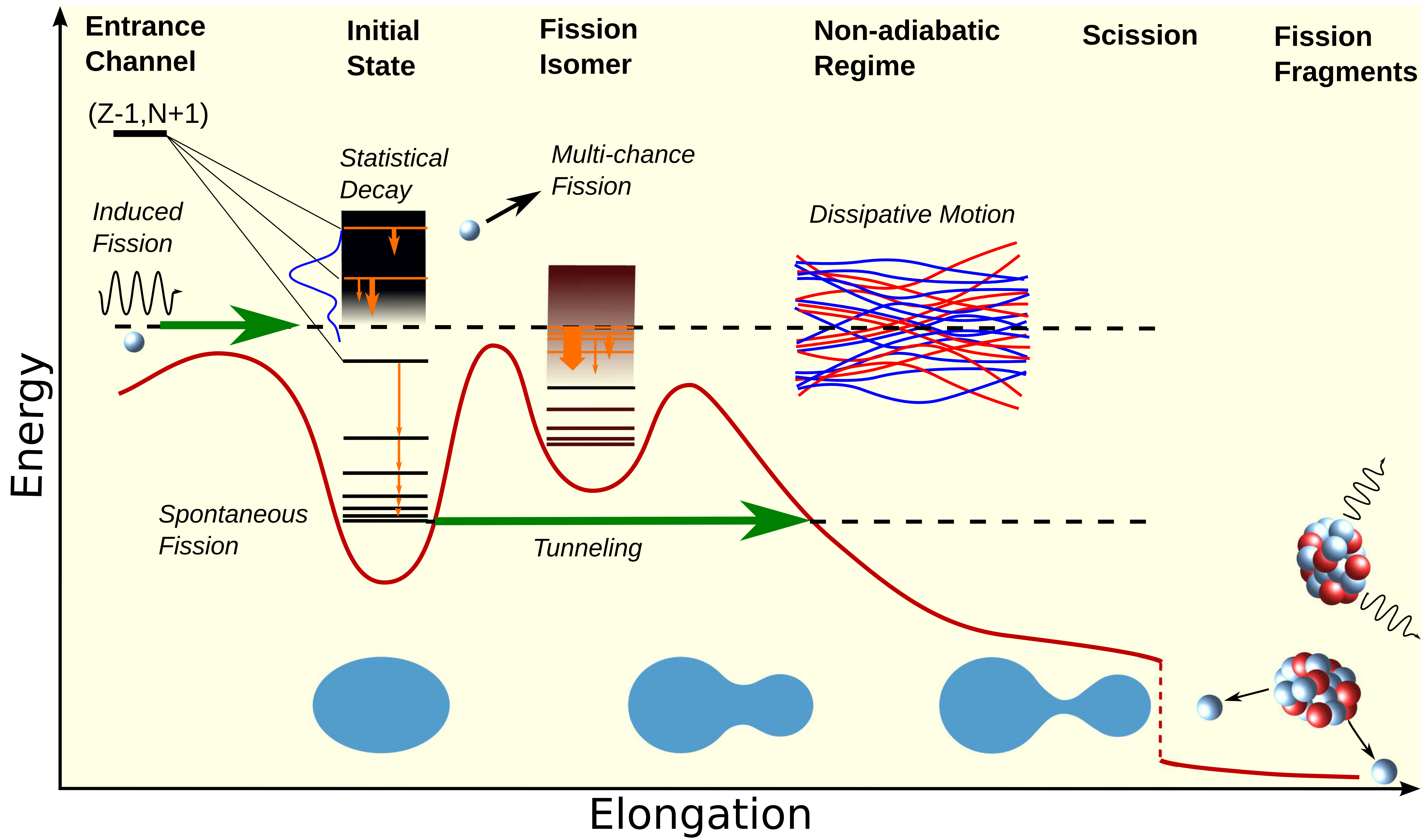
Microscopic Analysis of Induced Nuclear Fission Dynamics

Dario Vretenar
University of Zagreb

Sveučilište u Zagrebu
PMF
Ministarstvo regionalnog razvoja i fondova Europske unije
Ministarstvo znanosti i obrazovanja Republike Hrvatske
Europska unija
Zajedno do fondova EU
Europski strukturni i investicijski fondovi
Operativni program Konkurentnost i kohezija


Entrance Channel
Initial State
Fission Isomer
Non-adiabatic Regime
Scission
Fission Fragments
(Z-1,N+1)
Statistical Decay
Multi-chance Fission
Induced Fission
Dissipative Motion
Spontaneous Fission
Tunneling
Energy
Elongation

Two basic microscopic approaches to the description of induced fission dynamics:

The time-dependent generator coordinate method (TDGCM)

$$\left|\Psi(t)\right\rangle = \int_{\boldsymbol{q}\in E} \mathrm{d}\boldsymbol{q} \left|\phi(\boldsymbol{q})\right\rangle f(\boldsymbol{q}, t).$$

⇒ 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

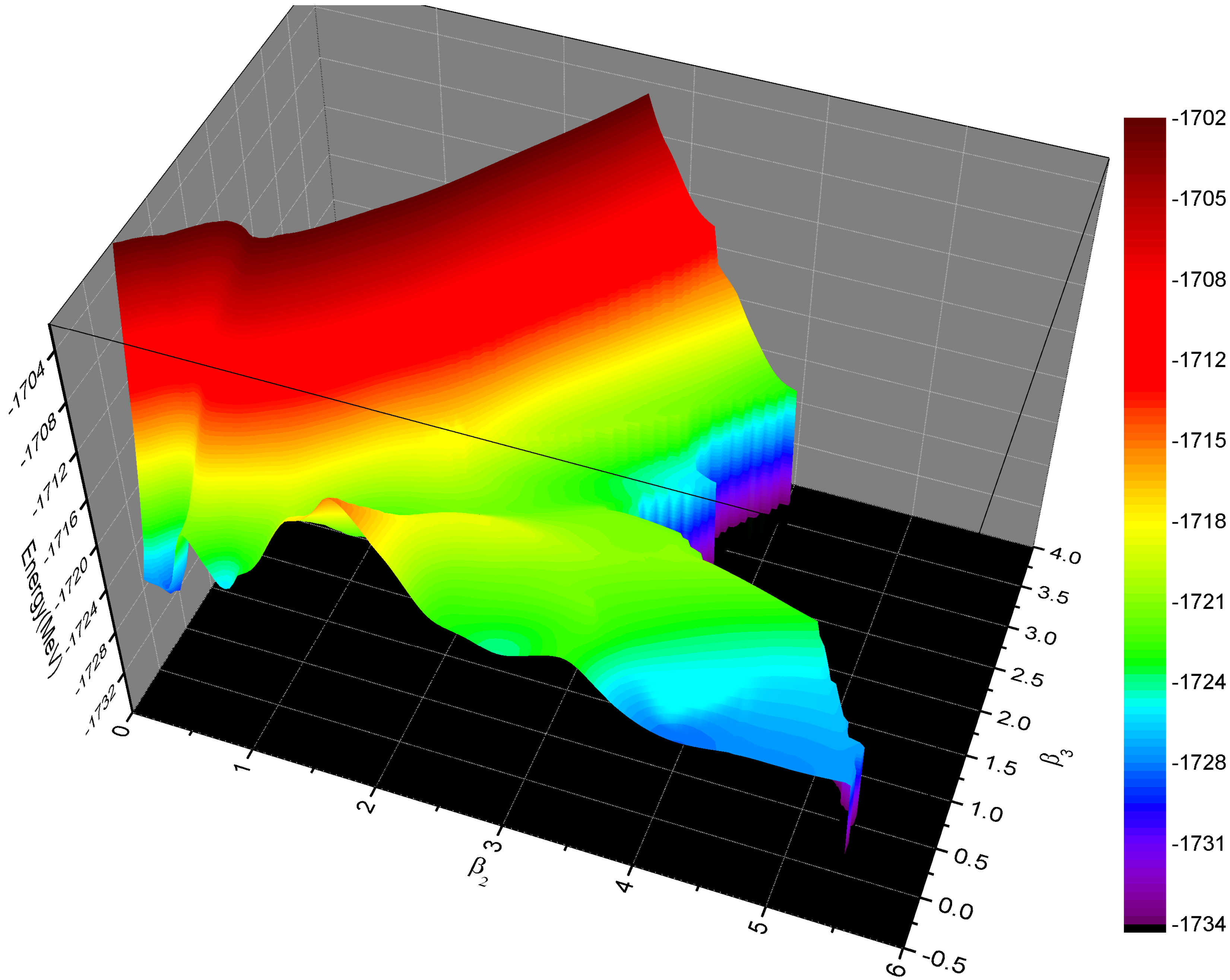
Time-dependent Schroedinger-like equation for fission dynamics (axial quadrupole and octupole deformation parameters as collective degrees of freedom):

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

RMF+BCS quadrupole and octupole constrained deformation energy surface of ^{226}Th in the $\beta_2 - \beta_3$ plane.

TAO, ZHAO, LI, NIKŠIĆ, AND VRETENAR

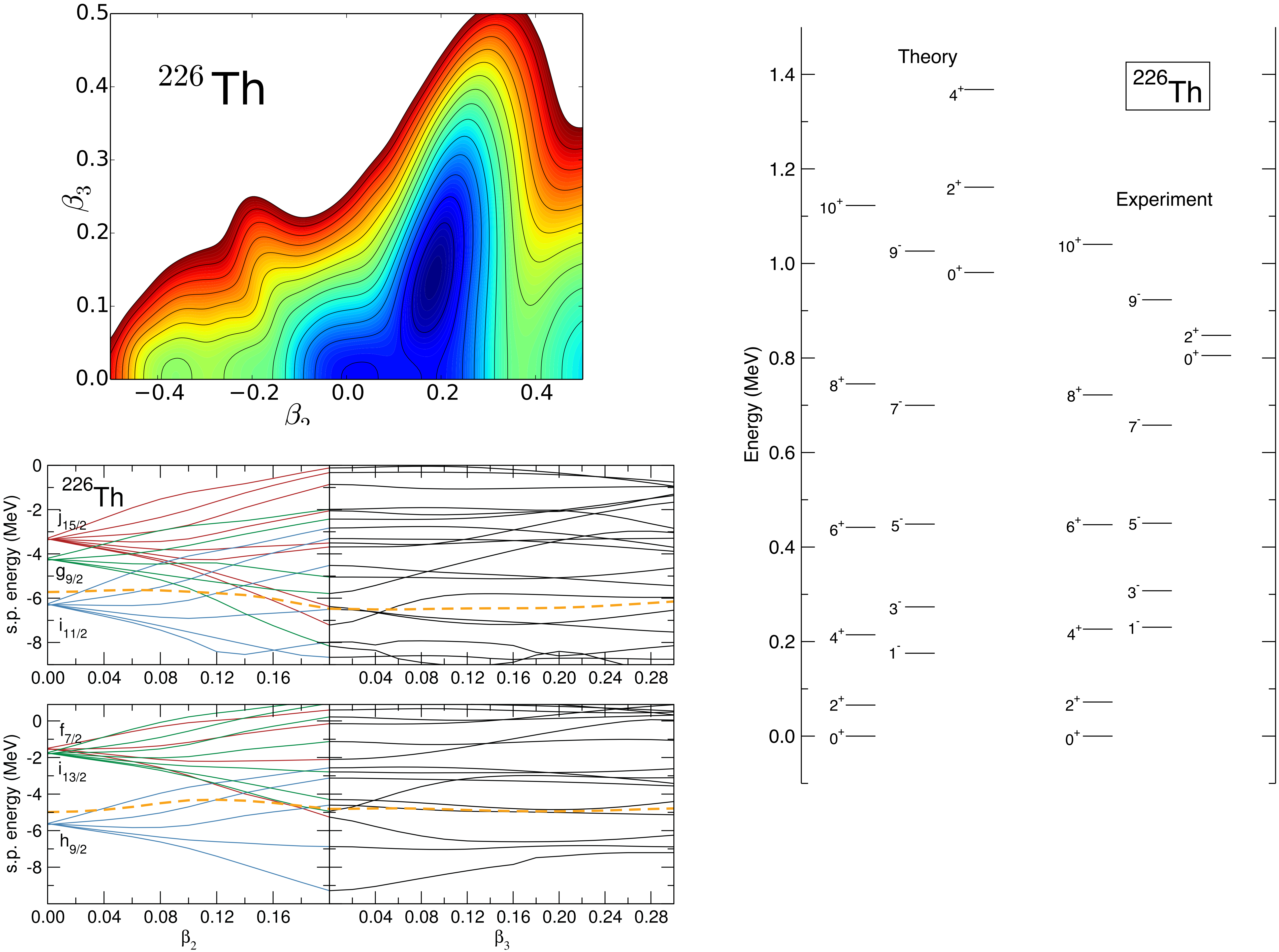
PHYSICAL REVIEW C **96**, 024319 (2017)



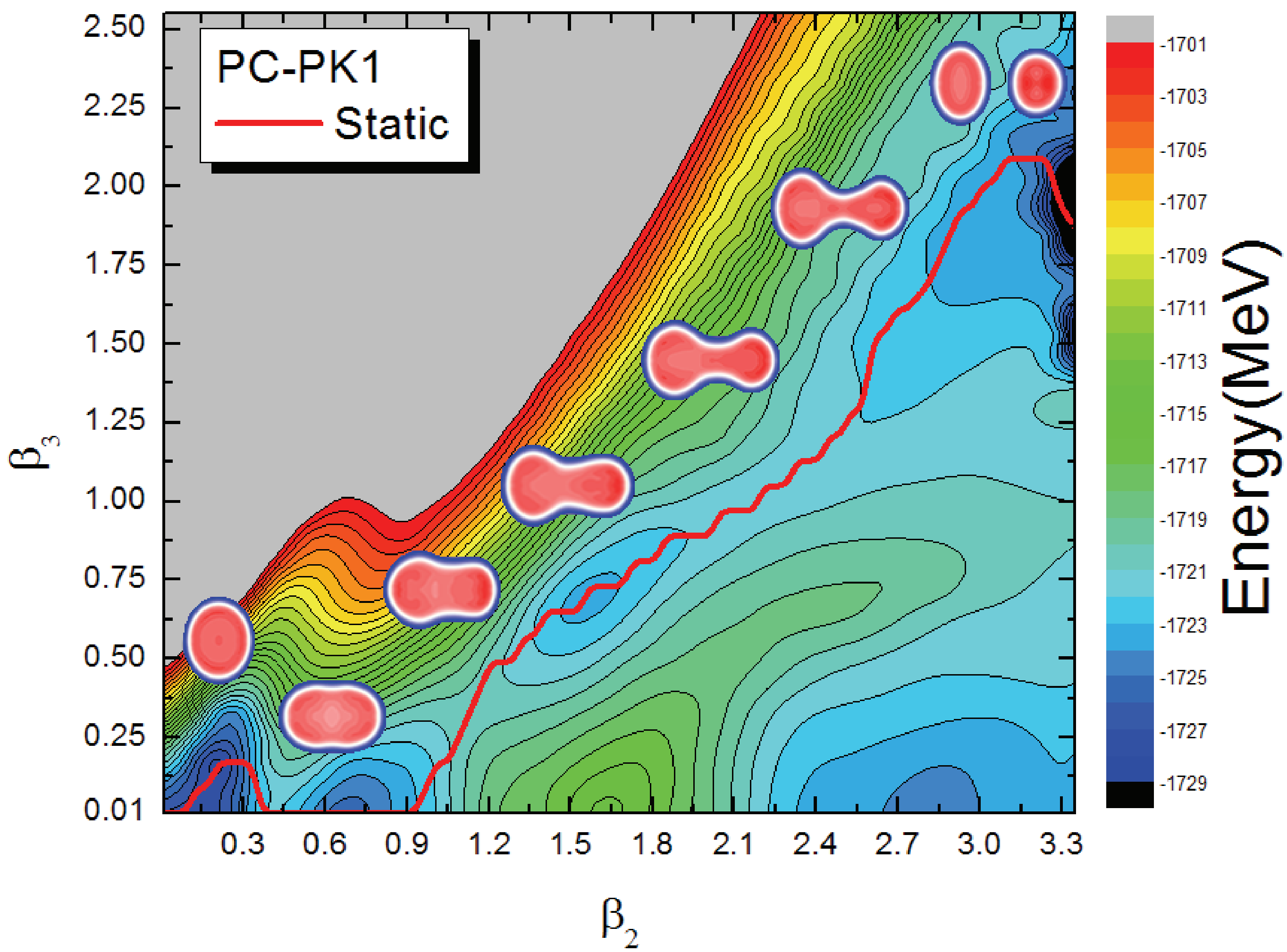
→ includes static correlations: deformations & pairing

→ does not include dynamic (collective) correlations that arise from symmetry restoration and quantum fluctuations around mean-field minima

PC-PK1 plus δ-force pairing



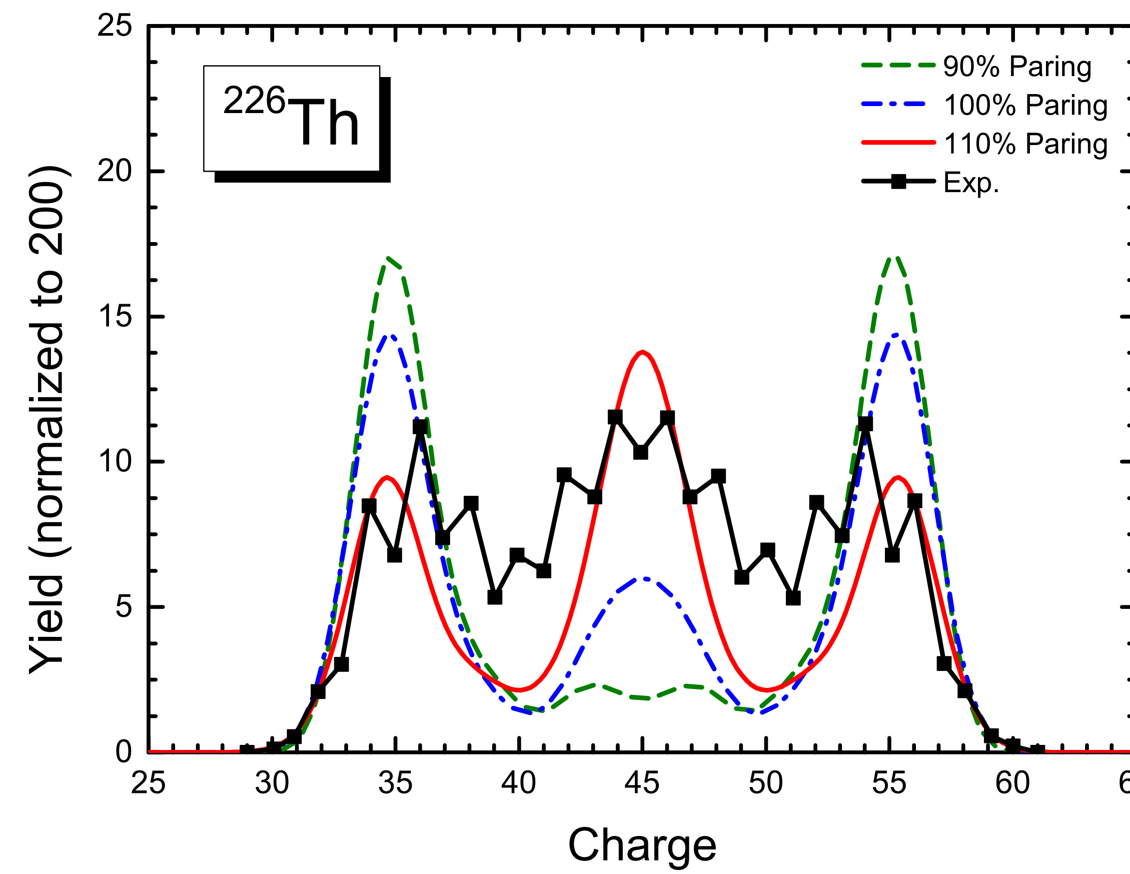
226 Th
β3
β2
0.5
0.4
0.3
0.2
0.1
0.0
−0.4
−0.2
0.0
0.2
0.4
226 Th
s.p. energy (MeV)
j15/2
g9/2
i11/2
f7/2
i13/2
h9/2
β2
β3
Theory
226 Th
Experiment
Energy (MeV)
10+
8+
6+
4+
2+
0+
9-
7-
5-
3-
1-
4+
2+
0+



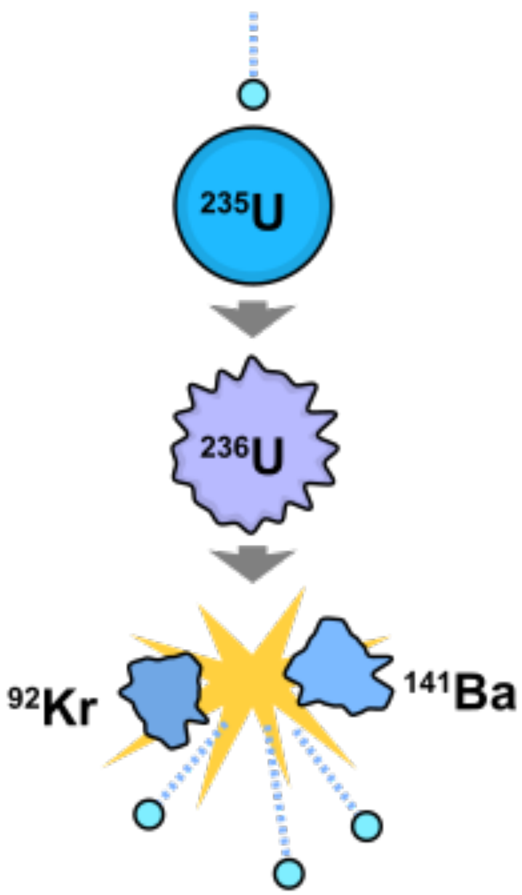
A triple-humped fission barrier is predicted along the static fission path, and the calculated heights are **7.10, 8.58, and 7.32 MeV** from the inner to the outer barrier.

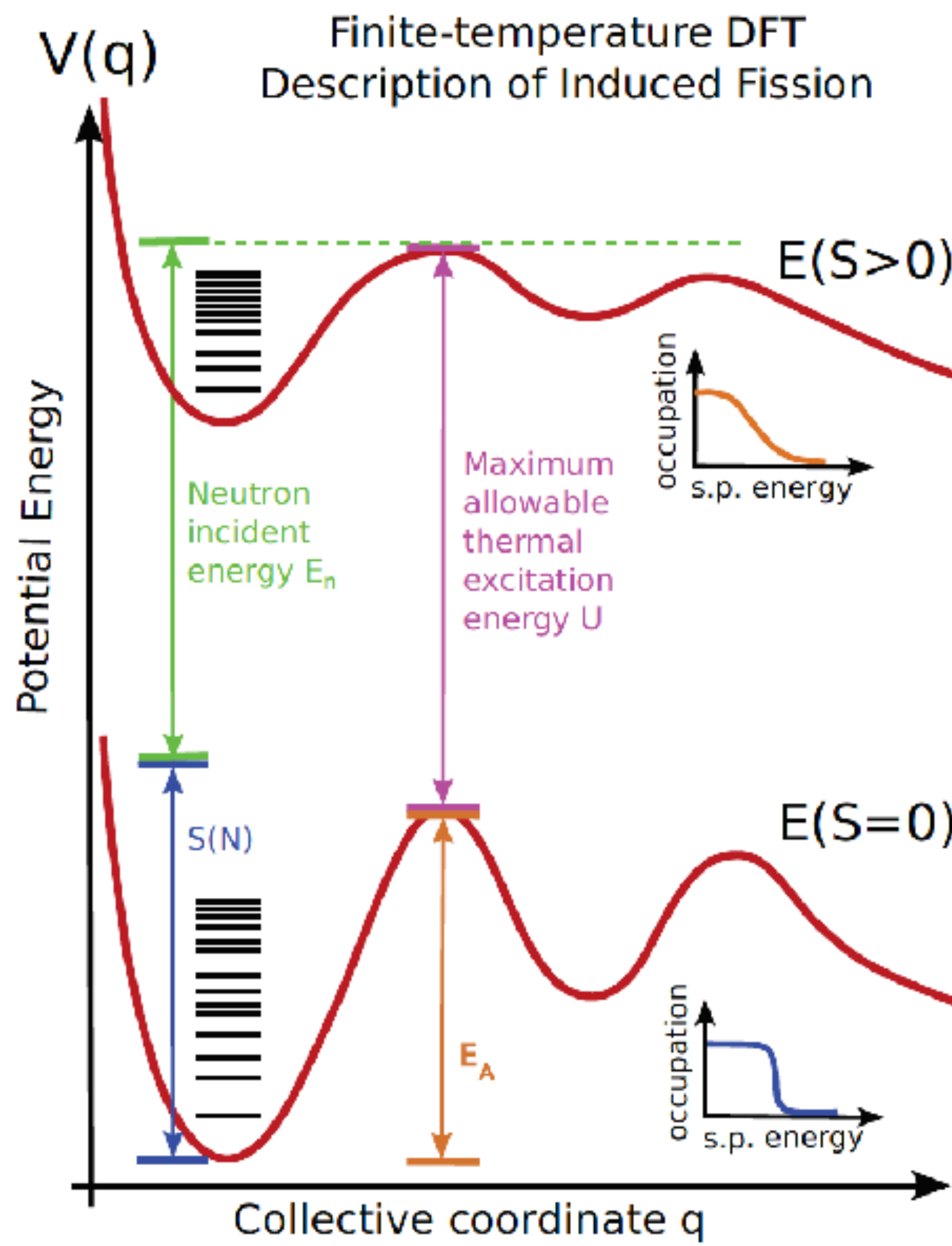
The height of the fission barriers (in MeV) with respect to the corresponding ground-state minima:

	B_I	B_{II}^{asy}	B_{III}^{asy}	B_{II}^{sym}	B_{III}^{sym}
90% pairing	8.23	9.47	7.74	15.64	6.38
100% pairing	7.10	8.58	7.32	14.21	5.72
110% pairing	5.92	7.78	7.09	12.72	5.17



Induced Fission - Finite Temperature Effects





N. SCHUNCK, D. DUKE, AND H. CARR
PHYSICAL REVIEW C 91, 034327 (2015)

Finite temperature effects:

$$i\hbar\frac{\partial g(\boldsymbol{q},t)}{\partial t} = \hat{H}_{\mathrm{coll}}(\boldsymbol{q})g(\boldsymbol{q},t)$$

$$\hat{H}_{\mathrm{coll}}(\boldsymbol{q}) = -\frac{\hbar^2}{2}\sum_{ij}\frac{\partial}{\partial q_i}B_{ij}(\boldsymbol{q})\frac{\partial}{\partial q_j} + V(\boldsymbol{q})$$

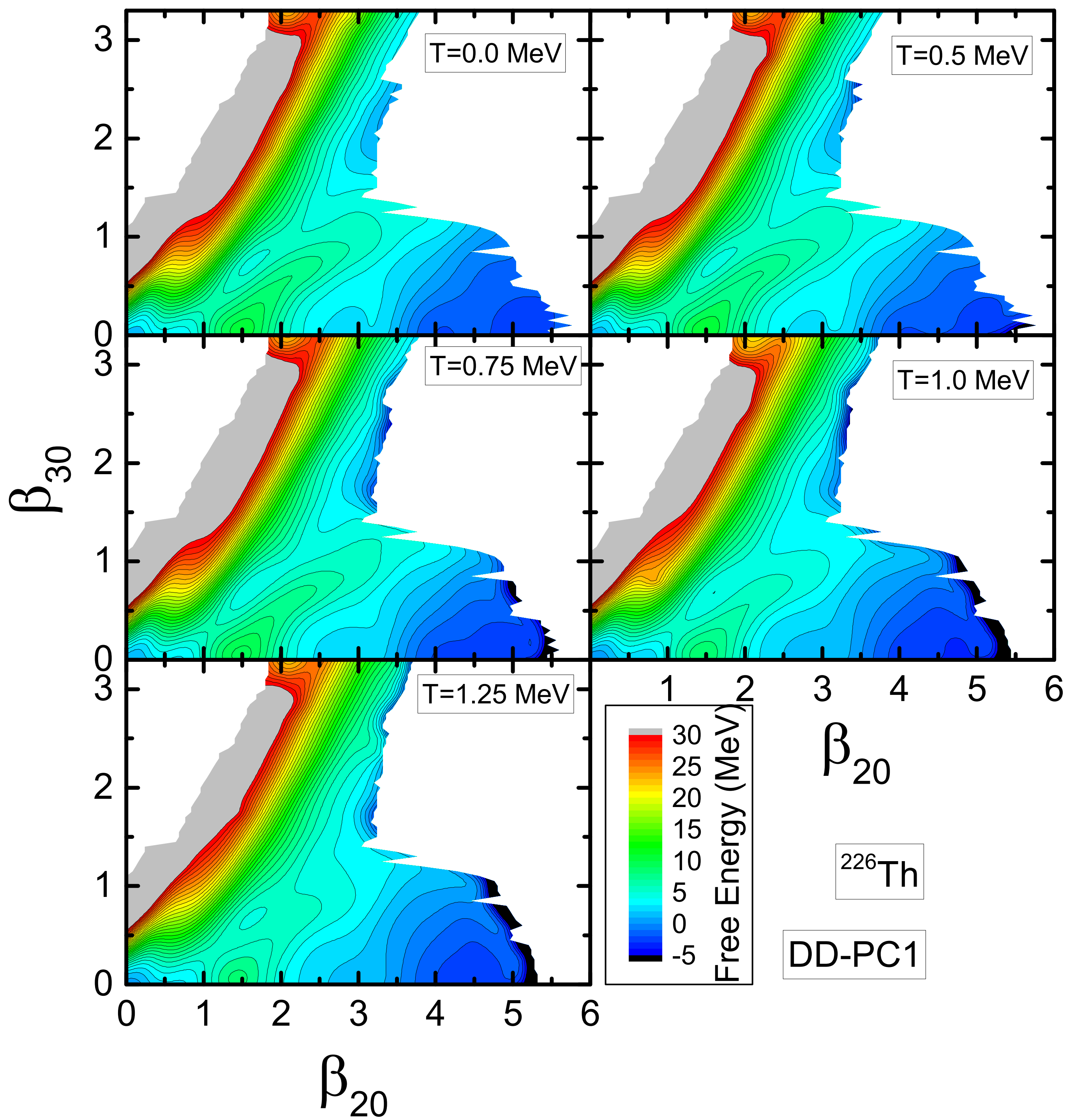
Helmholtz free energy: $F = E(T) - TS$

... entropy of the compound nuclear system:

$$S = -k_B\sum_k\left[f_k\ln f_k + (1-f_k)\ln(1-f_k)\right]$$

... thermal occupation probabilities:

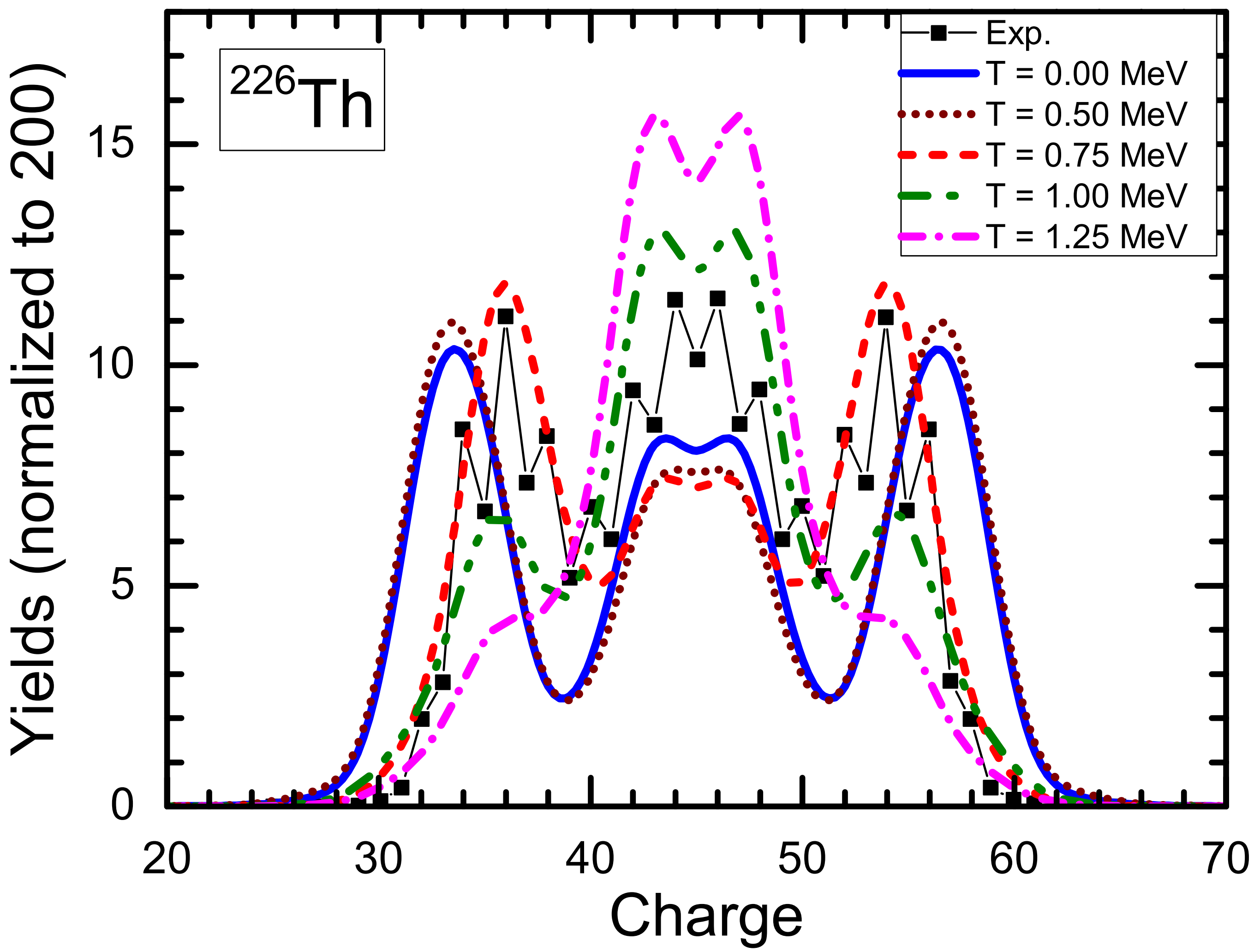
$$f_k = \frac{1}{1+e^{\beta E_k}}$$



Dynamics of induced fission

Zhao, Nikšić, Vretenar, Zhou
Phys. Rev. C **99**, 014618 (2019).

Charge yields:

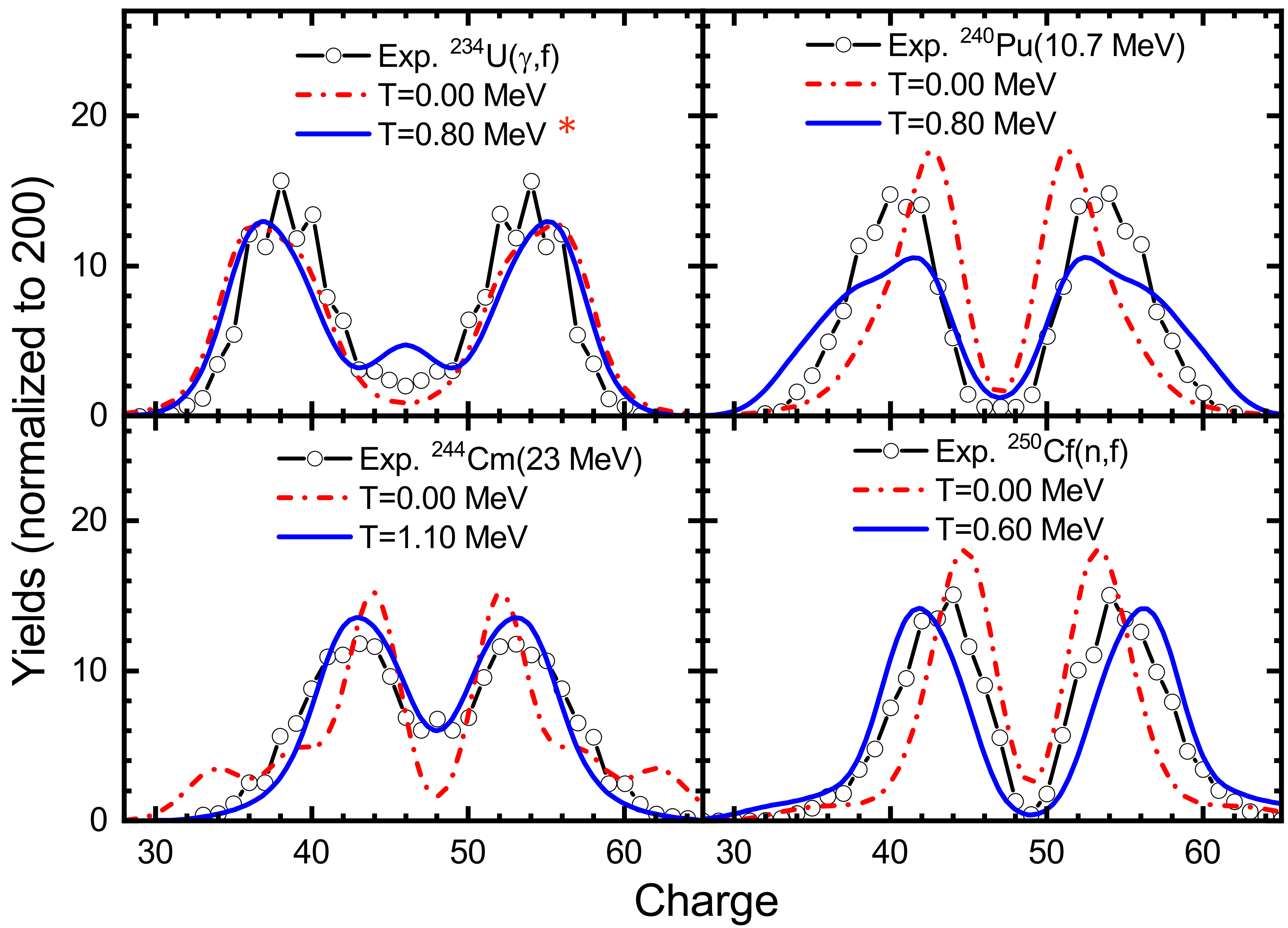


Experimental results ➠ photoinduced fission with photon energies in the interval 8 − 14 MeV, and a peak value Eγ = 11 MeV.

T = 0.5, **0.75**, **1.0**, and 1.25 MeV ➠ corresponding internal excitation energies E* are: 2.58, **8.71**, **16.56**, and 27.12 MeV, respectively.

Mass-asymmetric fission of actinides

Zhao, Xiang, Li, Nikšić, Vretenar, Zhou
Phys. Rev. C **99**, 054613 (2019).



*The temperature is adjusted so that the intrinsic excitation energy corresponds to the experimental exc. energy.

Induced fission: dynamical pairing degree of freedom

Zhao, Nikšić, Vretenar
Phys. Rev. C **104**, 044612 (2021).

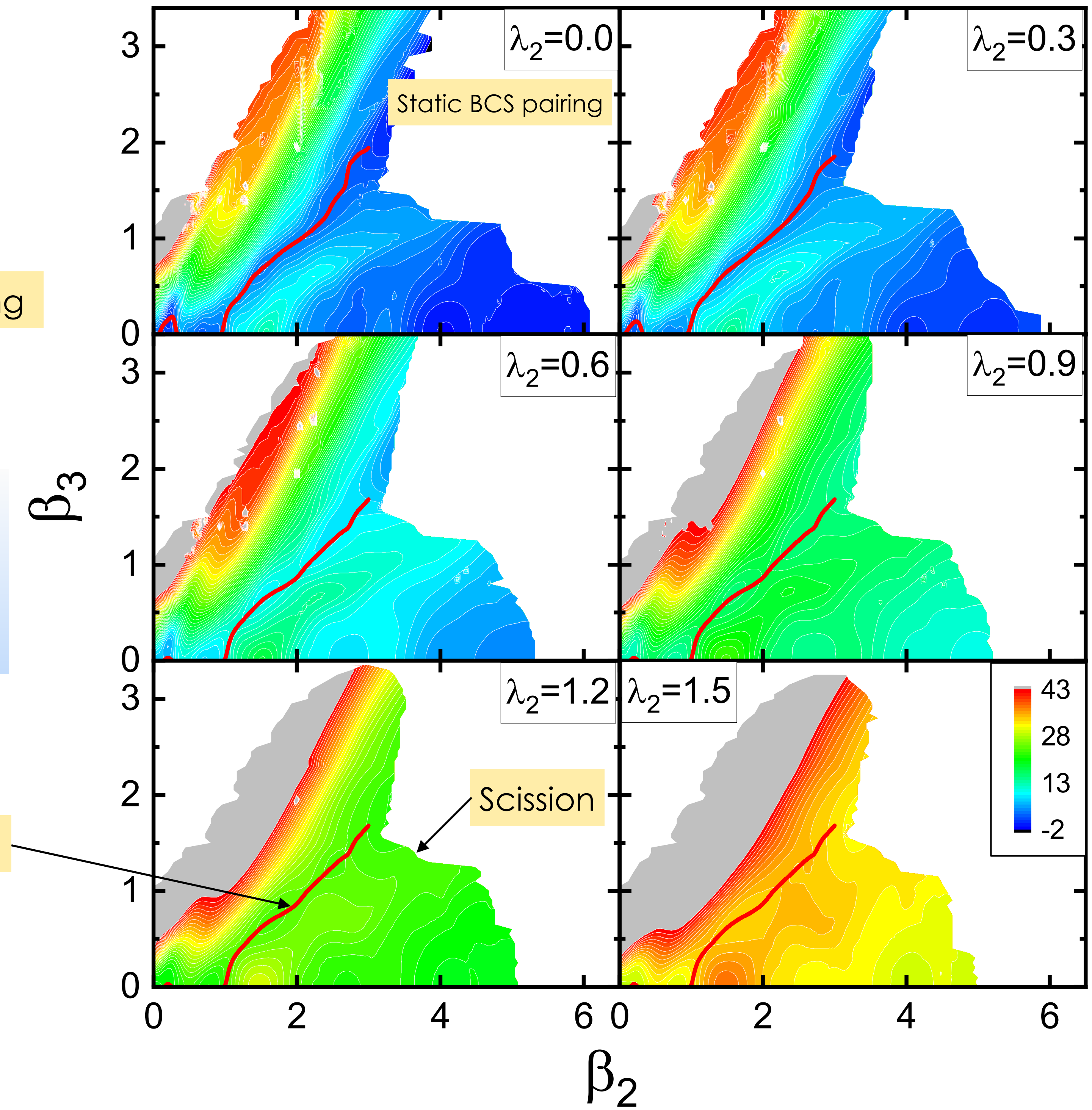
SCMF deformation energy surface ➠ constraints on the mass multipole moments and the particle-number dispersion operator: $\Delta\hat{N}^2 = \hat{N}^2 - \langle\hat{N}\rangle^2$.

... the Routhian:

$$E' = E_{\mathrm{RMF}} + \sum_{\lambda\mu} \frac{1}{2} C_{\lambda\mu} Q_{\lambda\mu} + \underbrace{\lambda_2 \Delta\hat{N}^2}_{\text{isoscalar dynamical pairing}}$$

2D projections of the deformation-energy manifold of ^{228}Th on the quadrupole-octupole axially symmetric plane, for selected values of the pairing coordinate λ_2.

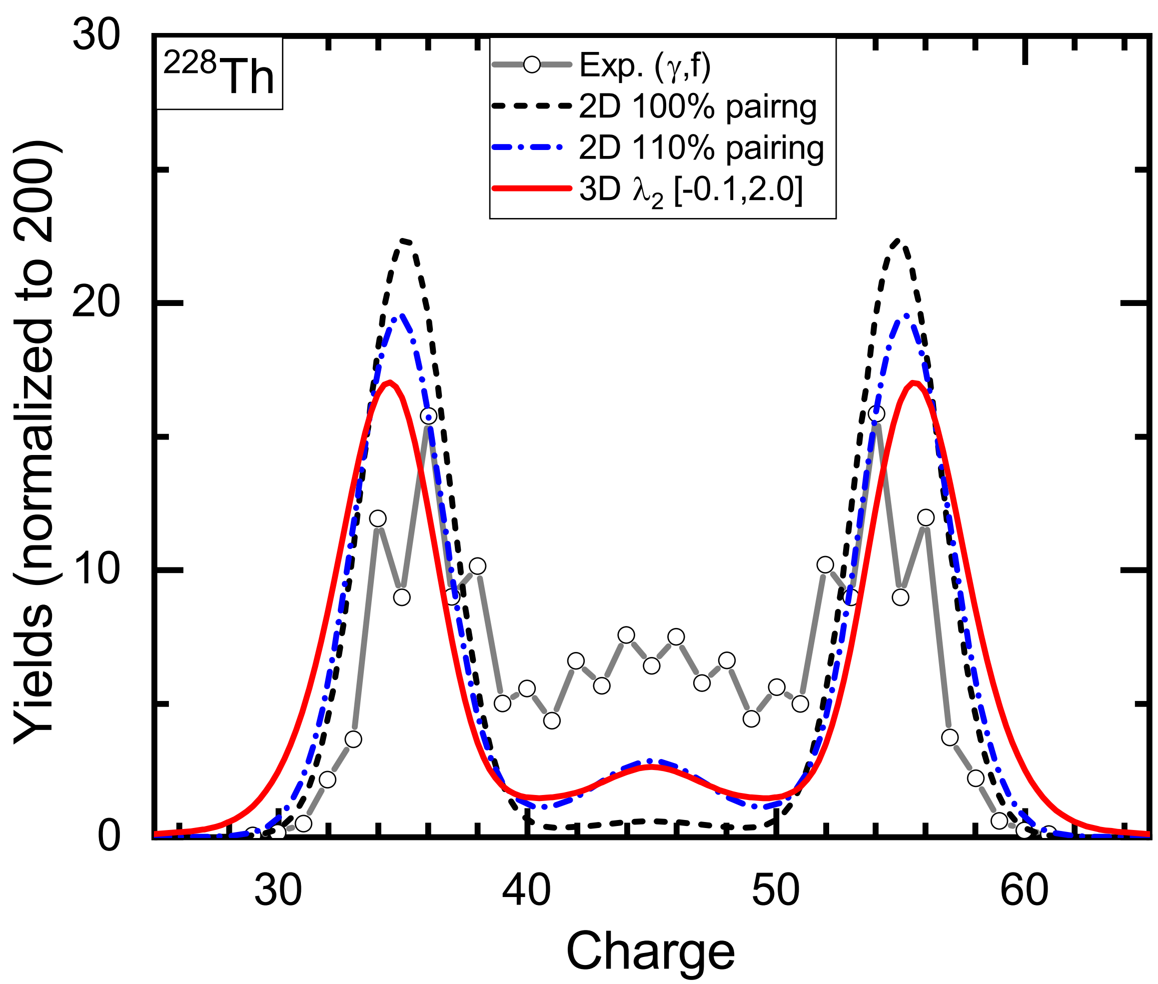
Static fission path of minimum energy

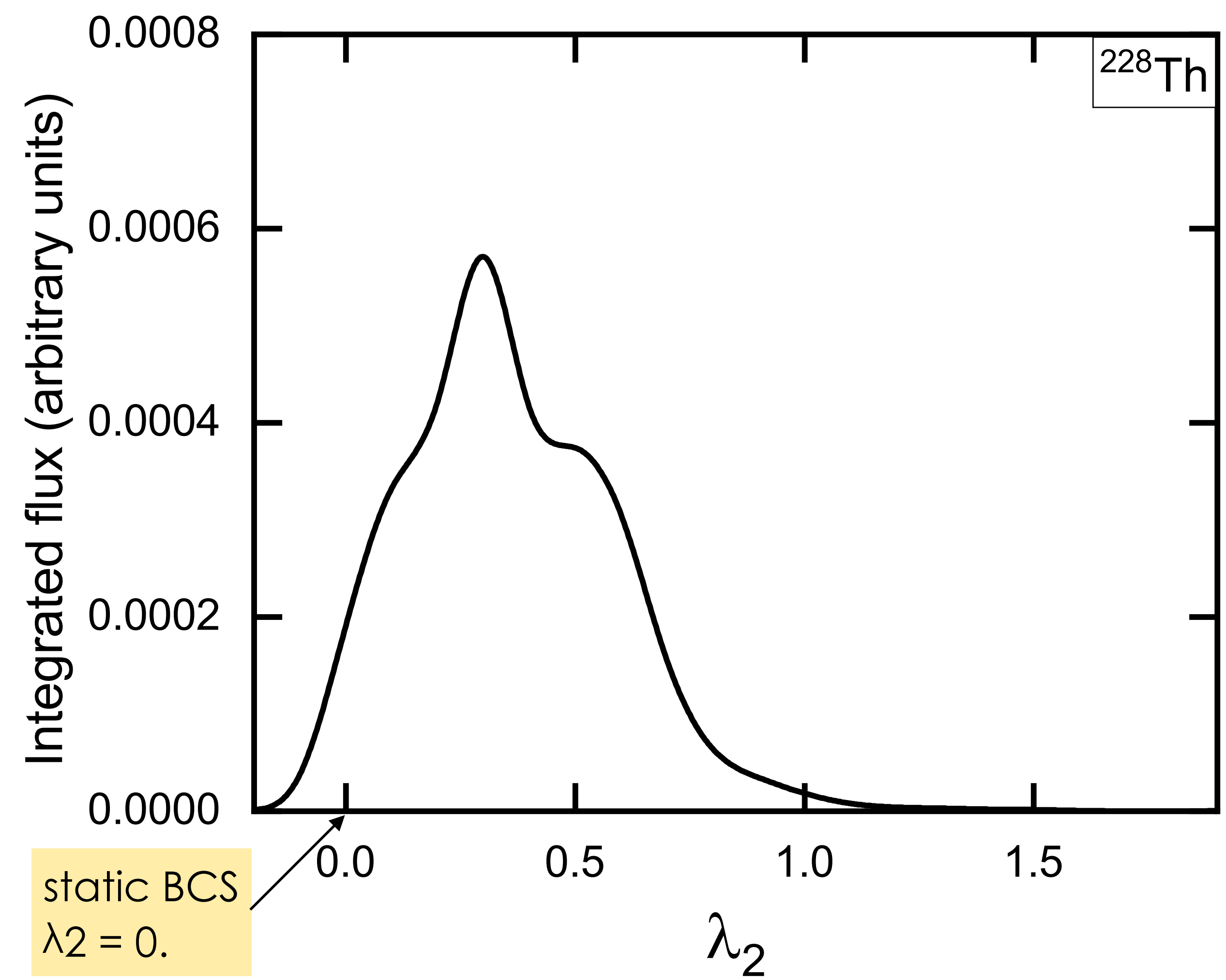


3D TDGCM+GOA calculation

$$\hat{H}_{\text{coll}}(\boldsymbol{q}) = -\frac{\hbar^2}{2}\sum_{ij}\frac{\partial}{\partial q_i}B_{ij}(\boldsymbol{q})\frac{\partial}{\partial q_j} + V(\boldsymbol{q})$$

$\mathbf{q} \equiv \{\beta_2, \beta_3, \lambda_2\}$





Charge yields calculated in the 3D collective space → deformation β2, β3 and dynamical pairing λ2 coordinates.

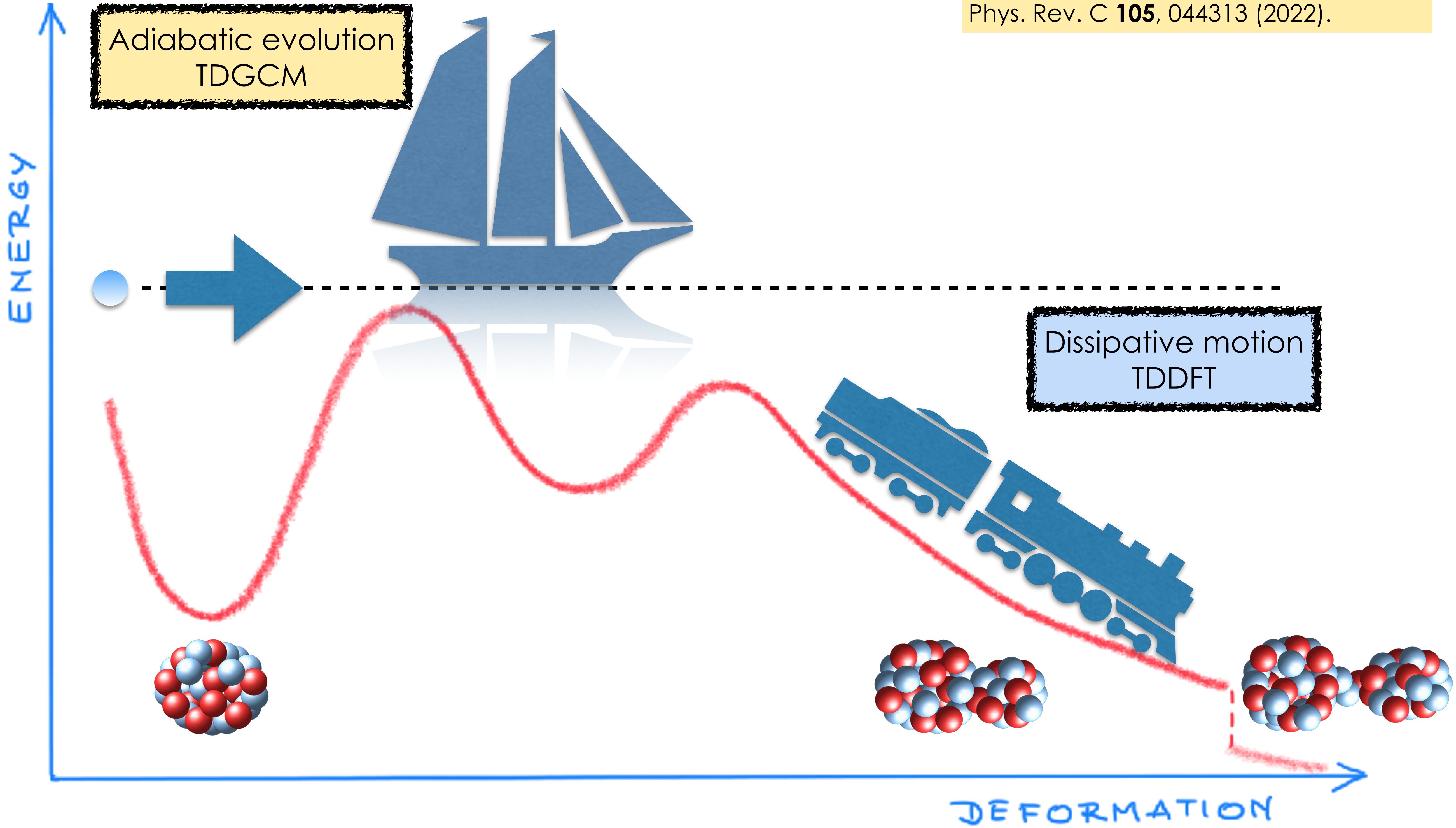
Effect of dynamical pairing on the flux of the probability current through the scission hyper-surface:

$$B(\lambda_2) \propto \sum_{\xi \in \mathcal{B}} \lim_{t\to\infty} F(\xi, \lambda_2, t).$$

→ time-integrated flux through the scission contour in the (β2, β3) plane, for a given value of the pairing collective coordinate λ2 .

Adiabatic evolution and dissipative dynamics

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



Time-dependent density functional theory (TDDFT)

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

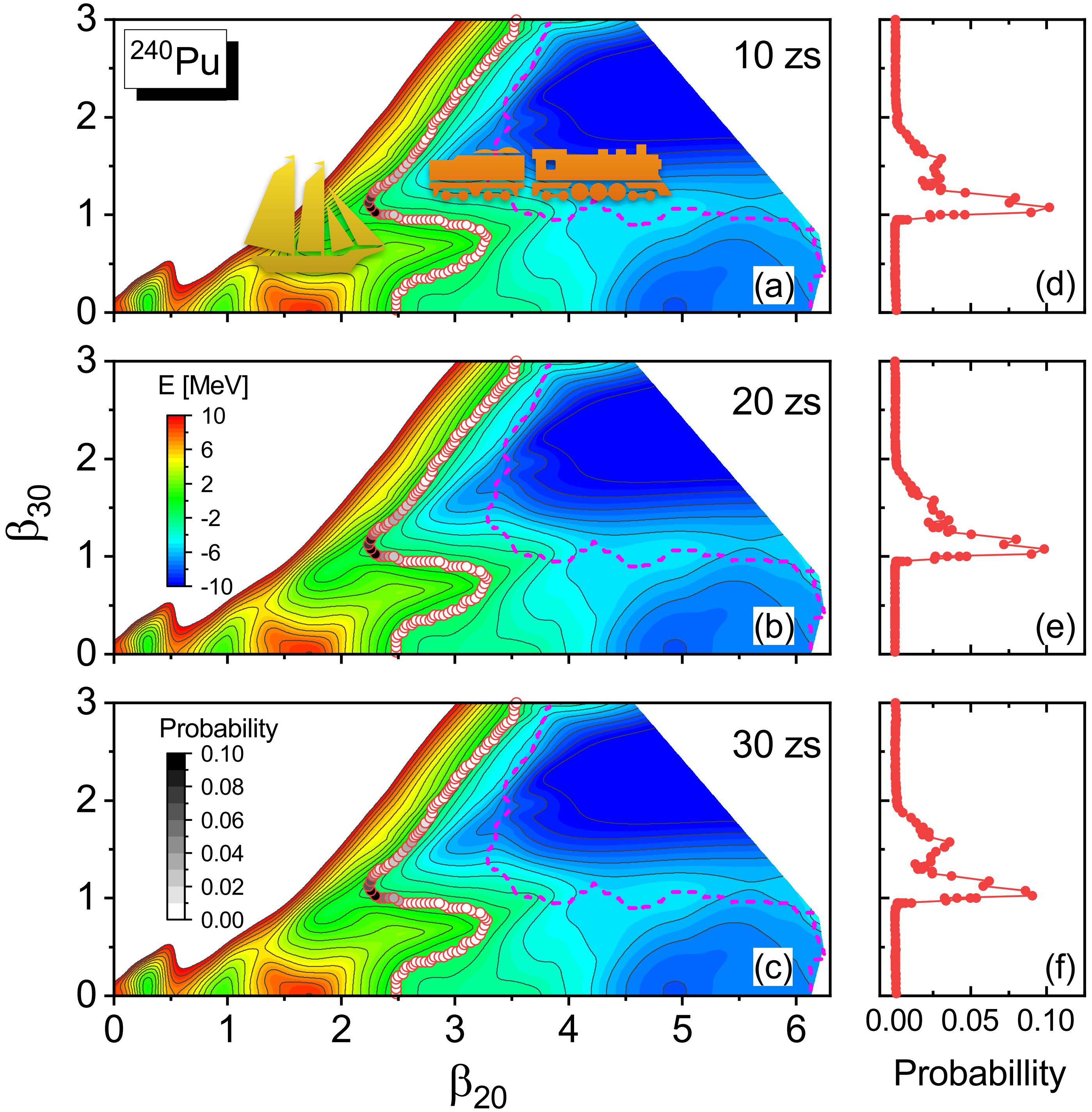
$$i\frac{d}{dt}n_k(t) = n_k(t)\Delta_k^*(t) - n_k^*(t)\Delta_k(t),$$

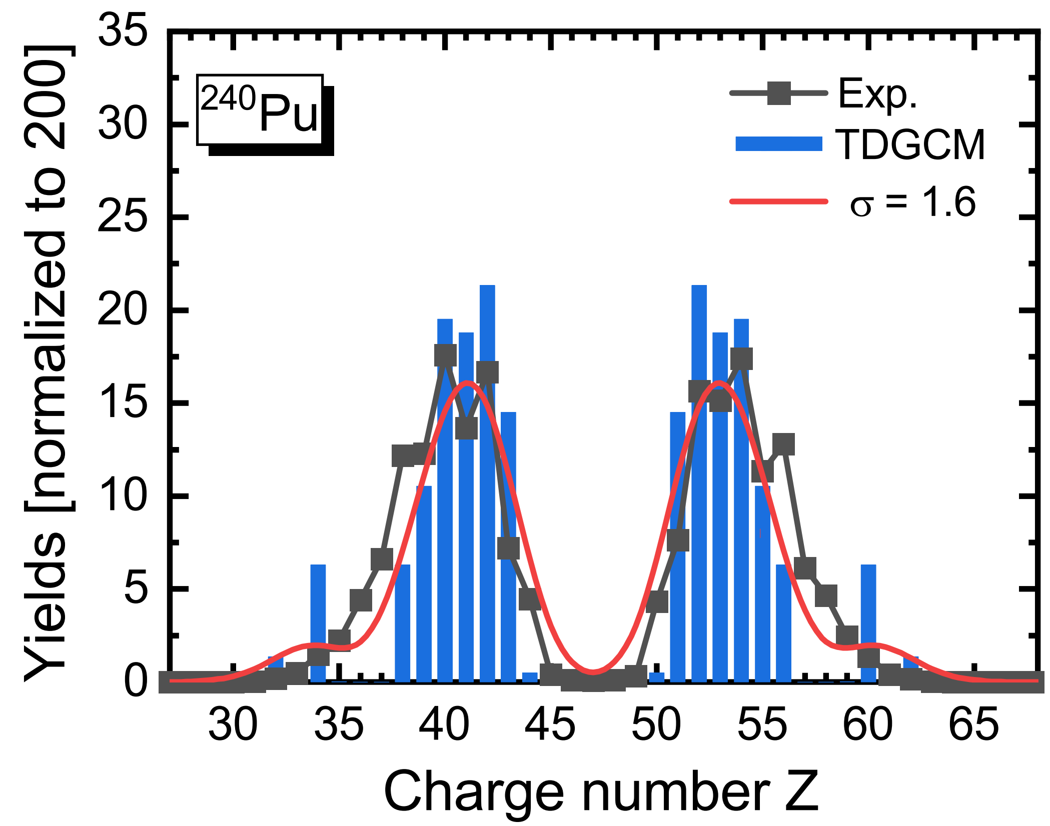
$$i\frac{d}{dt}\kappa_k(t) = [\varepsilon_k(t) + \varepsilon_{\bar{k}}(t)]\kappa_k(t) + \Delta_k(t)[2n_k(t) - 1].$$

⇒ 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.

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

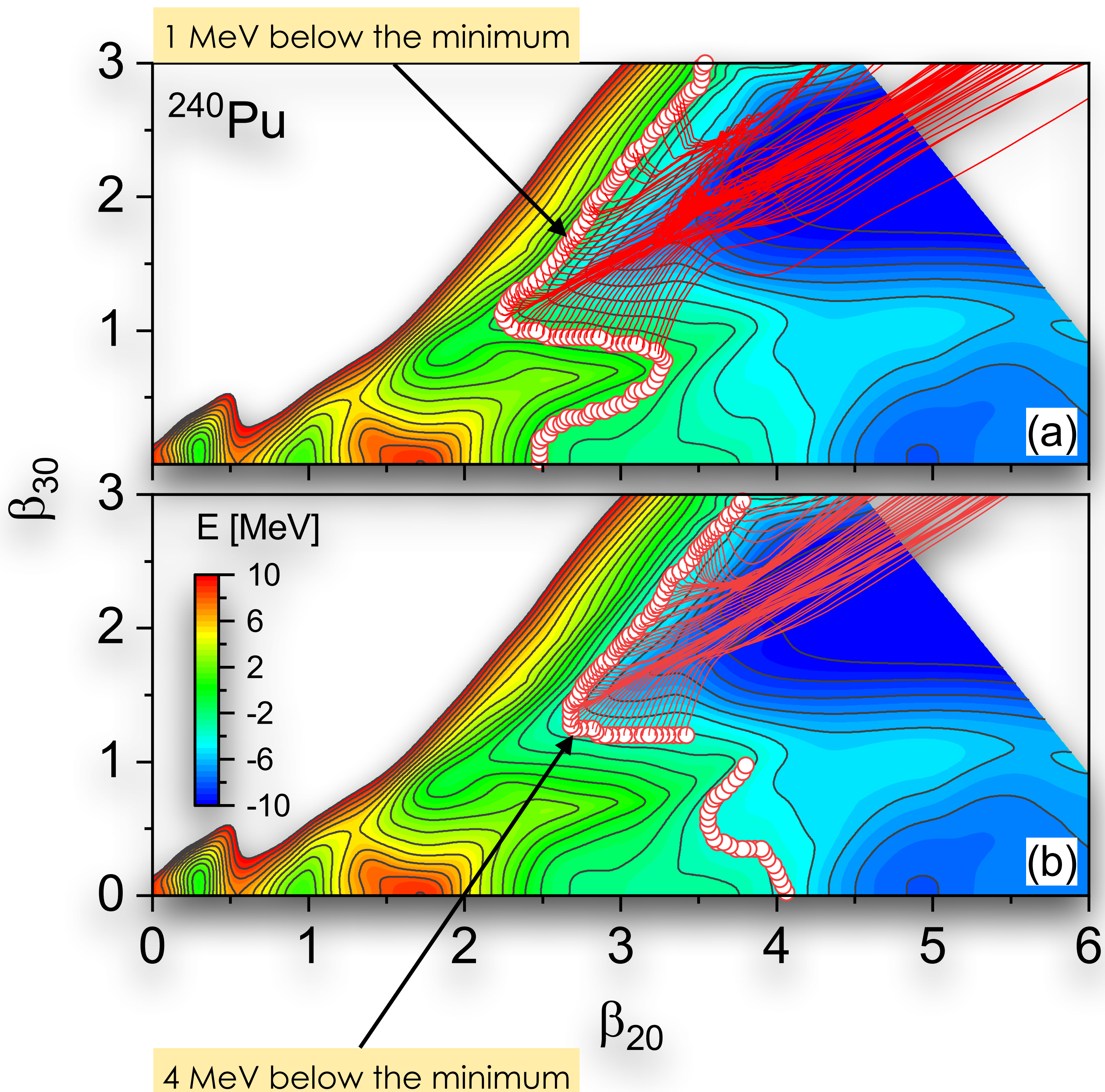
Negele et al. (1978) ➠ use an adiabatic model for the time interval in which the fissioning nucleus evolves from the quasi-stationary initial state to the saddle point, and a non-adiabatic method for the saddle-to-scission and beyond-scission dynamics.

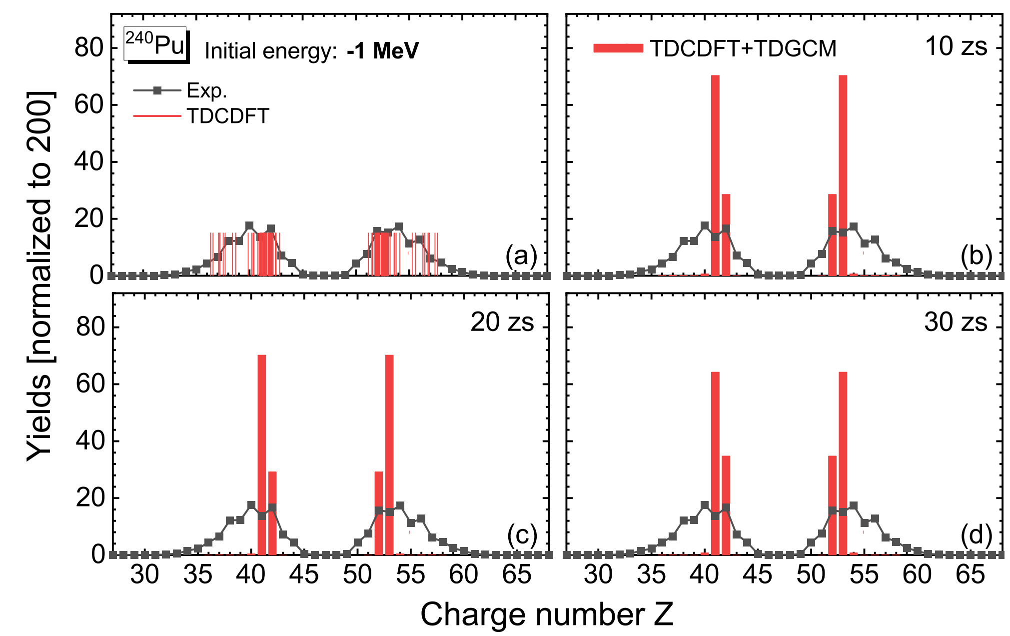


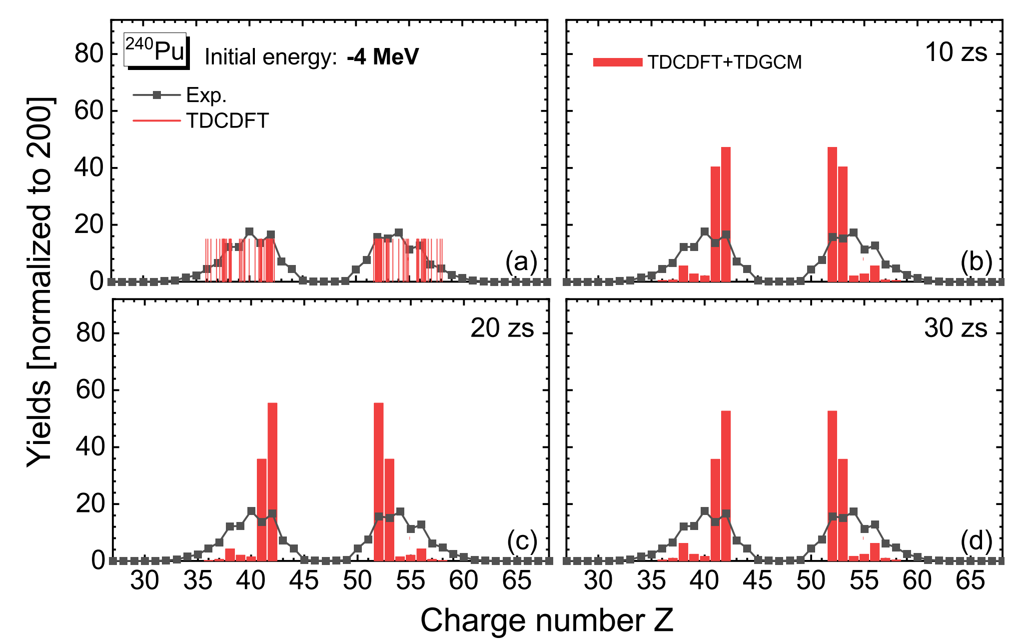


Ren, Zhao, Vretenar, Nikšić, Zhao, Meng
Phys. Rev. C **105**, 044313 (2022).

TDDFT fission trajectories







Total kinetic energies (TKEs) of the fragments

TDGCM+GOA

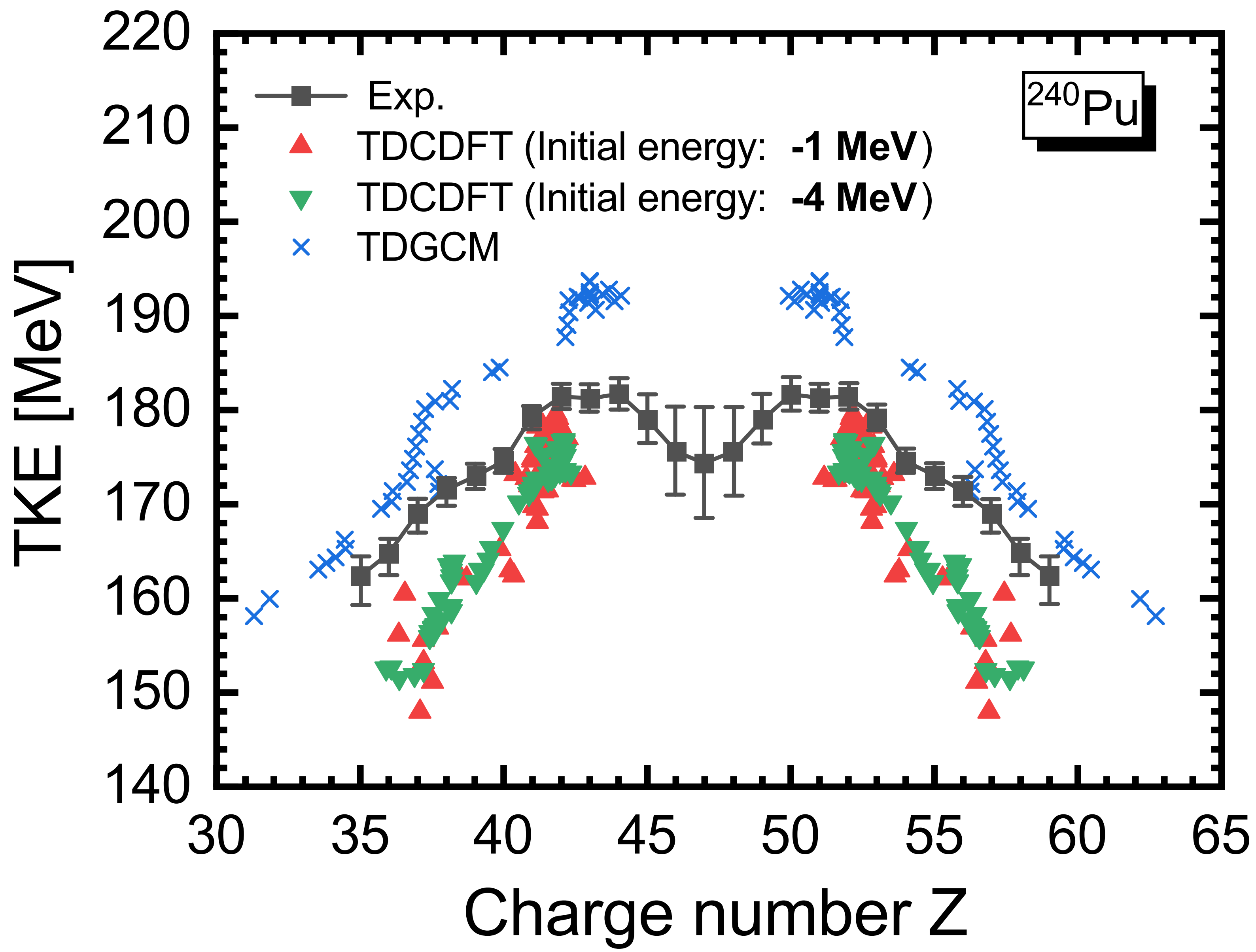
$$E_{\mathrm{TKE}} = \frac{e^2 Z_H Z_L}{d_{\mathrm{ch}}},$$

$d_{\mathrm{ch}} \rightarrow$ distance between centers of charge at the point of scission.

TDDFT

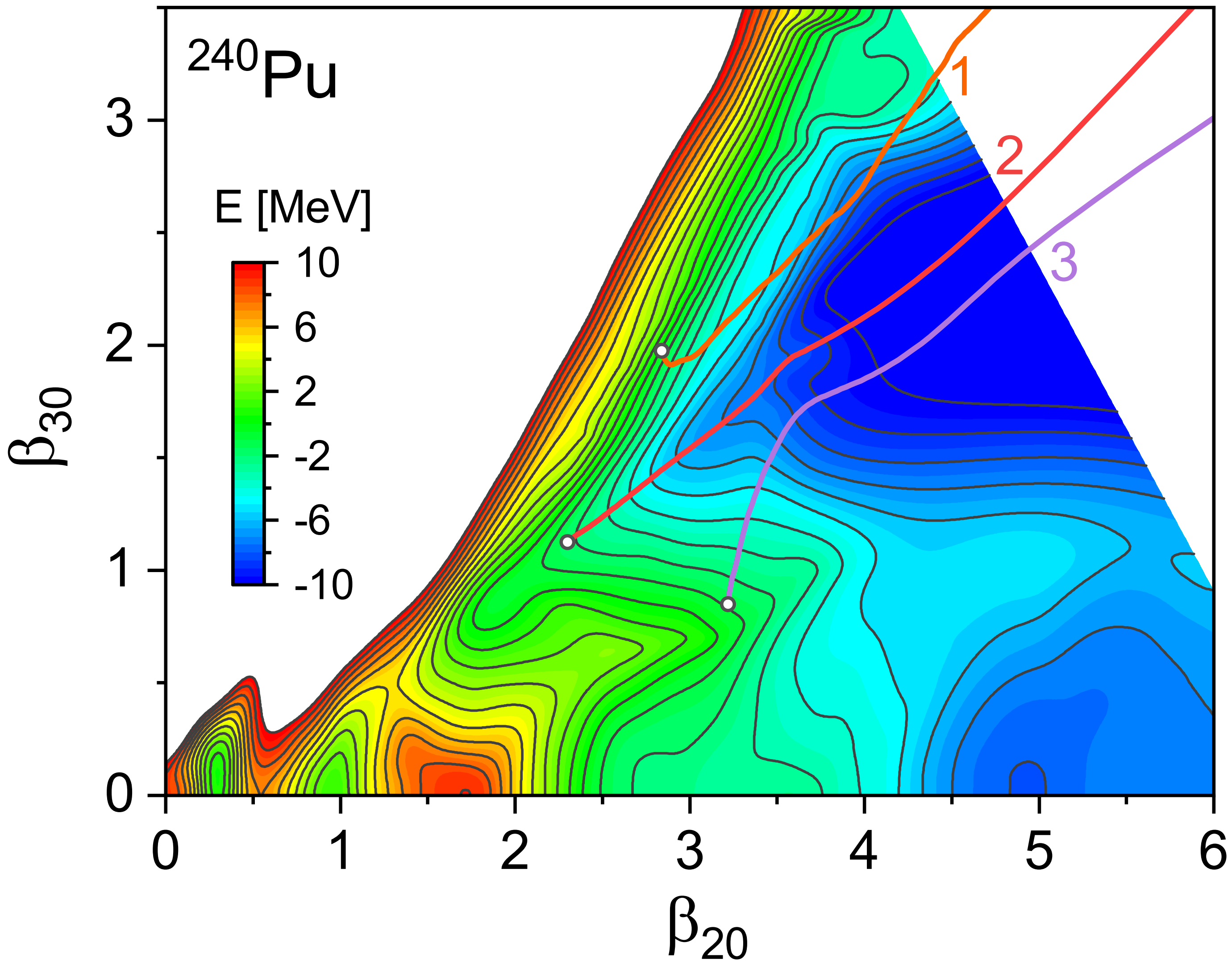
$$E_{\mathrm{TKE}} = \frac{1}{2} m A_{\mathrm{H}} \boldsymbol{v}_{\mathrm{H}}^2 + \frac{1}{2} m A_{\mathrm{L}} \boldsymbol{v}_{\mathrm{L}}^2 + E_{\mathrm{Coul}},$$

(≈ 25 fm, at which shape relaxation brings the fragments to their equilibrium shapes)

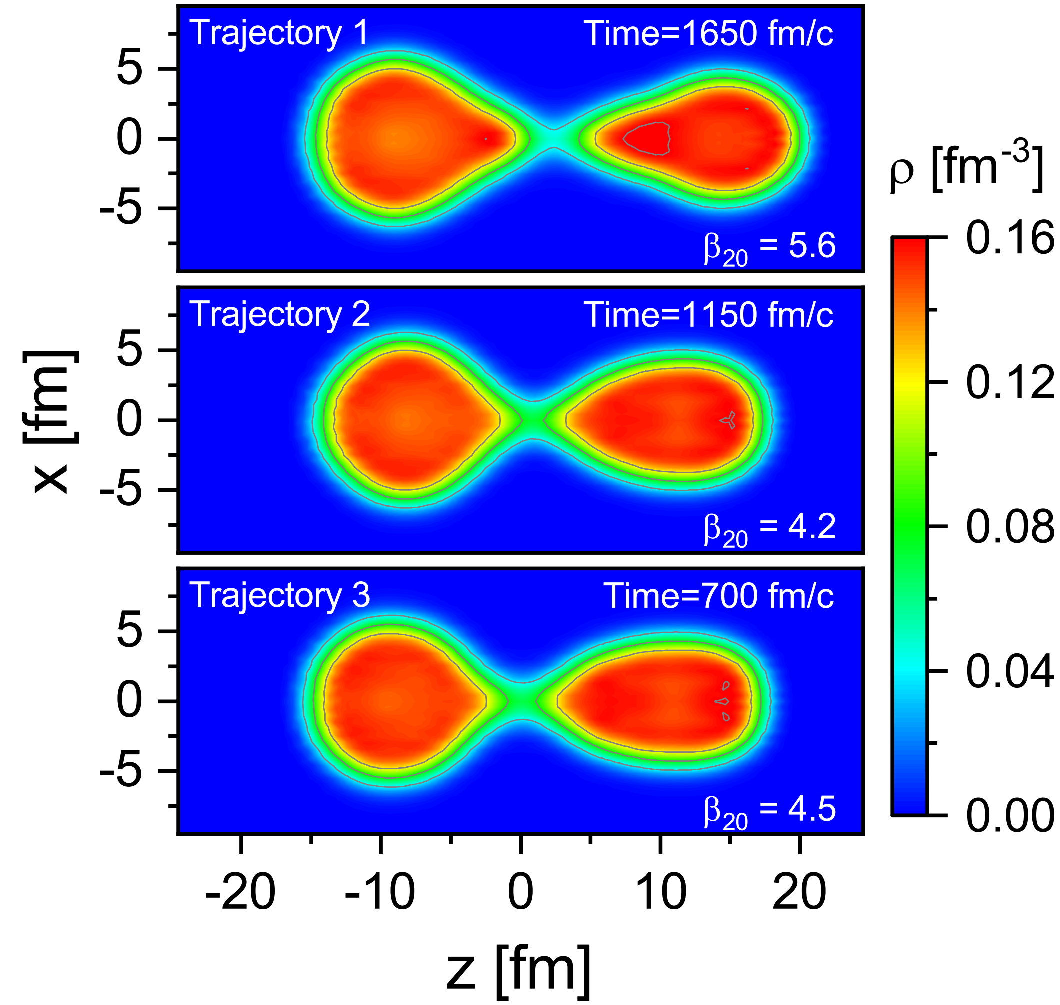


Dynamical synthesis of ^{4}He in the scission phase of nuclear fission

TDDFT fission trajectories



Density profiles at times immediately prior to the scission event.



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

Nucleon localization functions:

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

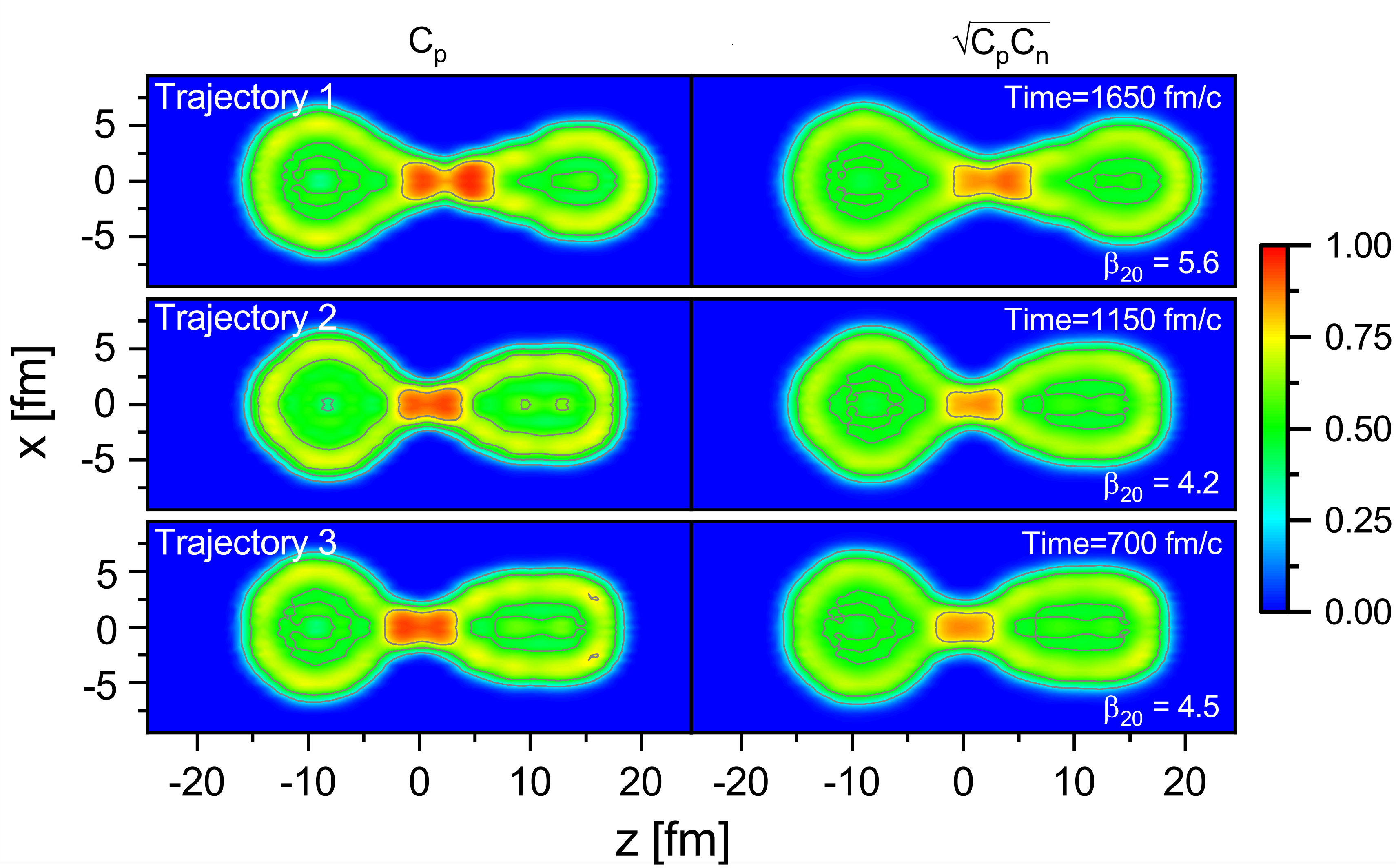
kinetic energy density, density, current density

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

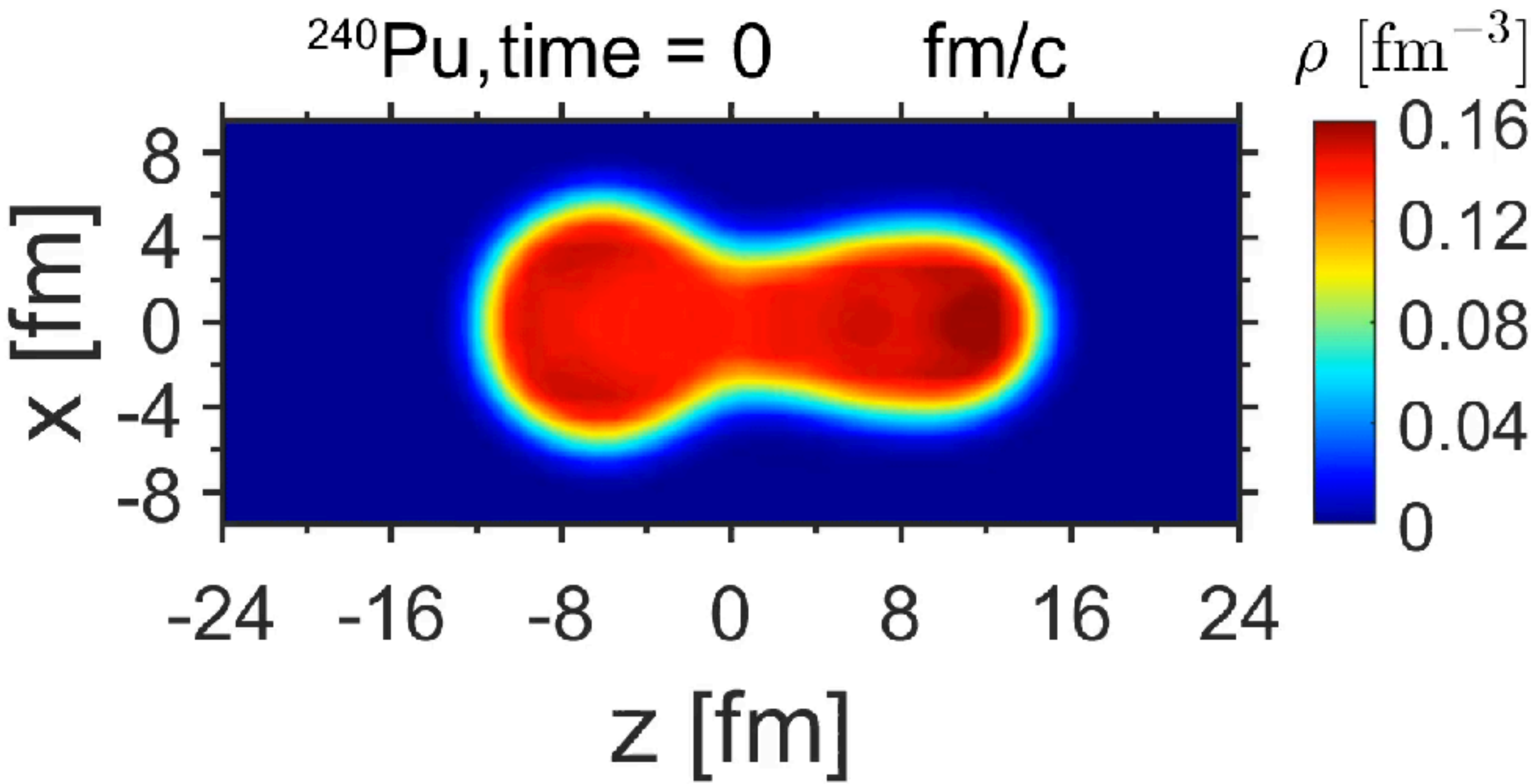
$$\tau^{\mathrm{TF}}_{q\sigma} = \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3}_{q\sigma}$$

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

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

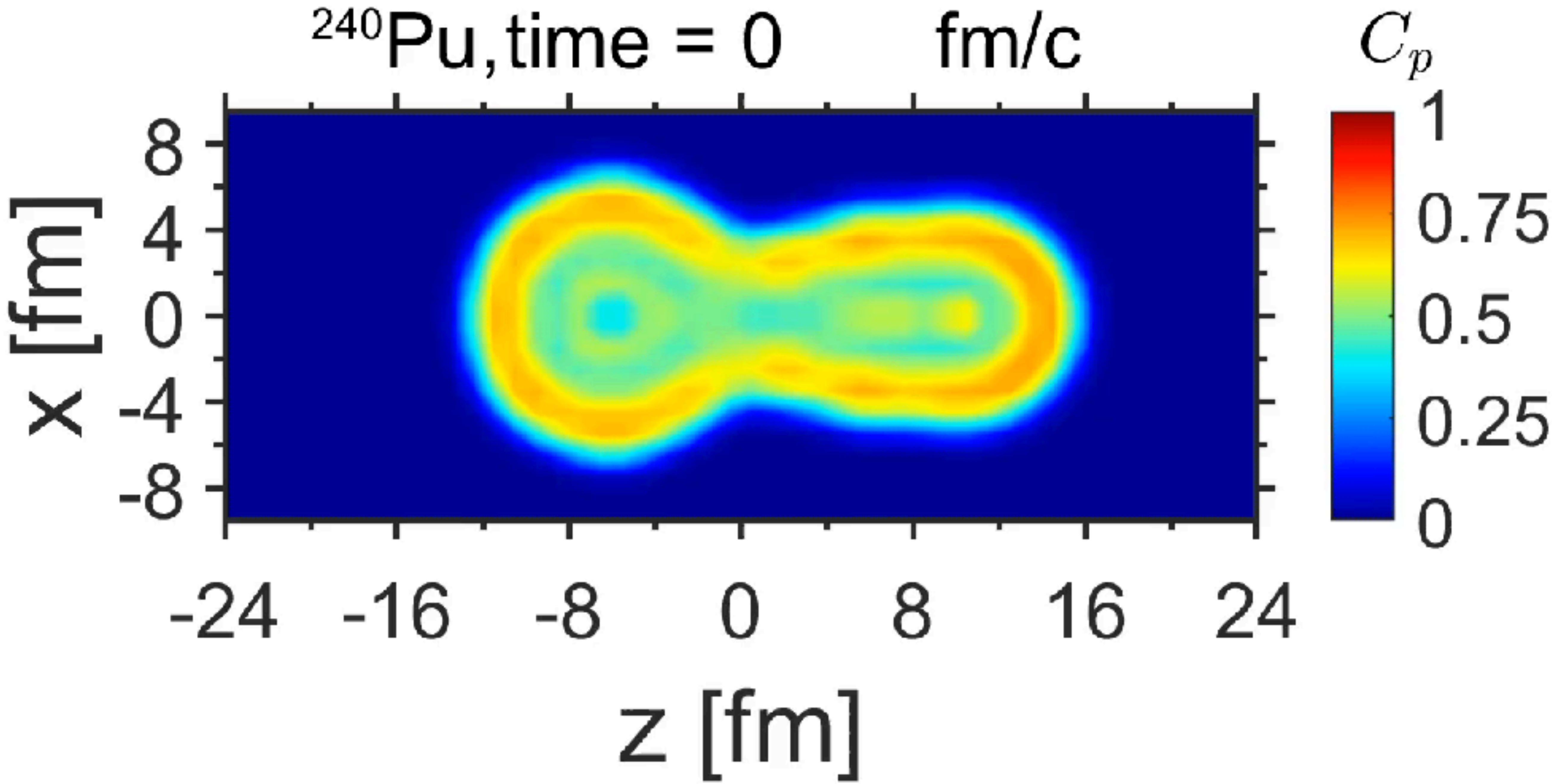


Trajectory 2



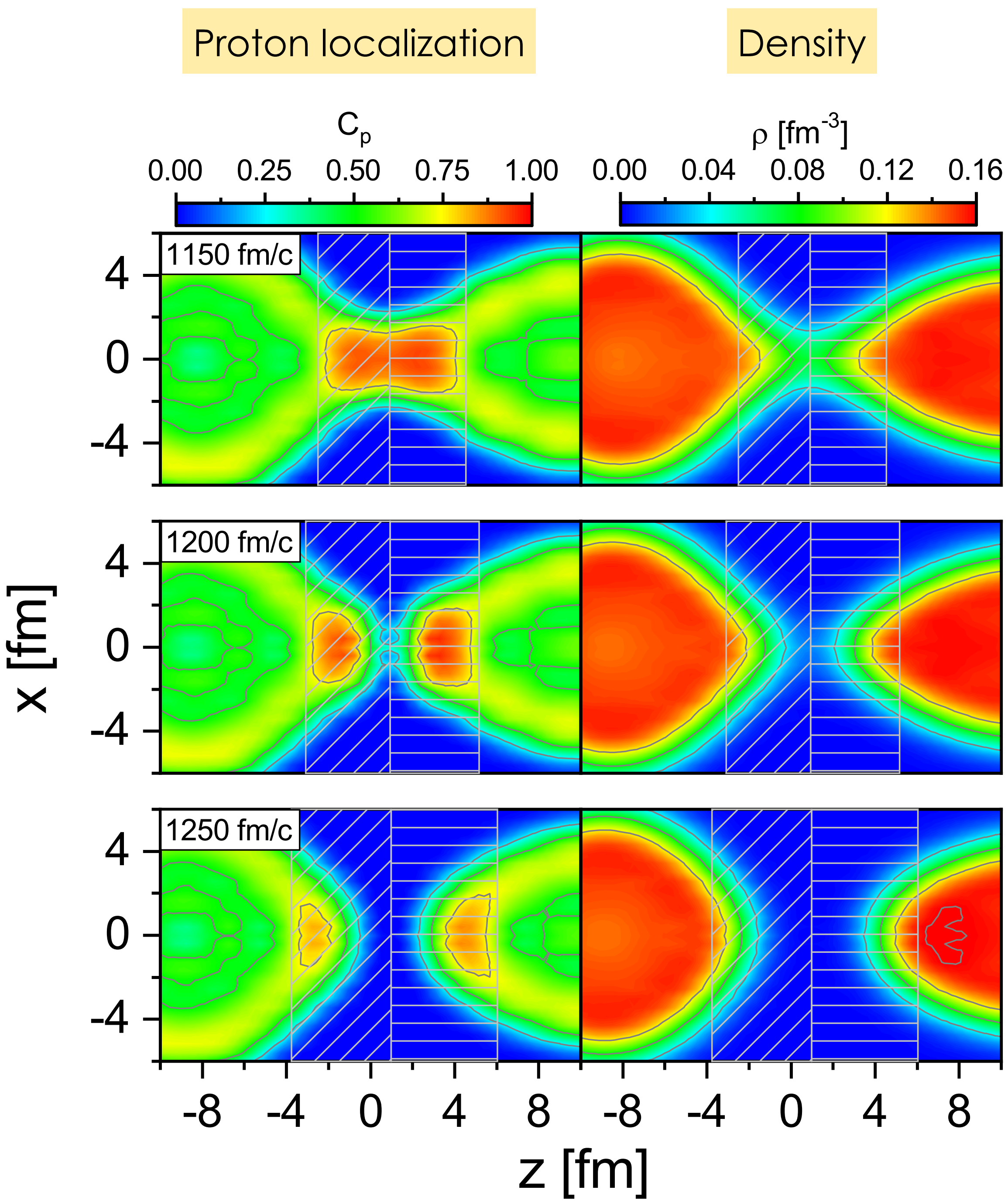
Ren, Vretenar, Nikšić, Zhao, Zhao, Meng, Phys. Rev. Lett. **128**, 172501 (2022).

Trajectory 2



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

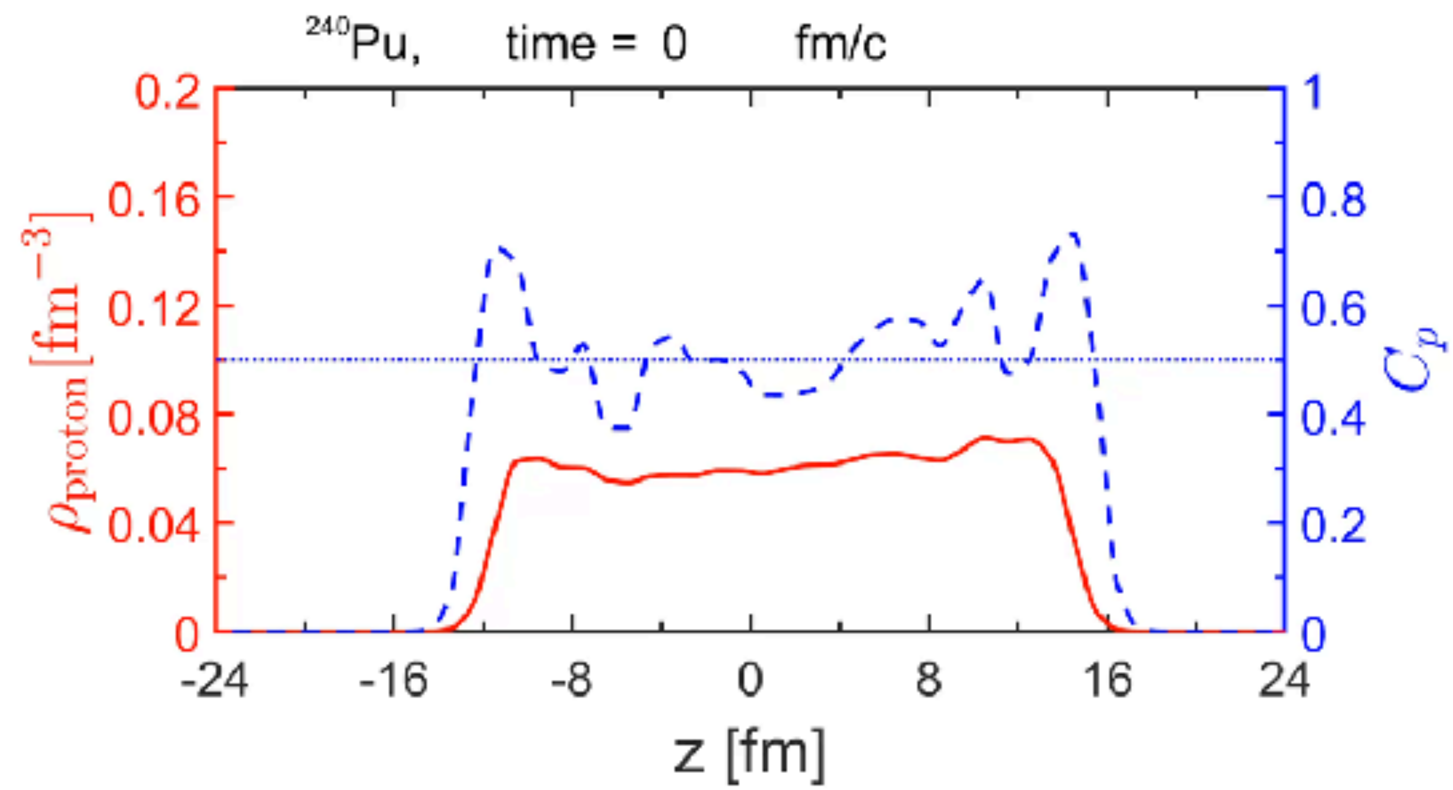
Trajectory 2



When are these light clusters formed?

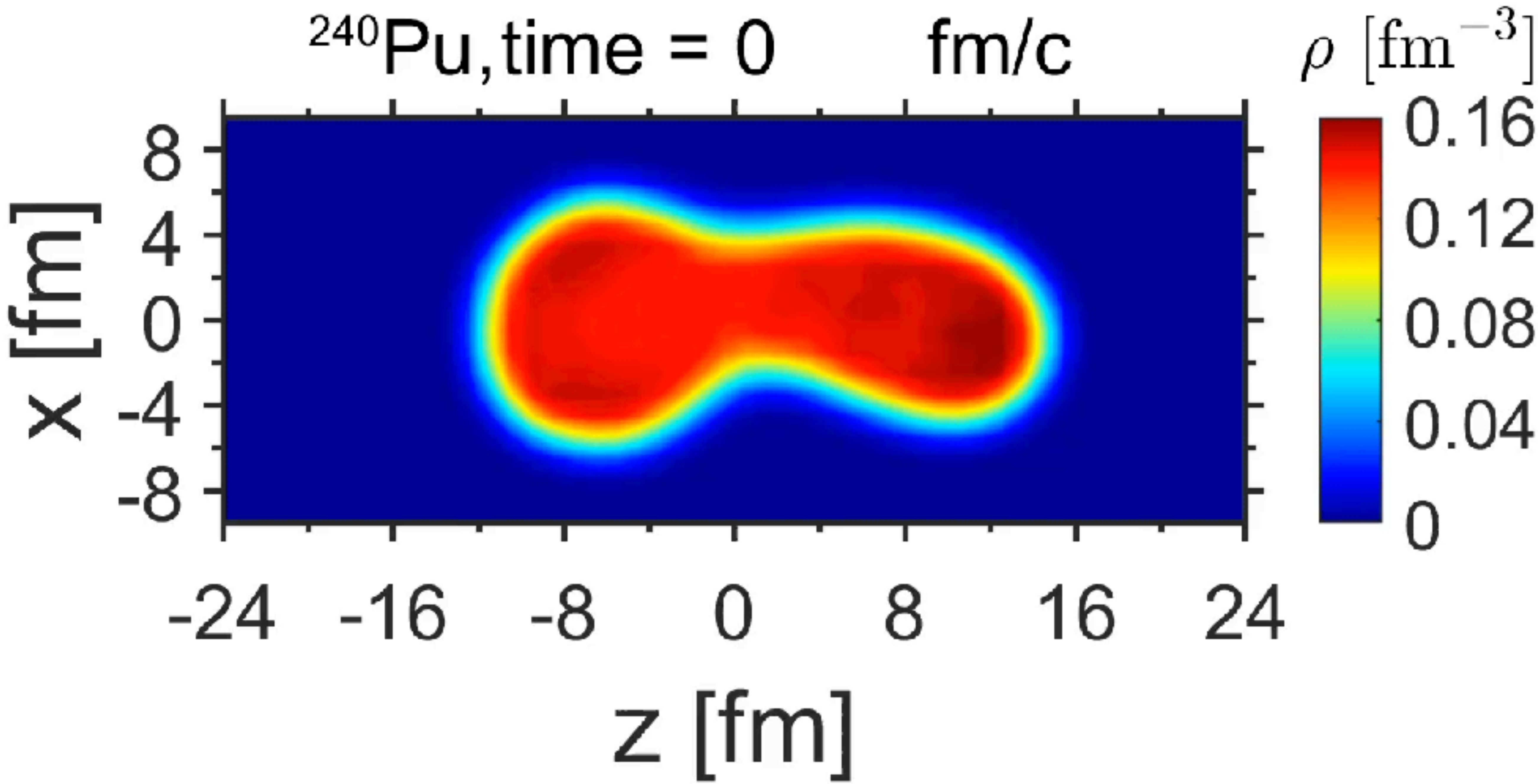
What is their structure?

What is their role in the scission mechanism?



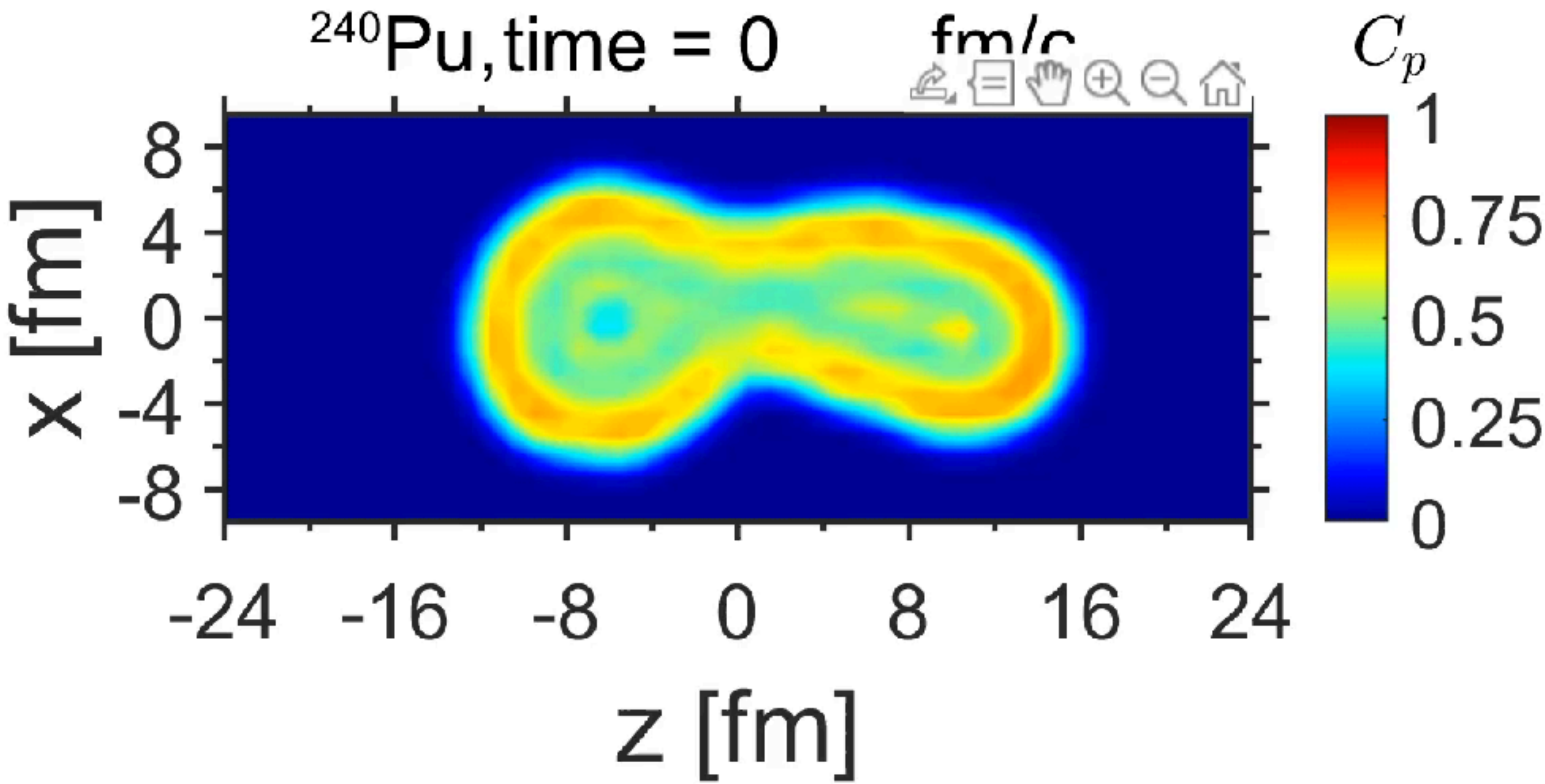
Ren, Vretenar, Nikšić, Zhao, Zhao, Meng, Phys. Rev. Lett. **128**, 172501 (2022).

Trajectory 2
Broken axial symmetry



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

Trajectory 2
Broken axial symmetry



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

Methods (TDGCM, TDDFT) based on the framework of universal Energy Density Functionals

✔ …accurate microscopic description of universal collective phenomena (fission) that reflect the organisation of nucleonic matter in finite nuclei.

- Finite temperature effects
- Energy dissipation and TKE of fragments
- Neck formation and scission mechanism
- Ternary fission
- Fragment angular momentum generation
- Symmetry restoration

Funding

This work was supported by the QuantiXLie Centre of Excellence, a project co-financed by the Croatian Government and European Union through the European Regional Development Fund - the Competitiveness and Cohesion Operational Program
(Grant KK.01.1.1.01.0004).

For more information please visit:
http://bela.phy.hr/quantixlie/hr/
https://strukturnifondovi.hr/

The sole responsibility for the content of this presentation lies with the Faculty of Science, University of Zagreb. It does not necessarily reflect the opinion of the European Union.

Europska unija
Zajedno do fondova EU

EUROPSKI STRUKTURNI
I INVESTICIJSKI FONDOVI

Operativni program
KONKURENTNOST
I KOHEZIJA

Co-financed by the European Union through the Eurpoean Regional Development Fund