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Microscopic description of fission properties for r-process nuclei

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Abstract. Fission properties of 886 even-even nuclei in the region 84 < Z < 120 and $118 \leq Z \leq 250$ were computed using the Barcelona-Catania-Paris-Madrid energy density functional. An extensive study of both the potential energy surfaces and collectives inertias was performed. Spontaneous fission half-lives are computed using the semiclassical Wentzel-Kramers-Brillouin formalism. By comparing these three quantities we found that the stability of the nucleus against the fission process is driven by the interplay between both the potential energy and the collective inertias. In our calculations, nuclei with relative long half-lives were found in two regions around Z = 120, N = 182 and Z = 104, N = 222.

1. Introduction and formalism

Fission is a crucial phenomenon to understand r-process nucleosynthesis [1, 2, 3]. Results coming from r-process simulations for matter ejected dynamically in neutron star mergers have been recently published [4, 5, 6]. In this specific astrophysical site the fission process determines how matter is recycled during the neutron irradiation and the production of superheavy nuclei. In ref. [5] was showed that fission fragments distributions have a strong impact in the final r-process distributions, specially in the region around the second r-process peak and the rare-earth subpeak. On the other hand, the accumulation of material in the fissioning region leads to a robust r-process pattern, as required by metal-poor star observations [6].

These simulations involve nuclei located far from the stability valley, where experimental data is not available. Despite of the great success in the synthesis of heavy nuclei, we are still far from having an exhaustive experimental data set able to provide all the required information for such kind of studies. Due to this, in the last decades a great number of studies were devoted to the description of the fission process within the Energy Density Functional model (EDF). This mean-field approach based in the Hartree-Fock-Bogoliubov (HFB) theory requires for a phenomenological effective interaction fitted to reproduce nuclear matter properties and/or equations of state (see [7] for a recent review and comparison with macroscopic-microscopic models). In this paper, we present the result of the fission properties obtained with the Barcelona-Catania-Paris-Madrid (BCPM) EDF. BCPM is a newly proposed EDF inspired by the Kohn-Sham theory [8]. Its free parameters were adjusted in order to reproduce the binding energy of the 518 even-even nuclei of the Audi and Wapstra 2003 mass table evaluation. In recent papers [9, 10] we explored the fission properties of this interaction, comparing our results

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with the available experimental data and the predictions obtained from other theoretical models. Following the same procedure described in [9, 10], we extended the calculations to nuclei with protons number $84 \le Z \le 120$ and neutrons number $118 \le N \le 250$. These calculations are an initial step towards the provision of a global and complete data set covering the major range of interest for the r-process nucleosynthesis.

2. Results

Spontaneous fission lifetimes are obtained using the semiclassical approach given by the WKB formalism. Within this approach, the half-lives (in seconds) can be written as:

$$t_{\rm sf} = 2.86 \times 10^{-21} (1 + \exp(2S)), \qquad (1)$$

where S is the action integral computed along the fission path s:

$$S = \int_{a}^{b} ds \sqrt{2B(s) \left[(V(s) - E_0) \right]} \,. \tag{2}$$

and E_0 is the zero-point energy. As it is shown in the expression above, the (spontaneous) fission process is driven by the interplay of two major quantities, namely the collective inertias B(s) and the potential energy V(s). Both quantities must be evaluated along the fission path s, where a and b are the classical turning points fulfilling the condition $V(s) = E_0$. In this work collective inertias were calculated with the Adiabatic Time Dependent HFB (ATDHFB) method [11]. The potential energy V(s) is given by the HFB theory corrected by both zero-point energy and rotational corrections, subtracting the energy of the ground-state [10].

The fission path is determined by minimizing the total energy as a function of the quadrupole moment operator $s = Q_{20}$. This approach, also known as static approximation, is required in order to reduce the computational time and allows the systematic calculation of the fission properties for a large set of nuclei. We should mention here that in recent papers extensive calculations studying the relevance of a multidimensional space with a dynamic determination of the fission path s were performed [12, 13]. However, despite the great interest that these studies deserve, their extension to a systematic calculation of the fission properties is nowadays unfeasible from the computational point of view.

From eq. (2) it is clear that the height of the fission barrier by itself does not provide a complete characterization of the fission process. A more complete picture of the fission properties can be obtained by studying the mean value of the potential energy $\overline{V}(Q_{20})$ and the collective inertias $\overline{B}(Q_{20})$. These quantities are obtained by averaging arithmetically the magnitude of $V(Q_{20})$ and $B(Q_{20})$ along the fission path, between the turning points *a* and *b*:

$$\overline{\mathcal{O}}(Q_{20}) \equiv \frac{1}{n} \sum_{i=a}^{b} \mathcal{O}(i) , \qquad (3)$$

being n the number of Q_{20} points along the fission path.

In Fig.1 the average values $\overline{V}(Q_{20})$ and $\overline{B}(Q_{20})$, depicted as a function of the protons and neutrons number, are compared with the spontaneous fission lifetimes $t_{\rm sf}$. Comparing these three panels we can conclude that for nuclei with $1.7 \leq \overline{V} \leq 4.5$ MeV collective inertias determine whether the nucleus will be stable, or not, against the spontaneous fission process. A clear example is given by the results obtained in the region around Z = 104 and N = 220. Nuclei close to this region show a similar value of $\overline{V} \sim 3.0$ MeV, while the lifetimes span a range of 15 orders of magnitude. The main reason of such a large variation in the lifetimes is the strong change in the inertias values \overline{B} between neighbor nuclei. Of course, the sensitivity with the collective inertias is reduced in regions where the \overline{V} is extremely low.

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Figure 1. Scatter plot of the mean potential energies $\overline{V}(Q_{20})$ (panel *a*), mean collective inertias $\overline{B}(Q_{20})$ (panel *b*) and spontaneous fission lifetimes $t_{\rm sf}$ (panel *c*) as a function of proton (*Z*) and neutron number (*N*). Stars in panel *c*) show nuclei that have been experimentally observed.

While it is not possible to extract a comprehensive information by just analyzing the fission barrier height, the quantity \overline{V} seems to provide a more general description of the fission properties of single nuclei. For example, comparing the values of \overline{V} of panel a) with the halflives of panel c), it is possible to conclude that almost all the nuclei with an average fission barrier below 1 MeV have fission lifetimes below 10^{-5} s. It is worth to mention that some of these nuclei show a fission barrier height well above this average value of 1 MeV, leading to a possible overestimation of the hindrance of the nucleus against the fission process. Finally, our calculations predict nuclei with relative long half-lives in the region around the protons number Z = 120 and the neutrons magic number N = 120. It should be noticed that this region is close to nuclei that were experimentally observed.

3. Conclusions

Using the BCPM EDF, we performed an extensive calculation of the potential energy surface, collective inertias and spontaneous fission lifetimes of 886 even-even nuclei in the region $84 \leq Z \leq 120$ and $118 \leq N \leq 250$. By comparing the half lives with the average value of $V(Q_{20})$ and $B(Q_{20})$ along the fission path, we found that the stability against the fission process is driven by the interplay of these two quantities. This result go against the common description, were

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the fission characteristics are determined only by the height of the fission barriers. The strong sensitivity of the fission lifetimes with the collective inertias point out the extreme importance of a proper calculation of B(s). In order to obtain a more realistic description of fission dynamics, both studies using a non perturbative calculation of the collective masses as well as a theory beyond the actual cranking approximation are required. Work in this direction is already in progress.

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