Evaluations "*à la BRC*"

APRENDE Experimentalists - Evaluators workshop (WP2-WP4)

CEA/DAM/DIF
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BRuyères-le-Châtel (BRC) Approach :

evaluations only based on models

with the TALYS code

$$a + A \longrightarrow C^* \longrightarrow B + b$$

$$A(a,b)B$$

$$\sigma_{a,b} = \frac{\pi}{k_a^2} \sum_{J,l_a,j_a,l_b,j_b} \frac{2J+1}{(2I_a+1)(2I_A+1)} \frac{T^{J\pi}_{l_a,j_a} T^{J\pi}_{l_b,j_b}}{\sum_{l_c,j_c} T^{J\pi}_{l_c,j_c}} \times W_{ab}$$

$$\sigma_{CN} = \sum_b \sigma_{a,b}$$ (Rappel : $\sigma_R = \sigma_{CN} + \sigma_{PE} + \sigma_{DI}$)

$\otimes \rightarrow T^{J\pi}_{l_a,j_a}$: $a = n$ $b = p, \cdots {}^4$He $\leftrightarrow$ **OMP+CCC OK** $\leftarrow \otimes$ **focus on this point**

and $b = \gamma \leftrightarrow$ **Kopecky-Uhl + Brink-Axel or QRPA OK**

$\otimes \rightarrow T^{J\pi}_{b=f} \rightarrow$ **fission exit channel ? ? ?** $\leftarrow \otimes$ **focus on this point**

BRuyères-le-Châtel (BRC) Approach :

evaluations only based

on phenomenological models

$\Updownarrow$

so we need experimental data

Evaluations only based

Pb : resolution of SE for scattering stationnary states

$$H(A+1)|\chi\rangle^{A+1} = E|\chi\rangle^{A+1} \text{ avec : } H(A+1) = H(A) + H(1)$$

Spherical Nuclei : Spherical optical Model

$$|\chi\rangle^{A+1} = |\phi\rangle_{lj} \otimes |0\rangle^{A} \text{ et : } H(A)|0\rangle^{A} = E_0|0\rangle^{A} = 0$$
$$H(1)|\phi\rangle_{lj} = \big(T(1) + U_{opt}(1)\big)|\phi\rangle_{lj} = E|\phi\rangle_{lj}$$

problem symmetries ($[H,\vec{L}^2] = 0$ et $[H,L_z] = 0 \Longrightarrow$) Solutions, $\forall l$:

$$\phi_{lj}(r,\theta) = \frac{1}{kr}\sum_{l=0}^{\infty}(2l+1)i^l y_l(r)P_l(\cos\theta)$$

Deformed Nuclei : Coupled Channels, ($[H,\vec{J}^2] = 0$ et $[H,J_z] = 0 \Longrightarrow$) Solutions, $\forall J$:

$$|\chi\rangle^{A+1} = (|\phi\rangle_{lj}\otimes|\Psi_I^A\rangle)_J \text{ et : } H(A)|\Psi_I^A\rangle = \epsilon_n|\Psi_I^A\rangle$$
$$H(1)(|\phi\rangle_{lj}\otimes|\Psi_I^A\rangle)_J = \big(T(1) + U_{opt}(1)\big)(|\phi\rangle_{lj}\otimes|\Psi_I^A\rangle)_J = (E-\epsilon_n)(|\phi\rangle_{lj}\otimes|\Psi_I^A\rangle)_J$$

$$|\chi\rangle^{A+1} = \frac{1}{r}\sum_{\substack{J,k,l_k,j_k,m_{j_k},\\ M_{I_k},m_{l_k},m_{s_k}}} R^J_{k,l_k,j_k}(r)\, C^{j_k m_{j_k}}_{l_k s_k m_{l_k} m_{s_k}}\, C^{JM}_{j_k I_k m_{j_k} M_{I_k}}\, i^{l_k}\, |l_k m_{l_k}\rangle |s_k m_{s_k}\rangle |k I_k M_{I_k}\rangle$$

$$\langle (l'j'I')_J | [U_r \otimes U_T]^{(0)} | (ljI)_J \rangle \neq 0$$

The scattering stationnary states can be written as :

$$|\Psi\rangle = \frac{1}{r} \sum_{J,k,l_k,j_k,m_{j_k},M_{I_k},m_{l_k},m_{s_k}} R^J_{k,l_k,j_k}(r) \langle j_k I_k m_{j_k} M_{I_k} | JM \rangle \times \langle l_k s_k m_{l_k} m_{s_k} | j_k m_{j_k} \rangle i^{l_k} |l_k m_{l_k}\rangle |s_k m_{s_k}\rangle |k I_k M_{I_k}\rangle$$

The Schrödinger equation solved for the scattering stationnary states, once projeted onto the different states $|l_i m_{l_i}\rangle |s m_s\rangle |i I_i M_{I_i}\rangle^J$, will give rise to a system of coupled equations as follows :

$$\left(-\frac{d^2}{dr^2} + \frac{l_i(l_i+1)}{r^2} + \frac{2\mu}{\hbar^2}(U^{diag}(r) + \epsilon_i - E)\right) R^J_{i,l_i,j_i}(r) + \frac{2\mu}{\hbar^2}\left(\sum_{k,l_k,j_k} {}^J\langle i I_i M_{I_i} | \langle s_i m_{s_i} | \langle l_i m_{l_i} | U^{coupl} | l_k m_{l_k} \rangle | s_k m_{s_k} \rangle | k I_k M_{I_k} \rangle^J R^J_{k,l_k,j_k}(r)\right) = 0 \quad ; \tag{1}$$

Here, the J exponent means "coupled to J", :

$$|l_k m_{l_k}\rangle |s_k m_{s_k}\rangle |k I_k M_{I_k}\rangle^J = \sum_{m_{l_k} m_{s_k} m_{j_k} M_{I_k}} i^{l_k} \langle j_k I_k m_{j_k} M_{I_k} | JM \rangle \langle l_k s_k m_{l_k} m_{s_k} | j_k m_{j_k} \rangle |l_k m_{l_k}\rangle |s_k m_{s_k}\rangle |k I_k M_{I_k}\rangle \tag{2}$$

This system of coupled equations can also be expressed in matrix form as :

$$\begin{pmatrix} R^{J\pi\,''}_{1,l_1,j_1} \\ \vdots \\ R^{J\pi\,''}_{i,l_i,j_i} \\ \vdots \\ R^{J\pi\,''}_{n,l_n,j_n} \end{pmatrix} - \begin{pmatrix} G^{J\pi}_{11} & \cdots & G^{J\pi}_{1k} & \cdots & G^{J\pi}_{1n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ G^{J\pi}_{i1} & \cdots & G^{J\pi}_{ik} & \cdots & G^{J\pi}_{in} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ G^{J\pi}_{n1} & \cdots & G^{J\pi}_{nk} & \cdots & G^{J\pi}_{nn} \end{pmatrix} \begin{pmatrix} R^{J\pi}_{1,l_1,j_1} \\ \vdots \\ R^{J\pi}_{i,l_i,j_i} \\ \vdots \\ R^{J\pi}_{n,l_n,j_n} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \qquad (3)$$

where the diagonal part of the previous equation (1) is written as :

$$G^{J\pi}_{ii} = \frac{l_i(l_i+1)}{r^2} + \frac{2\mu}{\hbar^2}\left(U^{diag}(r) + \epsilon_i - E\right), \qquad (4)$$

and the off-diagonal part ($i \neq k$) as :

$$G^{J\pi}_{ik} = \frac{2\mu}{\hbar^2}\left({}^{J}\langle i I_i M_{I_i}|\langle s_i m_{s_i}|\langle l_i m_{l_i}|U^{coupl}|l_k m_{l_k}\rangle|s_k m_{s_k}\rangle|k I_k M_{I_k}\rangle^{J}\right), \qquad (5)$$

After multipole expansion of the projectile-target interaction potential. :

$$U = \sum_{\lambda,\sigma,L} v_{\lambda,\sigma,L}(r) \left[[i^L Y^L \otimes Q^\sigma]^\lambda \otimes Q_T^\lambda \right]_0^0$$

$$\frac{\hbar^2}{2\mu} G_{ik}^{J^\pi} = \sum_{\lambda,\sigma,L} v_{\lambda,\sigma,L}(r)^J \langle i I_i M_{I_i} | \langle s_i m_{s_i} | \langle l_i m_{l_i} | \left[[i^L Y^L \otimes Q^\sigma]^\lambda \otimes Q_T^\lambda \right]_0^0 | l_k m_{l_k} \rangle | s_k m_{s_k} \rangle | k I_k M_{I_k} \rangle^J \quad (6)$$

$$\begin{aligned} \frac{\hbar^2}{2\mu} G_{ik}^{J^\pi} = \sum_{\lambda,\sigma,L} \sum_{m_{l_i} m_{s_i} m_{j_i} M_{I_i}} \sum_{m_{l_k} m_{s_k} m_{j_k} M_{I_k}} & i^{l_k - l_i} \frac{v_{\lambda,\sigma,L}(r)}{\sqrt{2\lambda+1}} \sum_\mu (-1)^{\lambda-\mu} \sum_{M_L,\nu} \langle L \sigma M_L \nu | \lambda \mu \rangle \\ & \times \langle j_i I_i m_{j_i} M_{I_i} | JM \rangle \langle l_i s_i m_{l_i} m_{s_i} | j_i m_{j_i} \rangle \\ & \times \langle j_k I_k m_{j_k} M_{I_k} | JM \rangle \langle l_k s_k m_{l_k} m_{s_k} | j_k m_{j_k} \rangle \\ & \times \langle l_i m_{l_i} | i^L Y_{M_L}^L | l_k m_{l_k} \rangle \langle s_i m_{s_i} | Q_\nu^\sigma | s_k m_{s_k} \rangle \langle i I_i M_{I_i} | Q_{(T)-\mu}^\lambda | k I_k M_{I_k} \rangle. \quad (7) \end{aligned}$$

$$\frac{\hbar^2}{2\mu} G_{ik}^{J\pi} = \sum_\lambda i^{l_k - l_i} (-1)^{J - s_i - I_k + l_i + l_k} v_\lambda(r) \times \sqrt{\frac{(2l_i+1)(2l_k+1)(2j_i+1)(2j_k+1)}{4\pi}} \times \langle I_i || Q^\lambda_{(T)} || I_k \rangle \langle l_i l_k 0 0 | \lambda 0 \rangle W(j_i I_i j_k I_k; J\lambda) W(l_i j_i l_k j_k; s_i \lambda). \tag{8}$$

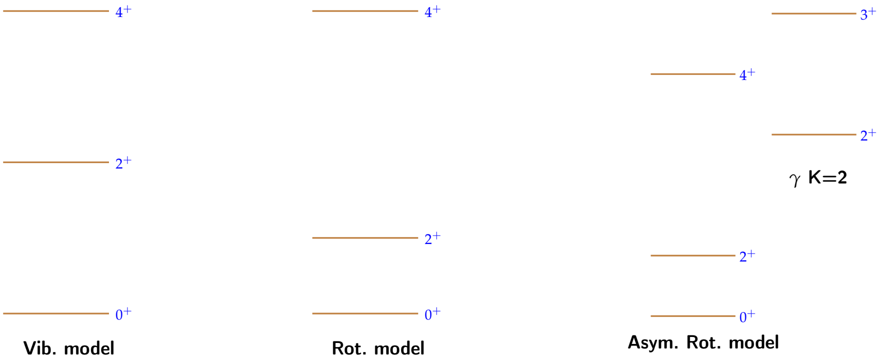
vibrational model (one phonon (surfon) excitation λ)

$$\langle I_i || Q^\lambda_{(T)} || I_k \rangle \longrightarrow \langle 0; 0 || Q^\lambda || 1; I_k \rangle = (-1)^{I_k} \beta_\lambda \delta_{\lambda I_k}. \tag{9}$$

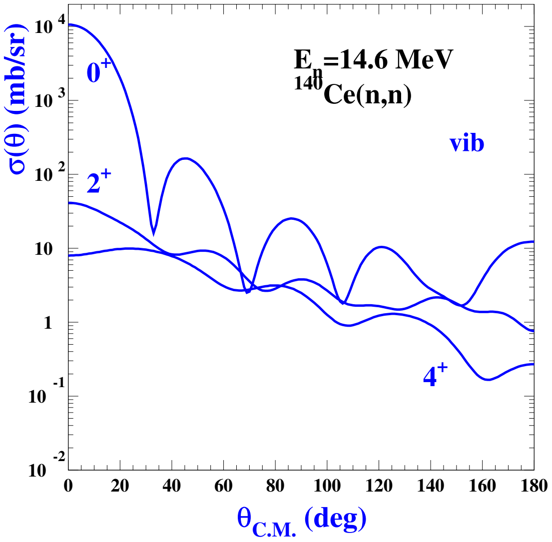
rotational symmetrical model

$$\langle I_i || Q^\lambda_{(T)} || I_k \rangle \longrightarrow \langle IK || \mathcal{D}^\lambda_0 || I' K' \rangle = \sqrt{2I'+1} \langle I' \lambda K 0 | IK \rangle \delta_{KK'} \tag{10}$$

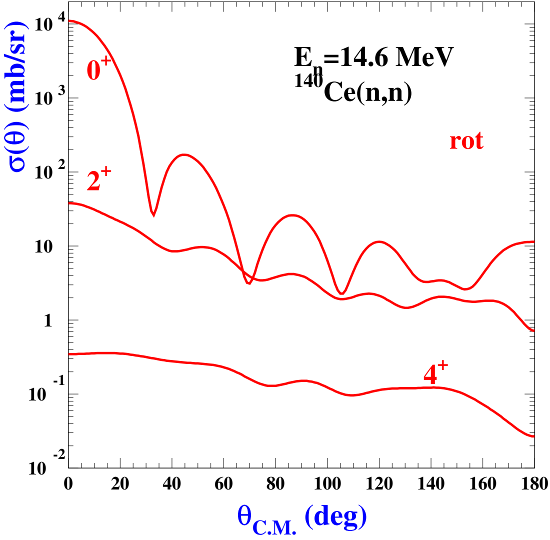
OMP - CCC ↔ which coupling scheme ?



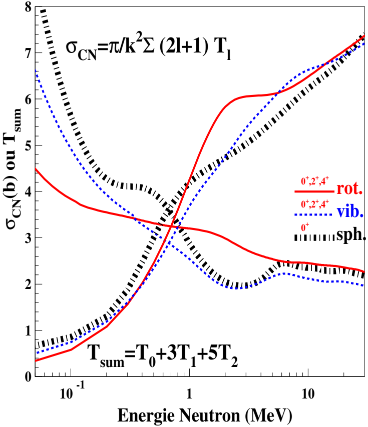
vibrationnal model

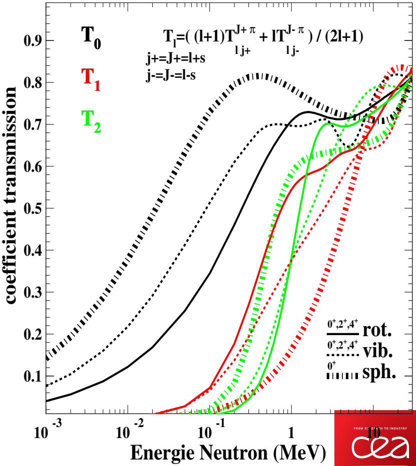


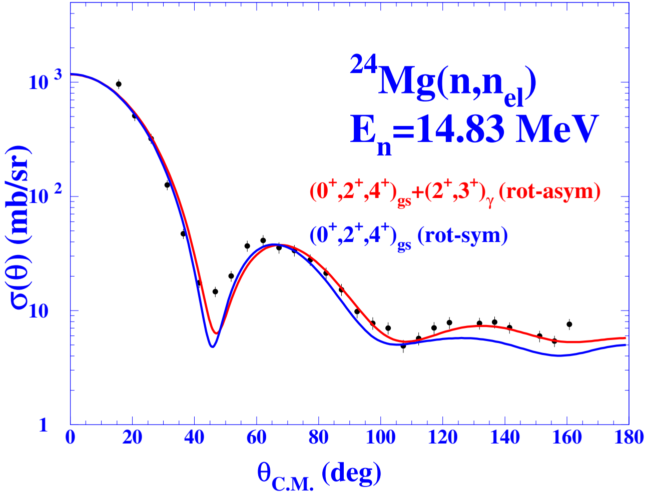
rotationnal model



Comparisons coeff. trans. and σ_{CN} vs coupling






^{24}Mg(n,n$_{el}$)
E$_n$=14.83 MeV
$(0^+,2^+,4^+)_{gs}+(2^+,3^+)_\gamma$ (rot-asym)
$(0^+,2^+,4^+)_{gs}$ (rot-sym)
σ(θ) (mb/sr)
$\theta_{C.M.}$ (deg)
1
10
10 2
10 3
0
20
40
60
80
100
120
140
160
180

$\mathbb{S}$ Matrix, σ_{tot}, σ_{SE}, σ_R et $T_{lj}^{J^\pi}$

Schrödinger Eq. (SE) solved by Numerov Method.

SE solutions y_α^J connected at $r \to +\infty$:
At $(R - h$ & $R + h : U_{nuc} = 0)$ with $\mathcal{F}_\alpha^J(r_i)$ & $\mathcal{G}_\alpha^J(r_i)$ functions related to Bessel spherical fonctions j_l et n_l :

$$y_\alpha^J(r_i) = \gamma_{lj}\left\{\underbrace{(\mathcal{G}_\alpha^J(r_i) - i\mathcal{F}_\alpha^J(r_i))}_{\text{FO ent.}} - \mathbb{S}_{\alpha\alpha'}^J \underbrace{(\mathcal{G}_{\alpha'}^J(r_i) + i\mathcal{F}_{\alpha'}^J(r_i))}_{\text{FO sor.}}\right\}$$

$$\alpha \equiv (l, j, I_A)$$

$$\sigma_{tot} = \frac{2\pi}{k^2}\sum_\alpha \frac{2J+1}{(2s+1)(2I_A+1)}(1 - Re(\mathbb{S}_{\alpha\alpha}^J))$$

$$\sigma_{SE} = \frac{\pi}{k^2}\sum_\alpha \frac{2J+1}{(2s+1)(2I_A+1)}|(1 - \mathbb{S}_{\alpha\alpha}^J)|^2$$

$$\sigma_R = \frac{\pi}{k^2}\sum_\alpha \frac{2J+1}{(2s+1)(2I_A+1)}(1 - \sum_{\alpha'}|\mathbb{S}_{\alpha\alpha'}^J|^2)$$

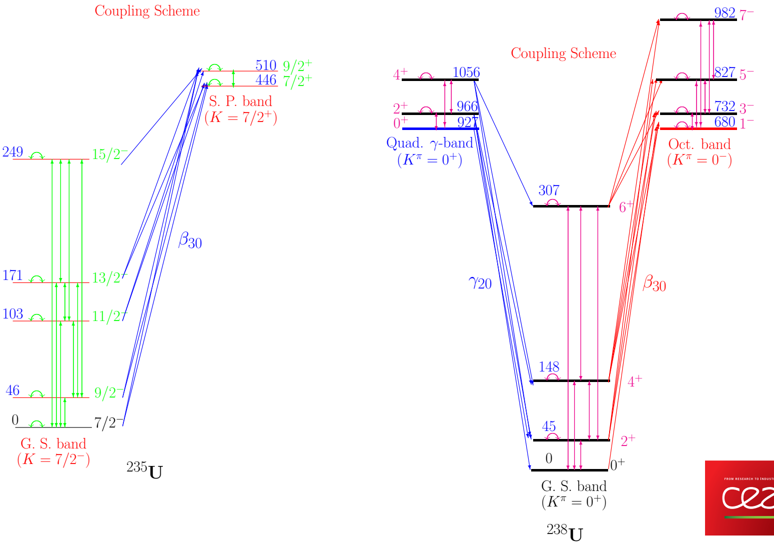
$$T_\alpha^{J^\pi} = 1 - \sum_{\alpha'}|\mathbb{S}_{\alpha\alpha'}^J|^2$$

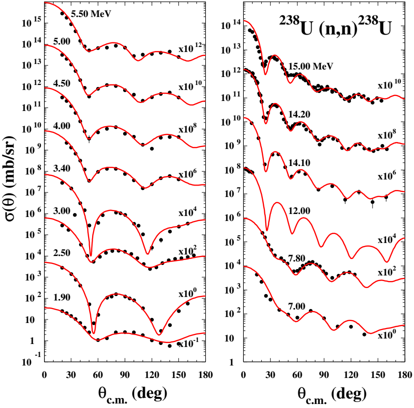
$\mathbb{S}$ Matrix :

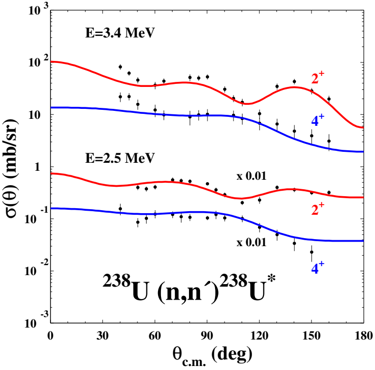
$$\sigma_{tot} = \sigma_{SE} + \underbrace{\sigma_R}_{T_{lj}^{J^\pi}}$$

$$U = V + iW$$

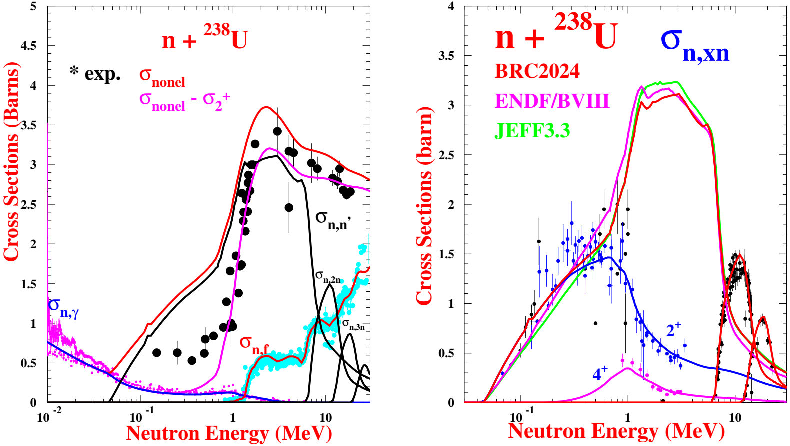
$$\sigma_R = (\sigma_{CN} + \sigma_{PE}) + \sigma_{DI}$$


Coupling Scheme
510 9/2+
446 7/2+
S. P. band
(K = 7/2+)
249 15/2−
171 13/2−
103 11/2−
46 9/2−
0 7/2−
β30
G. S. band
(K = 7/2−)
235U
Coupling Scheme
4+ 1056
2+ 966
0+ 927
Quad. γ-band
(Kπ = 0+)
307 6+
γ20
148 4+
45 2+
0 0+
G. S. band
(Kπ = 0+)
238U
982 7−
827 5−
732 3−
680 1−
Oct. band
(Kπ = 0−)
β30

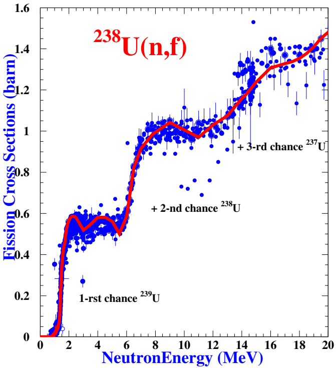

^{238}U (n,n)^{238}U
5.50 MeV
5.00
4.50
4.00
3.40
3.00
2.50
1.90
15.00 MeV
14.20
14.10
12.00
7.80
7.00
x10^{12}
x10^{10}
x10^{8}
x10^{6}
x10^{4}
x10^{2}
x10^{0}
x10^{-1}
σ(θ) (mb/sr)
θ$_{c.m.}$ (deg)

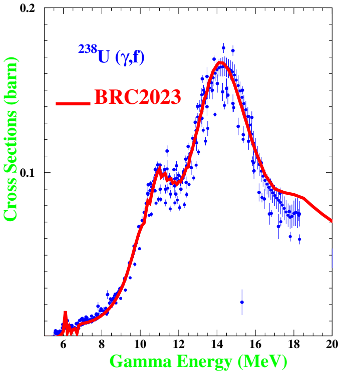

E=3.4 MeV
E=2.5 MeV
2^{+}
4^{+}
x 0.01
^{238}U (n,n´)^{238}U*
σ(θ) (mb/sr)
θ$_{c.m.}$ (deg)

(n,xn), (n,f), (n,γ) ^{238}U cross sections modeling with TALYS



Consistency between fission model parameters with other reactions





second chance n $+^{238}$U
third chance n $+^{238}$U

first chance γ $+^{238}$U
second chance γ $+^{238}$U

$\Longrightarrow$ test ^{238}U, ^{237}U fission parameters

Towards new models of fission modeling

If OMP modeling quite satisfactory

what about fission channel modeling ?

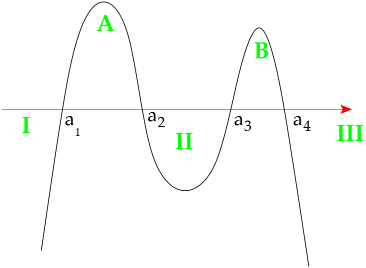
Until now, inverted parabolas have been used as fission barriers.

And transmission coefficients deduced from Hill-Wheeler formula :

$$T(E) = \frac{1}{1 + \exp\left[2\pi \frac{(B-E)}{\hbar\omega}\right]}$$

(= WKB approximation for this type of barriers)

The idea is to calculate the exact transmission coefficient of a given barrier, starting with one of this type :



using the Numerov's method

SE : $(H-E)u(r)=0 \iff u''(r)-\frac{2\mu}{\hbar^2}(V(r)-E)u(r)=0 \iff u''(r)-g(r)u(r)=0$

Taylor Expansion of u at $r+h$ and $r-h$:

$$u(r+h)=u(r)+hu'(r)+\frac{h^2}{2}u''(r)+\frac{h^3}{3!}u^{(3)}(r)+\frac{h^4}{4!}u^{(4)}(r)$$
$$u(r-h)=u(r)-hu'(r)+\frac{h^2}{2}u''(r)-\frac{h^3}{3!}u^{(3)}(r)+\frac{h^4}{4!}u^{(4)}(r)$$

and summing : $u(r+h)+u(r-h)=2u(r)+h^2u''(r)+\frac{h^4}{12}u^{(4)}(r)$

In the same way Taylor Expansion of u'' at $r+h$ and $r-h$:

$$\left.\begin{aligned} u''(r+h)&=u''(r)+hu^{(3)}(r)+\frac{h^2}{2}u^{(4)}(r) \\ u''(r-h)&=u''(r)-hu^{(3)}(r)+\frac{h^2}{2}u^{(4)}(r)\end{aligned}\right\} \Longrightarrow u^{(4)}(r)=\frac{u''(r+h)+u''(r-h)-2u''(r)}{h^2}$$

and summing : $u(r+h)+u(r-h)=2u(r)+h^2u''(r)+\frac{h^2}{12}\left(u''(r+h)+u''(r-h)-2u''(r)\right)$

and finally : $u(r+h)+u(r-h)=2u(r)+h^2g(r)u(r)+\frac{h^2}{12}\left(g(r+h)u(r+h)+g(r-h)u(r-h)-2g(r)u(r)\right)$

$$\Longrightarrow \left(1-\frac{h^2}{12}g(r+h)\right)u(r+h)=\left(2+\frac{5}{6}h^2g(r)\right)u(r)-\left(1-\frac{h^2}{12}g(r-h)\right)u(r-h)$$

$$\Longrightarrow u(r+h)=\left(1-\frac{h^2}{12}g(r+h)\right)^{-1}\left[\left(2+\frac{5}{6}h^2g(r)\right)u(r)-\left(1-\frac{h^2}{12}g(r-h)\right)u(r-h)\right]$$

Cowell's method

$$\Longrightarrow \quad \left(1-\frac{h^2}{12}g(r+h)\right)u(r+h)=\left(2+\frac{10}{12}h^2g(r)\right)u(r)-\left(1-\frac{h^2}{12}g(r-h)\right)u(r-h) \qquad \textbf{(11)}$$

$$\textbf{SE}: \quad (H-E)u(r)=0 \quad \Longleftrightarrow \quad u''(r)-\frac{2\mu}{\hbar^2}(V(r)-E)u(r)=0 \quad \Longleftrightarrow \quad u''(r)-g(r)u(r)=0$$

If no explicit need for $u(r)$ at any integration point, it can be replace by $\xi(r)=u(r)-\frac{\hbar^2}{12}u''(r)$ in (11), which will lead to the Numerov's method :

$$\xi(r+h)=u(r+h)-\frac{h^2}{12}u''(r+h)=2f(r)+\frac{10h^2}{12}u''(r)-u(r-h)+\frac{h^2}{12}u''(r-h),$$

equation that can be transformed into : $\xi(r+h)=2u(r)-2\frac{hr^2}{12}u''(r)+2\frac{h^2}{12}u''(r)+\frac{10h^2}{12}u''(r)-\xi(r-h)$, o become :

$$\xi(r+h)=2\xi(r)+\frac{12h^2}{12}u''(r)-\xi(r-h)=2\xi(r)-\xi(r-h)+\hbar^2u''(r). \qquad \textbf{(12)}$$

With $u''(r)=g(r)u(r)$: $\xi(r)=u(r)-\frac{h^2}{12}u''(r)=u(r)-\frac{h^2}{12}g(r)u(r)$, and to deduce :

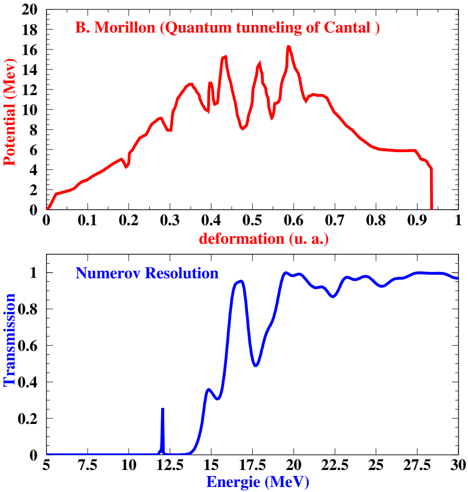
$$u(r)=\frac{1}{1-\frac{h^2}{12}g(r)}\xi(r) \qquad \text{et} \qquad u''(r)=g(r)u(r)=\frac{g(r)}{1-\frac{h^2}{12}g(r)}\xi(r),$$

and thus by posing : $\mathcal{U}(r)=h^2u''(r)=\frac{h^2g(r)}{1-\frac{h^2}{12}g(r)}\xi(r)$, $\quad ou \quad$ $\mathcal{V}(r)=h^2u''(r)=h^2g(r)\left(1+\frac{h^2}{12}g(r)\right)\xi(r)$

Equation (12)becomes Numerov or Numerov modified (J. Raynal) :

$$\xi(r+h)=2\xi(r)-\xi(r-h)+\mathcal{U}(r) \qquad ou \qquad \xi(r+h)=2\xi(r)-\xi(r-h)+\mathcal{V}(r).$$

(for these 2 methods : dependence on "potential" $g(r)$ at ONLY ONE point !!!)



Compared to previous formulas (2 inv. parab.) :

$$\frac{1}{T_2^{J\pi}} = \frac{1}{T_A^{J\pi}} + \frac{1}{T_B^{J\pi}} \Longrightarrow$$

$$T_2^{J\pi} = \frac{T_A^{J\pi} T_B^{J\pi}}{T_A^{J\pi} + T_B^{J\pi}}$$

with at resonance :

$$R_{I \longrightarrow II} T_2^{J\pi} = \frac{4 T_A^{J\pi} T_B^{J\pi}}{(T_A^{J\pi} + T_B^{J\pi})^2}$$

$$= T_2^{J\pi} \times \frac{4}{T_A^{J\pi} + T_B^{J\pi}}$$

Position-dependent collective inertia

When the collective inertia depends on position, the mass operator $M(X)$ is a function of position operator X, and does not commute impulse oprerator P. We are therefore led to define the kinetic energy term as the following form :

$$T = P\frac{1}{2M(X)}P = -\frac{\hbar^2}{2}\Big(\frac{d}{dx}(\frac{1}{m(x)})\frac{d}{dx}\Big)$$

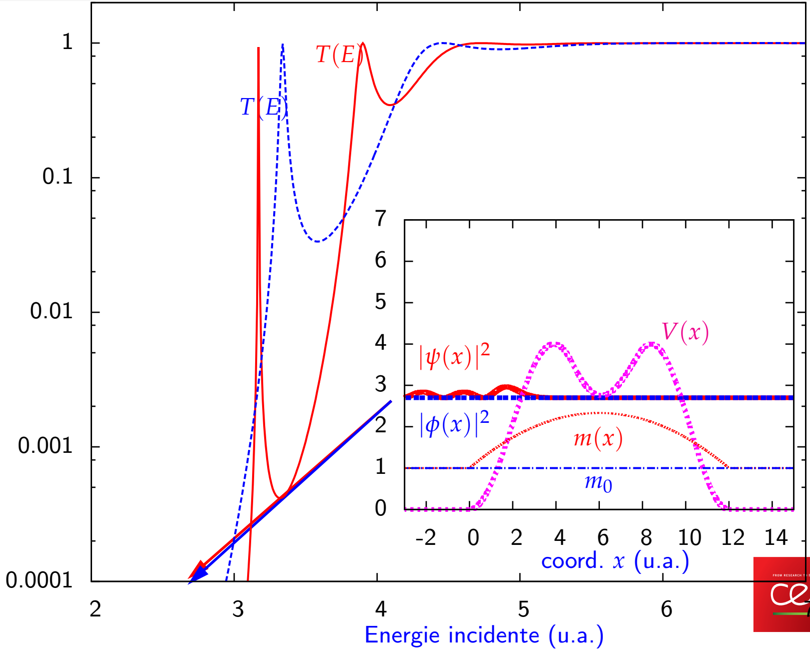
which leads to a Hamiltonian of the type :

$$H = -\frac{\hbar^2}{2m(x)}\frac{d^2}{dx^2} + \frac{\hbar^2}{2}\frac{m'(x)}{m^2(x)}\frac{d}{dx} + V(x), \quad (13)$$

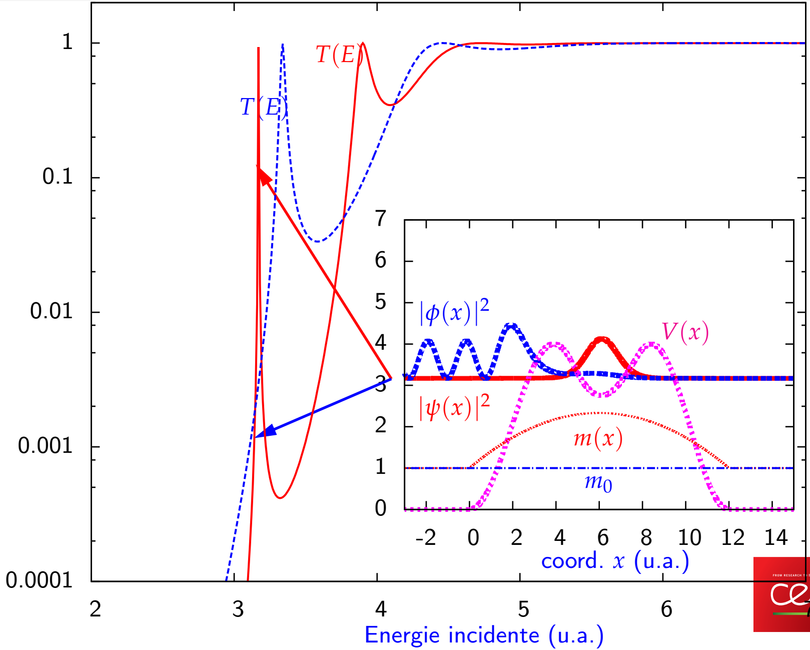
with a first derivative term.
It is then no longer possible to use Cowell's and Numerov's (modified) numerical methods. Nevertheless, at the beginning of the 2000s, V. I. Tselyaev succeeded in generalizing âtheseâ methods for this type of differential equation. :

$$y''(x) + g(x)y'(x) + f(x)y(x) = 0.$$

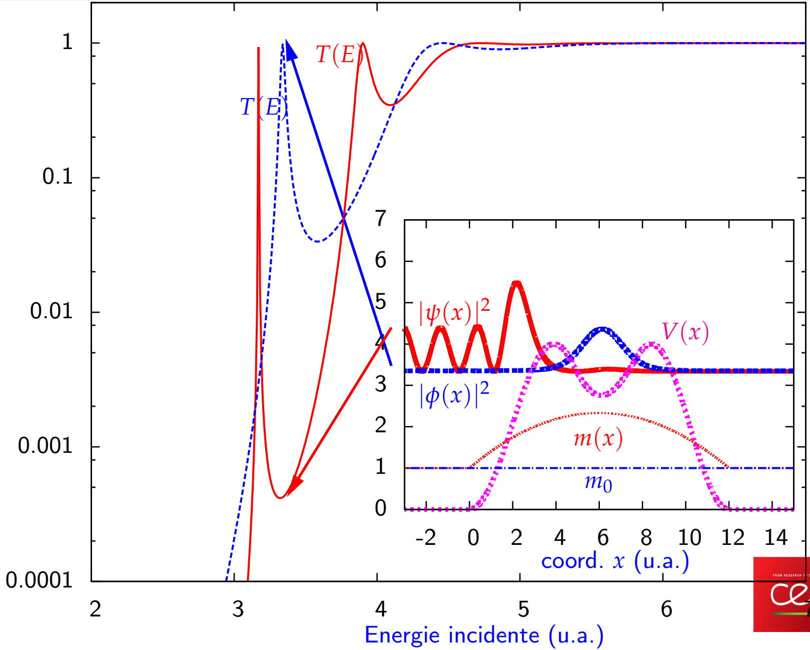
Position-dependent collective inertia

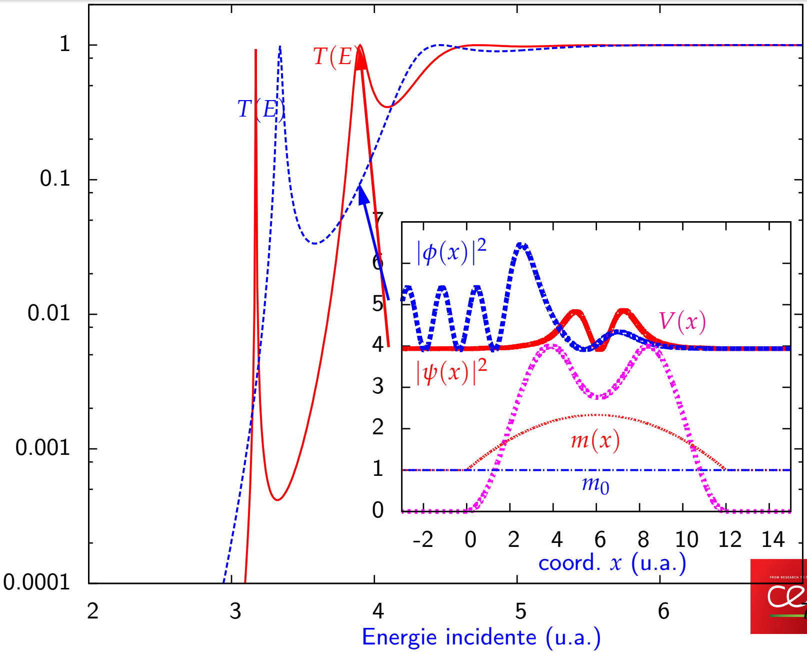


Position-dependent collective inertia

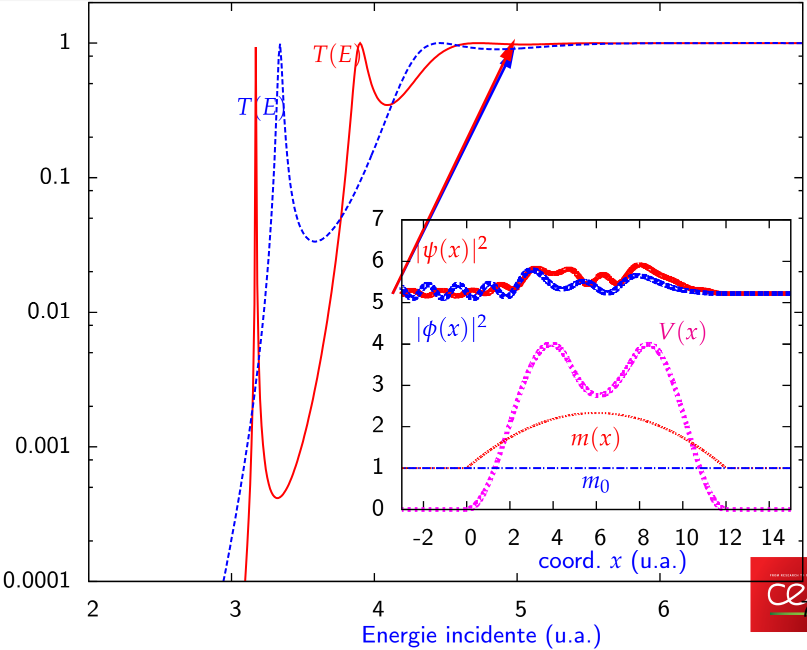


Position-dependent collective inertia




1
0.1
0.01
0.001
0.0001
2
3
4
5
6
T(E)
T(E)
|φ(x)|²
|ψ(x)|²
V(x)
m(x)
m₀
7
6
5
4
3
2
1
0
-2 0 2 4 6 8 10 12 14
coord. x (u.a.)
Energie incidente (u.a.)

Position-dependent collective inertia



7

What can we learn from experimental fission probabilities ?

Fission barriers distributions = interest of surrogate reactions

Like in heavy ions fusion reactions

it is very interesting to study the energy derivative :

$$\Downarrow$$

$$\frac{dP_{EC,f}}{dE} = D_f(E)$$

$$\Downarrow$$

$D_f(E)$ defines fission barriers distributions

Surrogate Reactions for fission barriers ?

$$D_f(E) = \frac{dP_f(E)}{dE}$$

$$\Downarrow$$

$$< B >= \frac{\int E D_f(E) dE}{\int D_f(E) dE}$$

$< B >$ (MeV)	reaction
6.512	n,f
6.542	γ,f
6.44 ± 0.11	SR

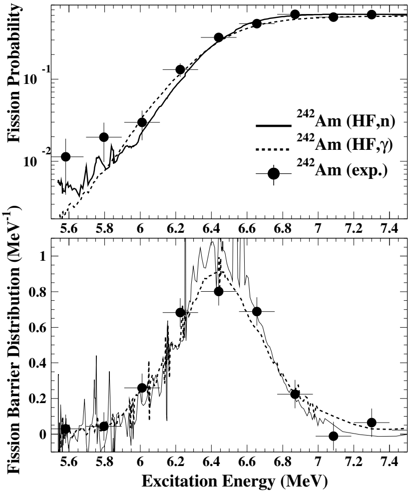
$SR = (^3\text{He}, \alpha f)$

consistency
between Entrance
Channels

$$\Downarrow$$

$$< B^{exp} >$$

completly exp.
using no model



Surrogate Reactions for fission barriers ?

$$D_f(E) = \frac{dP_f(E)}{dE}$$

$$\Downarrow$$

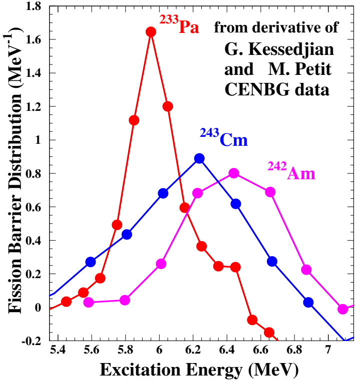
$$< B >= \frac{\int E D_f(E) dE}{\int D_f(E) dE}$$

$< B^{exp} >$ (MeV)	Bjørnholm & Lynn
6.44 ± 0.11	6.5 ± 0.2
5.98 ± 0.11	6.1 ± 0.3
6.15 ± 0.11	6.4 ± 0.3

$$\Downarrow$$

$$< B^{exp} >$$

completly exp. using no model



Surrogate Reactions for fission barriers ?

$$D_f(E) = \frac{dP_f(E)}{dE} \rightarrow < B > = \frac{\int E D_f(E) dE}{\int D_f(E) dE}$$

Consistency of $< B >$ values relatively to different Entrance Channels

Can we go a step further, and reconstruct a barrier shape ?

this means solving the Inverse Problem

Let's start by discussing the problem of classical mechanics posed and solved in 1826 by **Niels Henrik Abel (1802-1829)**, namely :

How to reconstruct the shape of a toboggan, knowing the total time of descent (frictionless) for a given starting height (without intial velocity) ?

Energy conservation (assuming $m = 2$)

$$\left(\frac{dx}{dt}\right)^2 + V(x) = E.$$

From this equation, the time of descent can be deduced :

$$\tau(E) = \int_{x(0)}^{0} \frac{dx}{\sqrt{E - V(x)}}.$$

Setting $u = V(x)$ and defining the inverse function of V as $x = W(u)$, we obtain then with the change of variables :

$$\tau(E) = -\int_{0}^{E} \frac{W'(u)du}{\sqrt{E - u}}.$$

$$\tau(E) = -\int_0^E \frac{W'(u)du}{\sqrt{E-u}}.$$

In this equation appears what is named now the **Abel Transform** :
Let $\mathcal{A}$ the linear operator defined for every continuous real function f on [0,b], by :

$$\forall y \in]0,b] \ : \ \mathcal{A}f(y) = \int_0^y \frac{f(x)dx}{\sqrt{y-x}} \quad \text{et} \quad \mathcal{A}f(0) = 0.$$

(This can be generalized to the fractionnal integration cases more precisely here : semi-integration $\mathcal{A} \equiv I_E^{\frac{1}{2}}$).

$$I_E^{\alpha}f(E) = \frac{1}{\Gamma(\alpha)} \int_{E_0}^{E} (E-E')^{\alpha-1} f(E')dE'$$

One of the Abel Transform property is the following :

$$\forall y \in]0,b] \quad : \quad \mathcal{A}(\mathcal{A}f)(y) = \pi \int_0^y f(x)dx$$

Indeed :

$$\mathcal{A}(\mathcal{A}f)(y) = \int_0^y \frac{1}{\sqrt{y-z}} \Big(\int_0^z \frac{f(x)dx}{\sqrt{z-x}} \Big) dz$$

which gives using Fubini Theorem :

$$\mathcal{A}(\mathcal{A}f)(y) = \int_0^y \Big(\int_x^y \frac{dz}{\sqrt{(y-z)(z-x)}} \Big) f(x)dx$$

and using the idententity : $\int_x^y \frac{dz}{\sqrt{(y-z)(z-x)}} = \pi$

we obtain then : $\mathcal{A}(\mathcal{A}f)(y) = \pi \int_0^y f(x)dx$

Now coming back to the Classical Mechanics problem posed by Abel we get :

$$\tau(E) = -\int_0^E \frac{W'(u)du}{\sqrt{E-u}} = -\mathcal{A}W'(E).$$

Applying a second Abel transform we get :

$$\mathcal{A}\tau(E) = -\mathcal{A}^2 W'(E) = -\pi \int_0^E W'(u)du = -\pi W(E).$$

from which :

$$W(E) = -\frac{1}{\pi}\mathcal{A}\tau(E)$$

We are now able to calculate W, and in fact the potential V from the τ function.

Initially O. Klein and R. Rydberg (1931,1932)
defined a method for the construction of potential energy curves
for diatomic molecules

Later J.A. Wheeler (1976)

If we consider the action integral :

$$S(E) = \int_{x_1}^{x_2} \sqrt{\frac{2m}{\hbar^2}[V(x) - E]}dx$$

used in the WKB approximation for the calculation of the potential barrier penetration coefficient :

$$T(E) = \frac{1}{1+e^{2S(E)}} \iff S(E) = \frac{1}{2}Log\left(\frac{1}{T(E)} - 1\right).$$

Applying the Abel transform to $-\frac{2}{\pi}\sqrt{\frac{\hbar^2}{2m}}\frac{dS(E)}{dE}$ **:**

$$\mathcal{A}\left(-\frac{2}{\pi}\sqrt{\frac{\hbar^2}{2m}}\frac{dS(E)}{dE}\right) = -\frac{2}{\pi}\sqrt{\frac{\hbar^2}{2m}}\int_E^B \frac{dS(E')}{dE'}\frac{dE'}{\sqrt{E'-E}}$$

$$\mathcal{A}\left(-\frac{2}{\pi}\sqrt{\frac{\hbar^2}{2m}}\frac{dS(E)}{dE}\right) = -\frac{2}{\pi}\sqrt{\frac{\hbar^2}{2m}}\int_E^B \frac{dS(E')}{dE'}\frac{dE'}{\sqrt{E'-E}}$$

$$= -\frac{2}{\pi}\int_E^B\int_{x_1}^{x_2} -\frac{1}{2}\frac{dx}{\sqrt{V(x)-E'}}\frac{dE'}{\sqrt{E'-E}}$$

$$= \frac{1}{\pi}\int_{x_1}^{x_2}\left(\int_E^B \frac{1}{\sqrt{V(x)-E'}}\frac{dE'}{\sqrt{E'-E}}\right)dx$$

$$= \int_{x_1}^{x_2} dx$$

$$= x_2(E) - x_1(E) = \Phi(E)$$

$$\mathcal{A}\left(-\frac{2}{\pi}\sqrt{\frac{\hbar^2}{2m}}\frac{dS(E)}{dE}\right) = x_2(E) - x_1(E) = \Phi(E) \qquad ???$$

$$T(E) = \frac{1}{1+e^{2S(E)}} \quad \Longleftrightarrow \quad S(E) = \frac{1}{2}Log\left(\frac{1}{T(E)} - 1\right)$$

$$\begin{aligned} \frac{dS}{dE} &= \frac{d}{dE}\left(\frac{1}{2}Log\left(\frac{1}{T(E)} - 1\right)\right) \\ &= \frac{1}{2} \times \frac{-\left(\dfrac{dT(E)/dE}{T^2(E)}\right)}{\left(\dfrac{1}{T(E)} - 1\right)} \\ &= -\frac{1}{2} \times \frac{D(E)}{T(E)[1-T(E)]} \end{aligned}$$

where we used : $\frac{dT(E)}{dE} = D(E)$ and defined $B =< B >= \frac{\int ED(E)dE}{\int D(E)dE}$, which finally gives :

$$x_2(E) - x_1(E) = \frac{1}{\pi}\sqrt{\frac{\hbar^2}{2m}}\int_E^B \frac{D(E')}{T(E')[1-T(E')]}\frac{dE'}{\sqrt{E'-E}}$$

$$x_2(E) - x_1(E) = \frac{1}{\pi}\sqrt{\frac{\hbar^2}{2m}} \int_E^B \frac{D(E')}{T(E')[1-T(E')]} \frac{dE'}{\sqrt{E'-E}}$$

There the advantage is that we know the barrier height $B = < B > = \frac{\int ED(E)dE}{\int D(E)dE}$.

Thickness :

$$\Phi(E) = x_2(E) - x_1(E)$$

OK, but not sufficient to define completely a potential barrier shape, how to go further ?

Need to use a second equation :

$$\Psi(E) = \psi\big(x_1(E), x_2(E)\big)$$

Assuming symmetrical barrier with respect to a line $x = x_0$

$$\Psi(E) = x_2 + x_1 = 2x_0$$

which leads to :

$$x_1(E) = \frac{1}{2}[\Psi(E) - \Phi(E)]$$

$$x_2(E) = \frac{1}{2}[\Psi(E) + \Phi(E)]$$

The potential is **known close to a x_0 translation.**

In the same way, using the same tricks, potential well can be reconstruct with :

$$\begin{aligned}
N(E) &= \int_{x_1}^{x_2} \sqrt{\frac{2m}{\hbar^2}[E - V(x)]}dx = \int pdx \\
&= Bohr - Sommerfeld = Weyl = WKB \\
&= (n(E) + 1/2)\pi \\
x_2(E) - x_1(E) &= \mathcal{A}\left(\frac{2}{\pi}\sqrt{\frac{\hbar^2}{2m}}\frac{dN(E)}{dE}\right) \\
&= \frac{2}{\pi}\sqrt{\frac{\hbar^2}{2m}}\int_{V_{min}}^{E}\frac{dN(E')}{dE'}(E - E')^{-1/2}dE'
\end{aligned}$$

Now (harmonic approximation) if we set $E \approx (n(E) + 1/2)\hbar\omega$ then we get :
$n(E) + 1/2 \approx \frac{E}{\hbar\omega} \approx \frac{N(E)}{\pi}$ from which :

$$\frac{dN(E)}{dE} \approx \frac{\pi}{\hbar\omega}$$

here V_{min} and $\hbar\omega$ were obtained using $D(E) = \frac{dT(E)}{dE}$
which allows to access at the peaks energy position and to get
part of the spectrum (E_n energies) inside the potential well and finally :

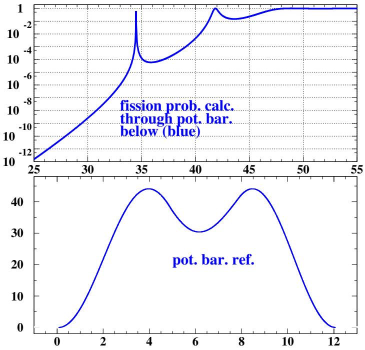
$$\hbar\omega = E_1 - E_0 \text{ and } V_{min} = E_0 - \frac{\hbar\omega}{2}.$$

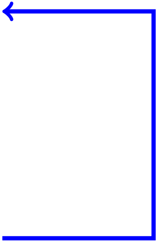
$$
\begin{aligned}
x_2(E) - x_1(E) &= \frac{2}{\pi}\sqrt{\frac{\hbar^2}{2m}} \int_{V_{min}}^{E} \frac{dN(E')}{dE'} (E - E')^{-1/2} dE' \\
&= 2\sqrt{\frac{\hbar^2}{2m}} \int_{V_{min}}^{E} \frac{1}{\hbar\omega} \frac{dE'}{\sqrt{E-E'}} \\
&= \Phi(E)
\end{aligned}
$$

In the Semiclassical Quantum theory the inverse of the potential is proportional to the half-derivative of the eigenvalues counting function $N(E)$

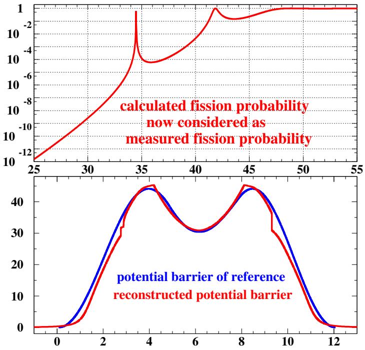
Always assuming symmetrical barrier with respect to a line $x = x_0$!

$$\Psi(E) = x_2 + x_1 = 2x_0$$





P_f obtained by Numerov method



$V(x)$ obtained solving Inverse Problem

HOW to reconstruct "true" fission barriers???

$$\Phi(E) = x_2(E) - x_1(E)$$

hump

$$\Phi(E) = \frac{1}{\pi}\sqrt{\frac{\hbar^2}{2m}} \int_E^B \frac{D(E')}{T(E')[1-T(E')]} \frac{dE'}{\sqrt{E'-E}}$$

$$B = < B > = \frac{\int ED(E)dE}{\int D(E)dE} \Longleftarrow \quad D(E) = \frac{dT(E)}{dE}$$

well

$$\Phi(E) = 2\sqrt{\frac{\hbar^2}{2m}} \int_{V_{min}}^E \frac{1}{\hbar\omega} \frac{dE'}{\sqrt{E-E'}}$$

$$\Longrightarrow \hbar\omega = E_1 - E_0$$

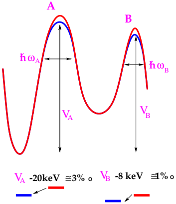
$$\Longrightarrow V_{min} = E_0 - \frac{\hbar\omega}{2}$$

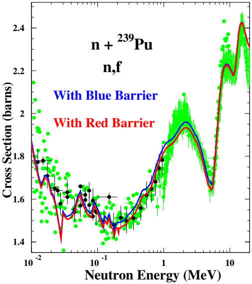
Here was assumed $\Psi(E) = x_1(E) + x_2(E) = cte$ only for symmetrical barriers $\Longrightarrow$ second equation needed :

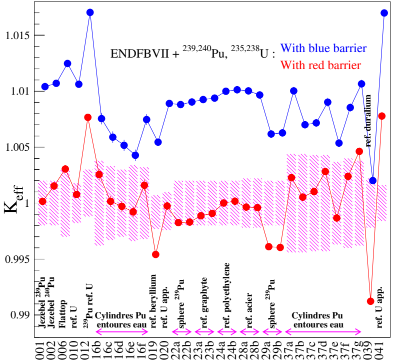
$$\Psi(E) = \psi\big(x_1(E), x_2(E)\big)$$

$$\lambda\Phi(E) \bigotimes \mu\Psi(E) \Longrightarrow x_1(E), x_2(E)$$

Surrogate Reactions for fission barriers ? BUT not so simple







BUT not so simple !