

Perspectives in Nuclear Fission Theory



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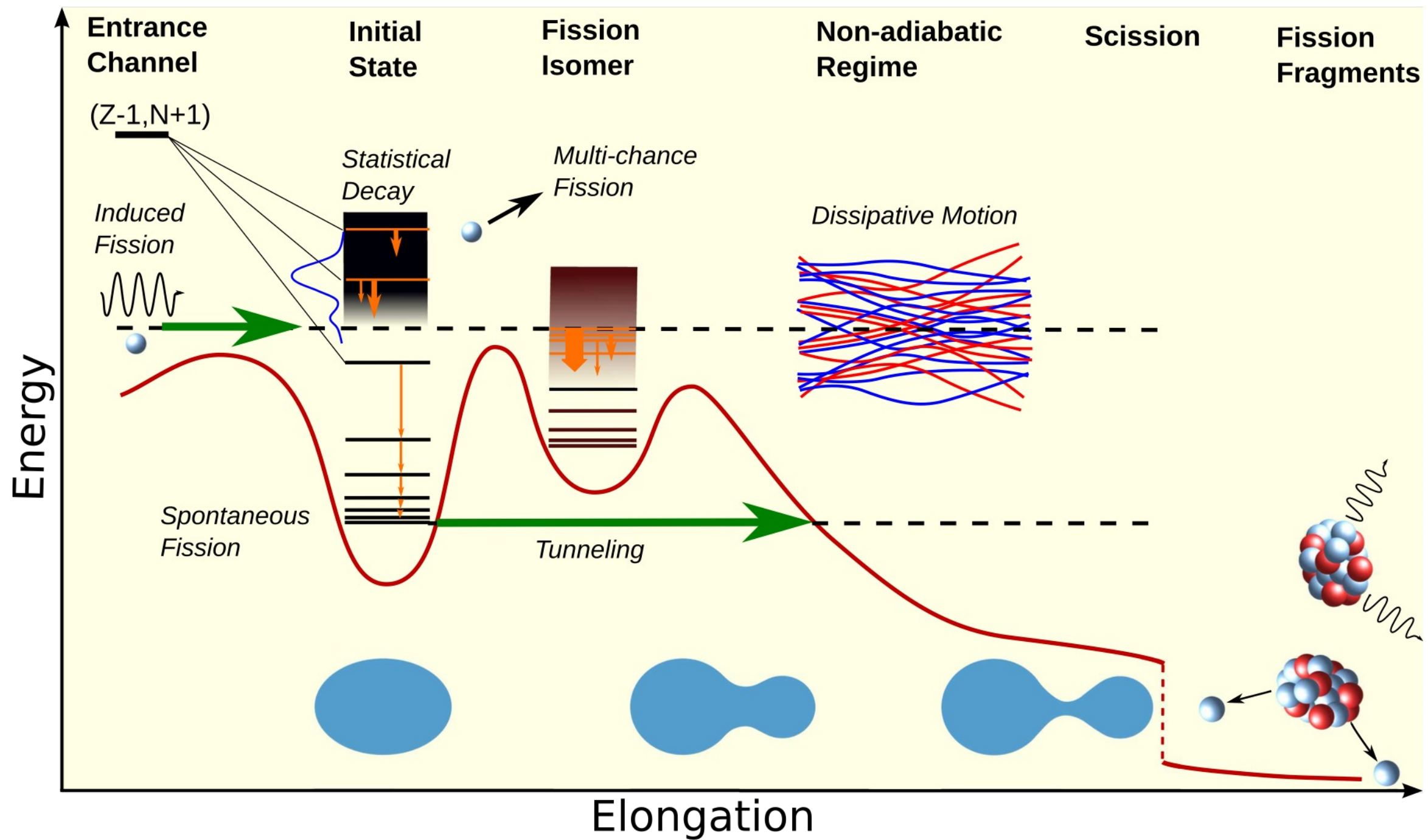
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Two basic microscopic approaches to the description of induced fission dynamics:

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

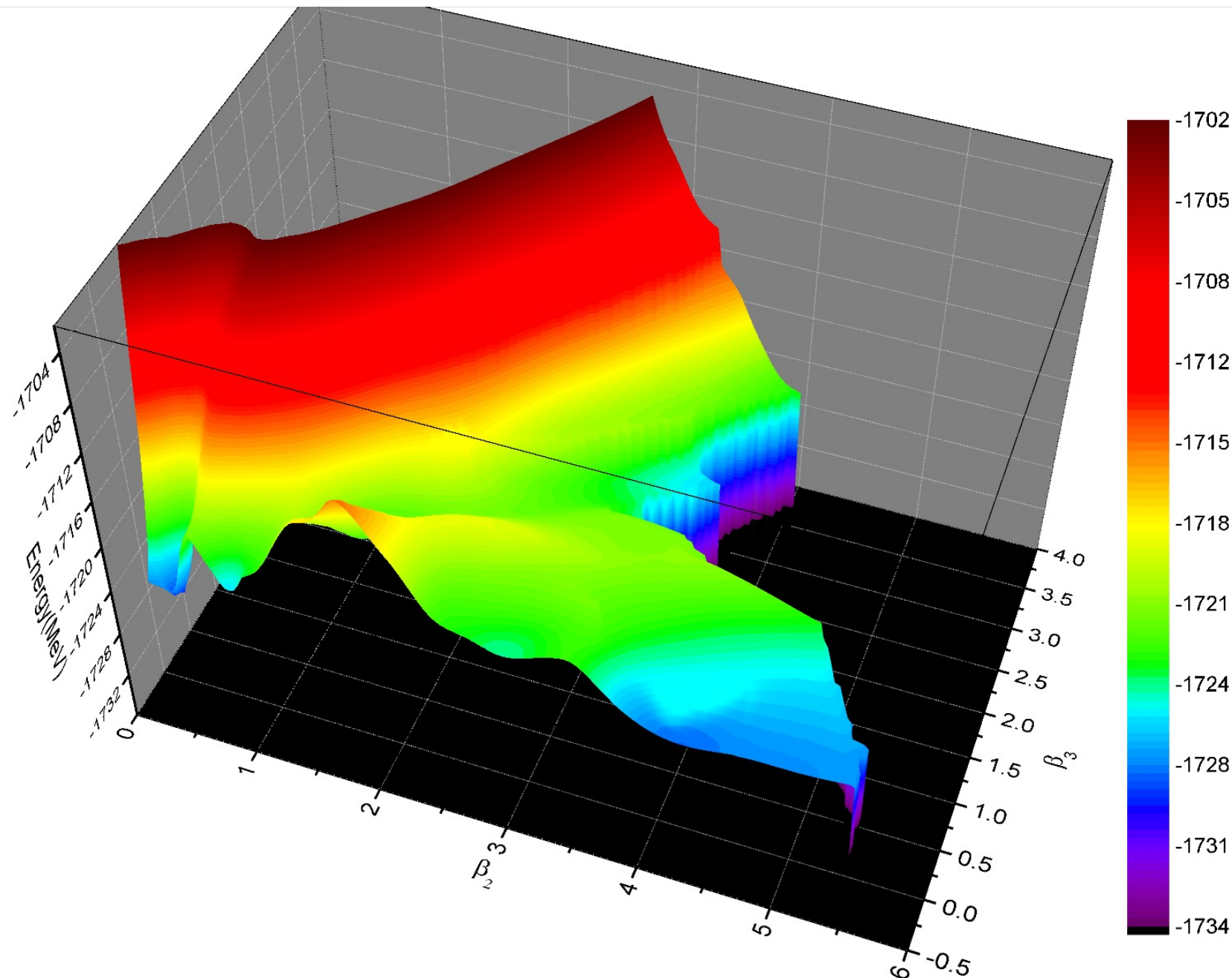
Time-dependent Schroedinger-like equation for fission dynamics (axial quadrupole and octupole deformation parameters as collective degrees of freedom):

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

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

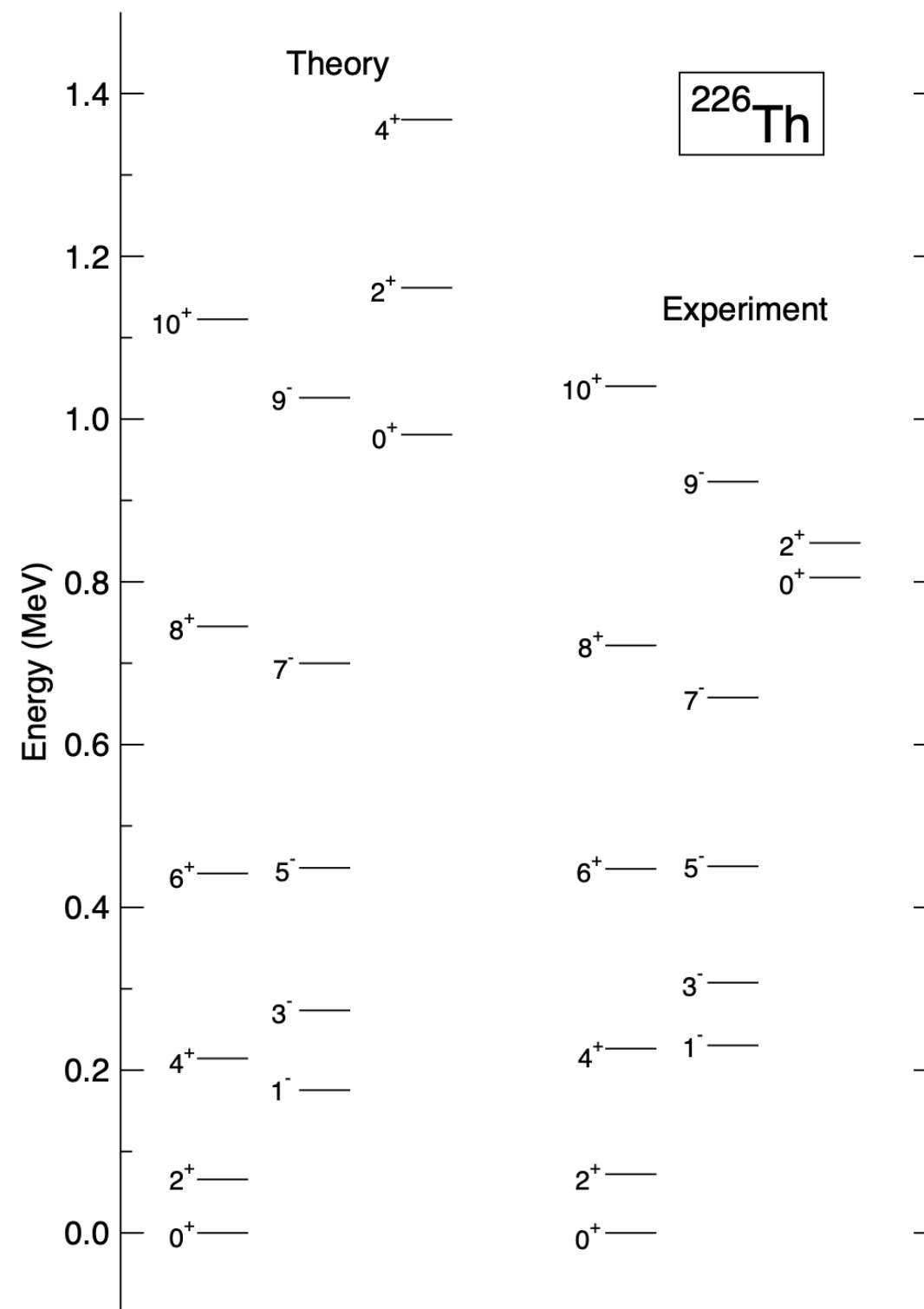
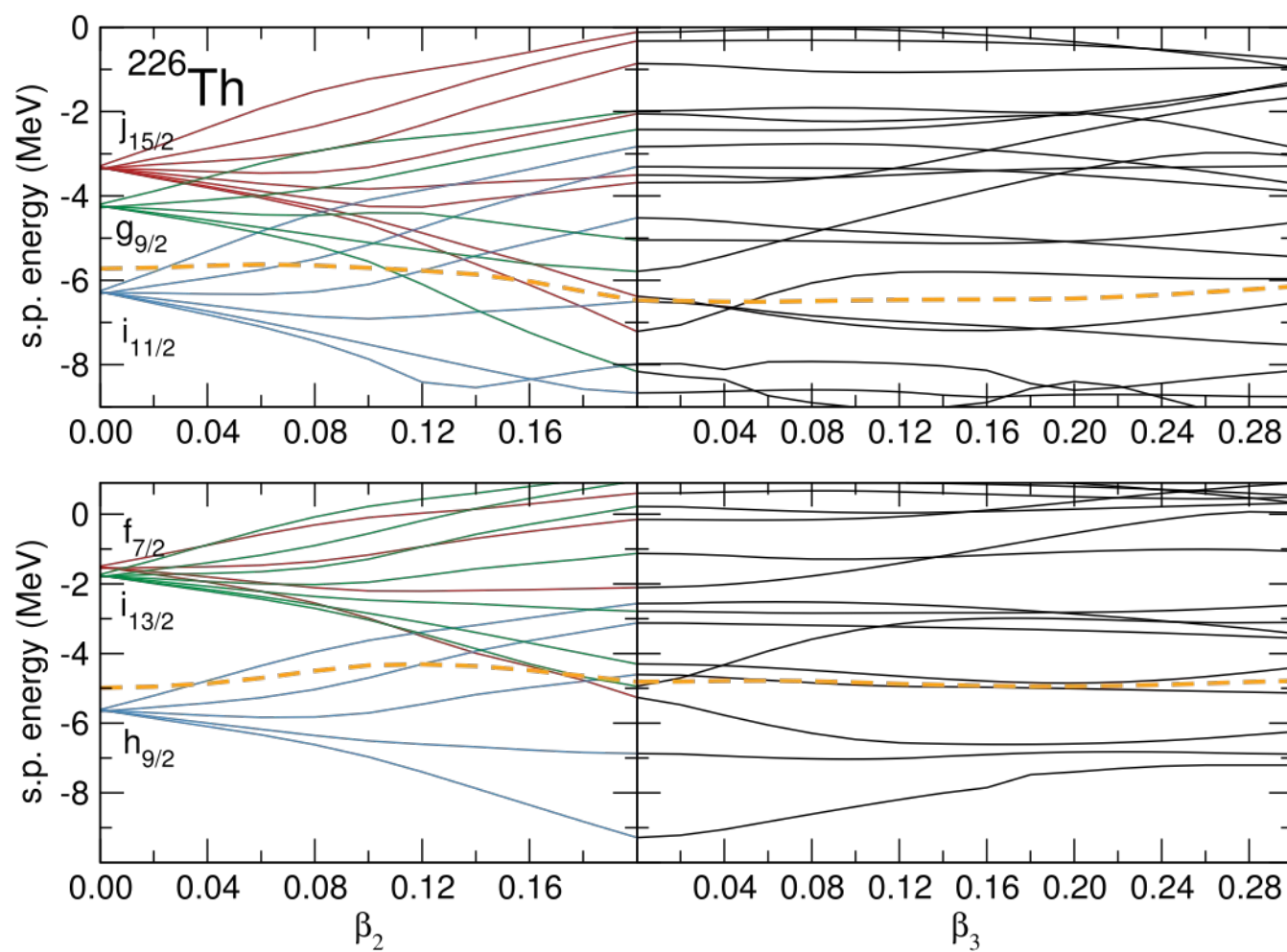
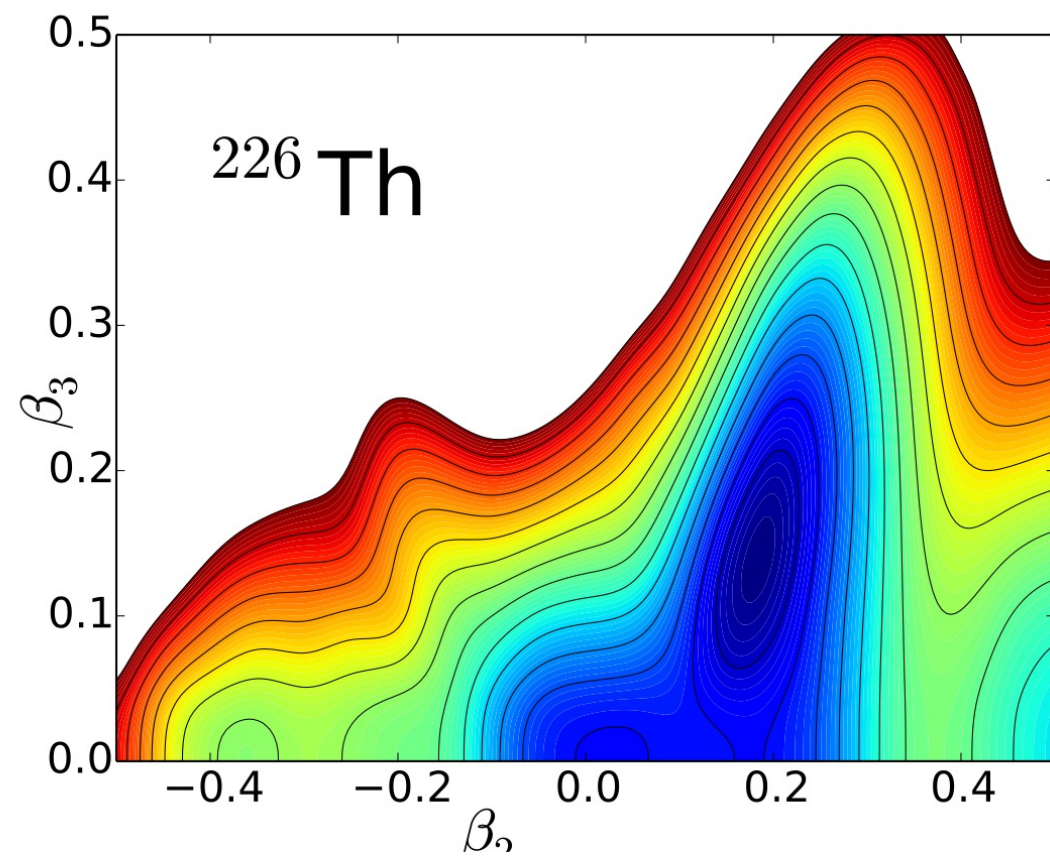
PHYSICAL REVIEW C **96**, 024319 (2017)

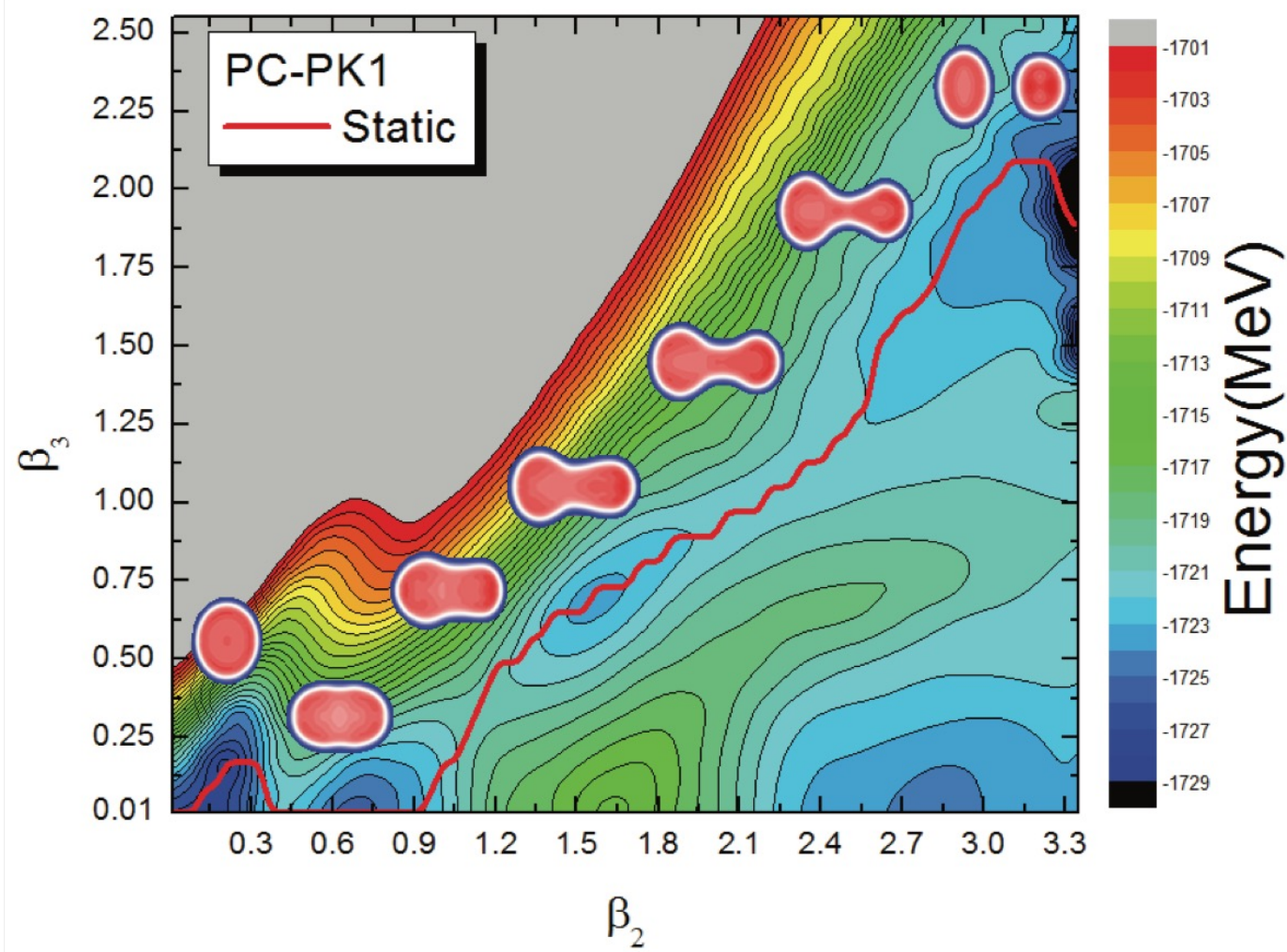


→ includes **static correlations**:
deformations & pairing

→ 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

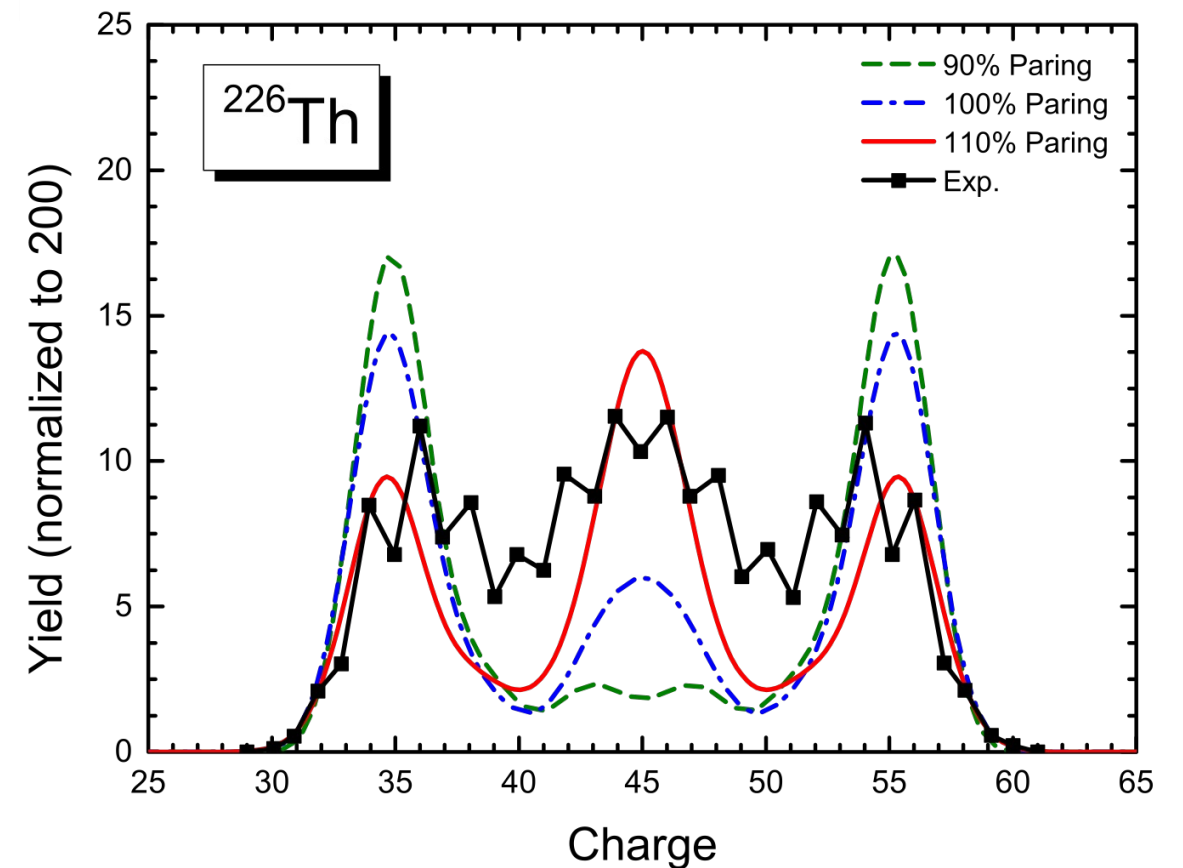




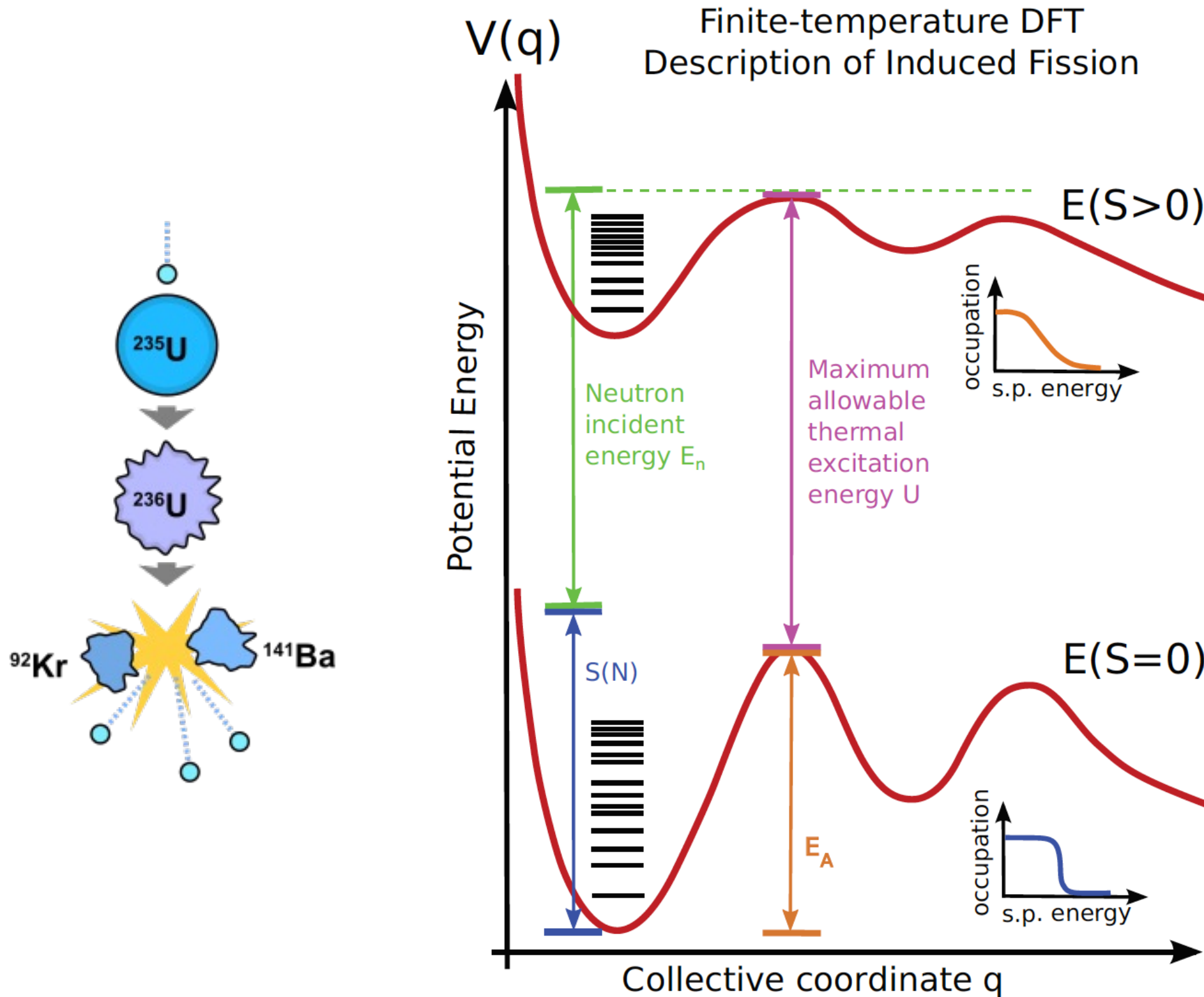
A triple-humped fission barrier is predicted along the static fission path, and the calculated heights are **7.10, 8.58, and 7.32 MeV** from the inner to the outer barrier.

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



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

Finite temperature effects:

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

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

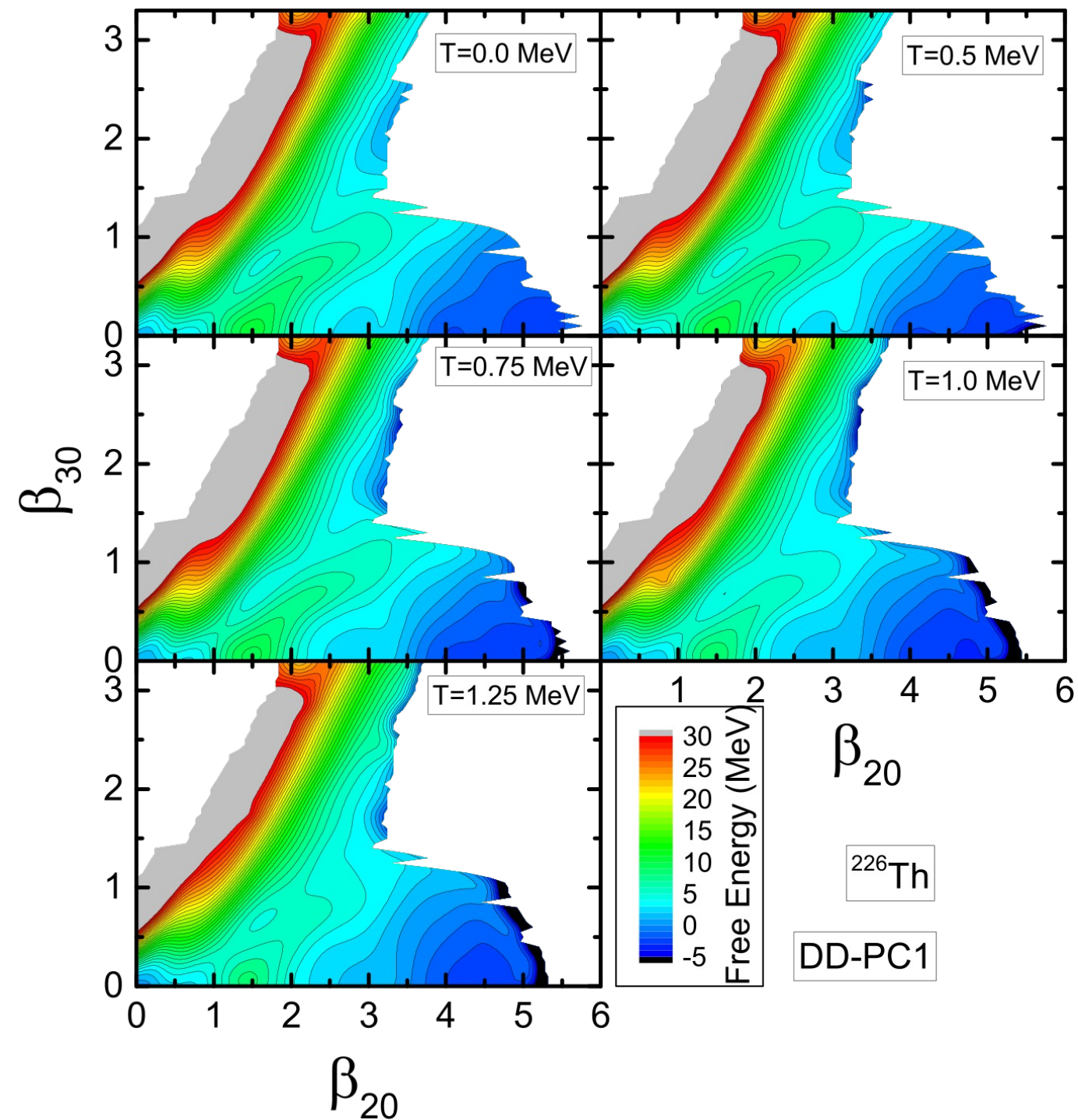
Helmholtz free energy: $F = E(T) - TS$

... 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:

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

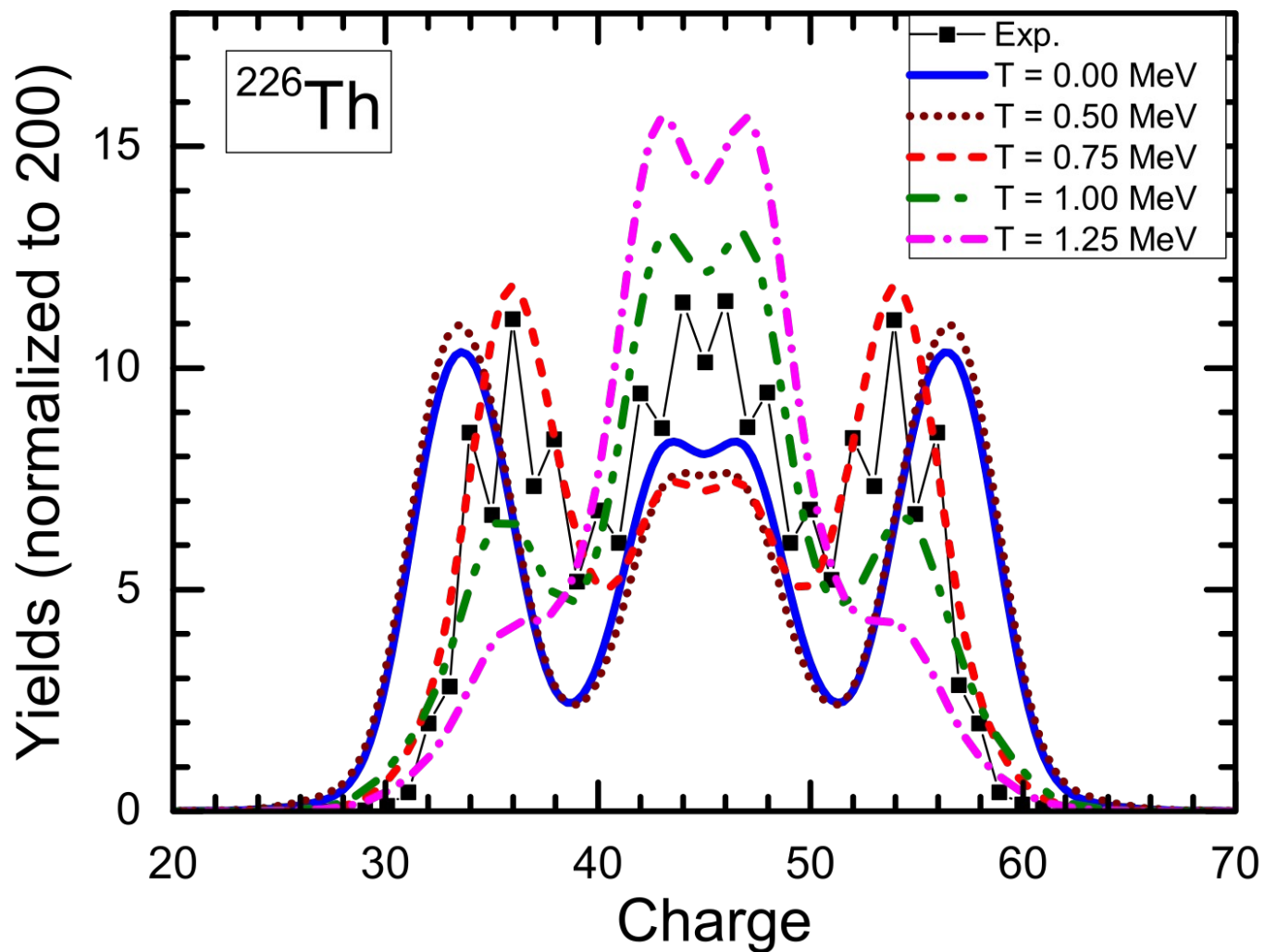


Dynamics of induced fission

Zhao, Nikšić, Vretenar, Zhou

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

Charge yields:



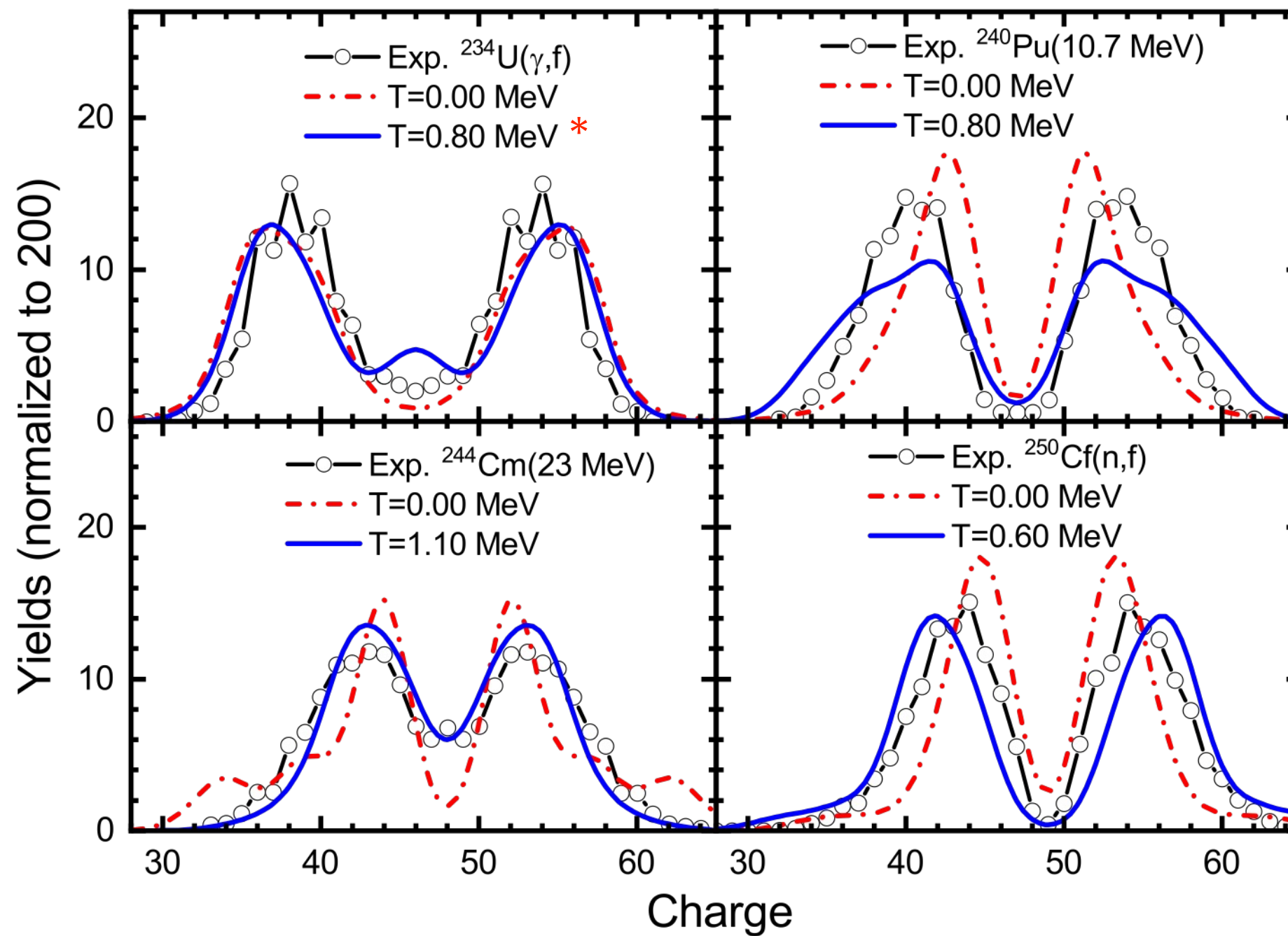
Experimental results \Rightarrow photoinduced fission with photon energies in the interval 8 – 14 MeV, and a peak value $E_\gamma = 11$ MeV.

$T = 0.5, \mathbf{0.75}, \mathbf{1.0}$, 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:

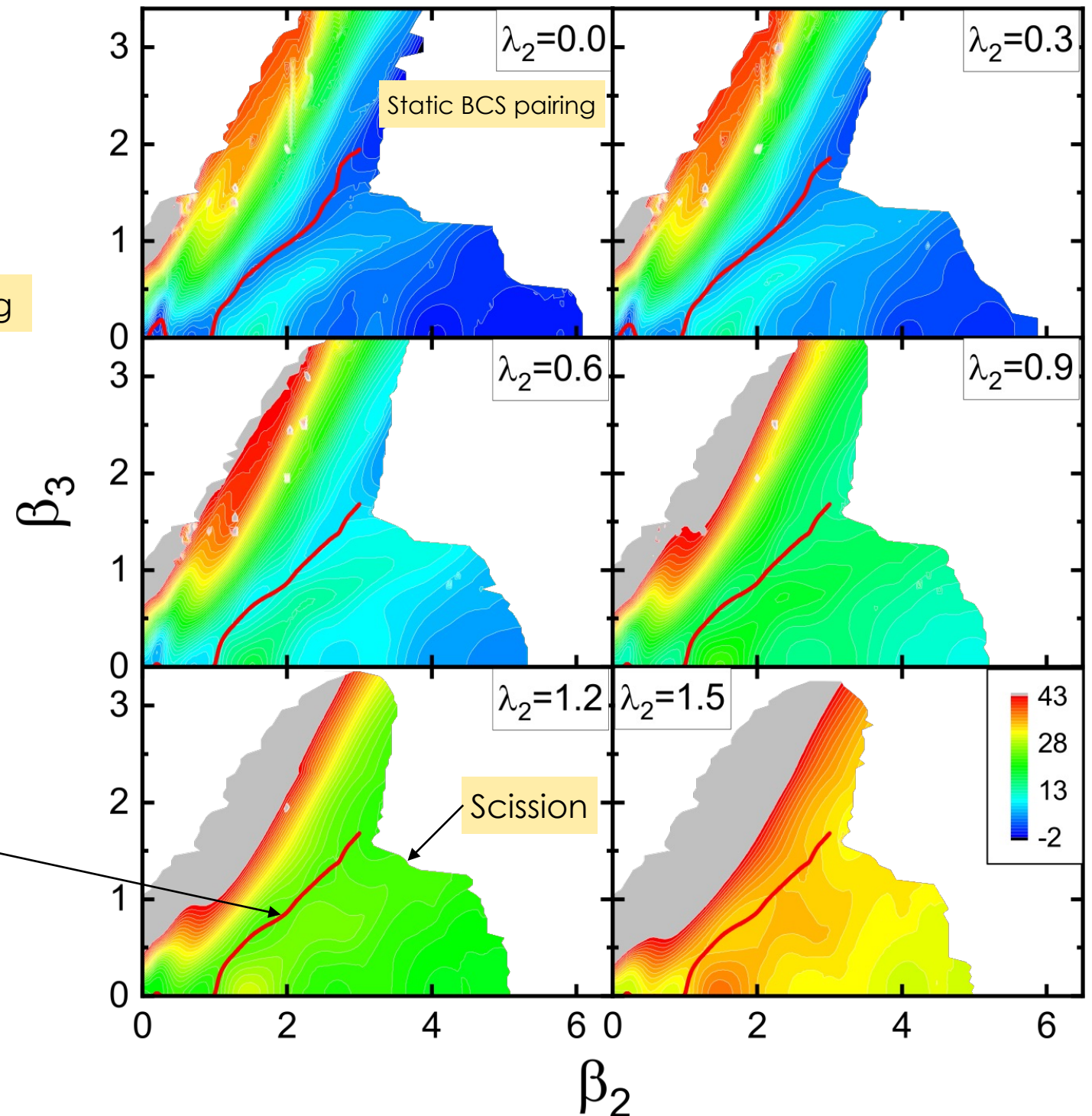
$$\Delta\hat{N}^2 = \hat{N}^2 - \langle\hat{N}\rangle^2.$$

... the Routhian:

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

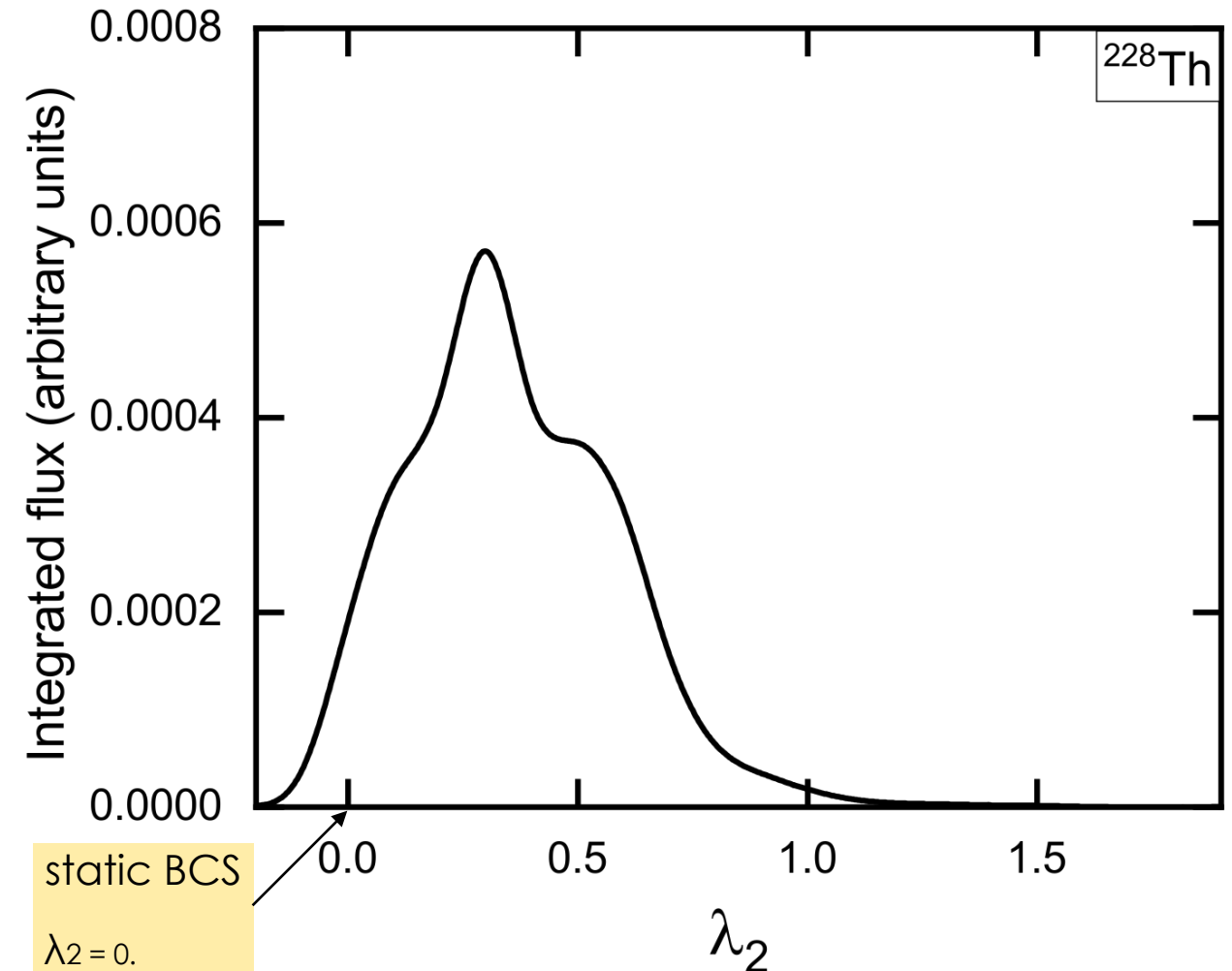
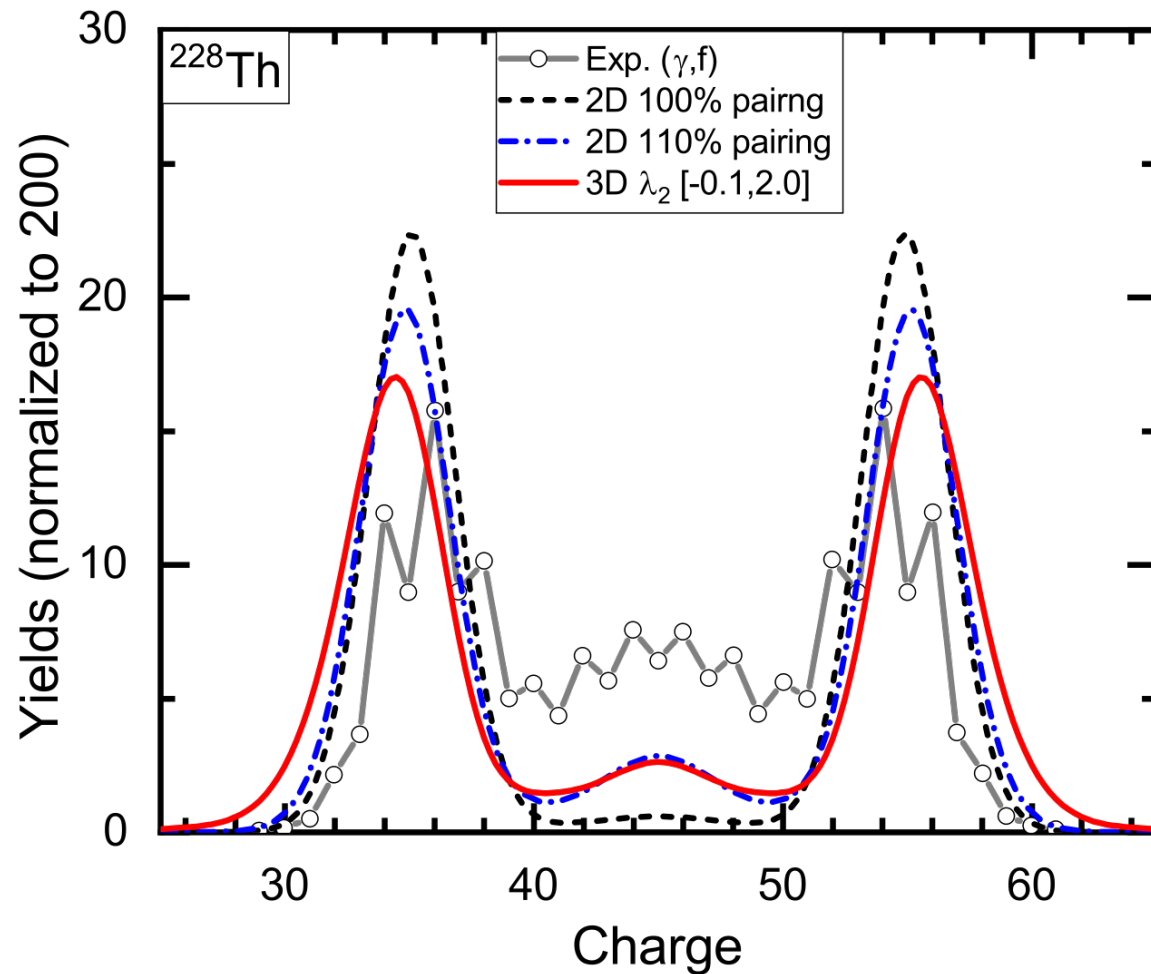
2D projections of the deformation-energy manifold of ^{228}Th on the quadrupole-octupole axially symmetric plane, for selected values of the pairing coordinate λ_2 .

Static fission path of minimum energy



3D TDGCM+GOA calculation

$$\hat{H}_{\text{coll}}(\mathbf{q}) = -\frac{\hbar^2}{2} \sum_{ij} \frac{\partial}{\partial q_i} B_{ij}(\mathbf{q}) \frac{\partial}{\partial q_j} + V(\mathbf{q}) \quad \mathbf{q} \equiv \{\beta_2, \beta_3, \lambda_2\}$$



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

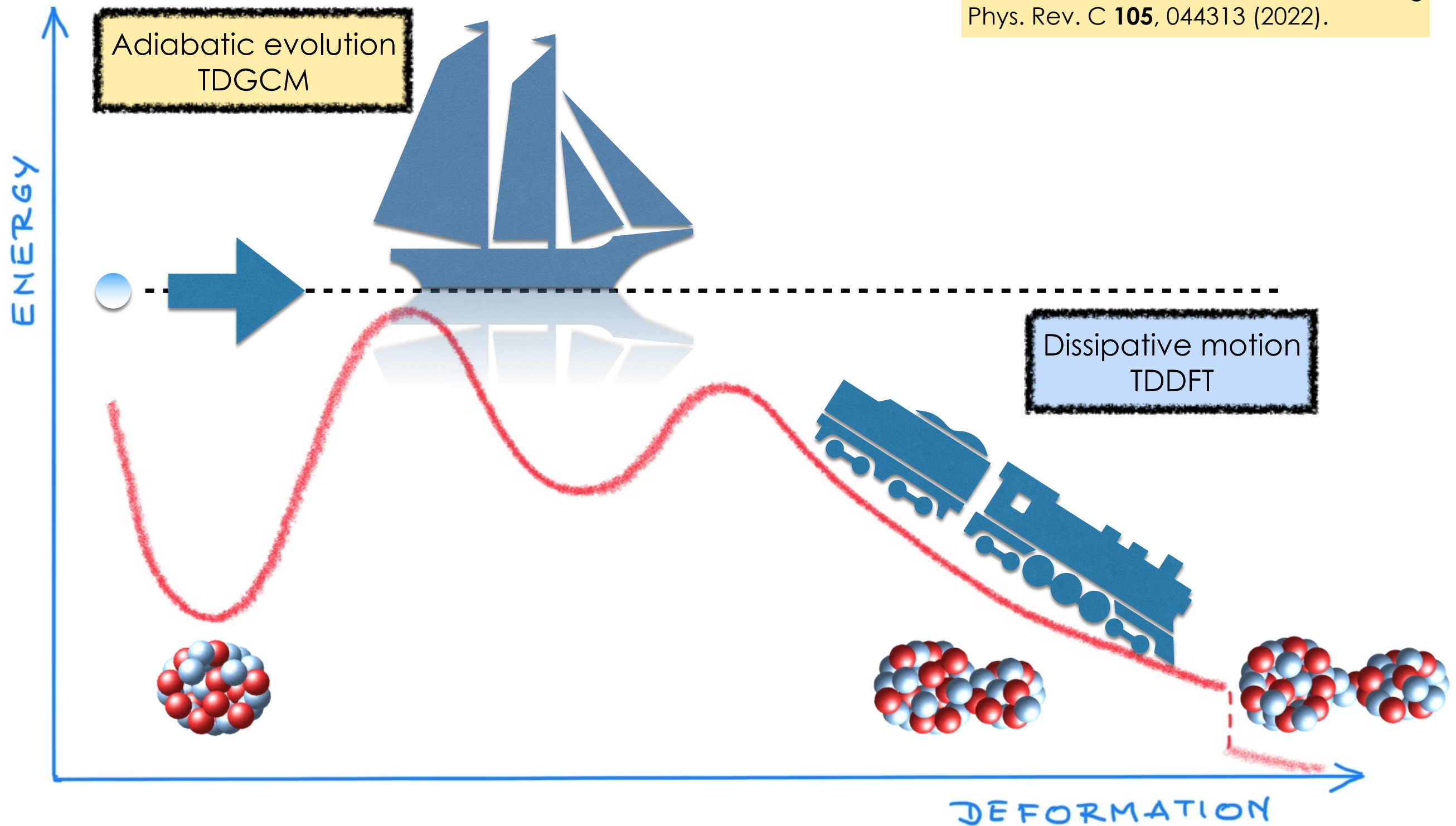
Effect of dynamical pairing on the flux of the probability current
through the scission hyper-surface:

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

→ 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)

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

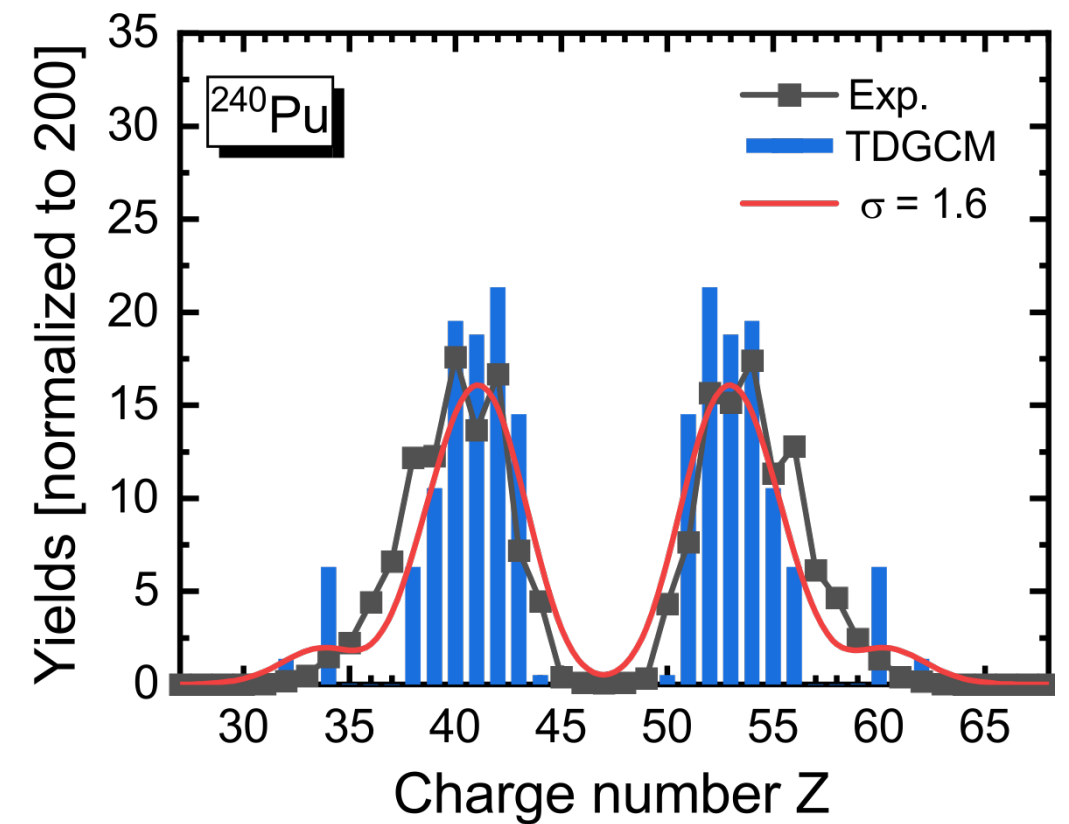
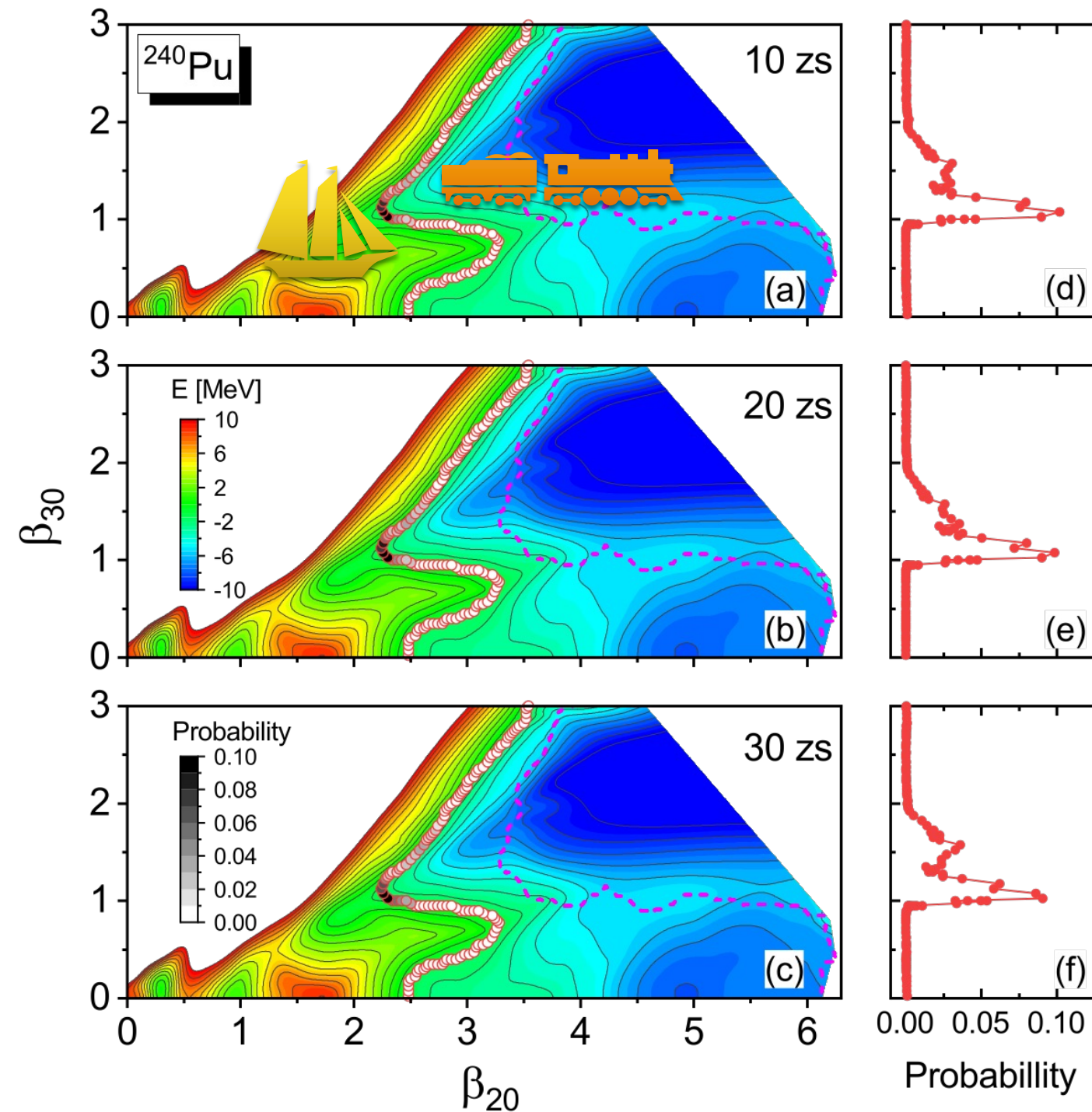
$$i \frac{d}{dt} n_k(t) = n_k(t) \Delta_k^*(t) - n_k^*(t) \Delta_k(t),$$

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

⇒ 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.

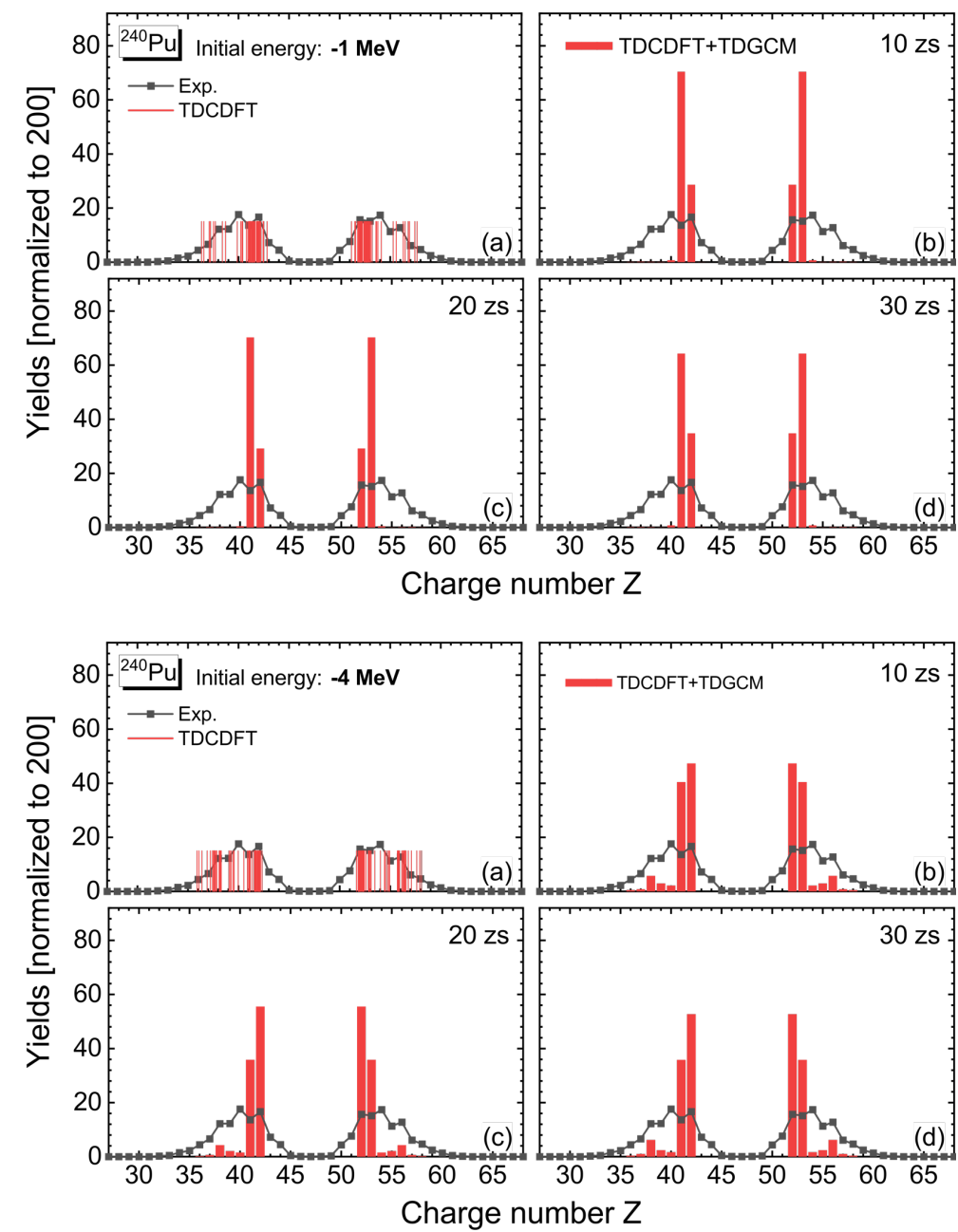
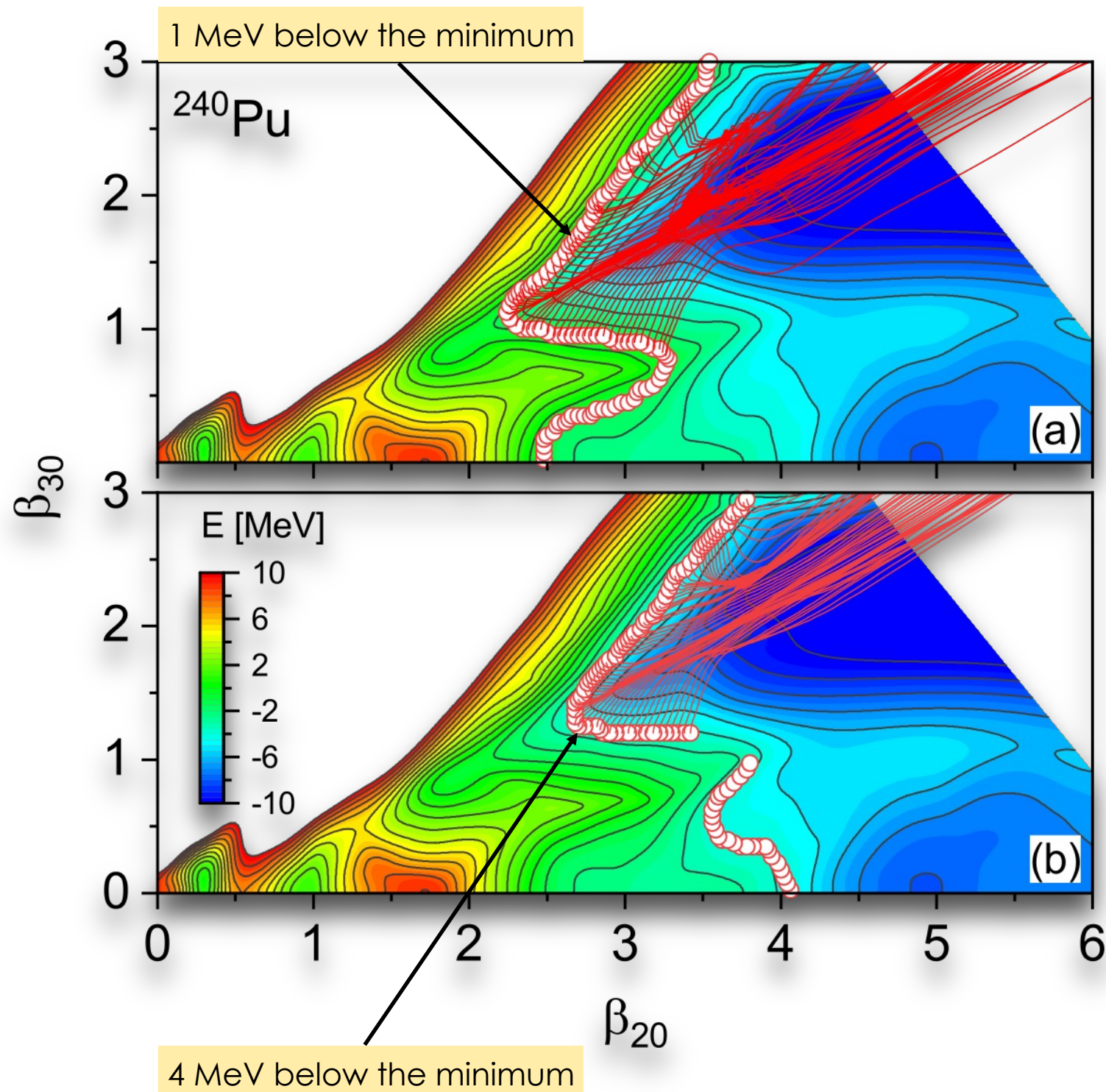
⇒ automatically includes the one-body dissipation mechanism, but can only simulate a single fission event by propagating the nucleons independently.

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

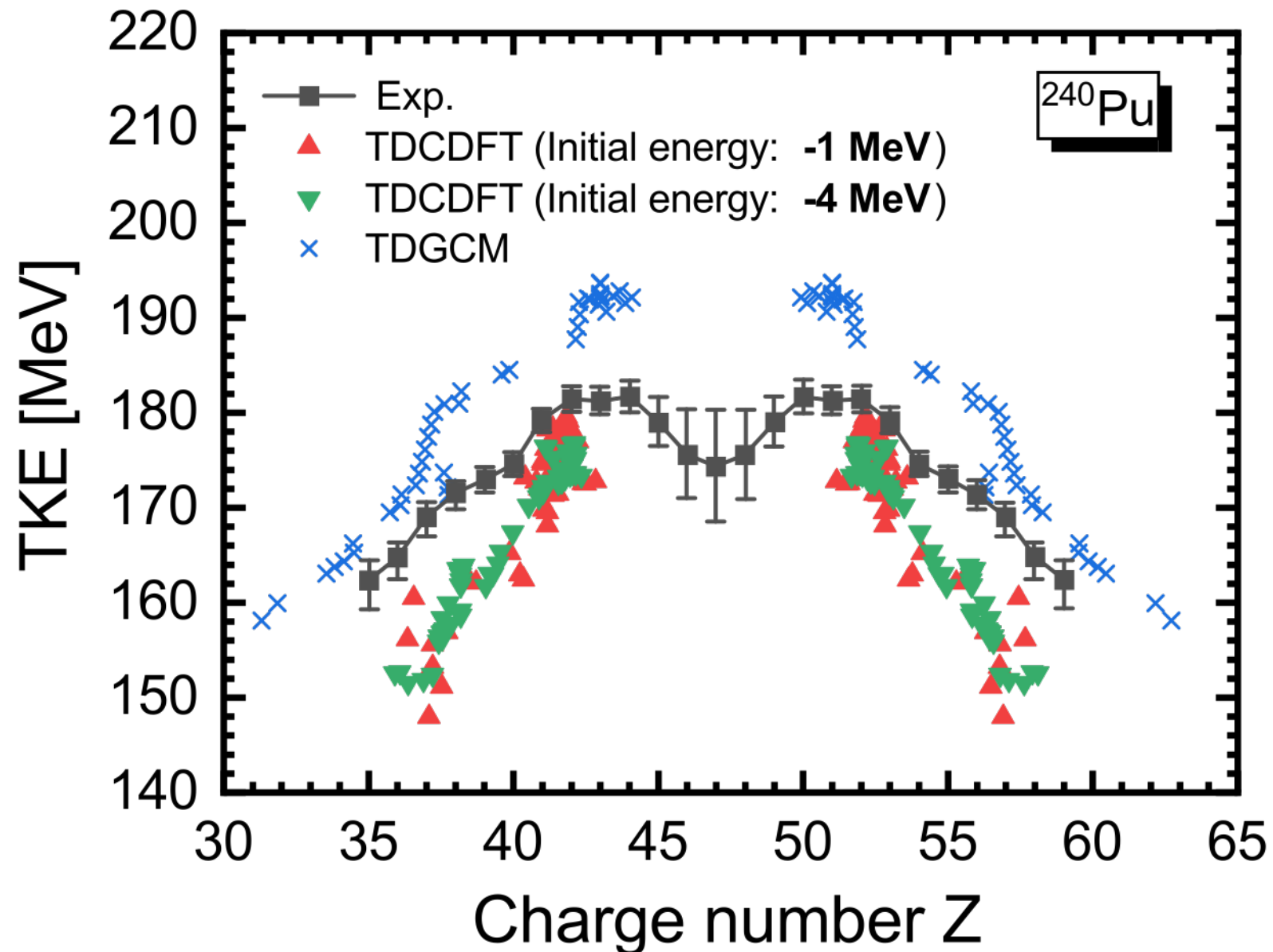
$$E_{\text{TKE}} = \frac{e^2 Z_H Z_L}{d_{\text{ch}}},$$

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

TDDFT

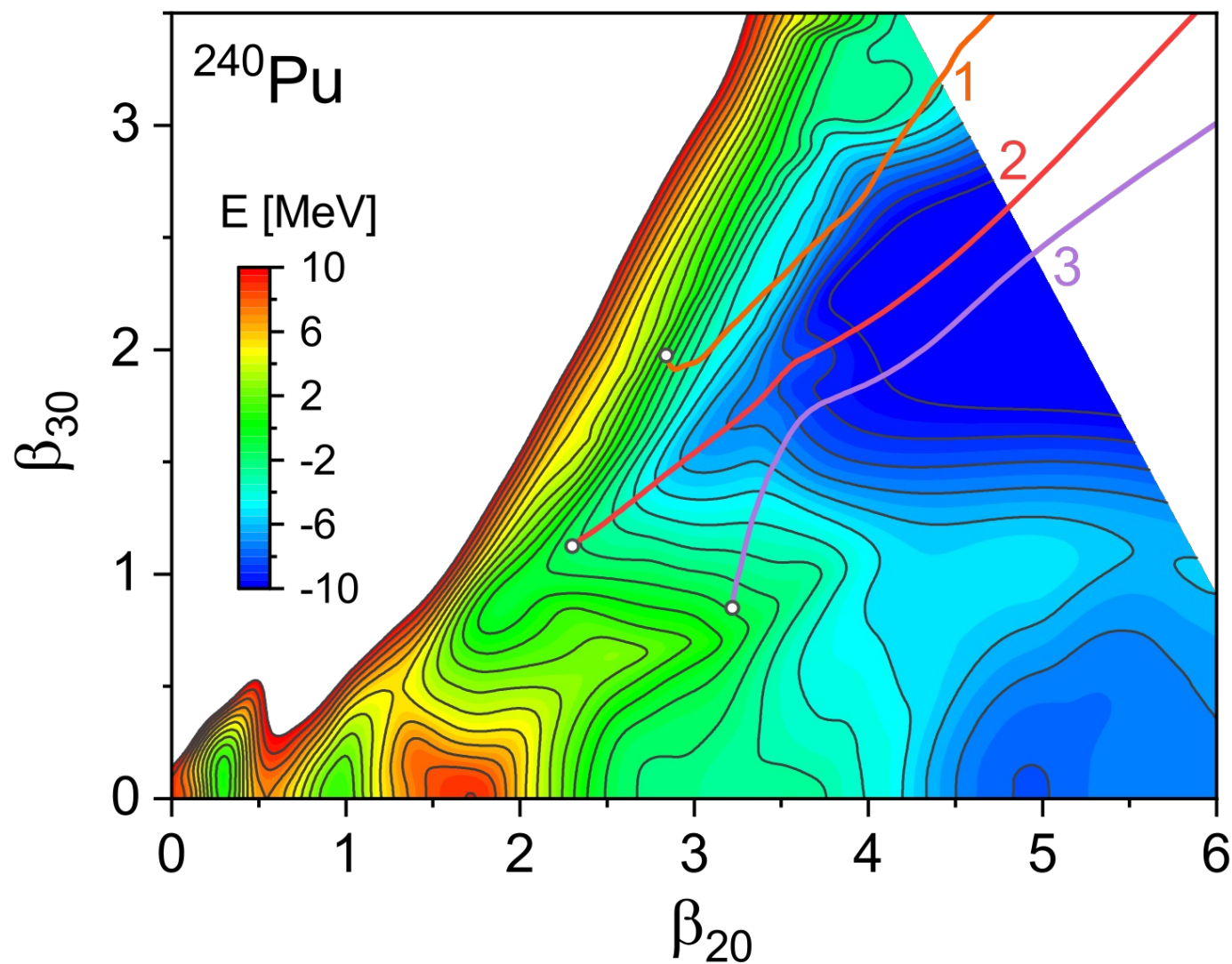
$$E_{\text{TKE}} = \frac{1}{2} m A_H \mathbf{v}_H^2 + \frac{1}{2} m A_L \mathbf{v}_L^2 + E_{\text{Coul}},$$

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

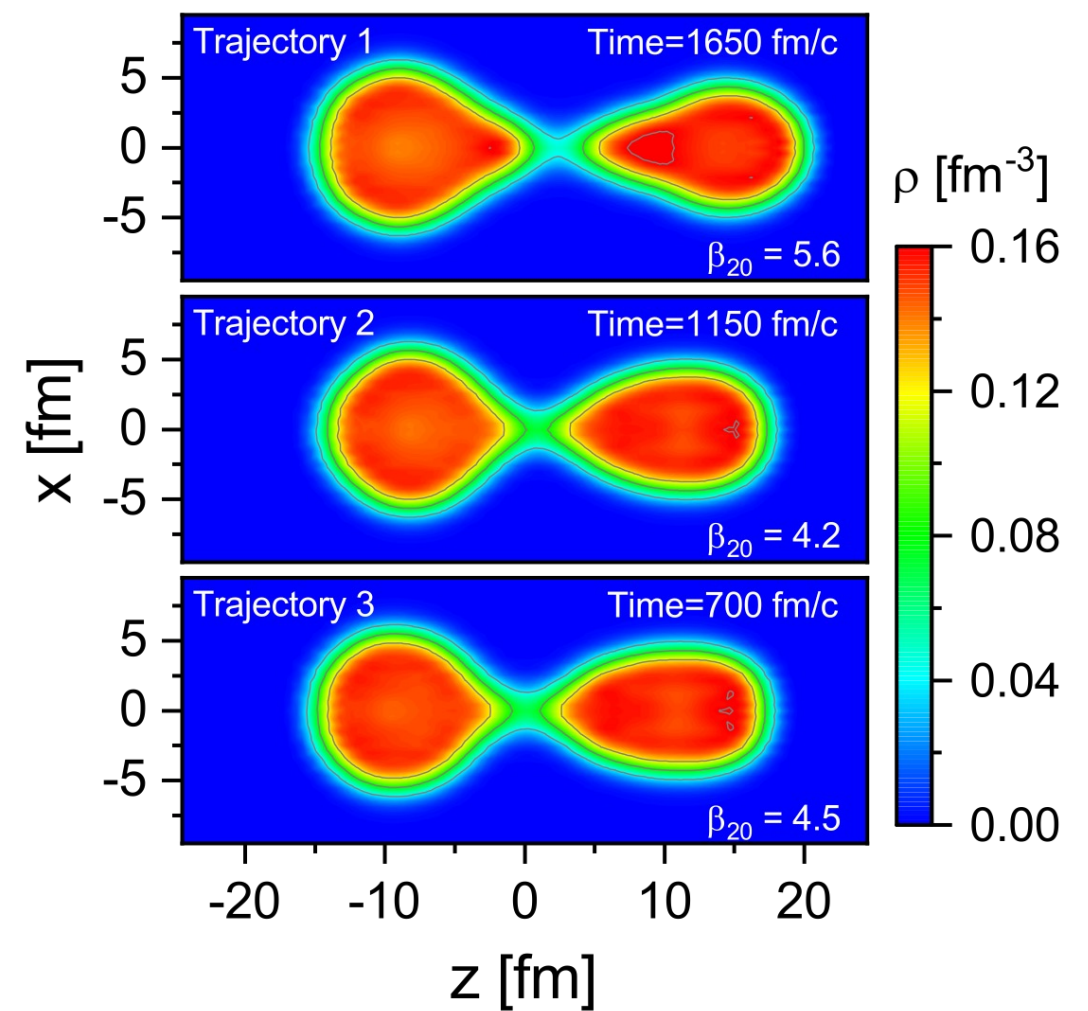


Dynamical synthesis of ^4He in the scission phase of nuclear fission

TDDFT fission trajectories



Density profiles at times immediately prior to the scission event.



Nucleon localization functions:

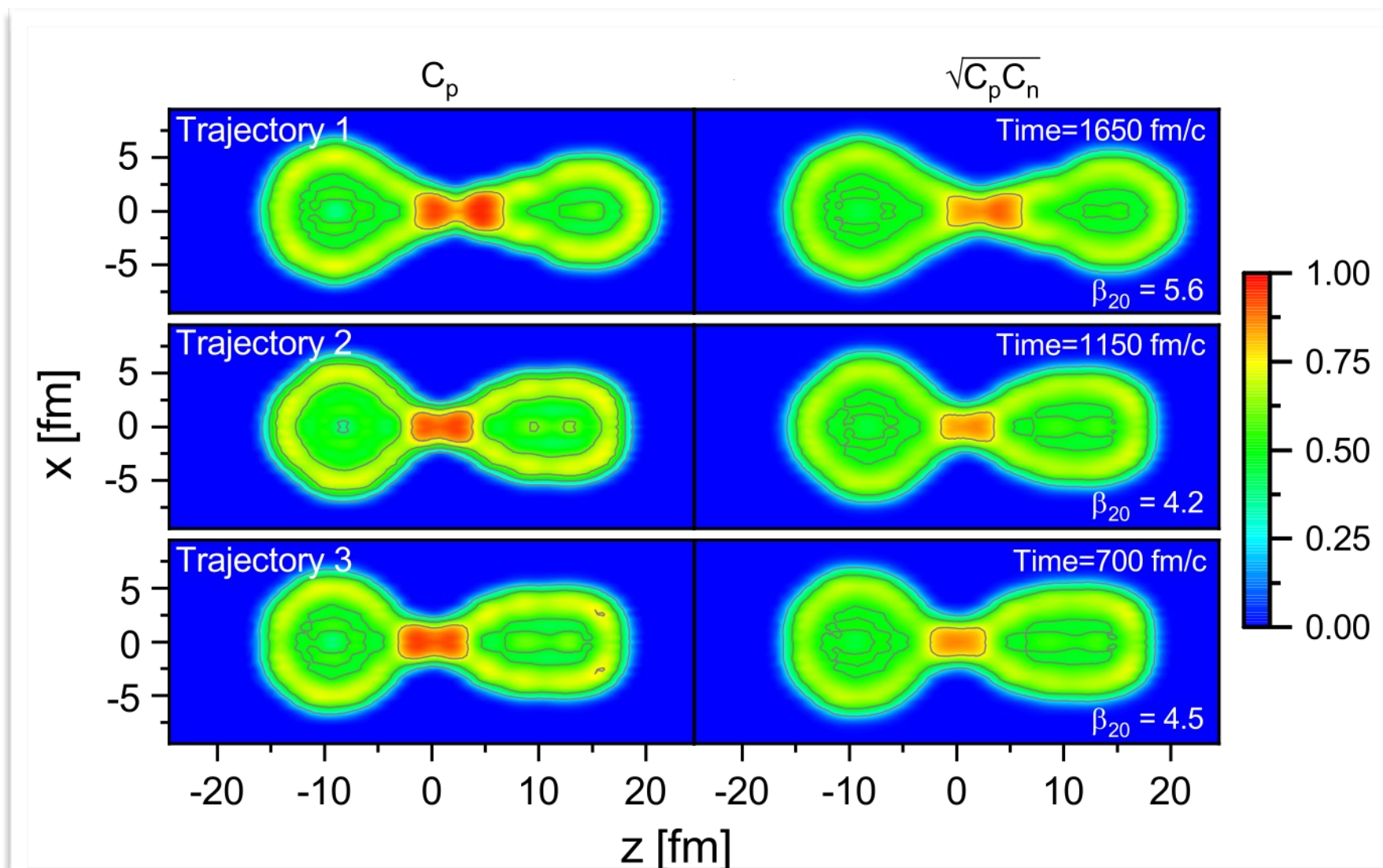
σ (\uparrow or \downarrow)
 q (n or p)

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

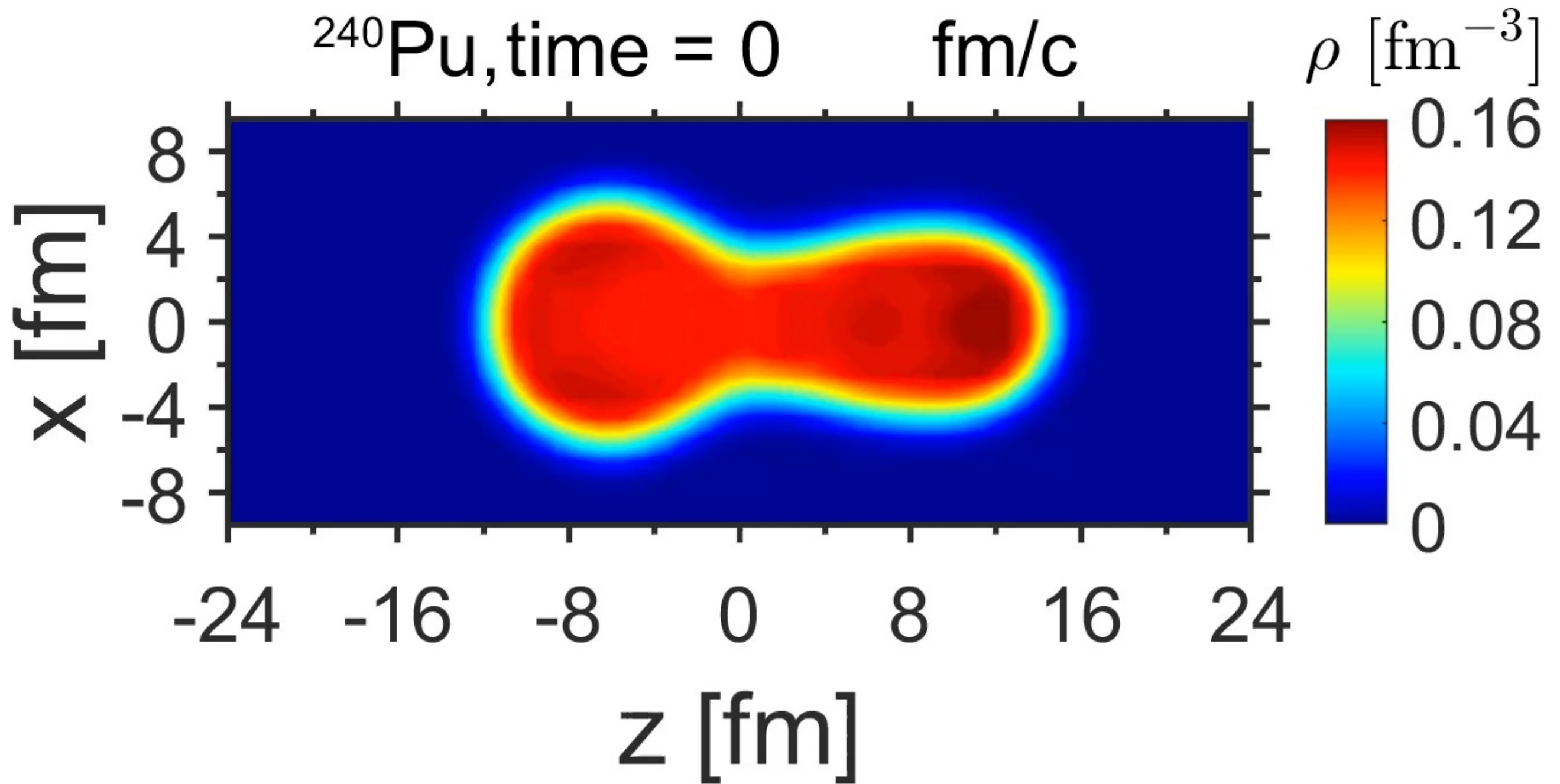
$$\tau_{q\sigma}^{\text{TF}} = \frac{3}{5}(6\pi^2)^{2/3}\rho_{q\sigma}^{5/3}$$

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

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

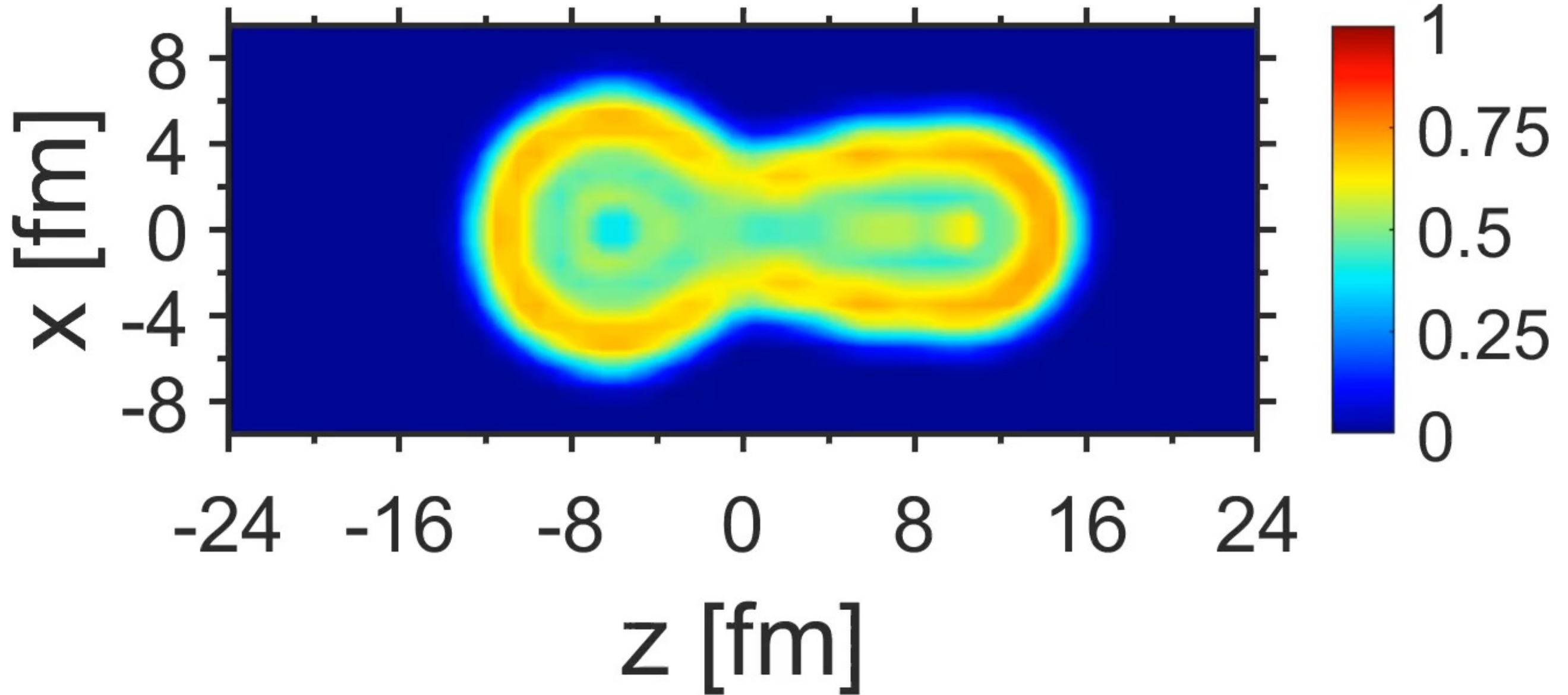


Trajectory 2



Trajectory 2

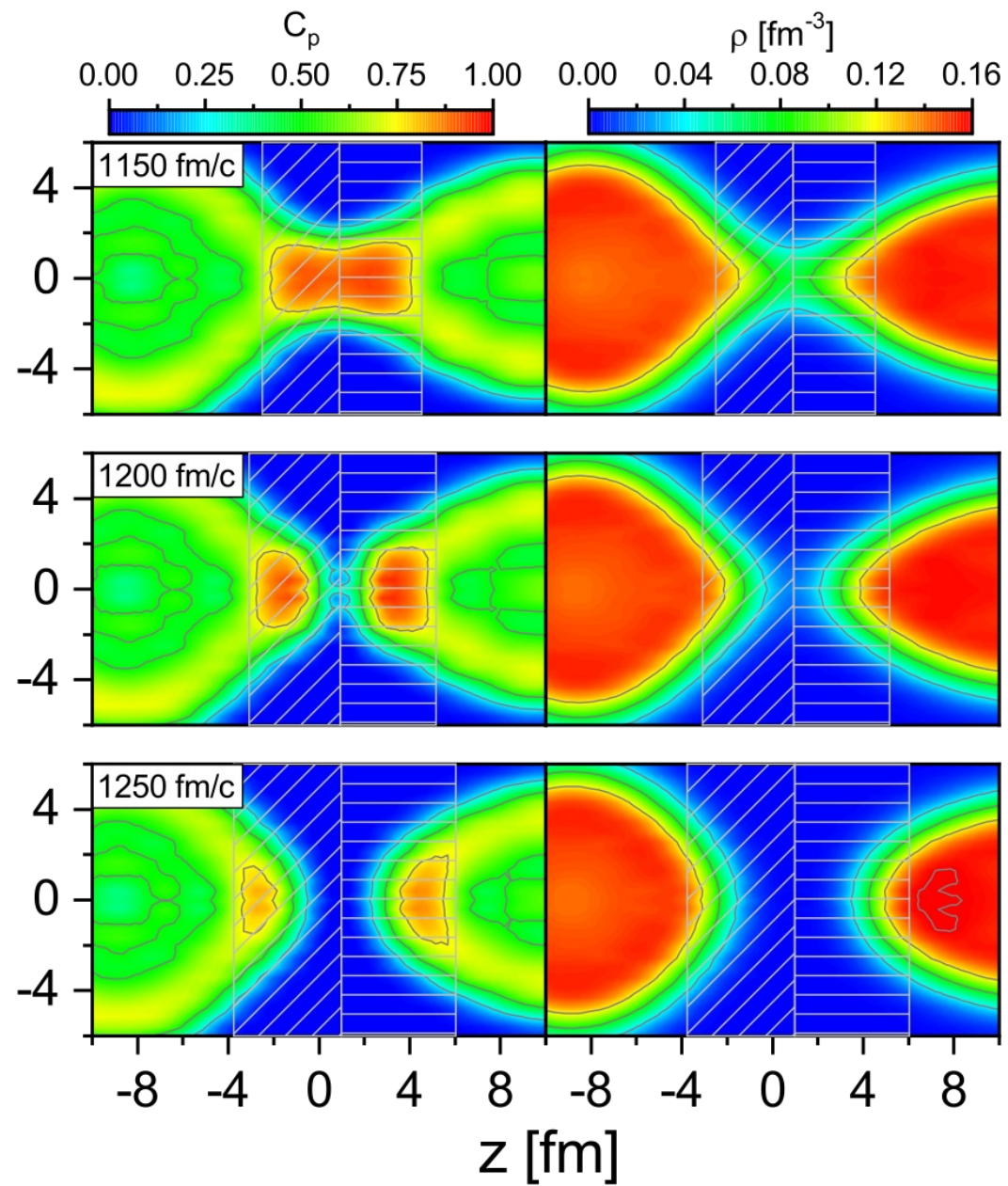
^{240}Pu , time = 0 fm/c



Trajectory 2

Proton localization

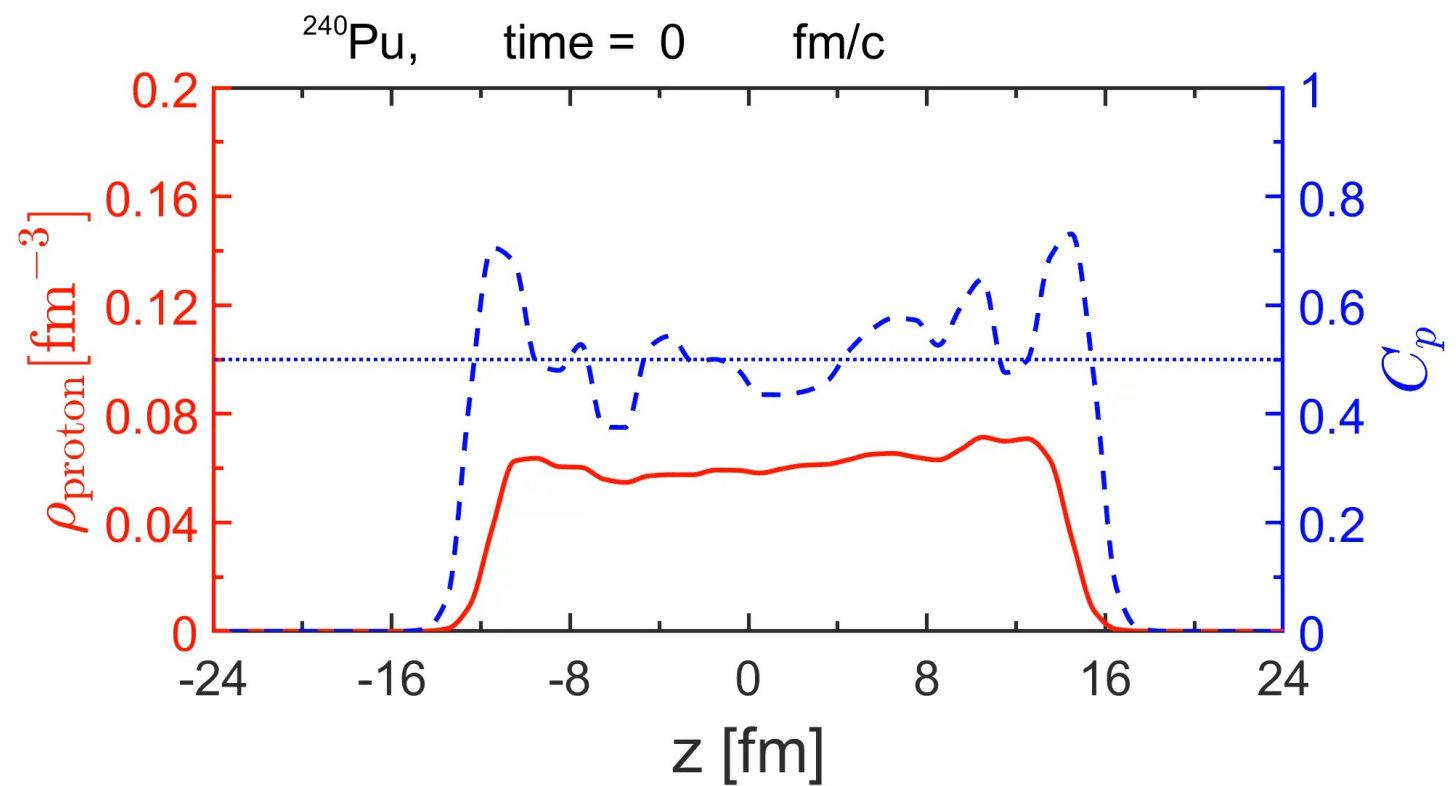
Density



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

Funding

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

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