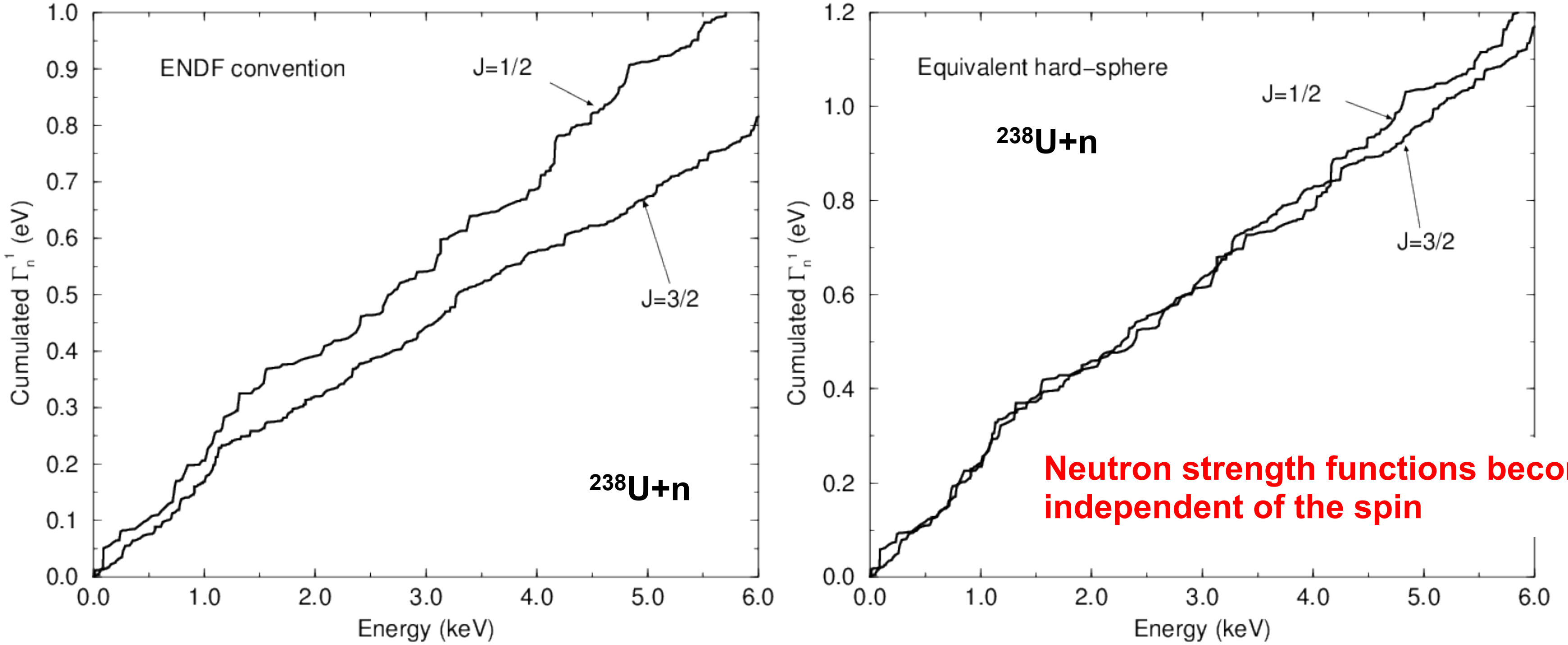
$$\sigma_p = \lim_{E \to 0} \sigma_{e_c}(E) = 4\pi R'^2$$

$$R' = a_0(1 - \overline{R}_0^\infty) \Rightarrow R' \approx a_0$$

? For ^{238}U+n $(\overline{R}_0^\infty \approx 0)$, the effectif radius and the channel radius are equivalent

Consequences on the p-wave neutron strength function

Staircase plot of the reduced neutron width for p-waves



Neutron strength functions become independent of the spin

? Hypothesis often used in Neutron Resonance Shape Analysis:

A. Michaudon « Contribution à l'étude par des méthodes du temps de vol de l'interaction des neutrons lents avec l'U235 », PhD thesis, Paris University, CEA Report R 2552, 1964

OPTMAN results

Equations of the SPRT method have been implemented in the OPTMAN code

Tests using a preliminary set of Optical Model Parameters for n+U238, n+U235 and n+Pu239

SPRT method from Delaroche and Lagrange (IAEA-190, 1976)

n+U238

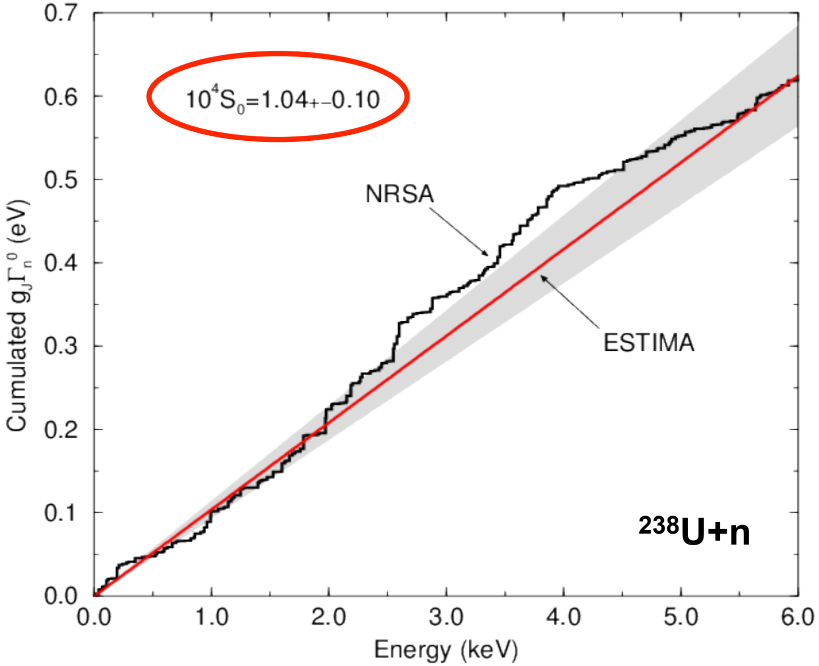
```
NEUTRON ENERGY =   0.005000
TOTAL  CR-SECT.= 17.749642
ELASTIC  CR-SECT.  = 11.357897
REACTION CR-SECT.  =  6.391744
REACTION CR-SECT. incl. coupled levels =  6.391744
SCATTERING RADIUS =  9.507012

 Nlev     Elev    Jpi          CR-SECT(Nlev)
  1     0.0000   0.0+            11.357897

                              STRENGTH  FUNCTIONS
SF0 =  0.1004878E-03         SF1 =  0.1808328E-03         SF2 =  0.1394003E-03

                         STRENGTH  FUNCTIONS FROM ESW
S0   =  0.1027956E-03         S1   =  0.2703804E-03         S2   =  0.1109824E-03

          Calculation time:   25 min 49 s
```

This work

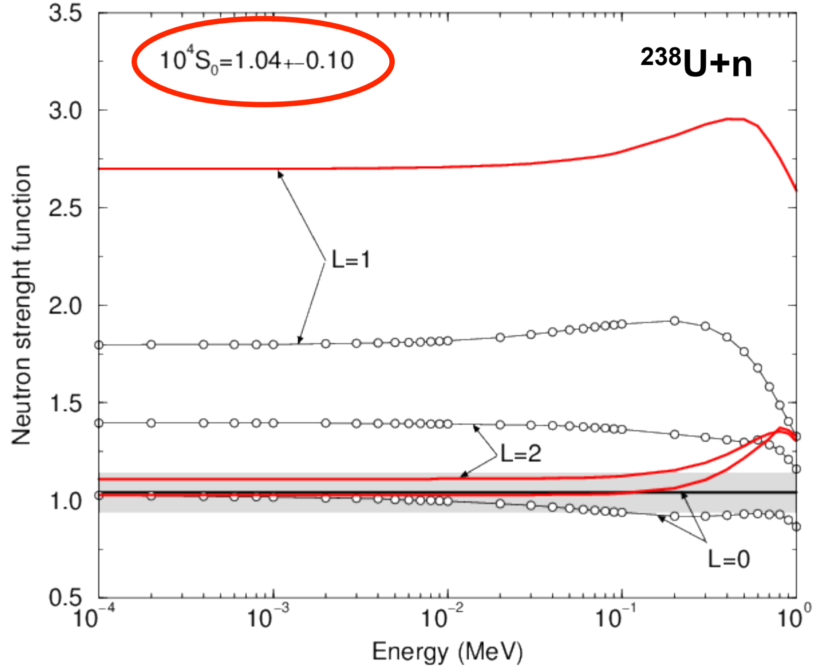
OPTMAN results

Comparison ESTIMA – SPRT analysis

Results from ESTIMA analysis



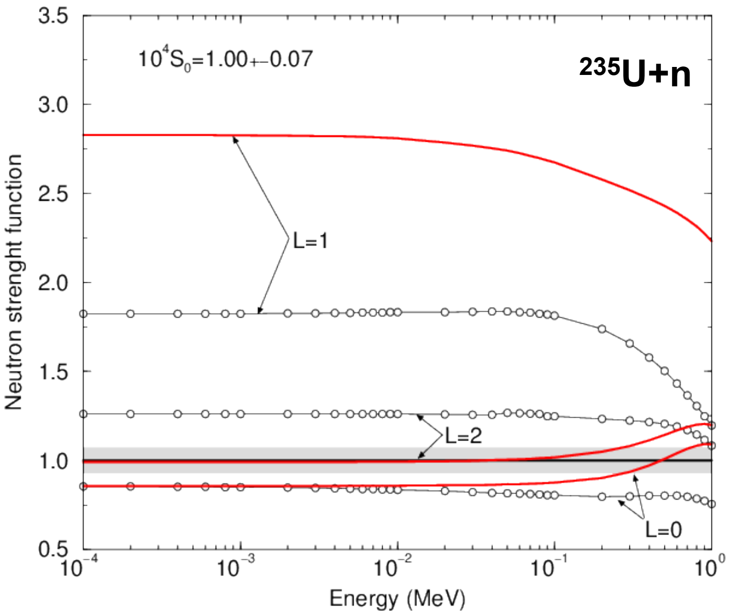
Results from SPRT analysis

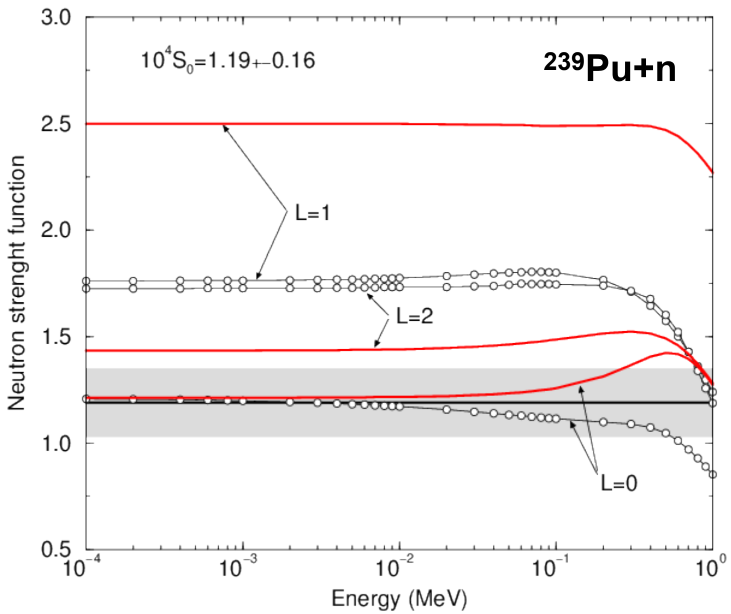


? Excellent agreement between ESTIMA and SPRT results for the s-wave and p-wave neutron strenght functions (OPTMAN gives $10^4 S_2$ = 1.10)

OPTMAN results

Comparison ESTIMA – SPRT analysis





? s-wave strenght function from OPTMAN calculations needs to be increased

? p-wave strenght function from OPTMAN calculations needs to be improved

Conclusions

The **equivalent hard-sphere radii** determined via the phase shift calculated by optical model seem to confirm several empirical rules and hypothesis:

•The neutron strength functions for L=0 and L=2 are likewize similar (S_0 [?] S_2)

•The effectif radius R' and the channel radius $a_{l=0}$ are equivalent

•The L-dependent neutron strength functions seem to be independent of the spin J

The present results indicate that S_0, R' and also S_2 can be used to establish a consisent set of optical model parameters.

The use of S_2 as an additional constraint could change the contribution of the compound nucleus cross section during the optimization procedure of the shape elastic and reaction cross sections

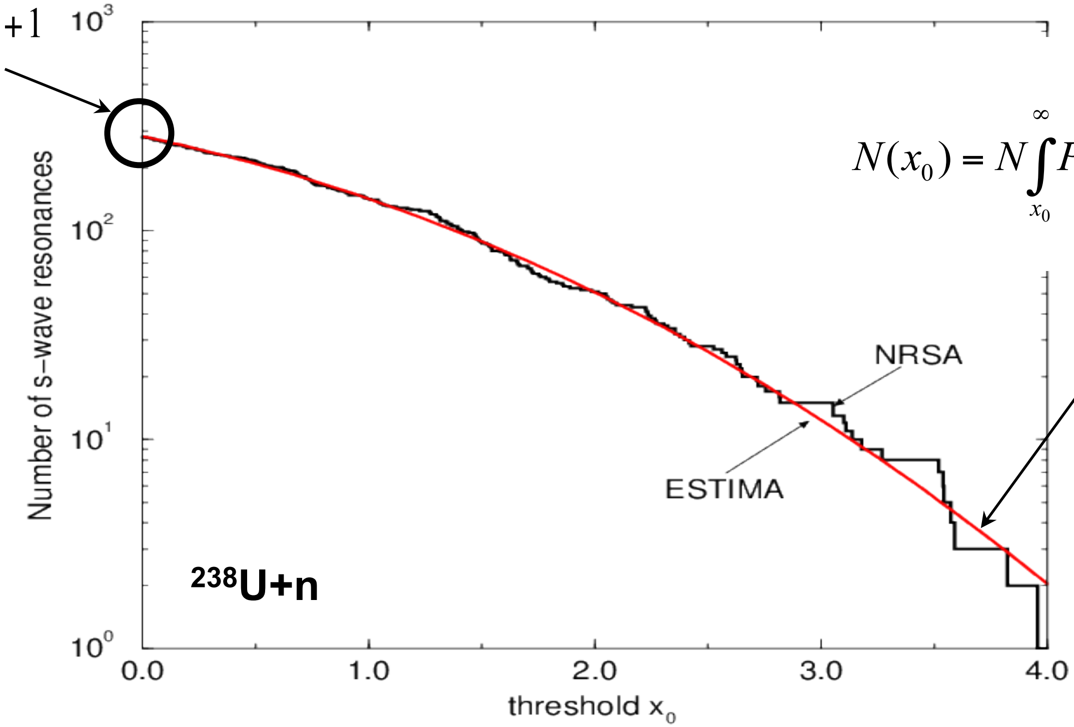
[?] impact on the partial cross sections (elastic, inelastic, fission cross sections) not yet tested.

Principle of the ESTIMA analysis

ESTIMA method (E.Fort, Cea Cadarache) for determining (S_0,D_0)

[?] The method determines simultaneously the most probable neutron strength function and mean level spacing for s-wave levels from the properties of the cumulative Porther-Thomas distribution of reduced neutron widths

$$N = \frac{E_{max} - E_{min}}{D_0} + 1$$



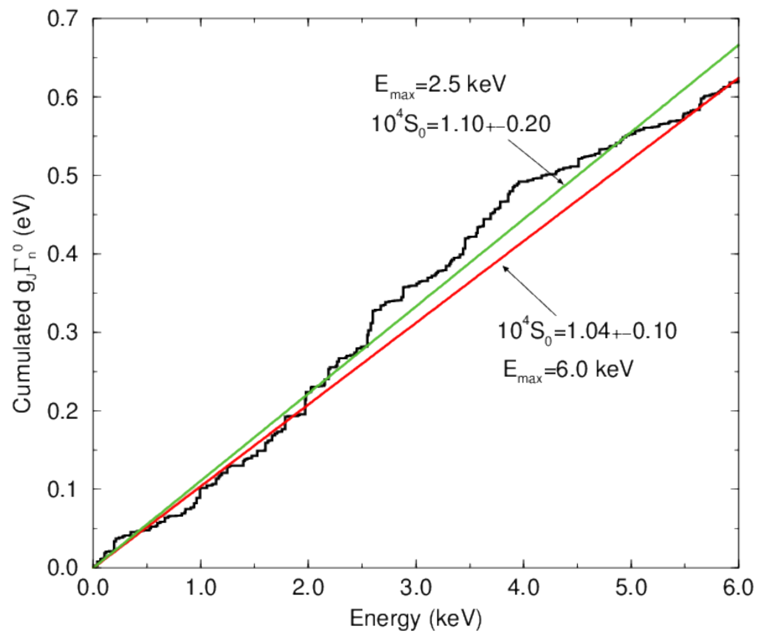
$$N(x_0) = N\int_{x_0}^{\infty} P(x)dx = N\ erfc\left(\sqrt{\frac{x_0}{2}}\right)$$

$$x_0 = \frac{g_J \Gamma_n}{D_0 S_0 \sqrt{E_\lambda}}$$

s-wave neutron strenght functions

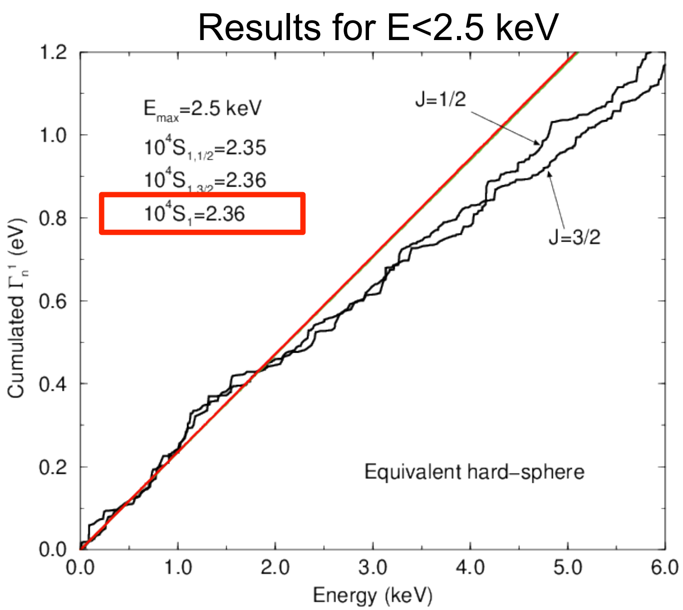
The s-wave neutron strength function for **U238+n** ranges from **1.04** to **1.10** depending on the criteria applied for the ESTIMA analysis

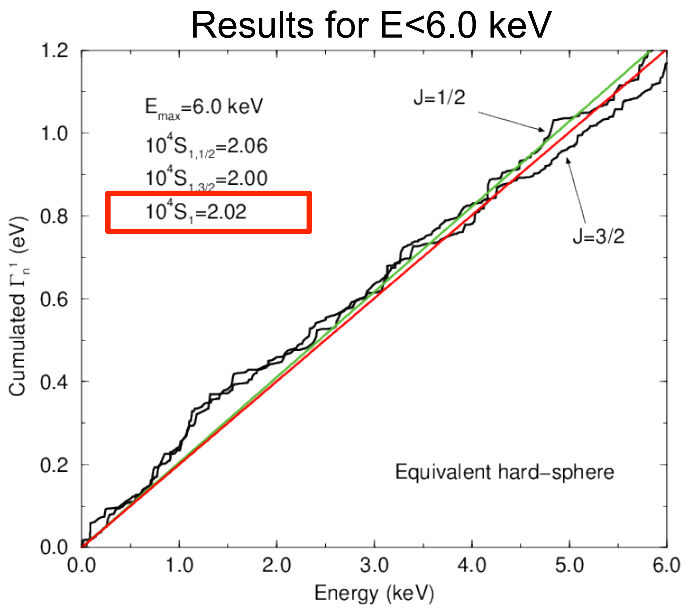
New resonance analysis between 2 keV and 5 keV is recommended



p-wave neutron strength function

Staircase plot of the reduced neutron width for p-waves





The p-wave neutron strength function for **U238+n** ranges from **2.02** to **2.36** depending on the criteria applied for the statistical analysis

Comparison ESTIMA – SPRT analysis

Summary of the results obtained for U238+n

		S_0	S_1	S_2
Compilation	**RIPL-3**	1.03±0.08	***1.2±0.2***	
	Atlas	***1.29±0.13***	2.17±0.19	
ESTIMA analysis (statistical analysis of the resonances)	**JEFF-3.1.1**	1.04±0.10	2.02-2.36	
	JEFF-3.3T2	1.03±0.10		
SPRT analysis with the OPTMAN code (with a set of preliminary optical model parameters)	**ENDF convention**	1.00	1.80	1.39
	Equivalent hard-sphere	1.03	2.70	1.11