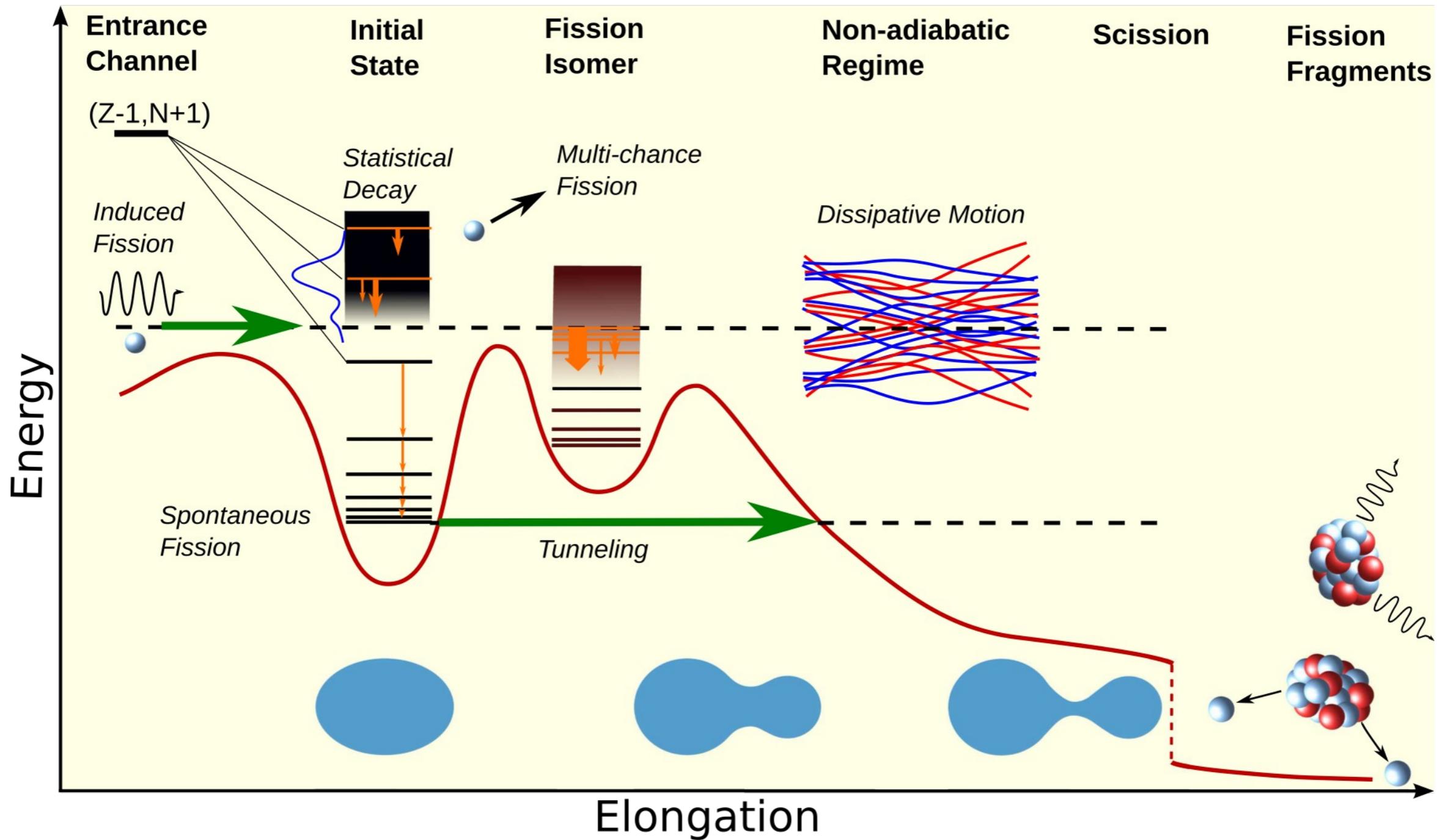


Perspectives in Nuclear Fission Theory



Dario Vretenar
University of Zagreb





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

The time-dependent generator coordinate method (TDGCM)

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

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

\Rightarrow no dissipation mechanism.

TDGCM in the Gaussian overlap approximation (TDGCM+GOA)

Example

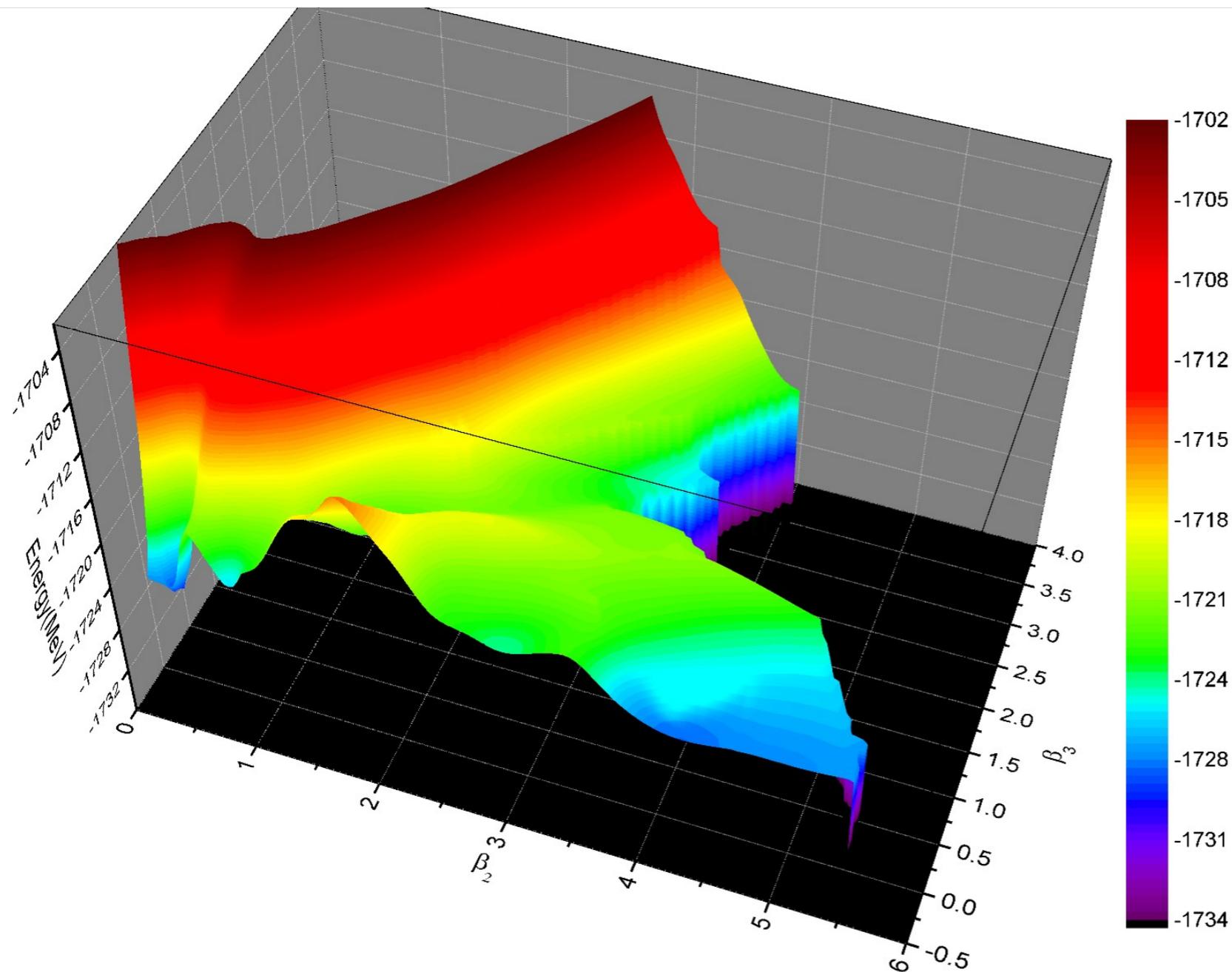
Time-dependent Schroedinger-like equation for fission dynamics (axial quadrupole and octupole deformation parameters as collective degrees of freedom):

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

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

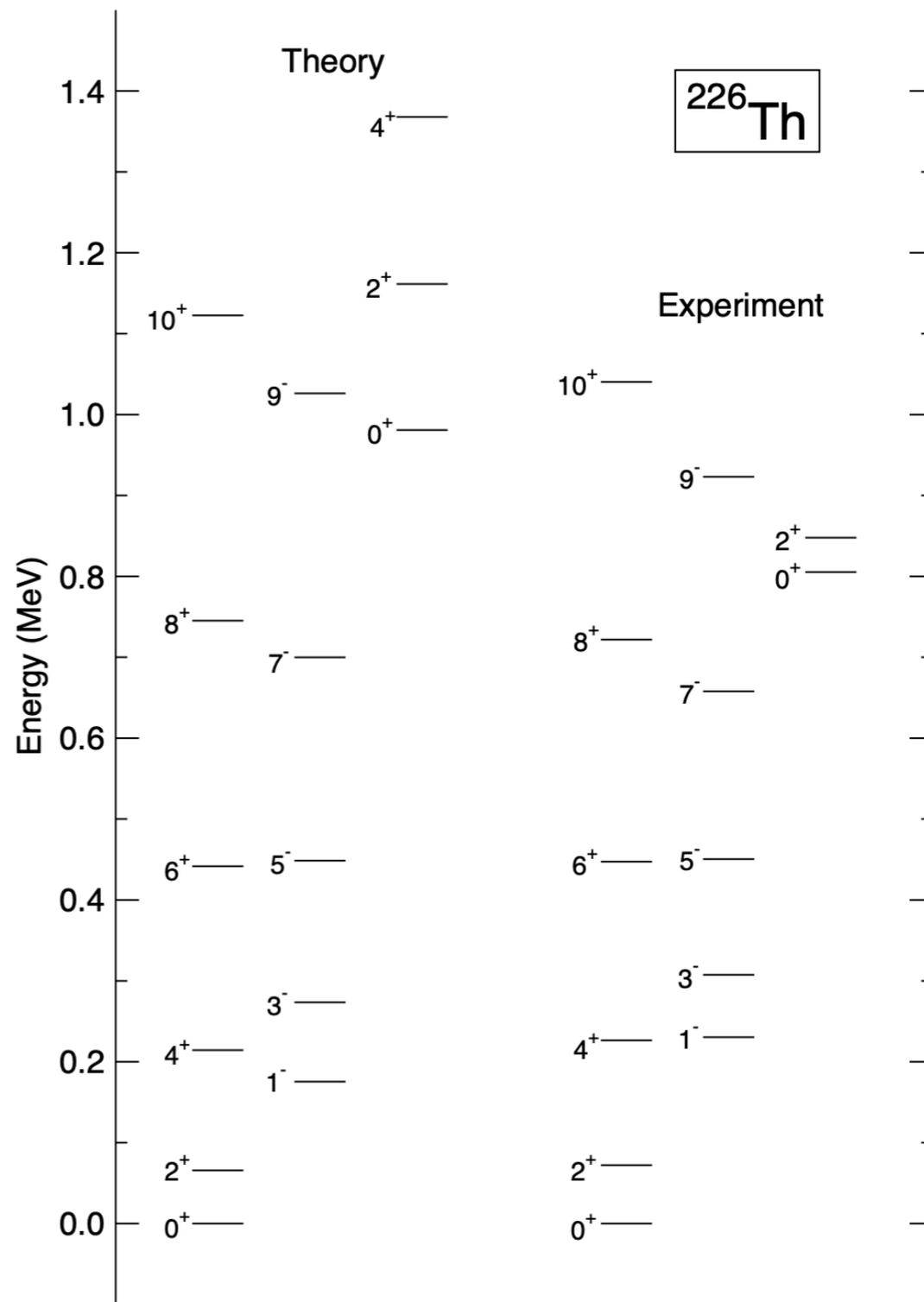
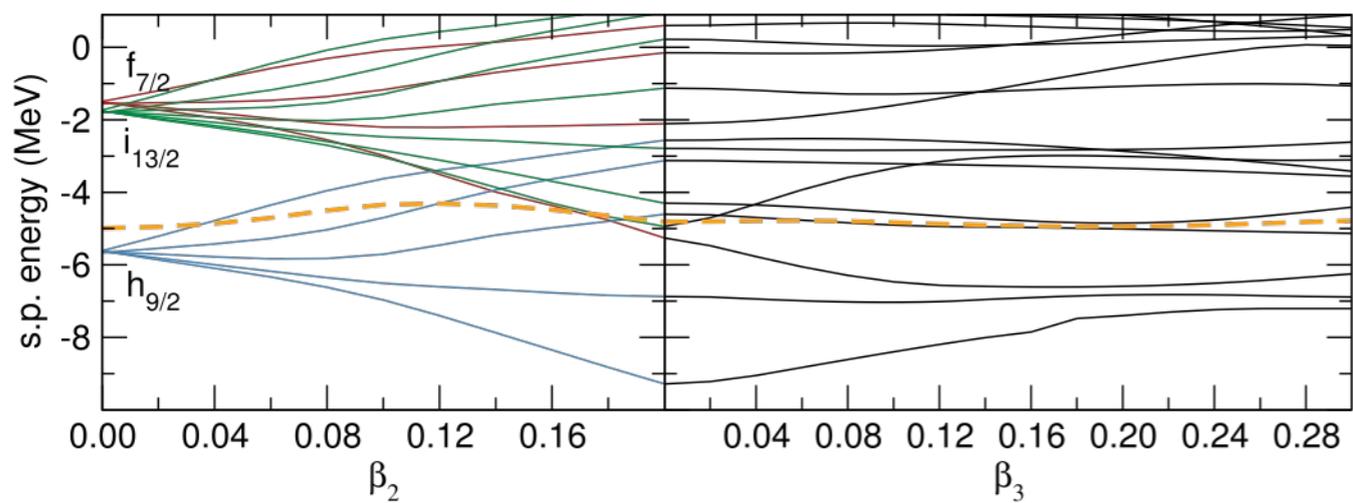
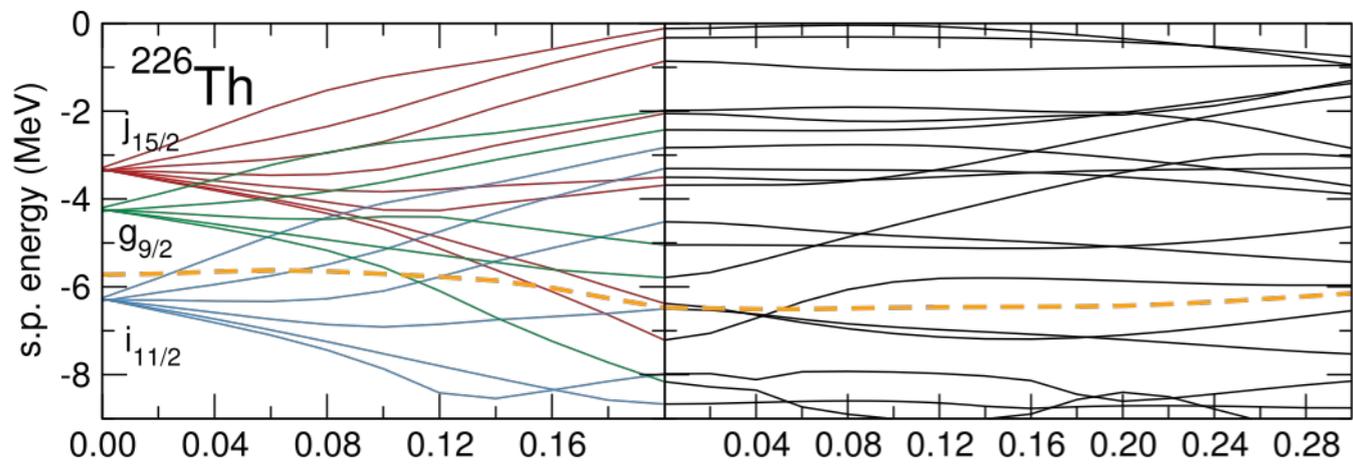
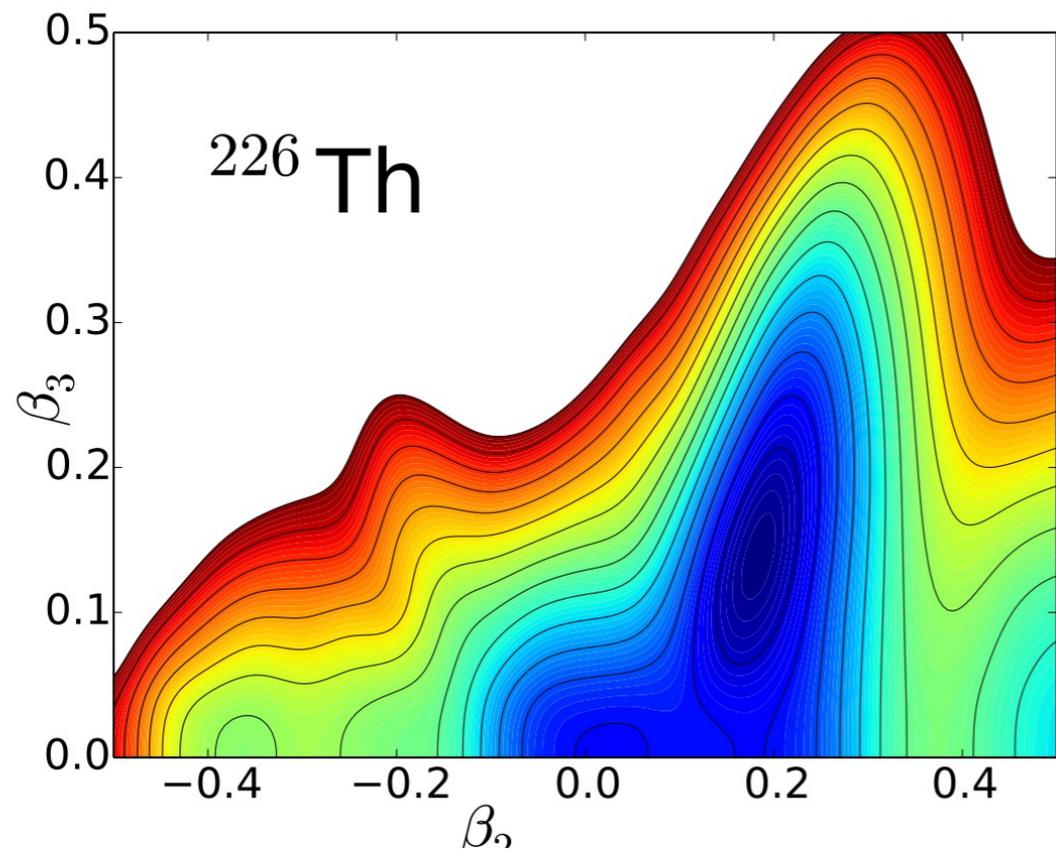
PHYSICAL REVIEW C **96**, 024319 (2017)

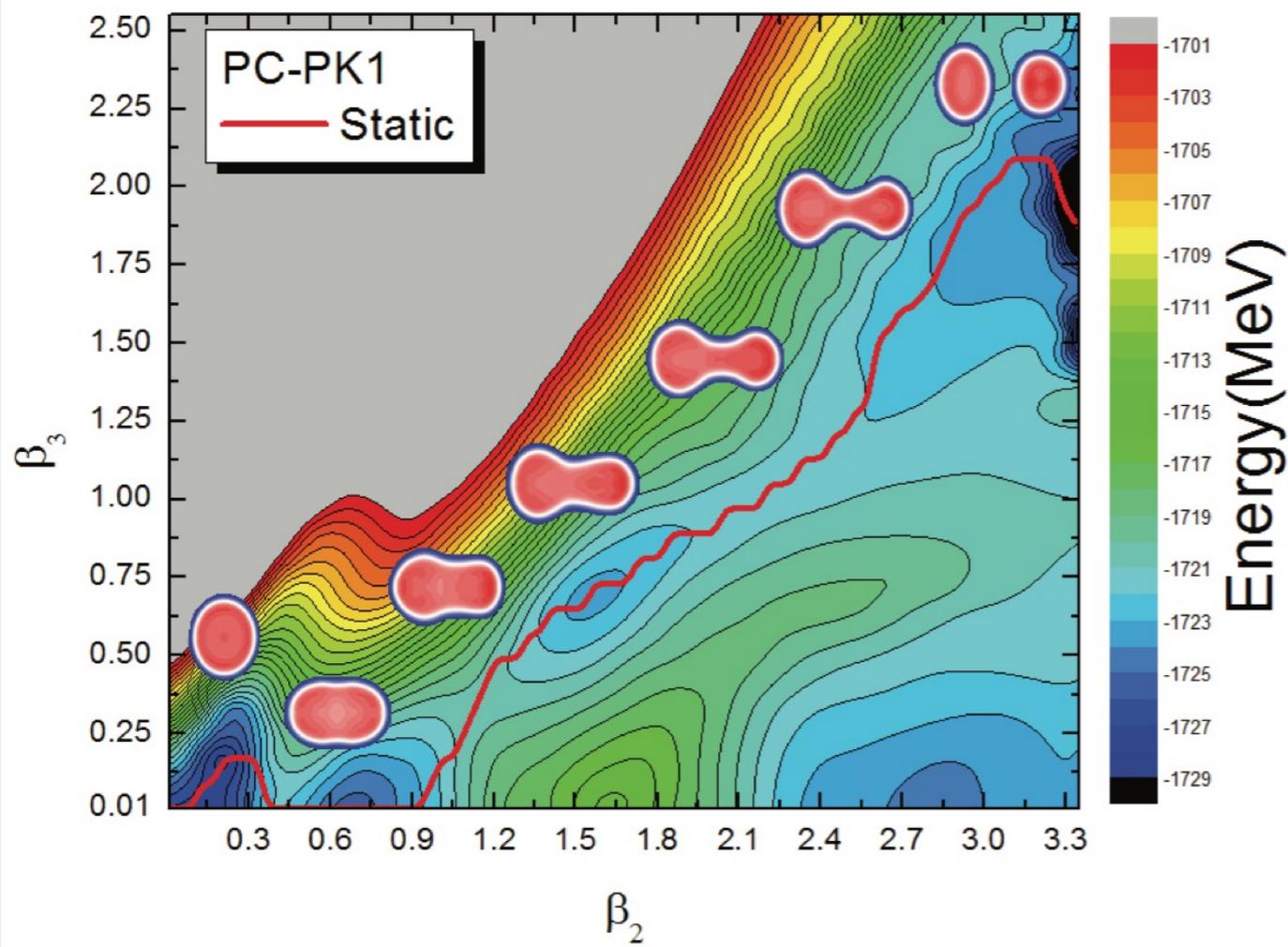


→ includes **static correlations**:
deformations & pairing

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

PC-PK I plus δ -force pairing

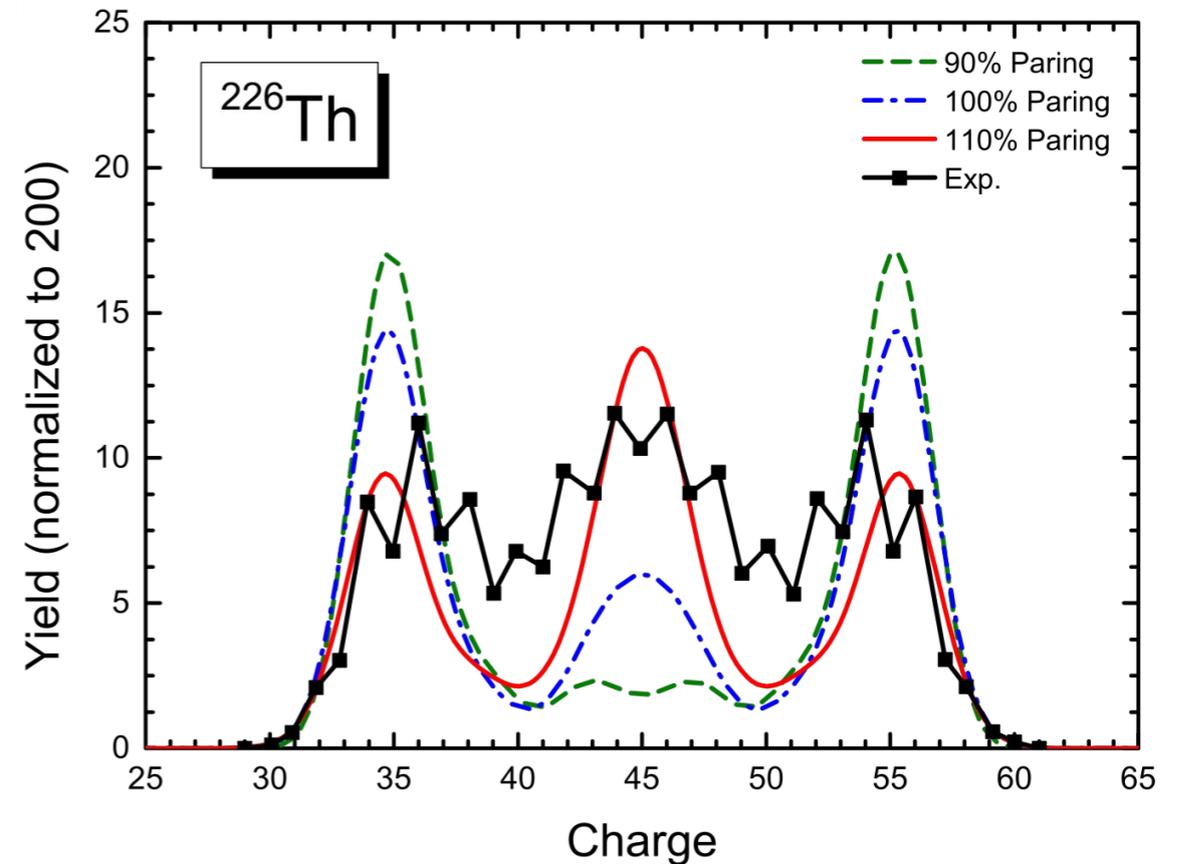




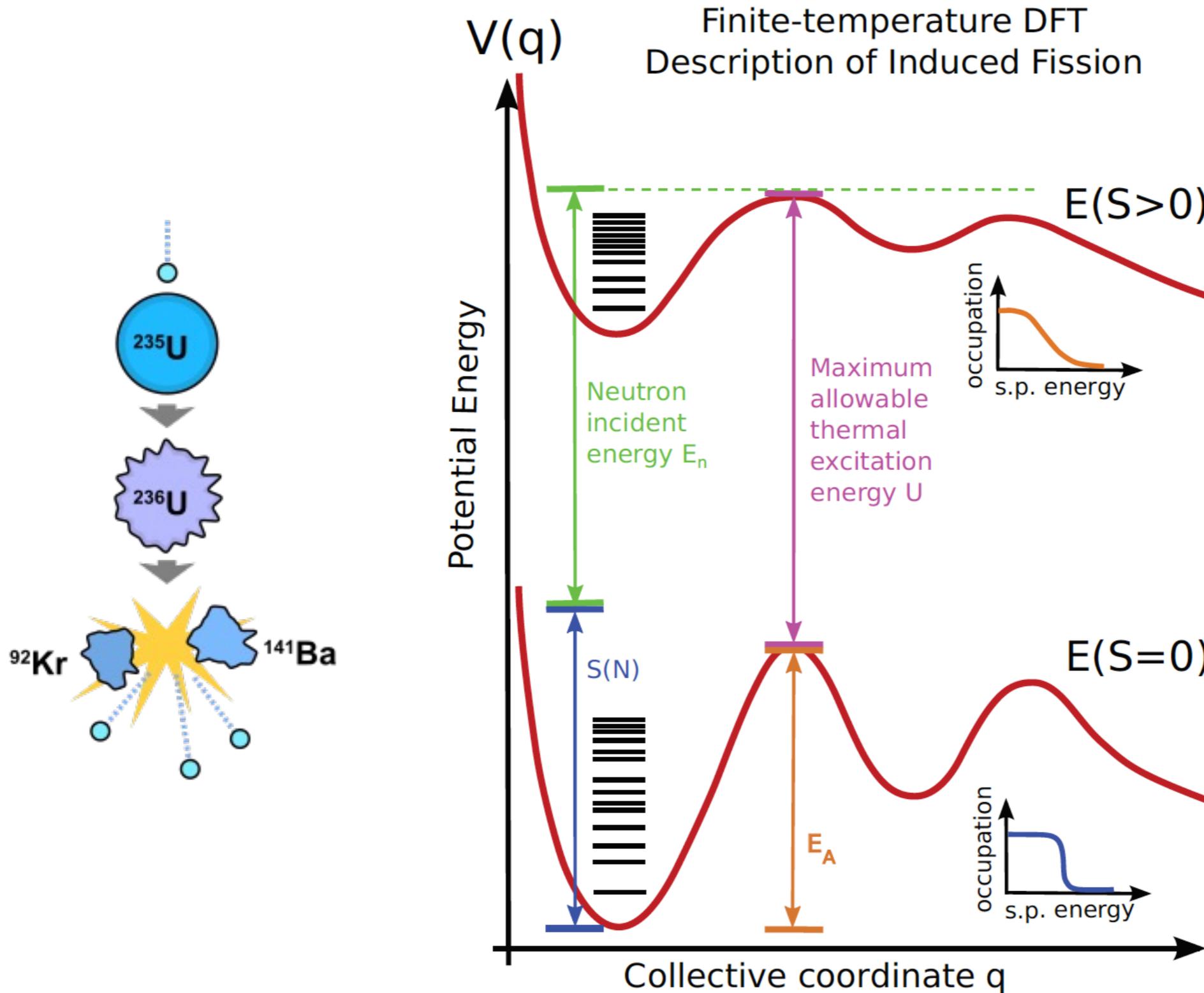
A triple-humped fission barrier is predicted along the static fission path, and the calculated heights are **7.10, 8.58, and 7.32 MeV** from the inner to the outer barrier.

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



Finite temperature effects:

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

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

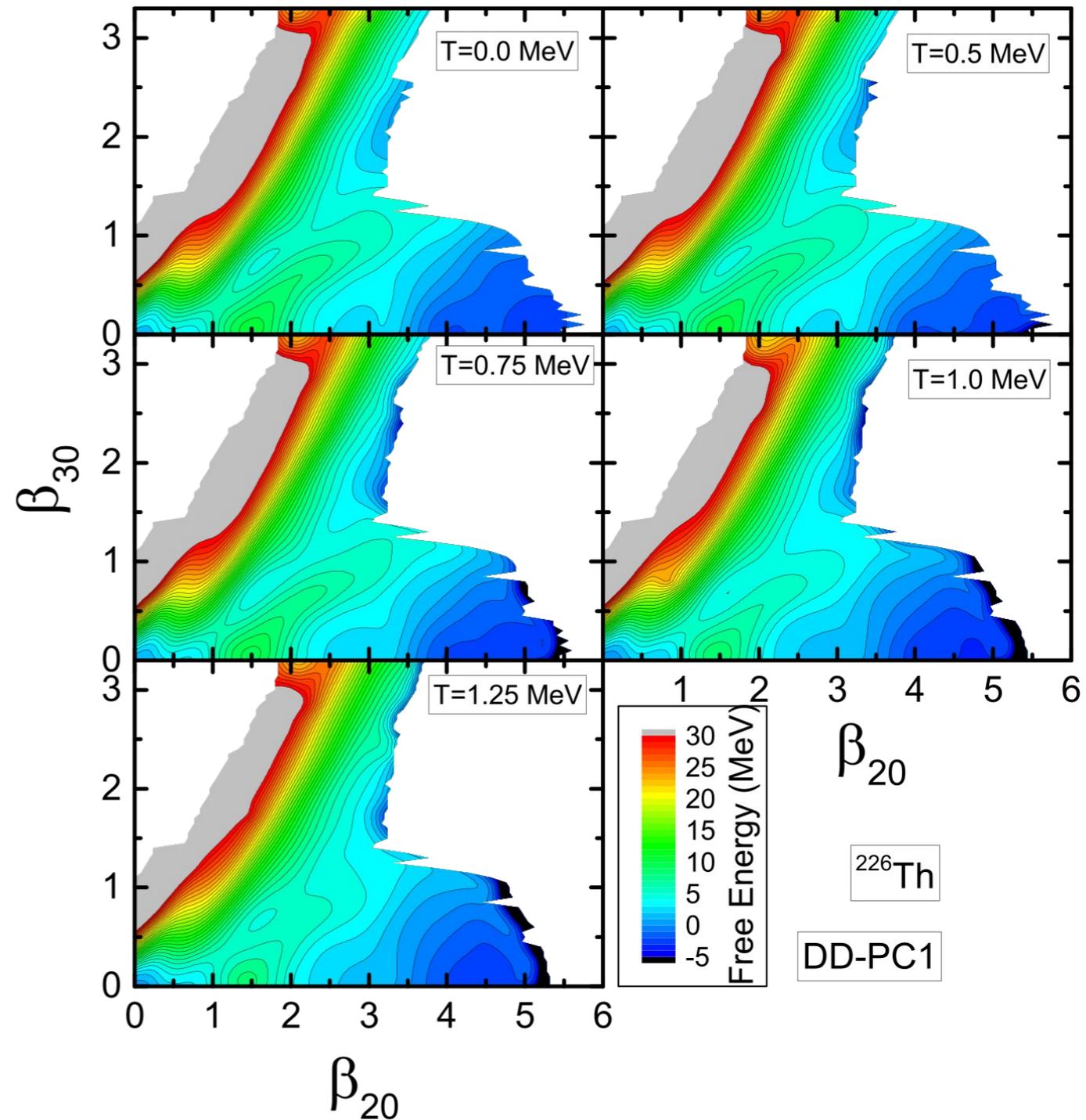
Helmholtz free energy: $F = E(T) - TS$

... entropy of the compound nuclear system:

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

... thermal occupation probabilities:

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

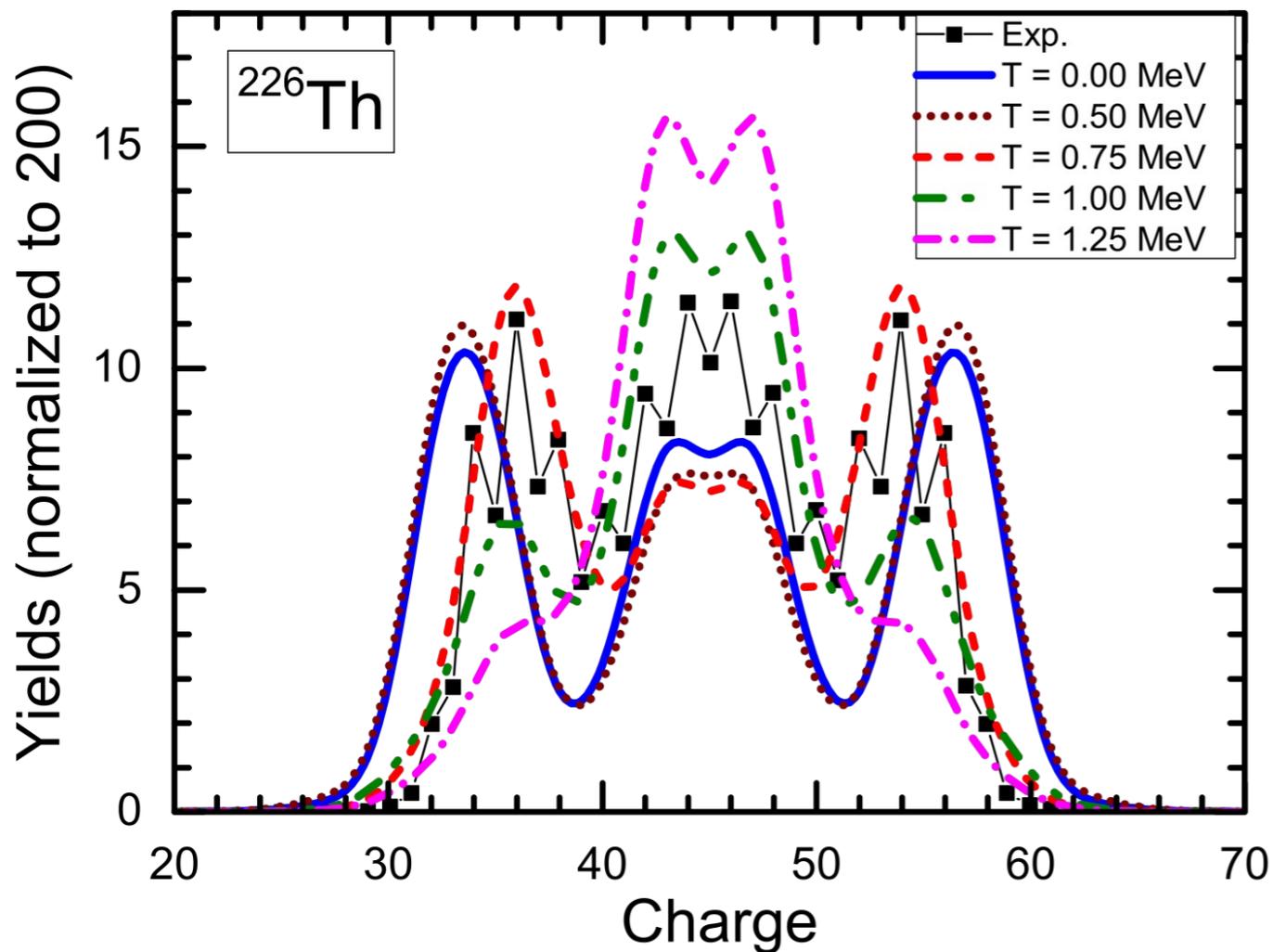


Dynamics of induced fission

Zhao, Nikšić, Vretenar, Zhou

Phys. Rev. C **99**, 014618 (2019).

Charge yields:

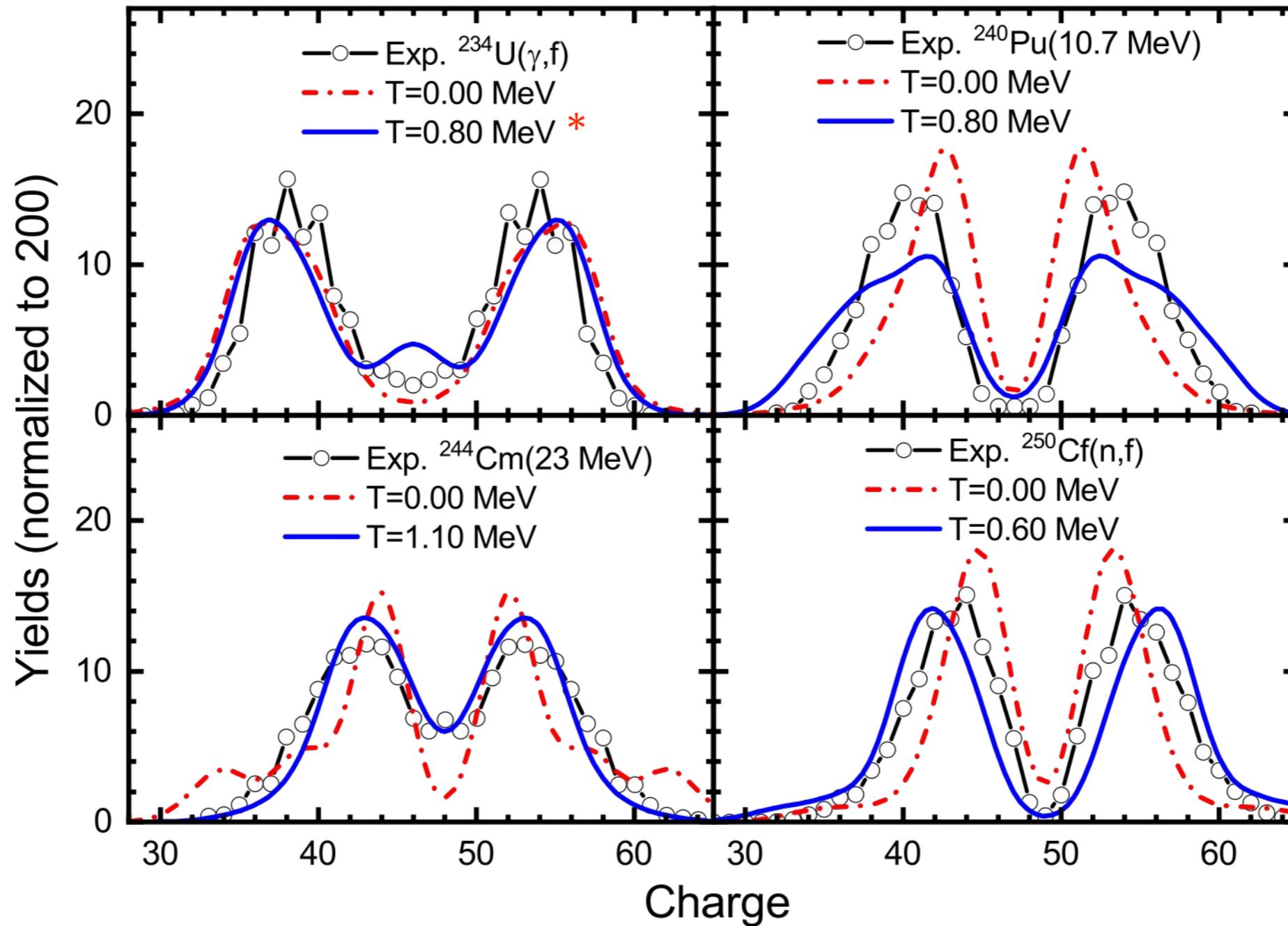


Experimental results \Rightarrow photoinduced fission with photon energies in the interval 8 – 14 MeV, and a peak value $E_\gamma = 11$ MeV.

$T = 0.5, 0.75, 1.0,$ and 1.25 MeV \Rightarrow 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 \Rightarrow constraints on the mass multipole moments and the particle-number dispersion operator:

$$\Delta\hat{N}^2 = \hat{N}^2 - \langle\hat{N}\rangle^2.$$

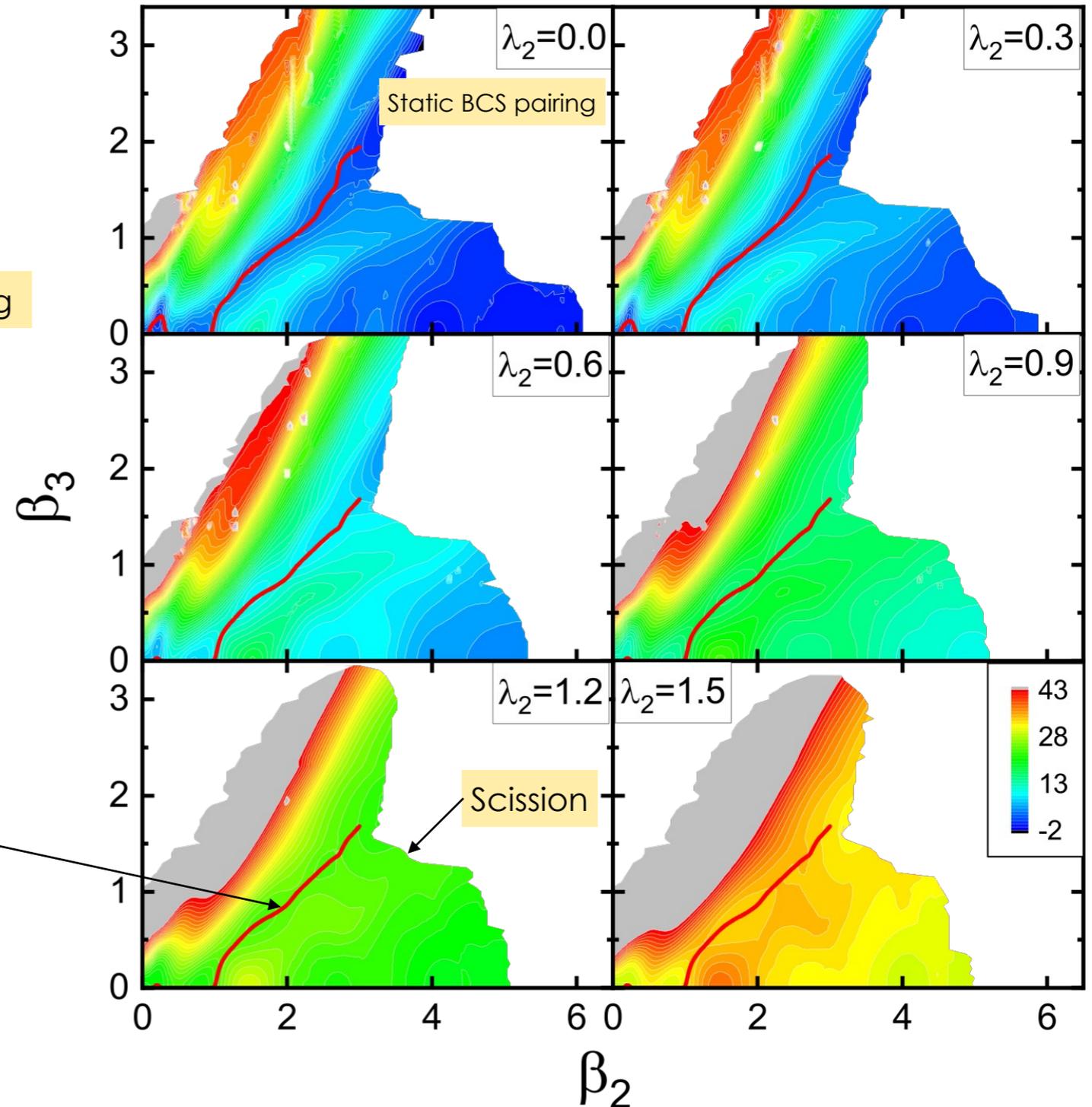
... the Routhian:

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

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 .

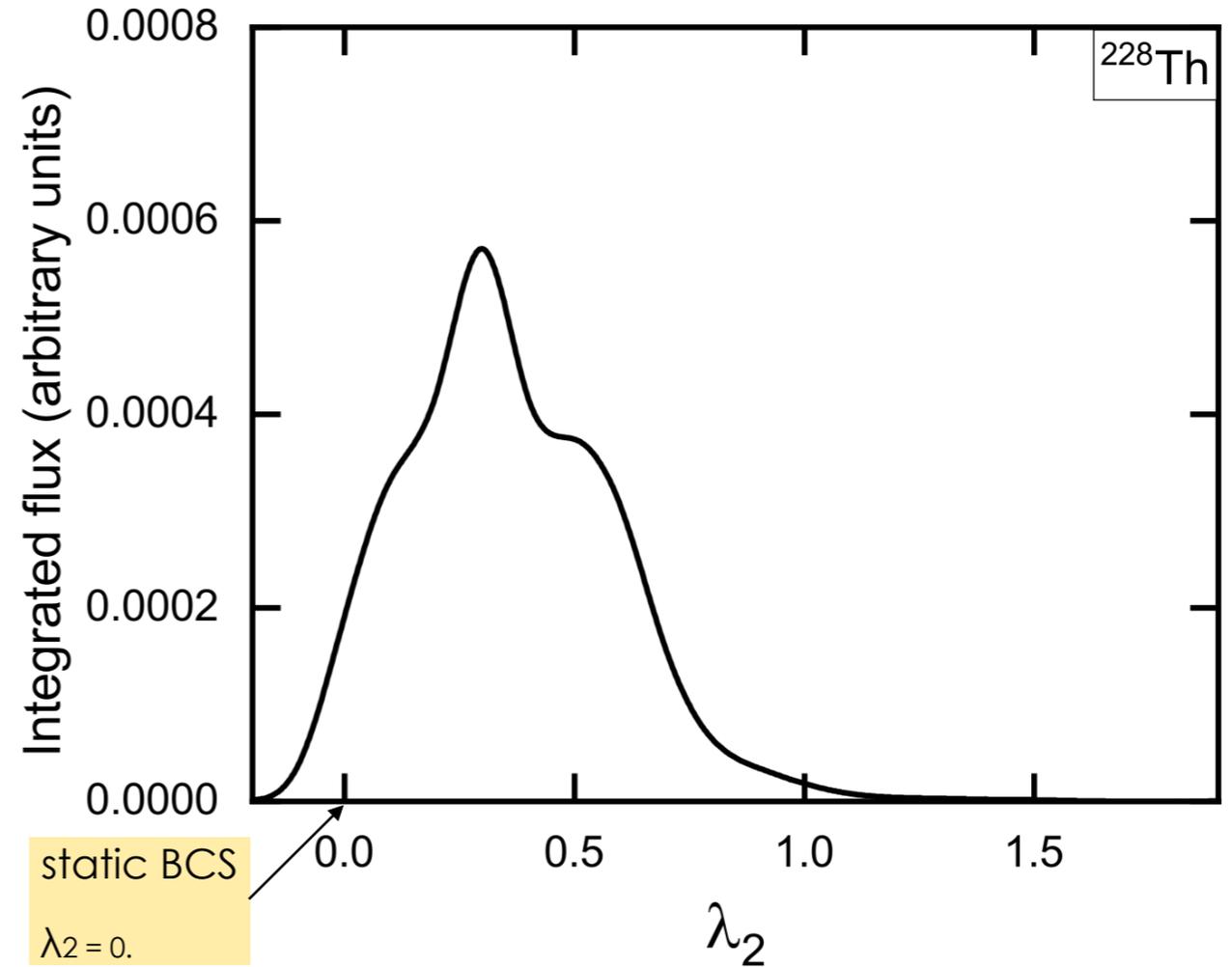
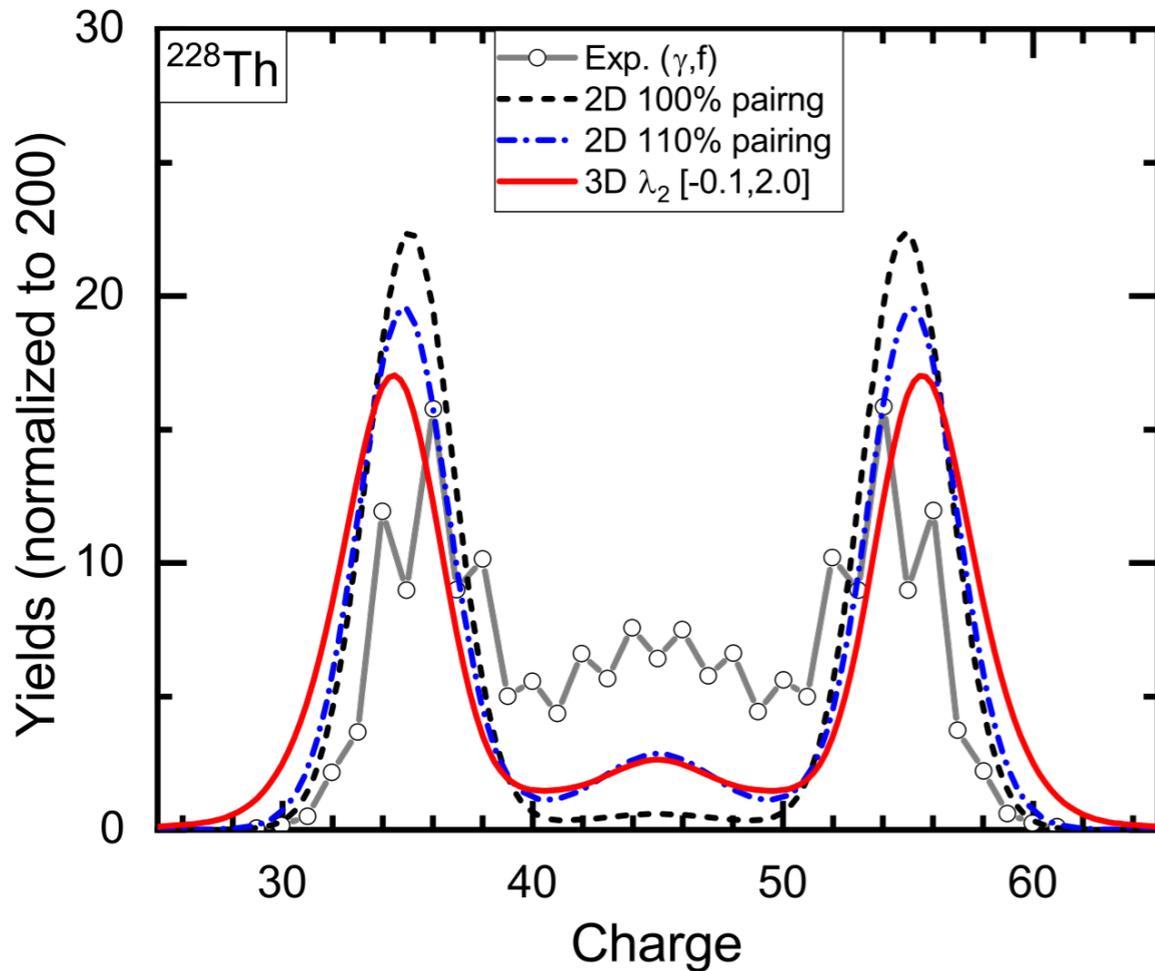
Static fission path of minimum energy



3D TDGCM+GOA calculation

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

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



Charge yields calculated in the 3D collective space
 → deformation β_2 , β_3 and dynamical pairing λ_2
 coordinates.

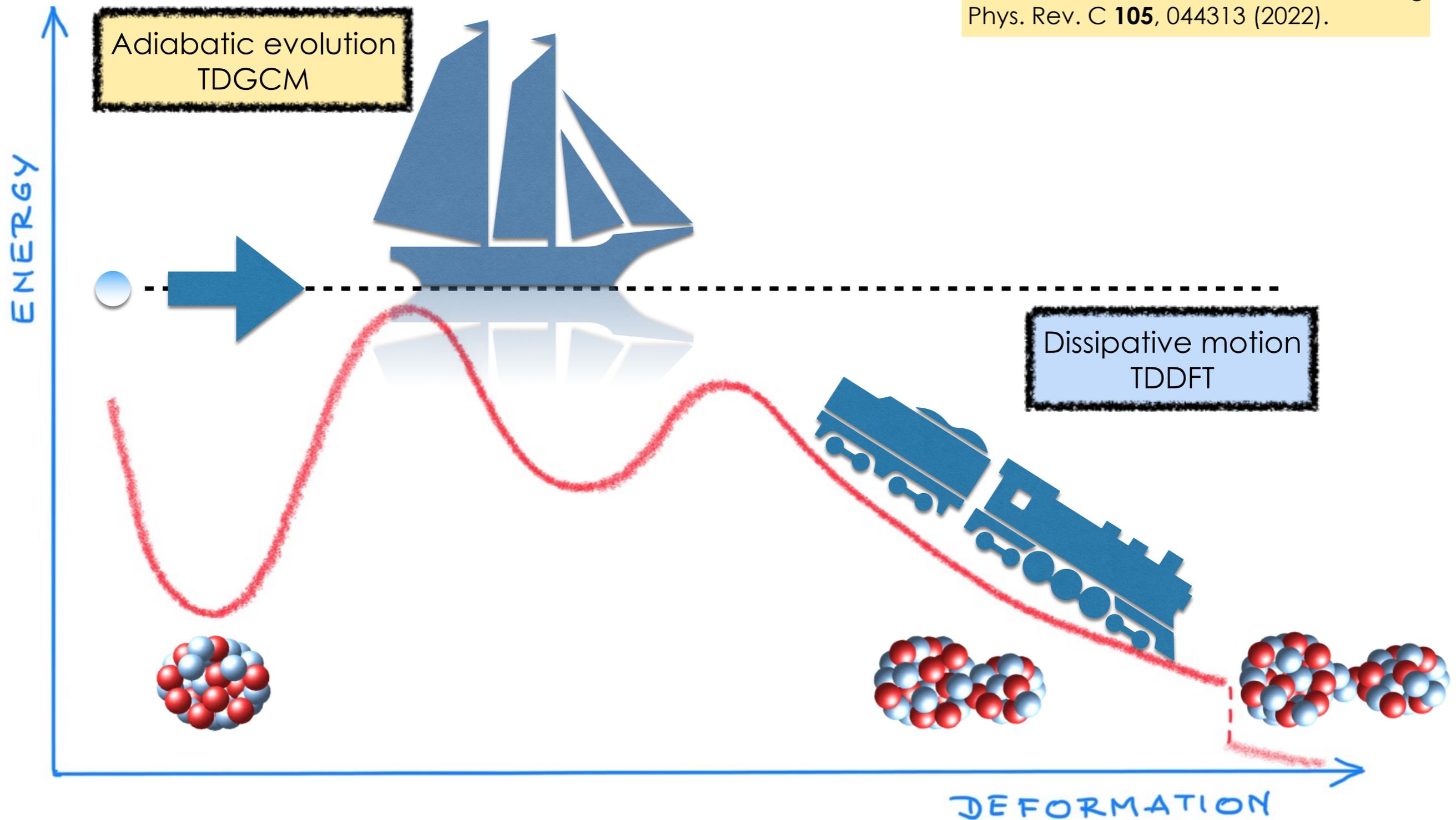
Effect of dynamical pairing on the flux of the probability current
 through the scission hyper-surface:

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

→ time-integrated flux through the scission contour in the (β_2, β_3)
 plane, for a given value of the pairing collective coordinate λ_2 .

Adiabatic evolution and dissipative dynamics

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



Time-dependent density functional theory (TDDFT)

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

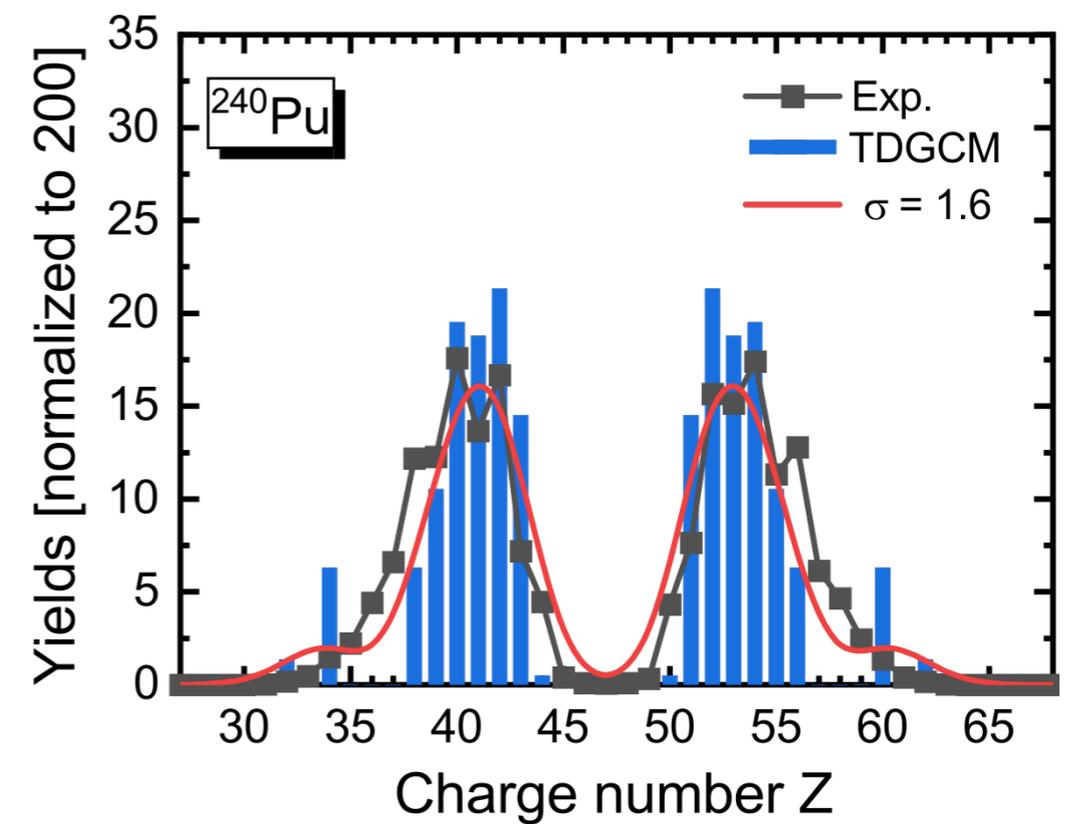
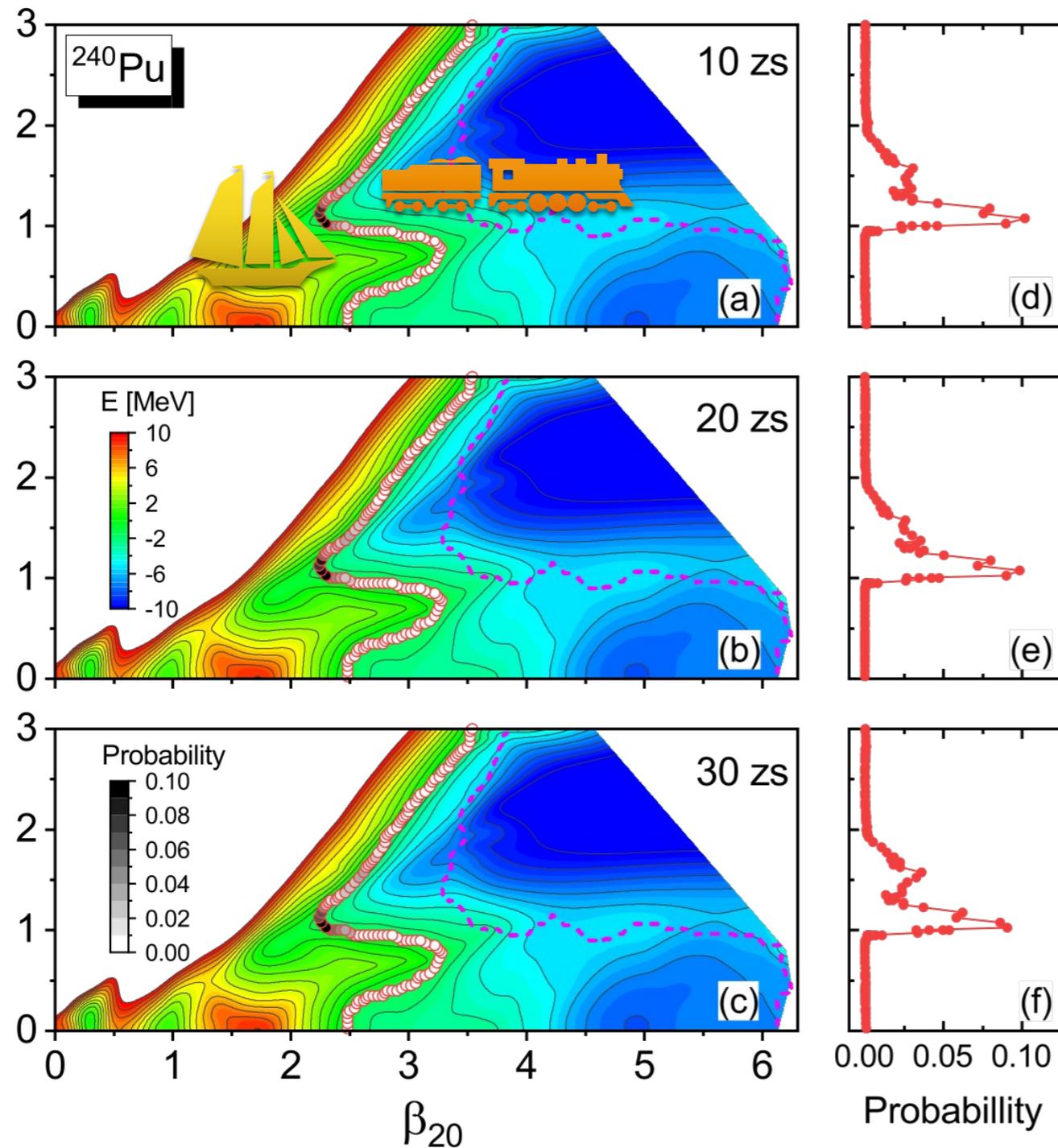
$$i \frac{d}{dt} n_k(t) = n_k(t) \Delta_k^*(t) - n_k^*(t) \Delta_k(t),$$

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

⇒ 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.

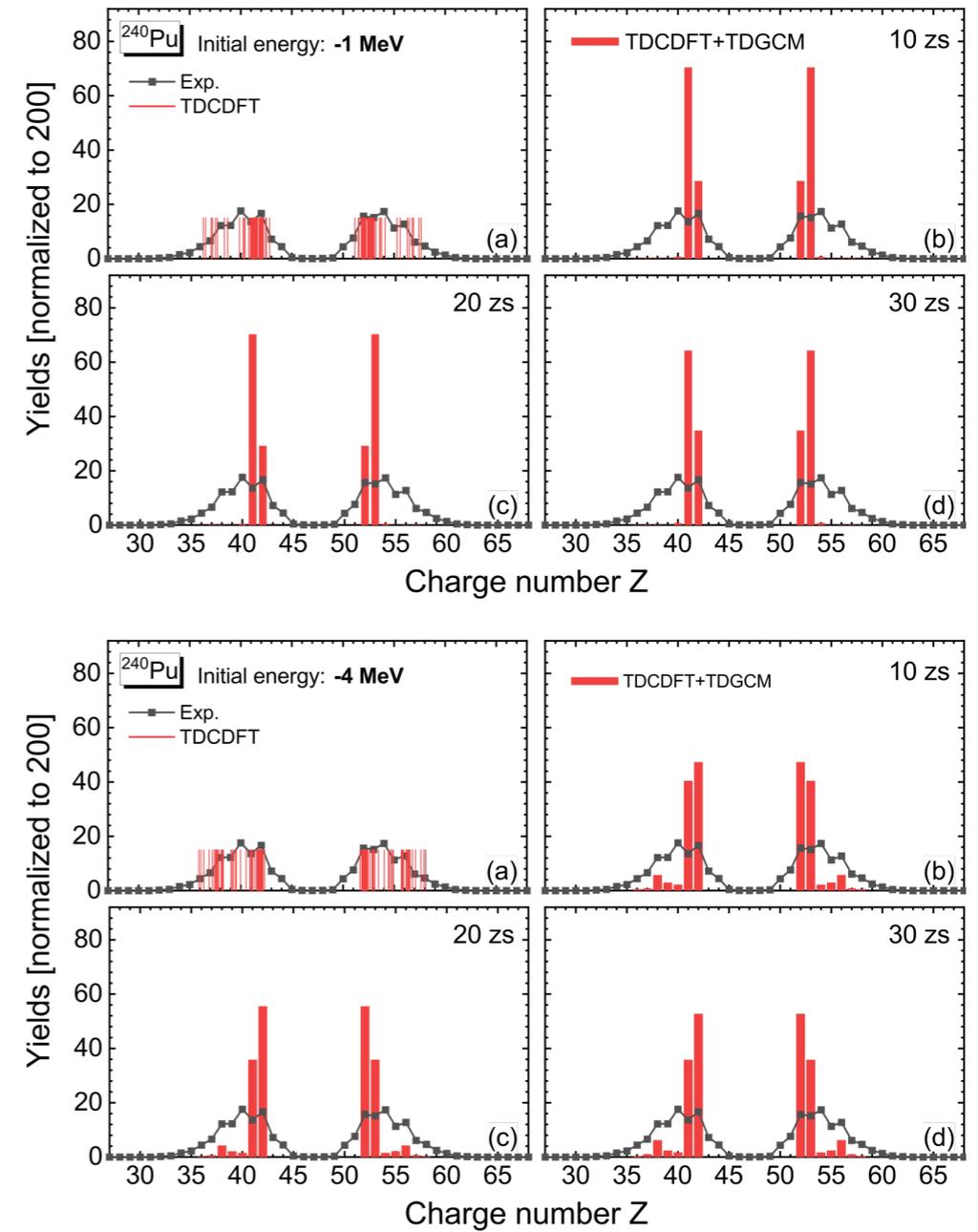
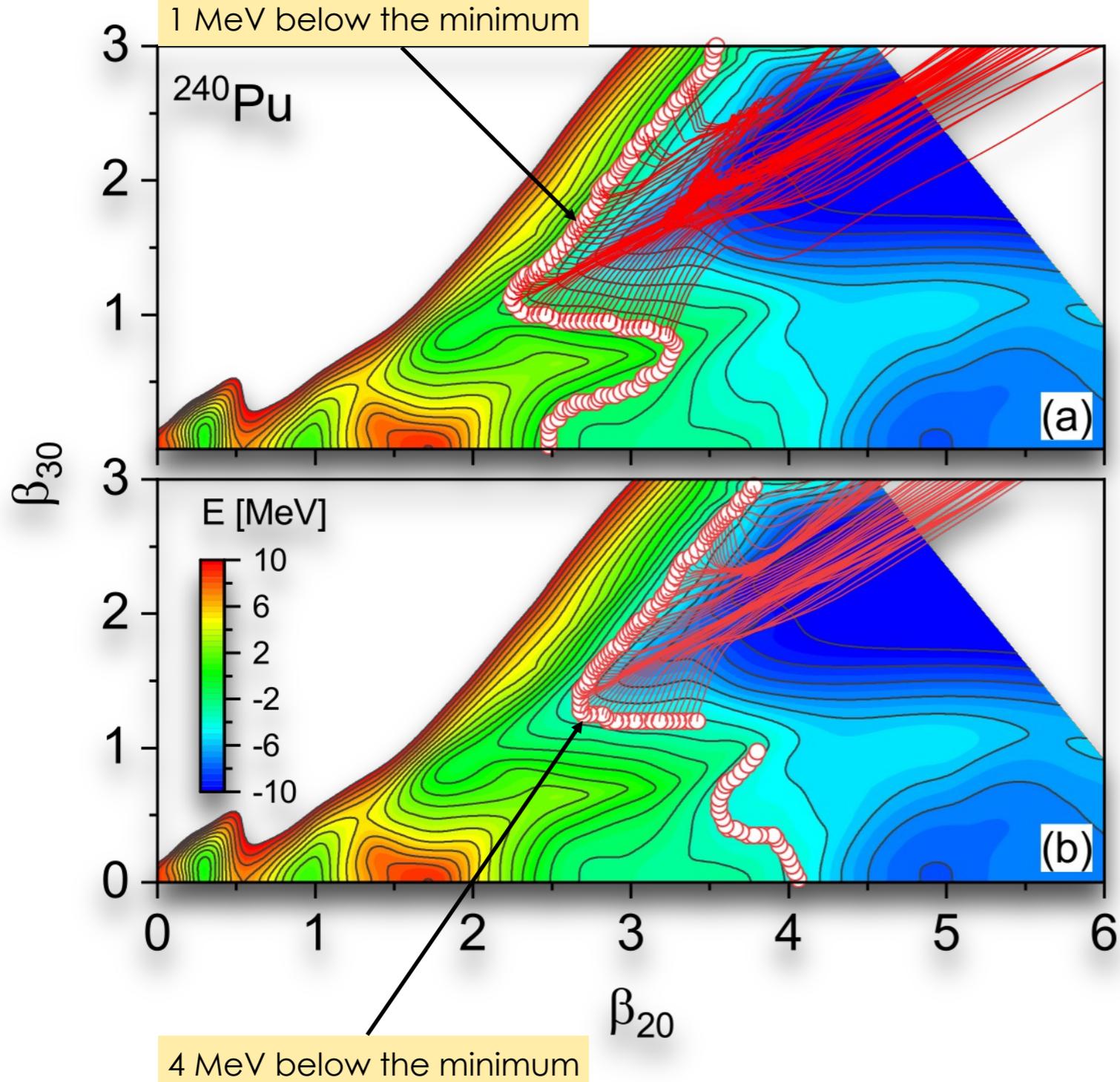
⇒ automatically includes the one-body dissipation mechanism, but can only simulate a single fission event by propagating the nucleons independently.

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

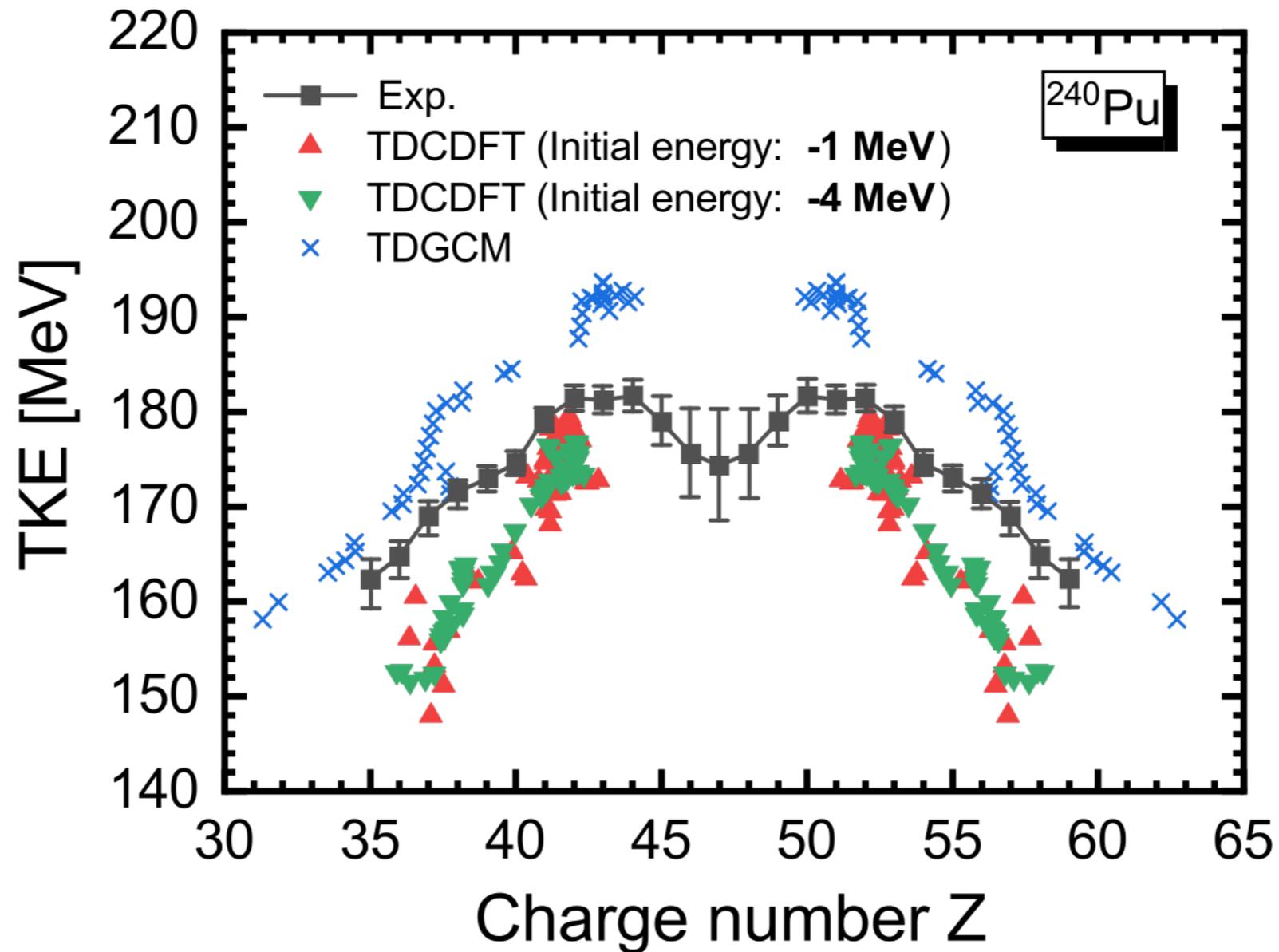
$$E_{\text{TKE}} = \frac{e^2 Z_H Z_L}{d_{\text{ch}}},$$

d_{ch} → distance between centers of charge at the point of scission.

TDDFT

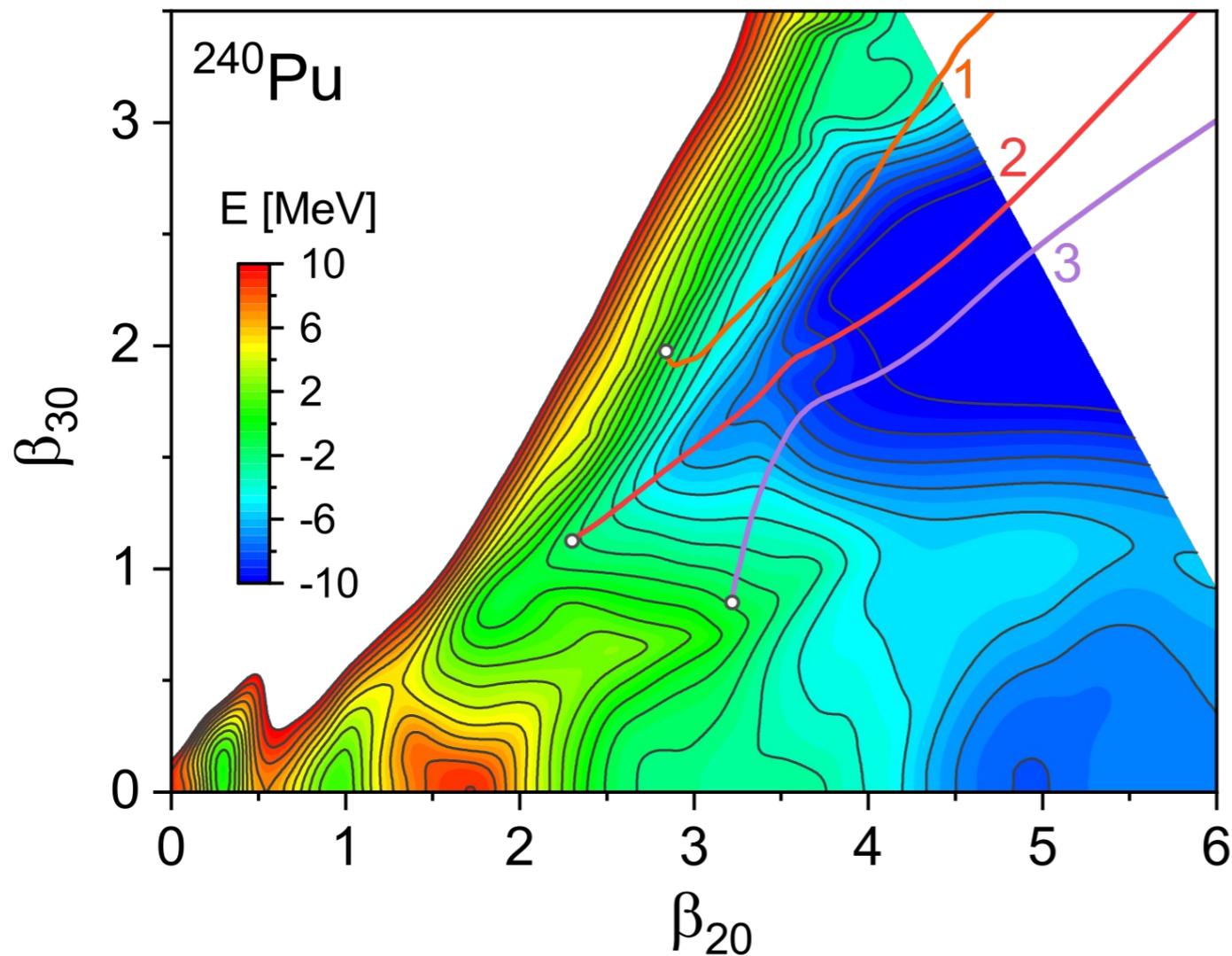
$$E_{\text{TKE}} = \frac{1}{2} m A_H v_H^2 + \frac{1}{2} m A_L v_L^2 + E_{\text{Coul}},$$

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

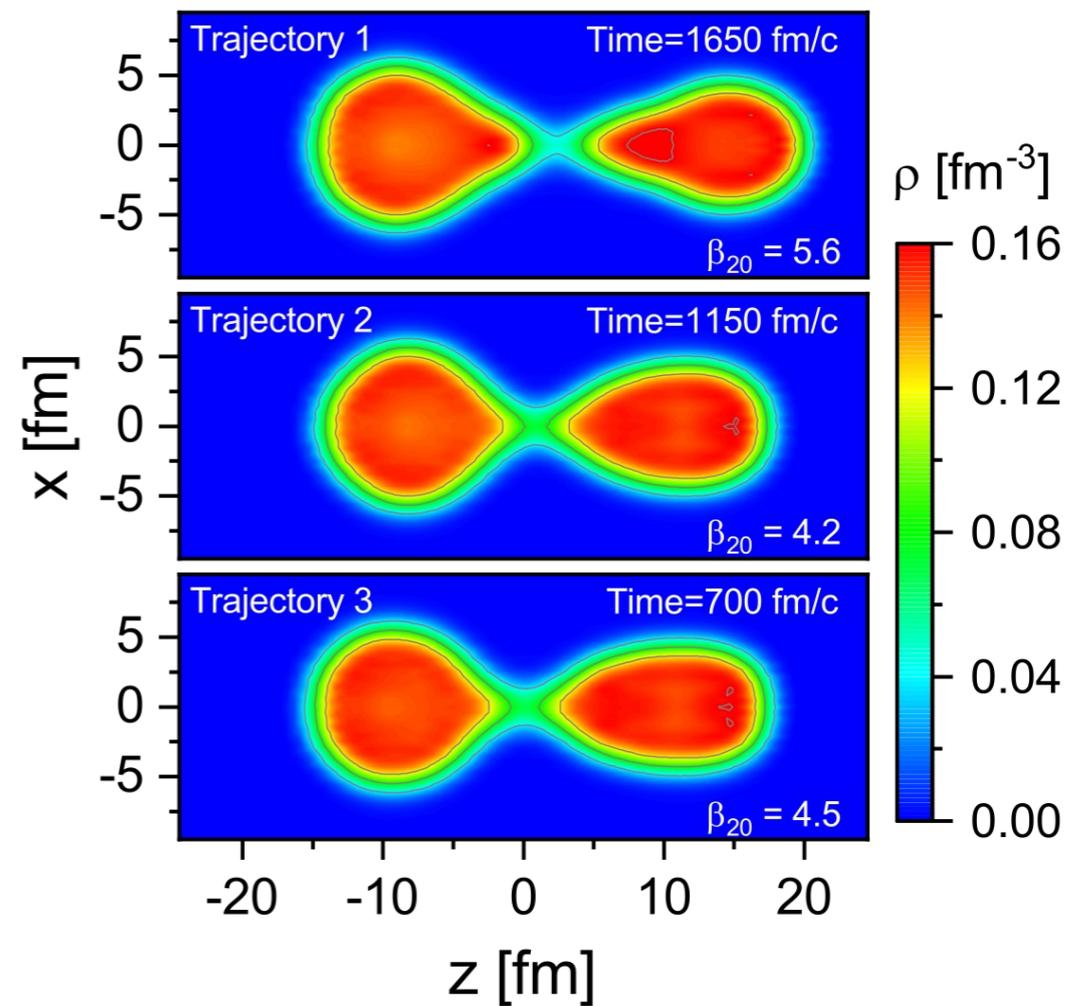


Dynamical synthesis of ^4He in the scission phase of nuclear fission

TDDFT fission trajectories



Density profiles at times immediately prior to the scission event.



Nucleon localization functions:

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

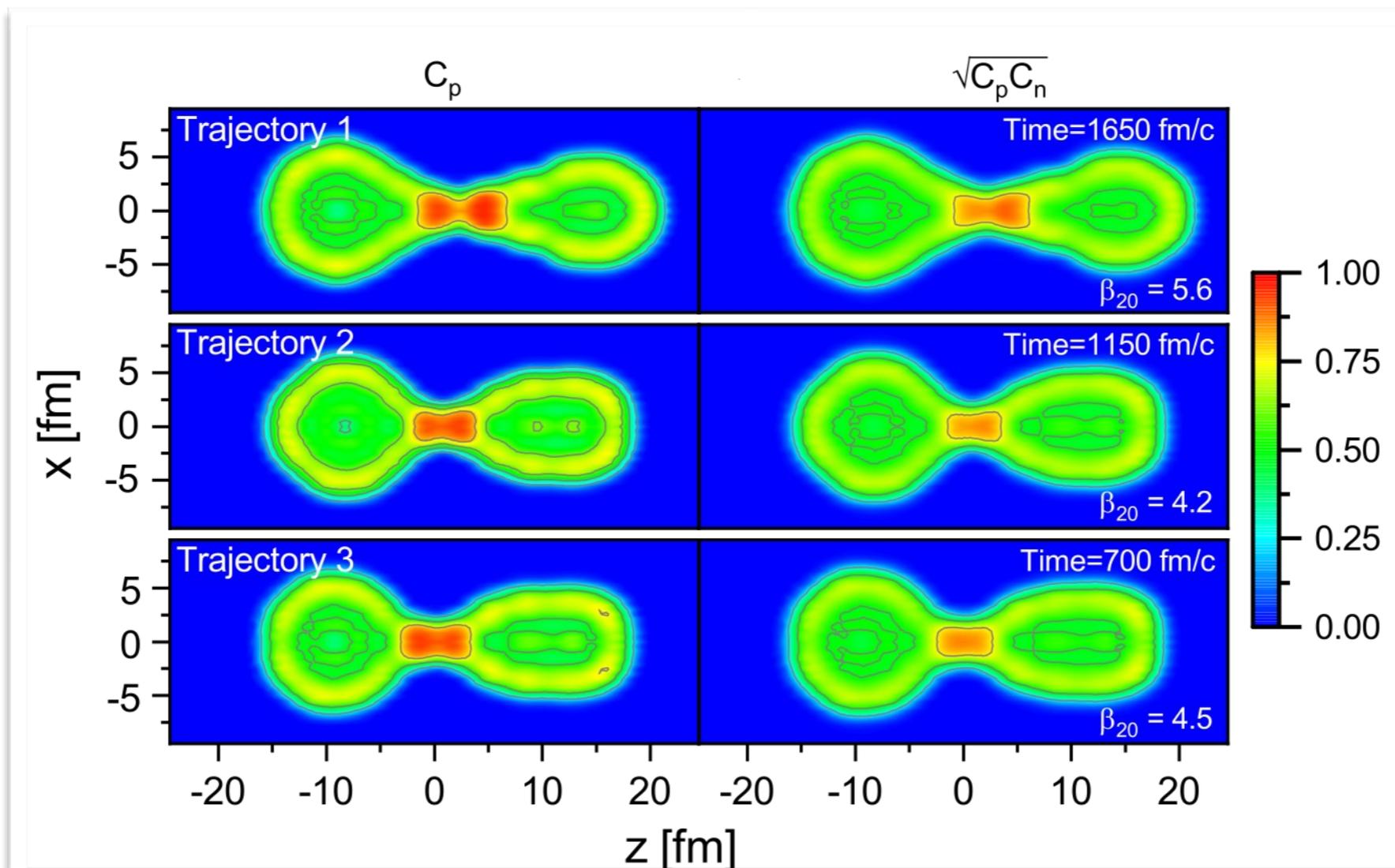
$$C_{q\sigma}(\vec{r}) = \left[1 + \left(\frac{\tau_{q\sigma} \rho_{q\sigma} - \frac{1}{4} |\vec{\nabla} \rho_{q\sigma}|^2 - \vec{j}_{q\sigma}^2}{\rho_{q\sigma} \tau_{q\sigma}^{\text{TF}}} \right)^2 \right]^{-1}$$

kinetic energy density
density
current density

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

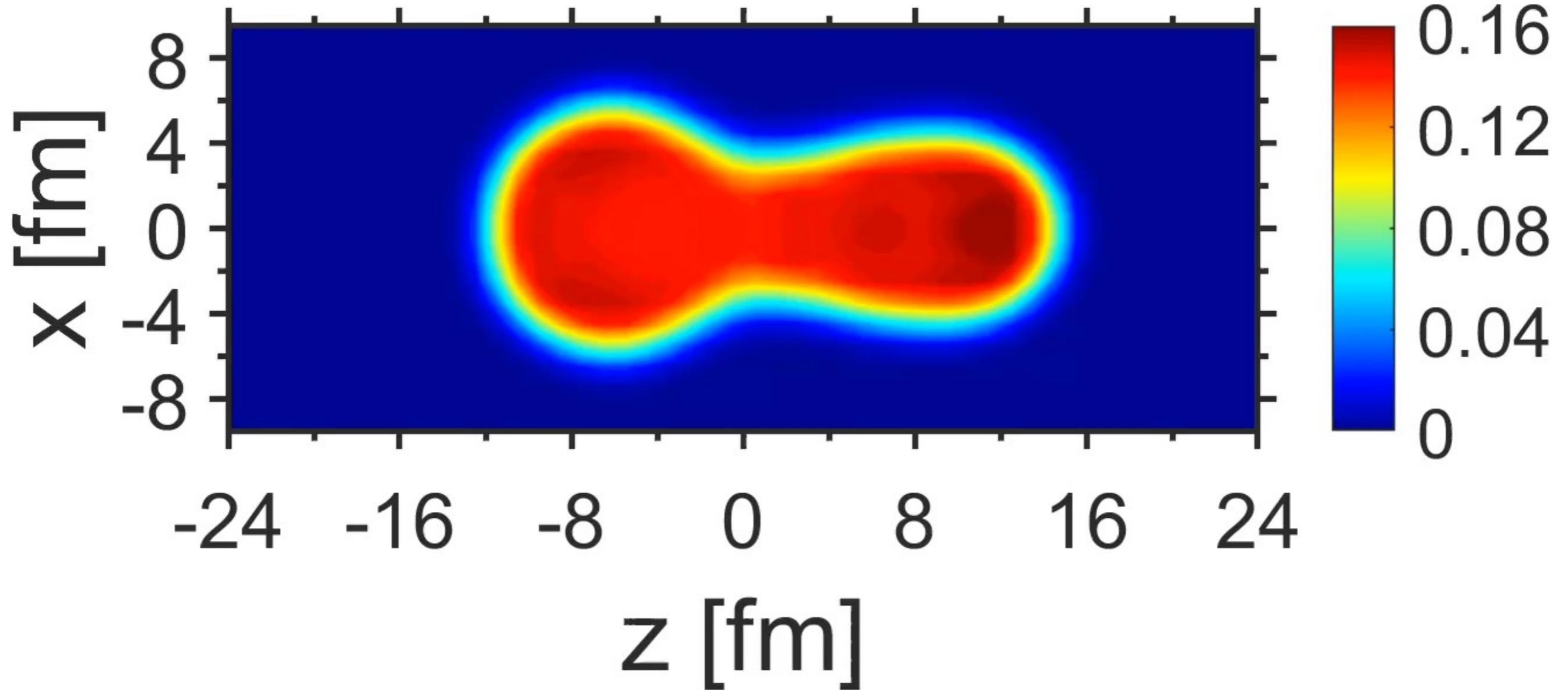
For homogeneous nuclear matter: $C_{q\sigma} = 1/2$

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



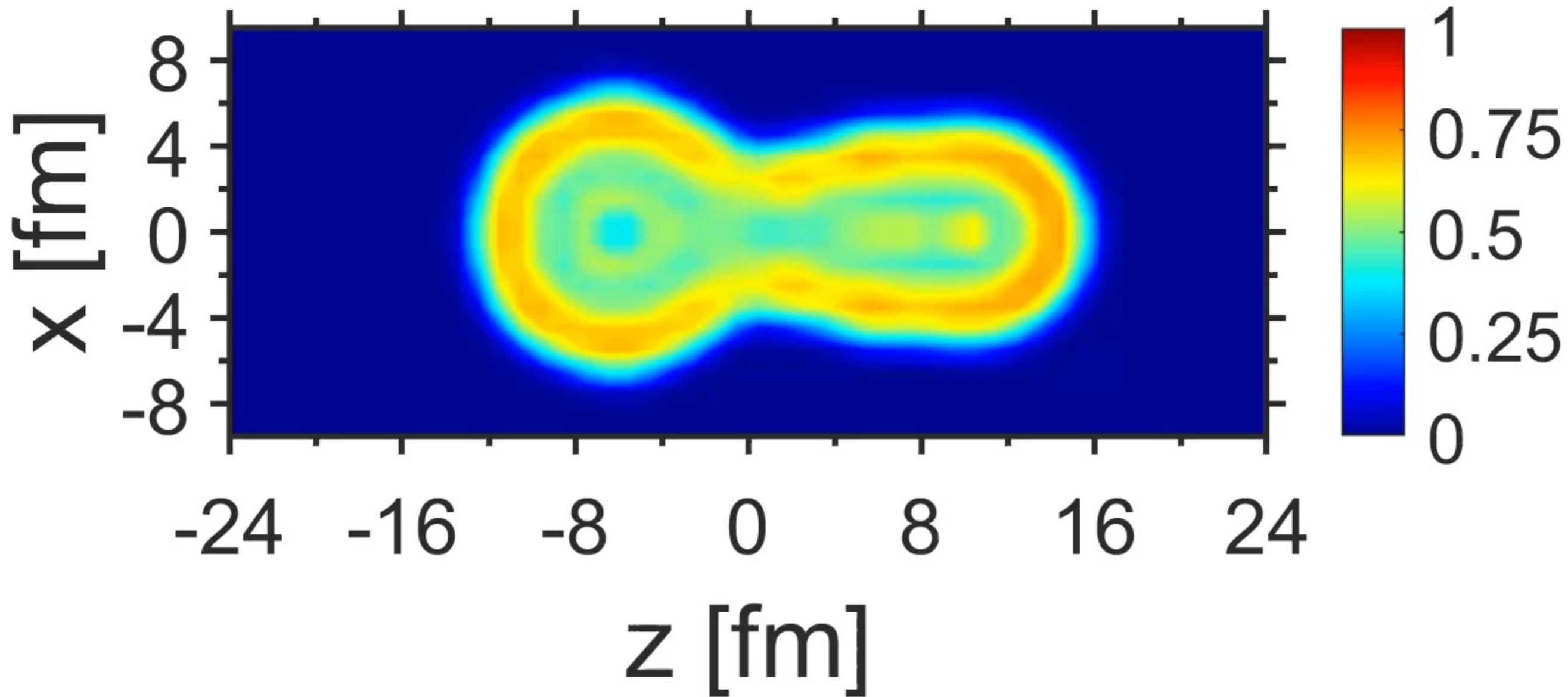
Trajectory 2

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

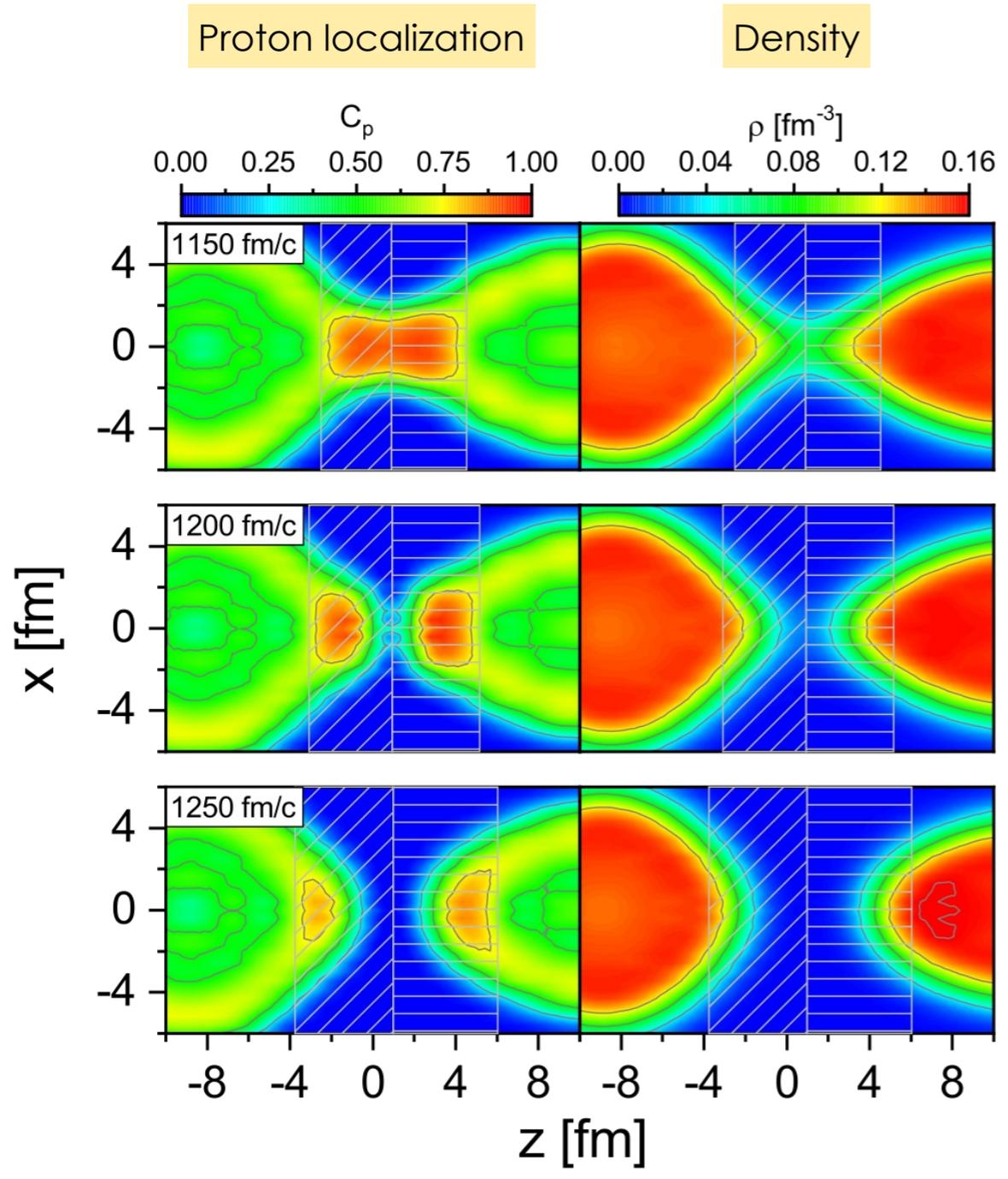


Trajectory 2

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



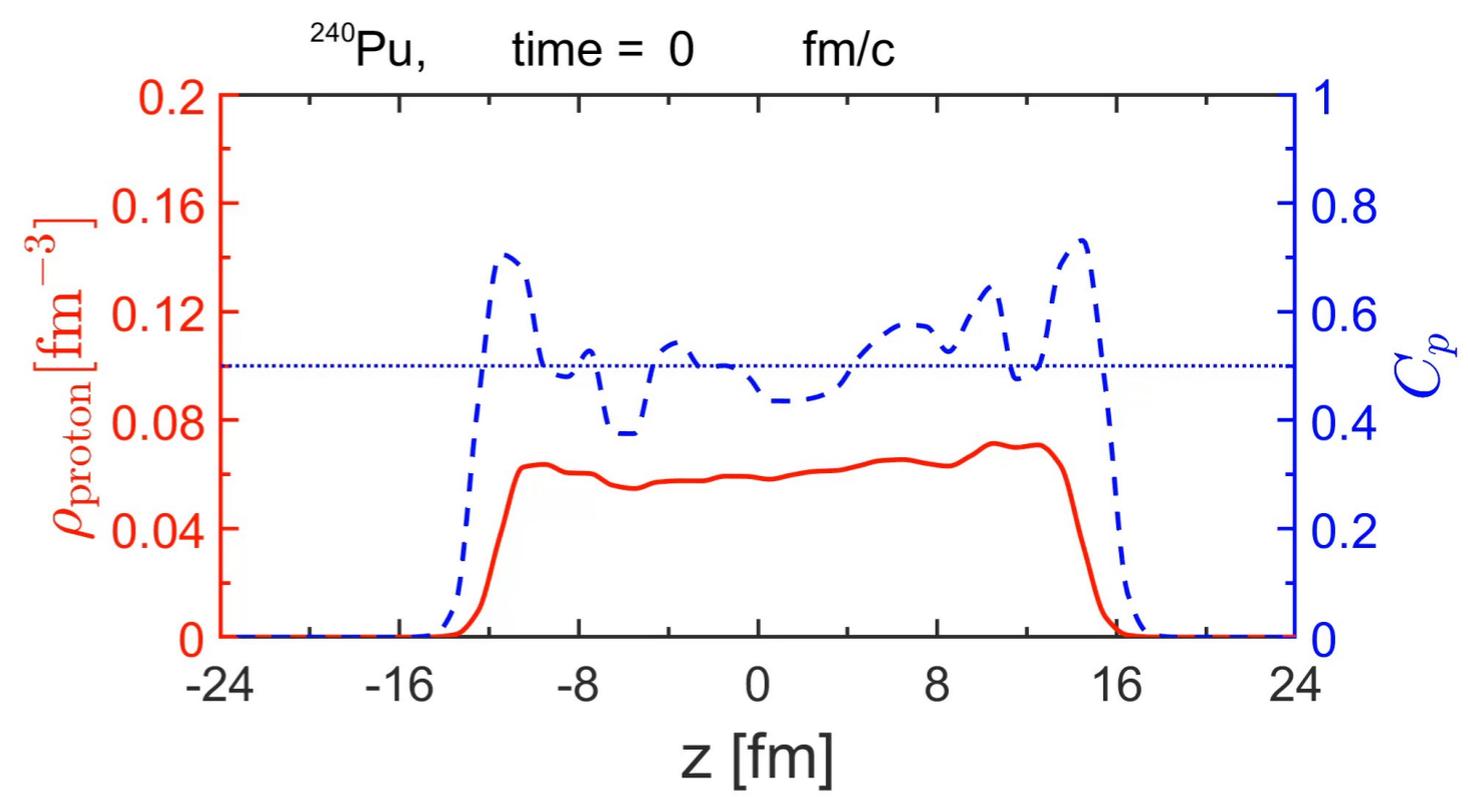
Trajectory 2



When are these light clusters formed?

What is their structure?

What is their role in the scission mechanism?



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

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

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