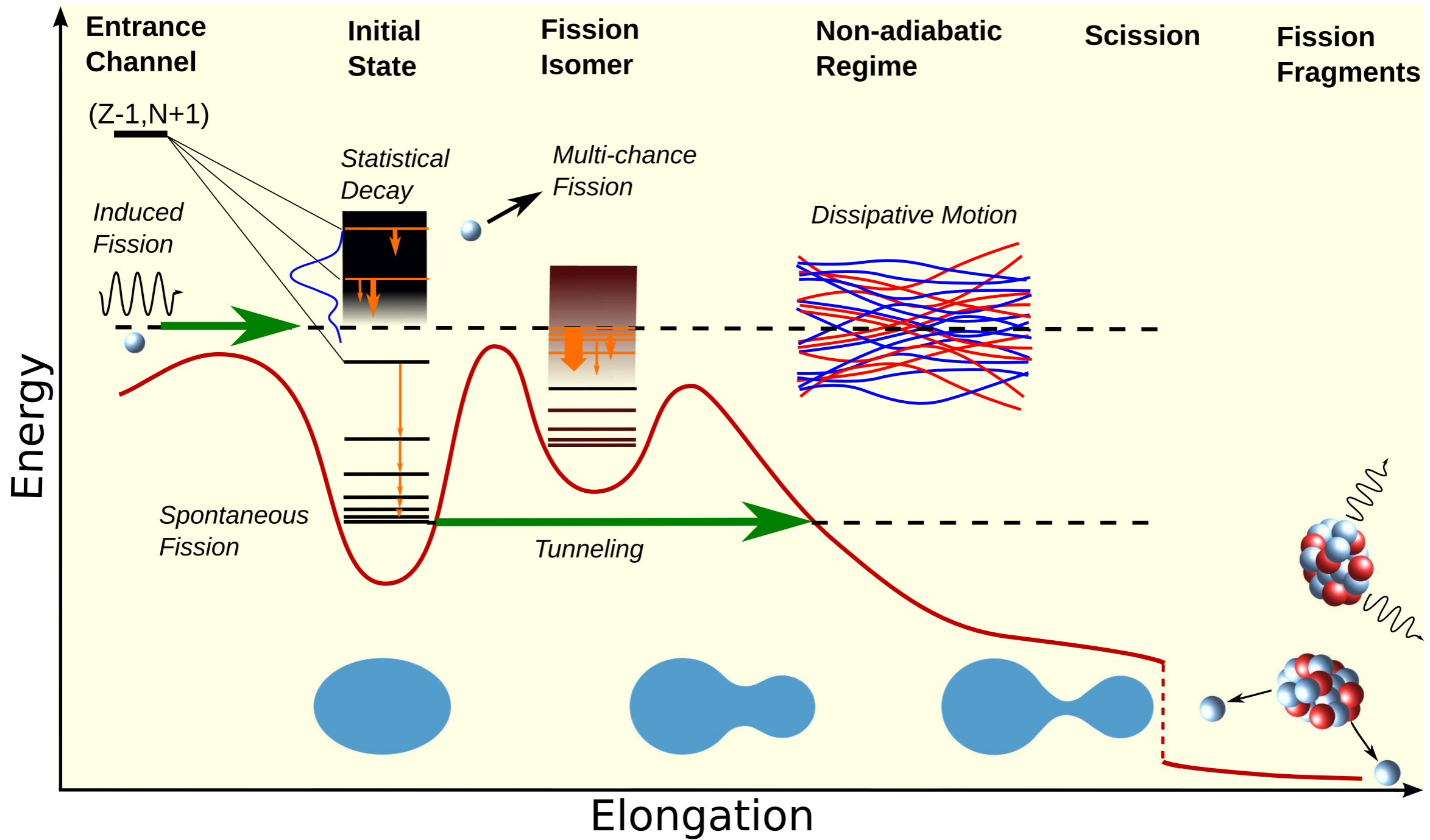


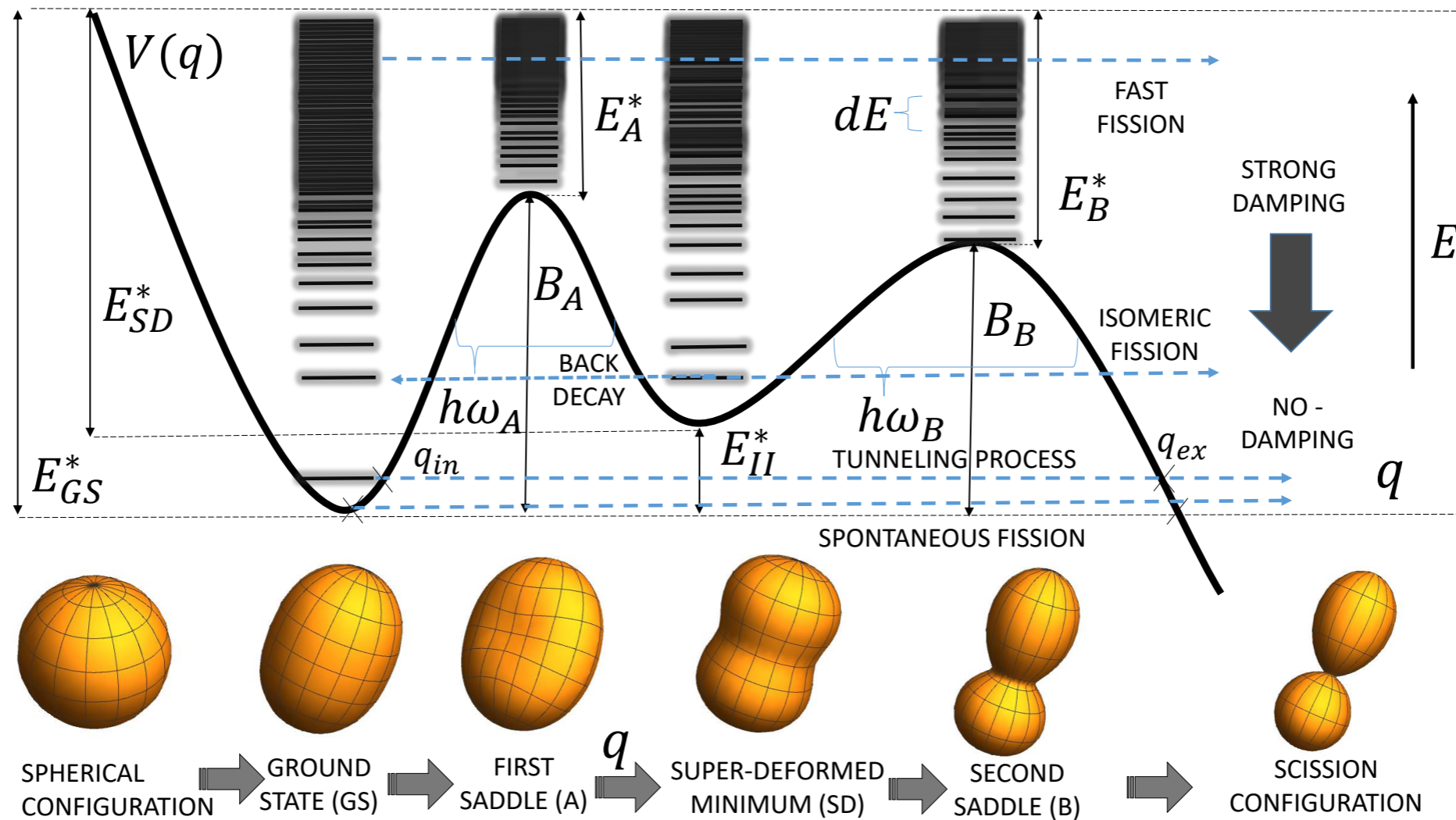
Microscopic Description of Fission Dynamics

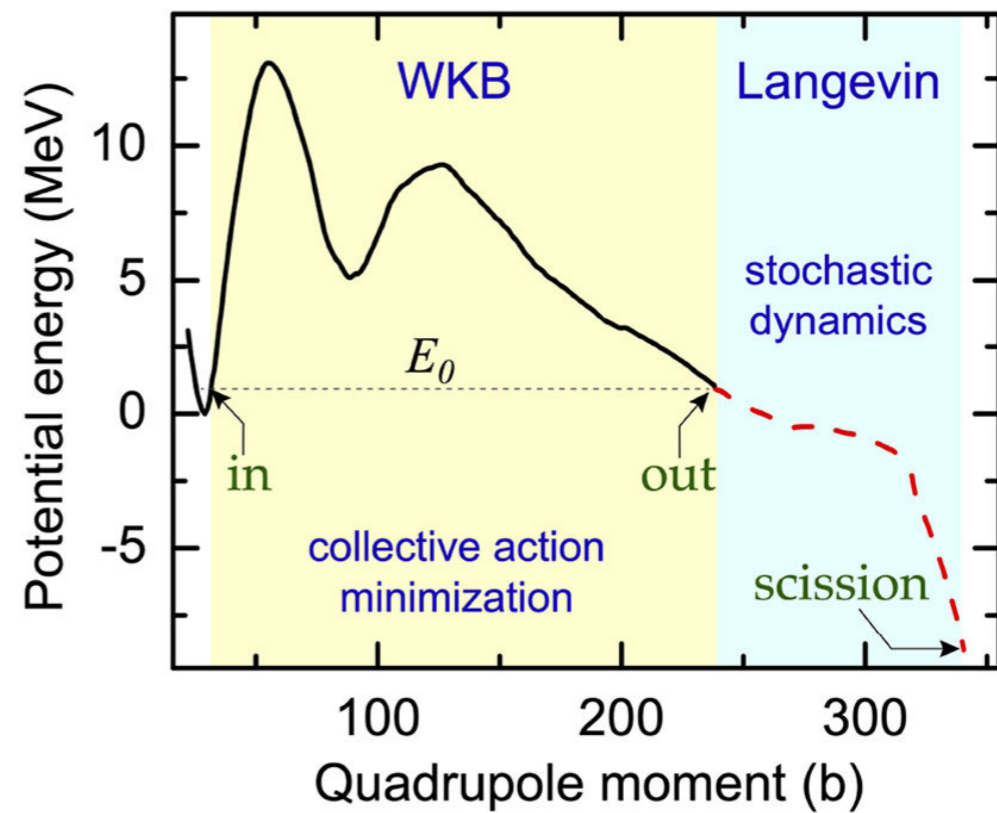
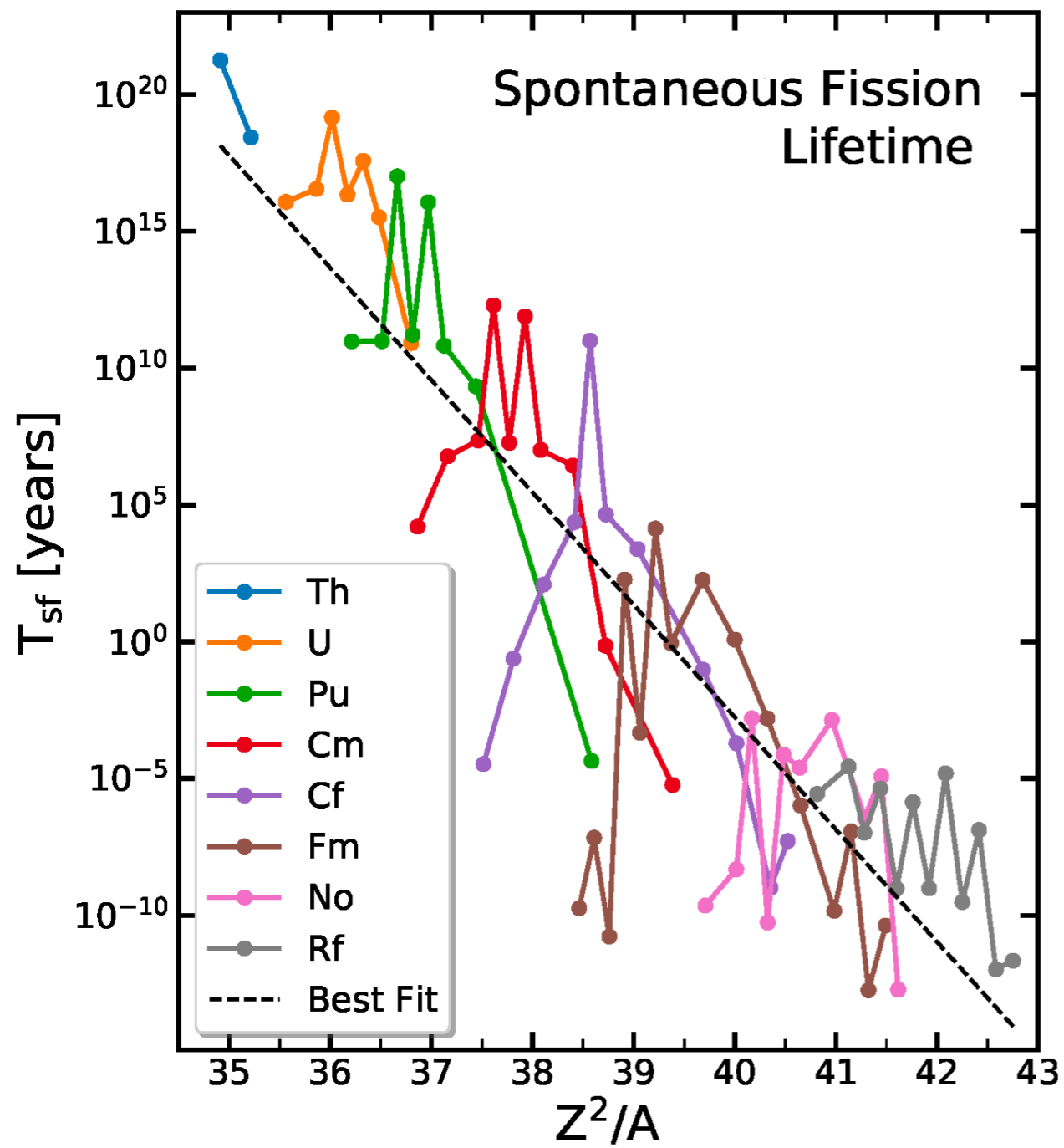


Dario Vretenar
University of Zagreb



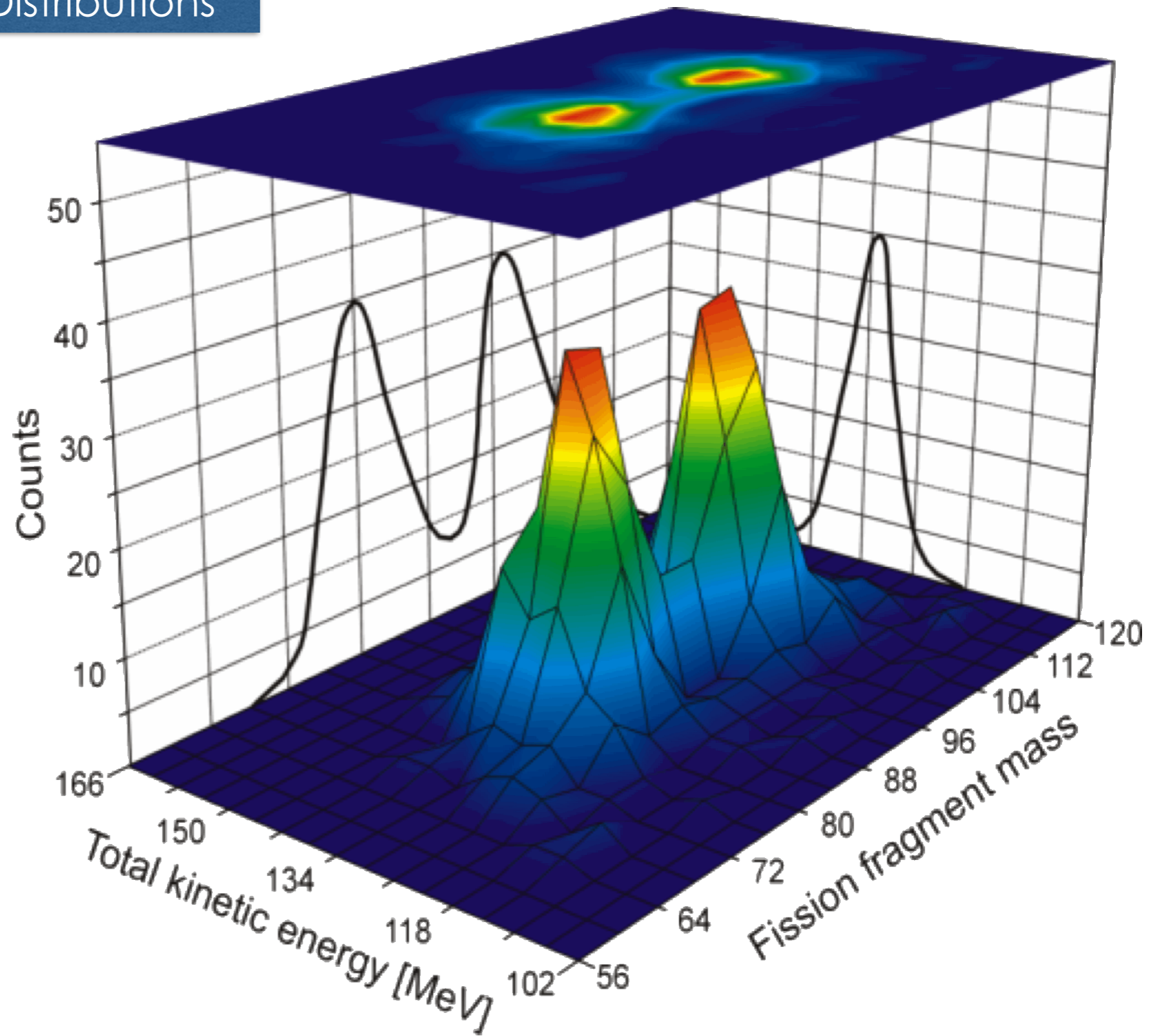
Fission Barrier Heights and Isomer Excitation Energies

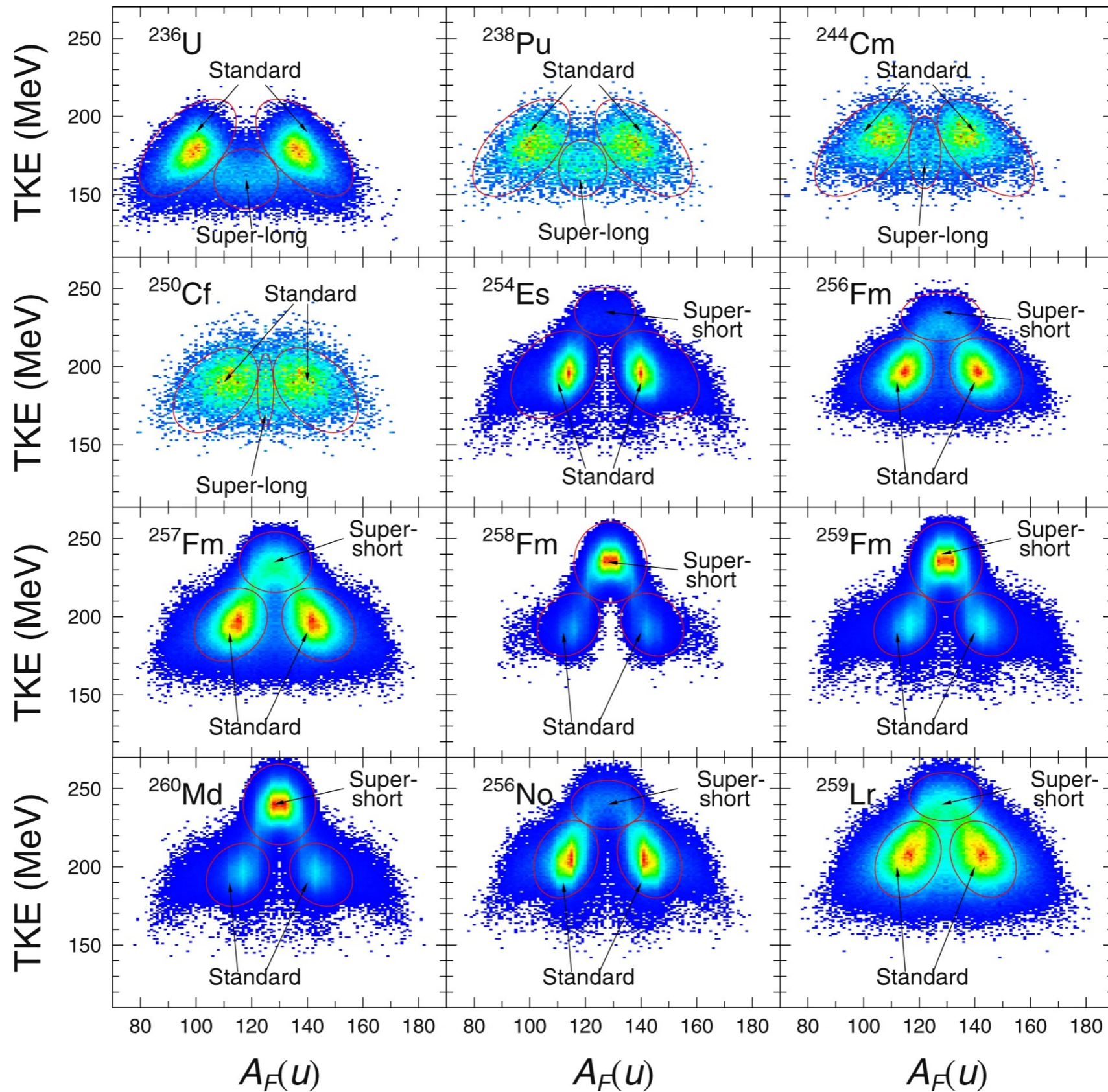




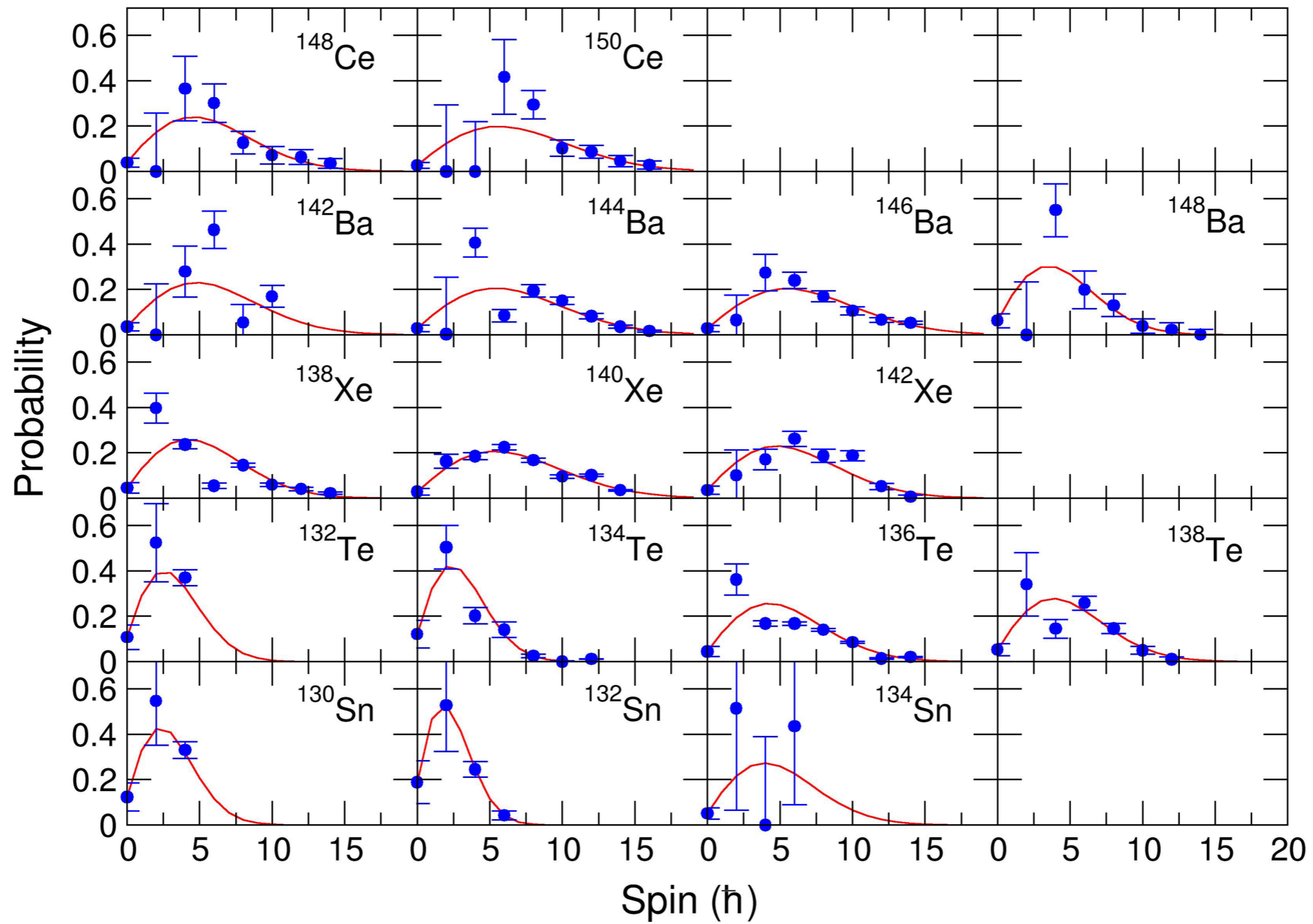
Sadhukhan J (2020) Microscopic Theory for Spontaneous Fission. *Front. Phys.* 8:567171.

Fragment Mass Distributions





Spin distribution of FFs



Microscopic Models

The time-dependent generator coordinate method (TDGCM)

$$|\Psi(t)\rangle = \int_{\mathbf{q} \in E} d\mathbf{q} |\phi(\mathbf{q})\rangle f(\mathbf{q}, t). \quad \rightarrow \text{represents the nuclear wave function by a superposition of generator states that are functions of collective coordinates.}$$

→ a fully quantum mechanical approach but only takes into account collective degrees of freedom in the adiabatic approximation.

→ no dissipation mechanism.

TDGCM in the Gaussian overlap approximation (TDGCM+GOA)

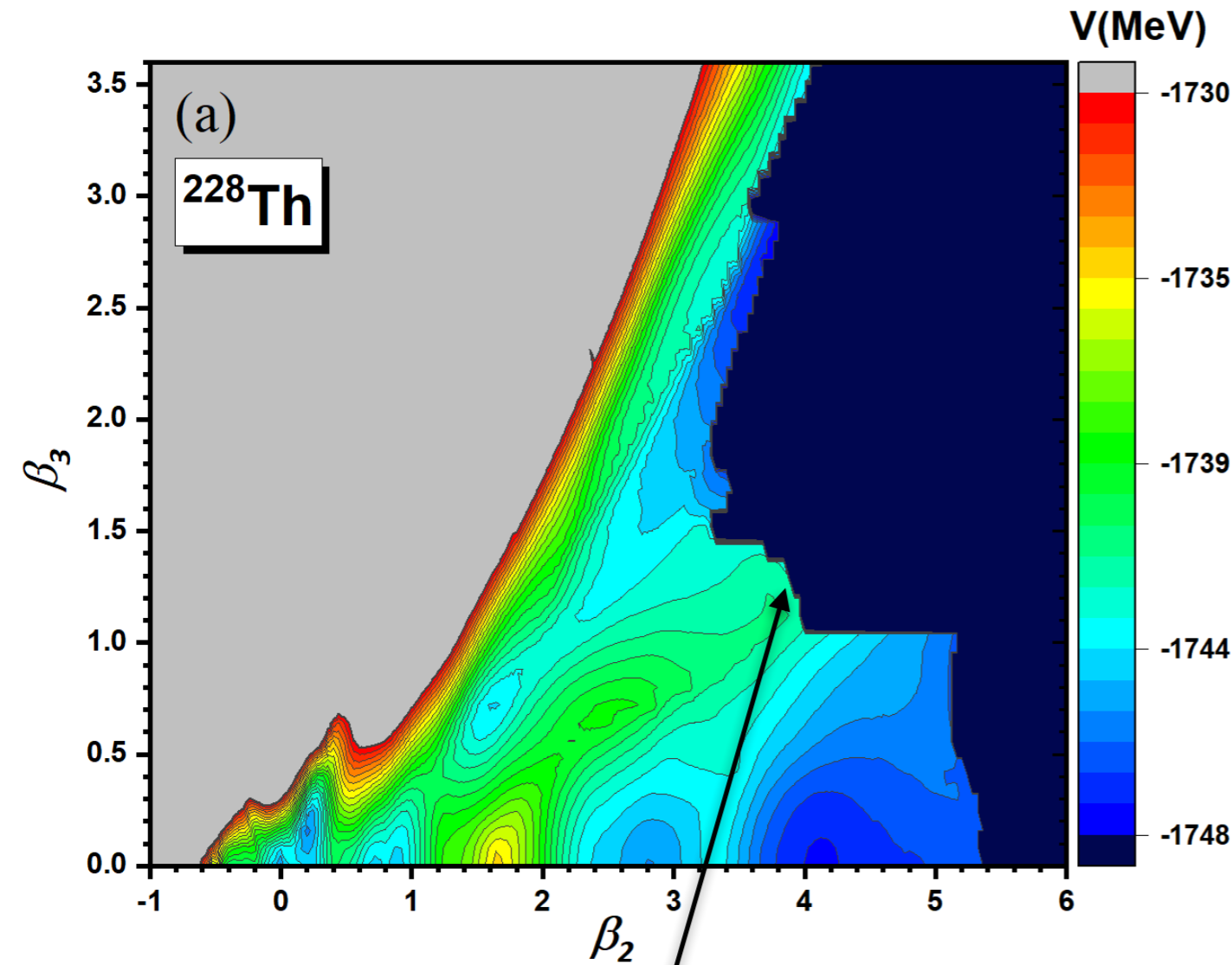
Example

Time-dependent Schroedinger-like equation for fission dynamics (axial quadrupole and octupole deformation parameters as collective degrees of freedom):

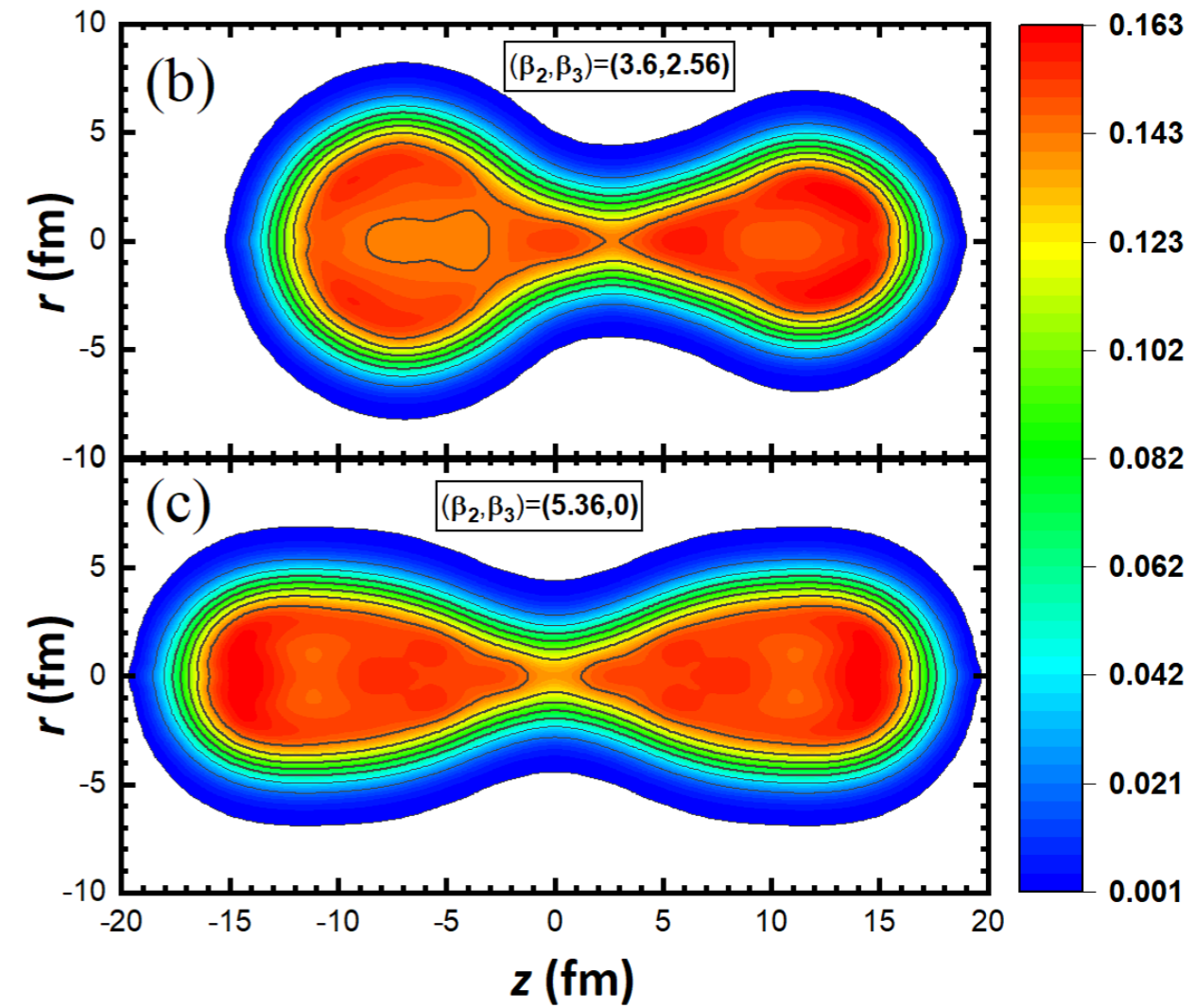
$$i\hbar \frac{\partial}{\partial t} g(\beta_2, \beta_3, t) = \left[-\frac{\hbar^2}{2} \sum_{kl} \frac{\partial}{\partial \beta_k} B_{kl}(\beta_2, \beta_3) \frac{\partial}{\partial \beta_l} + V(\beta_2, \beta_3) \right] g(\beta_2, \beta_3, t)$$

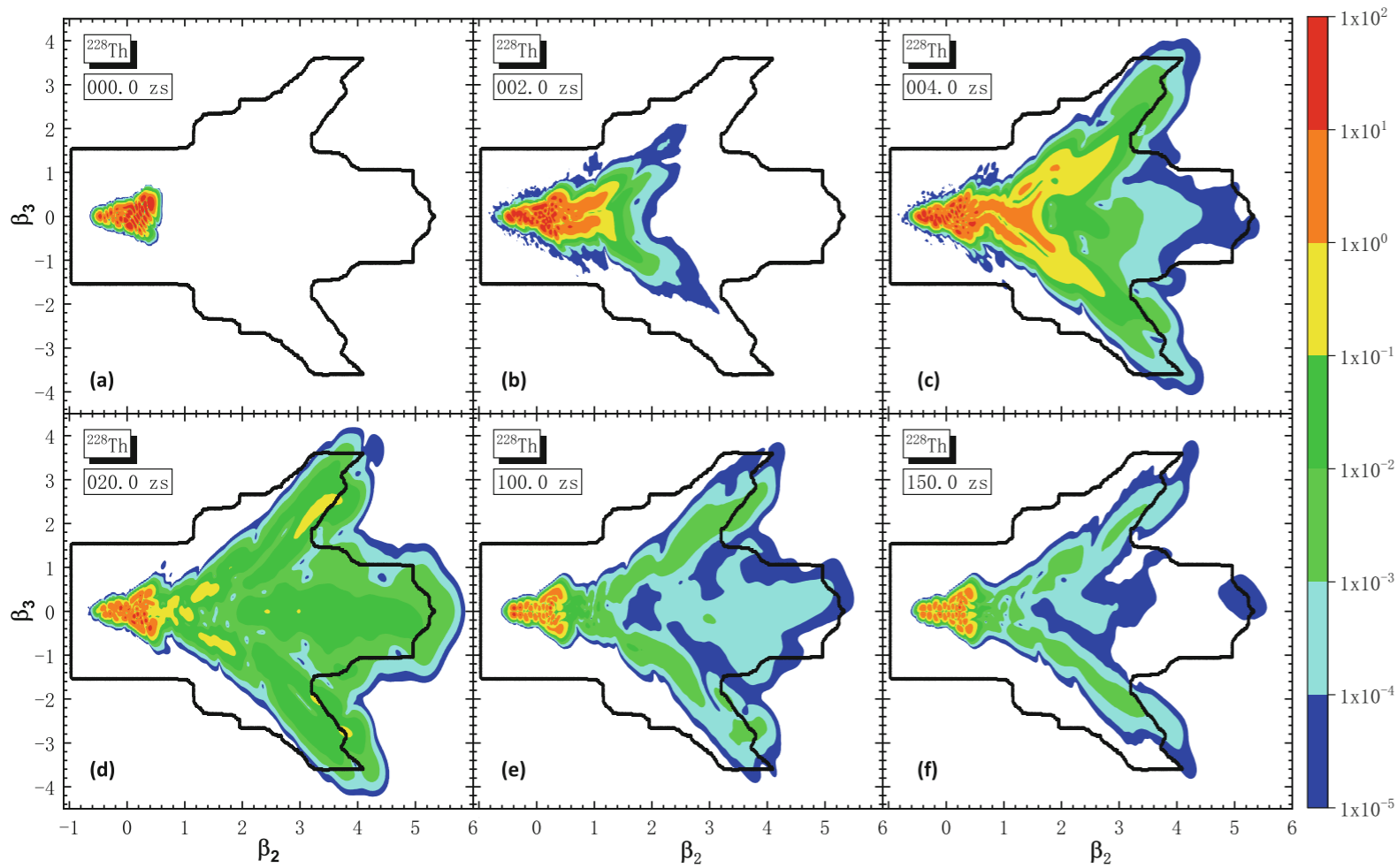
Quadrupole and octupole constrained deformation energy surface of ^{228}Th in the $\beta_2 - \beta_3$ plane.

Density profiles on the scission contour.



Scission contour





Time evolution of the probability density $|g|^2$ in the (β_2, β_3) plane. The solid line corresponds to the scission hypersurface.

...current

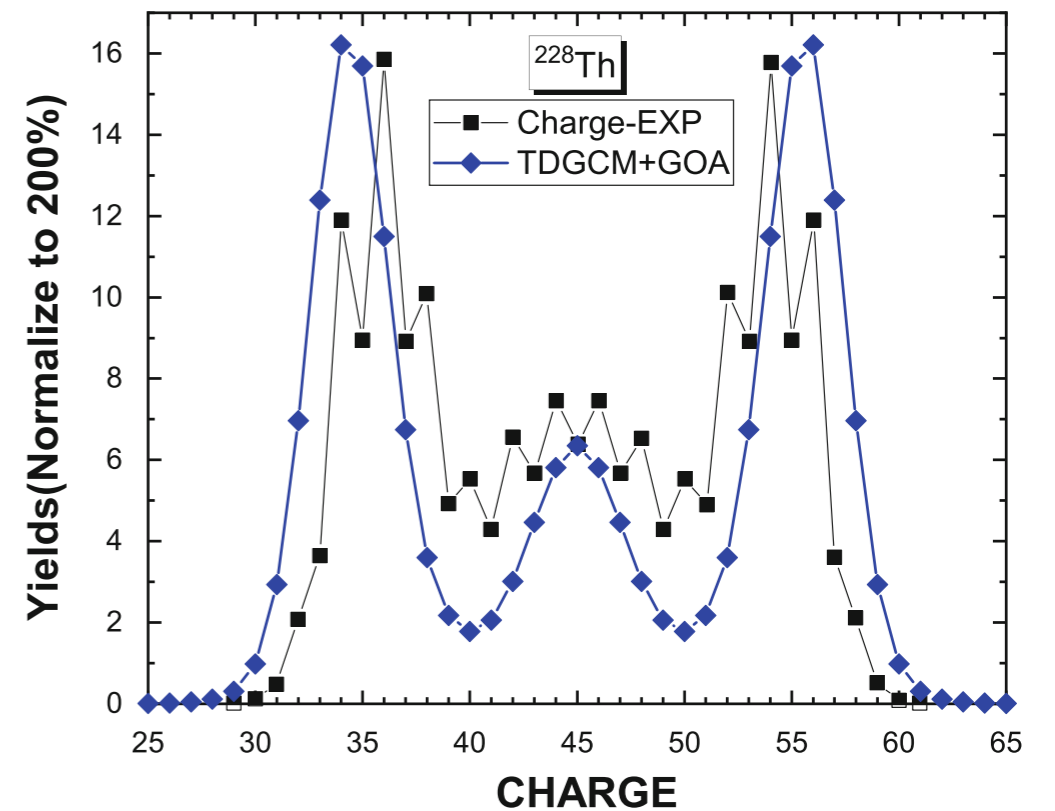
$$J_k(\beta_2, \beta_3, t) = \frac{\hbar}{2i} \sum_{l=2}^3 B_{kl}(\beta_2, \beta_3) \left[g^*(\beta_2, \beta_3, t) \frac{\partial g(\beta_2, \beta_3, t)}{\partial \beta_l} - g(\beta_2, \beta_3, t) \frac{\partial g^*(\beta_2, \beta_3, t)}{\partial \beta_l} \right].$$

...integrated flux

$$F(\xi, t) = \int_{t_0}^t dt' \int_{\{\beta_{20}, \beta_{30}\} \in \xi} \mathbf{J}(\beta_{20}, \beta_{30}, t') dS,$$

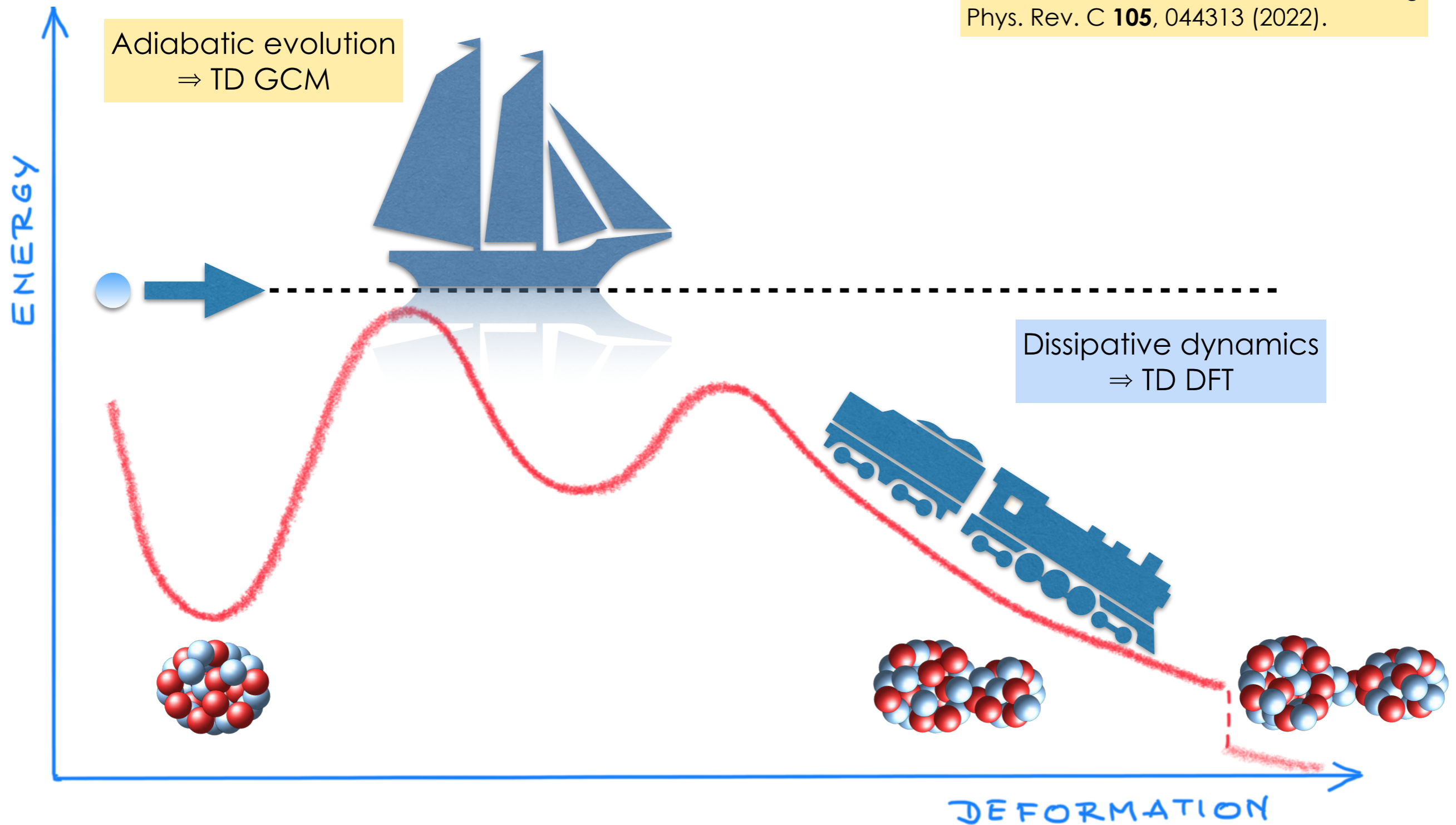
...charge yield

$$Y(Z) \propto \sum_{\xi \in \mathcal{A}} \lim_{t \rightarrow \infty} F(\xi, t).$$



Adiabatic evolution and dissipative dynamics

Ren, Zhao, Vretenar, Nikšić, Zhao, Meng
Phys. Rev. C **105**, 044313 (2022).



Time-dependent density functional theory (TD DFT)

$|\Psi(t)\rangle = |\phi(\mathbf{q}, t)\rangle \rightarrow$ single product state

$$i \frac{\partial}{\partial t} \psi_k(\mathbf{r}, t) = \left[\hat{h}(\mathbf{r}, t) - \varepsilon_k(t) \right] \psi_k(\mathbf{r}, t),$$

\rightarrow classical evolution of independent nucleons in mean-field potentials, cannot be applied in classically forbidden regions of the collective space, nor does it take into account quantum fluctuations.

$$i \frac{d}{dt} n_k(t) = n_k(t) \Delta_k^*(t) - n_k^*(t) \Delta_k(t),$$

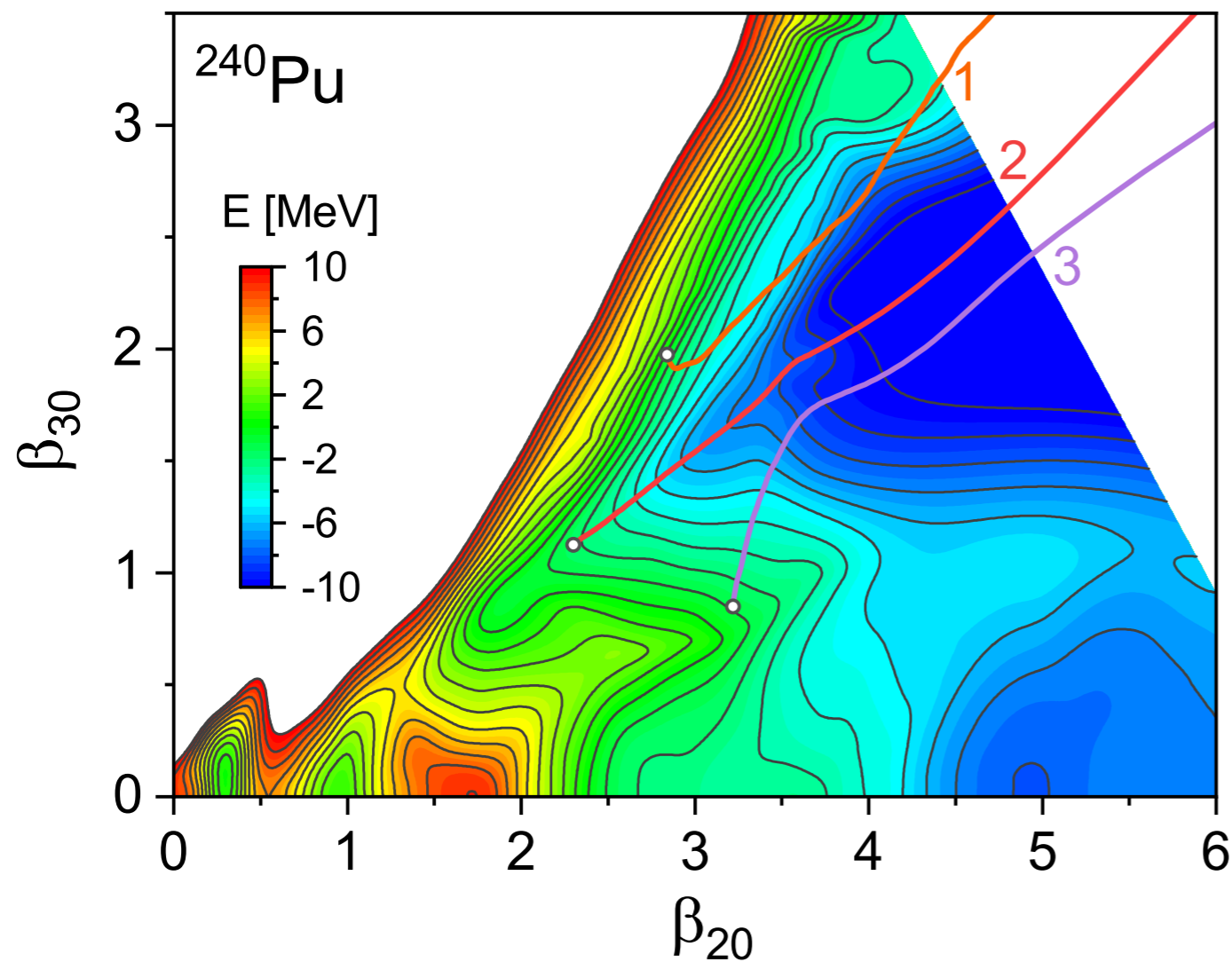
$$i \frac{d}{dt} \kappa_k(t) = [\varepsilon_k(t) + \varepsilon_{\bar{k}}(t)] \kappa_k(t) + \Delta_k(t) [2n_k(t) - 1].$$

\rightarrow automatically includes the one-body dissipation mechanism, but can only model a single fission event by propagating the nucleons independently.

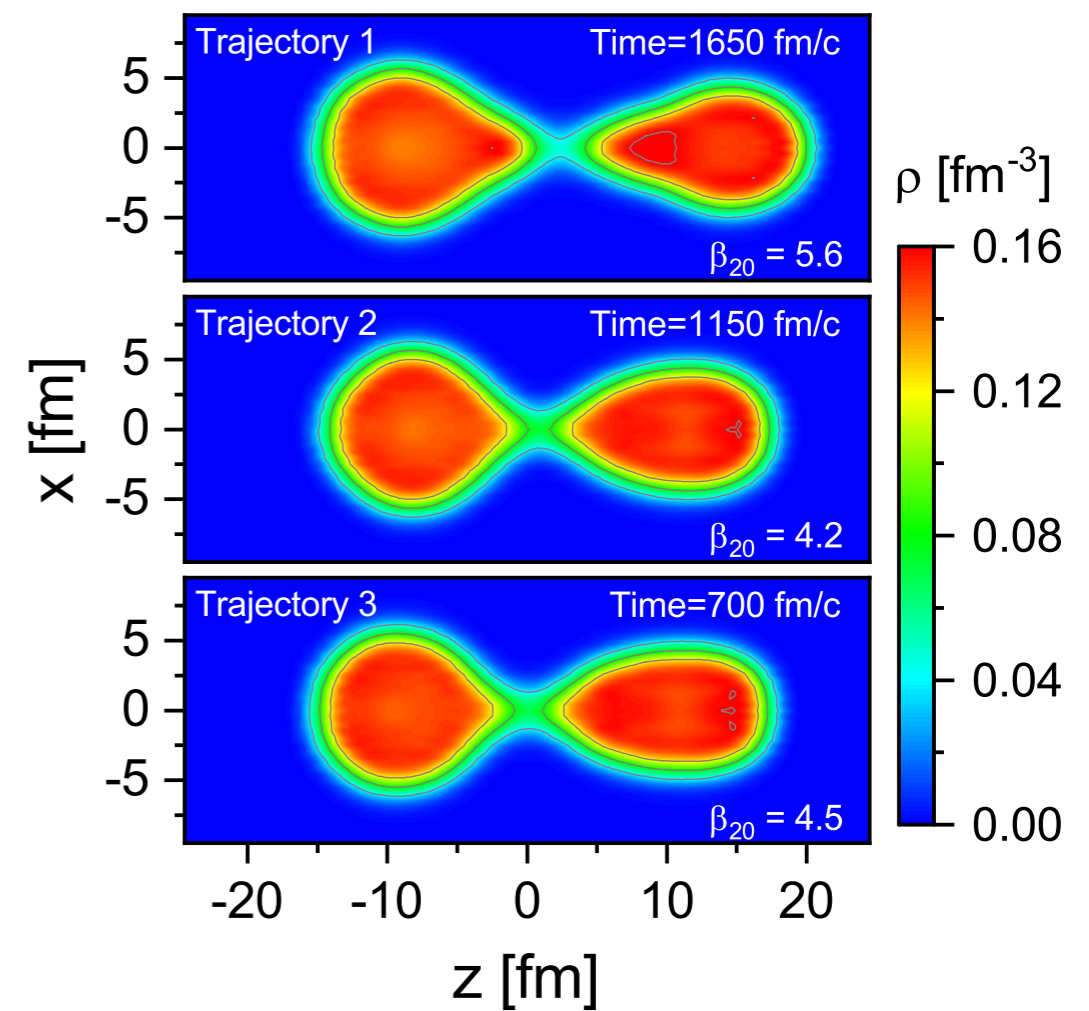
Dynamical synthesis of ^4He in the scission phase of nuclear fission

Ren, Vretenar, Nikšić, Zhao, Zhao, Meng, Phys. Rev. Lett. **128**, 172501 (2022).

TDDFT fission trajectories



Density profiles at times immediately prior to the scission event.



Nucleon localization functions:

σ (\uparrow or \downarrow)
 q (n or p)

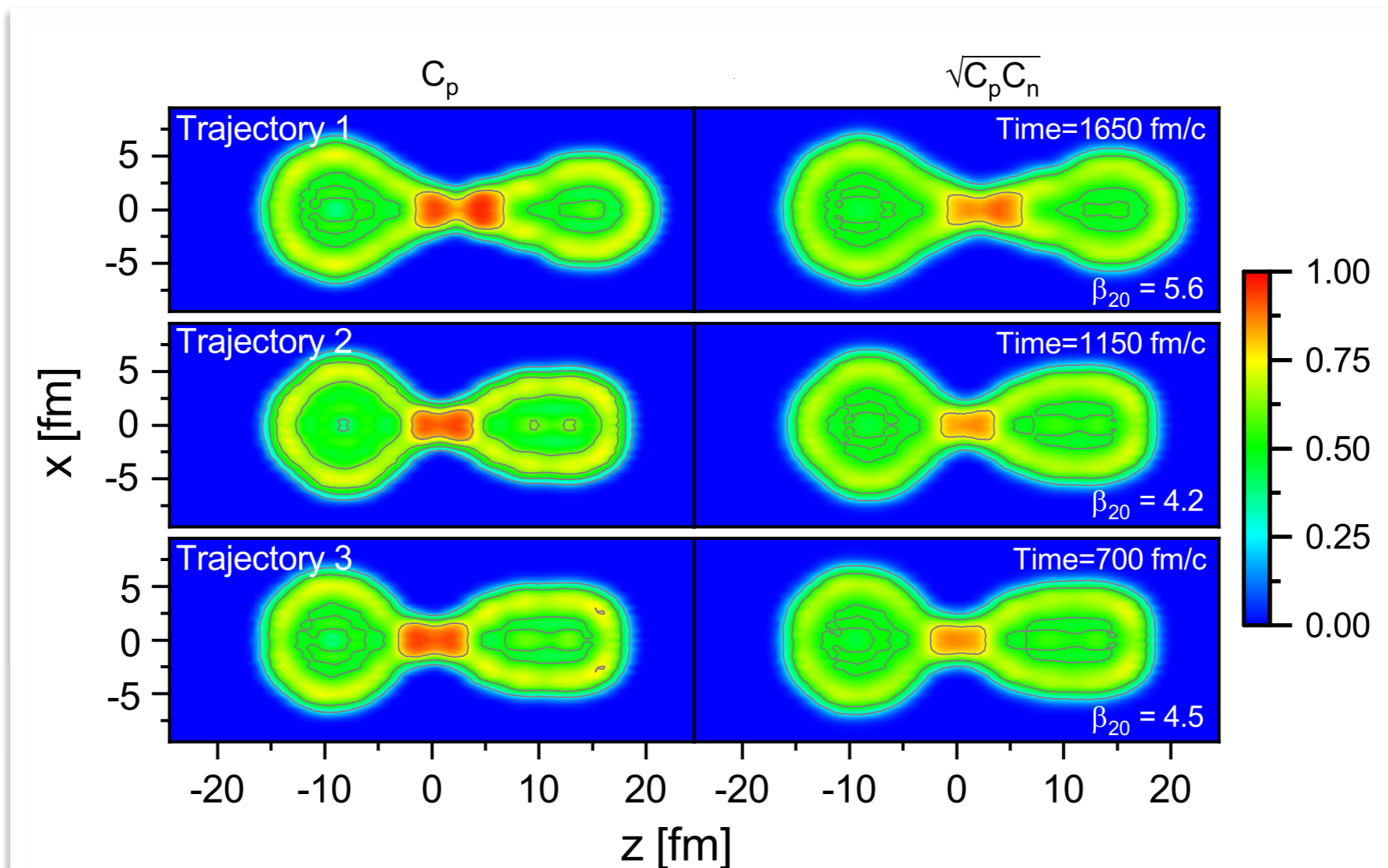
$$C_{q\sigma}(\vec{r}) = \left[1 + \left(\frac{\tau_{q\sigma} \rho_{q\sigma} - \frac{1}{4} |\vec{\nabla} \rho_{q\sigma}|^2 - j_{q\sigma}^2}{\rho_{q\sigma} \tau_{q\sigma}^{\text{TF}}} \right)^2 \right]^{-1}$$

kinetic energy density
density
current density

$$\tau_{q\sigma}^{\text{TF}} = \frac{3}{5} (6\pi^2)^{2/3} \rho_{q\sigma}^{5/3}$$

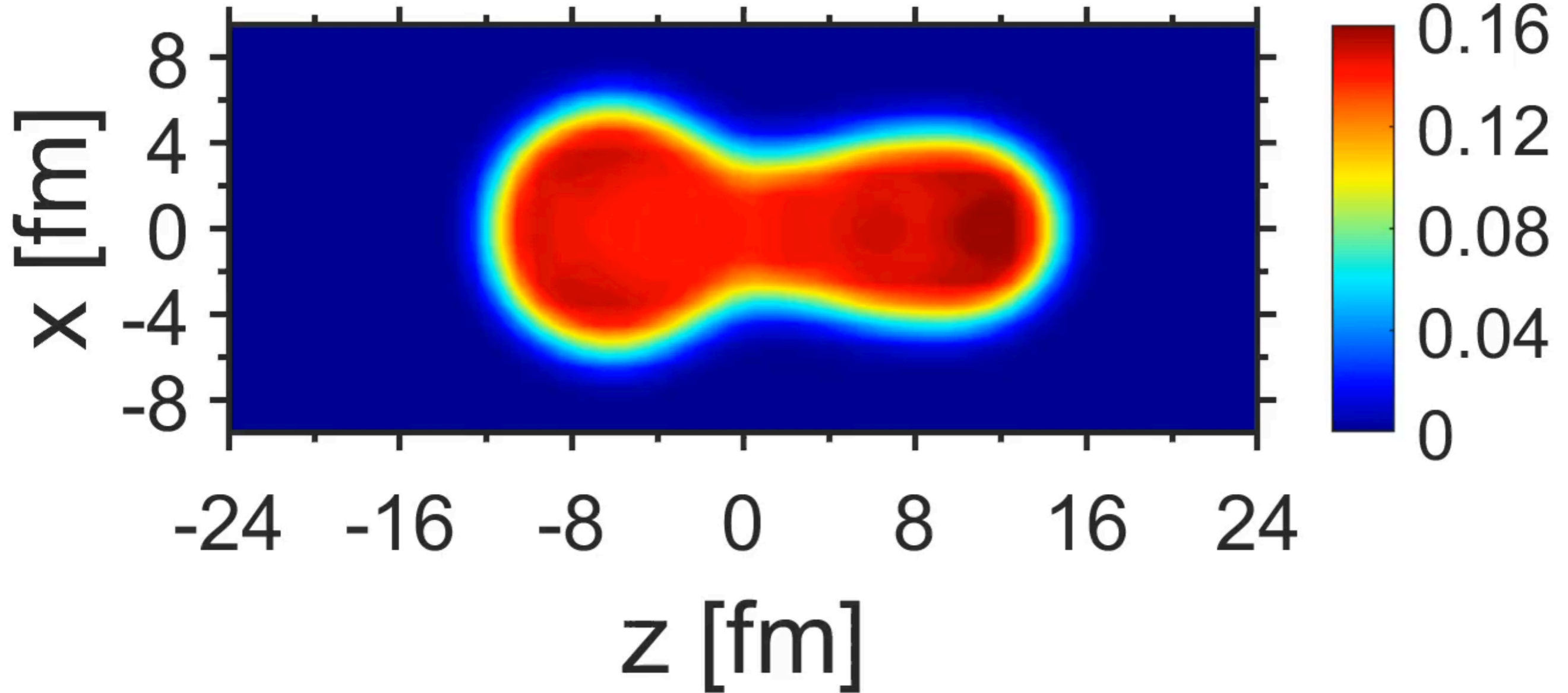
For homogeneous nuclear matter: $C_{q\sigma} = 1/2$

For the α -cluster of four particles: $C_{q\sigma}(\vec{r}) \approx 1$



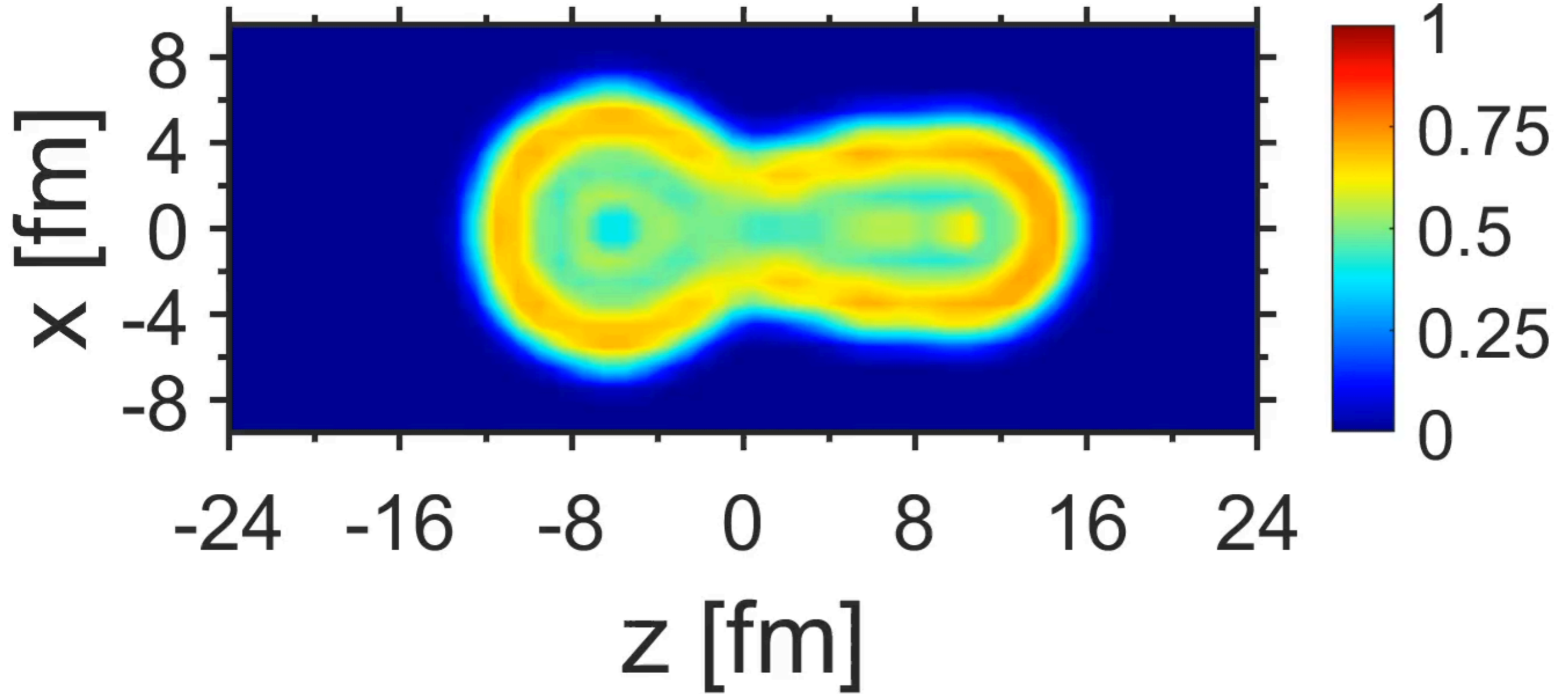
Trajectory 2

^{240}Pu , time = 0 fm/c

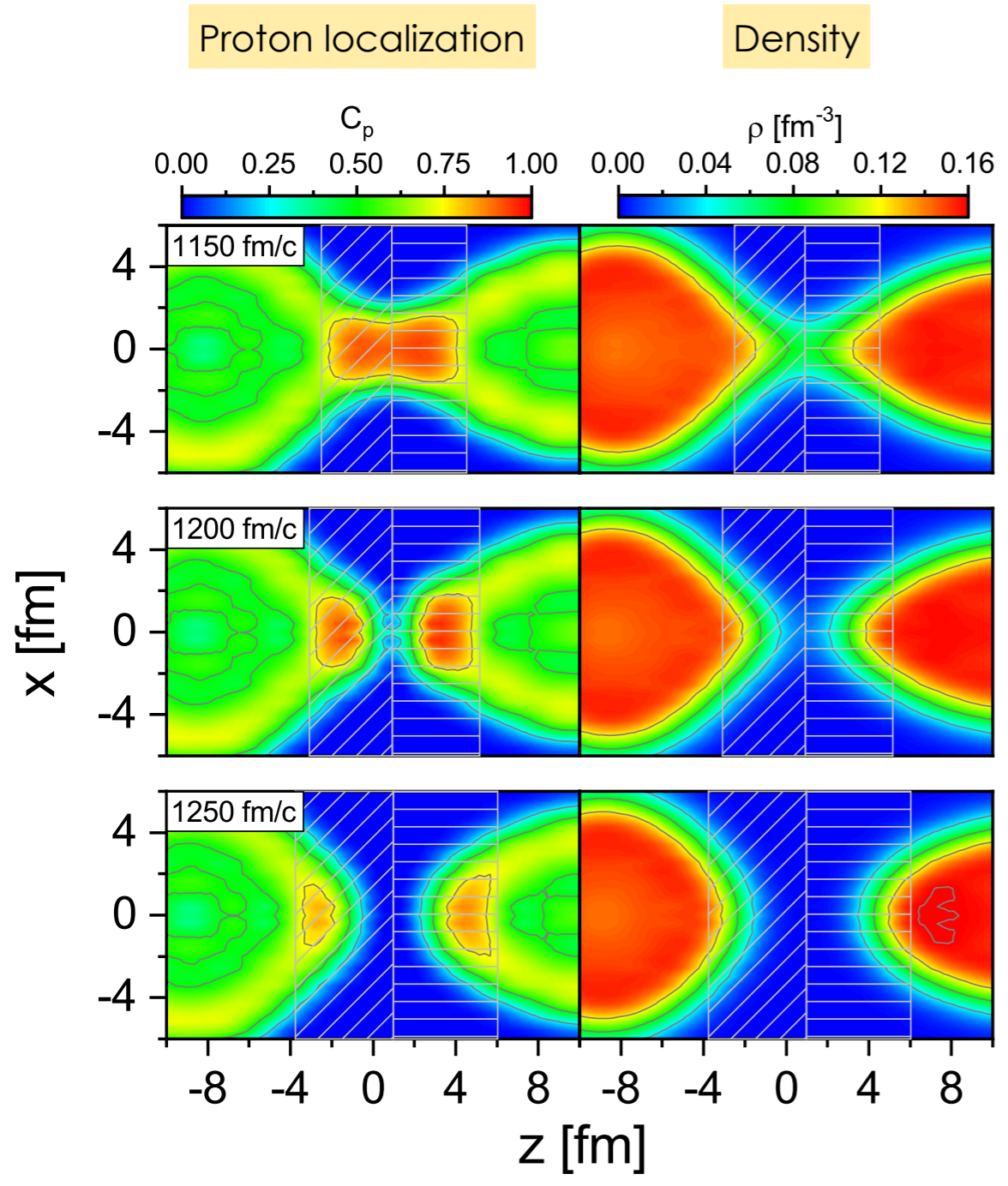


Trajectory 2

^{240}Pu , time = 0 fm/c



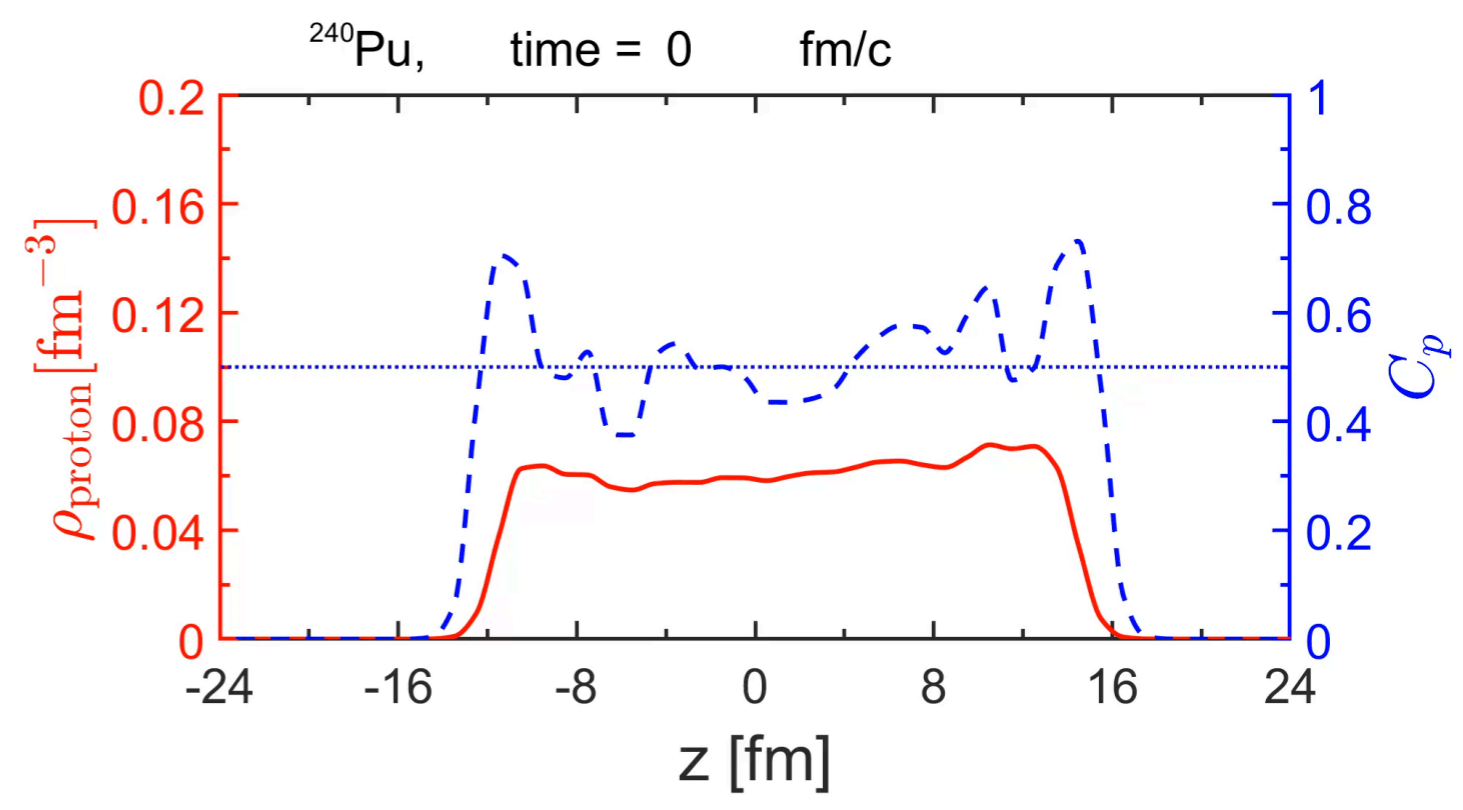
Trajectory 2



When are these light clusters formed?

What is their structure?

What is their role in the scission mechanism?

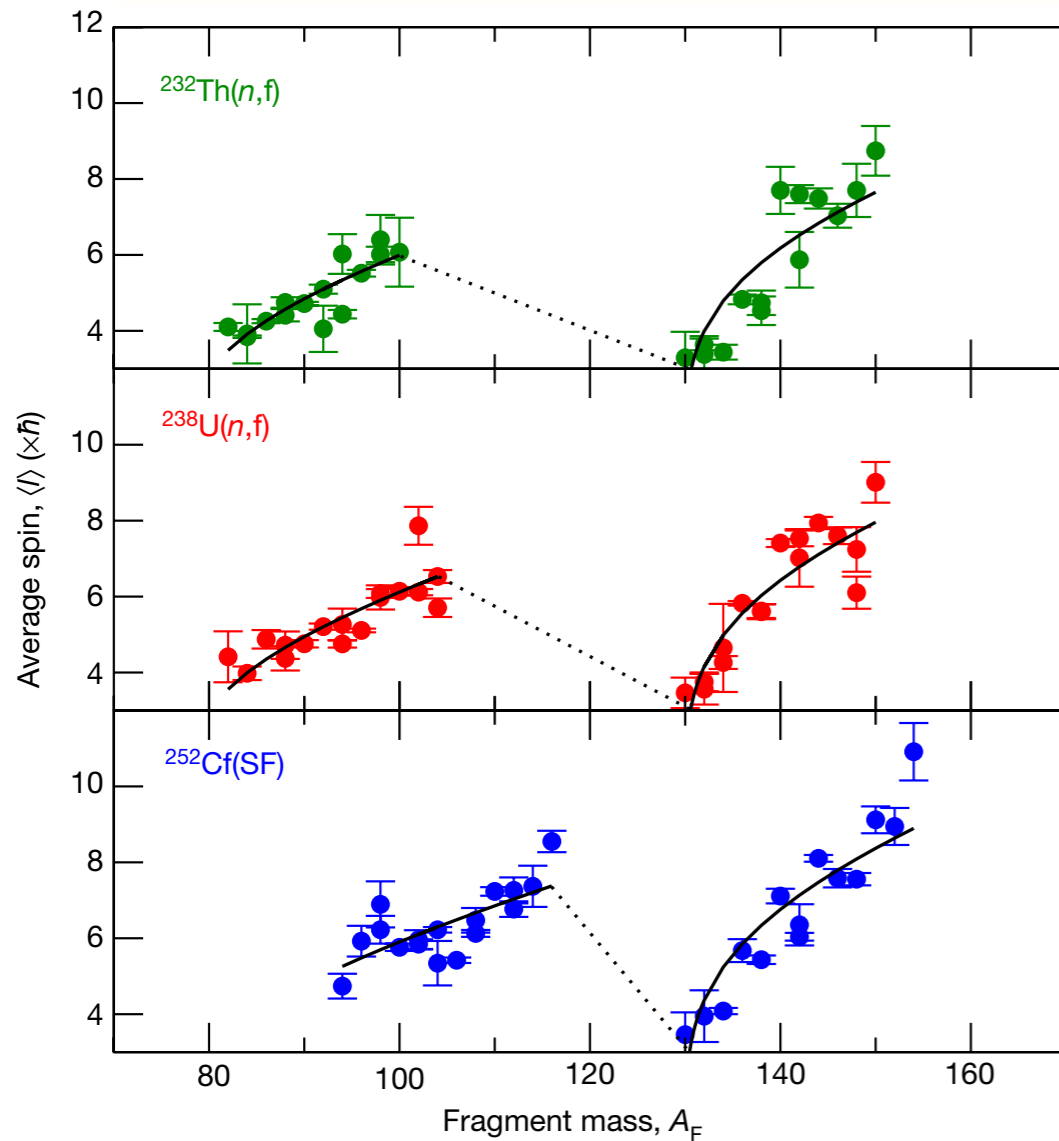


Generation and dynamics of FF angular momenta

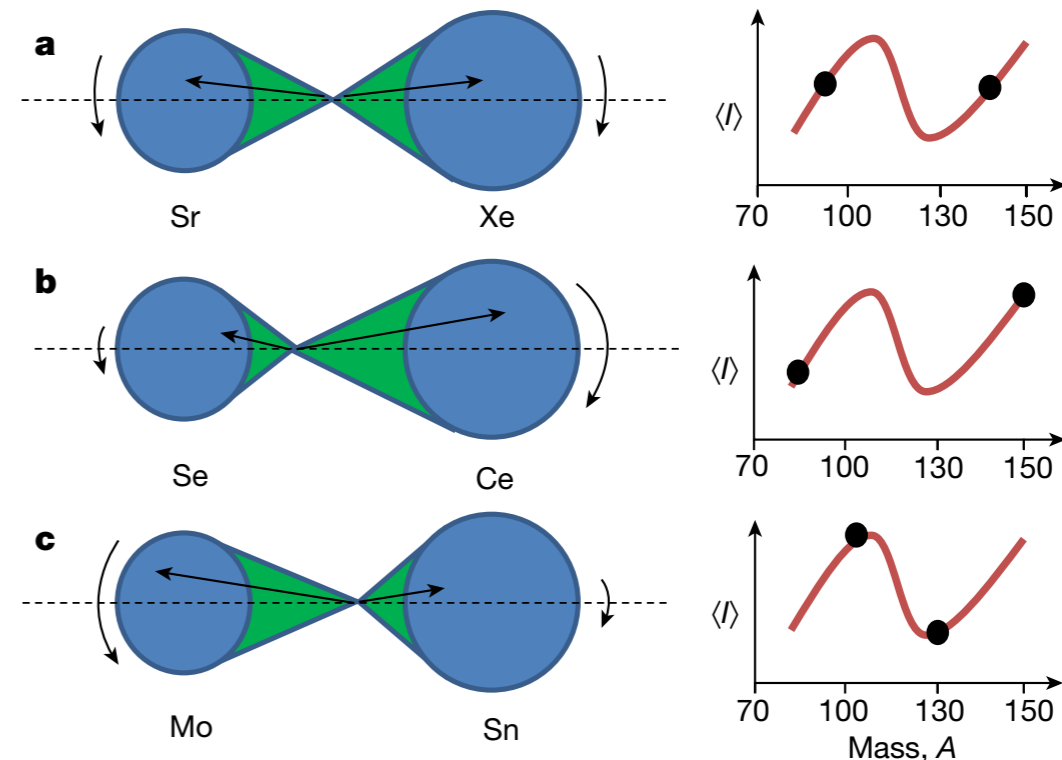
J. N. Wilson

566 | Nature | Vol 590 |

Dependence of average spin (after neutron emission) on fragment mass.



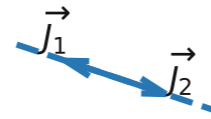
- no dependence of fragment spin on the mass or charge of the partner nucleus.
- no significant correlations between the spins of the fragment partners \rightarrow angular momentum is generated after the nucleus splits into fragments (post-scission).
- the collective motion of nucleons in the ruptured neck of the fissioning system generates two independent torques, analogous to the snapping of an elastic band.



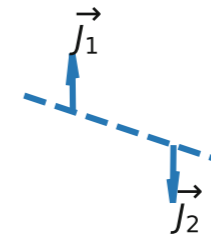
Microscopic studies based on TDDFT → the intrinsic spin dynamics of fission fragments is three-dimensional (3D) and all FF spin modes are active.

Conclusion → the average FF spin measured after statistical emissions is not necessarily connected with the scission mechanism.

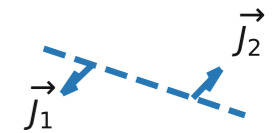
Twisting



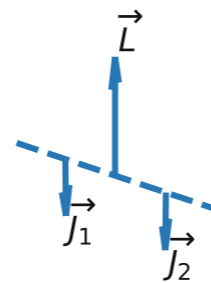
Bending



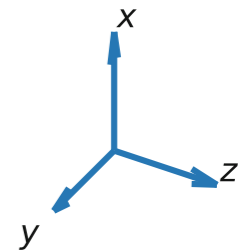
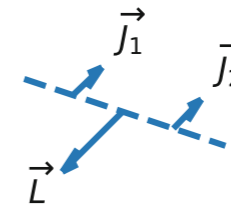
Bending



Wriggling



Wriggling

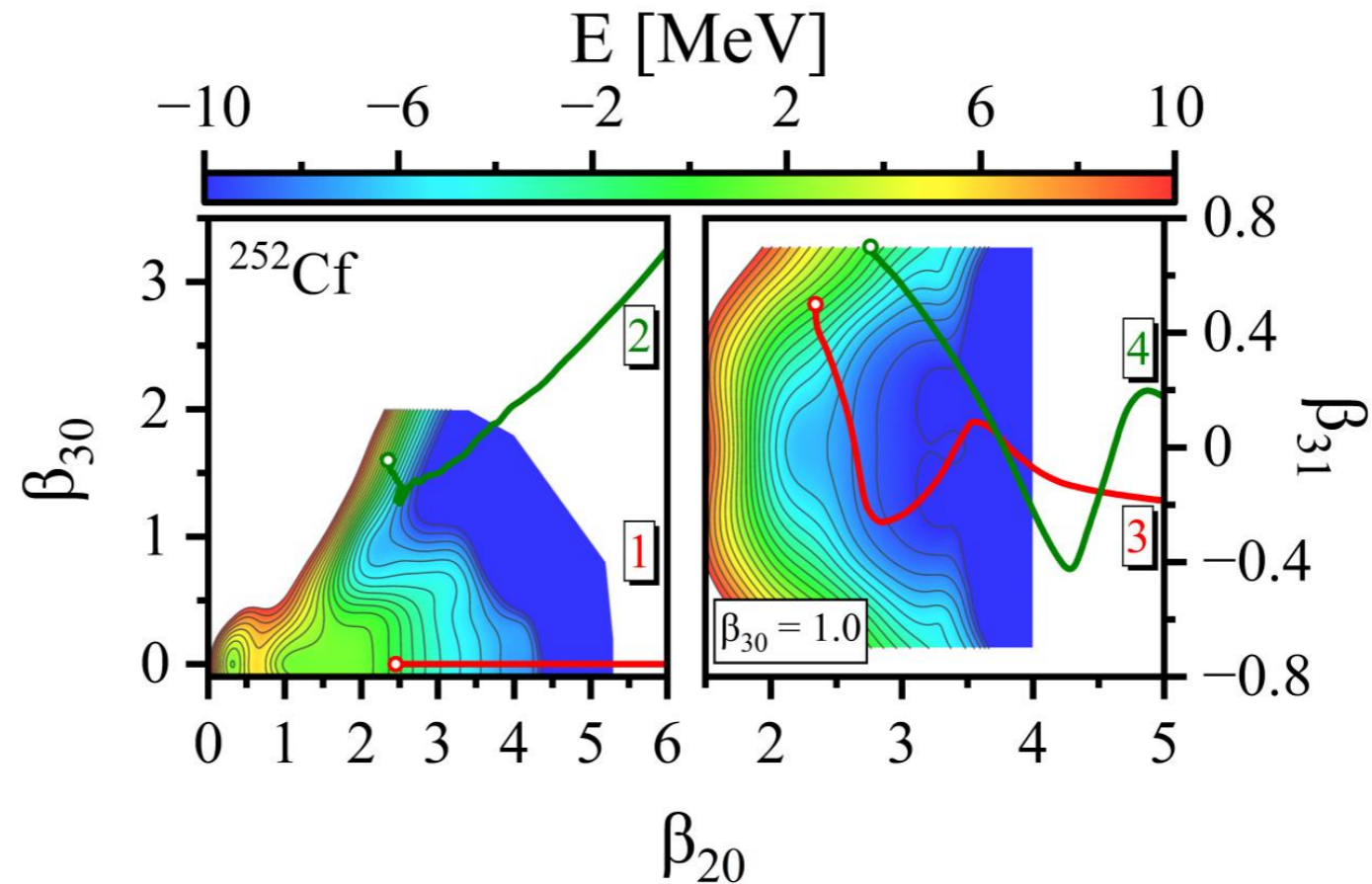


Intrinsic generation of angular momenta and entanglement in fission

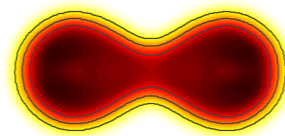
Li, Zhang, Vretenar, Nikšić, Zhao, Meng, Phys. Rev. Lett. (2026)

Spontaneous fission of ^{252}Cf

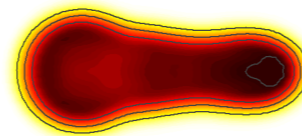
TD DFT trajectories:



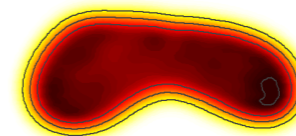
Initial state:



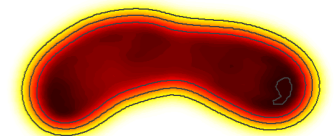
1



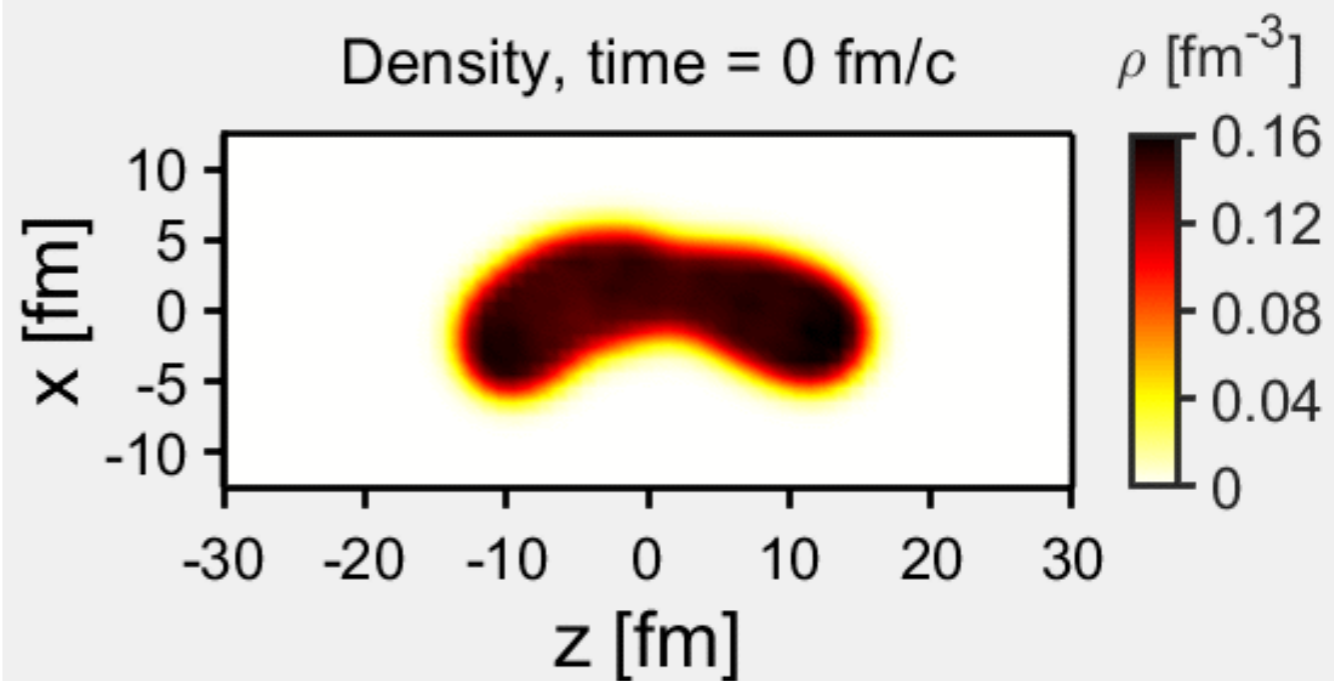
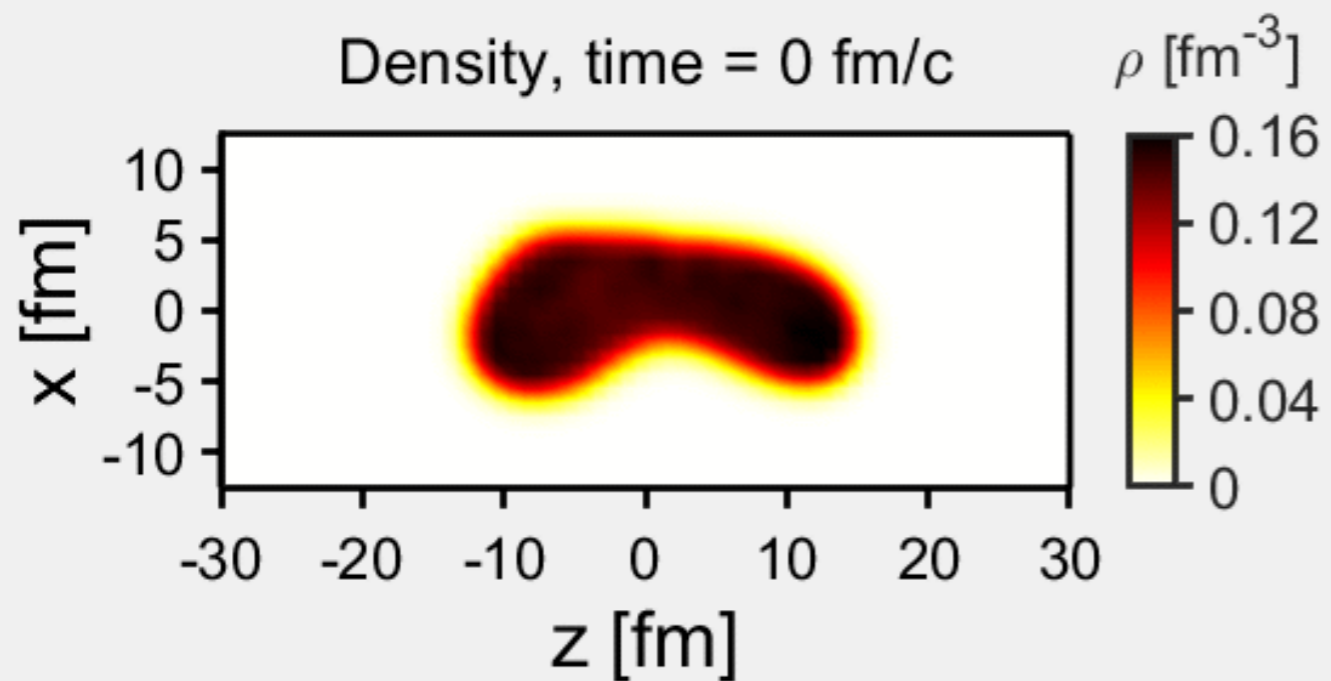
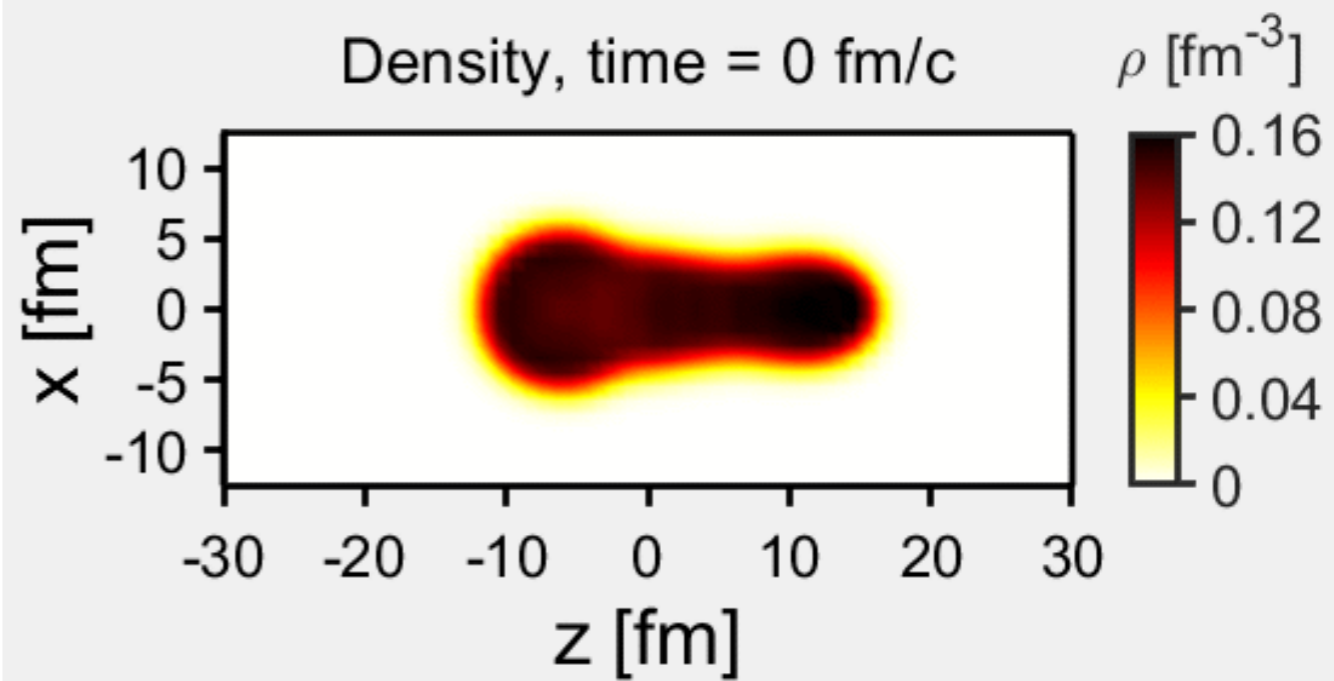
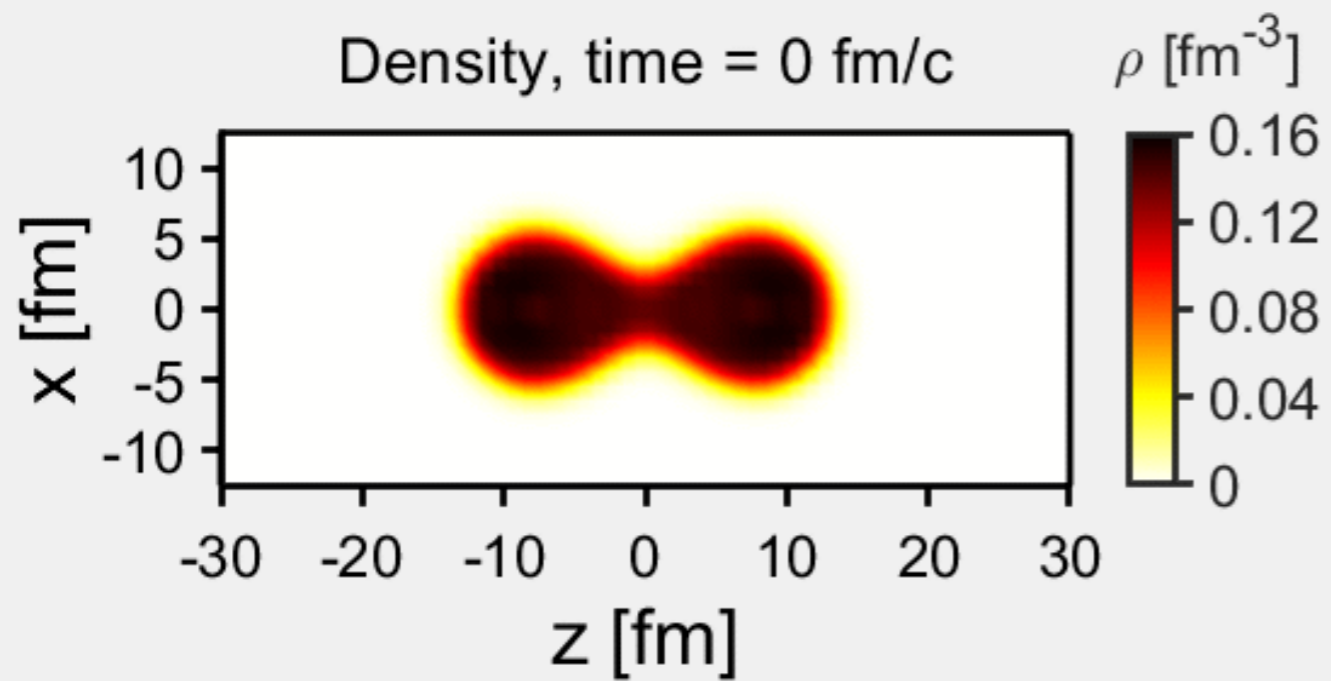
2



3

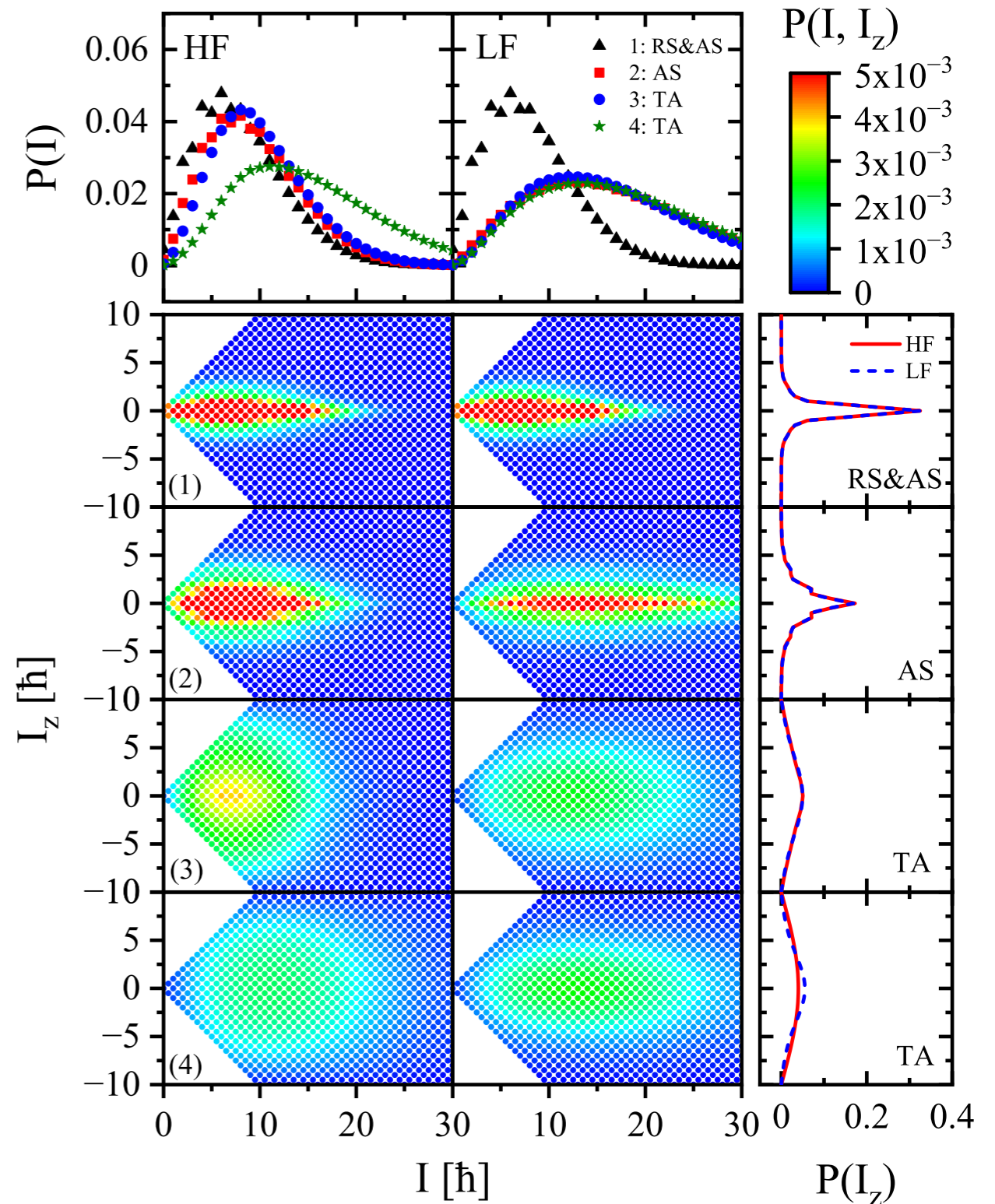
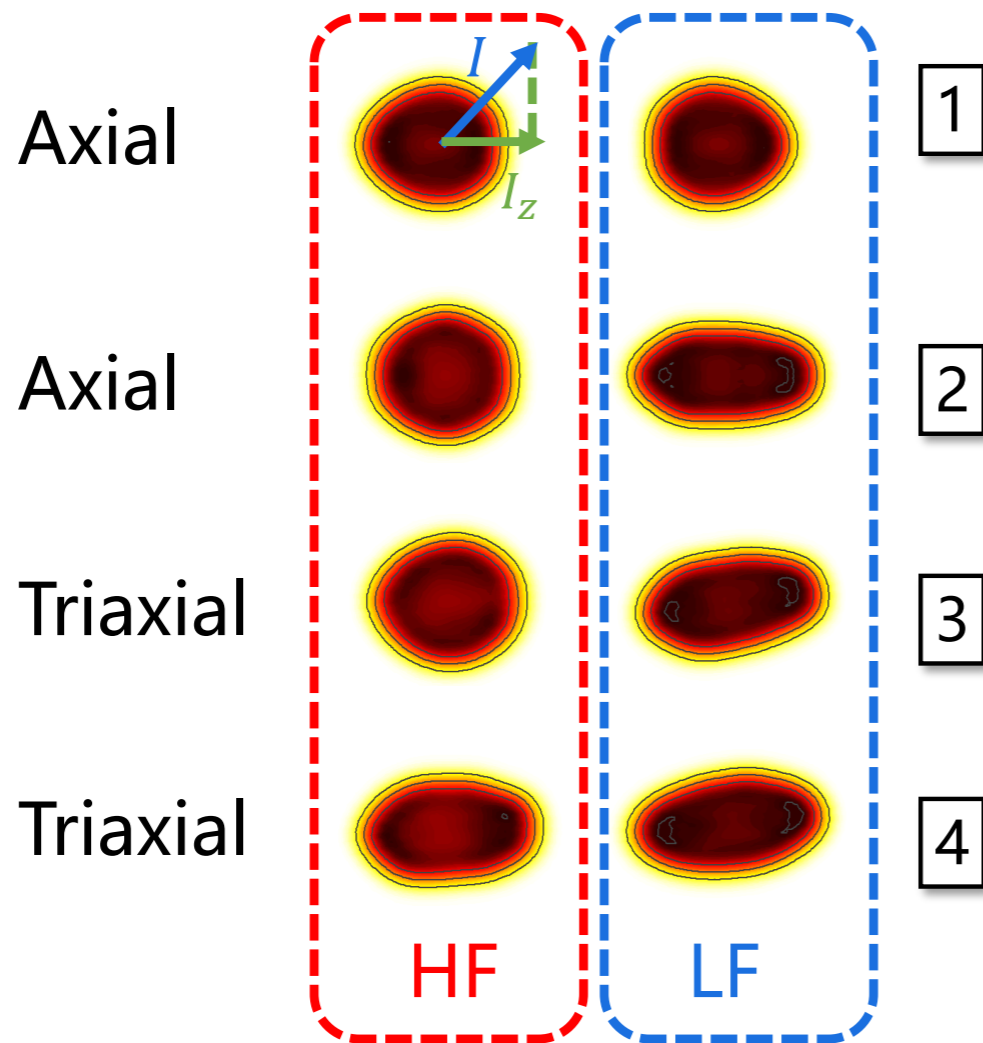


4



Spin distribution $P(I, I_z)$ for each fragment:

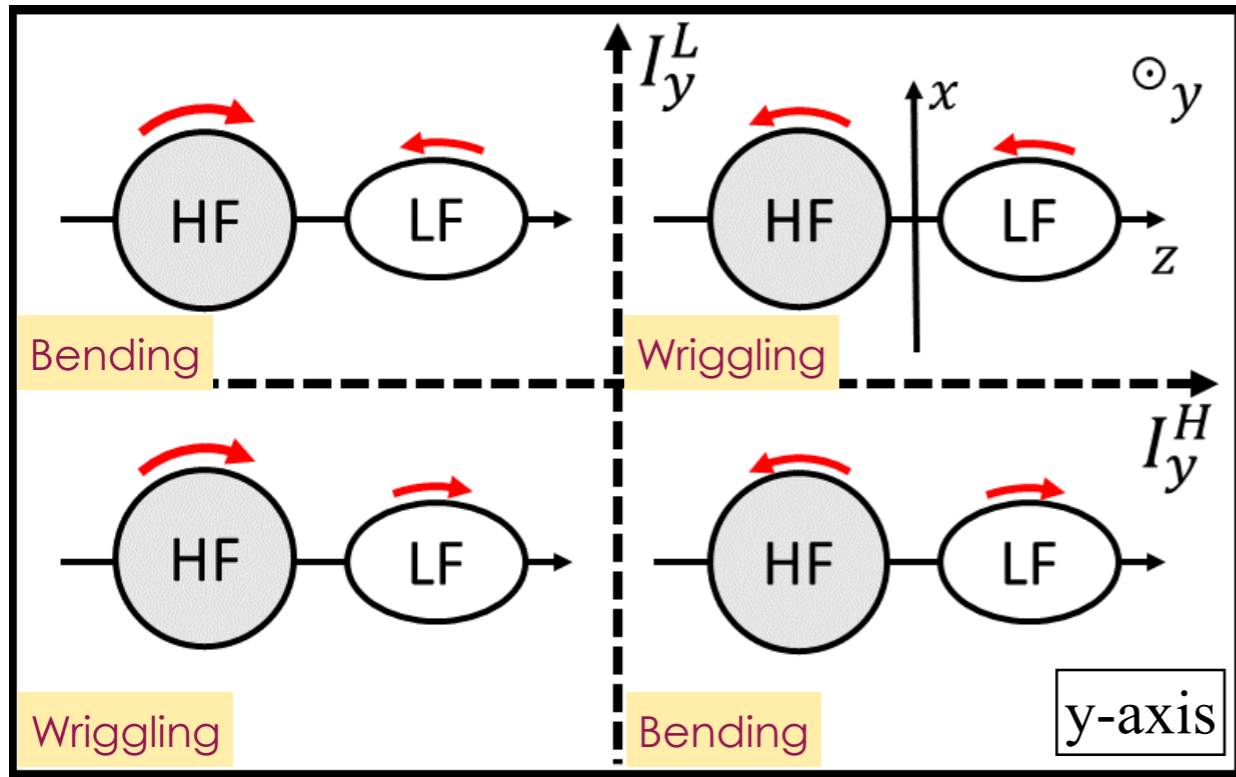
$$\begin{aligned}
 P(I, I_z) &= \langle \Psi | \hat{P}_{I_z I_z}^I | \Psi \rangle \\
 &= \frac{2I + 1}{16\pi^2} \int_0^{2\pi} d\alpha \int_0^\pi \sin \beta d\beta \int_0^{4\pi} d\gamma \\
 &D_{I_z I_z}^{I*}(\alpha, \beta, \gamma) \langle \Psi | e^{-i\hat{J}_z \alpha + i\hat{J}_y \beta + i\hat{J}_z \gamma} \Theta_{V_f}(\mathbf{r}) | \Psi \rangle,
 \end{aligned}$$



Correlations between the intrinsic angular momenta of the two FFs

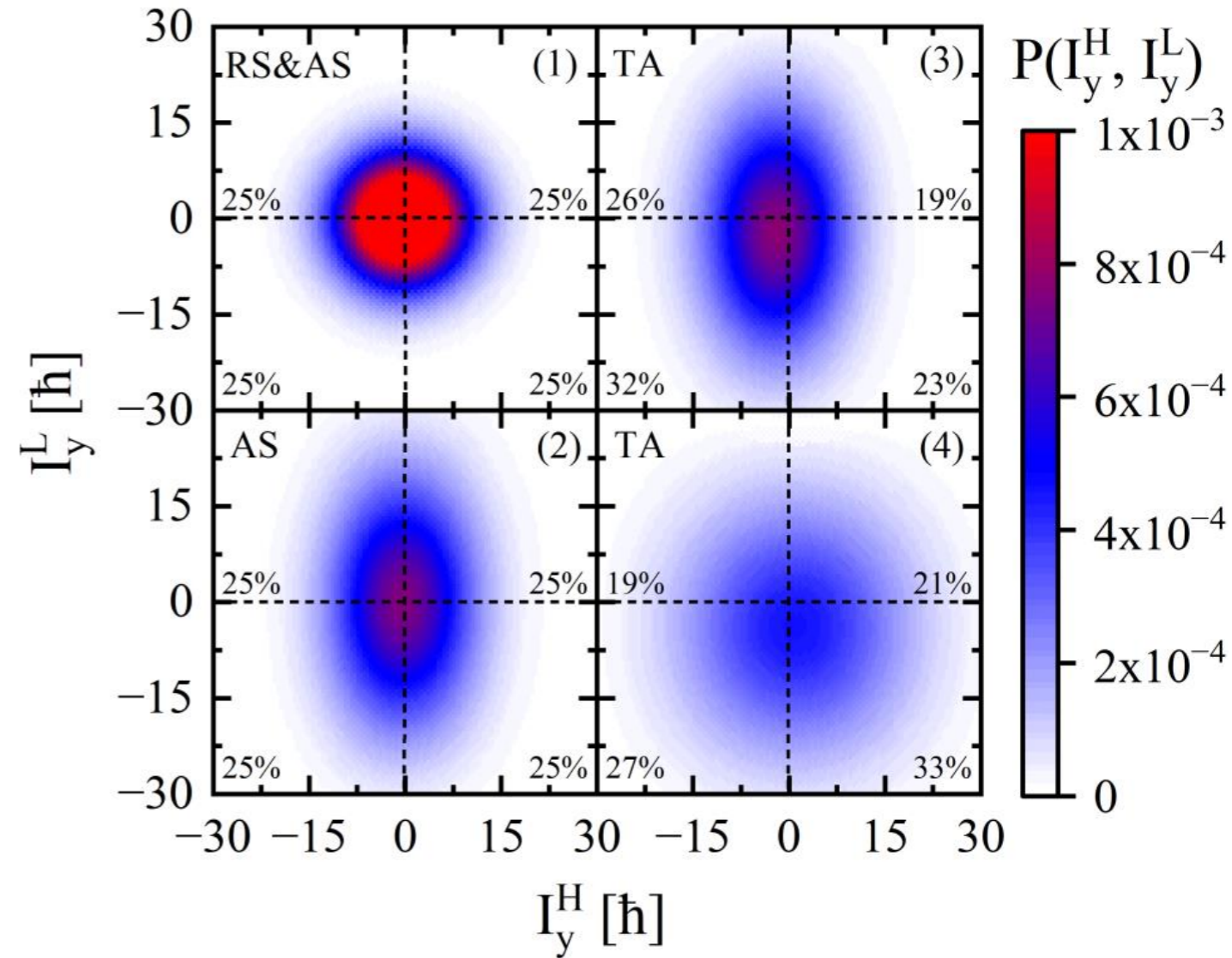
$$P(I_k^H, I_k^L) = \langle \Psi | \hat{P}_{I_k^H} \hat{P}_{I_k^L} | \Psi \rangle$$

Y-axis (perpendicular to the fission axis)



Axial

Triaxial

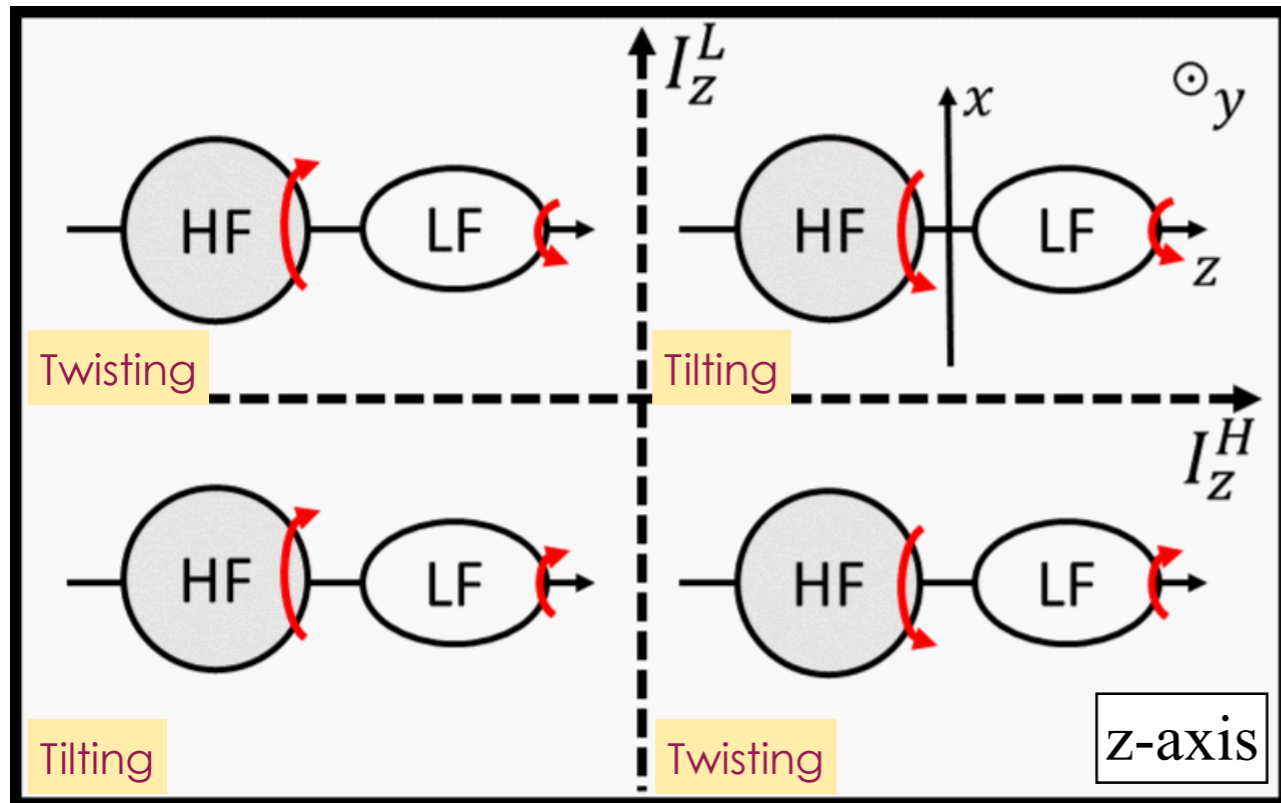


Triaxial degrees of freedom \Rightarrow the probabilities of bending and wriggling motion are not identical!

Correlations between the intrinsic angular momenta of the two FFs

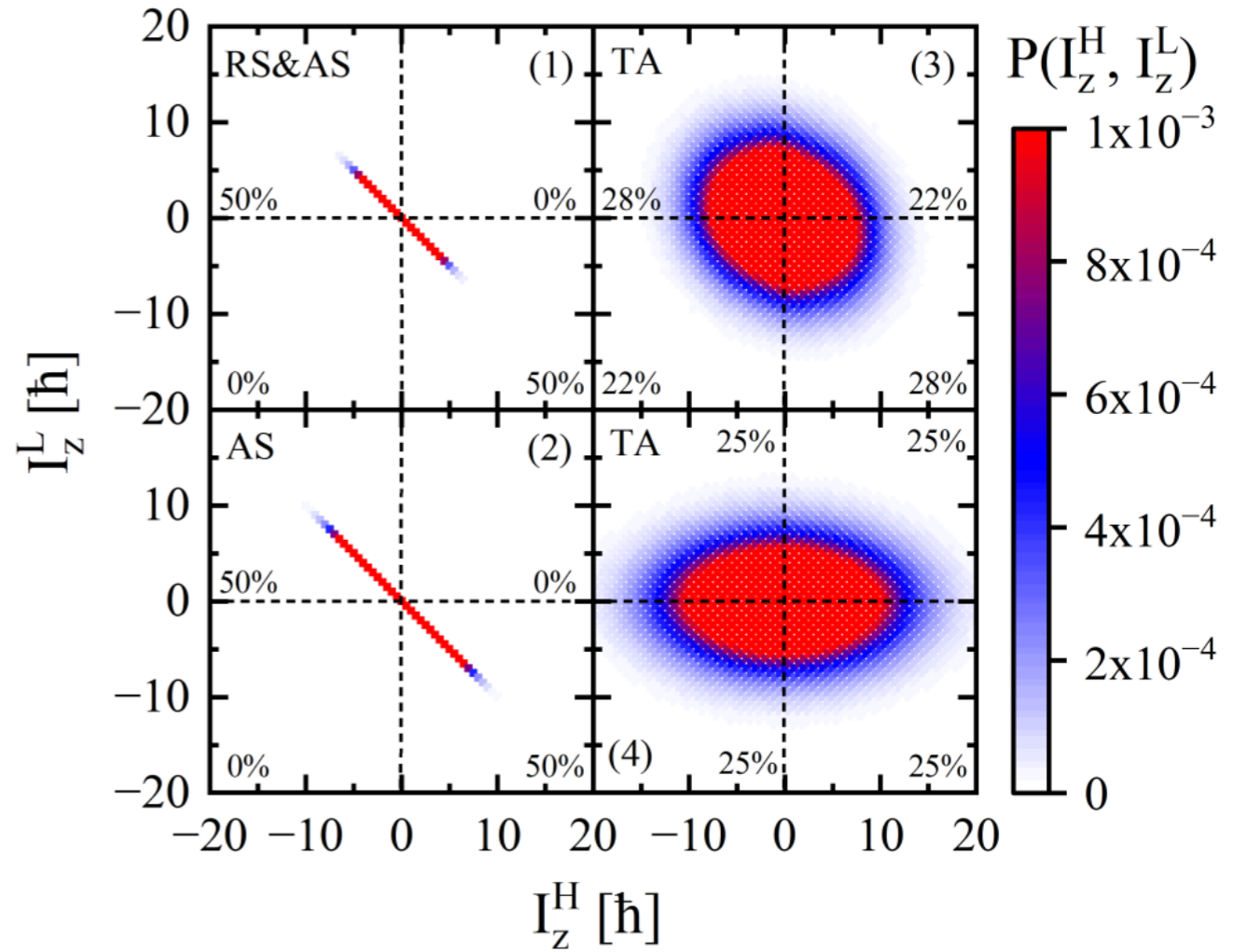
$$P(I_k^H, I_k^L) = \langle \Psi | \hat{P}_{I_k^H} \hat{P}_{I_k^L} | \Psi \rangle$$

Z-axis (fission axis)



Axial

Triaxial



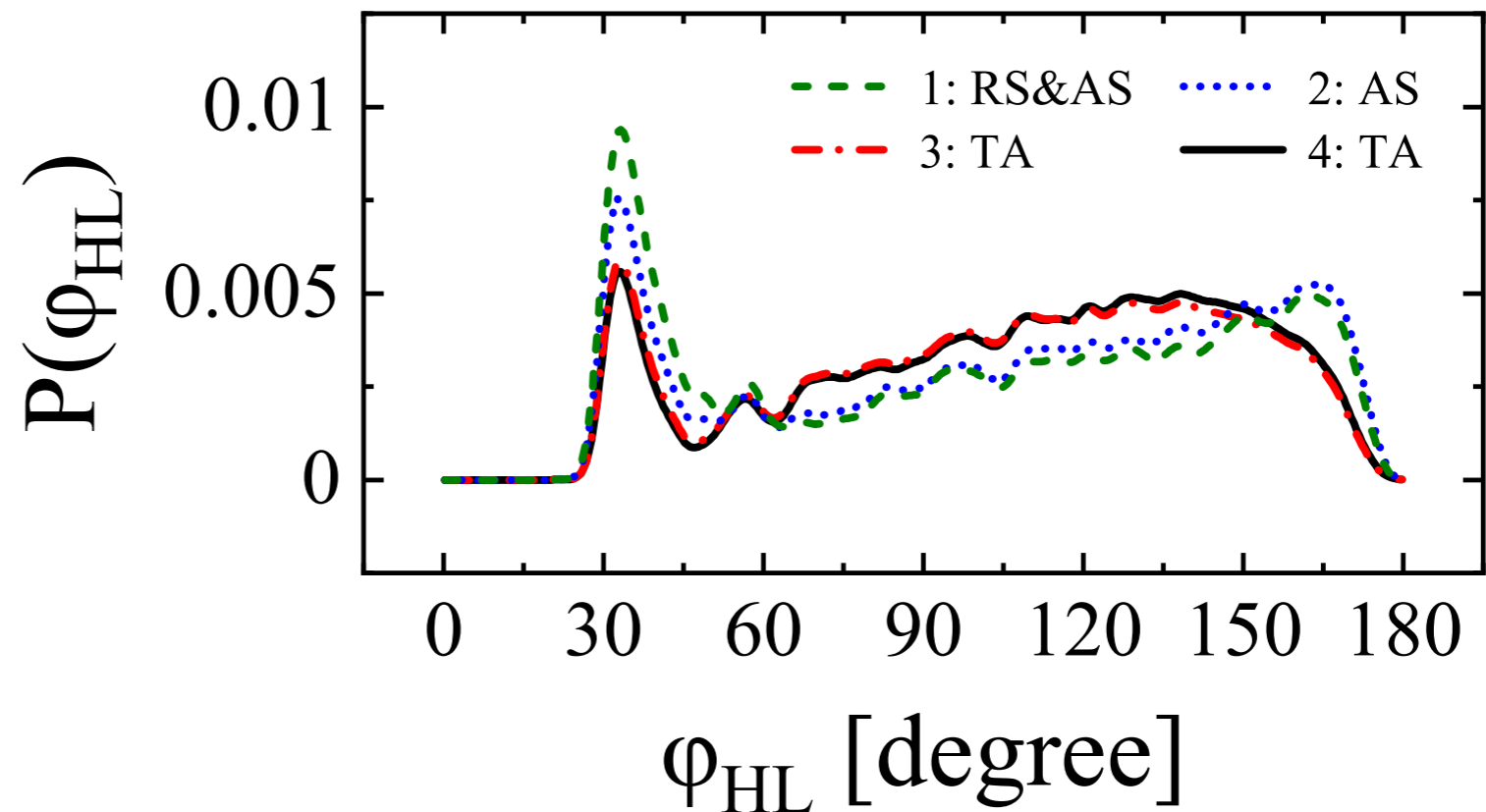
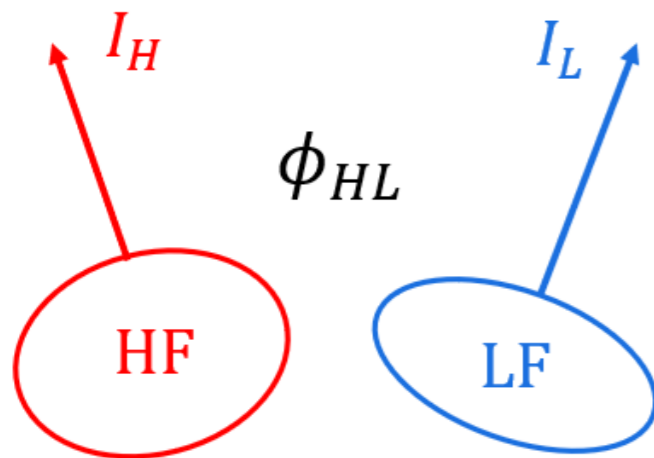
The opening angle ϕ_{HL} between the spins of the heavy and light FFs

The triple distribution $P(\Lambda, I_H, I_L)$:

$$P(\Lambda, I_H, I_L) = \sum_{\Lambda_z, I_z^H, I_z^L} \langle \Psi | \hat{P}_{\Lambda_z \Lambda_z}^\Lambda \hat{P}_{I_z^H I_z^H}^{I_H} \hat{P}_{I_z^L I_z^L}^{I_L} | \Psi \rangle$$

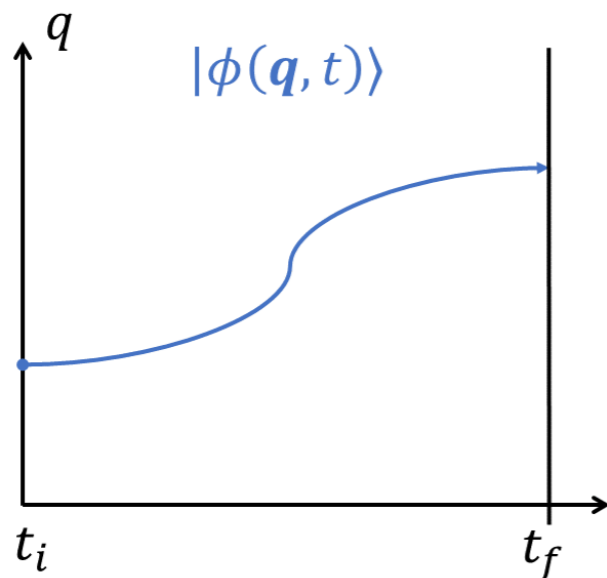
The opening angle:

$$\phi'_{HL}(\Lambda, I_H, I_L) = \arccos \left(\frac{\Lambda(\Lambda + 1) - I_H(I_H + 1) - I_L(I_L + 1)}{2\sqrt{I_H(I_H + 1)I_L(I_L + 1)}} \right)$$



TD DFT

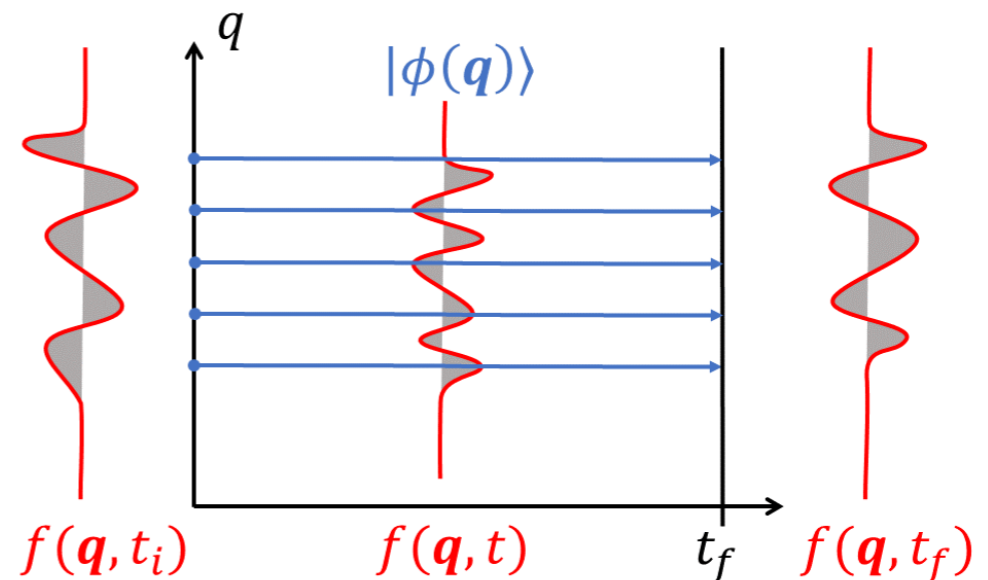
$$|\Psi(t)\rangle = |\phi(\mathbf{q}, t)\rangle$$



...one-body dissipation but no quantum fluctuations.

TD GCM

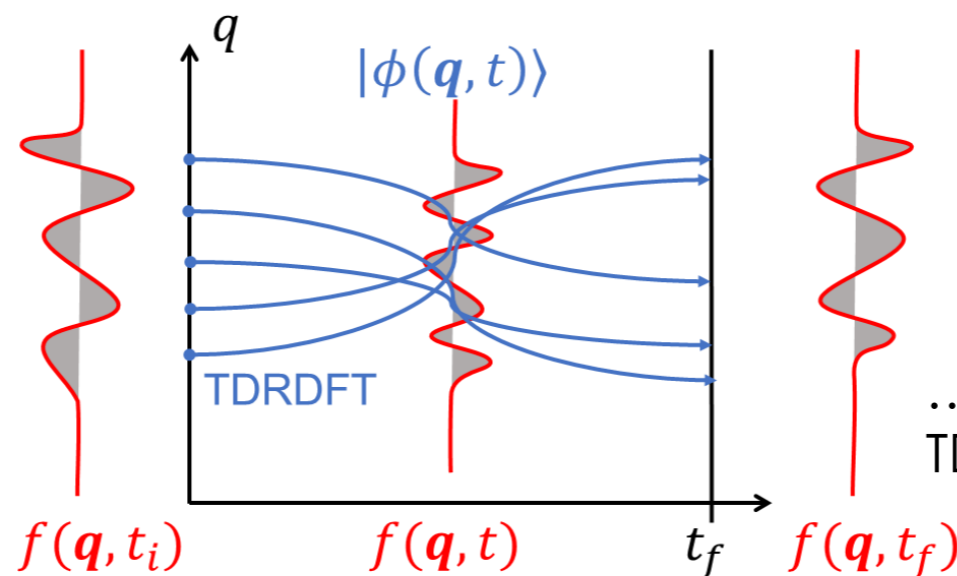
$$|\Psi(t)\rangle = \int_{\mathbf{q}} f(\mathbf{q}, t) |\phi(\mathbf{q})\rangle$$



...quantum fluctuations in collective coordinates but no dissipation mechanism.

Generalized TD GCM

$$|\Psi(t)\rangle = \int_{\mathbf{q}} f(\mathbf{q}, t) |\phi(\mathbf{q}, t)\rangle$$



...superposition of independent TD DFT trajectories.

Generalized time-dependent generator coordinate method

Li, Vretenar, Nikšić, Zhao, Meng, Phys. Rev. C **108**, 014321 (2023).

Li, Vretenar, Nikšić, Zhao, Zhao, Meng, Front. Phys. **19**, 44201 (2024).

The nuclear wave function: $|\Psi(t)\rangle = \sum_q f_q(t) |\Phi_q(t)\rangle \Rightarrow i\hbar\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$

\Rightarrow equation of motion for the weight functions: $\sum_q i\hbar\mathcal{N}_{q'q}(t)\partial_t f_q(t) + \sum_q \mathcal{H}_{q'q}^{MF}(t)f_q(t) = \sum_q \mathcal{H}_{q'q}(t)f_q(t)$

...time-dependent kernels:

$$\left\{ \begin{array}{l} \mathcal{N}_{q'q}(t) = \langle \Phi_{q'}(t) | \Phi_q(t) \rangle, \\ \mathcal{H}_{q'q}(t) = \langle \Phi_{q'}(t) | \hat{H} | \Phi_q(t) \rangle, \\ \mathcal{H}_{q'q}^{MF}(t) = \langle \Phi_{q'}(t) | i\hbar\partial_t | \Phi_q(t) \rangle, \end{array} \right.$$

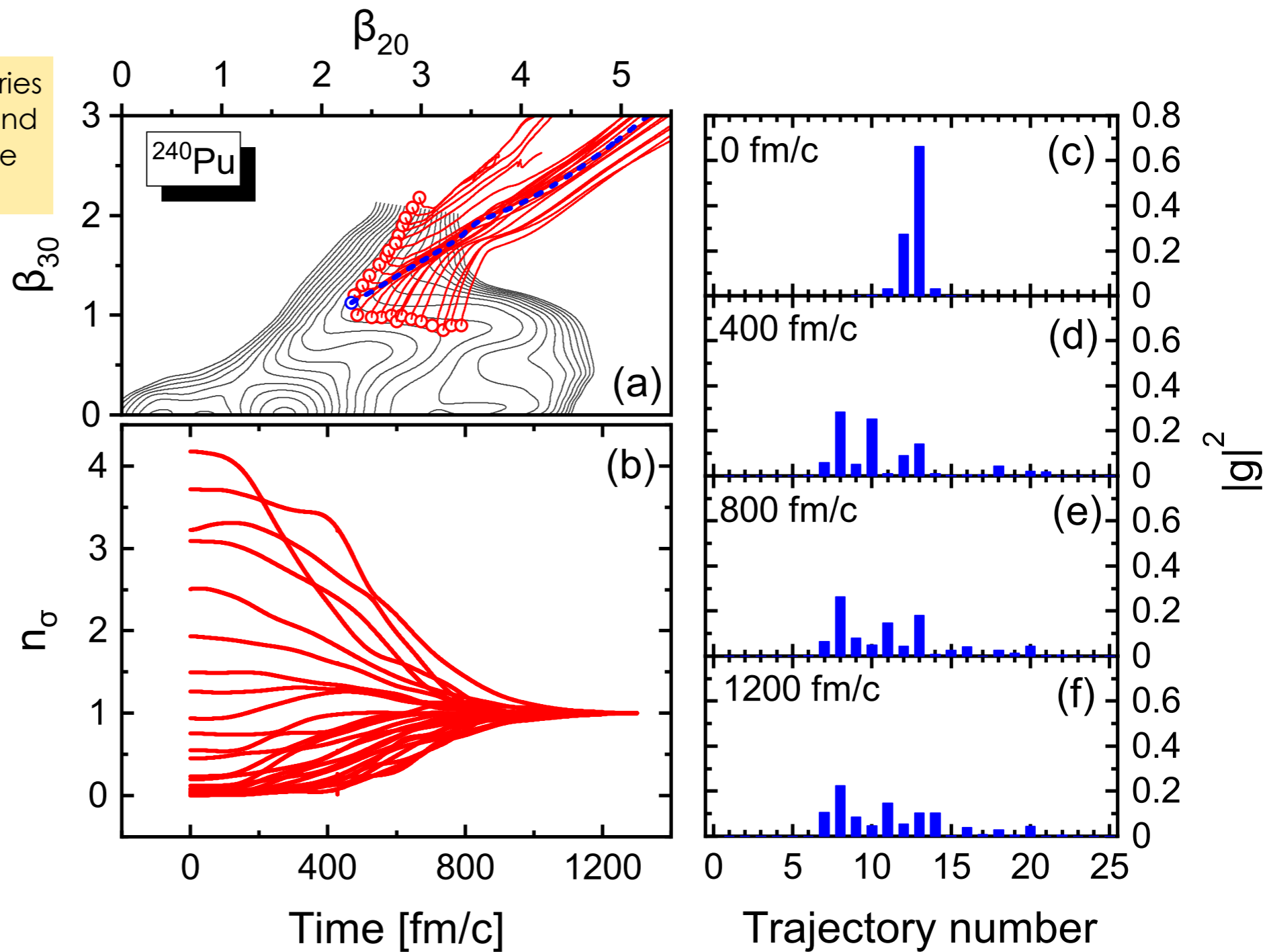
The time-dependent generator states are independent TDDFT fission trajectories on the PES.

...collective wave function: $g = \mathcal{N}^{1/2} f$

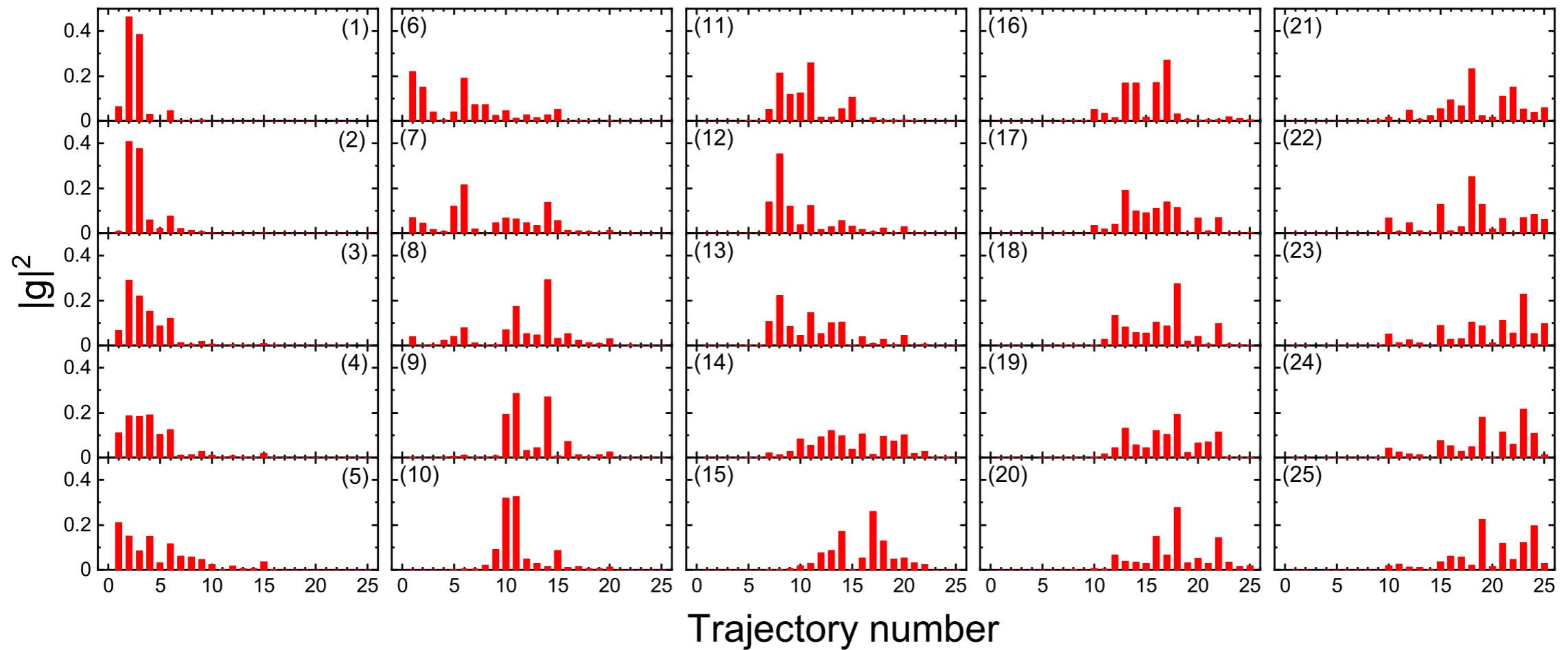
$$i\hbar\dot{g} = \mathcal{N}^{-1/2}(H - H^{MF})\mathcal{N}^{-1/2}g + i\hbar\dot{\mathcal{N}}^{1/2}\mathcal{N}^{-1/2}g.$$

Self-consistent TDDFT fission trajectories that start from the 25 initial points, and are used as a generator basis for the generalized TDGCM.

Time evolution of the eigenvalues of the norm kernel.



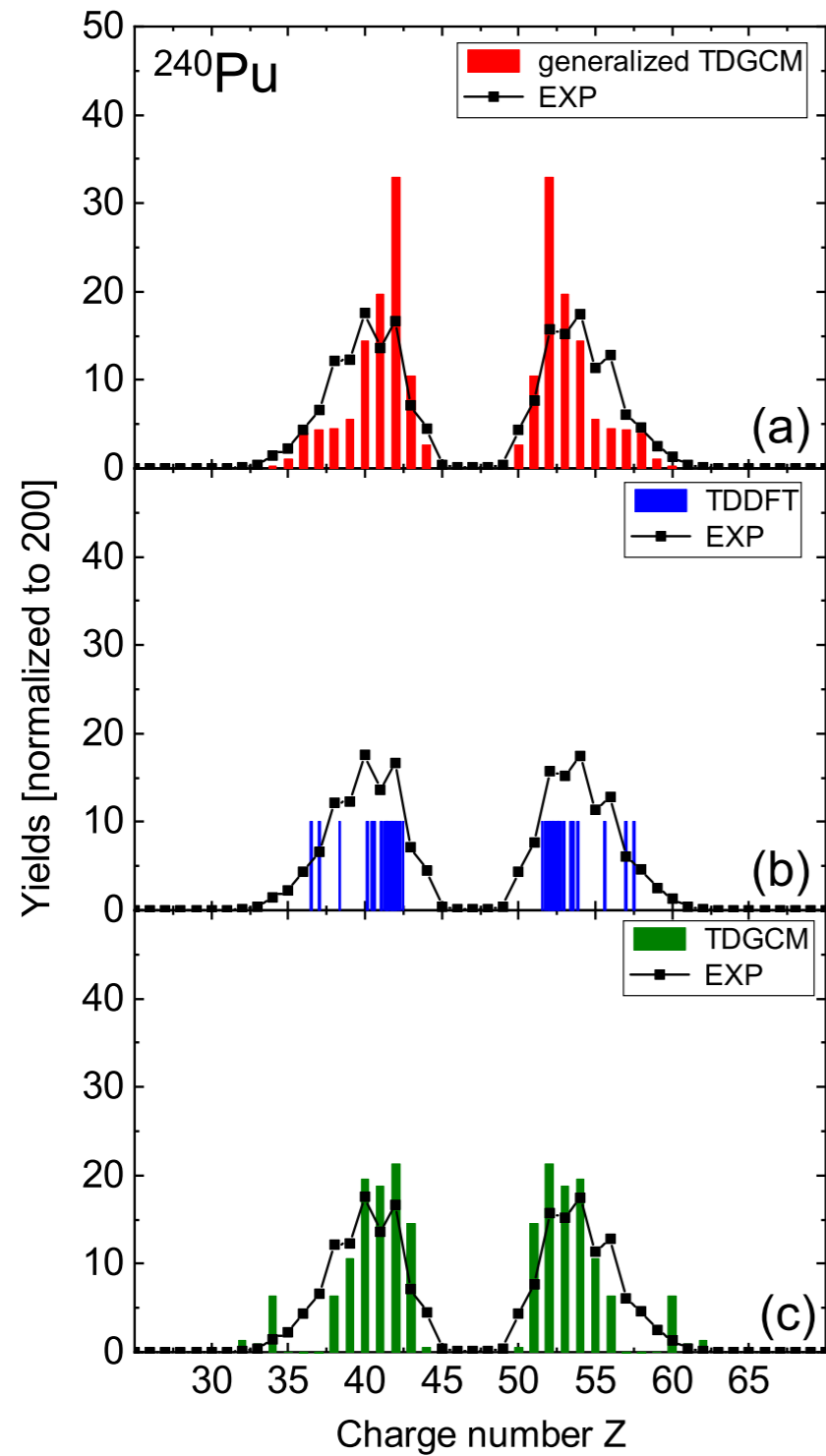
Square moduli of the components of the TDGCM collective wave function, that starts from the initial point $(\beta_{20}, \beta_{30}) = (2.30, 1.13)$ of trajectory number 13.



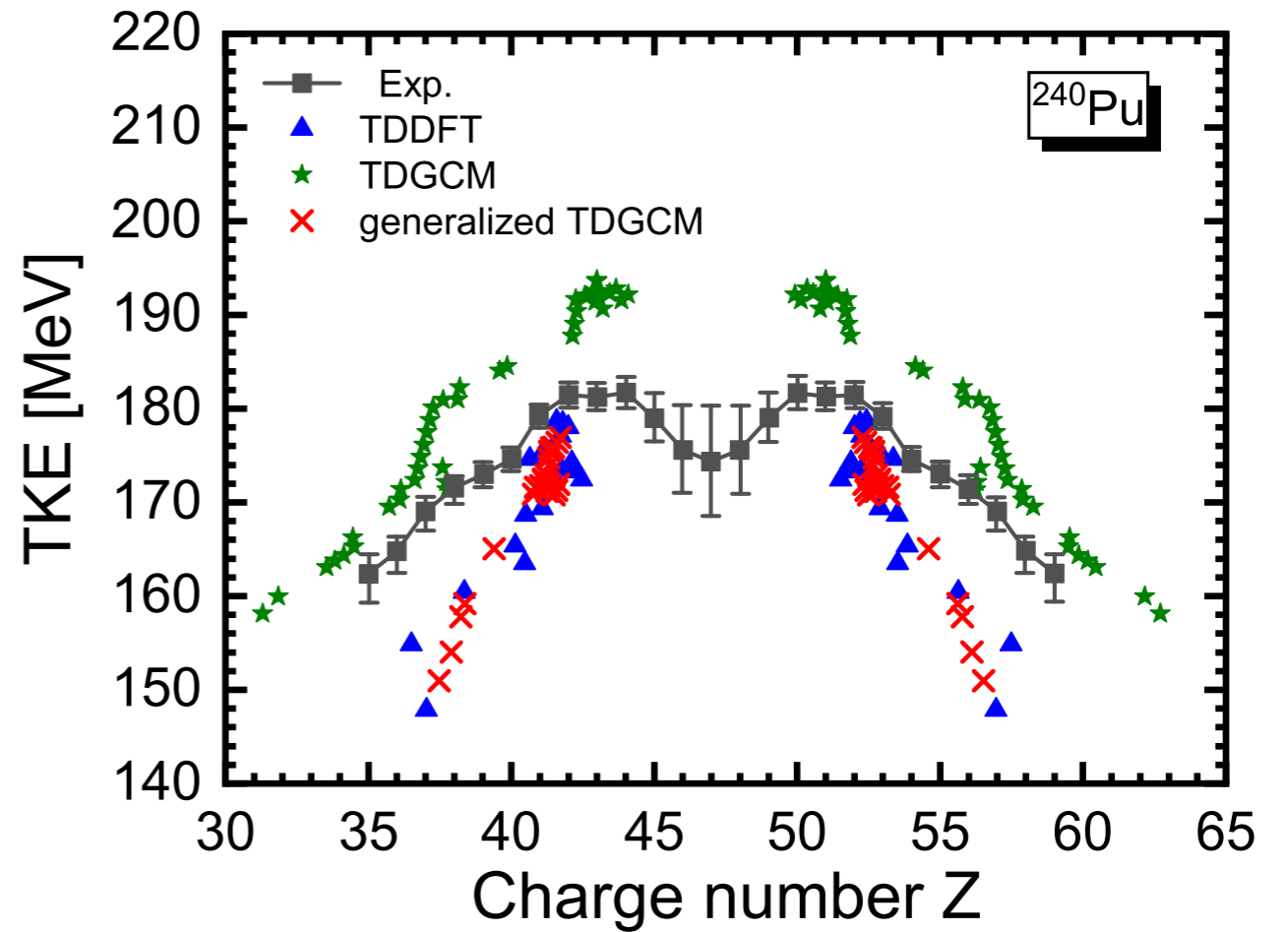
The square moduli of the 25 TDDFT components of the generalized TDGCM collective wave functions $|g|^2$, at time 1300 fm/c. The generalized TDGCM trajectories 1–25 start from the initial points 1–25.

Particle number projection \Rightarrow charge yields.

Charge yields for induced fission of ^{240}Pu .



Total kinetic energies of the emerging fragments.



Challenges for Fission Theory

- Microscopic description of tunneling (SF and low-energy induced fission)
- Extension of TDGCM to include finite temperature and dissipation
- Symmetry restoration (quantum numbers and observables)
- Microscopic Langevin approach
- A description of fission based on reaction theory

- Extend theory beyond even-even systems
- Neck formation, dynamics and scission mechanism
- Ternary fission
- Fragment angular momentum generation
- TKE distribution and fragment de-excitation
- Large-scale calculations for astrophysical applications