

Microscopic theory of angular momentum distributions across the full range of fission fragmentsPetar Marević ^{*}*Physics Department, Faculty of Science, University of Zagreb, HR-10000 Zagreb, Croatia*Nicolas Schunck [†]*Nuclear data and Theory Group, Nuclear and Chemical Science Division, Lawrence Livermore National Laboratory, Livermore, California 94550, USA*Marc Verriere [‡]*Nuclear data and Theory Group, Nuclear and Chemical Science Division, Lawrence Livermore National Laboratory, Livermore, California 94550, USA
and CEA, DAM, DIF, 91297 Arpajon, France*

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Modern nuclear theory provides qualitative insights into the fundamental mechanisms of nuclear fission and is increasingly capable of making reliable quantitative predictions. Most quantities of interest pertain to the primary fission fragments, whose subsequent decay is typically modeled using statistical reaction models. Consequently, a key objective of fission theory is to inform these models by predicting the initial conditions of the primary fragments. In this work, we employ a framework that combines joint angular momentum and particle number projection with time-dependent configuration mixing to calculate the angular momentum distributions of primary fragments. Focusing on the benchmark cases of neutron-induced fission of ^{235}U and ^{239}Pu , we predict—for the first time—microscopic angular momentum distributions for *all* fragments observed in experiments. Our results reveal a pronounced sawtooth pattern in the average angular momentum as a function of fragment mass, consistent with recent measurements. Additionally, we observe substantial variations in angular momentum distributions along isobaric chains, indicating that commonly used empirical formulas lack sufficient accuracy. We also quantify a strong correlation between the angular momentum and the deformation of the fragments at scission, and a weak correlation in the magnitude of the angular momentum between fragment partners. The generated data will enable estimation of the impact of microscopic distributions on fission spectra, paving the way toward fission modeling based on microscopic inputs.

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Nuclear fission was first observed more than 85 years ago [1,2], but a complete understanding of the phenomenon remains a major challenge to modern nuclear physics [3]. For most of its history, fission modeling has been phenomenological [4,5]. However, thanks to the unprecedented increase in computing capabilities, the past two decades have brought rapid developments of microscopic methods based on quantum-mechanical nuclear density functional theory (DFT) [6,7]. DFT models have been successful in describing numerous facets of fission, including the spontaneous fission half-lives [8–10], fragment mass and charge distributions [11–22], energy sharing among the fragments [23–26], the role of shell effects in fragment formation [27,28], and quantum entanglement between the fragments [29,30]. These advancements have ushered in an era where microscopic

models are finally competitive with phenomenological models and can offer new insights into the fission process.

One area where fission modeling has recently experienced a true renaissance concerns the angular momentum (AM) of fission fragments (FFs). The renewed interest in the subject was largely triggered by new high-resolution spectroscopy measurements at ALTO [31], which confirmed the sawtooth mass dependence of the average AM and found no correlation in magnitude between the AM of FF partners. Subsequent theoretical studies, based on both microscopic [32–38] and statistical [39–43] methods, have addressed various pertinent questions. Microscopic calculations found that the mass dependence is consistent with the sawtooth pattern [33], quantified the role of the relative orbital angular momentum [34], demonstrated the presence of tilting and twisting modes [38], and predicted a strong spatial correlation between the FF angular momenta [35,38]. Moreover, the studies of Refs. [32,33] independently found that light FFs typically carry more angular momentum than their heavy partners close to the most likely fragmentation, which was at odds with phenomenological models employed in popular FF decay models based on statistical reaction theory, such as FREYA [44] or CGMF [45].

^{*}Contact author: pmarevic@phy.hr[†]Contact author: schunck1@llnl.gov[‡]Contact author: marc.verriere@cea.fr

On the other hand, simulations of FF decay with these same codes have shown that statistical photons [33,40] and neutrons [40] can remove substantial angular momentum from primary FFs, challenging the assumptions often invoked to associate experimentally measured distributions to those in primary or postneutron FFs [31,46]. Other questions, such as the AM generation mechanism in FFs, are still under vigorous debate [31,34,36,37,39,42,43].

Currently, the modeling of FF decay is based on Weisskopf-Ewing [44] or Hauser-Feshbach [45,47–49] statistical reaction theories and will remain so for the foreseeable future. An essential ingredient of these models is a set of initial conditions corresponding to the properties of the primary FFs formed at scission. These include, among other quantities, the correlated distributions of their angular momentum, mass, charge, and excitation energies. Angular momentum distributions, in particular, are known to have a measurable impact on the decay process, causing the anisotropy of neutron emission and affecting photon multiplicities [50–54]. Despite the aforementioned recent progress by microscopic theories, calculations have not yet been able to scale to the full range in charge and mass of FFs required to make complete predictions of experimental observables. Consequently, reaction models still rely predominantly on phenomenological inputs, even though it was shown that using microscopic distributions for several fragmentations can substantially modify predictions for photon multiplicities [33].

In this work, we extend the framework of Ref. [33] by including simultaneous angular momentum projection (AMP) and particle number projection (PNP) in FFs, particle number projection in the whole nucleus, and configuration mixing with the time-dependent generator coordinate method. This approach enables us to predict, for the first time, angular momentum distributions across the full range of mass and charge in FFs. In addition, we provide unequivocal microscopic evidence of the sawtooth pattern in primary FFs, quantify the correlation between FF deformation and angular momentum, analyze the strong isobaric dependence of angular momentum distributions, and confirm the weak correlation in the magnitude of angular momentum between the FF partners. This benchmark study focuses on two fission reactions most relevant to applications: neutron-induced fissions of ^{235}U and ^{239}Pu .

The paper is organized as follows. Section II contains an overview of the theoretical framework: definition of scission configurations (Sec. II A); summary of projection methods (Sec. II B); reminder of the time-dependent generator coordinate method (Sec. II C); and summary of the model that combines the two methods to predict final distributions (Sec. II D). Sec. III presents the results for neutron-induced fission of ^{235}U and ^{239}Pu : properties of scission configurations (Sec. III A); predictions for primary FF yields (Sec. III B); and a comprehensive analysis of angular momentum distributions in FFs (Sec. III C). Concluding remarks are given in Sec. IV.

II. THEORETICAL FRAMEWORK

This section presents a comprehensive description of the theoretical framework used to obtain full angular momen-

tum distributions in FFs. The first step is to define a set of scission configurations in the even-even fissioning system, which represents an even- Z and odd- N nucleus that absorbed an incident neutron. This is described in Sec. II A. In Sec. II B, we show how projection techniques can be used to obtain combined angular momentum and particle number distributions in each scission configuration. In Sec. II C, we briefly recall how the probabilities of populating each scission configuration can be extracted from the time-dependent generator coordinate method. Finally, Sec. II D explains how the methods of the preceding sections are combined to predict, within a single theoretical framework, both the preneutron charge and mass yields and the angular momentum distributions for the full range of FF masses and charges.

A. Scission configurations

Scission configurations $|\Phi_q^S\rangle$ are determined by solving the constrained Hartree-Fock-Bogoliubov (HFB) equations of the nuclear DFT method [55,56], where q denotes all active constraints. Fission fragment configurations are determined in a three-step process: (i) defining an initial scission line, (ii) extending the scission line, (iii) identifying fission fragments in each configuration on the extended scission line.

1. Defining the scission line

By definition, the scission line separates nuclear configurations associated with the entire compound system from those associated with the fragments. However, this line is not accessible in approaches based on static calculations like ours, and a certain criterion needs to be adopted to determine an effective scission line [6].

This work uses the following procedure to define the scission line. We perform HFB calculations by imposing constraints on the expectation values of axially symmetric quadrupole (q_{20}) and octupole (q_{30}) moments, which describe, respectively, the elongation and the reflection asymmetry of the nuclear shape. This results in a two-dimensional potential energy surface (PES). Scission configurations form a line on this surface and can be probed using the neck operator,

$$\hat{Q}_N = \exp\left(-\frac{(\hat{z} - z_N)^2}{a_N^2}\right), \quad (1)$$

where z_N denotes the position along the symmetry axis at which the local one-body density reaches its minimum between the fragments, and the dispersion a_N is chosen to be equal to one nucleon. The expectation value of the neck operator in the HFB state $|\Phi_q\rangle$,

$$q_N \equiv \langle \Phi_q | \hat{Q}_N | \Phi_q \rangle, \quad (2)$$

then estimates the number of nucleons in a thin slice of matter connecting the two fragments [57]. This number is always nonvanishing in our approach; for fully separated fragments with $q_N = 0$, the static variational principle would yield two fragments in their ground states.

Our previous studies identified the scission line with a q_N isoline [12,17,18]. Here, we use a different criterion: We

first convert an existing, regularly spaced PES characterized by mesh sizes Δq_{20} and Δq_{30} in the q_{20} and q_{30} directions into a unit-1 grid by scaling all coordinates as $(q_{20}, q_{30}) \rightarrow (q_{20}/\Delta q_{20}, q_{30}/\Delta q_{30})$. In this PES with dimensionless axes, we can define topological balls (that is, circles, since we work in two dimensions) of radius R . A point on the PES is considered to belong to the scission line if $x\%$ of its neighbors within the ball of radius R have $q_N \leq q_N^{\text{sciss}}$, where x , R , and q_N^{sciss} are free parameters. The benefit of such an approach is that it allows the scission line to contain configurations with varying q_N values, potentially better reflecting the local topology of the PES and, therefore, the physics of scission. The final outcome of this step is a set of $\tilde{M}$ HFB configurations on the (q_{20}, q_{30}) scission line, each having a different q_N value.

2. Extending the scission line

Unfortunately, low-dimensional PESs such as the two-dimensional (q_{20}, q_{30}) PES contain discontinuities that separate prescission and postscission configurations [58]. This issue becomes particularly troublesome when a static model is combined with a dynamical model, as in the time-dependent generator coordinate method, where the collective wave packet evolves continuously towards scission [59]. In such cases, discontinuities connect different regions of the PES in a nonphysical manner. The generation of continuous PESs can be attempted by increasing the number of collective degrees of freedom to three or more; however, this approach quickly becomes computationally prohibitive without guaranteeing full continuity. A simple alternative would be to keep the value of q_N^{sciss} relatively large, e.g., $q_N^{\text{sciss}} \geq 4$ [12]. Such an approach worked rather well when calculating fission yields with [18] or without [12] particle number projection. However, an accurate description of angular momentum distributions requires lower q_N values [33].

In this work, we therefore adopt a different approach by expanding the set of configurations obtained in Sec. II A 1 through additional constrained calculations with reduced neck values. Specifically, for each of $\tilde{M}$ configurations, we constrain $\hat{Q}_N$ to several values with $1 \leq q_N \leq 3$, using the step size $\Delta q_N = 0.5$. This range was shown to yield a good description of angular momentum distributions [33]. However, not all of the additional calculations will converge to a stable solution. Therefore, at each of the $\tilde{M}$ points (q_{20}, q_{30}) of the scission line, we obtain a total of $n(q_{20}, q_{30})$ configurations with $1 \leq q_N \leq 3$. The final outcome is thus a set of $M > \tilde{M}$ configurations that span the scission line of the two-dimensional (q_{20}, q_{30}) PES and cover the range $1 \leq q_N \leq 3$ of neck values.

3. Identifying fission fragments

Each of the M scission configurations have axially symmetric density profiles and are dumbbellshaped. Consequently, they can be readily divided into left ($z < z_N$) and right ($z > z_N$) FFs, where z_N locates the minimum of density profile between the fragments for each configuration. It is useful to introduce a cutoff function $\Theta^F(z)$ that enables us to keep only

the relevant spatial region for each FF. It is defined as

$$\Theta^F(z - z_N) = \begin{cases} \mathcal{H}(-(z - z_N)) & \text{if } F = l, \\ \mathcal{H}(z - z_N) & \text{if } F = r, \end{cases} \quad (3)$$

for the left ($F = l$) and right ($F = r$) fragments, and $\mathcal{H}(z)$ is the Heaviside step function [60]. Alternatively, the fragments can be denoted as heavy ($F = H$) or light ($F = L$). In the present model, we consider scission configurations with positive octupole moments, where the heavy (light) fragment is typically identified with the left (right) fragment.

B. Projections in scission configurations

Due to spontaneous symmetry breaking, HFB configurations are not eigenstates of particle number or angular momentum operators. Therefore, projection techniques have been used in nuclear structure studies for decades to restore broken symmetries and recover good quantum numbers [55,56,61]. More recently, these techniques were extended to nuclear reactions and fission, particularly in the context of restoring good particle number [17,18,62–65] and angular momentum [32,33,38]. We start by outlining the angular momentum and particle number projections separately, before combining the two methods to obtain full-fledged angular momentum and particle number distributions in each scission configuration.

1. Angular momentum projection

The operator projecting on good angular momentum J_F in FFs reads

$$\hat{P}_{00}^{J_F} = \frac{2J_F + 1}{2} \int_0^\pi d\beta \sin \beta d_{00}^{J_F}(\beta) \hat{R}_y^F(\beta), \quad (4)$$

where

$$\hat{R}_y^F(\beta) = \exp(-i\beta \hat{J}_y^F) \quad (5)$$

is the operator performing a spatial rotation by an Euler angle β , $d_{00}^{J_F}(\beta)$ are Wigner matrix elements [66], and $\hat{J}_y^F$ is the y component of the angular momentum operator in FFs. Note that the operator (4) assesses only $K_F = 0$ configurations, where K_F is the projection of the FF angular momentum on fission axis, and that axial symmetry is assumed. In addition, projection is performed only for the FFs, and any effect of the relative orbital angular momentum [34] is presently neglected. The operators $\hat{J}_y^F$ have a support within the spatial region $\mathcal{S}^F$ containing each fragment [64,65]. They are computed from the associated kernels

$$J_y^F(\mathbf{r}, \sigma) = \Theta^{F*}(z - z_N) J_y(\mathbf{r}, \sigma) \Theta^F(z - z_N), \quad (6)$$

where $J_y(\mathbf{r}, \sigma) = L_y(\mathbf{r}) + S_y(\sigma)$ corresponds to the usual angular momentum operator that depends on spatial coordinates $\mathbf{r} \equiv (r_\perp, \phi, z)$ and the spin coordinate σ , and $\Theta^F(z)$ is the cutoff function (3). Note that the expression (6) preserves hermiticity of the original operator. In practice, the center of mass of each fragment is located at $\mathbf{r}_{\text{CM}}^F = (0, 0, z_{\text{CM}}^F)$. Therefore, we transform $\mathbf{r} \rightarrow \mathbf{r} - \mathbf{r}_{\text{CM}}^F$ in Eq. (6) to determine the angular momentum with respect to the center of mass of each fragment.

2. Particle number projection

The operator projecting on good particle number N^τ reads

$$\hat{P}^{N^\tau} = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \exp(-i\varphi N^\tau) \hat{R}_{N^\tau}(\varphi). \quad (7)$$

Here, N^τ can represent the total number of neutrons ($N^\tau \equiv N$) or protons ($N^\tau \equiv Z$) in the compound nucleus, as well as the number of neutrons ($N^\tau \equiv N_F$) or protons ($N^\tau \equiv Z_F$) in FFs. The rotation operator for gauge angle φ is defined as

$$\hat{R}_{N^\tau}(\varphi) = \exp(i\varphi \hat{N}^\tau), \quad (8)$$

where $\hat{N}^\tau$ are the particle number operators associated with different N^τ , which are mutually commuting. In particular, the neutron number operators in FFs can be defined as

$$\hat{N}^F = \sum_{\mathbf{r}, \sigma} \Theta^{F*}(z - z_N) a^\dagger(\mathbf{r}, \sigma) a(\mathbf{r}, \sigma) \Theta^F(z - z_N), \quad (9)$$

where $\{a^\dagger(\mathbf{r}, \sigma), a(\mathbf{r}, \sigma)\}$ denote single-neutron creation and annihilation operators, $\Theta^F(z)$ is the cutoff function, and $\sum$ represents the integration over spatial coordinates $\mathbf{r}$ and summation over spins σ . An equivalent definition holds for the proton number operator in FFs, $\hat{Z}^F$. Using (7) we can define a quadruple projection operator

$$\hat{P}_{N_F, Z_F}^{N, Z} = \hat{P}_{N_F}^N \hat{P}_{Z_F}^Z \hat{P}^N \hat{P}^Z. \quad (10)$$

This expression accounts for the fact that both the compound nucleus and the FFs are characterized by distributions in neutron and proton numbers. Similarly, we can introduce a quadruple rotation operator,

$$\hat{R}_{N_F, Z_F}^{N, Z}(\varphi) = \hat{R}_{N_F}(\varphi_N) \hat{R}_{Z_F}(\varphi_Z) \hat{R}_N(\tilde{\varphi}_N) \hat{R}_Z(\tilde{\varphi}_Z), \quad (11)$$

where $\varphi \equiv \{\varphi_N, \varphi_Z, \tilde{\varphi}_N, \tilde{\varphi}_Z\}$.

3. Combined quintuple projection

In the next step, we combine the angular momentum projection in FFs with the particle number projection in both the compound nucleus and FFs. We consider FFs in a scission configuration $|\Phi_q^S\rangle$, where $\mathbf{q} \equiv \{q_{20}, q_{30}, q_N\}$. The quintuple projection yields the probability for a fragment $F = l, r$ to have angular momentum J_F , neutron number N_F , and proton number Z_F , and for the compound nucleus to have neutron number N and proton number Z , given the configuration $\mathbf{q}$, that is

$$\mathbb{P}_F(J_F, N_F, Z_F, N, Z | \mathbf{q}) = \langle \Phi_q^S | \hat{P}_{00}^{J_F} \hat{P}_{N_F, Z_F}^{N, Z} | \Phi_q^S \rangle, \quad (12)$$

with the projection operators defined in Eqs. (4), (7), and (10). Using the Fomenko discretization [67] on N_φ mesh points for each PNP operator, Eq. (12) can be expanded as

$$\begin{aligned} \mathbb{P}_F(J_F, N_F, Z_F, N, Z | \mathbf{q}) &= \frac{2J_F + 1}{2} \frac{1}{N_\varphi^4} \int_0^\pi d\beta \sin \beta d_{00}^{J_F}(\beta) \\ &\times \sum_{l_N=1}^{N_\varphi} \sum_{l_Z=1}^{N_\varphi} e^{-iN_F \varphi_{l_N}} e^{-iZ_F \varphi_{l_Z}} \\ &\times \sum_{k_N=1}^{N_\varphi} \sum_{k_Z=1}^{N_\varphi} e^{-iN \tilde{\varphi}_{k_N}} e^{-iZ \tilde{\varphi}_{k_Z}} \\ &\times \mathcal{N}_q^F(\beta, \varphi_{l_N}, \varphi_{l_Z}, \tilde{\varphi}_{k_N}, \tilde{\varphi}_{k_Z}). \end{aligned} \quad (13)$$

The norm overlap kernel reads

$$\mathcal{N}_q^F(\beta, \varphi) = \langle \Phi_q^S | \mathcal{R}_y^F(\beta) \mathcal{R}_{N_F, Z_F}^{N, Z}(\varphi) | \Phi_q^S \rangle, \quad (14)$$

and it is separable in isospin,

$$\mathcal{N}_q^F(\beta, \varphi) = \mathcal{N}_q^{F(\tau=n)}(\beta, \varphi_{l_N}, \tilde{\varphi}_{k_N}) \mathcal{N}_q^{F(\tau=p)}(\beta, \varphi_{l_Z}, \tilde{\varphi}_{k_Z}), \quad (15)$$

where $\tau = n(p)$ stands for neutrons (protons). Since the HFB configurations are expanded in a basis that is not closed under rotation, the technique of symmetry restoration in incomplete bases needs to be employed [68–70]. The norm overlap kernel for isospin τ reads

$$\mathcal{N}_q^{F(\tau)}(\beta, \varphi, \tilde{\varphi}) = \sqrt{\det[\mathcal{A}_q^{F(\tau)}(\beta, \varphi, \tilde{\varphi})] \det[\mathcal{R}^F(\beta, \varphi, \tilde{\varphi})]}, \quad (16)$$

with

$$\begin{aligned} \mathcal{A}_q^{F(\tau)}(\beta, \varphi, \tilde{\varphi}) &= U_q^{(\tau)T} [(\mathcal{R}^F(\beta, \varphi, \tilde{\varphi}))^T]^{-1} U_q^{(\tau)*} \\ &+ V_q^{(\tau)T} \mathcal{R}^F(\beta, \varphi, \tilde{\varphi}) V_q^{(\tau)*}. \end{aligned} \quad (17)$$

Here, $U_q^{(\tau)}$ and $V_q^{(\tau)}$ are the HFB spinors and $\mathcal{R}^F(\beta, \varphi, \tilde{\varphi})$ is the matrix of the total (triple) rotation operator with $[(\mathcal{R}^F)^T]^{-1} \neq (\mathcal{R}^F)^*$.

In practice, we are interested only in the component of the total wave function that has the correct number of nucleons in the compound system, $N = N_0$ and $Z = Z_0$. In other words, we want to calculate the conditional probability that a fragment $F = l, r$ has the angular momentum J_F , the neutron number N_F , and the proton number Z_F , given that the compound nucleus has the correct number of neutrons ($N = N_0$) and protons ($Z = Z_0$) and the system is in configuration $\mathbf{q}$. This probability reads

$$\mathbb{P}_F(J_F, N_F, Z_F | N_0, Z_0, \mathbf{q}) = \frac{\langle \Phi_q^S | \hat{P}_{00}^{J_F} \hat{P}_{N_F, Z_F}^{N_0, Z_0} | \Phi_q^S \rangle}{\langle \Phi_q^S | \hat{P}^{N_0, Z_0} | \Phi_q^S \rangle}, \quad (18)$$

where $\hat{P}^{N_0}$ and $\hat{P}^{Z_0}$ are the single projection operators; cf. Eq. (7).

For each scission configuration $\mathbf{q}$ and each fragment $F = l, r$, the distribution (18) is normalized to 1,

$$\sum_{J_F, N_F, Z_F} \mathbb{P}_F(J_F, N_F, Z_F | N_0, Z_0, \mathbf{q}) = 1, \quad \forall \mathbf{q}. \quad (19)$$

Marginalizing over nucleon numbers gives the angular momentum distribution for each scission configuration,

$$\mathbb{P}_F(J_F | N_0, Z_0, \mathbf{q}) = \sum_{N_F, Z_F} \mathbb{P}_F(J_F, N_F, Z_F | N_0, Z_0, \mathbf{q}). \quad (20)$$

Similarly, marginalizing over angular momentum gives the distribution in nucleon numbers for each scission configuration,

$$\mathbb{P}_F(N_F, Z_F | N_0, Z_0, \mathbf{q}) = \sum_{J_F} \mathbb{P}_F(J_F, N_F, Z_F | N_0, Z_0, \mathbf{q}). \quad (21)$$

For any given J_F, N_F, Z_F , there can be several scission configurations $\mathbf{q}$ for which (18) is nonzero. In other words, to obtain the full probability distribution that the fission fragment has angular momentum J_F , and particle numbers N_F and Z_F ,

we must sum the contributions from all scission configurations. In the next step, we recall how to determine population probabilities of different scission configurations.

C. Dynamical population of scission configurations

In this work, we model the dynamical population of scission configurations with the time-dependent generator coordinate method (TDGCM) under the Gaussian overlap approximation (GOA). In the following, we only recall the basic elements of the method; see, e.g., [59,71] for a more detailed presentation of the theory.

1. Dynamical equation of motion

At any given time t , the wave function of a fissioning nucleus is given by the linear combination

$$|\Psi(t)\rangle = \int d\mathbf{q} f_{\mathbf{q}}(t) |\Phi_{\mathbf{q}}\rangle, \quad (22)$$

where $f_{\mathbf{q}}(t)$ is a complex-valued mixing function and $|\Phi_{\mathbf{q}}\rangle$ are constrained HFB states. In our case, $\mathbf{q} \equiv \{q_{20}, q_{30}\}$. Applying the time-dependent variational principle with the ansatz (22) gives the Hill-Wheeler-Griffin non-local equation of motion. This equation can be reduced into a local Schrödinger-like equation of motion with the GOA,

$$i\hbar \frac{\partial g_{\mathbf{q}}(t)}{\partial t} = [H_{\mathbf{q}}^{\text{coll}} + iA_{\mathbf{q}}^{\text{coll}}]g_{\mathbf{q}}(t), \quad (23)$$

where the complex-valued functions $g_{\mathbf{q}}(t)$ are related to $f_{\mathbf{q}}(t)$ and contain all the information about the nuclear dynamics, while $A_{\mathbf{q}}^{\text{coll}}$ is a real-valued field added to avoid reflection on the boundaries of the deformation domain [72]. The collective Hamiltonian $H_{\mathbf{q}}^{\text{coll}}$ is a linear operator that acts on $g_{\mathbf{q}}(t)$. It depends on the collective inertia tensor $B_{\mu\nu}(\mathbf{q})$, the potential energy $V(\mathbf{q})$, the metric $\gamma(\mathbf{q})$, and a zero-point energy correction $\varepsilon(\mathbf{q})$. All these quantities can be calculated from the knowledge of the energy density functional and the generator states $|\Phi_{\mathbf{q}}\rangle$ [6]. In practice, Eq. (23) is solved using the FELIX solver [72] and the generator states are determined with the HFBTHO solver [73].

2. Initial conditions

To solve Eq. (23), we first need to define an initial collective wave packet, representing the compound nucleus just after the absorption of the incident neutron. Here, we follow the recipe of [12,74] by calculating the set of quasibound states $g_{\mathbf{q}}^k$,

$$\mathcal{H}_{\mathbf{q}}^{\text{coll}} g_{\mathbf{q}}^k = E_k g_{\mathbf{q}}^k, \quad (24)$$

where $\mathcal{H}_{\mathbf{q}}^{\text{coll}}$ is obtained by replacing the potential $V(\mathbf{q})$ in the original collective Hamiltonian $H_{\mathbf{q}}^{\text{coll}}$ with a potential extrapolated from the inner potential barrier using a quadratic form. The initial state can then be built as a Gaussian superposition of quasibound states,

$$g_{\mathbf{q}}(t=0) = \sum_{k=1}^{n_{\text{max}}} \exp\left(-\frac{(E_k - \tilde{E})^2}{2\sigma^2}\right) g_{\mathbf{q}}^k, \quad (25)$$

where σ is the parameter controlling the energy spread of the wave packet. Given σ , the parameter $\tilde{E}$ is iteratively determined so that the binding energy of the initial wave packet is equal to some E_0 . Ideally, this energy can be determined from the one-neutron separation energy S_n and the energy of the incoming neutron E_n : $E_0 = S_n + E_n$. However, in the actinides considered here, the one-neutron separation energy is approximately equal to the fission barrier height E_B . Thus, we use the approximate relation $E_0 \approx E_B + E_n$ to define the energy of the initial state relative to the fission barrier height rather than the one-neutron separation energy. This approach allows us to partially simulate the effect of different incident neutron energies but it does not account for modifications of deformation properties with excitation energy. Extension of the formalism that take such modifications into account have been proposed in [19,22,75,76]. To avoid misunderstandings, we will be referring to E_n as an equivalent incident neutron energy.

3. Probability of populating scission configurations

As time passes, the collective wave packet progressively spreads and finally escapes the simulation domain, exiting through the scission line. In our two-dimensional calculation, the initial scission line is determined using the criterion outlined in Sec. II A and can be parametrized with a single coordinate ξ , i.e., $\mathbf{q}(\xi)$, with $\mathbf{q} = \{q_{20}, q_{30}\}$. Analogously, the modified set of scission configurations can be parametrized with η , i.e., $\mathbf{q}(\eta)$, with $\mathbf{q} = \{q_{20}, q_{30}, q_N\}$. The population of scission configurations is obtained by integrating the flux density $\phi(\xi, t)$ [12,18]. In particular, we assume that the probability of exiting through the point $\mathbf{q}(\xi)$ is proportional to the time-integrated flux density, defined as [18]

$$F(\xi) = \lim_{t \rightarrow \infty} \int_{\tau=0}^{\tau=t} d\tau \phi(\xi, \tau). \quad (26)$$

In practice, each point $\mathbf{q}(\xi)$ is associated with a probability $F(\mathbf{q}(\xi))$ such that the total probability is normalized to one. Here, we make an additional assumption that, for a fixed (q_{20}, q_{30}) , the probability $F(\mathbf{q}(\xi))$ is partitioned among the $n(q_{20}, q_{30})$ configurations obtained by the constrained reduction of the neck size value. To limit the number of parameters, we assume this partition is uniform across different scission configurations at $\mathbf{q}(\xi)$. This results in the probability of populating each scission configuration, $F(\mathbf{q}(\eta))$, which is normalized to 1,

$$\int d\eta F(\mathbf{q}(\eta)) = 1. \quad (27)$$

D. Angular momentum, mass, and charge distributions in FFs

In Secs. II B and II C we calculated the angular momentum and particle number distributions in scission configurations [cf. Eq. (18)] and the population probability for each scission configuration, respectively. In this section, we combine the two results to obtain the angular momentum and particle number distributions in actual fission fragments. We demonstrate how the same framework can be used to calculate angular

momentum distributions in FFs and preneutron mass and charge yields.

1. Distributions in fragments

Folding the results of the previous two sections gives

$$\mathbb{P}_F(J_F, N_F, Z_F | N_0, Z_0) = \int d\eta F(\mathbf{q}(\eta)) \mathbb{P}_F(J_F, N_F, Z_F | N_0, Z_0, \mathbf{q}(\eta)), \quad (28)$$

which is the probability for a fragment $F = l, r$ to have an angular momentum J_F , and numbers of neutrons N_F and protons Z_F , given that the compound nucleus has the correct number of neutrons and protons. Due to Eqs. (19) and (27), this distribution is also normalized to 1,

$$\sum_{J_F, N_F, Z_F} \mathbb{P}_F(J_F, N_F, Z_F | N_0, Z_0) = 1. \quad (29)$$

The final distribution is obtained by summing the distributions for $F = l, r$,

$$\mathbb{P}(J_F, N_F, Z_F | N_0, Z_0) = \mathbb{P}_l(J_F, N_F, Z_F | N_0, Z_0) + \mathbb{P}_r(J_F, N_F, Z_F | N_0, Z_0), \quad (30)$$

and it is normalized to 2.

2. Angular momentum distribution in FFs

Starting from the full distribution (30), it is straightforward to determine the angular momentum distribution in a FF with fixed $N_F = N_F^0$ and $Z_F = Z_F^0$,

$$\mathbb{P}(J_F | N_F^0, Z_F^0, N_0, Z_0) = \frac{\mathbb{P}(J_F, N_F^0, Z_F^0 | N_0, Z_0)}{\sum_{J_F} \mathbb{P}(J_F, N_F^0, Z_F^0 | N_0, Z_0)}, \quad (31)$$

Note that, in principle, Eq. (31) enables us to access the fragmentations that have a non-negligible component in at least one scission configuration $|\Phi_q^S\rangle$ with a non-negligible population probability $F(\mathbf{q}(\eta))$. In practice, as will be demonstrated, we are able to account for a very wide range of FF masses and charges.

From the distribution (31), we can estimate the average magnitude of angular momentum in the FF [32,33],

$$\bar{J}_F(\bar{J}_F + 1) = \sum_{J_F} J_F(J_F + 1) \mathbb{P}(J_F), \quad (32)$$

where $\mathbb{P}(J_F)$ is short for $\mathbb{P}(J_F | N_F^0, Z_F^0, N_0, Z_0)$.

3. Preneutron mass and charge yields

Starting from Eq. (30), marginalization over angular momentum J_F gives the distribution in neutron and proton numbers in FFs,

$$\mathbb{P}(N_F, Z_F | N_0, Z_0) = \sum_{J_F} \mathbb{P}(J_F, N_F, Z_F | N_0, Z_0), \quad (33)$$

i.e., the preneutron fission yields. This work considers only binary fission. As a consequence, we normalize the fission yields to 2. Introducing the total number of particles in a fragment $A_F = N_F + Z_F$, we can easily relate (33) to the

two-dimensional (2D) isotopic yields, $Y(A_F, Z_F)$. Furthermore, the distribution in one isospin can be obtained through marginalization over the complementary isospin,

$$\mathbb{P}(N_F | N_0, Z_0) = \sum_{Z_F} \mathbb{P}(N_F, Z_F | N_0, Z_0), \quad (34a)$$

$$\mathbb{P}(Z_F | N_0, Z_0) = \sum_{N_F} \mathbb{P}(N_F, Z_F | N_0, Z_0). \quad (34b)$$

Equivalently, the mass distribution can be readily evaluated as

$$\mathbb{P}(A_F | N_0, Z_0) = \sum_{N_F, Z_F} \mathbb{P}(N_F, Z_F | N_0, Z_0) \delta_{N_F + Z_F, A_F}. \quad (35)$$

This quantity corresponds to the calculated preneutron mass yield, $Y(A_F)$.

III. RESULTS

In this section, the theoretical framework is applied to the neutron-induced fission of ^{235}U and ^{239}Pu . In Sec. III A we discuss the generation and properties of scission configurations in the compound systems ^{236}U and ^{240}Pu . In Sec. III B, we examine the predictions of the model for primary FF mass yields and 2D isotopic yields. Finally, Sec. III C contains a comprehensive analysis of angular momentum distributions in FFs, including the range of obtained FFs, the role of shell structure in inducing the sawtooth pattern, the correlation between FF angular momentum and deformation, the isobaric dependence of AM distributions, and the correlation in magnitude of angular momentum between the FF partners.

A. Properties of scission configurations

1. Generation and average properties of scission configurations

The potential energy surfaces of ^{236}U and ^{240}Pu are generated by performing constrained HFB calculations and are shown in panels (a) and (b) of Fig. 1. The SkM* parametrization [77] of the Skyrme energy density functional is employed in the particle-hole channel, while pairing is modeled with a mixed volume-surface contact force [78], with the pairing strength parametrization proposed in [79]. The calculations are performed with the HFBTHOSolver [73], in a deformed harmonic oscillator basis of 1200 states from up to 30 major shells. In the pairing channel, the usual cutoff in the quasiparticle space is set at $E_{\text{cut}} = 60$ MeV.

Initial scission configurations in the (q_{20}, q_{30}) plane are generated according to the procedure outlined in Sec. II A by setting the values of $x = 90$, $q_N^{\text{sciss}} = 0.5$, and $R = 10$. This means that a point in the PES is considered as belonging to the scission line if, in the associated PES with dimensionless axes, 90% of its neighbors within a ball of radius 10 have $q_N \leq 0.5$. The obtained scission lines are then extended by constraining the neck values to $q_N \in [1.0, 3.0]$ with $\Delta q_N = 0.5$. This gives 1773 configurations in ^{236}U and 2344 configurations in ^{240}Pu . To decrease the computational cost of subsequent projected calculations, we further reduce the size of these sets. In particular, we use the fact that each configuration is characterized by the average FF mass $\langle A_F \rangle$ and charge $\langle Z_F \rangle$. These values can be calculated by integrating the one-body total density $\rho(\mathbf{r})$

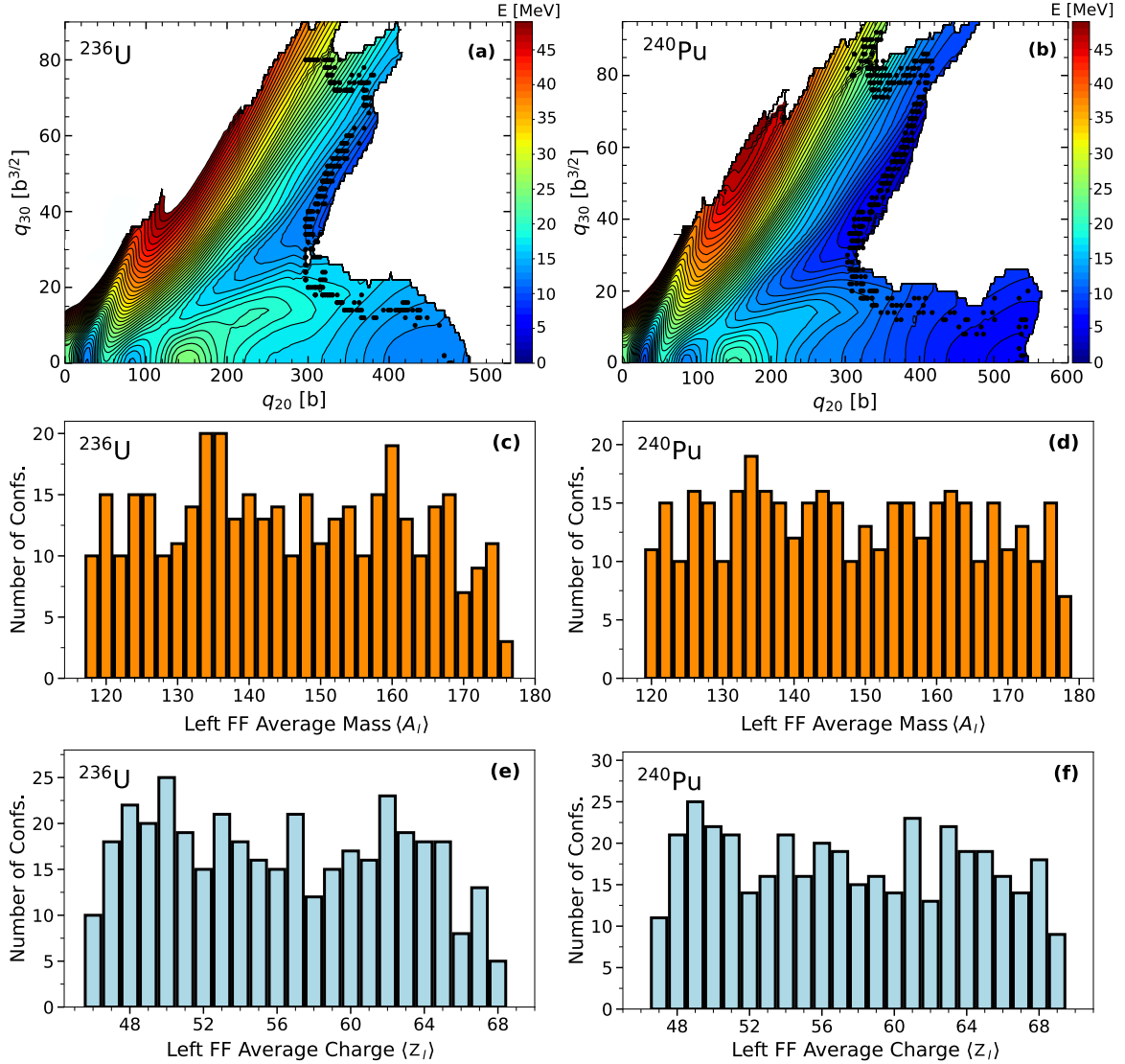


FIG. 1. Properties of $N_{\text{conf}} = 384$ scission configurations in ^{236}U (left column) and $N_{\text{conf}} = 404$ scission configurations in ^{240}Pu (right column). Panels (a) and (b) show each configuration as a black point in the (q_{20}, q_{30}) PES. Note that there are typically several neck values q_N per each (q_{20}, q_{30}) value. Panels (c) and (d) show the distributions in left FF average mass $\langle A_l \rangle$, Eq. (36a), with a bin width of 2. Panels (e) and (f) show the distributions in left FF average charge $\langle Z_l \rangle$, Eq. (36b), with a bin width of 1. The relevant ranges of (q_{20}, q_{30}) , $\langle A_l \rangle$, and $\langle Z_l \rangle$ in both nuclei are properly covered by the chosen sets.

and the one-body proton density $\rho_p(\mathbf{r})$, respectively, over the space corresponding to each FF,

$$\langle A_F \rangle = \int d^3\mathbf{r} \rho(\mathbf{r}) \Theta^F(z - z_N), \quad (36a)$$

$$\langle Z_F \rangle = \int d^3\mathbf{r} \rho_p(\mathbf{r}) \Theta^F(z - z_N), \quad (36b)$$

where $\langle A_l \rangle + \langle A_r \rangle = A_0$ and $\langle Z_l \rangle + \langle Z_r \rangle = Z_0$, where A_0 (Z_0) is the mass (charge) of the compound system. The final sets are determined through the following filtering procedure:

- (1) We define two-dimensional bins $(\langle A_l \rangle, \langle Z_l \rangle)$ of width of 1 nucleon along each dimension.
- (2) We parse all configurations with $\langle A_r \rangle \geq 60$ for ^{236}U and $\langle A_r \rangle \geq 62$ for ^{240}Pu and assign them to the relevant

bin; if this bin contains less than 5 configurations, the current one is retained, otherwise it is discarded.

- (3) To minimize bias and ensure balanced coverage in the (q_{20}, q_{30}) plane, the order of processing configurations is randomized.

This procedure yields 384 scission configurations in ^{236}U and 404 scission configurations in ^{240}Pu . As can be seen in panels (a) and (b) of Fig. 1, the chosen sets cover a broad range of (q_{20}, q_{30}) deformations and span most of the physically relevant scission line. Most importantly, the distributions in the left FF mass [panels (c) and (d)] and charge [panels (e) and (f)] also cover the relevant ranges comprehensively and evenly. Of course, the same conclusion applies to the right FF distributions. In addition, the neck values q_N are also quite evenly distributed over the interval $[1.0, 3.0]$. For ^{236}U , there are 69 con-

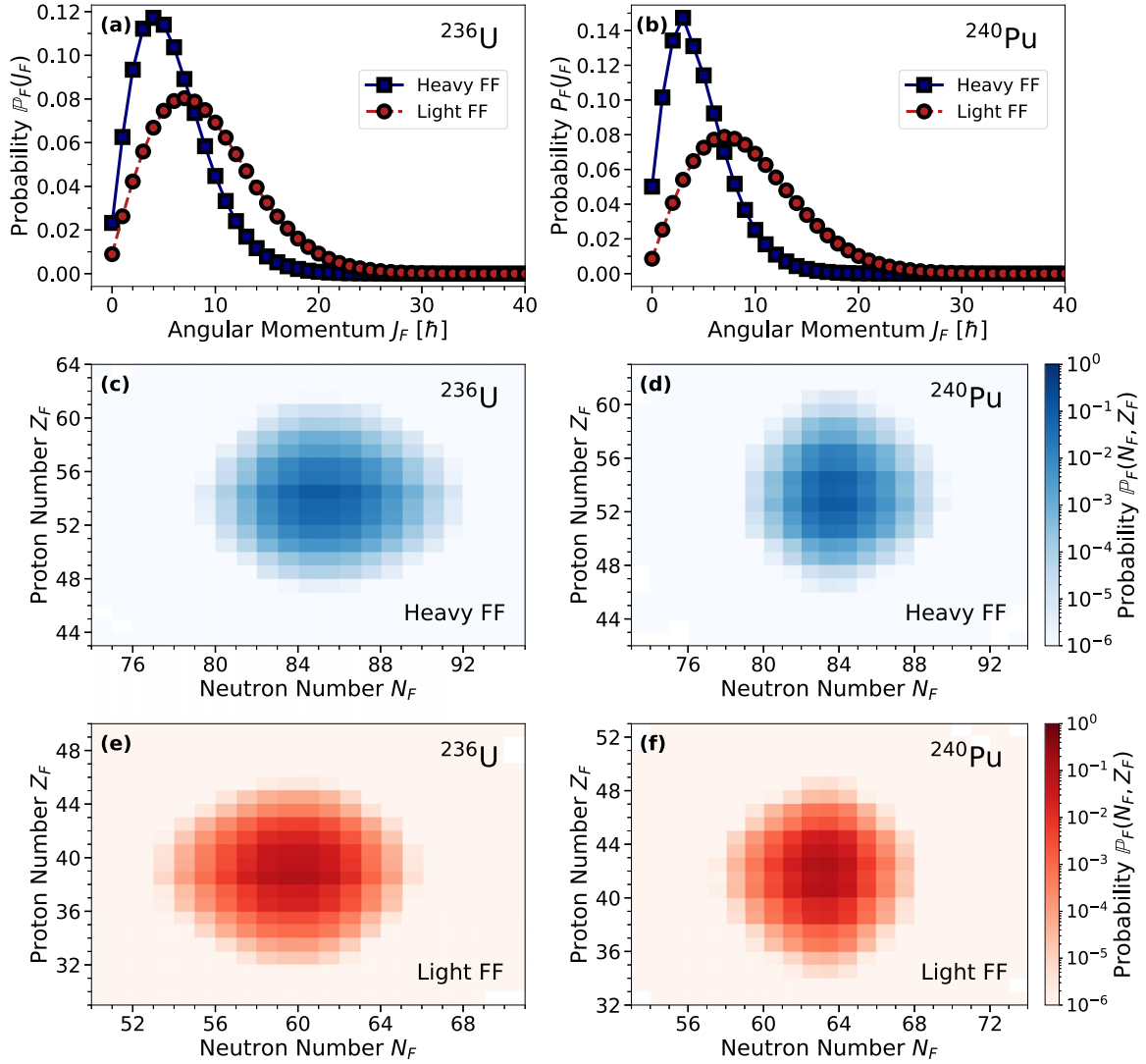


FIG. 2. Quantum number distributions in two scission configurations of ^{236}U (left column) and ^{240}Pu (right column) near the most likely fragmentation; see text for more details. Panels (a) and (b) show the angular momentum distributions in both FFs, obtained by marginalizing the full distribution over nucleon numbers [Eq. (20)]. Panels (c) and (d) show the neutron and proton number distributions in heavy FFs, obtained by marginalizing the full distribution over angular momentum [Eq. (21)]. Panels (e) and (f) show the same for light FFs. Note the logarithmic scale on panels (c)–(f).

figurations with $q_N = 1.0$, 71 with $q_N = 1.5$, 60 with $q_N = 2.0$, 72 with $q_N = 2.5$, and 112 with $q_N = 3.0$. For ^{240}Pu , there are 75 configurations with $q_N = 1.0$, 78 with $q_N = 1.5$, 80 with $q_N = 2.0$, 79 with $q_N = 2.5$, and 92 with $q_N = 3.0$.

2. Illustrative quantum number distributions

In Fig. 1, scission configurations were associated with the corresponding average mass and charge numbers in FFs. However, each configuration is in fact characterized by a full distribution $\mathbb{P}_F(J_F, N_F, Z_F|N_0, Z_0, \mathbf{q})$ in FF angular momentum J_F , neutron number N_F , and proton number Z_F , for both FFs. These distributions can be extracted using the projection techniques presented in Sec. II B. As an illustrative example, in each nucleus, we consider the following configuration, which is located near the maximum of the TDGCM + GOA population probability: $(q_{20}, q_{30}, q_N) = (306 \text{ b}, 40 \text{ b}^{3/2}, 3.0)$

for ^{236}U and $(q_{20}, q_{30}, q_N) = (321 \text{ b}, 36 \text{ b}^{3/2}, 2.5)$ for ^{240}Pu . The corresponding average mass and charge numbers of the left (heavy) FF are $(\langle A_H \rangle, \langle Z_H \rangle) = (138.3, 53.5)$ for ^{236}U , and $(\langle A_H \rangle, \langle Z_H \rangle) = (136.1, 52.7)$ for ^{240}Pu . The AMP is performed with $N_\beta = 64$ rotational angles and all PNPs with $N_\varphi = 31$ gauge angles. This choice of parameters ensures excellent convergence of the projected calculations and is used for all calculations in the paper.

In the upper two panels of Fig. 2 we show the angular momentum distributions in both FFs for the two configurations, obtained by marginalizing the full distributions over nucleon numbers according to Eq. (20). In agreement with previous studies [32,33], the light FF near the most likely fragmentation carries more angular momentum than its heavy counterpart. For ^{236}U , we obtain the average AM values $\bar{J}_H = 6.8\hbar$ and $\bar{J}_L = 10.2\hbar$. These values are somewhat higher than those

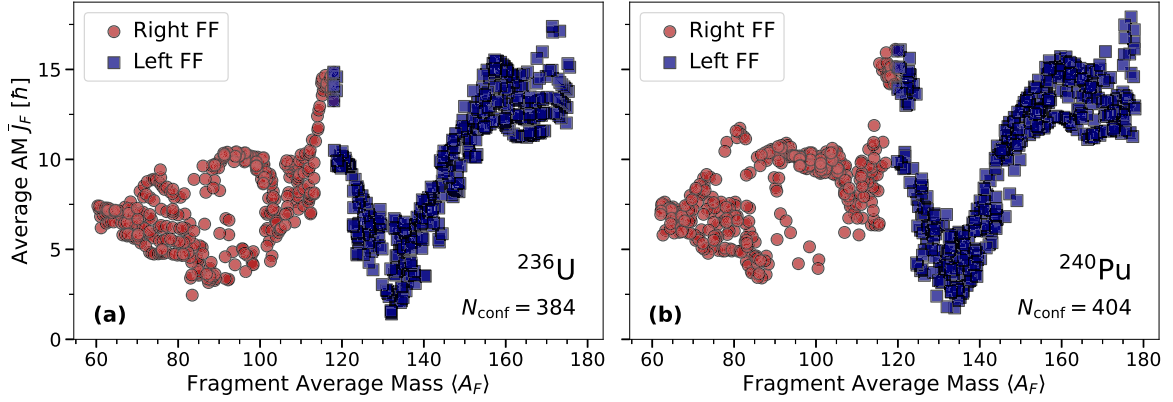


FIG. 3. Average angular momentum magnitude [Eq. (32)] of left FFs (blue squares) and right FFs (red circles) in all scission configurations for ^{236}U [panel (a)] and ^{240}Pu [panel (b)], as a function of the average FF mass [Eq. (36a)]. A sawtooth pattern is apparent in both nuclei.

obtained with time-dependent HFB (TDHFB) using the same Skyrme functional, $\bar{J}_H = 6.3(0.7)\hbar$ and $\bar{J}_L = 8.6(0.6)\hbar$ [32]. However, note that reducing q_N typically lowers angular momentum; e.g., the $(q_{20}, q_{30}, q_N) = (312 \text{ b}, 40 \text{ b}^{3/2}, 2.0)$ configuration, which is the second most likely populated in our simulation, has $\bar{J}_H = 5.1\hbar$ and $\bar{J}_L = 9.9\hbar$. Furthermore, for ^{240}Pu we obtain $\bar{J}_H = 5.4\hbar$ and $\bar{J}_L = 10.4\hbar$, which is comparable to $\bar{J}_H = 5.8(0.5)\hbar$ and $\bar{J}_L = 9.4(0.4)\hbar$ obtained with TDHFB [32].

In the middle (lower) panel of Fig. 2 we show the combined distribution in neutron and proton number for the heavy (light) FF, obtained by marginalizing the full distribution over angular momentum according to Eq. (21). For both nuclei, the distributions are centered close to the average mass and charge numbers. In ^{236}U (left column), the maxima are found at $(A_H^{\text{max}}, Z_H^{\text{max}}) = (138, 54)$ and $(A_L^{\text{max}}, Z_L^{\text{max}}) = (98, 38)$. In ^{240}Pu (right column) they are found at $(A_H^{\text{max}}, Z_H^{\text{max}}) = (135, 52)$ and $(A_L^{\text{max}}, Z_L^{\text{max}}) = (105, 42)$. However, the distributions are generally rather wide and various (N_F, Z_F) components contribute to the total distribution.

3. Mass dependence of the average angular momentum

Using Eq. (20), we can calculate the average angular momentum of the full set of scission configurations as a function of their average mass $\langle A_F \rangle$. In Fig. 3 we show the results for ^{236}U and ^{240}Pu , both exhibiting a clear sawtooth pattern. This finding is consistent with our previous study in ^{240}Pu [33], which combined the AMP in FFs with a simple interpolation to obtain angular momentum distributions in 24 fragmentations with integer particle numbers. It is also consistent with measurements by Wilson *et al.* [31], which have established a universal sawtooth pattern for average AM of FFs after the prompt emissions. A more detailed analysis of the sawtooth pattern for FFs with integer nucleon numbers is given in Sec. III C 2.

B. Primary fission fragment yields

Calculations of fission fragment distributions were performed with the FELIX solver [72]. Like the calculations of Ref. [18], the collective dynamics with FELIX is characterized by a time step of $\Delta t = 2 \times 10^{-4}$ zs and is simulated up to

a time $t_f = 20$ zs. The initial wave packet (25) is characterized by an energy spread $\sigma = 0.5$ MeV and a number of states $n_{\text{max}} = 100$. The absorption field A_q^{coll} in Eq. (23) is expressed by Eq. (28) of [72] with rate $r = 8$ MeV and width $w = 10$. The mesh size is $\Delta q_{20} = 2 \text{ b}$ and $\Delta q_{30} = 1 \text{ b}^{3/2}$. The collective inertia is computed at the GCM approximation and the GCM zero-point energy correction is included in the potential energy. We used Gauss-Legendre quadratures for the integration of the H matrix and Gauss-Lobatto quadratures for the integration of the M matrix; see [72] for details. The state-of-the-art microscopic description of fission yields includes combining the PNP in FFs with the adiabatic TDGCM + GOA framework [7,18]. Consequently, a model that combines the PNP and AMP in FFs with TDGCM should, in principle, predict the yields with similar accuracy. However, the choice of q_N range in scission configurations turns out to have a substantial impact on the quality of results. In this section, we briefly discuss the predictions of the present model for primary FF mass yields and isotopic 2D yields in ^{236}U and ^{240}Pu , and outline the main limitations.

In Fig. 4 we show (green squares) the primary FF mass distribution in ^{236}U , calculated from Eq. (35) and using the full set of 384 scission configurations with $q_N \in [1, 3]$. An equivalent quantity was calculated in [18], using the PNP + TDGCM model with different parameters, including a set of configurations with fixed $q_N = 4$. Therein, it was demonstrated that PNP smooths out the odd-even staggering effects which characterize yields obtained in the HFB + TDGCM model [12]. On the other hand, despite employing PNP, the results shown in Fig. 4 still exhibit a clear staggering. The equivalent results for ^{240}Pu are smoother, but nevertheless with some staggering effects.

The root cause of this can, to a large extent, be traced back to the choice of scission configurations. In fact, in [18] it was also shown that considering small q_N values induces odd-even staggering effects, especially in the charge yields. Indeed, if we consider only the 112 configurations from the full set with $q_N = 3$, the resulting yields (grey triangles in Fig. 4) are significantly smoother and closer to the predictions of [18]. Unfortunately, a proper description of angular momentum in FFs requires considering neck values smaller than $q_N = 4$. Eventually, this should be achieved by considering either a small- q_N scission line defined on a discontinuity-free energy

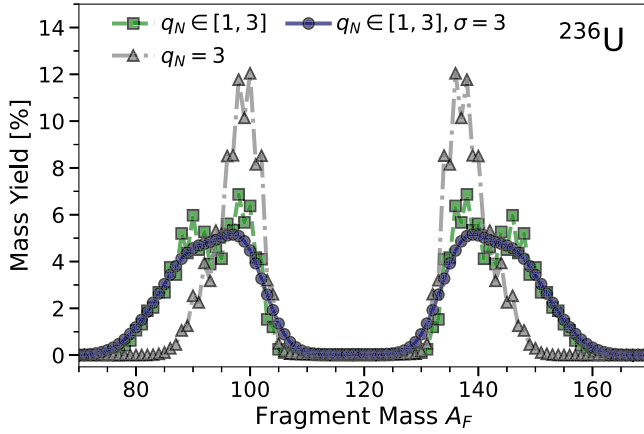


FIG. 4. Primary FF mass distribution (normalized to 200) in ^{236}U , for three different cases. The distribution obtained from the full set of scission configurations with $q_N \in [1, 3]$, as described in Sec. III A 1, is shown with green squares. The distribution obtained using only the $q_N = 3$ configurations is shown with grey triangles. The distribution obtained from the full set of scission configurations with $q_N \in [1, 3]$ by additionally applying a Gaussian folding with $\sigma = 3$ is shown with blue circles.

hypersurface, or by employing a model such as TDHFB that does not require using a somewhat ambiguous concept of the scission line. In the meantime, to account for the theoretical dispersion induced by considering an arbitrary range of q_N , the yields calculated with the present model should be smoothed with a Gaussian. Furthermore, when comparing the model to experiment, an equivalent smoothing should be used to account for the fact that the extraction of pre-neutron yields from measured yields is model dependent, typically leading to uncertainties of about 3–4 mass units. A single Gaussian folding can be performed to account for both these effects; such a smoothed distribution is shown with blue circles in Fig. 4.

In Fig. 5, we show the calculated mass distribution of primary FFs in ^{236}U (left) and ^{240}Pu (right), in comparison to experimental data [80–88]. The distributions are calculated at $E_n = 1$ MeV and additionally folded with a $\sigma = 3$ Gaussian, as explained above. In ^{236}U , the position of the peaks of the distribution is reproduced, even if the absolute yield is underestimated. The proportion of more symmetric

configurations is somewhat underestimated, while the highly asymmetric configurations are overestimated. In ^{240}Pu , the peaks are slightly shifted to smaller A_H , but the absolute yield is rather close to experiment. Furthermore, the antisymmetric configurations are generally underestimated in ^{240}Pu , while the symmetric configurations are populated with larger probability than experimentally observed. Note that the minor bump at $A_H \approx 160$ is not physical and likely stems from a part of the flux artificially exiting and reentering the simulation domain within the TDGCM + GOA calculation.

For completeness, in Fig. 6 we show the full (raw) isotopic 2D yields, cf. Eq. (33), in both ^{236}U and ^{240}Pu , at equivalent incident neutron energies of $E_n = 1, 2, 5, 10$ MeV. In ^{236}U , the symmetric configurations are increasingly more populated with increasing E_n , as expected. On the other hand, the isotopic yields of ^{240}Pu are somewhat less sensitive to E_n in the present calculations.

Overall, the model provides reasonable predictions for primary FF yields. Their quality could be enhanced by including a more refined treatment of scission, as well as by improving the TDGCM + GOA description of nuclear dynamics (continuity of PES, complete absorption at the boundary). However, these improvements are beyond the scope of this paper.

C. Angular momentum distributions in FFs

1. Mass and charge range of FFs

The present model is able to account for angular momentum distributions in the full range of FF masses and charges. For ^{236}U , at $E_n = 1$ MeV we obtain a total of 1494 fragments: 381 even-even, 360 odd-odd, and 753 odd-even or even-odd fragments. This number depends weakly on the equivalent neutron incident energy; for example, at $E_n = 2, 5, 10$ MeV we obtain 1495, 1543, and 1619 fragments, respectively. Similarly, for ^{240}Pu at $E_n = 1$ MeV we obtain a total of 1611 fragments: 412 even-even, 401 odd-odd, and 798 odd-even or even-odd fragments. The corresponding numbers for $E_n = 2, 5, 10$ MeV are 1601, 1635, 1695, respectively.

It is worth recalling that the model, by construction, provides the $\mathbb{P}(J_F)$ probabilities for integer J_F . This means that the distributions obtained for even-even and odd-odd FFs, which have integer angular momenta, can be readily used. On the other hand, the results for even-odd or odd-even FFs may

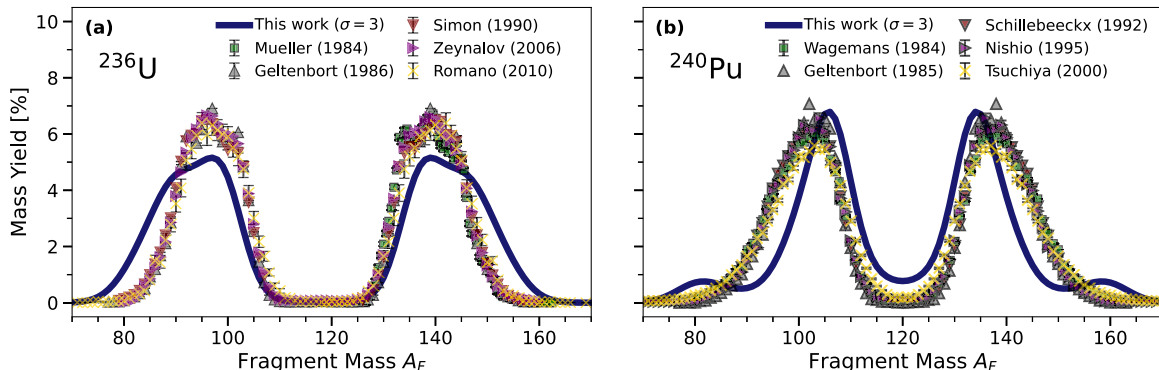


FIG. 5. Primary FF mass distribution (normalized to 200) in ^{236}U (left) and ^{240}Pu (right). The predictions of the model, calculated at $E_n = 1$ MeV, are compared to experimental data [80–88].

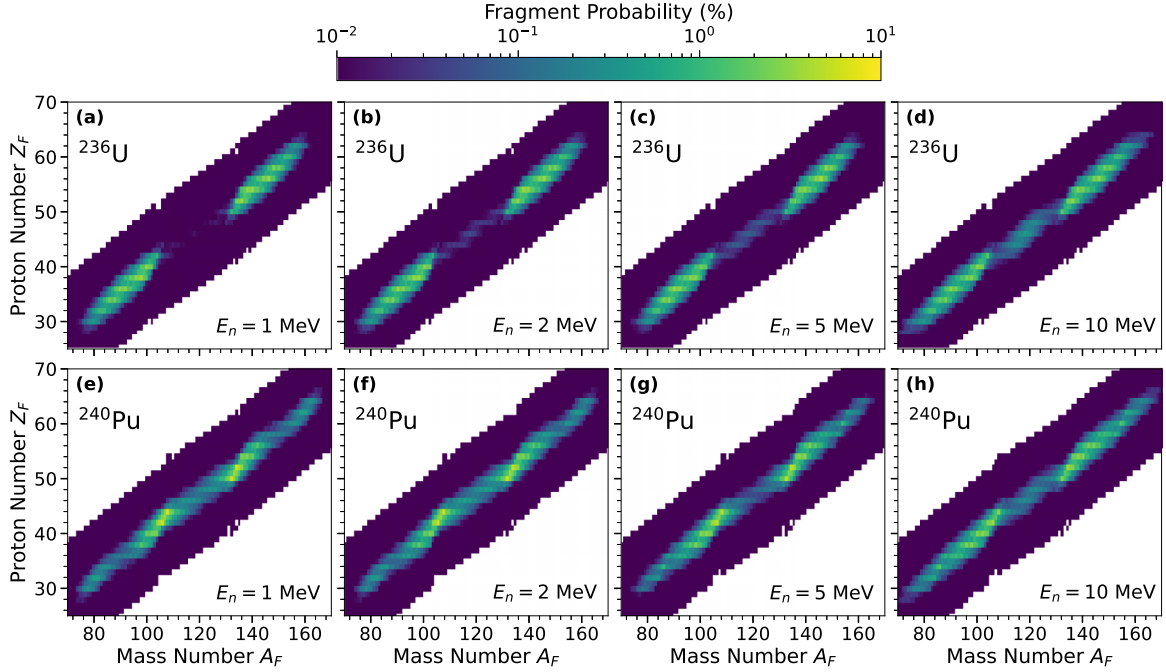


FIG. 6. Isotopic yields (normalized to 200) in ^{236}U (upper panel) and ^{240}Pu (lower panel), calculated at equivalent incident neutron energies $E_n = 1, 2, 5, 10$ MeV. Note the logarithmic scale on all panels.

be used in a more phenomenological manner, by interpolating the obtained distributions to half-integer J_F values. In the remainder of the paper, however, we will generally be focusing on the even-even FFs.

2. Sawtooth pattern and shell effects

The high-precision measurements at ALTO have established a sawtooth dependence of the average angular momentum of FFs on their mass, for both spontaneous and neutron-induced fission [31]. This feature was experimentally inferred for FFs *after* the emission of prompt particles. On the other hand, microscopic theory can only model properties of primary FFs, that is, *before* any emission takes place. Nevertheless, it is interesting to examine whether such models predict the occurrence of a sawtooth pattern. The robustness of this pattern with respect to prompt emissions can then be examined using statistical reaction models [44,45].

In Ref. [33], a microscopic model based on AMP in FFs predicted mass dependence of the average AM that is consistent with a sawtooth pattern. However, the model did not consider PNP or dynamic population of scission configurations, and was therefore able to approximately assess only 24 fragmentations. In Fig. 7 we show the average AM of *all* even-even FFs as a function of their mass, for both ^{236}U and ^{240}Pu . A clear sawtooth pattern is present in both nuclei at $E_n = 1$ MeV. Moreover, within our model, the pattern persists up to $E_n = 10$ MeV. We note that including FFs with odd number of neutrons and/or protons does not affect the pattern. To the best of our knowledge, this is the first unequivocal evidence of a sawtooth pattern in primary FFs, for two reactions, based on microscopic theory.

To demonstrate the role of shell structure in the formation of a sawtooth pattern, in Fig. 8 we show the average angular momentum of heavy FFs as a function of their neutron number for several isotopic chains in ^{236}U . As can be seen in the left panel, the isotopes of Sn ($Z = 50$), Te ($Z = 52$), Xe ($Z = 54$), and Ba ($Z = 56$) all exhibit a pronounced minimum at $N_F = 82$ shell closure. The absolute minimum, as expected, is found for the doubly magic ^{132}Sn . The particular value at 1 MeV is $\bar{J}_F \approx 2.2\hbar$, in decent agreement with recent FIFRELIN results obtained by combining experimental data with statistical modeling [89]. Since the present model only partially captures the effect of varying incident neutron energy, the increase with E_n is rather modest compared to FIFRELIN estimates: $\bar{J}_F \approx 2.3\hbar$ at 10 MeV.

In addition to the absolute minimum at $A_F \approx 130$, the model predicts a local minimum in the $A_F \approx 165$ – 170 region, in both ^{236}U and ^{240}Pu . In the right panel of Fig. 8 we show the average angular momentum of heavy FFs in the rare earth region: Sm ($Z = 62$), Gd ($Z = 64$), Dy ($Z = 66$), and Er ($Z = 68$). Interestingly, all four isotopic chains exhibit a shallow minimum for $N_F = 100$ – 104 . We note that it is precisely in this region that some experiments [90] and nuclear structure calculations [91,92] have suggested the appearance of a deformed shell closure. This phenomenon is particularly relevant as a possible contributor to the observed rare-earth peak of r -process abundances in the solar system [93,94]. However, it should be noted that these fragmentations are found at the far tail of fission yields (see Fig. 5) and probing this effect experimentally would be a rather challenging task.

3. Deformation of FFs

The deformation of FFs largely determines their ability to acquire angular momentum [95]. Moreover, their deformation

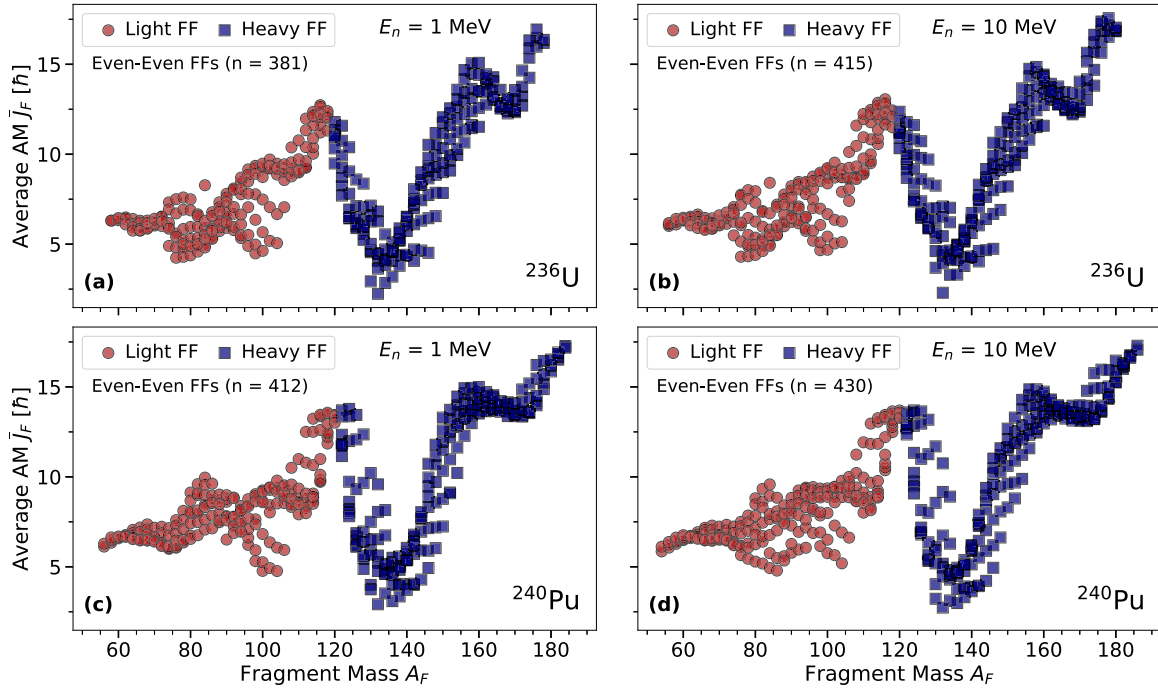


FIG. 7. Average angular momentum magnitude of heavy FFs (squares) and light FFs (circles) in all even-even FFs for ^{236}U and ^{240}Pu , at equivalent incident neutron energies $E_n = 1$ MeV and $E_n = 10$ MeV. Fragments with $A_F = A_0/2$ are marked as heavy by convention. A sawtooth pattern is apparent in both nuclei and at both energies.

at scission is generally different from their ground-state deformation, which substantially impacts AM distributions [33]. A proper treatment of FF deformation is also crucial for predictions of statistical models; for example, only by including the deformation effects are they able to reproduce the sawtooth pattern [54].

A major strength of microscopic models such as the present one is that the deformation of FFs is determined self-consistently. In particular, the axial quadrupole deformation parameter $\beta_2^F(\mathbf{q})$ of a fragment $F = l, r$ in a scission configuration $\mathbf{q}$ can be calculated as $\beta_2^F(\mathbf{q}) = (4\pi)/(3A_F R_F^2) q_{20}^F(\mathbf{q})$,

where $R_F = 1.2A_F^{1/3}$ fm and $q_{20}^F(\mathbf{q})$ is the quadrupole moment of the FF [33]. The average quadrupole deformation of a FF with integer (N_F, Z_F) can then be estimated as

$$\bar{\beta}_2^F(N_F, Z_F) = \frac{\int d\mathbf{q} F(\mathbf{q}) \beta_2(N_F, Z_F, \mathbf{q})}{\int d\mathbf{q} F(\mathbf{q}) s(N_F, Z_F, \mathbf{q})}, \quad (37a)$$

$$\beta_2(N_F, Z_F, \mathbf{q}) = \mathbb{P}_l(N_F, Z_F | N_0, Z_0, \mathbf{q}) \beta_2^l(\mathbf{q}) + \mathbb{P}_r(N_F, Z_F | N_0, Z_0, \mathbf{q}) \beta_2^r(\mathbf{q}), \quad (37b)$$

$$s(N_F, Z_F, \mathbf{q}) = \mathbb{P}_l(N_F, Z_F | N_0, Z_0, \mathbf{q}) + \mathbb{P}_r(N_F, Z_F | N_0, Z_0, \mathbf{q}), \quad (37c)$$

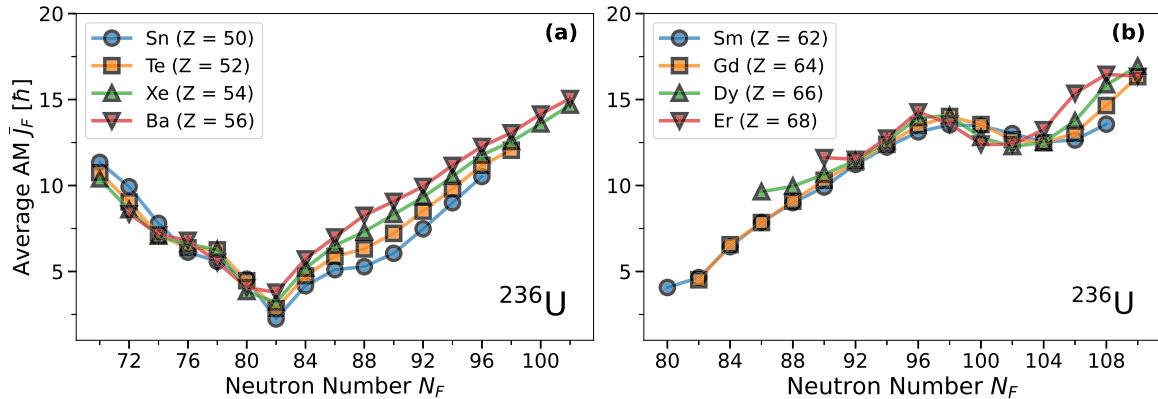


FIG. 8. Average angular momentum magnitude $\bar{J}_F$ of heavy FFs as a function of their neutron number N_F , for several isotopic chains: Sn ($Z = 50$), Te ($Z = 52$), Xe ($Z = 54$), and Ba ($Z = 56$) (left panel); and Sm ($Z = 62$), Gd ($Z = 64$), Dy ($Z = 66$), and Er ($Z = 68$) (right panel). Neutron shell closure at $N_F = 82$ and a potential deformed shell closure in the $N_F = 100$ – 104 region affect the ability of FFs to acquire angular momentum. The results are shown for FFs in ^{236}U at $E_n = 1$ MeV.

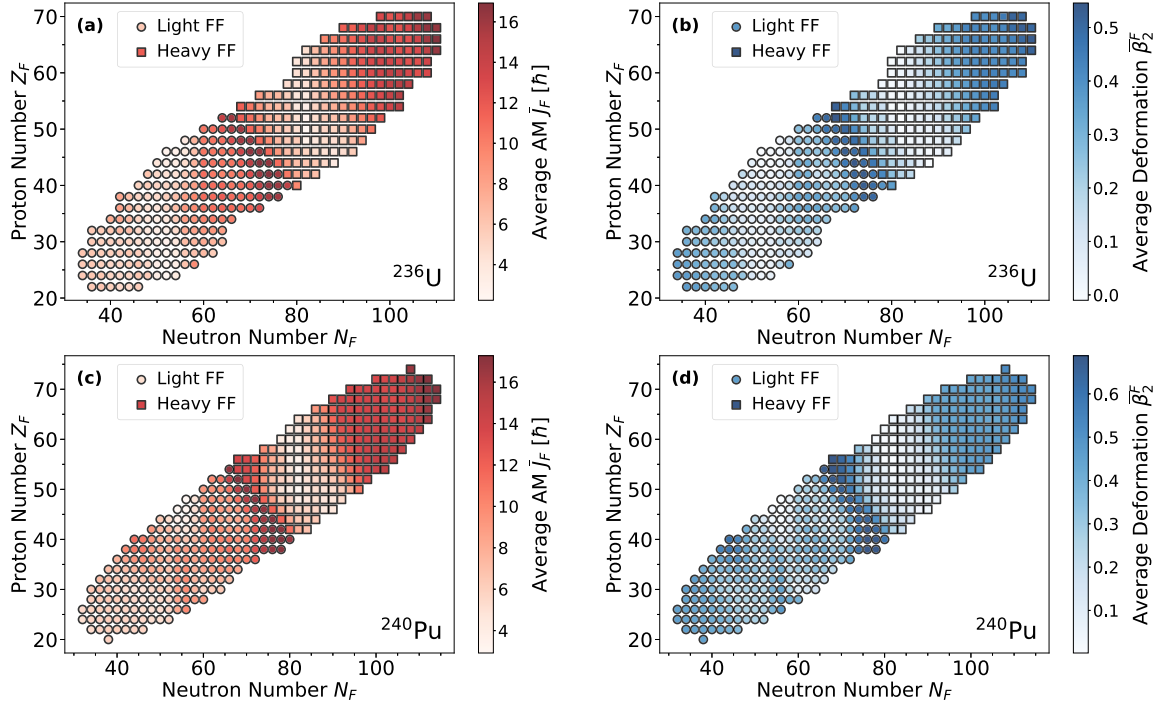


FIG. 9. Average angular momentum magnitude $\bar{J}_F$ [panel (a)] and axial quadrupole deformation $\bar{\beta}_2^F$ [panel (b)] of even-even FFs in ^{236}U as a function of their neutron number N_F and proton number Z_F , at $E_n = 1$ MeV. Panels (c) and (d) show the same for ^{240}Pu .

where $\mathbb{P}_F(N_F, Z_F | N_0, Z_0, \mathbf{q})$ is defined in Eq. (21), $F(\mathbf{q})$ is given by Eqs. (26) and (27), and the integration is performed over the entire set of scission configurations.

In Fig. 9, we show the average angular momentum $\bar{J}_F$ and the average quadrupole deformation $\bar{\beta}_2^F$ of even-even FFs as functions of their neutron and proton numbers, in both ^{236}U and ^{240}Pu . For both nuclei, a sawtoothlike pattern in the diagonal direction is also visible in the 2D (N_F, Z_F) plot of $\bar{J}_F$. The pattern for FF deformations is very similar and they span a rather wide range, from nearly spherical heavy FFs in the vicinity of the double shell closure to $\bar{\beta}_2^F \approx 0.5$ – 0.6 for light FFs near symmetric fragmentation and extremely heavy FFs.

To quantify the correlation between $\bar{J}_F$ and $\bar{\beta}_2^F$, we calculate the Pearson correlation coefficient, which corresponds to the covariance of the two variables divided by the product of their standard deviations. We obtain 0.67 in ^{236}U and 0.64 in ^{240}Pu . The coefficients are similar for the two nuclei and point to a strong correlation between $\bar{J}_F$ and $\bar{\beta}_2^F$. We note that the present model does not allow for intrinsic excitation of FFs, and all excitation energy is stored as FF deformation energy. Consequently, allowing for intrinsic excitations in FFs may somewhat modify the correlation estimate.

4. Isobaric dependence of angular momentum distributions

Statistical reaction theory models typically sample the primary FF angular momentum from a distribution of the form

$$p(J_F) \propto (2J_F + 1) \exp\left(-\frac{1}{2} \frac{J_F(J_F + 1)}{B^2(Z_F, A_F, T_F)}\right), \quad (38)$$

where $B^2(Z_F, A_F, T_F)$ encodes a possible dependence on FF charge, mass, and temperature, and includes adjustable parameters that are fixed by fitting the model predictions for fission spectra to experimental measurements. However, with the exception of CGMF [45], such models typically consider only variations of B^2 with A_F and T_F , while any isobaric dependence is entirely disregarded.

In Fig. 10, we revisit this assumption by showing the full angular momentum distributions for three heavy FF isobaric chains in ^{236}U at $E_n = 1$ MeV: $A_H = 130$ [panel (a)], $A_H = 140$ (b), and $A_H = 150$ (c). The evolution of corresponding average angular momentum $\bar{J}_F$ with FF neutron number N_F is shown as an inset in each panel.

The $A_H = 130$ isobaric chain starts far from the neutron shell closure, at $N_F = 74$. The corresponding angular momentum distribution is rather spread out and the average angular momentum is $\bar{J}_F > 7\hbar$. Changing protons for neutrons leads to a systematic decrease of $\bar{J}_F$, and the maximum of $\mathbb{P}(J_F)$ is shifted toward smaller J_F . For the magic $N_F = 82$ isobar, we get $\bar{J}_F \approx 2.9\hbar$ and $\mathbb{P}(J_F = 0) \approx 0.46$. Further increase of N_F leads again to the increase of $\bar{J}_F$ and lowering of $\mathbb{P}(J_F = 0)$. Furthermore, for $A_H = 140$ we start with $N_F = 80$, 82 isobars that have $\bar{J}_F \approx (4.0\text{--}4.5)\hbar$ and $\mathbb{P}(J_F = 0) \approx 0.22$. Here, the increase of N_F also at first leads to the increase of $\bar{J}_F$. However, a local minimum of $\bar{J}_F \approx 6\hbar$ is found for the $N_F = 90$ isobar, which lies at the $Z_F = 50$ proton shell closure. Moving away from magicity again increases $\bar{J}_F$. Finally, the $A_H = 150$ chain does not contain any nuclei with magic numbers. Consequently, $\bar{J}_F$ increases rather monotonically with N_F , reflecting a systematic spreading of the $\mathbb{P}(J_F)$ toward larger J_F values.

Overall, these results demonstrate a strong dependence on Z_F and N_F of AM distributions within an isobaric chain of

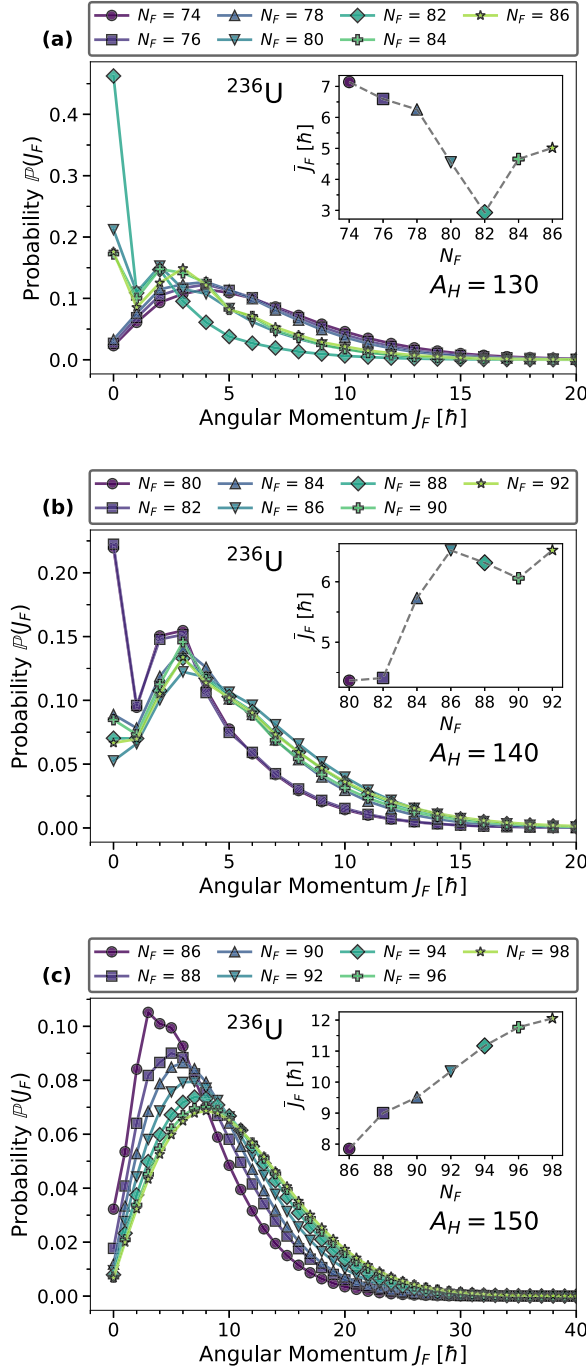


FIG. 10. Angular momentum distributions in three heavy FF isobaric chains for fission of ^{236}U , at $E_n = 1$ MeV: $A_H = 130$ [panel (a)], $A_H = 140$ (b), and $A_H = 150$ (c). The corresponding average angular momenta $\bar{J}_F$ as functions of the FF neutron number N_F are shown as insets in each panel. The results demonstrate a pronounced isobaric dependence of angular momentum distributions.

primary FFs. Pronounced qualitative variations are found in the $A_H = 130$ and $A_H = 140$ isobars, whose distributions are largely driven by the $N_F = 82$ shell closure. However, even far from magicity, at $A_H = 150$, the variation of $\bar{J}_F$ within the isobaric chain can be larger than $5\hbar$. Other isobaric chains exhibit pronounced variations as well. Taking these effects

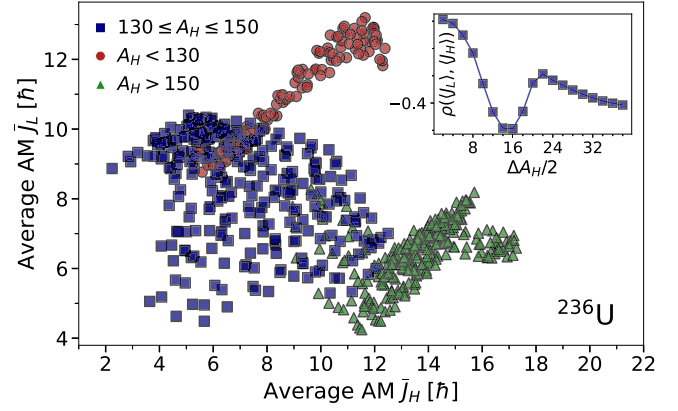


FIG. 11. Average angular momentum magnitude of light FFs as a function of the average angular momentum magnitude of their heavy partners. The results are shown for all FF pairs in ^{236}U at $E_n = 1$ MeV. Fragmentations with $A_H < 130$ (nearly symmetric configurations, red), $130 \leq A_H \leq 150$ (most strongly populated configurations, blue), and $A_H > 150$ (highly asymmetric configurations, green) are shown separately. Additionally, the inset shows the correlation coefficient as a function of the $\pm \Delta A_H / 2$ window of included configurations around the $A_H^{\text{peak}} = 140$. Angular momentum magnitudes of FFs for the most strongly populated configurations are only weakly correlated.

into account may improve the predictive power of models based on statistical reaction theory.

5. Correlation between FF angular momenta

The ALTO measurements also probed the correlation in magnitudes of AM between the two FFs [31]. This was achieved by measuring the AM of one FF while constraining the partner population to increasingly higher AM. For six most populated FFs in $^{238}\text{U}(n, f)$, no significant correlation was found. This finding was interpreted as an argument for a postscission generation mechanism of AM in FFs. Unfortunately, the present model does not allow for probing the correlation in an entirely analogous manner. However, for the large set of obtained fragmentations, we can examine how the average AM of light FF $\bar{J}_L$ depends on the average AM of its heavy partner $\bar{J}_H$.

In Fig. 11, we show $\bar{J}_L$ as a function of $\bar{J}_H$ for all pairs of FFs in ^{236}U at 1 MeV. We classify the fragmentations into three groups according to their mass asymmetry. The first group contains fragmentations in the $130 < A_H < 150$ range, covering more than 95% of experimental mass yields [81–83]. The remaining two groups contain nearly symmetric configurations ($A_H \leq 130$) and highly asymmetric configurations ($A_H \geq 150$). To quantify correlations, the Pearson coefficient is calculated for each group separately.

For the set of strongly populated configurations, we obtain $\rho(\bar{J}_L, \bar{J}_H) = -0.33$, which is considered a weak negative correlation. Note that the correlation is estimated before any prompt emission takes places. On the other hand, experiments can only assess FFs after prompt emissions, which are expected to have a further decorrelating effect. Furthermore, the Pearson coefficient for highly asymmetric configurations

is $\rho = 0.43$, indicating a moderate positive correlation. On the other hand, the nearly symmetric configurations are very strongly correlated, with $\rho = 0.97$. This is entirely expected because the two FFs become identical in the limit $A_H \rightarrow 118$.

Since the aforementioned division into groups is somewhat arbitrary, in the inset of Fig. 11 we also examine how the correlation coefficient of the most strongly populated configurations changes as we increase the $\pm\Delta A_H/2$ window of included configurations around the $A_H^{\text{peak}} = 140$ mass yields peak. From $\Delta A_H/2 = 2$ to $\Delta A_H/2 = 6$ the correlation is essentially negligible, $|\rho| < 0.1$. Note that the six most strongly populated heavy FFs and light FFs from [31] lie within 8 and 10 mass units, respectively. In our calculation, the correlation coefficient peaks at $\Delta A_H/2 = 16$, and then it systematically drops as the $118 \leq A_H \leq 124$ configurations are gradually included. Further inclusion of asymmetric configurations leads to a slight increase of correlation, and the coefficient finally settles at $\rho = -0.41$ for the full set of fragmentations.

Overall, the AM magnitudes of strongly populated FFs are weakly correlated in the present model: $\rho = -0.33$ for $130 \leq A_H \leq 150$ and $|\rho| < 0.1$ for $134 \leq A_H \leq 146$. Similar results are obtained for ^{240}Pu . We note, however, that the model is not best suited to probe this correlation, since the distributions are obtained by separate AM projections in the two FFs. Nevertheless, it is interesting to observe that a strong correlation can be absent even in a model whose AM generation mechanism is explicitly *not* of postscission origin.

IV. CONCLUSION

In this paper, we report the first microscopic calculations of angular momentum distributions across the full range of fission fragments. The theoretical framework is based on the combined projection on particle number (in both the compound nucleus and the fission fragments) and angular momentum (in the fragments only) for a chosen set of scission configurations. The TDGCM + GOA model is used to estimate the weight of each scission configuration in setting the final angular momentum distribution of each fragment. We present results for the two benchmark reactions of $^{235}\text{U}(n,f)$ and $^{239}\text{Pu}(n,f)$.

In both reactions, we observe a clear sawtooth pattern in the relationship between the average angular momentum magnitude of fission fragments and the fragment mass. Since the model implicitly assumes that all excitation energy is collective, we find little dependence of the angular momen-

tum on the incident neutron energy. In contrast, shell effects manifest themselves strongly, hindering the ability of heavy fragments to carry angular momentum close to the double shell closure. Importantly, we also find that angular momentum distributions can vary substantially along isobaric chains. This suggests that the commonly used statistical model formula, which typically depends on the mass but not the charge of the fragment, is not sufficiently accurate. Furthermore, we quantify a strong correlation between the deformation and angular momentum of fragments, and observe a weak correlation in angular momentum magnitude between the fragment partners for the most strongly populated configurations. Finally, we demonstrate that the primary fission fragment yields can be calculated within the same framework, even if a more rigorous treatment of scission configurations will be needed to improve the quality of predictions.

The calculated set of angular momentum distributions can be used to perform full-fledged fragment decay simulations. This would enable us to estimate the impact of microscopic distributions on fission spectra, paving the way toward fission modeling based on microscopic inputs. Such a database of distributions could also be valuable for informing phenomenological models that parametrize the angular momentum distribution using formulas from statistical models. Further extensions of the model should include a more refined treatment of scission and a proper incorporation of nuclear excitation effects.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [96].

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