Multiplicity of Scision Neutrons from Density Functional Scission Dynamics

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Plan

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Motivation

The most important feature of nuclear fission is that it is accompanied by emission of prompt neutrons (PFN).
Two PFN sources have been discussed so far:
1) Neutrons evaporated from fully-accelerated excited fragments (EVN).
2) Neutrons dynamically released at scission (SN) due to the diabatic coupling between the neutron degree of freedom and the rapidly changing neutron-nucleus potential.
The relative intensities of these two components are completely unknown. It is very difficult to separate them experimentally since the gross features of PFN can be accounted for by both hypotheses.

Motivation-2

While the 1st component depends on the excitation and extra deformation with which the fission fragments are born (Madland-Nix 1982), the 2nd depends on the dynamical evolution of the system during the scission process (Carjan-Rizea 2012). Therefore a simple stationary approach suffices for EVN but a more complicated dynamical approach is needed for SN. There are three parameters in the dynamical scission model: the nuclear shapes just before (α_i) and immediatelly after (α_f) scission and the duration ΔT of the transition between these two shapes. Since these quantities were unknown, in the past we have used educated guesses.

Motivation-3

At present reliable values for these quantities are available from the density functional theory (DFT) applicable to superfluid systems (usually named the superfluid local density approximation or SLDA), within a time-dependent extension (TD-SLDA) (Bulgac et al. 2016). Among the many nuclear energy density functionals we choose the one based on the Skyrme force SkM* (Bartel et al. 1982) that reproduces the fission barriers in ^{240}Pu. We extract these three quantities and calculate the multiplicity of the neutrons released at scission and emitted immediately after (i.e., during the acceleration of the fragments).
Finally we estimate the energy available to emit prompt γ-rays and evaporate neutrons: E^*_{sc} + ΔE_{def}

Dynamical Scission Model (DSM)

To simulate the evolution of the neutron wave functions from α_i to α_f lasting ΔT, the two-dimensional time-dependent Schrödinger equation (TDSE2D) with a time-dependent potential (TDP) is solved. The distribution of final wave packets $\hat{\Psi}^i$(ΔT) (that correspond at t = 0 to the eigenstates $\hat{\Psi}^i$ of α_i) over the eigenstates $\hat{\Psi}^f$ of α_f:

$$a_{if} = \langle \hat{\Psi}^i(\Delta T) | \hat{\Psi}^f \rangle. \tag{1}$$

constitutes the core of DSM. All wave functions have an implicit dependence on the cylindrical coordinates (ρ, z). a_{if} is $\neq$ 0 only if $|\hat{\Psi}^i\rangle$ and $|\hat{\Psi}^f\rangle$ have the same projection Ω of the total angular momentum along the symmetry axis.

DSM-2

The rapid change of the potential in which the nucleons move produces, by means of a diabatic coupling, their excitation and eventual emission.
The a_{if} coefficients are used to calculate the scission neutron multiplicity ν_{sc} in a simple and intuitive way. It is given by the sum of the probabilities P_{em}^i that a neutron occupying a given bound-state i is emitted:

$$P_{em}^i = v_i^2 (\textstyle\sum_f |a_{if}|^2)$$

$$\nu_{sc} = 2 \sum_i P_{em}^i \tag{2}$$

i-sum is over bound states while f-sum is over unbound states. v_i^2 is the occupation probability of the state i.

DSM-3

Similarly, the excitation energy in which the fragments are left immediately after scission is given by

$$E^*_{sc} = 2 \times (\sum_f V_f^2 e_f - \sum_f v_f^2 e_f), \tag{3}$$

where $V_f^2 = \sum_i v_i^2 |a_{if}|^2$ is the probability that an eigenstate $|\hat{\Psi}^f\rangle$ of the final configuration α_f is occupied after the sudden transition and e_f is its eigen-energy. The i and f sums are over the bound states of the initial and final nuclear configurations, respectively. The nuclear shapes involved are described by Cassini ovals (Pashkevich 1971) with two parameters: α (the overall deformation) and α_1 that fixes the mass asymmetry.

TD-SLDA

In SLDA, the nuclear system is described by a density functional $\mathcal{E}(n(\vec{r}), \nu(\vec{r}), \vec{j}(\vec{r}), \ldots)$, where n is the normal (number) density, ν is the anomalous density, $\vec{j}$ is the current density, etc. They are defined in terms of the $u_{k\uparrow(\downarrow)}$ and $v_{k\uparrow(\downarrow)}$ components of the quasiparticle wave functions (qpwfs). The dynamics of the nucleus is followed in real time by solving a system of time-dependent Schrödinger-like equations

TD-SLDA-2

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k\uparrow} \\ u_{k\downarrow} \\ v_{k\uparrow} \\ v_{k\downarrow} \end{pmatrix} = \tag{4}$$

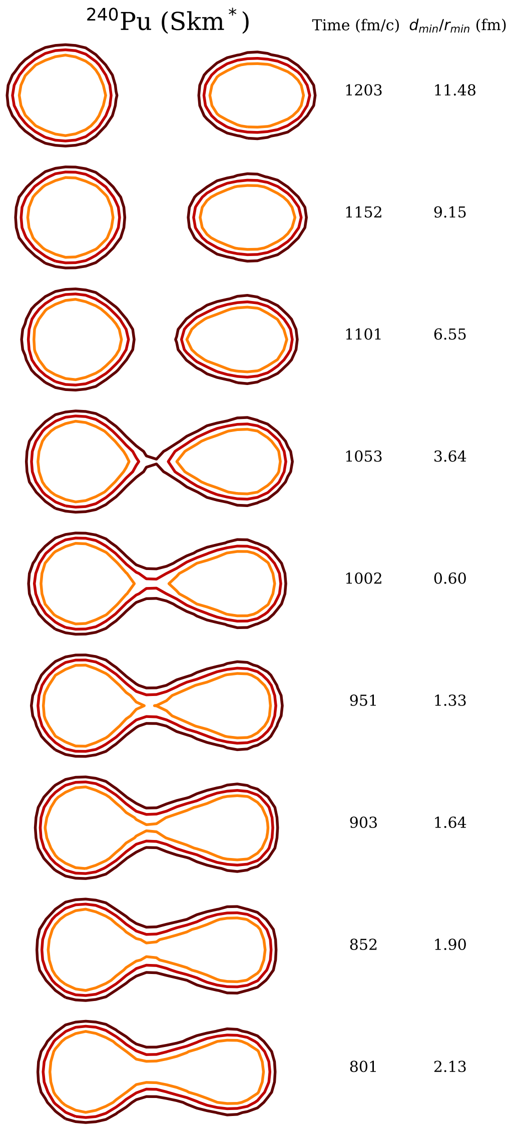
$$\begin{pmatrix} h_{\uparrow\uparrow}-\mu & h_{\uparrow\downarrow} & 0 & \Delta \\ h_{\downarrow\uparrow} & h_{\downarrow\downarrow}-\mu & -\Delta & 0 \\ 0 & -\Delta^* & -(h^*_{\uparrow\uparrow}-\mu) & -h^*_{\uparrow\downarrow} \\ \Delta^* & 0 & -h^*_{\downarrow\uparrow} & -(h^*_{\downarrow\downarrow}-\mu) \end{pmatrix}\begin{pmatrix} u_{k\uparrow} \\ u_{k\downarrow} \\ v_{k\uparrow} \\ v_{k\downarrow} \end{pmatrix},$$

with the dependence on the spacial coordinates and time not shown explicitly. The one-body Hamiltonian $h = \partial\mathcal{E}/\partial v^*$ and the pairing field Δ depend on the densities and currents constructed from the qpwfs at the time t.

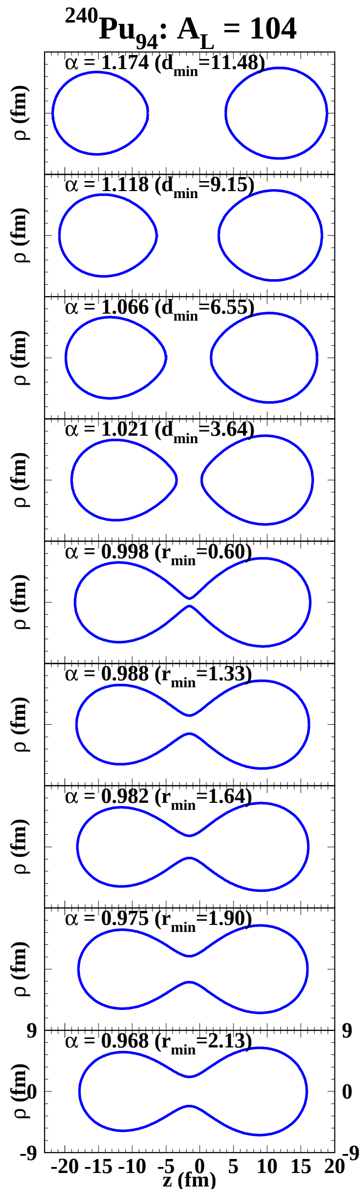
TD-SLDA scission dynamics

We calculate at each time the number density $n(\vec{r},t) = \sum_k (|v_{k\uparrow}(\vec{r},t)|^2 + |v_{k\downarrow}(\vec{r},t)|^2)$ shown in the next slide at several times before and after scission in ^{240}Pu. This trajectory leads to a mass asymmetry of the fragments defined by A_L=104 (A_H=136) close to the most probable experimental mass division in the reaction $^{239}Pu(n_{th},f)$. The middle equidensity line is the half density n_0/2 with n_0=0.16 fm^{-3}. It is equivalent with the equipotential line V_0/2 of the deformed Woods-Saxon potential used in DSM. V_0 is the potential depth. These equipotential lines are shown for comparison on the same slide. The similarity is good.

Time evolution of the density and of the potential

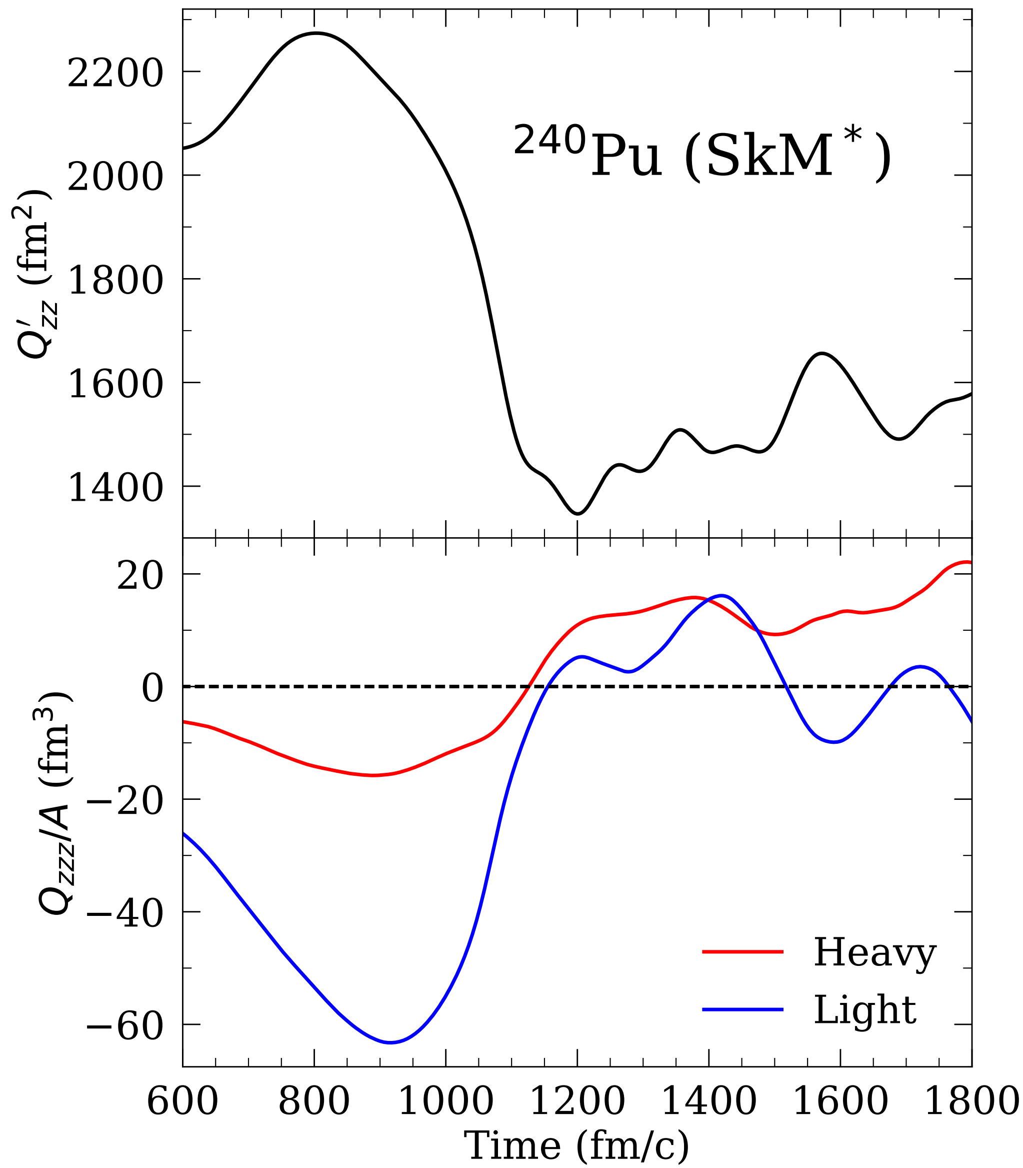


nuclear density

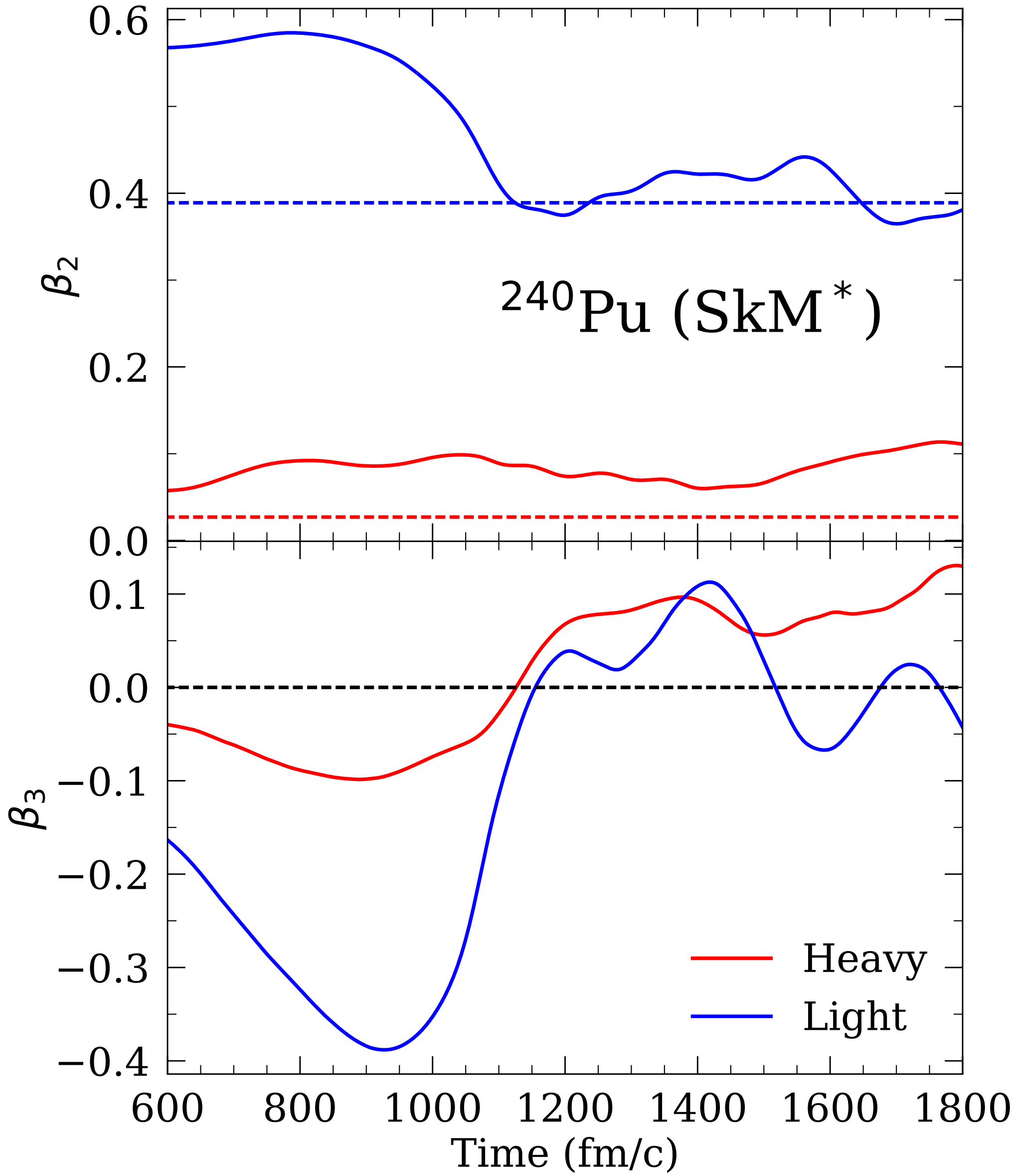


nuclear potential

Quadrupole (nucleus) and Octupole (fragments) Moments



β_2 and β_3 deformations of the nascent fragments



SCN multiplicities

The deformations of the Cassini ovals that have the same r_{min} and d_{min} values are found to be α_i = 0.968 and α_f = 1.174 respectively. We therefore calculate the evolution of all neutron wave functions from α_i to α_f keeping the mass asymmetry fixed at A_L=104 with the help of the parameter α_1. The duration of the transition is ΔT=13.4 10^{-22} sec.

Table 1: *Scission neutron multiplicity:* $240Pu, A_L = 104$, $0.968 >> 1.174$, $\Delta T = 13.4 \times 10^{-22}$ *sec*

Ω	$1/2$	$3/2$	$5/2$	$7/2$	$9/2$	$11/2$	$\Sigma(\Omega)$
ν_{sc}	0.833	0.465	0.037	0.005	0.006	0.001	1.347

SCN, EVN and γ-rays

The results are presented for each set of wave functions of given Ω. ν_{sc} decreases with Ω, the contribution of Ω=1/2 being more then 50$\%$. In the case of ^{240}Pu the multiplicity summed over all Ω values is found to be 1.347, i.e., half of the prompt fission neutrons measured in the reaction $^{239}Pu(n_{th},f)$ are released at scission.
In addition of being promoted to positive energy states at the end of the scission process, the neutrons are also promoted to states between the Fermi and the "zero" level producing excitation in the primary fragments. Eq (3) gives E^*_{sc} = 12.59 MeV.

Post-scission fragments' deformation

Finally we estimate the extra deformation energy ΔE_{def} of the primary fragments. From the slides with the time evolution of Q_{zz} and Q_{zzz} of each fragment, one can extract their deformations β_2 and β_3 and from this we calculate their post-scission deformation energies (P. Möller et al.)

Table 2: *Deformation parameters of the primary fragments and their extra deformation energy:* $240Pu, A_L = 104$

Z	A	β_2	β_3	ΔE_{def}
41	104	0.39	0.10	$0.79 MeV$
53	136	0.10	0.10	$2.27 MeV$

The total energy is balanced

On one side we have the estimated total excitation energy
E^*_{sc} + ΔE_{def} = 15.65 MeV
that will be used to emit prompt γ rays and evaporate neutrons.
On the other side we have $< E_\gamma >$ = 6.70 MeV measured (Knitter et al.) and 1.52 neutrons to evaporate. With S_n = 4.97 MeV and 3.78 MeV for the L and H fragments, the latter requires 6.65 MeV. So the sum is 13.35 MeV.

Discussion and Conclusions

- We give a first plausible answer to a long-standing question regarding the emission of prompt fission neutrons: is the percentage of neutrons emitted at scission and during acceleration significant? YES!
- We use DSM to calculate ν_{sc} and E^*_{sc} In this phenomenological model the dynamics of the neck rupture determines how many unbound neutrons and how much excitation we have at the end.
- Implementing the scission dynamics given by TD-SLDA into DSM, we obtain ν_{sc}= 1.347 (half of the PFN originate at scission) and E^*_{sc} = 12.59 MeV.
- From the deformations of the primary fragments predicted by TD-SLDA, we calculated their extra deformation energies ΔE_{def} =3.06 MeV.
- The total energy balance is fulfilled