Dynamic versus static fission paths with realistic interactions

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The properties of dynamic (least action) fission paths are analyzed and compared to the ones of the more traditional static (least energy) paths. Both the Barcelona-Catania-Paris-Madrid and Gogny D1M energy density functionals are used in the calculation of the Hartree-Fock-Bogoliubov (HFB) constrained configurations providing the potential energy and collective inertias. The action is computed as in the Wentzel-Kramers-Brillouin method. A full variational search of the least-action path over the complete variational space of HFB wave functions is cumbersome and probably unnecessary if the relevant degrees of freedom are identified. In this paper, we consider the particle number fluctuation degree of freedom that explores the amount of pairing correlations in the wave function. For a given shape, the minimum action can be up to a factor of 3 smaller than the action computed for the minimum energy state with the same shape. The impact of this reduction on the lifetimes is enormous and dramatically improves the agreement with experimental data in the few examples considered.

I. INTRODUCTION

The description of fission in the atomic nucleus (see Ref. [1] for a recent account) is the subject of a renewed interest as a consequence of potential applications both at the level of fundamental science and industrial applications. The mechanism of fission involves a delicate balance between quantum mechanical effects inherent to the quantum many-body problem and properties of the nuclear interaction that are not well understood yet. Deepening our understanding of fission is therefore important in order to understand both aspects of the dynamics of the atomic nucleus. Fission is also relevant to other areas outside traditional nuclear physics like astrophysics, where the understanding of the nucleosynthesis of heavy elements in explosive galactic environments through the r-process is of great relevance. A deeper understanding of fission is also of interest in safe energy production in the new generation of nuclear reactors or in novel mechanisms to degrade radioactive waste. The theoretical interpretation of fission is based on two properties of the parent nucleus: the evolution of the energy as the system traverses from its ground state to scission and the inertia associated with the collective motion along that path. To improve in the former, properties of the fission energy landscape as the inner and outer barrier heights have been considered as a physical constraint in the fitting protocol of several energy density functionals (EDFs) [2–5]. On the other hand, an

effort to improve the description of the collective inertias is underway [6,7]. The gross features of fission can be understood rather well from a microscopic perspective using the mean field Hartree-Fock-Bogoliubov (HFB) theory [8] along with effective phenomenological interactions of different kinds. Therefore, it is not surprising that there have been numerous studies devoted to this subject with Skyrme interactions [5,9–11], Gogny ones [2,12–21], or those based on the relativistic mean field [22–24] or other kind of energy density functionals recently proposed [25,26].

The traditional paradigm in fission is to describe the path to the scission configuration by looking at the minimum energy in multidimensional energy landscapes. Several deformation parameters associated with multipoles of different orders are routinely used in those calculations. Surprisingly the role played by pairing in the dynamical aspects of the theory has attracted little attention and only recently the uncertainties associated with that degree of freedom in the values of fission observables have been explored [20,21,26]. The static (minimum energy) description is an approximation of the more quantal approach where the action of the collective degrees of freedom is the quantity driving the dynamics (the dynamical description). Assuming a static description simplifies the computational problem and, in addition, it was argued [27] that both approaches give equivalent results when shape degrees of freedom alone are considered as collective degrees of freedom (see [28] for a recent result). On the other hand, that pairing is a fundamental ingredient for fission dynamics was already pointed out 40 years ago by Moretto and Babinet [29] in a seminal paper where the impact of pairing correlations on the action was analyzed in a simple, yet realistic, model.

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The main conclusion of this paper is that the competition between the collective inertia, decreasing as the square of the inverse pairing gap [30,31], and the energy, increasing as the square of the pairing gap, lead to a minimum of the action at a pairing gap twice as large as the one of the minimum energy. The importance of pairing vibrations in nuclear dynamics was emphatized by Bés *et al.* [32] in the context of the cranking model and by Gozdz *et al.* [33–35] in the generator coordinate method (GCM) framework. The idea of coupling pairing vibrations to nuclear fission dynamics was pursued further by the Lublin school [35] in a series of papers where realistic fission calculations seeking for the minimum of the action were performed; see [36] for a recent overview and additional references. When pairing was included as dynamical variable they observed reductions of a few orders of magnitude (up to 8 in Cm isotopes) in the spontaneous fission lifetimes t_{SF} as compared to the minimum energy results. In nuclei with higher and broader barriers (like the ones considered here) the reduction is expected to be larger.

In this paper we study the predictions for spontaneous fission lifetimes when considering the minimum action scheme instead of the minimum energy one. We will consider pairing as a relevant degree of freedom in the parameter space used in the minimum action search. Calculations with effective, yet realistic, interactions including finite range ones (Gogny D1M [37,38]) and pure energy density functionals like the Barcelona-Catania-Paris-Madrid (BCPM) functional [25] will be considered. We will restrict ourselves to several isotopes of uranium where experimental data are available. The main reason for this choice is the large discrepancies observed between theory and experiment that are due to too high and too wide fission barriers.

II. METHODS

The path from the ground state to the scission point is assumed to be driven by the least-action principle, where the action is computed as

$$S = 2 \int_a^b ds \sqrt{2B(s)[V(s) - E_0]}. \tag{1}$$

The variable s is used to parametrize the fission path, and all the relevant collective degrees of freedom depend upon it. The inertia is given by the general expression

$$B(s) = \sum_{ij} B_{ij} \frac{dq_i}{ds} \frac{dq_j}{ds}, \tag{2}$$

where the $q_i(s)$ are the values along the fission path of the relevant degrees of freedom like the axial quadrupole (Q_{20}), octupole (Q_{30}), and hexadecapole (Q_{40}) moments and in our case the particle number fluctuation ΔN^2. The B_{ij} are the collective inertias for each pair of degrees of freedom and computed using the perturbative cranking approximation [7,39]. Both the expressions obtained in the adiabatic time dependent HFB (ATDHFB) or the GCM approximations will be used. The potential $V(s)$ is given by the HFB energy, with corrections from beyond mean field effects included, as

$$V(s) = E_{HFB}(s) - \epsilon_{ROT}(s) - \epsilon_{fluc}(s). \tag{3}$$

The most important is the rotational energy correction $\epsilon_{ROT}(s)$ which is the correlation energy gained by restoring angular momentum quantum numbers. It is proportional to quadrupole deformation and can reach several MeV and therefore has the potential to substantially reduce the fission barrier heights. It has been computed using a well performing approximation to the exact quantity [40]. Less important for fission are the zero point energy corrections $\epsilon_{fluc}(s)$ associated with quantum fluctuations of the collective variable s. The E_0 is the ground state energy computed as the minimum of $V(s)$ plus a zero point energy corresponding to quadrupole fluctuations and taken, for simplicity, as a constant value of 1 MeV.[1] Details on how all those quantities are evaluated are given in [26]. The constrained HFB wave functions obtained with state-of-the-art semiphenomenological energy density functionals of the Gogny and BCPM type are used in the calculations. Axial symmetry is preserved in the calculation but reflection symmetry is allowed to break at any stage of the calculations.

For this exploratory calculation we have made several simplifying assumptions:

(i) Separated proton and neutron pairing correlations are not considered. Instead, a single constraint in the total particle number fluctuation is considered. This simplification reduces the computational cost by a factor of a few tens (depending on the number of $\langle \Delta N^2 \rangle$ values considered).

(ii) The fission path is parametrized by the mass quadrupole moment. As customary in fission calculations based in the minimum energy principle, the coupling with other degrees of freedom in the evaluation of the inertia [Eq. (2)] is neglected and only the quadrupole inertia is considered.

(iii) As a consequence, the determination of the minimum action path does not require sophisticated linear programming techniques. It reduces to a simple minimization for fixed quadrupole moments of the integrand in the action considered as a function of the other degrees of freedom.

The constrained HFB wave functions $|\varphi(Q_{20}, \langle \Delta N^2 \rangle)\rangle$ are obtained using an approximate second-order gradient method [41] with the HFBAXIAL code [42]. Two EDFs will be used in the calculation to make sure that the conclusions are independent of the details of the nuclear interaction. First we use the Gogny [37] force with the D1M [38] parametrization, whose main characteristic is its finite range, which allows a consistent treatment of pairing correlations using the same two-body force that determines de particle-hole Hartree-Fock potential. Although D1M was specifically tailored to describe binding energies, it has been shown in a series of papers [20,21,43–46] that D1M provides good results for many low-energy nuclear observables. The other EDF used is the recently proposed BCPM EDF [25] with its density-dependent

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[1]Much in the same way as the one-dimensional harmonic oscillator ground state energy is given by the sum of the potential energy at the minimum plus half of the oscillator frequency times $\hbar$.
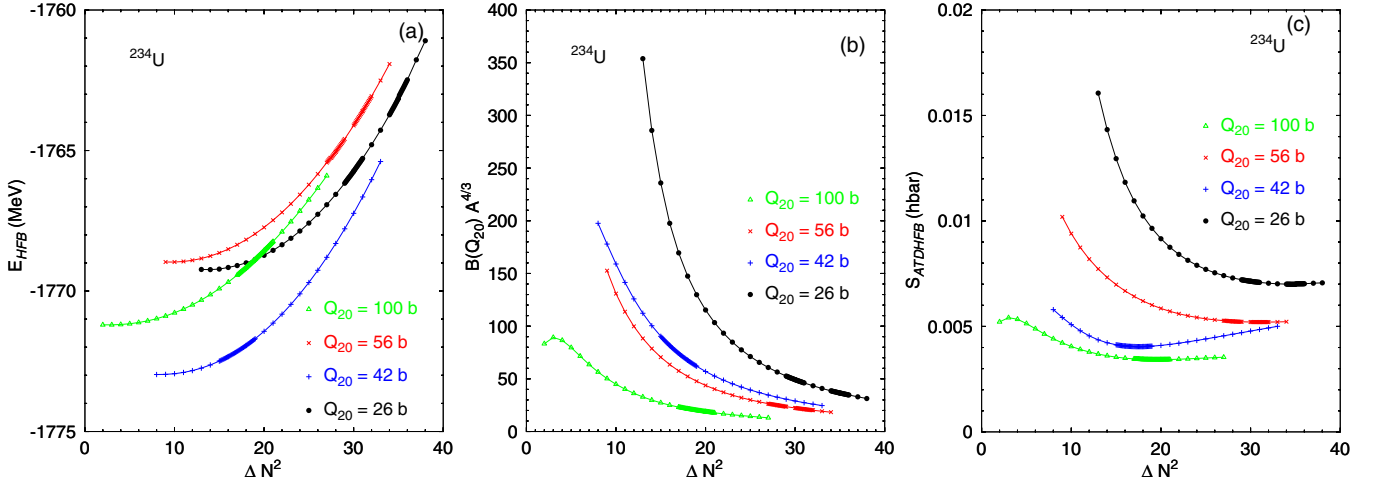
FIG. 1. (Color online) (a) HFB energy, (b) collective inertia, and (c) action represented as functions of particle number fluctuation ΔN^2 for several relevant Q_{20} values (given in barns). All the curves start at the ΔN^2 values of the minimum energy solutions.

pairing and effective mass equal to unity. Again BCPM has been fitted to reproduce binding energies but has proved to produce consistent low-energy results in a variety of cases [25] including fission [26].

III. RESULTS

To illustrate the procedure, we will focus on the nucleus ^{234}U whose fission properties were thoroughly studied in [26] using the BCPM and Gogny D1M functionals. For both functionals, the nucleus presents its ground state minimum at $Q_{20} = 12$ b. Also for both functionals, the first fission barrier is located at $Q_{20} = 26$ b, the fission isomer minimum is at $Q_{20} = 42$ b, and the second fission barrier is at $Q_{20} = 62$ b. As discussed thoroughly in [26] the main difference between the two functionals is the inertia, which is roughly three times larger for BCPM. This is probably a consequence of its larger effective mass and the different pairing interactions used.

To find the $\langle \Delta N^2 \rangle$ value minimizing the action, we carry out constrained HFB calculations starting at the $\langle \Delta N^2 \rangle$ value minimizing the energy for each Q_{20} value of the fission path. In this way we obtain curves for the relevant physical quantities as a function of $\langle \Delta N^2 \rangle$ for each value of Q_{20}. An example of such curves is shown in Fig. 1 for the Q_{20} values corresponding to the first and second fission barriers and to the fission isomer, and at $Q_{20} = 100$ b, which was chosen as a characteristic value for very large elongations. We observe in Fig. 1(a) an almost parabolic behavior for the energy as a function of $\langle \Delta N^2 \rangle$ with the minimum located at the self-consistent solution. In Fig. 1(b) the decrease of the inertia with the inverse of $\langle \Delta N^2 \rangle^2$ (corresponding to the law $B \approx 1/\Delta^2$ [30,31]) is noticed. Finally, the integrand in the action S of Eq. (1), computed with the ATDHFB version of the inertia is plotted in Fig. 1(c). It shows a minimum at $\langle \Delta N^2 \rangle$ values much larger than the ones of the minimum energy solution. The minimum value of the action integrand does not coincide with the value obtained (self-consistently) from the minimization of the energy, because the latter is up to a factor of 3 larger. This large quenching reduces considerably

the action [Eq. (1)] that appears in the exponential of the WKB formula. Therefore, the impact on the t_{SF} values is large. In this case we obtain 0.18×10^{23} and 0.21×10^{19} s depending on the choice of the collective mass, ATDHFB or GCM, respectively. Those values have to be compared with the ones obtained minimizing the energy, namely, 0.81×10^{43} and 0.70×10^{30} s. We observe a reduction of 20 and 11 orders of magnitude, which brings the theoretical predictions in much closer agreement with experiment. Another beneficial side effect of the action minimization is that results are much less sensitive to the approach used to compute the inertias. This remarkable reduction was observed in previous calculations [36] by the Lublin group in other heavy nuclei.

The minimum action solutions have $\langle \Delta N^2 \rangle$ values much larger than the minimum energy configurations and therefore have stronger pairing correlations. In [20,21,26] we analyzed the impact on t_{SF} of modifying the pairing strength and a strong influence was observed. We have repeated those calculations but now computing the lifetimes using the minimum action principle. The results obtained with BCPM [26] (the ones for Gogny D1M are similar [20]) are shown in Fig. 2 as a function of the factor η used to modify the pairing strength.

We observe that the strong dependence of t_{SF} with η in the minimum energy calculation gets severely reduced in the minimum action case. This is not so surprising because in the minimum action case we are already exploring the appropriate amount of pairing correlations in the search for the minimum action configuration. This search can somehow compensate for the changes induced by the varying interaction strength. It is also noteworthy to mention that now both the ATDHFB and GCM results are in much closer agreement than in the minimum energy case.

Recently, fission calculations based on the minimum action principle and using one of the Skyrme variants have been presented [28]. The variables considered are the axial Q_{20} and triaxial Q_{22} multipole moments. The main conclusion of that work is that minimum energy and minimum action results are essentially the same. Obviously, the result is not in contradiction with ours since different degrees of freedom
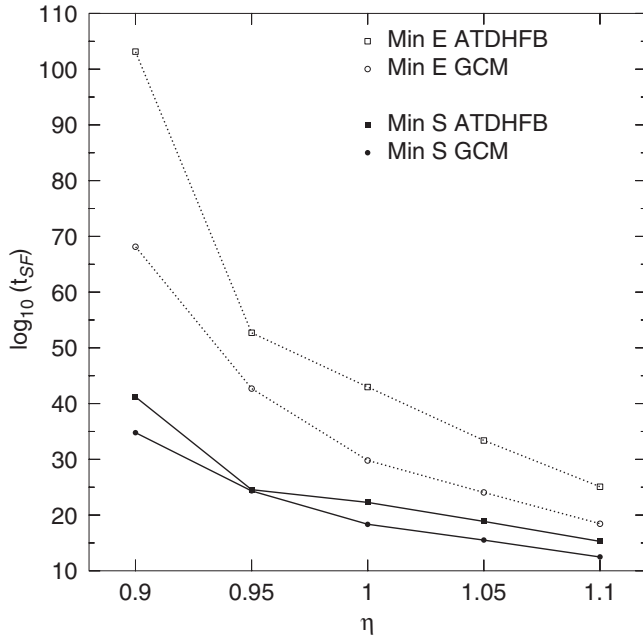
FIG. 2. Spontaneous fission lifetimes of ^{234}U obtained with different approaches as a function of the η factor multiplying the pairing interaction strength.

TABLE II. Spontaneous fission lifetimes for several uranium isotopes obtained using the minimum action principle with the ATDHFB (A) and GCM (G) variants of the collective inertias.

	Gogny D1M		BCPM		Expt.
	S_{min} (A)	S_{min} (G)	S_{min} (A)	S_{min} (G)	
^{232}U	5.4×10^{20}	1.5×10^{17}	8.6×10^{19}	8.2×10^{16}	2.5×10^{21}
^{234}U	7.3×10^{21}	2.7×10^{18}	1.7×10^{22}	2.1×10^{18}	4.7×10^{23}
^{236}U	2.8×10^{23}	9.9×10^{19}	1.9×10^{22}	1.2×10^{18}	7.8×10^{23}
^{238}U	1.6×10^{24}	6.7×10^{20}	6.1×10^{21}	6.2×10^{17}	2.6×10^{23}

Finally, we show in Table II a summary of the t_{SF} obtained minimizing the action and using the two EDFs considered and the two variants of the collective inertia for several isotopes of uranium. When compared with the results obtained minimizing the energy [20,21,26], the action minimization results show a much better agreement with experiment as well as a much reduced dispersion with the interaction used and the variant of the collective mass considered. This is a very important result because the theoretical interpretation of fission was hampered by the large variability in the t_{SF} values depending on the pairing strength [20,21,26].

are considered. To further investigate this aspect we have carried out action minimization calculations considering the pairs of collective variables (Q_{20}, Q_{30}) and (Q_{20}, Q_{40}) to explore the minimum action trajectory. The results obtained with BCPM are summarized in Table I. The results obtained considering Q_{30} and Q_{40} in the minimization of the action are much closer to the ones obtained minimizing the energy than the results obtained using pairing correlations as a relevant collective variable in the action. This result can be understood as a consequence of the weak dependence of the collective inertia $B(Q_{20})$ with Q_{30} and Q_{40} and agrees with previous results also considering multipole moments in the action minimization [27,28]. It is worth recalling that the coupling between collective variables as in Eq. (2) is not considered in the present calculation. It could lead to a stronger dependence of the inertia on those variables and therefore to a larger difference with the energy minimization results. However, based on the difference of many orders of magnitude observed in the pairing results, we can conclude that the pairing degree of freedom is more relevant for the action minimization calculations than the other multipole moment variables.

IV. CONCLUSIONS

The main conclusion of the paper is that the scheme in which the minimum action principle is used to compute t_{SF} and the amount of pairing correlations is considered as a collective variable gives results that strongly differ from the ones where the fission path is determined by energy minimization. The spontaneous fission lifetimes computed minimizing the action are several orders of magnitude smaller than the ones obtained from the traditional minimization of the energy. This decrease improves dramatically the agreement with the experimental data. In addition, the minimum action results show a weaker dependence with the ingredients of the calculation than the minimum energy ones. This is an important result for the credibility of mean field techniques to adequately reproduce fission observables. It is also shown that considering other variables in the minimization of the action such as the multipole moments Q_{30} and Q_{40} has little impact on the results being equivalent to the energy minimization ones.

TABLE I. Spontaneous fission lifetimes computed with the ATDHFB and GCM approximations to the collective inertias. Results for different sets of collective variables used to search for the minimum of the action are given.

Method	t_{SF} (ATDHFB)	t_{SF} (GCM)
E_{min}	0.81×10^{43}	0.70×10^{30}
$S_{min}(Q_{20}, \Delta N^2)$	0.18×10^{23}	0.21×10^{19}
$S_{min}(Q_{20}, Q_{30})$	0.44×10^{42}	0.64×10^{29}
$S_{min}(Q_{20}, Q_{40})$	0.12×10^{43}	0.10×10^{29}

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