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Monte Carlo simulation of transfer reactions using extended R-matrix theory picturing surrogate-type WFCF features

Olivier H. Bouland[a]

CEA, DEN, DER, SPRC, Physics Studies Laboratory, Cadarache, F-13108 Saint-Paul-lez-Durance, France

Abstract. This article supplies an overview of issues related to the interpretation of surrogate measurement results for neutron-incident cross section predictions; difficulties that are somehow masked by the historical conversion route based on Weisskopf-Ewing approximation. Our proposal is to handle the various difficulties by using a more rigorous approach relying on Monte Carlo simulation of transfer reactions with extended *R*-matrix theory. The multiple deficiencies of the historical surrogate treatment are recalled but only one is examined in some details here; meaning the calculation of in-out-going channel Width Fluctuation Correction Factors (WFCF) which behavior witness partly the failure of Niels Bohr's compound nucleus theoretical landmark. Relevant WFCF calculations according to neutron-induced surrogate- and cross section-types as a function of neutron-induced fluctuating energy range [*0 - 2.1 MeV*] are presented and commented in the case of the $^{240}Pu^{*}$ and $^{241}Pu^{*}$ compound nucleus isotopes.

1 Introduction

The aim of this paper is to supply an overview of issues related to the conversion of surrogate measurements to neutron-induced cross sections; difficulties that are somehow masked by persistent use of the so-called Weisskopf-Ewing approximation (WE). The difficulties will be enlightened by using the more rigorous approach developed in our AVXSF-LNG (AVerage CROSS Section Fission – Lynn and Next Generation) code [1] at CEA Cadarache in collaboration with LANL/T2. Our code is based on Monte Carlo simulation of transfer reactions (also referred as surrogates) and makes use of extended *R*-matrix theory.

Surrogate measurements are substitute technique to determine reaction cross sections for compound nuclei that are difficult to measure directly by neutron physics spectroscopy (NPS) or to predict with some degree of confidence from 'systematics' or theory. The surrogate method comes as an alternative to form the compound nucleus (CN), let say *C**, usually formed in NPS as [*n+target*→ *C*]*. Alternatively another projectile-target combination, more accessible experimentally, can be involved such that [*projectile* + *Surrogate_Target* → *C**+ *ejectile*]. By measuring the number of coincidences between the ejectile and the observable that identifies the desired exit reaction channel (*c'*), normalized to total number of measured surrogate events (i.e; how many times the selected CN is formed), the experimental probability, let's say $\beta_{sp,c'}^{CN}(E^{*})$, related to CN formation at excitation

[a] Corresponding author: olivier.bouland@cea.fr

energy E^* by given surrogate reaction (labeled '*sp*' since the CN entrance channel is of single-particle type) and subsequent decay in reaction channel c', is obtained experimentally. Combination (see later in the text) of $\beta^{CN}_{sp,c'}(E^*)$ with calculated neutron-induced CN formation cross section is then routinely carried out using the WE frame and benchmarked, whenever possible, with neutron-incident cross sections that were directly measured.

2 Historical surrogate modeling

The starting point and appropriate formalism for describing CN reactions is Hauser-Feshbach (HF) statistical theory [2], meaning the pure Hauser-Feshbach equation (as stated by equation 1 of Ref. [1]) that carries 'Niels Bohr's hypothesis' of independence of formation and decay of the CN [3] in first order. A more realistic picture involves $W_{c,c'}$, the in-out-going channel WFCF. The formulation for the average partial reaction cross section, $\sigma_{c,c'}(E_c)$, according to entrance channel *c* and exit channel c' applied to neutron-induced reactions at given neutron energy E_n is then addressed as

$$\sigma_{n,c'}(E_n) = \sum_{J^\pi} \sigma_n^{CN}(E_n, J, \pi) \sum_{s'=|I'-i'|}^{|I'+i'|} \sum_{l'=|J-s'|}^{|J+s'|} \frac{T_{c'}^{J^{\pi}(l's')}(E_{c'})}{\sum_{c''} T_{c''}^{J^{\pi}(l"s")}(E_{c''})} \times W_{n,c'}^{J^\pi} \ , \tag{1}$$

where $\sigma_n^{CN}(E_n, J, \pi)$ is the neutron-induced compound nucleus formation cross section for given (J,π) couple; the expression of which is,

$$\sigma_n^{CN}(E_n, J, \pi) = \pi \lambda\!\!\!^{-2} g_J \sum_{s=|I-\frac{1}{2}|}^{|I+\frac{1}{2}|} \sum_{l=|J-s|}^{|J+s|} T_n^{J^{\pi}(ls)}(E_n), \tag{2}$$

with g_J, the statistical spin factor or weight according to CN total angular momentum *J* as $g_J = (2J+1)/(2(2I+1))$ and where $T_n^{(J^\pi ls)}$ are the neutron entrance transmission coefficients.

Historical surrogate treatment assumes that customary in-out-going channel WFCF can be neglected (i.e ; $W_{c,c} \approx 1$) although, by matter of fact, we know that this correction is substantial [4] for any open channels for excitation energies up to *2 MeV* above neutron emission threshold (S_n) as far as actinide nuclides are concerned. According to fission decay, the amount of average cross section correction depends on both the number of fission channels involved and the magnitude of their average widths. The larger the sub-barrier effect is (case of fertile heavy isotopes), the larger the amount of fluctuations ($W_{n,f} \approx$ *35%* compared to *20%* at 1 keV neutron-incident energy respectively for fertile and fissile isotopes [5]). Obviously $W_{n,f}$ tends to unity as the total number of open channels increases. The absence of WFCF in the cross section formulation is then the first step leading to the WE limit of HF theory. **Equation 1** then switches back to pure HF that can be re-written in a concise manner as,

$$\sigma_{n,c'}(E_n) = \sum_{J^\pi} \left[\sigma_n^{CN}(E_n, J, \pi) \times P_{c'}^{J^\pi}(E_{c'}) \right] , \tag{3}$$

where $P_{c'}^{J^\pi}(E_{c'})$, the individual CN decay probability into reaction channel c', is also commonly referred as branching ratio (BR) to channel c' in associated surrogate literature. Equation 3 can be factorized such that,

$$\sigma_{n,c'}(E_n) = \sigma_n^{CN}(E_n) \sum_{J^\pi} \left[\frac{\sigma_n^{CN}(E_n, J, \pi)}{\sigma_n^{CN}(E_n)} \times P_{c'}^{J^\pi}(E_{c'}) \right], \tag{4}$$

to make provision for $\sigma_n^{CN}(E_n, J, \pi) / \sigma_n^{CN}(E_n)$, the fraction of CN excited states formed with *(J, π)* couple that is commonly labeled as $F_{sp}^{CN}(E^*, J, \pi)$ in surrogate literature. This gives us the opportunity to unfold the experimental (coincidence) surrogate probability accordingly such that writing,

$$\beta_{sp,c'}^{CN}(E^*) = \sum_{J^\pi} \left[F_{sp}^{CN}(E^*, J, \pi) \times P_{c'}^{J^\pi}(E_{c'}) \right], \tag{5}$$

Straightforward connection can be made under the so-called WE limit of the Hauser-Fechbach theory between neutron-induced cross section data and $\beta_{sp,c'}^{CN}$; the actually observed surrogate probability that is mostly measured as a function of a single variable meaning the CN excitation energy (E^*). This probability involves the additional crude simplification that BR quantities are independent of spin and parity, meaning substituting $P_{c'}^{J^\pi}(E_{c'})$ by $P_{c'}(E_{c'})$. In the framework of independence between formation and decay processes in compound nucleus system supplemented by the latter hypothesis, branching ratios are automatically pulled off the spin-parity summation in **Eqs. 3** and **5**. The replacement of $P_{c'}(E_{c'})$ in the **Eq. 3** by its equivalence given by **Eq. 5** returns the well-suited and well-known WE expression that is,

$$\sigma_{n,c'}^{WE}(E_n) = \left[\sum_{J^\pi} \sigma_n^{CN}(E_n, J, \pi) \right] \times \beta_{sp,c'}^{CN}(E^*), \tag{6}$$

$$\text{since } \left[\sum_{J^\pi} F_{sp}^{CN}(E^*, J, \pi) \right] = 1. \tag{7}$$

3 Refined transfer reaction data modeling based on extended *R*-matrix Monte Carlo simulations

At first sight, this WE strategy (**Eq. 6**) supplies a suitable and quick estimate of the desired neutron-induced cross section, inaccessible from NPS, without any need to extract individual CN decay reaction probabilities, $P_{c'}^{J^\pi}(E_{c'})$, from surrogate data using both **Eq. 5** and input simulations of the $F_{sp}^{CN}(E^*, J, \pi)$ direct-reaction CN population fractions. The retrieval procedure of Eq. 6 assumes, of course, that the neutron-induced total formation cross section, $\sum_{J^\pi} \sigma_n^{CN}(E_n, J, \pi)$ is ideally computed using convenient optical potential. Unfortunately this WE strategy (**Eq. 6**) has shown its limits over the last decade especially in terms of neutron-induced capture cross section predictions [6] from associated surrogate-reaction measurements although it worked surprisingly pretty well in terms of fission cross section retrieval [7]. Thinking about the conceptual differences between **Eqs. 4** and **5** and according to **Eq. 1**, we realize that

A/ the absence of WFCF prevents at least from dealing with the genuine outgoing channel width correlations; meaning in the case of observed fission, correlations between the fission and total CN decay widths. However, the absence of WFCF can also alter the surrogate data conversion to neutron cross section data since we expect conceptual differences in WFCF calculations between surrogate- and neutron-type measurements; this question being the purpose of this short paper, B/ the use of the unitary property (**Eq. 7**) washes out *(J,π)* population fraction differences encountered between neutron-induced and surrogate reactions. This is equivalent to state that final results are not sensitive to the actual entrance spin-parity probability distribution although many prospective calculations, spread over four decades (already in Ref. [8]), have shown that distribution patterns are strongly spin-parity reaction dependent and this, at least for nucleus excitation energies up to $(S_n + 2)$ *MeV*.

In consequence of the WE strategy expected deficiencies, we have chosen an approach free of the WE assumption for simulating $\beta^{CN}_{sp,c'}$, the surrogate probability actually measured. This more rigorous method is implemented in our AVXSF-LNG code and relies in particular on a Monte Carlo simulation of the transfer reactions using extended *R*-matrix theory. An article in preparation [9] will supply more details. However a refined analytical formulation of the fission channel, allowed also by our code, can illustrate our purpose. This calculates $\beta^{CN}_{sp,f}$ as

$$\beta_{sp,f}(E^*) = \sum_{J^\pi} \left[F^{CN}_{sp}(E^*, J, \pi) \times \left[\sum_{\mu \in J^\pi} P^\mu_f(E_{c'}) W^\mu_{II} \right] \times W^{J^\pi}_{sp,f} \right], \tag{8}$$

where $P^\mu_f(E_{c'})$ and W^μ_{II} are respectively the individual CN fission decay probability over given Aage Bohr [1] transition channel μ and appropriate class-II compound nucleus state WFCF; the behavior and the effect of latter being detailed in [5].

Equation 8 enlightens the importance of the in-out-going channel WFCF although this latter might be inadequately calculated using its customary definition as remembered by the following,

$$\left\langle \frac{\Gamma^{J^\pi}_c \Gamma^{J^\pi}_{c'}}{\sum_{c''} \Gamma^{J^\pi}_{c''}} \right\rangle = \frac{\left\langle \Gamma^{J^\pi}_c \right\rangle \left\langle \Gamma^{J^\pi}_{c'} \right\rangle}{\sum_{c''} \left\langle \Gamma^{J^\pi}_{c''} \right\rangle} \times W_{c,c'} \ , \tag{9}$$

where $\Gamma^{J^\pi}_c$ and $\Gamma^{J^\pi}_{c'}$ are respectively channel widths corresponding to the c entrance and c' exit channels.

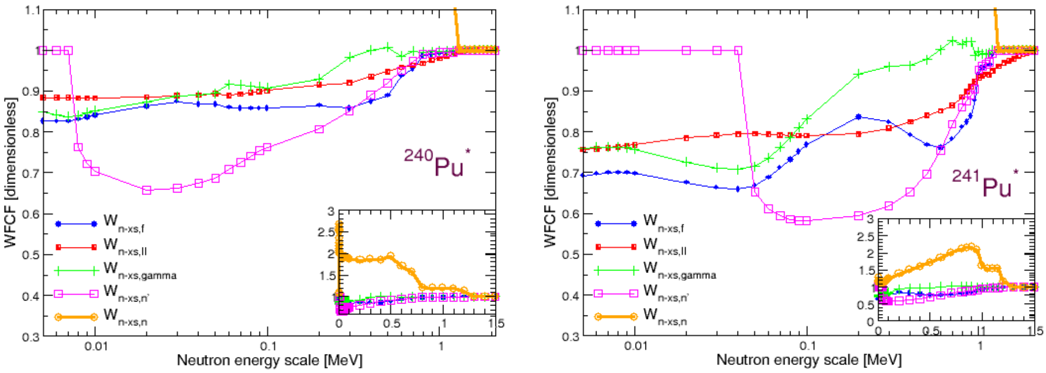
4 Expected WFCF differences between surrogate- and neutron-induced-type measurements

Straight application of **Eq. 9** to the fissile $^{240}Pu^*$ and fertile $^{241}Pu^*$ compound nucleus isotopes in the case of neutron-induced reaction carried out analogously to the general single variable integral established by Dresner [10] (see also [1] for practical details) can be visualized respectively under **Figs. 1** and **2**. In both cases, we recognize the well-known enhancement of the elastic cross section (greater than +100% as symbolized by the solid-orange-opened circle curve on both graphic insets) whereas the inelastic channel is strongly depreciated (at least of -30%) when neutron inelastic threshold is crossed at $S_n + 7$ *keV*.

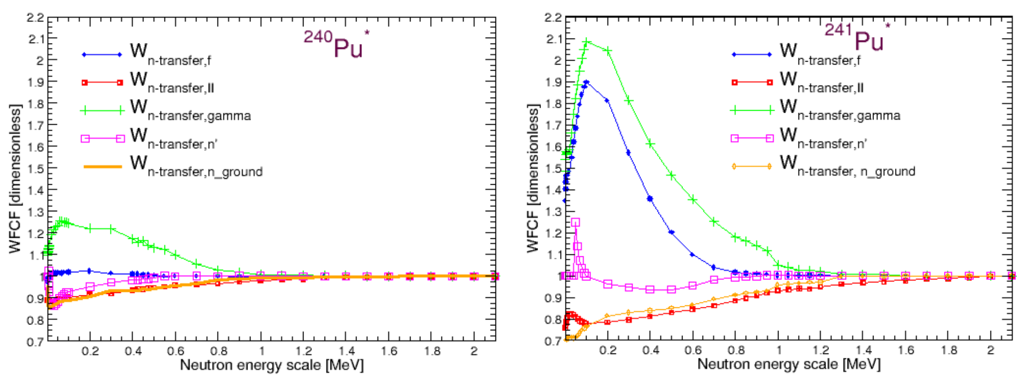
We can wonder whether this conventional WFCF prescription remains valid when surrogate reactions are involved and more precisely when a direct reaction is the first stage leading ultimately to CN formation. Considering the very different nature of the entrance channel in the latter case compared to neutron-induced reactions, we might consider the extreme case of no correlation between CN formation and decay widths as it is suggested in Ref.[9] according to *(t,pf)* surrogate measurements. **Eq. 9** then reduces to the following

$$\left\langle \frac{\Gamma^{J^\pi}_{sp} \Gamma^{J^\pi}_{c'}}{\sum_{c''} \Gamma^{J^\pi}_{c''}} \right\rangle \equiv \Gamma^{J^\pi}_{sp} \frac{\left\langle \Gamma^{J^\pi}_{c'} \right\rangle}{\sum_{c''} \left\langle \Gamma^{J^\pi}_{c''} \right\rangle} \times W_{sp,c'} \ , \tag{10}$$

where $\Gamma_{sp}^{J\pi}$ is the entrance channel width related to the single particle stripped from the incident light particle (e.g; a dineutron for a *(t,p)* entrance vector) and transferred into corresponding sp-orbit of target nucleus that carries two neutrons less than the formed CN.



Figures 1 (left side) and 2 (right side): customary WFCF curves (**Eq. 9**) as a function of neutron incident energy respectively for the fissile ^{240}Pu* and fertile ^{241}Pu* CN isotopes. WFCF curves are related respectively to overall fission ($W_{n\text{-}xs,f}$), class-II CN state intrinsic properties ($W_{n\text{-}xs,II}$), gamma emission ($W_{n\text{-}xs,\gamma}$), neutron elastic scattering ($W_{n\text{-}xs,n}$) and inelastic emission ($W_{n\text{-}xs,n'}$). Customary WFCF behavior manifests by an amount of flux taken from each exit channel that is not also an entrance channel (fission, gamma and inelastic neutron emission) and redistributed to the entrance-exit channel (meaning the neutron channel according to a neutron elastic reaction).



Figures 3 (left side) and 4 (right side). Analogous WFCF numerical Dresner calculations as **Figs. 1** and **2** except that in-out-going channel width correlation is assumed to be negligible in transfer reaction treatment as addressed by **Eq. 10**. For genuine comparisons to the WFCF cross section-type calculations, same J^{π} CN state populations have been supplied according to a neutron entrance channel configuration.

Figures 3 and **4** supply a quick overview of how modified are WFCF as assumed in the surrogate extreme limit (**Eq. 10**) of none in-out-going channel width correlation but with preservation of channel width correlations between the various CN exit channels. By analogy to the customary situation, each WFCF tends to unity when the total number of channels becomes very large (in practice above *(S_n +1.5) MeV* of excitation energy for these plutonium isotopes). However the absence of elastic reaction prevents any elastic enhancement (since no exit channel is similar by nature to the direct reaction entrance channel) but it happens that both radiative and fission decays now endorse the role of the enhanced channel. In this picture, the WFCF coefficients related to $^{241}Pu^{*}$ carry the maximum of strength (up to a factor 2.1 for the γ-decay probability – **Fig. 4 -** $W_{n\text{-transfer},\gamma}$) because of the $^{241}Pu^{*}$ neutron-incident sub-threshold fission nature that maintains at high level partial cross section fluctuations. By reciprocity, neutron emission channels are depreciated accordingly to the total amount of reaction rate redistributed. This statement can be materialized as

$$\left(WFCF_{sp,f} \times P_f + WFCF_{sp,\gamma} \times P_\gamma\right) \equiv \left| \sum_i \left(WFCF_{sp,n_i} \times P_{n_i}\right) \right|$$

where n_i corresponds to given CN neutron emission channel i including the channel corresponding to the residual nucleus left in its ground state.

5 Summary

This paper clearly recalls the four key ingredients, $F_{sp}^{CN}(E^*, J, \pi)$, $P_f^{\mu}(E_{c'})$, $W_{sp,f}^{J^\pi}$ and W_{II}^{μ}, which full knowledge is crucial for any valuable comparison between predicted and observed surrogate probabilities over low excitation energy range ($4.0 < E^*\ [MeV] < S_n+2.0$) as it was suggested by recent measured γ-decay surrogate-type probabilities. This paper acknowledges in particular the dedicated behavior of surrogate WFCF as assumed in the extreme limit (**Eq. 10**) of none in-out-going channel width correlation but with preservation of channel width correlations between the various CN exit channels. This special behavior is worth to be noted since we are not usually accustomed to deal with it. In particular we realize that both radiative and fission decays can now endorse the role of the enhanced channel. The enhancement factor observed on both fission and γ-decay probabilities is especially strong (up to +100%) for fertile heavy isotopes in the energy range above S_n although the actual consequence of wrong prediction on small fission decay probability (of *0.1* magnitude) for fertile nuclides remains limited in neutron reactor applications. On the opposite, this might have great importance for neutron-induced capture cross section retrievals. As conclusion, we own nowadays some capability for more precise surrogate-type probability calculations preventing the fragile use of the historical Weisskopf-Ewing assumption that especially does not include the calculation of WFCF.

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