Proposed Updates to Improve Resonance Parameter Evaluations for Fissile Actinides

M.T. Pigni Nuclear Data Criticality Safety Oak Ridge National Laboratory, USA

IAEA International Nuclear Data Evaluation Network (INDEN)

Vienna, Austria, May 2018





ORNL is managed by UT-Battelle for the US Department of Energy

Outline

- ²³⁵U
 - Effects of the inclusion of higher partial waves (*p* and *d*-wave) coupled to the treatment of the (n,f) reaction channel with three fission widths
 - Inclusion of the first inelastic state
 - Attempt to describe energy-dependent fluctuating $\bar{v}(E)$ coupled to resonance parameters (RPs)
- ²³⁵U and ²³⁹Pu
 - $\bar{v}(E)$ fluctuations and RPs

Open issues

- Generation of a validated experimental database
- Statistical treatment of RPs
- High-resolution measured data needs for neutron energy in the keV range



- The inclusion of *p* and *d*-waves increased the number of incident *neutron* channels and outgoing *fission* channels
 - *s*-, *d*-waves are present for channel spins $s = 3^{-}$ and $s = 4^{-}$
- Γ_n is affected by the magnitude of the related penetrability factors (see figures below). This does not happen for the Γ_f (unitary penetrability)





- Test on the fitted RPs when *s* and *d*-waves are included in the sequential fit of three reaction channels: (n,tot), (n,f), and (n,γ)
 - Specific case for three levels with total angular momentum $J = 4^-$ is in the neutron energy range 15–17 eV
 - Based on the values of the total cross section at the energy peaks, (n,el) is about 30%
 - Comparison between values of RPs is fitted by using channels with both *s* and *d*-wave and channels with only *s*-wave
 - The test was performed with three fission widths (Γ_{f1} , Γ_{f2} , Γ_{f3}) for total angular momentum $J = 4^-$ and leads to comparable fits
 - The test shows the impact of the incoming neutron *d*-wave channels on other channels such as capture and fission



	$\ell = 0$						$\ell=2$							
			$s = 4^{-}$				s = 3 ⁻				$s = 4^{-}$			
l	E(eV)	Γγ	Γ_n	Γ_{f_1}	Γ_{f_2}	Γ_{f_3}	Γ_{n}	Γ_{f_1}	Γ_{f_2}	Γ_{f_3}	Γ_{n}	Γ_{f_1}	$\Gamma_{\rm f_2}$	Γ_{f_3}
S	15.4	47.4	0.22	1.1	51.6	2.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
s,d ^a	15.4	46.5	0.15	2.3	15.5	13.4	0.07	5.13	7.71	8.88	0.0	0.0	0.0	0.0
s,d^b	15.4	46.3	0.10	3.2	7.9	7.6	0.05	5.17	6.80	5.97	0.067	5.6	5.5	5.7
S	16.1	37.5	0.33	-0.05	17.2	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
s,d ^a	16.1	37.5	0.22	0.05	5.3	7.3	0.11	2.94	3.27	2.84	0.0	0.0	0.0	0.0
s,d^b	16.1	38.8	0.11	0.61	0.94	1.1	0.19	3.69	2.77	3.34	0.036	3.48	3.31	3.32
S	16.6	36.6	0.24	8.0	105.3	0.003	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
s,d ^a	16.6	36.3	0.14	5.7	22.3	51.0	0.10	2.2	12.75	15.23	0.0	0.0	0.0	0.0
s,d^b	16.6	34.5	0.04	7.9	14.7	10.5	0.09	12.2	12.0	12.1	0.114	12.0	12.1	12.4

^(a) RPs for $J = 4^{-}$ set to small values, i.e., 10^{-5} meV

 $^{(b)}$ RPs for all J are considered

Note : Starting values of the RPs were set to 1 meV for incoming neutron channels and to 10 meV for outgoing fission channels







Energy-dependent fluctuations in $\bar{v}(E)$

- The average number of neutrons from fission, \bar{v}_p , is a key observable used to calculate the reactivity of nuclear materials and is the one requested with the most stringent accuracy, typically 0.25–0.5%
- $\bar{v}_p \equiv \bar{v}_p(E)$ depends on the incident energy *E* of the neutron causing the fission event, and in the low-energy range, it is usually evaluated as a linear function of *E*:

$$\bar{\mathbf{v}}_p(E) = \mathbf{v}_c + \frac{\partial \mathbf{v}}{\partial E} E$$

 However, departures from linear behavior have been shown in several measurements of *ν̄_p* in the resonance regime; fluctuations in *ν̄_p* were experimentally observed and inter- preted as a *spin effects* and a result of the competition of the (n,γf) process and the (n,f) direct fission process:

$$\bar{\boldsymbol{\nu}}_p(E) = \boldsymbol{\nu}^{\text{spin}}(E) - \Delta \boldsymbol{\nu}^{(n,\gamma f)}(E)$$
(1)

- Predominant in the epithermal range, the spin effect progressively decreases, and in the keV region, the reduction of $\bar{v}_p(E)$ is due to the (n, γ f) process only
- The effect of the $(n,\gamma f)$ process is a reduction of the energy available for fission by the emission of a primary γ -ray, and hence is a reduction of \bar{v}_p (negative sign in Eq. 1)
- In general, the impact of these fluctuations on reactivity coefficients can be significant



On the $(n, \gamma f)$ reaction



Figure 1: Schematic diagram of the $(n,\gamma f)$ reaction (Lynn 1965). After the emission of a primary γ -ray (e.g., E1, M1,..), the compound nucleus may still be in a highly excited state that may decay by fission as an alternative to secondary γ -ray emission. In the two-stage decay, the compound nucleus can be in an intermediate state that differs from the initial state depending on the multipolarity of the transition.



Experimental evidence of $(n, \gamma f)^1$





¹Picture taken from Phys. Rev. C 10, 1402 (1974).

Calculating spin effect and $(n, \gamma f)$

- Based on Fort et al., this formalism can define and compute the fluctuating behavior of prompt neutrons based on the competition of $(n, \gamma f)$ and direct fission (n, f) processes
- The first and second term of Eq. 1 can be defined as

$$\boldsymbol{v}^{\text{spin}}(E) = \left[\sum_{J} \boldsymbol{v}_{c,J} \sum_{k_J} \boldsymbol{\sigma}_{f,k_J}(E)\right] / \boldsymbol{\sigma}_{\text{f}}(E)$$
$$\Delta \boldsymbol{v}^{(n,\gamma f)}(E) = \left[\sum_{J} C_J \sum_{k_J} \boldsymbol{\sigma}_{f,k_J}(E) / \Gamma_{f,k_J}\right] / \boldsymbol{\sigma}_{\text{f}}(E),$$

where the quantities $v_{c,J}$ and C_J are deduced by a least-squares of the measured data

- The resonance fission widths Γ_{f,k_J} (taken from ENDF/B-VIII.0) for each resonance are used in SAMMY to calculate the partial energy-dependent fission cross section $\sigma_{f,k_J}(E)$:
 - The coefficients $C_J = (\partial v_J / \partial E) \Gamma_{\gamma,f} \cdot E_{\gamma,f}$ are deduced from the linear dependence of \bar{v}_p for the direct process, assuming that $\Gamma_{\gamma,f}$, $E_{\gamma,f}$ are constant due to the large number of independent channels involved
 - For ²³⁹Pu (having spins $J = 0^+, 1^+$), the parameters used in the calculations are

$$v_{c,0^+} = 2.8819 \pm 0.005$$

 $v_{c,1^+} = 2.8689 \pm 0.0023$
 $C_{0^+} = (0.66 \pm 0.091) \cdot 10^{-3} \text{ eV}$
 $C_{1^+} = (0.629 \pm 0.067) \cdot 10^{-3} \text{ eV}$



Examples: ²³⁹Pu up to 15 eV



Figure 2: The \bar{v}_p in the incident neutron energy up 15 eV plotted together with spin effect component. Calculations performed with SAMMY and based on Fort's formalism Eqs.2–2.



Example: ²³⁹Pu 15–30 eV



Figure 3: The \bar{v}_p in the incident neutron energy 15–30 eV plotted together with spin effect component. Calculations performed with SAMMY and based on Fort's formalism Eqs.2–2.



Example: ²³⁹Pu 30–50 eV



Figure 4: The \bar{v}_p in the incident neutron energy 30–50 eV plotted together with spin effect component. Calculations performed with SAMMY and based on Fort's formalism Eqs.2–2.



Comparison with ENDF/B-VIII.0



Figure 5: The \bar{v}_p in the incident neutron energy up to 100 eV. Calculations (in red) performed with SAMMY and based on Fort's formalism Eqs.2–2, along with ENDF/B-VIII.0 β_5 evaluation (in black).



Current situation for ²³⁹Pu in ENDF/B-VIII.0

- The new IAEA STD2017 values (σ_f =752.4±2.2) are discrepant at thermal energy for fission cross sections, i.e., about 2 σ lower (747.4 b)
- The ²³⁹Pu $\bar{v}_{tot}(E_{th})$ is 2.8749 slightly lower than the recommended thermal neutron constant (TNC)
- For ²³⁹Pu measured α value at the thermal by Lounsbury (as corrected by Beer) is equal to α =0.3558±0.0057
- *α* (ENDF/B-VIII.0): 0.3614
- *α* (IAEA/STD 2017): 0.3585
- Softer thermal (neutron induced) PFNS was described in Nuclear Data Sheets 131, 1 (2016)



Why \bar{v} fluctuations very small for ²³⁵U?

- ²³⁵U has a much smaller level spacing than ²³⁹Pu. For close fission resonances with large $\Gamma_{\rm f}$ widths, interference effects might decrease the effect of (n, γ f) reaction
- ²³⁵U has a spin $I = 7/2^{-}$ that gives channel spin resonances with $J = 3^{-}$ and $J = 4^{-}$. The $\Gamma_{\gamma f}^{J}$ widths are theoretically estimated to be in the range of 1–3 meV against 7–8 meV for ²³⁹Pu. The statistical quality of the current measured data is too low to permit any firm conclusion to be drawn
- The spin effect for ²³⁵U might be small because the two spin states $J = 3^-$ and $J = 4^-$ couple to two octupole channels $K = 1^-, 2^-$ with very similar properties (both symmetric). Under these conditions, the fission properties do not vary much from resonance to resonance, but these small variations will not necessarily be correlated with the spin of the resonances



Example: ²³⁵U up to 50 eV



Figure 6: The \bar{v}_p in the incident neutron energy up to 50 eV. Calculations (in red) performed with SAMMY and based on Fort's formalism Eqs.2–2



Experimental data needs

- Generation of selected experimental data (values and related covariance information)
- Experimental data certified and compatible with other data sets, i.e., same reference
- High-resolution measurement for neutron energies in the keV region for all reaction channels (total, fission, capture)



Conclusions

- Effects of the inclusion of *d*-wave channels for spin group $J = 3^-, 4^-$ were investigated
 - When the large value of the relative centrifugal barrier penetrability of *s*-wave is compared with the same barrier of *d*-wave, the results of the fit show the RPs are affected also by *d*-wave
- Studies on the effects to include the first excited state are ongoing
- The first attempt to couple resonance evaluation to fluctuations in the \bar{v}_p was initiated for ²³⁵U and ²³⁹Pu isotopes
- Emphasis was on a validated and certified experimental database
- High-resolution measurement is needed to improve fit in the neutron energies in the keV region



Acknowledgments

This work was partially supported by the US Department of Energy (DOE) Nuclear Criticality Safety Program (NCSP) funded and managed by the National Nuclear Security Administration for DOE.

Thank you!

