NUCLEAR FISSION MODELLING WITH SPY*

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A precise knowledge of the impact of the compound nucleus characteristics on fission fragments properties like fission yield or kinetic energy is a big challenge. Since we are not able to track a nucleus splitting from compound nucleus to the fragments formation, we need a theoretical laboratory to study the fission mechanism and to have access to the correlation between the fragments properties and their nuclear structure, such as shell correction, pairing or collective degrees of freedom. To bring some answers, a new model named SPY (Scission Point Yields) has been developed to determine fission fragments characteristics using a statistical description of the fission process at the scission point. The most important property of the model relies on the nuclear structure of the fragments which is derived from full quantum microscopic calculations. This approach allows computing the fission final state of extremely exotic nuclei which are inaccessible by most of the fission model available on the market.

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1. Introduction

Although discovered 75 years ago, nuclear fission is still under investigation. Indeed, the understanding of this phenomenon still presents theoretical difficulties due to its complexity. This requires a good understanding of the structure of atomic nucleus and, at the same time, a detailed description of the mechanisms driving the evolution of a fissioning system. To what extent the system dynamics or fragments nuclear structure play a role in fragments formation at the scission point? This is the main question that the SPY (Scission Point Yields) model wants to investigate by studying the role of fragments nuclear structure in the fission process.

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2. SPY model features

The SPY model consists in a statistical description of the fission process at the so-called scission point. At this point, fragments are completely formed and well separated with fixed properties. As a previous model by Wilkins [1], the fissioning system at scission is modelled by two deformed coaxial fragments with sharp frontiers and separated by a fixed intersurface distance d (taken here at 5 fm). They have well defined characteristics such as proton, neutron number or shape deformation. For example, in thermal neutron induced fission or spontaneous fission of actinides, there are around one thousand energetically possible fragmentations. Using a statistical microcanonical description of the system, the probability of a given fragmentation is proportional to the number of available states. A state is reachable only if the system owns enough available energy to populate this state.

At scission, the available energy of a given fragmentation is the difference between the total energy of the excited compound nucleus $(E_{\rm CN}^{\rm tot})$ and the formation energy of this fragmentation, depending on the fragments deformation. This last term is composed of the individual energy of both fragments from microscopic calculation [4] $(E_{\rm ind})$ taking into account its nuclear structure, and nuclear interaction energy $(E_{\rm nucl})$ and mostly Coulomb interaction energy $(E_{\rm coul})$ between the fragments. Then, for an energetically reachable fragmentation, its Available Energy (AE) is defined by (1)

$$AE = \left| E_{\text{ind1}} + E_{\text{ind2}} + E_{\text{coul}} + E_{\text{nucl}} - E_{\text{CN}}^{\text{tot}} \right| \,. \tag{1}$$

The number of Available States (AS) of a given fragmentation at a given deformation and at a given energy partition between the two fragments is the product of individual state densities of the two fragments which are considered as isolated. Each fragment is considered like a Fermi gas, where the fragment state density is: $\rho(U) = \frac{\sqrt{12}}{\pi} \frac{e^{2\sqrt{aU}}}{a^{1/4}U^{5/4}}$ where U is excitation energy and a the level density parameter. Fermi gas state density has no dependence on nuclear structure contrary to the individual energy. For a given fragmentation at given deformation, the number of available states is obtained by summation on all possible available energy sorting between the two fragments (2)

$$AS = \int_{0}^{1} \rho_1(xAE)\rho_2((1-x)AE) \, dx \,. \tag{2}$$

3. Results

Generally, a nucleus can split in two fragments with comparable masses (symmetric fission) or with rather different masses (asymmetric fission). The transition from symmetric to asymmetric fission is clearly observed experimentally (Fig. 1) for thorium, palladium and uranium isotopic chain and depends mainly on the neutron number of the fissioning system. SPY reproduces fairly well this transition due to the fragmentation 132 Sn (doubly magic) and its counterpart which become more favourable than symmetric fragmentation.



Fig. 1. Charge yield, in black: exp. data from [5], in dark grey/red: SPY model.

Thanks to its very fast computation time, the SPY model was able to compute the fission yields of almost 3000 fissioning systems from Z = 80to Z = 109 and from proton to neutron drip line. From the isobaric fission yield, a peak multiplicity has been calculated with a fit procedure to extract a global trend on the evolution from symmetric to asymmetric fission. As shown in Fig. 2, nucleus splitting is mainly driven by its neutron number. The asymmetric fission of actinides is reproduced as well as the symmetric fission of light nuclei and the asymmetric fission of very light nuclei like ¹⁸⁰Hg [2]. Heavy nuclei split symmetrically however we observe less usual one for $N_{\rm CN} \approx 165$ where symmetric and asymmetric fission are in competition. Finally, a new fission "mode" is predicted for $N_{\rm CN} \approx 180$ where an asymmetric fission and a very asymmetric one are in competition (4 peaks). These nuclei play an important role in solar abundance of heavy elements [3].



Fig. 2. Peak multiplicity in isobaric yield of around 3000 fissioning systems.

4. State densities improvement

The description of state density of fragments can be improved, because Fermi-like state densities do not take into account any nuclear structure. Using combinatorial method on single-particle level scheme issued from HFB calculation, nuclear structure of fragments were taken into account in their state densities. For example, in doubly magic nuclei ¹³²Sn, there is an energy gap in the single-particle level scheme for spherical deformation due to proton and neutron shell closure that implies a drop of state density around sphericity (see Fig. 3). These new state densities counterbalance strong shell effects in available energy balance. Indeed, a fragmentation with ¹³²Sn is generally the most energetically favoured fragmentation. In the case of a



Fig. 3. State density of ¹³²Sn depending on deformation parameter \tilde{q} and excitation energy U. Left: Fermi gas model, right: combinatorial calculation.

Fermi gas description, state densities have smooth behaviour as a function of proton and neutron number so fission yields are directly linked to the available energy and, therefore, the fragmentation $^{132}\text{Sn} + ^{A_{\text{CN}}-132}X$ is the most probable (see Fig. 4, dashed/red curve). For the spontaneous fission of californium, the microscopic state densities improve significantly the fission yields description. Peaks width is close to experimental one without any impact on fission dynamics (see Fig. 4, thick solid/green curve). Even if in the uranium case, the addition of microscopic state densities is not as good as that in the californium case, it gives encouraging results.



Fig. 4. Isobaric fission yield distribution $^{252}Cf(sf)$.

5. Conclusion

SPY is a new scission-point model based on a static and statistical description of the fission process that makes use of one of the most up-to-date microscopic description of the nuclear structure. The interesting results are obtained for the fission of light nuclei, actinides and exotic ones. Moreover, new microscopic state densities partially counterbalance the too strong nuclear shell effects of fragments around magicity. The SPY model is still under development and even if state densities need to be improved, it provides very encouraging results on the role of nuclear structure in the fission process.

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