Spontaneous fission lifetimes from the minimization of self-consistent collective action

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The spontaneous fission lifetime of 264Fm has been studied within nuclear density functional theory by minimizing the collective action integral for fission in a two-dimensional quadrupole collective space representing elongation and triaxiality. The collective potential and inertia tensor are obtained self-consistently using the Skyrme energy density functional and density-dependent pairing interaction. The resulting spontaneous fission lifetimes are compared with the static result obtained with the minimum-energy pathway. We show that fission pathways strongly depend on assumptions underlying collective inertia. With the non-perturbative mass parameters, the dynamic fission pathway becomes strongly triaxial and it approaches the static fission valley. On the other hand, when the standard perturbative cranking inertia tensor is used, axial symmetry is restored along the path to fission; an effect that is an artifact of the approximation used.

Introduction.—The spontaneous fission (SF) of a nucleus plays important role in many areas of science and applications [1–3]. In particular, it determines the stability of the heaviest and superheavy elements [4–6] and it impacts the formation of heavy elements at the final stages of the r-process through the recycling mechanism [6–8]. Therefore, a capability of theory to predict SF lifetimes in a reliable way is essential.

The main ingredients for a theoretical determination of SF lifetimes are the collective potential and inertia tensor. For heavy systems, these quantities can be calculated by using the self-consistent mean field theory based on the energy density functional [9]. The potential energy surface (PES) is obtained by solving constrained Hartree-Fock-Bogoliubov equations (HFB) in a multidimensional space of collective coordinates. The collective inertia (or mass) tensor is obtained from the self-consistent densities by employing the adiabatic time-dependent HFB approximation (ATDHFB) [10–12]. Since SF is a quantum-mechanical tunneling process and the fission barriers are usually both high and wide, the SF lifetime is obtained semi-classically by minimizing the fission action integral in the collective space.

The main objective of this work is to study SF by combining the microscopic density functional input with the sophisticated action minimization techniques. We demonstrate that the predicted SF pathway strongly depends on the choice of the collective inertia. In particular, in the commonly used perturbative cranking approximation, the variations of mass parameters due to level crossings (configuration changes) are underestimated; this results in an artificial restoration of axial symmetry in the region of the first barrier that is broken in a static and non-perturbative approaches.

Model.—In a semi-classical approximation, the SF half-life is given by [13, 14] \[ T_{1/2} = \ln 2 / (n P) \]

where \( n \) is the number of assaults on the fission barrier per unit time and \( P \) is the penetration probability given by \[ P = (1 + \exp [2 S(L)])^{-1}. \]

In Eq. (1) \( S(L) \) is the fission action integral calculated along the one-dimensional fission path \( L(s) \) pre-selected in the multidimensional collective space:

\[
S(L) = \int_{s_{\text{in}}}^{s_{\text{out}}} \frac{1}{\hbar} \sqrt{2M_{\text{eff}}(s)(V_{\text{eff}}(s) - E_0)} ds,
\]

where \( V_{\text{eff}}(s) \) and \( M_{\text{eff}}(s) \) are the effective potential energy and inertia along the fission path \( L(s) \), respectively. \( V_{\text{eff}} \) can be obtained by subtracting the vibrational zero-point energy \( E_{\text{ZPE}} \) from the total Hartree-Fock-Bogoliubov energy \( E_{\text{tot}} \). Integration limits \( s_{\text{in}} \) and \( s_{\text{out}} \) are the classical inner and outer turning points, respectively, defined by \( V_{\text{eff}}(s) = E_0 \) on the two extremes of the fission path. The collective ground state energy is \( E_0 \), and \( ds \) is the element of length along \( L(s) \). A one-dimensional path \( L(s) \) can be defined in the multidimensional collective space by specifying the collective variables \( q_i(s) \) as functions of path’s length \( s \). The most probable fission path corresponds to the minimum of \( S(L) \) [15, 16]. The expression for \( M_{\text{eff}} \) is [13, 14, 17]:

\[
M_{\text{eff}}(s) = \sum_{ij} M_{ij} \frac{dq_i}{ds} \frac{dq_j}{ds},
\]
where $M_{ij}$ are the components of multidimensional collective inertia tensor.

In this pilot study, we consider the SF of $^{264}$Fm. This nucleus is predicted to undergo a symmetric fission due to shell effects in the doubly magic nucleus $^{132}$Sn \[18\]. Consequently, we consider a two-dimensional collective space of mass (isoscalar) quadrupole moments $Q_{20} \equiv Q_1$ (elongation) and $Q_{22} \equiv Q_2$ (triaxiality) defined as in Table 5 of Ref. \[19\]. To compute the total energy $E_{\text{tot}}$ and inertia tensor $M_{ij}$, we employed the symmetry-unrestricted HFB solver HFODD (v2.49) \[20\].

Throughout this work, we closely follow Refs. \[5, 12\]. Namely, in the particle-hole channel we use the Skyrme energy density functional SkM* \[21\]. The particle-particle interaction was approximated by the density-dependent mixed pairing force \[22\].

The zero-point energy was estimated by using the Gaussian overlap approximation \[5, 23, 24\]. The collective masses \[26\] have been widely used \[5, 17, 28–35\] to calculate SF lifetimes.

It is important to remark that rapid variations in $M_{ij}$ are expected in the regions of configuration changes (level crossings) due to strong variations of density derivatives in \[7\] associated with structural rearrangements. Such variations are quenched in perturbative moment tensors \[7\] as the matrix elements $\langle 0|Q_i|\alpha\beta\rangle$ are actually reduced in level-crossing regions.

**Results.**—The energies $E_{\text{tot}}$ and $E_{\text{ZPE}}$ for $^{264}$Fm are shown in Fig. 1. It is seen that in the range of deformations considered, the zero-point energy varies between 0 and -0.9 MeV; hence, it only slightly renormalizes the topology of $E_{\text{tot}}$. The triaxial deformations are important around the fission barrier, and they reduce the fission barrier height by over 2 MeV.

Since the three individual components of the quadrupole inertia tensor are difficult to interpret, in Fig. 2 we show the square-root-determinants of inertia tensors \[4\] and \[6\], defined as $|M|^{1/2} = (M_{11}M_{22} - M_{12}^2)^{1/2}$. These quantities are invariant with respect to two-dimensional rotations in the space of collective coordinates and well illustrate the overall magnitudes of collective masses. Figure 2 also shows the square-root-determinants of energy-weighted moment tensors $M^{(1)}$ and $M^{(3)}$ \[7\] that define the perturbative-cranking inertia tensor $M^{C_p}$. For $|M^{C_p}|^{1/2}$, we notice rapid variations as a function of collective coordinates, and similar trends are also evident for $|M^{(3)}|^{1/2}$ and $|M^{(1)}|^{1/2}$. However, in $M^{C_p}$, which depends on the ratio \[6\] of $M^{(3)}$ and $M^{(1)}$, variations in $Q_{20}, Q_{22}$ are quenched.

Large fluctuations of mass parameters are manifestations of crossings of single-particle levels at the Fermi level, see, e.g., Ref. \[33\]. To illustrate this, Fig. 3 displays single-particle energies for $^{264}$Fm along two straight lines in the collective space, given by $Q_{22} = 0$ and $Q_{20} = 61$ b. It is clearly visible, that multiple level crossings appear very close to the Fermi energy, at deformations where $M^{C_p}, M^{(1)}$, and $M^{(3)}$ exhibit rapid variations.

Before we proceed, we demonstrate the numerical accuracy of the calculated inertia tensors. To this end, we compute the effective quadrupole inertia \[3\] along the negative $Q_{20}$ axis, which corresponds to $\gamma = 180^\circ$. In this case, the $z$-axis is a symmetry axis and nuclear shape has an oblate deformation. Here, only $M_{11}$ component contributes to $M_{\text{eff}}$ as $d\gamma_2/ds = 0$. Next, nuclear densities were rotated in space, so that the $y$-axis becomes the
symmetry axis and $\gamma = 60^\circ$. Along this path, all $M_{ij}$ components are nonzero. Nevertheless, the new path proceeds through exactly the same sequence of shapes; hence, the effective quadrupole inertia must be identical in both cases. This is demonstrated in Fig. 4: the agreement between $\gamma = 180^\circ$ and $\gamma = 60^\circ$ results is indeed excellent.

We determined the minimum-action paths by following two different numerical techniques: the dynamic-programming method (DPM) [13] and Ritz method (RM) [14]. For DPM, we discretized the quadrupole surface into a two-dimensional mesh. Then, the fission path is calculated by connecting those mesh points that contribute minimum value for $S(L)$ out of all possible combinations. In case of comparatively large distances between two successive mesh points, we further divided the corresponding path length into small segments. This is essential in case of non-perturbative inertia as $M_{ij}$ varies quite nonlinearly in certain regions of the deformation plane. In case of RM, trial paths are expressed as Fourier series of collective coordinates and the coefficients of different Fourier components are then extracted by minimizing the action integral [4]. For both methods, different possible values of turning points $s_{\text{in}}$ and $s_{\text{out}}$ have been considered to obtain the minimum action path.

In Fig. 5 we show dynamical minimum-action paths determined for $M_C$ and $M_C^p$ and compare them with the static path corresponding to the minimized collective potential. To obtain the static path, we proceed from one point to the next point on the path by searching the minimum potential on the circumference of a tiny circle centered around the previous point. Evidently, the static path traverses the longest distance through the two-dimensional collective space. For perturbative inertia, there is a strong dynamical hindrance that prevents the
paths from departing towards large triaxial shapes: the collective mass $\mathcal{M}_{C}^{\text{cr}}$ favors near-axial shapes. This observation is consistent with findings of previous Refs. [31–35] that the effects of triaxial shapes on the fission process are weakened by the inertia tensor. In the barrier region, all the components of $\mathcal{M}_{C}^{\text{cr}}$ increase smoothly with $Q_{22}$, and this offsets the reduction of $V_{\text{eff}}$ in the action integral \( \mathcal{M}_{\text{eff}} \). Consequently, as discussed in Ref. [33], the fission path remains fairly straight in order to achieve minimum action by minimizing the path’s length.

This is not true for the non-perturbative inertia. Here, localized large variations in $\mathcal{M}_{C}^{\text{cr}}$ due to level crossings push the fission path substantially towards triaxial deformations. Interestingly, the resulting non-perturbative trajectory appears fairly close to the static fission valley. Both of these trajectories indeed try to minimize the single particle level density along the fission path by avoiding the regions of level crossing shown in Fig. 2.

For completeness, the dynamical path corresponding to constant mass parameter (“const”), fixed at the ground state value of $\mathcal{M}_{111}^{\text{cr}}$, is shown in Fig. 5. As expected, this path also appears close to the static fission valley. Values of the action integral and fission half-lives corresponding to different fission paths are summarized in Table I. They indicate strong structural dependence of the spontaneous fission on collective dynamics. (It is worth emphasizing that in the present theoretical work, the values of $T_{1/2}$ are calculated only for a comparative study and they are not intended to relate to experimental systematics.)

**TABLE I. Values of the action integral** \( \mathcal{M}_{\text{eff}} \) **and half-lives for different spontaneous fission paths shown in Fig. 4.**

| path | $S(L)$ | $\log(T_{1/2}/\text{yr})$ |
|------|--------|-----------------|
| Static+$\mathcal{M}_{C}$ | 23.4 | -7.7 |
| Static+$\mathcal{M}_{C}^{\text{cr}}$ | 20.8 | -10.0 |
| DPM+$\mathcal{M}_{C}$ | 19.1 | -11.4 |
| RM+$\mathcal{M}_{C}$ | 18.9 | -11.6 |
| DPM+$\mathcal{M}_{C}^{\text{cr}}$ | 16.8 | -13.4 |
| RM+$\mathcal{M}_{C}^{\text{cr}}$ | 16.8 | -13.4 |

**Conclusions.**—In conclusion, SF lifetimes have been studied within a dynamic approach based on the minimization of the fission action in a two-dimensional quadrupole collective space of elongation and triaxiality. Strong dynamical effects have been predicted. In the perturbative picture, the collective inertia $\mathcal{M}_{C}^{\text{cr}}$ drives the system towards near-axial shapes, consistent with Refs. [31–35]. We believe that this effect is an artifact of the perturbative approximation employed that underestimates the role of level crossings. The most important conclusion of this study is that, strong triaxial effects are indeed predicted with the more appropriate non-perturbative cranking inertia, in agreement with static calculations. This indicates that the localized structural properties of collective mass parameter, present in $\mathcal{M}_{C}$, play a crucial role in determining the SF dynamics. Presently, the inertia tensors are calculated within the cranking variant of ATDHFB [12]. The calculation of the full ATDHFB inertia is in progress, also developments are initiated in the context of dynamical effects due to the competition between triaxial and reflection asymmetric degrees of freedom.

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