Microscopic description of fission in Uranium isotopes with the Gogny energy density functional

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(Dated: May 27, 2014)

The most recent parametrizations D1S, D1N and D1M of the Gogny energy density functional are used to describe fission in the isotopes $^{232-280}$U. Fission paths, collective masses and zero point quantum corrections, obtained within the constrained Hartree-Fock-Bogoliubov approximation, are used to compute the systematics of the spontaneous fission half-lives $t_{SF}$, the masses and charges of the fission fragments as well as their intrinsic shapes. The Gogny-D1M parametrization has been benchmarked against available experimental data on inner and second barrier heights, excitation energies of the fission isomers and half-lives in a selected set of Pu, Cm, Cf, No, Rf, Hs and Fl nuclei. It is concluded that D1M represents a reasonable starting point to describe fission in heavy and superheavy nuclei. Special attention is also paid to understand the uncertainties in the predicted $t_{SF}$ values arising from the different building blocks entering the standard semi-classical Wentzel-Kramers-Brillouin formula. Although the uncertainties are large, the trend with mass or neutron numbers are well reproduced and therefore the theory still has predictive power. In this respect, it is also shown that modifications of a few per cent in the pairing strength can have a significant impact on the collective masses leading to uncertainties in the $t_{SF}$ values of several orders of magnitude.

PACS numbers: 24.75.+i, 25.85.Ca, 21.60.Jz, 27.90.+b, 21.10.Pc

I. INTRODUCTION.

Nuclear fission is, at the same time, one of the most distinctive phenomenon in the physics of the nucleus and one of the most elusive to a theoretical description. It takes place mostly in heavy and superheavy nuclei and involves the evolution of the initial parent system from its ground state to scission through a sequence of intrinsic shapes labeled by some sort of deformation parameter [1–3]. Once the scission configuration is reached, the system splits in two daughter nuclei. The occurrence of fission is the result of the competition between the nuclear surface energy coming from the strong interaction and the Coulomb repulsion of the nuclear charge density [4]. In fact, nuclear fission was originally described [4] in terms of the liquid-drop model where the surface tension plays an essential role. However, experimental and theoretical evidences emphasize the stabilizing role of shells effects [5–8] and therefore much effort has been laid on the development of models that incorporate those effects to the semi-classical liquid-drop model description [9–11]. The outcome of these models (see, for example, Refs. [12, 13] and references therein) is a potential energy surface, expressed in terms of several deformation parameters, showing a quite involved topography (direct consequence of shell effects) with minima, valleys, ridges and saddle points. In this picture, fission is the journey along this complicated landscape from the ground state to the scission point (an elusive concept to be discussed later). In spite of their success in describing some fission observables, these models lack essential quantum mechanisms like tunneling through a classically forbidden barrier or a sound description of the inertia associated to the collective degrees of freedom used to describe fission.

From a more fundamental point of view, fission could be regarded as a quantum mechanical problem describing the evolution from some given initial quantum state to a final state with two fragments and involving tunneling through a potential barrier defined in a multi-dimensional space. The initial state can be the parent nucleus ground state in spontaneous fission or a highly excited state (usually described as a statistical admixture by assuming thermal equilibrium) in induced fission. Although several attempts to deal with this problem in a path-integral framework involving instantons and other sophisticated concepts have been considered [14, 15] in the past, it has not been possible to establish a computationally feasible framework capable to describe real nuclei with realistic interactions. Therefore, it is customary to use a more phenomenological approach where the dynamical changes involved in the transition from a single nucleus to two fragments are usually described in the framework of the (constrained) self-consistent mean-field approximation [6, 16] based on a given non-relativistic Energy Density Functional (EDF) of the Gogny [17–21]
In the last decades there has been a renewed interest in microscopic fission studies due to the wealth of information in actinide nuclei, the huge progress in the production of superheavy elements, via cold and hot fusion reactions, and the new possibilities opened up by heavy-ion collisions with radioactive ion beams (see, for example, Refs. 17–55 and references therein). In particular, the theoretical description of fission in superheavy elements is quite relevant to better understand both the shell structure evolution and the appearance of new proton and/or neutron magic numbers in heavy nuclei 56, 57. Superheavy elements are also produced during the r-process and their properties determine the upper end of the nucleosynthesis flow 58.

In addition, it should be kept in mind that, as a decay mode, spontaneous fission competes with α-decay 59 and determines the stability of heavy and superheavy elements. It is therefore, highly desirable to devote systematic microscopic studies, based on different effective EDFs, to the prediction of the spontaneous fission $t_{\text{sp}}$ and α-decay $t_{\alpha}$ half-lives (see, for example, Refs. 25, 29). This is particularly relevant, taking into account the large uncertainties 38 associated with the different building blocks entering the Wentzel-Kramers-Brillouin (WKB) formula 60, 61 used to compute the $t_{\text{sp}}$ values.

Although the theoretical uncertainties in the determination of the absolute values of the fission observables are presumed to be large 38, the behavior of quantities as a function of mass number and/or along isotopic chains is reasonably well reproduced. Therefore, one expects to obtain a reasonable theoretical description of the physics of fission along isotopic chains extending up to the neutron dripline. Those regions are the territories where the fate of the nucleosynthesis of heavy nuclei is determined.

To study the fission of neutron-rich nuclei we have used a mean-field framework with the Gogny-EDF in the Uranium isotopic chain up to the neutron dripline 240U. The three most relevant parametrizations of the Gogny-EDF 39, namely DIS 17, DIN 62 and DIM 63, have been used in the calculations. The DIS parametrization is the oldest among the three and its fitting protocol included fission properties of 240Pu. Along the years, DIS has built itself a strong reputation given its ability to reproduce a large collection of low-energy data all over the periodic table 17, 18, 23, 25, 39, 64–81. In particular, the parametrization DIS has already been successfully applied to the microscopic description of fission in heavy and superheavy nuclei (see, for example, Refs. 18, 23, 25 and references therein) and, for this reason, it is taken as a reference in the present study. However, DIS is not specially good in reproducing masses specially when moving away from the stability valley.

To cure this deficiency the D1N parametrization was introduced. It provides a good fit to realistic neutron matter equation of state (EoS) and therefore its fitting protocol included fission properties of 240Pu. Along the years, DIS has built itself a strong reputation given its ability to reproduce a large collection of low-energy data all over the periodic table 17, 18, 23, 25, 39, 64–81. In particular, the parametrization D1S has already been successfully applied to the microscopic description of fission in heavy and superheavy nuclei (see, for example, Refs. 18, 23, 25 and references therein) and, for this reason, it is taken as a reference in the present study. However, D1S is not specially good in reproducing masses specially when moving away from the stability valley.
FIG. 1: (Color online) The HFB plus the zero point rotational energies obtained with the D1S, D1N and D1M EDFs are plotted in panel a) as functions of the quadrupole moment $Q_{20}$ for the nucleus $^{240}$U. For each EDF, both the one (1F) and two-fragment (2F) solutions are included in the plot. The pairing interaction energies are depicted in panel b) for protons (thick lines) and neutrons (thin lines). The octupole and hexadecapole moments corresponding to the 1F and 2F solutions are given in panel c). The collective masses obtained within the ATDHF approximation are plotted in panel d). For more details, see the main text.

The paper is organized as follows. In Sec. II we briefly outline the theoretical formalism used in the present work. The results of our calculations are discussed in Sec. III. First, in Sec. III A we illustrate the methodology employed to compute the fission paths and other fission-related quantities in the case of $^{240}$U. The same methodology has been used for all the nuclei studied in this paper. In Sec. III B we discuss the D1M results for the nuclei $^{212}$–$^{238}$U, $^{238}$–$^{244}$Pu, $^{210}$–$^{218}$Cm, $^{250}$–$^{252}$Cf, $^{250}$–$^{256}$Fm, $^{252}$–$^{256}$No, $^{256}$–$^{260}$Rf, $^{258}$–$^{262}$Sg, $^{264}$Hs and $^{286}$Fl and compare them with available experimental data [87–91]. This section is mainly intended to validate D1M for fission studies. The systematics of the fission paths, spontaneous fission half-lives and fragment mass in the isotopes $^{232}$–$^{280}$U is presented in Sec. III C. We will compare the results obtained with the D1S, D1N and D1M parametrizations to demonstrate the robustness of the predicted trends in $^{232}$–$^{280}$U with respect to particular choices of parametrizations. One of the main advantages of all the considered Gogny-EDFs is that they provide a self-contained approach to pairing correlations [22]. Due to the differences in the corresponding fitting protocols [17, 62, 63], each of the EDFs displays a different pairing content [65]. This, by itself, provides some insight into the impact of pairing correlations on fission properties in $^{232}$–$^{280}$U. However, in Sec. III D we explicitly discuss the impact of pairing correlations on the predicted $t_{SF}$ values for $^{232}$–$^{280}$U by increasing artificially the pairing strengths by 5 and 10%, respectively. Finally, Sec. IV is devoted to the concluding remarks and work perspectives.
II. THEORETICAL FRAMEWORK

The mean-field approximation [6] based on wave functions \(|\Phi_{HFB}\rangle\) of the HFB type has been used in the present study. Constraints in the mean value of the axially symmetric quadrupole \(Q_{20}\), octupole \(Q_{30}\) as well as the necking \(Q_{Neck}(20, C_0)\) operators have been used. The last constraint, as discussed in Sec. III A, allows us to reach two-fragment (2F) solutions starting from the one-fragment (1F) ones [23, 24, 38]. As a consequence of the axial symmetry imposed on our HFB wave functions one-fragment (1F) ones [23, 24, 38]. For each of the considered nuclei and each of the constrained configurations \((Q_{20}, Q_{30}, Q_{Neck}, \ldots)\) the two lengths \(b_2\) and \(b_+\) characterizing the HO basis have been optimized so as to minimize the total HFB energy. With the choice of basis size and the minimization of the energy with the oscillator lengths, the relative energies determining the dynamics of the fission process are well converged. For the solution of the HFB equations, an approximate second order gradient method [93] has been used. The method is very robust and the typical number of iterations to converge is quite small (a few tens) as compared to other methods. In addition, the complexity in the handling of constraints does not increase with its number.

Concerning the different interaction terms, the two-body kinetic energy correction has been fully taken into account (including exchange and pairing channels) in the variational procedure. On the other hand, the Coulomb exchange term is considered in the Slater approximation [44] while the Coulomb and spin-orbit contributions to the pairing field have been neglected.

The spontaneous fission half-life is computed (in seconds) with the WKB formalism [42] as

\[ t_{SF} = 2.86 \times 10^{-21} \times (1 + e^{28}) \]  

where the action \(S\) along the quadrupole constrained fission path reads

\[ S = \int_a^b dQ_{20} \sqrt{2B(Q_{20}) (V(Q_{20}) - (E_{GS} + E_0))}. \]

Here the integration limits \(a\) and \(b\) are the classical turning points [42] below the barrier and corresponding to the energy \(E_{GS} + E_0\). The potential \(V(Q_{20})\) is given by the HFB energy corrected by the zero point energies stemming from the restoration of the rotational symmetry \(\Delta E_{ROT}(Q_{20})\) and the fluctuations in the quadrupole moment \(\Delta E_{vib}(Q_{20})\). The rotational correction \(\Delta E_{ROT}(Q_{20})\) has been computed, in terms of the Yoccoz moment of inertia, according to the phenomenological prescription discussed in Refs. [45, 57]. This correction plays a key role to determine the shape of the potential \(V(Q_{20})\) as it can be as large as \(6 - 7\) MeV and its value is proportional to the degree of symmetry breaking, i.e., the value of the deformation \(Q_{20}\) [78].

For the evaluation of the collective mass \(B(Q_{20})\) and the vibrational energy correction \(\Delta E_{vib}(Q_{20})\) two methods have been used. One is the cranking approximation [44, 45] to the Adiabatic Time Dependent HFB (ATD-HFB) scheme [8]. In this case

\[ B_{ATDHFB}(Q_{20}) = \frac{1}{2} \frac{\mathcal{M}_{-3}(Q_{20})}{\mathcal{M}_{-1}(Q_{20})} \]  

where the moments \(\mathcal{M}_{-n}(Q_{20})\) of the generating quadrupole field read

\[ \mathcal{M}_{-n}(Q_{20}) = \sum_{\mu\nu} \frac{\langle \hat{Q}_{20}^{\mu\nu} \rangle^2}{(E_{\mu} + E_{\nu})^n}. \]
and $Q_{20}$ is the 20-component of the quadrupole operator in the quasiparticle representation \[6\]. The quasiparticle energies $E_\mu$ are the ones obtained in the solution of the HFB equations. The ATDHFB zero point vibrational correction $\Delta E_{vib}(Q_{20})$ is given by

$$\Delta E_{vib, ATDHFB}(Q_{20}) = \frac{1}{2} G(Q_{20}) B_{ATDHFB}(Q_{20})$$ \hspace{1cm} (6)

where

$$G(Q_{20}) = \frac{1}{M_{20}} \frac{M_{20}(Q_{20})}{M_{-1}(Q_{20})}$$ \hspace{1cm} (7)

is the width of the overlap between two configurations with similar quadrupole moments.

The second method is based on the Gaussian Overlap Approximation (GOA) to the GCM \[6\]. Here, the collective mass reads

$$B_{GCM}(Q_{20}) = \frac{1}{2} M_{-2}(Q_{20}) \frac{M_{-1}(Q_{20})}{M_{20}(Q_{20})}$$ \hspace{1cm} (8)

and $\Delta E_{vib, GCM}(Q_{20})$ is given by Eq. (6) but replacing the ATDHFB mass with the GCM one. We have evaluated the spontaneous fission half-life $t_{SF}$ Eq. (2) with the two schemes outlined above. The reason is that the ATDHFB masses are typically around 1.5 to 2 times larger than the GCM ones \[38, 95\]. As a consequence, the action in the exponent defining $t_{SF}$ is, in the ATDHFB case, between 20 and 40 % larger than the GCM one. Depending on the value of the action, this increase can represent a difference of several orders of magnitude in the $t_{SF}$ results. We also have to keep in mind that the inertias are computed in the so-called "perturbative cranking approximation" that is known to underestimate the real inertia values by a factor as small as 0.7 implying a reduction of a typical 15 % in the action. For a thorough comparison of different forms of the collective inertia in the framework of Skyrme-like EDFs, including the ones in Eqs. \[31\] and \[33\], and including also the different computational schemes the reader is referred to Ref. \[97\].

In Eq. (3), the parameter $E_0$ accounts for the true ground state energy once the zero point quadrupole fluctuations are considered. Although it is not difficult to estimate its value using the curvature of the energy around the ground state minimum and the values of the collective inertias \[30\] we have followed the usual recipe \[23, 38\] of considering it as a free parameter that takes four different values (i.e., $E_0=0.5, 1.0, 1.5$ and 2.0 MeV). In this way we can estimate its impact on the predicted spontaneous fission half-lives.

To summarize the previous discussions, we conclude that the $t_{SF}$ values obtained within our computational scheme are subject to several uncertainties related to the following items:

1. The characteristics of the different parametrizations of the Gogny-EDF considered.

2. The impact of triaxiality in the fission path. It is well known that the configurations around the top of the inner barrier can reduce their energies when triaxiality is allowed. It is also possible in some superheavy nuclei that their oblate ground state evolves towards fission through a triaxial path. In our case, we have kept axial symmetry as a self-consistent symmetry along the whole fission path in order to reduce the already substantial computational effort. However, for a few selected configurations around the inner barrier we have allowed triaxiality to set in as to study the reduction of the inner barrier height. Typically, the lowering represents at most a few MeV when triaxial shapes are allowed \[18, 32\]. However, the lowering of the inner barrier comes together with an increase of the collective inertia \[31, 96\] that tends to compensate in the final value of the action. Therefore, the impact of triaxiality in the final value of $t_{SF}$ is very limited and it has not been considered in the present study. In addition, previous studies \[31\] analyzing the dynamical path to fission have corroborated the insignificant role played by triaxiality to determine lifetimes.

3. The value of the parameter $E_0$. This is particularly relevant in the case of long-lived isotopes with wide and high fission barriers since the different $E_0$ values provide different classical turning points $a$ and $b$ \[see, Eq. (3)\] and therefore modify in a substantial way the final value of the action integral.

4. The assumptions involved in the computation of the collective masses as well as the zero point corrections to the HFB energies. Note that, for example, within the "perturbative cranking" scheme \[44, 46\], only the zero-order approximation is used instead of the full linear-response matrix.

5. Pairing correlations. They play a key role in the computation of both the zero point energies associated to quantum fluctuations and the collective masses. In fact, as we will see in Sec. \[11, 13\] (see also Ref. \[38\]), changes of 5 or 10 % in the pairing strengths of the original Gogny-D1M EDF can modify the predicted $t_{SF}$ values by several orders of magnitude.

As a consequence the predicted $t_{SF}$ values will have large theoretical error bars spanning several orders of magnitude implying that their absolute values cannot be used with confidence. However, the experimental isotopic and/or isotonic trends are reproduced with much higher accuracy giving us confidence on the validity of our predictions in that respect.

Finally, we have computed the $\alpha$-decay half-lives using the parametrization \[97\]

$$\log_{10} t_\alpha = \frac{AZ + B}{\sqrt{Q_\alpha}} + CZ + D$$ \hspace{1cm} (9)
of the phenomenological Viola-Seaborg formula \[59\]. The \( Q_\alpha \) value (in MeV) is obtained from the calculated binding energies for Uranium and Thorium isotopes as

\[
Q_\alpha = E(Z, N) - E(Z - 2, N - 2) - E(2, 2) \quad (10)
\]

In Eqs. \[9\] and \[10\], \( Z \) and \( N \) represent the proton and neutron numbers of the parent nucleus. On the other hand, \( E(2, 2) = -28.295674 \text{ MeV} \) \[98\] while \( A = 1.64062, B = -8.54399, C = -0.19430 \) and \( D = -33.9054 \) \[97\].

III. DISCUSSION OF THE RESULTS

In this section, we discuss all the results obtained. First, in Sec. III A we illustrate the methodology used to compute the fission observables in the case of \( ^{240}\text{U} \). In Sec. III B we discuss the Gogny-D1M results for a set of U, Pu, Cm, Cf, Fm, No, Rf, Sg and Fl nuclei for which experimental data are available \[87–91\]. The aim of these calculations is to validate D1M as a reasonable parameter set for fission studies. The systematics, provided by the D1S, D1N and D1M Gogny-EDFs, for the fission paths, \( t_{SF} \) and \( t_\alpha \) values as well as the fragment mass in the Uranium chain \( ^{232–280}\text{U} \) is presented in Sec. III C. Finally, in Sec. III D we explicitly discuss the impact of pairing correlations on the predicted \( t_{SF} \) values for \( ^{232–280}\text{U} \) using a modified Gogny-D1M EDF in which the pairing interaction strengths are increased by 5 and 10 \%, respectively.

A. An illustrative example: the nucleus \( ^{240}\text{U} \)

In Fig. \( \text{I(a)} \), the evolution of the energy as a function of the mass quadrupole moment for the nucleus \( ^{240}\text{U} \) as the system evolves from its ground state to very elongated shapes is shown. The results obtained with the D1S, D1N and D1M parametrizations are depicted. The energies shown in the plot are the HFB energies plus the ones coming from the zero point rotational motion \( E_{HFB} + \Delta E_{\text{ROT}} \). The zero point vibrational energies \( \Delta E_{\text{vib}} \) (not included in the plot) are always considered in the evaluation of the lifetimes. The curves labeled D1S(1F), D1N(1F) and D1M(1F), respectively, correspond to 1F solutions of the HFB equations. In order

![Density contour plots for the nucleus \( ^{240}\text{U} \) at the quadrupole deformations \( Q_\alpha = 80 \text{ b} \) [panel a] and \( Q_\alpha = 138 \text{ b} \) [panels b) and c)]. The density profiles in panels a) and b) correspond to 1F configurations while the one in panel c) represents a 2F solution. Results are shown for the parametrization D1M of the Gogny-EDF. Densities are in units of \( \text{fm}^{-3} \) and contour lines are drawn at 0.01, 0.05, 0.10 and 0.15 \( \text{fm}^{-3} \).
TABLE I: The heights of the inner $B_{1}^{th}$ and second $B_{1}^{th}$ barriers as well as the excitation energies $E_{1}^{th}$ of the fission isomers, predicted with the Gogny-D1M EDF, are compared with the available experimental values $B_{1}^{exp}$, $B_{1}^{exp}$ and $E_{1}^{exp}$ [5, 52]. The $B_{1}^{th}$ values obtained in the framework of triaxial calculations are given in parenthesis. All the theoretical results have been obtained from the rotational corrected HB energies. For more details, see the main text.

| Nucleus | $B_{1}^{th}$ | $B_{1}^{exp}$ | $E_{1}^{th}$ | $E_{1}^{exp}$ |
|---------|-------------|--------------|-------------|--------------|
| $^{234}$U | 7.60 | 4.80 | 3.32 | 8.09 | 5.90 |
| $^{236}$U | 8.33 | 5.00 | 3.17 | 2.75 | 8.69 | 5.67 |
| $^{238}$U | 9.06 | 6.30 | 3.37 | 2.55 | 9.54 | 5.50 |
| $^{238}$Pu | 8.77 | 5.60 | 3.20 | 2.40 | 7.75 | 5.10 |
| $^{240}$Pu | 9.45 | 6.05 | 3.36 | 2.80 | 8.57 | 5.15 |
| $^{242}$Pu | 9.90 | 5.85 | 3.57 | 2.20 | 9.18 | 5.05 |
| $^{244}$Pu | 10.16 | 5.70 | 3.83 | - | 9.60 | 4.85 |
| $^{240}$Cm | 8.98 | - | 2.55 | 2.00 | 6.13 | - |
| $^{242}$Cm | 9.78 | 6.65 | 2.77 | 1.90 | 6.99 | 5.00 |
| $^{244}$Cm | 10.38 | 6.18 | 3.02 | 2.20 | 7.70 | 5.10 |
| $^{246}$Cm | 10.75 | 6.00 | 3.29 | - | 8.13 | 4.80 |
| $^{248}$Cm | 10.68 | 5.80 | 3.32 | - | 8.28 | 4.80 |
| $^{250}$Cf | 11.38 | - | 2.81 | - | 7.09 | 3.80 |
| $^{252}$Cf | 10.96 | - | 1.37 | - | 6.79 | 3.50 |

An important point to be discussed later on in Sec. III C is the presence of a second fission isomer around $Q_{20} = 86$ b with its associated third fission barrier. As will be discussed later on in Sec. III C such second fission isomers are also found in the 1F curves of several Uranium isotopes regardless of the Gogny-EDF employed [15]. Coming back to the second fission barrier, its height takes the values 8.41, 8.91 and 10.21 MeV, for D1S, D1N and D1M, respectively. In this case, the trend observed in Ref [71] relating the height of the second barrier with $a_{s}$ (larger $a_{s}$ leads to larger barrier heights) is not fulfilled. A possible explanation is that at such large elongation the exchange properties of the interactions are more relevant than the surface properties. For the largest values of the quadrupole moment, the D1S and D1N curves show a similar decline due to the decreasing of Coulomb repulsion. In this region the D1S curve is a couple of MeV lower in energy than D1N. This is not consistent with the behavior observed in [71] for D1 and D1S and attributed there to the $a_{s}$ values of the two interactions. For D1, with an $a_{s}$ coefficient 1.2 MeV larger than D1S, the HFB energy was around 10 MeV higher than for D1S. Finally, D1M shows a gentler decline than the ones provided by the D1N and D1S functionals. This points to a larger value of $a_{s}$ than for D1N and D1S but the first barrier height values point in the opposite direction of a lower surface energy coefficient for D1M. These results do not follow the neat trend observed in [17, 71] in the comparison between the D1 and D1S parametrizations. This problem deserves further study, although a possible explanation is that the properties of the region beyond the first barrier are driven by quantum effects (exchange and shell effects) rather than macroscopic properties like the surface energy coefficient $a_{s}$.

In Fig. 2 the 1F $E_{HFB} + \Delta E_{ROT}$ energies obtained in the axially symmetric calculations for the nucleus $^{240}$U are compared with the ones obtained in the framework of triaxial calculations (see [52] for a thorough discussion of the framework and results with D1M). The curves depicted correspond to the D1M parametrization only, but
similar results are obtained for the other parametrizations. The inclusion of the $\gamma$ degree of freedom leads to the lowering of the energies in the $18\ b \leq Q_{20} \leq 32\ b$ range with $\gamma = 12^\circ$ being the largest value in the region. Compared with the axially symmetric one (i.e., 9.47 MeV) the height 7.51 MeV of the triaxial inner barrier in $^{240}\text{U}$ displays a reduction of 1.96 MeV.

Coming back to Fig. 1 (a), very steep curves labeled D1S(2F), D1N(2F) and D1M(2F) are depicted. They correspond to solutions with two well separated fragments and their energy corresponds to the quasifission channel for the corresponding fragments. These 2F solutions can be reached, starting from the 1F ones, by constraining the hexadecapole moment $Q_{40}$ \cite{17, 24}. Alternatively, one can resort to a constraint in the mean value of the necking operator $\bar{Q}_{\text{Neck}}(z_0, C_0)$ \cite{23, 58}. For the nucleus $^{240}\text{U}$, the 2F curves seem to intersect the 1F ones around $Q_{20}=130\ b$ and exhibit a quasilinear decrease in energy for increasing values of the quadrupole moment $C_0$. The intersection of the 1F and 2F curves, appears as a consequence of projecting multi-dimensional paths into a one-dimensional plot. Actually, there is a minimum action path with a ridge connecting the 1F and 2F curves in the collective space. As the determination of this path is quite cumbersome and its contribution to the action Eq. (4) is small, we have neglected its contribution to the action. Within this approximation we take the 2F curves, for which the charge and mass of the fragments lead to the minimum energy, as really intersecting the 1F ones. In practice, we have obtained the 2F curves by constraining the number of particles in the neck of the parent nucleus to a small value and then releasing the constraint in a self-consistent HFB calculation. To assess the stability of the procedure a set of calculations with different values of the neck parameters $z_0$ and $C_0$ \cite{33} is performed to make sure that the same minimum is always reached. The steep decrease in the energy of the 2F solutions is a consequence to the direct relationship that exists in this case between $Q_{20}$ and the fragments’ separation distance $R$. As the quadrupole...
(d). Their evolution, as functions of $Q_{20}$, is well correlated with the one of the pairing interaction energies shown in Fig. 1 (b). A similar pattern is found for the GCM masses (not shown in the plot) though their values are always smaller than the ATDHFB ones. For example, for $Q_{20}=18$ b we have obtained the ratios $B_{ATDHFB}/B_{GCM}=1.97, 1.98$ and 1.85 for the D1S, D1N and D1M parametrizations, respectively.

With all the previous ingredients at hand, we have computed the spontaneous fission half-lives using Eq. (2). Since we take the 1F and 2F curves as intersecting ones and do not include the effect of triaxiality on the inner barriers, our $t_{SF}$ values should be regarded as lower bounds [38] to the real values. For the nucleus $^{240}$U, we have obtained ($E_0 = 1.0$ MeV) $t_{SF} = 2.612 \times 10^{27}$ s, $2.161 \times 10^{35}$ s and $3.215 \times 10^{42}$ s in the framework of the ATDHFB scheme for the D1S, D1N and D1M parametrizations, respectively. The large differences in the predicted fission half-lives can be attributed to the differences in the fission paths and ATDHFB masses provided by the considered EDFs. To disentangle the different contributions we have taken the D1S fission path and the D1N (D1M) ATDHFB mass to obtain $6.1 \times 10^{26}$ s ($1.5 \times 10^{24}$ s) instead of the nominal value $2.612 \times 10^{27}$ s. We conclude that the main effect is to be attributed to the different fission paths. The impact of the wiggles in the masses has also been estimated by replacing the mass by a smoothed out mass (using a three point filter) and the half life changes by a factor 1.2 which is irrelevant in the present context. Using the GCM inertias, we obtain (again, $E_0 = 1.0$ MeV) smaller values $t_{SF} = 4.089 \times 10^{20}$, $3.764 \times 10^{26}$ and $3.552 \times 10^{32}$ s. Larger ATDHFB $t_{SF}$ values as compared with the GCM ones is, as discussed in Sec. III C, a general trend for all the studied Uranium isotopes regardless of the particular functional employed. We thus see, how the differences in the ATDHFB and GCM masses, can have a strong impact on our predictions for fission observables. This is the reason why, for each Gogny-EDF, both kinds of collective masses have been considered in the computation of the spontaneous fission half-lives. On the other hand, increasing $E_0$ leads to smaller $t_{SF}$ values in either the ATDHFB or GCM frameworks (see below for a more quantitative assessment of the effect).

Finally the density contour plots corresponding to the nucleus $^{240}$U at the quadrupole deformations $Q_{20}=80$ and 138 b are shown in Figs. 3 (a), (b) and (c). Results are shown only for the Gogny-D1M EDF but similar ones have been obtained for the other parametrizations. For $Q_{20}=138$ b two plots are presented corresponding to 1F and 2F solutions, respectively. The 2F solution in Fig. 3 (c) consists of a spherical $^{132}$Sn fragment plus an oblate and slightly octupole deformed $^{108}$Mo fragment with $\beta_2 = -0.22$ and $\beta_3 = 0.03$ (referred to the fragment’s center of mass). As we will see later on in Sec. III C oblate deformed fragments also appear as a result of fissioning other Uranium isotopes. Similar results have been obtained in a recent study [38] based on the BCPM-
EDF. They deserve further analysis, as it is usually assumed \[12, 13\] that fission fragments only exhibit prolate deformations. In our calculations, the deformed oblate fragment acquires this shape in order to minimize a large Coulomb repulsion of 195.19 MeV. The 2F solution shown is the one that minimizes the energy with the given quadrupole constraint. This does not necessarily mean that this is the configuration obtained after scission. In fact, it is observed experimentally that the mass number of the heavy fragment is close to 140 instead of the \(^{132}\)Sn obtained as the minimum energy solution. Successful theories of scission \[100\] postulate that the breaking of the nucleus takes place when the neck between fragments reaches some critical value. If we consider the rupture point as the position where the neck reaches its smallest width we obtain for the heavy fragment the values \(Z = 51.9\) and \(N = 84.5\) which are close to \(Z = 50\) and \(N = 82\) of \(^{132}\)Sn but lead to a mass of 136.4 which is closer to the experimental value. It has to be stressed that the values obtained should be taken as an approximation to the peaks of the mass distribution of the fragments. Obviously, in order to reproduce the broad mass fragment distribution observed experimentally a dynamical theory considering the quantum mechanic evolution like, for instance, the one of Ref. \[101\] is required.

**B. Heavy nuclei with known experimental data**

In this section, the results obtained with the Gogny-D1M EDF for the set of nuclei 232–238U, 238–244Pu, 240–248Cm, 250–252Cf, 252–256Fm, 252–256No, 256–260Rf, 258–262Sg, 261Hs and 266Fl are discussed. The selected nuclei correspond to those where experimental data are available \[87–89\]. Previous theoretical results, based on the parametrization D1S, have already been presented in Refs. \[18, 23, 25\].

In Table I, we compare the predicted heights for the inner \(B^i_{th}\) and outer \(B^o_{th}\) barriers as well as the excitation energies \(E^i_{th}\) of the fission isomers with the experimental ones \(B^i_{th}, E^i_{th}\) and \(E^o_{th}\). The theoretical values have been obtained from the corresponding energies \(E_{HF} + \Delta E_{ROT}\) by looking at the energy differences between the ground state energy and the energies of the corresponding maxima and minima. The axial \(B^i_{th}\) values are larger than the experimental ones \[57\] reaching a maximal deviation \(B^i_{th} - B^i_{th}^{exp} = 4.88\) MeV in \(^{248}\)Cm. In order to explore the impact of the \(\gamma\) degree of freedom, for all the nuclei reported in Table I, we have performed triaxial calculations for configurations with \(10 \leq Q_{ax} \leq 40\) b. The parameter \(\gamma\) takes on the values \(0^\circ \leq \gamma \leq 12^\circ\) in this range of quadrupole deformations. As can be seen from panels (a) to (n) of Fig. 4 and the numerical values given in parenthesis in the table, the triaxial inner barriers are systematically lower than the axial ones by up to 3.18 MeV in \(^{248}\)Cm. They also display the position of the top of the barrier shifted to higher quadrupole deformations. The triaxial heights still overestimate the experimental ones. However, having in mind that the Gogny-D1M EDF has not been fine tuned to fission data and the large uncertainties in the extraction of the experimental inner barrier heights (a 1 MeV error bar is usually presumed), it is more important that the global trend observed in the experiment and other theoretical models (see, for example, Refs. \[26, 33, 38\] and references therein) is reasonably well reproduced. The D1M values for \(B^i_{th}\) are consistent with the ones obtained in the framework of Gogny-D1S calculations \[18\].

In the case of the outer barriers, the inclusion of reflection-asymmetric shapes leads to a reduction of a few MeV. However, we still observe deviations of up to \(B^o_{th} - B^o_{th}^{exp} = 4.75\) MeV with respect to the experimental data. As no significant effects are expected from triaxiality ours, as well as previous Gogny-D1S results \[18\], seem to indicate that other effects not related to the mass moments may be required to further decrease the predicted \(B^o_{th}\) values. Whether it is the pairing degree of freedom or effects associated to symmetry restoration or the collective dynamics is something that remains to be

**FIG. 6:** (Color online) In panel a), the proton \((Z_1, Z_2)\), neutron \((N_1, N_2)\) and mass \((A_1, A_2)\) numbers of the two fragments resulting from the fission of \(^{238–244}\)Pu, \(^{248}\)Cm, \(^{250, 252}\)Cf, \(^{252–256}\)Fm, \(^{252–256}\)No, \(^{256–260}\)Rf, \(^{258–262}\)Sg, \(^{261}\)Hs and \(^{266}\)Fl [see, panel b)] are shown as functions of the fissility parameter \(Z^2/A\) in the parent nucleus. Results have been obtained with the Gogny-D1M EDF. The magic proton \(Z = 50\) and neutron \(N = 82\) numbers are highlighted with dashed horizontal lines to guide the eye.
explored. However, we have to keep in mind the model dependent character of the experimental data for outer barriers heights that makes those quantities less reliable than the corresponding fission half-lives for a comparison with theoretical values. In the case of the fission isomer excitation energy, the largest difference observed $E_{II}^{th} - E_{II}^{exp}$ of 1.37 MeV occurs for $^{242}$Pu.

In Fig. 5 we compare the Gogny-D1M $t_{SF}$ values, obtained for the nuclei $^{232}$U, $^{240}$Pu, $^{248}$Cm, $^{256}$Fm, $^{252}$No, $^{256}$Rf, $^{258}$Sg, $^{260}$Hs and $^{268}$Fl within the GCM and ATDHFB schemes, with the experimental data [80]. Results are shown for $E_0=0.5$, 1.0, 1.5 and 2.0 MeV, respectively (see, Sec. II). The effect of triaxiality has not been taken into account in the calculations. The experimental fission half-lives expand a range of 27 orders of magnitude. The theoretical predictions display a larger variability depending on whether the GCM or ATDHFB scheme is used as well as on the $E_0$ parameter. For example, differences of up to 12, 9, 7 and 5 orders of magnitude occur in $^{232}$U, $^{238}$U, $^{238}$Pu, $^{248}$Cm and $^{256}$Fm, for $E_0=0.5$ MeV. Such differences become smaller for the heavier Fm, No, Rf, Sg, Hs and Fl nuclei. On the other hand, increasing $E_0$ leads to smaller $t_{SF}$ in either of the two schemes. This reduction is particularly pronounced in the case of nuclei with higher and wider fission barriers. It is satisfying to observe that both the GCM and ATDHFB Gogny-D1M schemes capture the large reduction of $t_{SF}$ observed experimentally when going from $^{232}$U to $^{286}$Fl.

The comparison along isotopic chains reveals that the trend with neutron number is also reasonably well described. For the nuclei depicted in Fig. 5 both our Gogny-D1M and previous [23, 25] Gogny-D1S calculations exhibit a similar trend as a function of the fissibility parameter $Z^2/A$. However, larger $E_0$ values are required in our case to improve the comparison with the experimental data. This is not surprising, as in most cases the Gogny-D1M 1F curves display a gentler decline for the largest deformations.

The proton ($Z_1, Z_2$), neutron ($N_1, N_2$) and mass ($A_1, A_2$) numbers of the 2F solution leading to the minimum energy for a given quadrupole moment and corresponding to the nuclei $^{238}$−$^{244}$Pu, $^{238}$−$^{244}$Cm, $^{250}$−$^{256}$Fm, $^{252}$−$^{256}$No, $^{256}$−$^{260}$Rf, $^{258}$−$^{262}$Sg, $^{264}$Hs and $^{268}$Fl are shown in Fig. 6 as functions of the fissibility parameter $Z^2/A$ of the parent nucleus. Fragment properties have been obtained from the 2F solutions and for the largest $Q_{20}$ values available as to guarantee that those properties are nearly independent of the quadrupole moment (which is equivalent to fragment’s separation for 2F solutions) considered. In our calculations, the proton and neutron numbers in the fragments are mostly dominated by the $Z = 50$ and $N = 82$ magic numbers. Experimentally [90, 11], the average masses $\overline{A}_H$ of the heavy fission fragments in $^{238}$−$^{244}$Pu, $^{238}$−$^{244}$Cm, $^{250}$−$^{256}$Fm and $^{254}$−$^{258}$Fm are nearly constant with a value around $\overline{A}_H = 140$ and deviations of 1 or 2 mass units. As mentioned before, the 2F solution discussed here is determined by the minimum energy requirement and according to several models of scission this is not necessarily the configuration obtained after the break up of the parent nucleus. In the previous section, we briefly mentioned that if the breakup point is taken as the point where the well developed neck attains its minimum width then the mass distribution becomes closer to the experimental values. However, a more microscopic model including quantum-mechanical effects like the one of Ref. [101] should be used for a sounder theoretical description. As this kind of dynamical model is very involved computationally we will not dwell on this and we just keep in mind that the mass distribution of the two fragments leading to the minimum energy at the HFB level underestimates the mass of the heavier fragment by a few units. In addition to this general consideration we can encounter locally examples where our model is not able to reproduce the delicate balance between macroscopic and shell effects that lead, for example, to mass asymmetric splittings in the heavy Fm isotopes. As an example, let us mention that a symmetric splitting is obtained in $^{256}$Fm in disagreement with the rather large mass asymmetry $\overline{A}_L/\overline{A}_H = 112/141$ observed experimentally. Similar results have been obtained in previous calculations with the Gogny-D1S EDF [23]. On the other hand, the ratio $\overline{A}_L/\overline{A}_H = 124/136$ predicted for $^{260}$Rf coincides with the one reported in Ref. [23].

To summarize the conclusions of this section, it has been shown that in spite of large theoretical uncertainties in the choice of the models to describe the relevant quantities, the Gogny-D1M [63] HFB framework provides a reasonable description of the tendencies with mass number of the physical observables. This validates the use of this parametrization to study the systematics of fission paths and other relevant quantities in the isotopes $^{232}$−$^{280}$U that is presented in the next section. Results obtained with the DIS and D1N parameter sets will also be discussed to quantify the typical uncertainties associated to the employed Gogny-EDF.

C. Systematics of fission paths, spontaneous fission half-lives and fragment mass in Uranium isotopes

In Figs. 7, 8 and 9 we have plotted the energies $E_{HF B} + \Delta E_{ROT}$, obtained with the DIS, D1N and D1M Gogny-EDFs, for the nuclei $^{232}$−$^{256}$U [panel (a)] and $^{258}$−$^{280}$U [panel (b)]. Both the 1F (full lines) and 2F (dashed lines) curves are shown in the plots. Starting from $^{232}$U ($^{258}$U) in panel (a) [in panel (b)] all the curves have been successively shifted by 15 MeV in order to accommodate them in a single plot. Before commenting on more quantitative aspects of the results it is worth to notice that, regardless of the functional employed, the shapes of the 1F and 2F curves in $^{232}$−$^{280}$U look rather similar pointing to equivalent liquid drop and shell effect properties of the three EDFs considered.

As the neutron number increases, we observe a gradual decrease in the deformations corresponding to the abso-
FIG. 7: The HFB plus the zero point rotational energies obtained with the Gogny-D1S EDF are plotted in panel a) for the nuclei $^{232-256}\text{U}$ and in panel b) for the nuclei $^{258-280}\text{U}$ as functions of the quadrupole moment $Q_{20}$. Both the one (1F) and two-fragment (2F) solutions are shown in the plot with continuous and dashed lines, respectively. Starting from $^{232}\text{U}$ ($^{258}\text{U}$) in panel a) [in panel b)] all the curves have been successively shifted by 15 MeV in order to accommodate them in a single plot. Note, that the energy scales span different ranges in each panel. For more details, see the main text.

An increase in the height of the inner fission barriers and the widening of the 1F curves is noticed in all the considered Gogny-EDFs as the two-neutron dripline is approached. As a consequence, an increase in the spontaneous fission half-lives for the heavier Uranium isotopes is expected. It is also worth mentioning, the existence of second fission isomers in several of the considered nuclei. For example, in $^{240-252}\text{U}$ they exhibit quadrupole deformations $Q_{20} \approx 86-96$ b. The second fission isomers are also visible in the 1F curves of heavier isotopes though in some cases the situation is not as well defined due to the presence of several shallow minima. Similar results have been recently obtained with the BCPM-EDF [38].

In order to explore the role of the $\gamma$ degree of freedom, we have performed Gogny-D1M triaxial calcula-
tions, for the isotopes $^{232-240, 248, 254, 260, 272-280}\text{U}$. The corresponding results for $^{240}\text{U}$ and $^{234-238}\text{U}$ have already been shown in Figs. 2 and 4 respectively, but they are included again in Fig. 8 for the sake of completeness. For the heavier nuclei $^{248, 254, 260, 272-280}\text{U}$, we have performed triaxial calculations for $4 \leq Q_{20} \leq 50$ b, with $\gamma = 20^\circ$ being the largest value considered. The corresponding energies are shown in Fig. 9 and thin lines visible in the neighborhood of the first fission barrier.

In order to better understand the trends in binding energies for the Uranium isotopes the two neutron separation energies ($S_{2N}$) are plotted in Fig. 10 for the three sets of calculations. We observe that whereas the D1N and D1M $S_{2N}$ are rather similar, the D1S values are typically 1 MeV lower than the previous ones. These low values for D1S were reported in previous large-scale calculations [102] and show up as a systematic drift in the differences between the experimental and theoretical binding energies in heavy nuclei. In fact, the effort to correct this drift in the quest for an accurate mass table based on the Gogny-EDF led to the proposal of both D1N [62] and D1M [63]. Previous studies [62, 63, 65, 82–85] suggest that, while improving the description of nuclear masses, both the D1N and D1M sets still have the same essential predictive power to describe low-energy nuclear structure properties as the Gogny-D1S EDF. Nevertheless, more calculations are still required to substantiate this conclusion. The main features observed in the $S_{2N}$ are the plateau between $N = 166$ and $N = 174$ and the sudden drop at $N = 186$ that signals the magic number character of $N = 184$.

In Fig. 11 the excitation energies of the first $E_I$ fission...
isomers are plotted along with the first barrier height $B_I$ in panel a). In panel b) the same quantities but referred to the second isomeric well are shown. The results for the three EDFs show a similar behavior with neutron number for the first barrier height $B_I$. A sudden drop is observed at $N = 164$ that is correlated with the plateau observed in the $S_{2N}$ plot. The excitation energies of the first fission isomer remain more or less constant with a value around 3 MeV up to $N = 164$ where they show a change of tendency and start to increase linearly with neutron number. At $N = 184$ there is a sudden drop accompanied by a drop in $B_I$ characteristic of the filling of a new major shell. As previously mentioned, for D1M triaxial calculations in the neighborhood of the inner fission barriers have been carried out. Triaxiality reduces the $B_I$ by 0.55, 0.59, 1.33, 1.60 and 1.96 MeV in the case of $^{232-240}$U, respectively. In spite of this reduction the theoretical predictions still overestimate the experimental data \cite{87,88} for $^{234-238}$U (see, also Table I). On the other hand, the axial barrier heights 8.30, 8.02, 8.44, 12.71, 13.32, 11.42 and 9.54 MeV in the nuclei $^{248,254,260,272-280}$U are reduced by 2.70, 1.75, 0.56, 1.33, 0.86, 1.04, 1.01 and 0.88 MeV, respectively.

For the second isomeric well the behavior is more erratic and we can even observe the lack of second isomeric well in some nuclei. It is also worth noticing the similar predictions for $B_{II}$ from the three EDFs and the large dispersion in the predicted $E_{II}$ values.

With all the previous ingredients at hand, we have computed the spontaneous fission half-lives Eq. (2) for...
the considered Uranium isotopes. The effect of triaxiality, is not taken into account in the calculations. The $t_{\text{SF}}$ values, predicted within the GCM and ATD-HFB schemes, are plotted in Fig. 12 as a function of the neutron number. Results have been obtained with the Gogny-D1S [panel (a)], Gogny-D1N [panel (b)] and Gogny-D1M [panel (c)] EDFs. For each parametrization, we have carried out calculations with $E_0$ = 0.5, 1.0, 1.5 and 2.0 MeV, respectively. The experimental $t_{\text{SF}}$ data for $^{232-238}$U are included in the plot.

The $t_{\text{SF}}$ values predicted within the ATDHF approximation are always larger than the GCM ones for a given $E_0$. For example, for $E_0$ = 0.5 MeV, differences of up to 12 orders of magnitude are obtained for the lighter isotopes. Such differences increase with increasing neutron number reaching 23, 31 and 26 orders of magnitude in the nucleus $^{276}$U with the parametrizations D1S, D1N and D1M, respectively. Increasing $E_0$ leads always to a decrease in $t_{\text{SF}}$. It is satisfying to observe that all the parametrizations lead to the same trend in $t_{\text{SF}}$, even though D1M provides the largest absolute values in half-lives and, as already discussed in Sec. III B, larger $E_0$ values are required to improve the agreement with the available experimental data. This is a consequence of the shape of the 1F curves provided by the Gogny-D1M EDF for the considered Uranium isotopes that are wider than for the other EDFs. Regardless of the EDF employed, we observe a steady increase in the spontaneous fission half-lives for neutron numbers $N \geq 166$ reaching a maximum at $N = 184$, which is predicted to be a magic neutron number in our calculations.

In Fig. 12, we have also plotted the $\alpha$-decay half-lives computed with a parametrization [27] of the Viola-Seaborg formula [28], Eq. (10). To this end, we have used the binding energies obtained for the corresponding Uranium and Thorium isotopes [see, Eq. (10)]. Here, we stress that, at variance with the Gogny-D1S [17], both the D1N [62] and D1M [63] parametrizations have been tailored to give a better description of the nuclear masses and therefore their $\alpha$ decay half-lives are expected to be much more realistic than the D1S ones. In all cases, a steady increase is observed in $t_\alpha$ as a function of the neutron number. Though the precise value depends on the selected EDF (i.e., $N = 144$ for D1S, $N = 150$ for D1N and $N = 156$ for D1M), it is clearly seen that for increasing neutron number fission turns out to be faster than $\alpha$-decay.

Our predictions compare well with the semiclassical results of Ref [105] using the Extended Thomas-Fermi method for a Skyrme interaction. In that calculation very high barriers are predicted for $N = 184$ in the uranium isotopic chain contrary to some liquid drop models. The barrier heights in those neutron rich nuclei are correlated to the surface symmetry energy coefficient $a_{ss}$, an effect that deserves further study for the Gogny class of energy functionals.

The proton ($Z_1, Z_2$), neutron ($N_1, N_2$) and mass ($A_1, A_2$) numbers of the 2F solutions for $^{232-280}$U are shown in Fig. 13 as functions of the neutron number of the parent nucleus. Results have been obtained with the Gogny-D1S [panel (a)], Gogny-D1N [panel (b)] and Gogny-D1M [panel (c)] EDFs. Exception made of the
number in the parent nucleus except for the case of the light isotopes, agrees well with the experimental \(\alpha\) addition, magic number in one of the fragments is always close to the neutron number in the parent nucleus. The proton number for one of the fragments is always close to the magic number \(Z\) while for the other fragment it increases as a function of \(Z\) stabilizes at \(262\) nuclei. The neutron number in one of the fragments always corresponds to the magic number \(N\) for \(232\)–\(238\)\(^{232}\)–\(238\)\(^{238}\) and \(268\)–\(280\)\(^{268}\)–\(280\) which, in the case of the light isotopes, agrees well with the experimental results and the ones discussed in Sec. IIIA, we conclude that the Gogny-D1M EDF represents a reasonable starting point to describe fission properties in the isotopes \(232\)–\(238\)\(^{232}\)–\(238\) and other heavy nuclei. With this in mind, we will proceed to explicitly discuss the impact of pairing correlations in the next Sec. IIIID.

The results discussed in this section, show that the same trends are obtained with the D1S, D1N and D1M parametrizations. This gives us confidence in the robustness of our predictions with respect to the version of the Gogny-EDF employed. In particular, from the previous results and the ones discussed in Sec. IIIB we conclude that the Gogny-D1M EDF represents a reasonable starting point to describe fission properties in the isotopes \(232\)–\(280\)\(^{232}\)–\(280\) and other heavy nuclei. With this in mind, we will proceed to explicitly discuss the impact of pairing correlations in the next Sec. IIIID.

D. Varying pairing strengths in Uranium isotopes

In this section, we discuss the impact of the strength of pairing correlations on the predicted spontaneous fission half-lives and other relevant fission properties in \(232\)–\(280\)\(^{232}\)–\(280\). To this end, we have carried out self-consistent calculations with a modified Gogny-D1M EDF in which, a multiplicative factor \(\eta\) has been introduced in front of the HFB pairing field \(\Delta_{\text{hf}}\). The corresponding pairing...
interaction energy reads

\[ E_{pp}(\eta) = -\frac{\eta}{2} \text{Tr} (\Delta \kappa^*) \]  

(11)

For simplicity, we have considered the same \( \eta \)-factor for both protons and neutrons. In addition to the normal Gogny-D1M EDF (i.e., \( \eta = 1 \)), calculations have then been carried out with \( \eta = 1.05 \) and \( 1.10 \), respectively. Our main reason to consider different pairing strengths is that they are key ingredients in the computation of both the collective masses and the zero point energies. For example, it has already been shown \[12, 43\] that the collective mass is inversely proportional to some power of the pairing gap, i.e., the stronger the pairing correlations are the smaller the collective masses become. Similar \( \eta \)-factors have been recently used in Ref. \[38\] as well as to describe pairing and rotational properties of actinides and superheavy nuclei in the framework of the RMF approximation (see, for example, Ref. \[105\] and references therein).

A typical outcome of our calculations is shown in Fig. 13(a) where, we compare the three fission profiles obtained for the nucleus \( ^{240}\text{U} \) using the normal (\( \eta = 1.00 \)) and modified (\( \eta = 1.05 \) and 1.10) Gogny-D1M EDFs. For each \( \eta \) value, both the 1F and 2F solutions are included in the plot. Exception made of the corresponding energy shifts, the 1F and 2F curves in \( ^{240}\text{U} \) and all the other Uranium isotopes, exhibit rather similar energy shapes. The ground state in \( ^{240}\text{U} \) located around \( Q_{20} = 14 \) b and its deformation decreases with increasing \( \eta \). Increasing the pairing strength by 5 and 10 % we gain 1.11 and 2.29 MeV in binding energy, respectively. These quantities have to be compared to the HFB pairing correlation energy of 1.92 MeV obtained by subtracting the HFB energy to the Hartree-Fock one. We observe an increase of around 60% in correlation energy for \( \eta = 1.05 \) which is consistent with the exponential dependence of the correlation energy on the pairing strength. In spite of the large impact on correlation energies other quantities considered to fix the pairing strength like two neutron separation energies do not change significantly when \( \eta \) is increased justifying the range of \( \eta \) values considered. On the other hand, the heights of the inner barriers (8.76 MeV for \( \eta = 1.05 \) and 8.00 MeV for \( \eta = 1.10 \)) display a reduction of 720 KeV and 1.47 MeV when compared to the one obtained using the normal Gogny-D1M EDF. The excitation energy of the first fission isomer, located at \( Q_{20} = 42 \) b, is lowered by 50 KeV (\( \eta = 1.05 \)) and 140 KeV (\( \eta = 1.10 \)).

The proton (dashed lines) and neutron (full lines) pairing interaction energies are depicted in Fig. 15(b). They display similar trends as functions of the quadrupole moment though, as expected, they become larger with increasing \( \eta \) values. Concerning the multipole moments \( Q_{20}(1F), Q_{30}(1F), Q_{20}(2F) \) and \( Q_{30}(2F) \) shown in panel c), one observes that they lie on top of each other, for all the considered \( \eta \) values.

In Fig. 16(d), the collective inertia \( B_{ATDHFB} \) is depicted. The behavior as a function of the quadrupole moment is similar in the three cases but the actual values are clearly correlated with the \( \eta \) factor. This is a direct consequence of the inverse dependence of the collective mass with the square of the pairing gap \[12, 43\]. In particular, for \( \eta = 1.05 \) (\( \eta = 1.10 \)) the ATDHFB mass is reduced, on the average, by 28 % (46 %). The GCM masses (not shown in the plot) are reduced by 28 and 35 %, respectively. These reductions have a significant impact on the predicted fission half-lives. For example, for \( E_0 = 1.0 \) MeV we have obtained, within the ATDHFB scheme, \( t_{SF} = 3.215 \times 10^{42}, 3.051 \times 10^{31} \) and \( 2.575 \times 10^{23} \) s for \( \eta = 1.00, \eta = 1.05 \) and \( \eta = 1.10 \), respectively.
FIG. 14: (Color online) Density contour plots for the nuclei $^{234}\text{U}$ [panel a], $^{256}\text{U}$ [panel b] and $^{280}\text{U}$ [panel c]. The density profiles correspond to $2\text{F}$ solutions at the quadrupole deformations $Q_{20}=150$, 150 and 220 $b$, respectively. Results are shown for the parametrization D1M of the Gogny-EDF. The density is in units of fm$^{-3}$ and contour lines correspond to densities 0.01, 0.05, 0.10 and 0.15 fm$^{-3}$.

half-lives $t_{\text{SF}}$, predicted within the GCM and ATDHFB schemes, for the isotopes $^{232-280}\text{U}$ as functions of the neutron number. Results have been obtained with the normal and modified Gogny-D1M EDFs. Calculations have been carried out with $E_0=0.5$ [panel (a)], 1.0 [panel (b)], 1.5 [panel (c)] and 2.0 MeV [panel (d)], respectively. The experimental $t_{\text{SF}}$ values for the nuclei $^{232-238}\text{U}$ are included in the plot. In addition, $\alpha$-decay half-lives are plotted with short dashed lines.

On the one hand, the results shown in Fig. 16 illustrate the strong impact that pairing correlations have on the fission half-lives in the considered Uranium isotopes. Increasing $\eta$, leads to a reduction in both $B_{\text{ATDHFB}}$ and $B_{\text{GCM}}$. As a consequence, for a given $E_0$, we observe a significant decrease in $t_{\text{SF}}$ in either the ATDHFB or the GCM schemes. For example, for $E_0=0.5$ MeV and within the GCM scheme, increasing the pairing strength by 5 \% (10 \%) leads to a reduction in $t_{\text{SF}}$ of up to 9 (16) orders of magnitude in the light isotopes. Such a reduction becomes even more pronounced for the heavier isotopes reaching 23 (42) orders of magnitude in the case of $^{270}\text{U}$. Note, that our results for $^{232-238}\text{U}$ agree reasonably well with the experimental data. However, it is more important that, in spite of the large variability in the predicted $t_{\text{SF}}$ values due to pairing correlations, the same global features discussed in the previous Sec. III C (see, Fig. 12) still hold: 1) a steady increase in the spontaneous fission half-lives is observed for $N \geq 166$ reaching a maximum at $N = 184$; 2) beyond $N=166$ the Uranium isotopes can be considered stable with respect to spontaneous fission; 3) for increasing neutron number fission turns out to be faster than $\alpha$-decay, with the transition point being around $N = 144 - 150$.

Once again, we stress that the results discussed in this and the previous Sec. III C point to the robustness of the overall trend predicted for the spontaneous fission half-lives in $^{232-280}\text{U}$ using the more recent parametrizations of the Gogny-EDF. They suggest the use of experimental fission data, instead of the more traditional odd-even staggering, to fine tune the pairing strengths in those EDFs commonly employed in microscopic studies. They also point to the relevance of beyond mean correlations associated with the interplay between pairing fluctuations and particle number symmetry restoration in the description of fission. Given the large uncertainties in the predicted $t_{\text{SF}}$ values, in ours and other the-


IV. CONCLUSIONS

In the present work, we have considered the evaluation of fission observables within the constrained HFB approximation based on Gogny-like EDFs. We have presented a detailed description of the methodology employed to obtain the fission paths in the studied nuclei. Besides the proton \( Z \) and neutron \( N \) number operators, we have considered constraints on the axially symmetric quadrupole \( Q_{20} \), octupole \( Q_{30} \) and \( Q_{10} \) operators. In some instances, we have explored the role of the \( \gamma \) degree of freedom by means of triaxial calculations with simultaneous constraints on both the \( Q_{20} \) and \( Q_{32} \) components of the quadrupole moment. On the other hand, HFB solutions corresponding to separated fragments have been reached with the help of the necking operator \( Q_{Neck}(z_0, C_0) \). The \( 1F \) curves obtained in this way exhibit a rich topography including the ground state minimum, the inner and outer barriers as well as the first and second fission isomers. For larger deformations we have found \( 2F \) curves displaying a quasi-linear decrease in energy for increasing values of the quadrupole moment. Zero point quantum corrections have always been added to each of the mean-field solutions \( a posteriori \). In particular, the rotational correction has been computed in terms of the Yoccoz moment of inertia while two different schemes (i.e., the ATDHFB and GCM ones) have been employed in the calculation of both the collective inertia and the vibrational corrections. We have thoroughly discussed the uncertainties in the predicted spontaneous fission half-lives \( t_{SF} \) arising from different building blocks affecting the WKB formula.

We have carried out Gogny-D1M calculations for a selected set of actinides and superheavy elements. The comparison between the theoretical and experimental inner and second barrier heights as well as the excitation energies of fission isomers shows that the global trend observed in the experiment is reasonably well reproduced. The same is true in the case of the spontaneous fission half-lives, regardless of whether the ATDHFB or GCM masses are used. In particular, our results demonstrate that the Gogny-D1M HFB framework captures the severe experimental \( t_{SF} \) reduction between \( ^{232}\text{U} \) and \( ^{288}\text{Fl} \) as well as the trend along different isotopic chains. Another relevant source of information is the mass and charge of the resulting fission fragments, which are determined by the nuclear shape in the neighborhood of the scission point. In our calculations the proton and neutron numbers of the fragments are determined by energetic considerations and therefore they are mostly dominated...
In addition, the analysis of the masses and charges of the fission fragments reveals, the key role played by the $Z = 50$ and $N = 82$ shell closures in the splitting of the considered Uranium isotopes. Interesting enough, oblate deformed fragments are predicted in our calculations that deserve further attention as it is usually assumed that fission fragments exhibit prolate deformations.

In the present study special attention has been paid to the impact of pairing correlations on the fission properties in $^{232-280}$U. To this end, we have also considered a modified Gogny-D1M EDF in which the pairing strengths are increased by 5 and 10 %, respectively. On the one hand, our calculations further corroborate the robustness of the predicted spontaneous fission half-lives systematics. On the other hand, they also illustrate that modifications of such a few per cent in the pairing strength can have a dramatic impact on the collective masses therefore altering the absolute values of the fission half-lives by several orders of magnitude. Within this context, we advocate the use of experimental fission data, instead of the more traditional odd-even staggering, to fine tune the pairing strengths in those EDFs commonly employed in microscopic studies. Our results also point, to the relevance of beyond mean correlations associated with the interplay

- beyond $N = 166$ the Uranium isotopes can be considered stable with respect to spontaneous fission
- as a decay mode fission becomes faster than $\alpha$-emission for increasing neutron number.

by the $Z = 50$ and $N = 82$ magic numbers. Those values, however, underestimate by several mass units the experimental values pointing to the need of a better dynamical theory to describe post-fission phenomena. The results obtained validate the D1M Gogny-EDF, originally tailored to better reproduce nuclear masses, for the study of fission properties in heavy and superheavy nuclei.

We have performed a systematic study of the fission properties in Uranium nuclei, including very neutron-rich isotopes up to $^{280}$U. In order to verify the robustness of our predictions, when extrapolated to very exotic $N/Z$ ratios, calculations have been carried out with the three most recent incarnations of the Gogny-EDF, i.e., the parametrizations D1S, D1N and D1M. The well known under-binding of the heavier isotopes characteristics of the Gogny-D1S EDF is clearly visible in our calculations. Nevertheless, the fission paths still exhibit rather similar shapes regardless of the functional employed. An increase in the height of the inner fission barriers and the widening of the 1F curves appear as common features as we approach the two-neutron dripline. Second fission iso-

- a steady increase in the spontaneous fission half-lives is observed for $N \geq 166$ with a peak at the neutron magic number $N = 184$
between pairing fluctuations and particle number symmetry restoration in the description of nuclear fission.

Last but not least, let us also comment on a more methodological issue. Given the present state of affairs in the microscopic computation of spontaneous fission half-lives, even in the case of state-of-the-art approximations, it is highly desirable to explore new avenues in which the minimization of the action $S$ (see, Eq. [10]) acquires a central role. The first steps, within the Skyrme-EDF framework, have been undertaken very recently [106]. The action is proportional to the square root of the collective inertia and therefore any degree of freedom having an impact on it, will play an essential role. In this respect, pairing correlations should be incorporated as an important degree of freedom, in addition to the more traditional quadrupole and octupole moments. Work along these lines is in progress and will be reported elsewhere.

**Acknowledgments**

Work supported in part by MICINN grants Nos. FPA2012-34694, FIS2012-34479 and by the Consolider-Ingenio 2010 program MULTIDARK CSD2009-00064. This work was completed while one of the authors (LMR) participated at the INT13-3 program. The warm hospitality of the Institute for Nuclear Theory and the University of Washington is greatly acknowledged.
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