Towards prediction of fission cross section on the basis of microscopic nuclear inputs

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Almost all the evaluations of the neutron-induced fission cross section for nuclei involved in nuclear applications rely on phenomenological ingredients. For instance, the shapes of the fission barriers are usually approximated by inverted parabolas with specified heights and widths, and the required nuclear level densities are also based on highly-parameterized phenomenological expressions. If such approaches enable to fit available experimental data, their predictive power is clearly poor, and they can not be recommended for applications requiring a proper description of fission for nuclei far from stability.

In contrast, microscopic Hartree-Fock-Bogolyubov (HFB) calculation can provide all the nuclear ingredients required to describe the fission path from the equilibrium deformation up to the nuclear scission point with, in principle, a higher predictive power. The aim of this contribution is to test such microscopic information to calculate neutron-induced fission cross sections on selected actinide nuclei. This approach includes not only the details of the energy surface along the fission path, but also the estimate of the nuclear level density derived within the combinatorial approach on the basis of the same HFB single-particle properties, in particular at the fission saddle points.

It is shown that a satisfactory estimate of the fission cross section for non-energy applications can be achieved with a global renormalization of the barrier heights and the microscopic nuclear level densities at the fission saddle points. Good agreement with experimental data can be obtained if both the fission barrier heights and level densities are independently renormalized.

I. INTRODUCTION

Since its discovery, nuclear fission has always been an active field of research both as purely theoretical challenge as well as for its practical applications. From the theoretical point of view, the main challenge consists in understanding how the nucleus goes from an equilibrated shape to such a highly deformed shape that it finally splits into lighter fragments. The fragments' charge and mass distributions, the energy released, the fragments' deformations and excitation energies are among the questions not yet fully understood theoretically. In practical applications, it remains of major importance to be able to estimate accurately the probability that fission occurs when competing with other decay channels or the number of neutrons released during the fission process. All these questions are generally addressed on the basis several approximate models depending on parameters tuned to fit available experimental fission cross sections. If such approaches respond to the needs of nuclear power applications achieving an improved description of the neutron induced fission cross sections [1, 2], their predictive power remains poor and they cannot be used in applications requiring a blind description of fission for experimentally unknown nuclei, as for example nuclear astrophysics.

To our knowledge, a link between the modern microscopic tools usually employed to study the purely theoretical aspects of fission and the fission cross section prediction has never been established or at least tested through the comparison of calculated and measured fission cross sections. The goal of the present work is thus to establish such a "bridge", or, in other words, to use the outputs of the microscopic methods to produce the ingredients which are necessary to perform fission cross section calculations. Such an approach follows naturally previous microscopic studies related to the calculation of nuclear reaction ingredients such as nuclear level densities (NLD) [3], gamma-ray strength functions [4], nuclear masses and fission barriers [5] or optical model potentials [6] in view

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of being able to perform cross section predictions far from the valley of stability based on sound physical bases. We indeed believe that such (semi)-microscopic approaches have higher predictive power than usually employed extrapolations of phenomenological formulae adjusted on a very narrow range of nuclei in the valley of stability. This being said, it is clear that a fair study of the predictive power of a microscopic fission cross section calculation implies that such predictions should be compared to what is obtained using standard analytical methods (i.e. global sets of parameters for all the key ingredients entering the fission description) without any fine tuning as, for instance those that can be found in the Reference Input Parameter Library (RIPL2) [7].

In the present work, new ingredients to the fission cross section calculations are tested. These concern the static fission path (including the barrier height and width) and the NLD, both being obtained coherently within the same mean field model. The impact of the optical potential will not be studied since it is expected to be constrained without calling for any fission information. After recalling in Sect. II the various nuclear reaction models used to predict fission cross sections, we will discuss the nuclear models adopted to derive the corresponding ingredients in Sect. III. A sensitivity analysis is conducted in Sect. IV before performing a more global analysis of the fission cross section prediction on the basis of microscopic nuclear models (Sect. V). Conclusions and outlook are finally given in Sect. VI.

II. FISSION CROSS SECTION CALCULATIONS

The prediction of nuclear reaction cross sections above the resonance region, depends on several nuclear reaction models chained together [8]. The starting model is the optical model which essentially provides the total cross section and enables to separate it between the reaction and the elastic cross section. If the incident energy is high enough, the excited nucleus decays first through the pre-equilibrium process and, later on, through the emission from the compound nucleus (CN). Both emission mechanisms contribute to the description of the light particle and photon emission, while fission is treated solely as an outgoing channel of the CN decay.

In practice, the CN decay only depends on two main quantities, namely the transmission coefficients and the NLDs. For light ejectiles, the transmission coefficients are a subproduct of the optical model potential mentioned above, and for emitted photons, they are given by gamma-ray strength functions. The need for NLD depends on the outgoing channel. While for γ and light particle emission, the knowledge of the NLD to which the decay occurs in the residual nucleus is required, fission is a very specific process. Indeed, if transmission coefficients are obtained by calculating a probability of tunneling through a given potential (fission barrier) which is somehow an equivalent of the optical model potential for light particles, it does not involve NLD related to any residual nucleus for which minimum information might be available. In contrast, the fission transmission coefficient should be theoretically determined by summing the penetrabilities through all the fission barriers that might be tunneled through, which would require that one is able to describe all these barriers. This turns out to be impossible since (i) the number of such barriers is too large and (ii) they cannot be described correctly one by one. This is the reason why it is a usual practice to introduce on top of each barrier the so-called transition states supposed to be associated with a fission barrier, so that the fission transmission coefficient reads

$$T(E,J,\pi) = \sum_d P(E-\varepsilon_d^{J,\pi}) + \int_{E_d}^{E} P(E-\varepsilon)\rho(\varepsilon,J,\pi)d\varepsilon \ , \quad (1)$$

where P is the tunneling probability and the first sum runs over all the discrete transition levels $\varepsilon_d^{J,\pi}$ having the same spin J and parity π as those of the decaying compound nucleus with excitation energy E, and where the integration runs over the transition levels' continuum described by the NLD ρ. This NLD function corresponds to the density of levels on top of the fission barrier and is called the saddle-point NLD. The barriers are generally described by inverted parabolas enabling the analytical determination (Hill-Wheeler approximation) of P [8] and it is generally assumed that their shapes remain unchanged whatever the transition state energy is, so that the tunneling probability through the barrier associated with the transition state of energy ε is that of the ground state barrier calculated for the energy $E-\varepsilon$. Another usually adopted approximation consists in introducing multiple-humped barriers (at least double-humped and sometimes triple-humped) considered as completely independent (decoupled) in the simplest approaches or coupled in more advanced descriptions [1] which also deal with barriers' wells properties introducing resonant states to further improve the fit of measured fission cross sections. For simplicity, we will only consider here the case of double humped fission barrier described as if the two humps were decoupled (classically referred to as the full damping limit or the strong absorption limit [9]) and write the total fission transmission as

$$T(E,J,\pi) = \frac{T_A T_B}{T_A + T_B} \ , \quad (2)$$

where both transmission coefficients through the first (T_A) and the second (T_B) barriers are determined using Eq.(1), which requires the NLD on top of each barrier as well as the barrier penetrabilities.

Considering the situation described before, it is clear that the number of possible sources of uncertainties in fission cross section calculations is by far larger than for any other competing channel. This large number of free parameters enables to perform accurate fits of experimental data but also explains why the predictive power remains rather poor for the fission channel.

III. MICROSCOPIC INGREDIENTS FOR FISSION CROSS SECTION CALCULATION

As clearly indicated in the previous section, two major ingredients are needed to predict fission cross section, the fission barriers and the saddle point NLDs. Two cases are going to be considered. On the one hand we will use phenomenological barriers described by inverted parabolas as provided in the RIPL2 library together with a Fermi-gas type closed formula for the NLDs, and, on the other hand, we will use the full fission path as calculated in Ref. [5] within the HFB approach, together with the microscopic NLD derived within the HFB plus combinatorial model [10].

For the fission barriers, as can be seen in Fig. 1, the HFB-14 predictions for the Pu isotopes close to the valley of β stability (for more details, see [5]) rather look like traditional double-humped barriers. But for exotic neutron-rich isotopes (right panel) the fission path cannot, in general, be simply approximated by a double-humped barrier with parabolic shapes. To estimate the transmission coefficients with fission barriers deviating from the simple inverted parabolic picture, the full WKB approximation [8] needs to be employed.

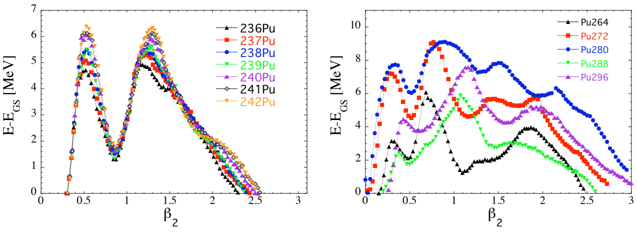

FIG. 1: Fission path (total energy with respect to the ground state energy E_{GS}) as a function of the quadrupole deformation parameter β_2 for various Pu isotopes.

Concerning the NLDs, an important effort has recently been made to improve the quality of microscopic models [10] and analytical parameterizations [11]. Both types of NLD have been adjusted to obtain, simultaneously, the best description of the low energy cumulative discrete level schemes and the mean s-wave resonances spacing whenever available. These adjustments can only be performed for the so-called ground-state NLD associated with nuclei in their equilibrium deformation. These NLD models are considered as global as they reproduce observables for all nuclei in a very satisfactory way. Since they have been adjusted on model-independent data, no attempt will be made in the present study to modify them to improve the description of fission cross section. In contrast, the saddle level densities suffer from a much more severe lack of experimental information because of their large sensitivity to the nucleus deformation and to the breaking of additional symmetries around the saddle points. Nevertheless, as predicted by mean field calculations [12], we consider here that the inner barrier is triaxial and the outer left-right asymmetric and take into account the corresponding enhancement factors as determined in Ref. [13]. These enhancement factors are used to multiply the microscopic NLDs determined with the same method as in Ref. [10], making a coherent use of the corresponding HFB predictions for the single-particle level scheme and pairing strength at the corresponding deformation. It should however be mentioned that if the NLD is rather well constrained by the HFB structure properties (though still affected by the complicated task to determine the saddle point deformation), the inclusion of the phonon excitations is still subject to a rather large uncertainty. Due to the lack of observables, the same prescription is used for the saddle points as for the ground state : a total of 3 phonons are coupled to the excitation configurations having a maximum of 4 particle-holes and the phonons' energies are assumed identical to those of the ground state. The comparison of microscopic HFB plus combinatorial NLD with the back-shifted Fermi gas model (BSFG) (see Fig. 2) used in the present work [7] displays three major differences. First, at very low energies, the phonon excitations included in the HFB model significantly enhance the NLD. Second the HFB vibrational damping, already discussed, affects the energy dependence of the NLD and third, the NLD at the outer saddle point is significantly larger than the ground-state NLD in contrast to the BSFG case.

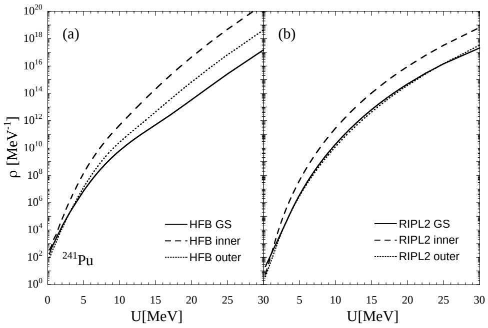

FIG. 2: ^{241}Pu total NLD at the ground state (GS) and at inner and outer saddle points determined within the HFB plus combinatorial method (left panel) and with the BSFG model [7].

IV. SENSITIVITY ANALYSIS

We now present the cross section calculations obtained with the recent HFB model for the fission path and the NLD determined at the corresponding saddle point within the HFB plus combinatorial method. As already mentioned, the incident channel is here assumed to be properly described by the dispersive coupled-channel optical model given in Refs [14, 15] and the final sensitivity to this ingredient will not be further discussed here. Note that all calculations in the present work have been performed either with the TALYS [16] or EMPIRE [17] reaction codes. Both codes provide similar results whenever the nuclear inputs are identical.

While the fission cross section is known to be extremely sensitive to the barrier height, it is less clear to what extent it is affected by the fission barrier shape. To test it, we compare in Fig. 3 the ^{238}Pu and ^{240}Pu neutron-induced fission cross sections obtained with two different descriptions of the potential energy surfaces. The first one corresponds to the HFB fission path and therefore involves the WKB treatment while the second one corresponds to the parabolic approximation fitted to the HFB path around both the inner and outer maxima. Consequently, both calculations uses the same barriers heights and widths at maximum. It can be seen in Fig. 1 that if the shape of the inner barrier of these two Pu isotopes can be properly reproduced by an inverted parabola, this is not the case for the outer barrier. The impact of these differences can be seen in Fig. 3 to be the largest in the low-energy regime, where the width of the barrier dominates the tunneling effects. For the same reason, the shape of the barrier essentially affects the fission cross section of fertile nuclei.

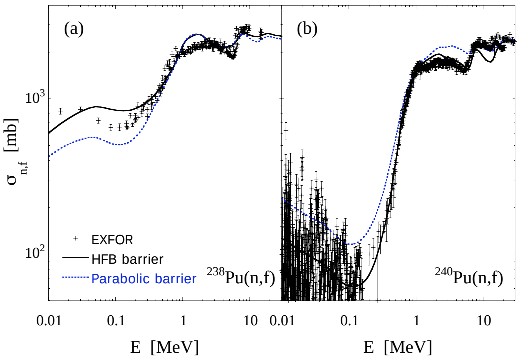

FIG. 3: Neutron-induced fission cross section of ^{238}Pu (left panel) and ^{240}Pu (right panel) obtained with the HFB fission path (solid line) and the double-humped inverted parabolas approximation (dotted line). In the ^{240}Pu case, for both calculations, the HFB fission barrier height has been renormalized, as described in Sect. V. Both calculations are performed with the combinatorial NLD. Experimental data are taken from the EXFOR library to guide the eye. [18].

Transition state densities are known to play a crucial role in the prediction of fission cross sections. This is illustrated in Fig. 4 by the ^{238}Pu and ^{240}Pu fission cross section obtained using the HFB plus combinatorial method and BSFG prescriptions for the NLDs at equilibrium and saddle configurations. The BSFG model is employed with and without inclusion of the discrete transitions states prescribed by Ref. [7], but because of the non-universal character of the phenomenology used to determine these transitional states, they are not included when calculating the cross section with the HFB plus combinatorial NLD. As can be observed, including such states clearly leads to an increase of the cross section at low energies. This comparison also clearly shows that analytical NLD approximations at the saddle points are strongly associated with the barrier heights and widths determined through a cross section fit, but are also dependent on all the specificities of the reaction model considered (in particular the inclusion of discrete transitional states). For this reason, it remains difficult to reproduce fission calculations obtained by other groups, if all the recipes and input parameters are not precisely given.

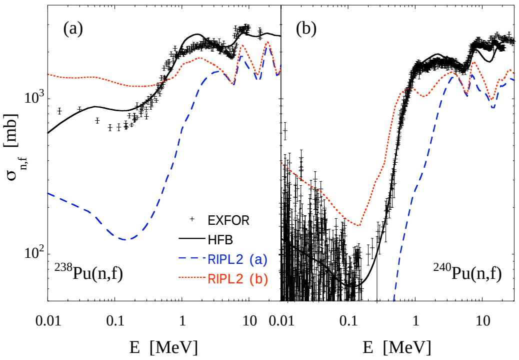

FIG. 4: Neutron-induced fission cross section of ^{238}Pu (left panel) and ^{240}Pu (right panel) obtained with the combinatorial NLD (solid line) and the back-shifted Fermi gas model [7] without (dashed line: RIPL2 (a)) and with (dotted line: RIPL2 (b)) the inclusion of discrete transition states of Ref. [7]. The calculations are performed with the HFB fission path and the WKB approximation for the penetrability. Experimental data are taken from the EXFOR library [18].

V. FISSION CROSS SECTIONS PREDICTIONS

We now turn to the global calculation of neutron-induced fission cross section. As mentioned in Sect. II, we restrict ourselves to the simple framework of the full damping approximation with two barriers and without inclusion of class-II states. Our purpose here is not to perform a fit to experimental data by tuning all possible parameters of relevance but rather to estimate to what extent fission cross sections can nowadays be predicted and what is the global accuracy that can be expected.

We compare in Fig. 5 the experimental neutron-induced fission cross sections for 9 different isotopes of U, Np and Pu with the calculation based on the raw microscopic nuclear models for the HFB fission path and the combinatorial NLD. As can be observed, the uncertainty on the fission path and more specifically on the barrier heights gives rise to a cross section that can hardly be estimated better than within a factor of roughly 10 for energies below some few MeV. Only for ^{237}Np and ^{238}Pu is the cross section overestimated, showing that the HFB model overestimates most of the barriers' height.

Before considering a possible renormalization of the HFB fission path, it is interesting to perform the similar

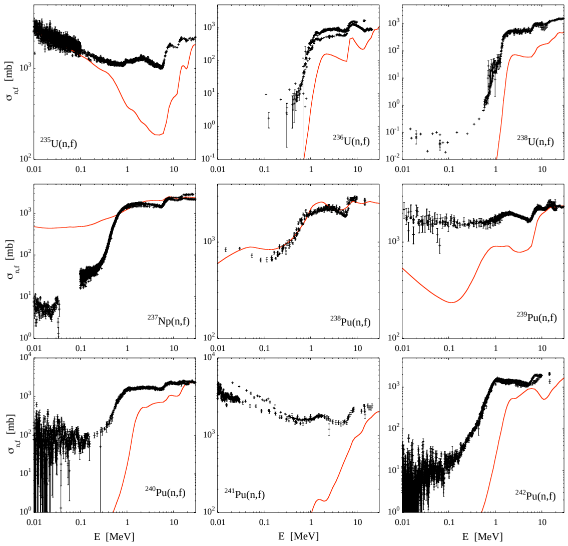

FIG. 5: Neutron-induced fission cross sections obtained with the microscopic HFB fission path and HFB plus combinatorial NLD without any renormalization (solid line).

predictions keeping the NLDs untouched but using this time the barrier heights and widths (extracted from a data evaluation) recommended in Ref. [7]. The obtained results are plotted in Fig. 6. As can be seen, the agreement has been clearly improved with respect to the previous calculation (Fig. 5) but nevertheless remains globally unsatisfactory. Note that we did not renormalize the RIPL2 barriers here. This comparison confirms the correlation between the saddle point NLDs and barrier height, or, in other words, that the barrier heights are NLD-dependent. It also gives a first hint that the combinatorial model provides reasonable NLDs for the fission saddle points.

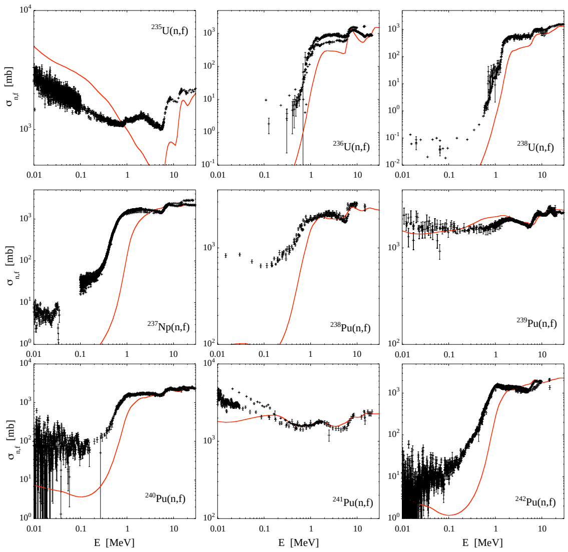

FIG. 6: Neutron-induced fission cross sections obtained with the HFB plus combinatorial NLD and the RIPL2 fission barriers used with the Hill-Wheeler approximation.

Now turning to the HFB fission path, it remains to be studied if renormalizing the barrier height can improve the description of the cross section using the same HFB plus combinatorial NLD. We have therefore globally renormalized the HFB energy surface (Fig. 1) by a deformation-independent parameter b adjusted on experimental cross sections within the $0.01 \leq E \leq 10$ MeV energy range for each reaction. The corresponding cross sections are shown in Fig. 7. As can be seen, the impact of the renormalization on the fission cross section is drastic and the agreement with experimental data significantly improved. In some cases, the agreement is very satisfactory, like e.g. in some Pu isotopes, at least for the nuclear applications that do not require too much of an accuracy. Note that no attempt has been made to fit the second-chance or third-chance fission by additionally tuning the fission barriers of the residual nuclei separately.

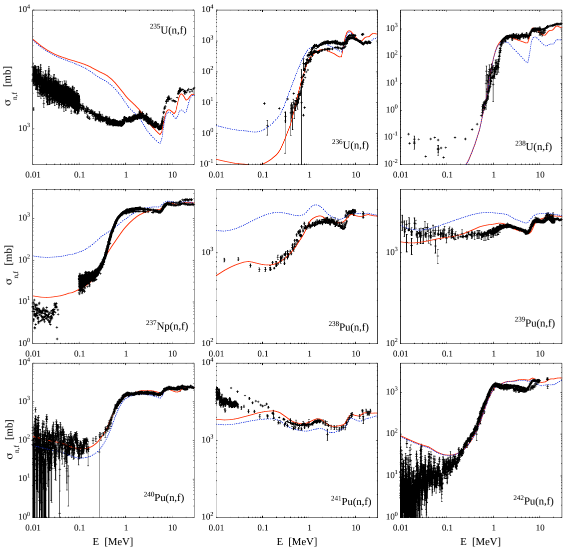

FIG. 7: Neutron-induced fission cross sections obtained with the microscopic HFB fission path and combinatorial NLD when the fission paths are globally renormalized by a deformation-independent parameters b (solid line) or by the systematics given in the text (dotted line).

To improve the predictive power using the microscopic fission paths, a systematics as been deduced for the renormalization b-factor, though no charge or isospin dependence can be extracted due to the small size of the sample. In view of a clear odd-even effect, different factors have been determined depending on the oddness of the nucleon number and we finally found that the fit can be optimized with a constant b factor amounting to 0.86, 0.89, 0.94 and 1.02 for even-even, even-odd, odd-even and odd-odd nuclei, respectively. Using this systematics, it can be seen in Fig. 7 that the reproduction of experimental data is significantly improved with respect to the default calculation (Fig. 5) : the overall default deviation by a factor of more than 10 is now reduced to less than a factor of 3, in particular at low energies.

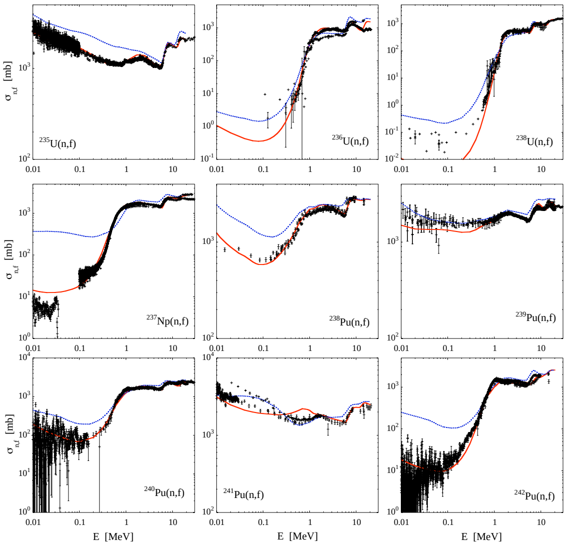

FIG. 8: Neutron-induced fission cross sections (solid line) obtained with renormalized HFB fission path (independently for the inner and outer barriers) and renormalized HFB plus combinatorial NLD. The dotted line corresponds to cross sections estimated with all the RIPL-2 recommendations.

Finally, it is possible to tune the nuclear inputs a step further to still improve the fit to experimental cross sections. In particular, the inner and outer barrier heights can be tuned independently and the NLD at each saddle points renormalized (as described in Ref.[10]). The results obtained in this case are shown in Fig. 8 together with the cross sections obtained using all the RIPL-2 recommendations [7] for barrier heights and widths and NLD at both ground state and saddle points (discrete transitions states are also included). A very nice fit can then be achieved with the renormalized microscopic ingredients.

VI. CONCLUSIONS

A consistent and complete modeling of the fission cross section remains a challenge in nuclear physics since prediction of fission cross section is far from being satisfactory. The present study has evaluated the quality of microscopic inputs, such as fission barriers (or more generally fission path) and NLD at the fission saddle points, in the calculation of fission cross section. Since the barrier heights can not be predicted with an accuracy better than typically 20%, fission cross sections remain affected by uncertainties of the order of a factor 10 or so. However, the use of the full HFB fission path and the corresponding WKB calculation of the probability to penetrate the fission barrier clearly provides a more reliable way to estimate fission cross section than what would be deduced out of a phenomenological model, in particular if we renormalize globally the height of the fission path (using the raw corresponding set of NLD at the fission saddle) according to a systematics. We then globally reproduce the experimental fission cross section within less than a factor of 3.

It will remain difficult to improve in a near future the accuracy on the prediction of fission barrier height, but it must remain a field of intense research due to the fundamental property they represent. Similarly, even if the HFB plus combinatorial method has proven to give satisfactory results when consistently used with renormalized HFB fission path, since some uncertainties still affect these microscopic ingredients, there is still place for improvement. Finally, to be able to further improve the prediction of fission cross section, a continued effort needs to be devoted to better predict not only the fission path and corresponding NLD but also the deformed optical model potential as well as transition and class II/III states.

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