Microscopic Analysis of Induced Nuclear Fission Dynamics

Dario Vretenar
University of Zagreb

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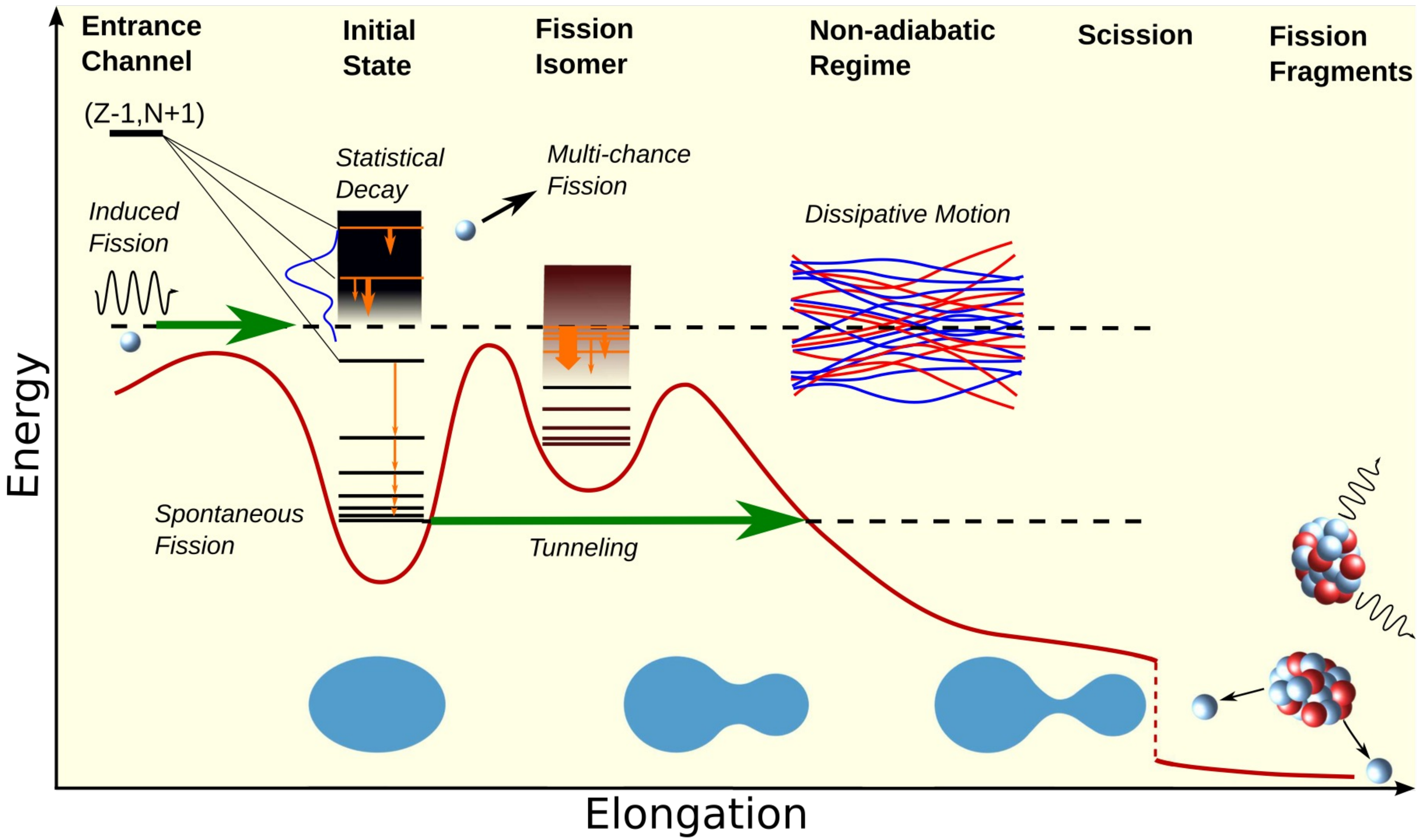
Future of nuclear fission theory

J. Phys. G: Nucl. Part. Phys. **47** (2020) 113002



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

The time-dependent generator coordinate method (TDGCM)

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

⇒ 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

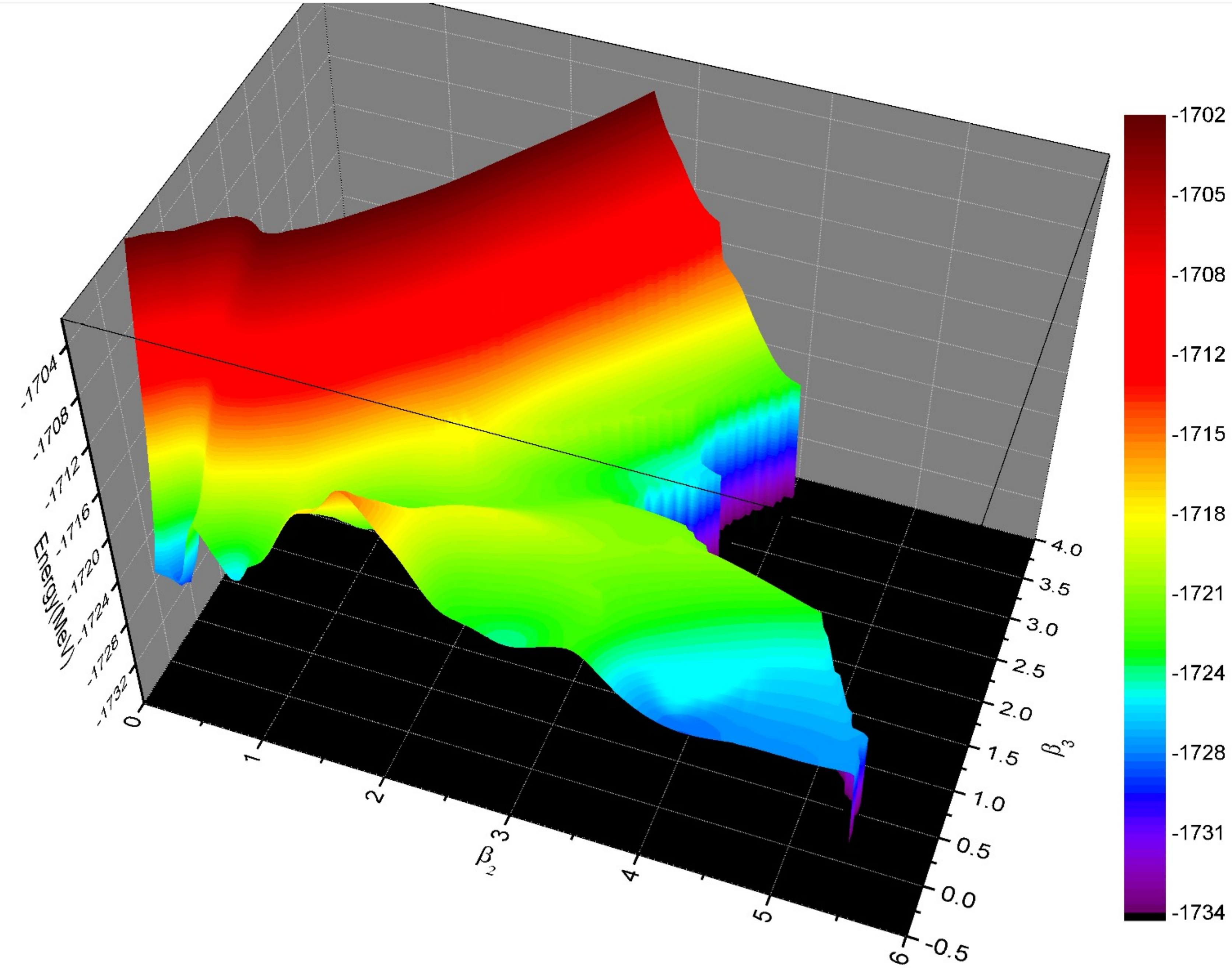
Time-dependent Schroedinger-like equation for fission dynamics (axial quadrupole and octupole deformation parameters as collective degrees of freedom):

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

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

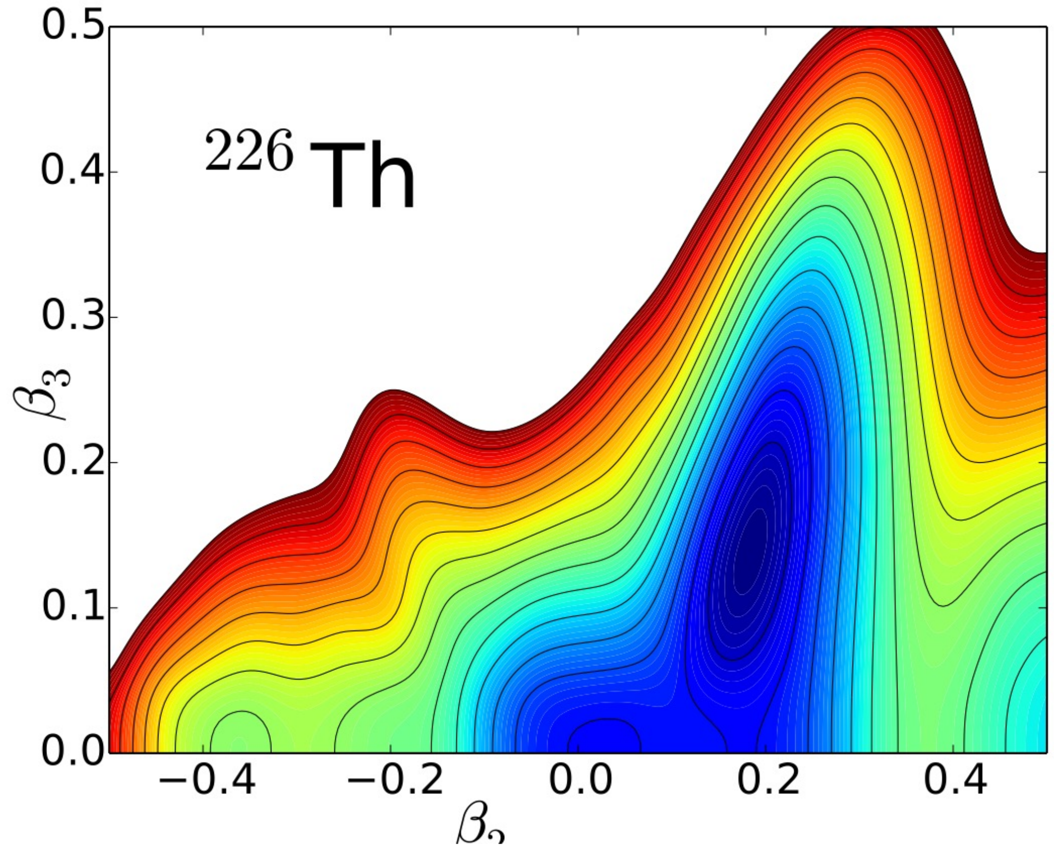
PHYSICAL REVIEW C **96**, 024319 (2017)



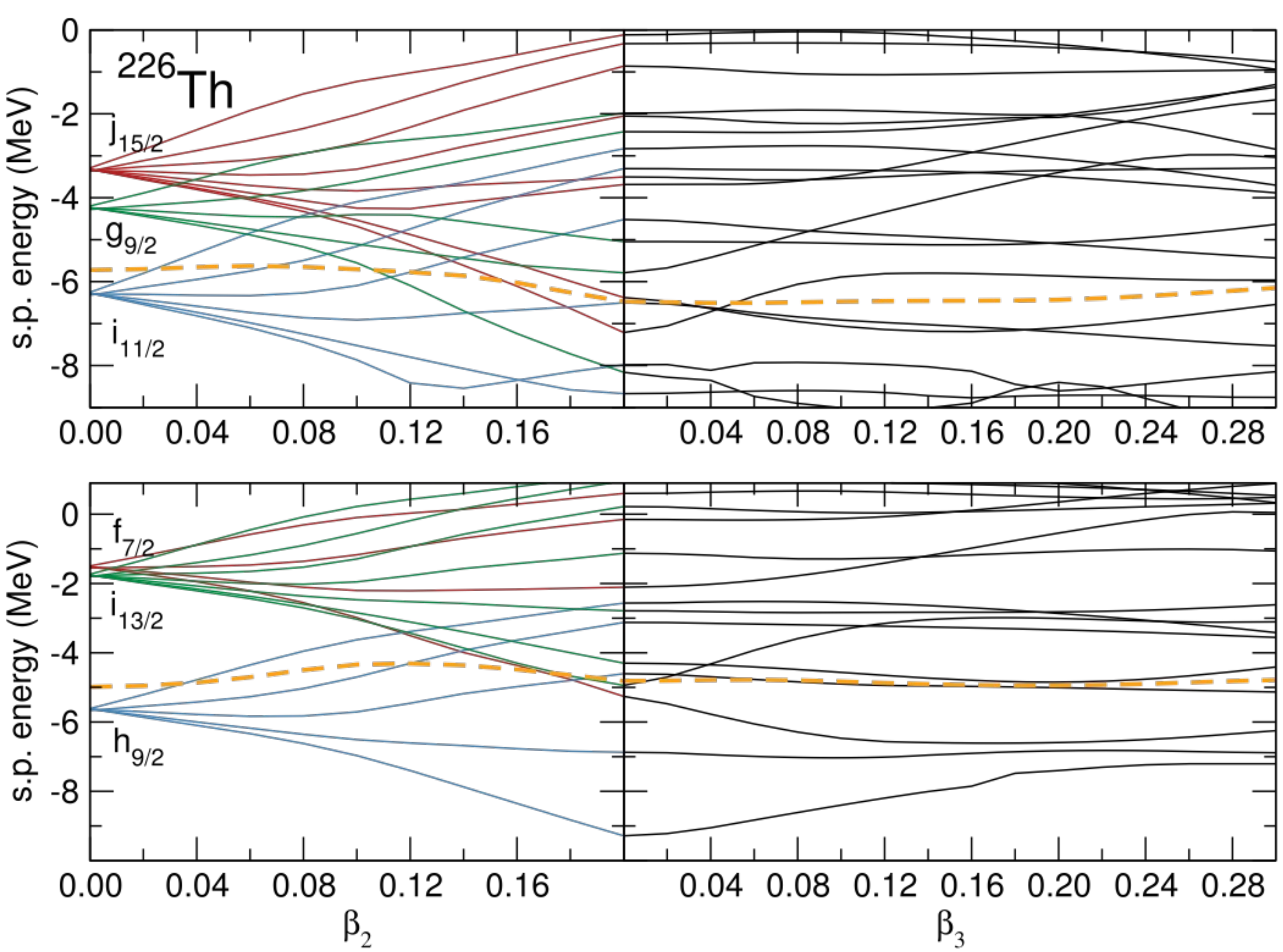
→ includes static correlations: deformations & pairing

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

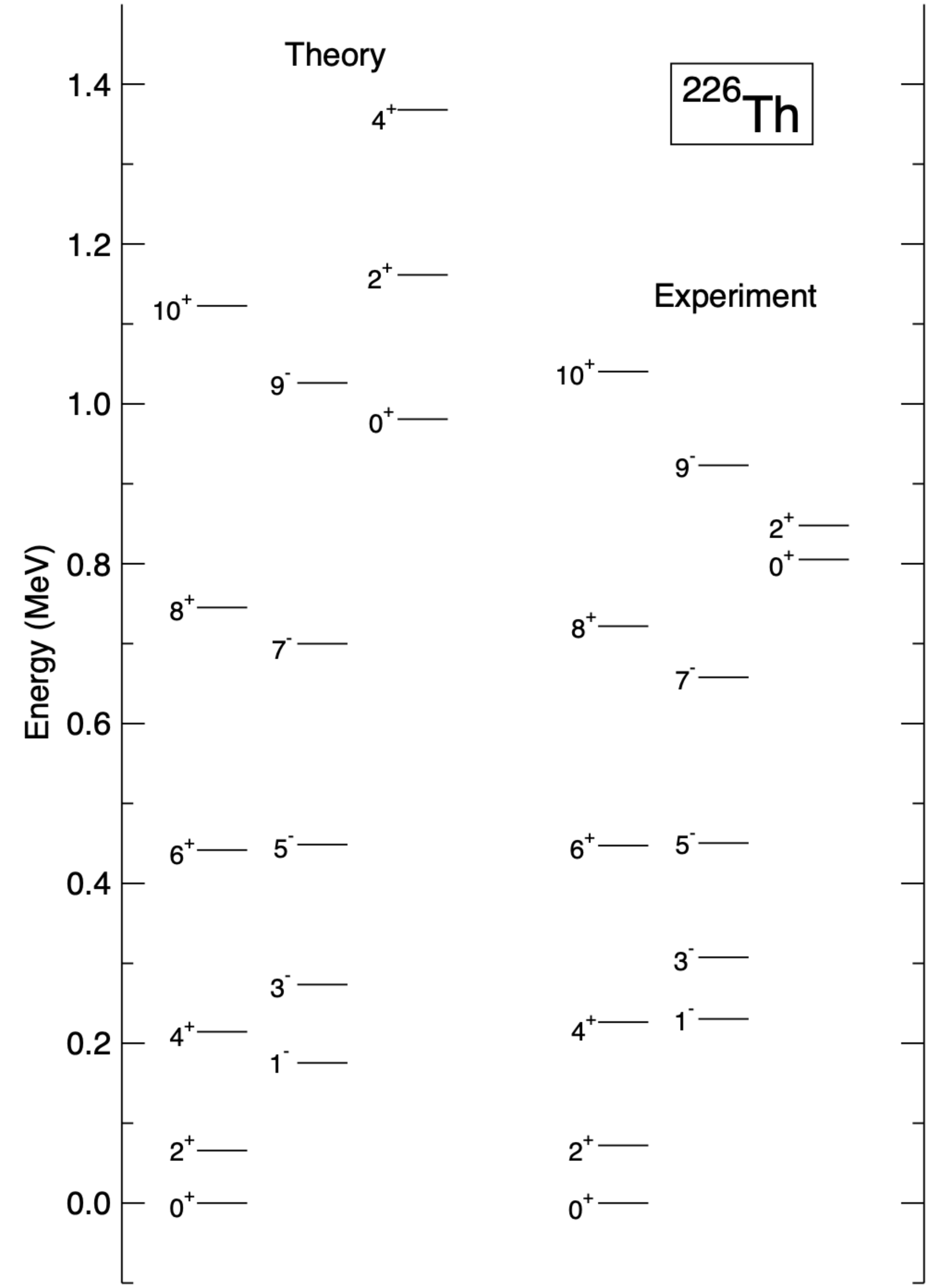
PC-PK1 plus δ-force pairing



^{226}Th
β_3
β_2
0.0
0.1
0.2
0.3
0.4
0.5
−0.4
−0.2
0.0
0.2
0.4



^{226}Th
s.p. energy (MeV)
$j_{15/2}$
$g_{9/2}$
$i_{11/2}$
$f_{7/2}$
$i_{13/2}$
$h_{9/2}$
β_2
β_3
0.00
0.04
0.08
0.12
0.16
0.20
0.24
0.28
0
-2
-4
-6
-8



Theory
^{226}Th
Experiment
Energy (MeV)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0^+
2^+
4^+
6^+
8^+
10^+
1^-
3^-
5^-
7^-
9^-
0^+
2^+
4^+
0^+
2^+
4^+
6^+
8^+
10^+
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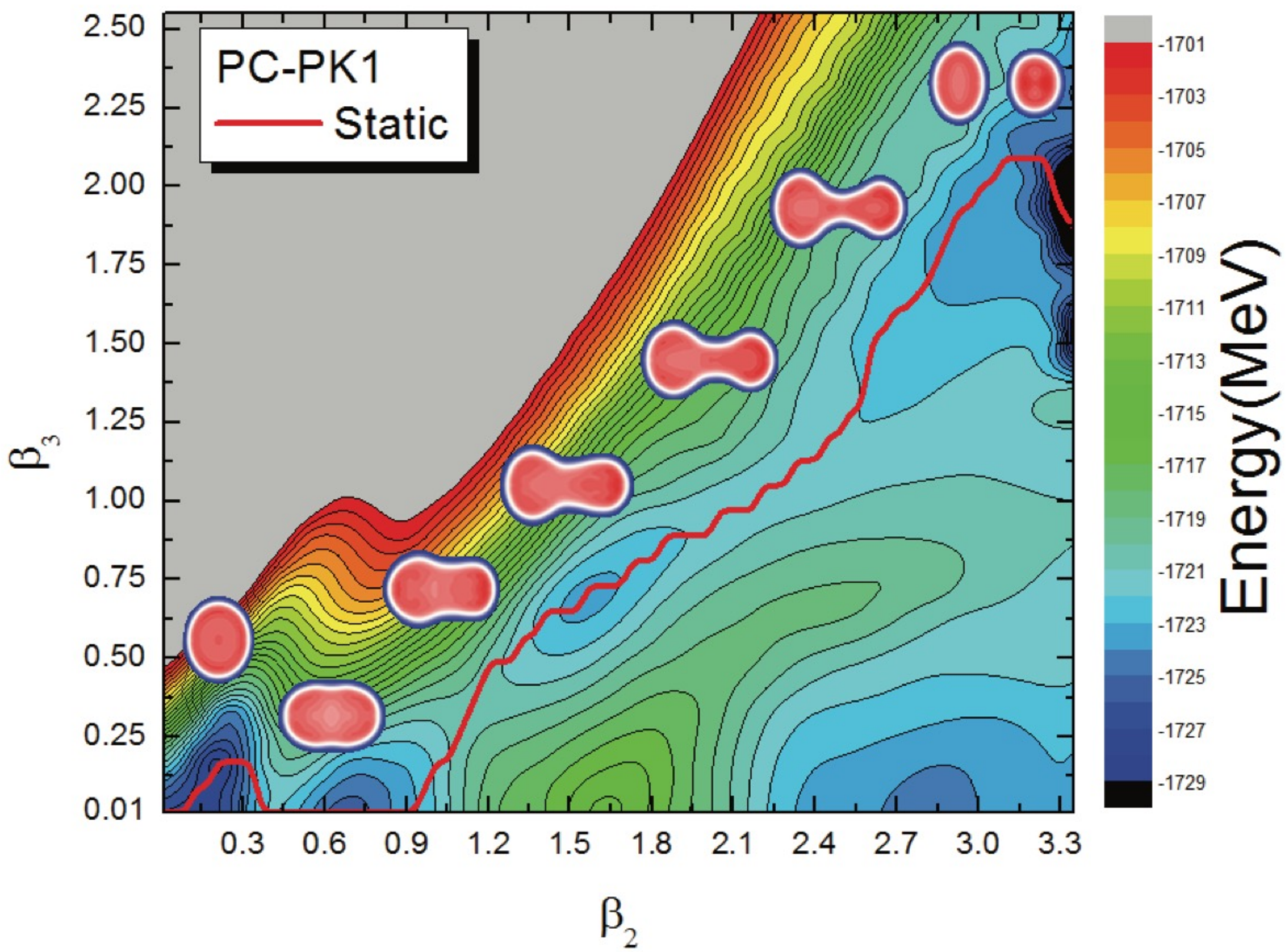
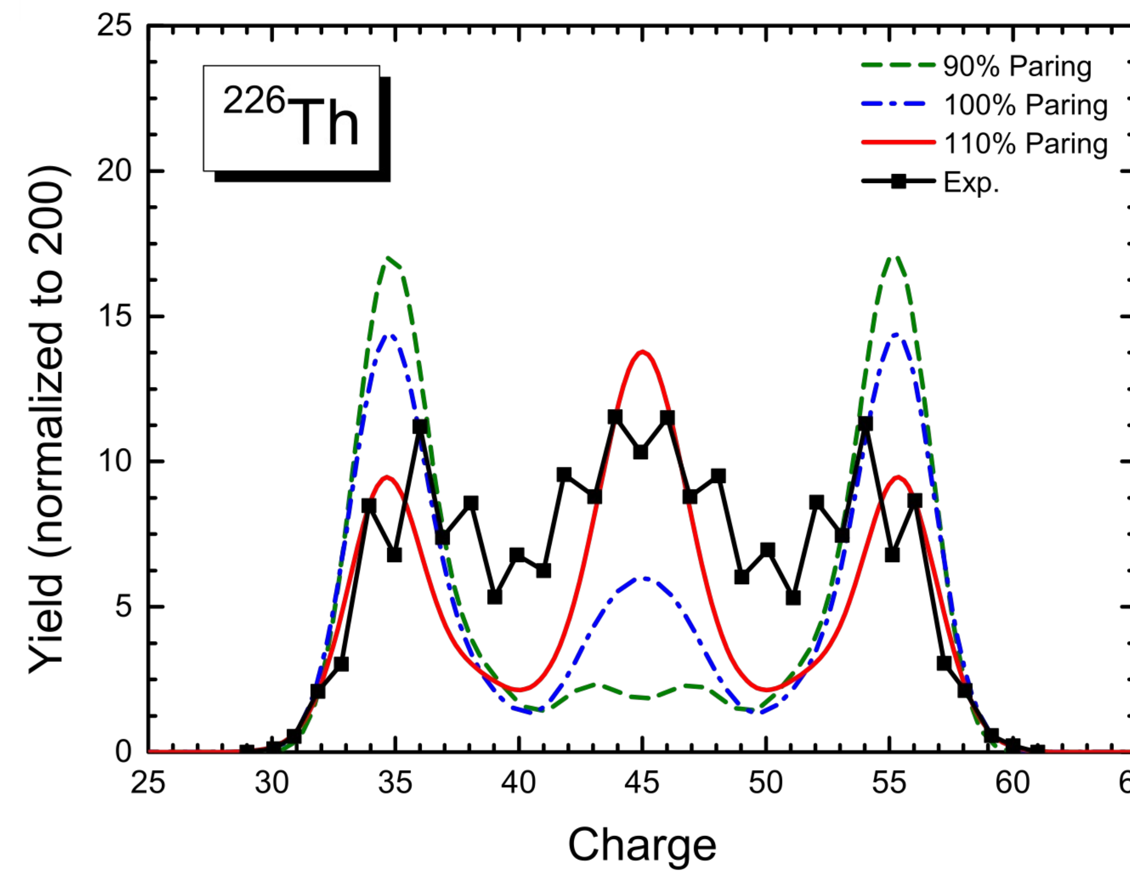
3^-
5^-
7^-
9^-
0^+
2^+



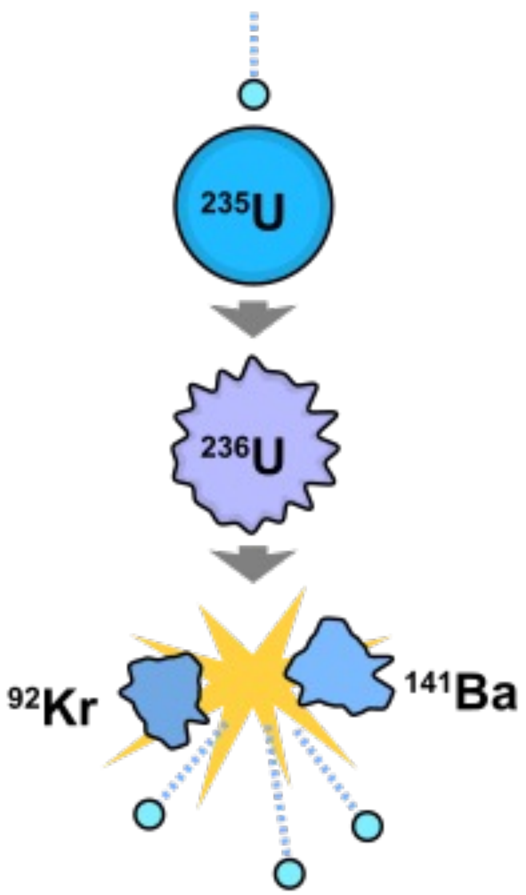
A triple-humped fission barrier is predicted along the static fission path, and the calculated heights are **7.10, 8.58, and 7.32 MeV** from the inner to the outer barrier.

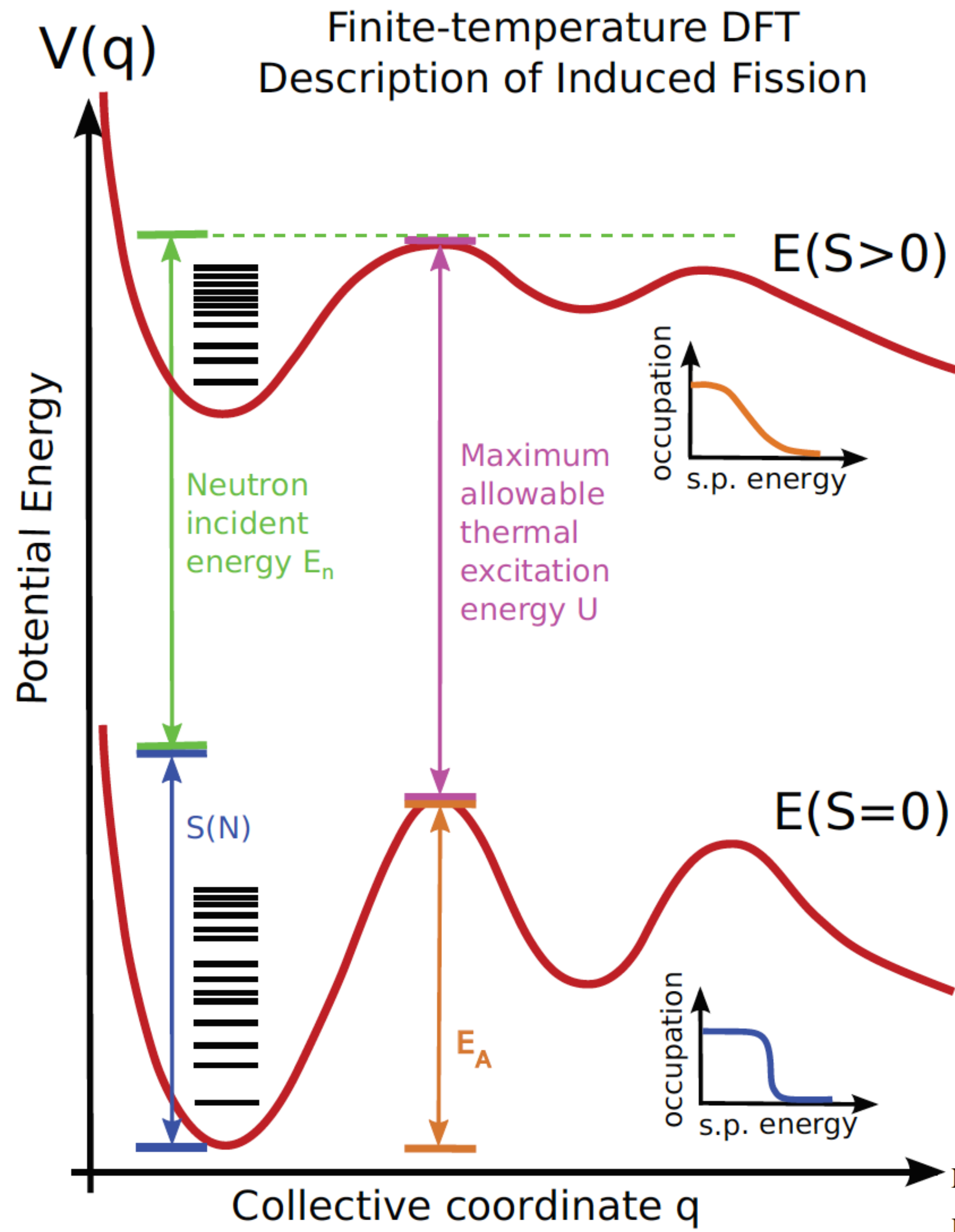
The height of the fission barriers (in MeV) with respect to the corresponding ground-state minima:

	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:

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

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

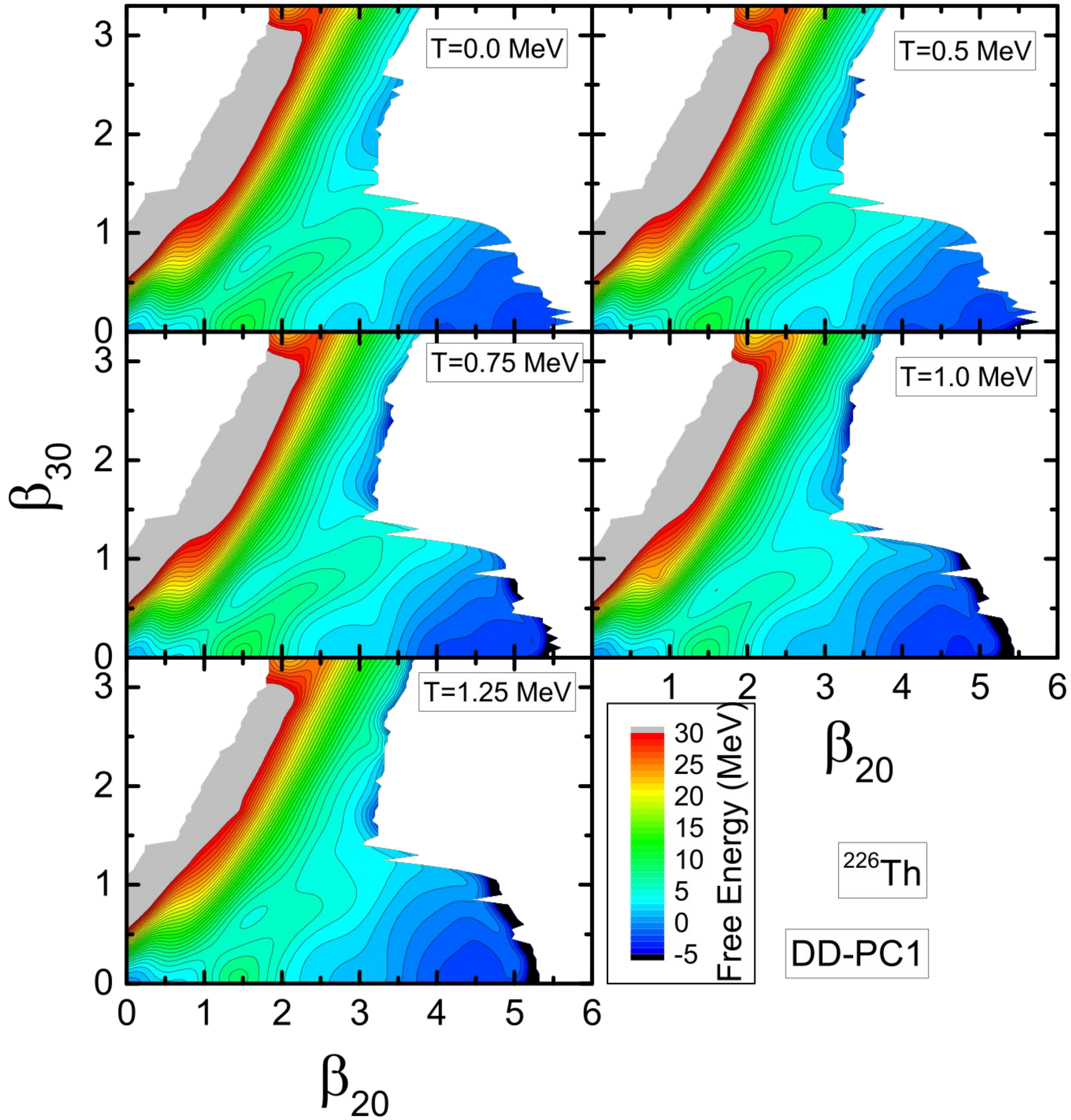
Helmholtz free energy: $F = E(T) - TS$

... entropy of the compound nuclear system:

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

... thermal occupation probabilities:

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

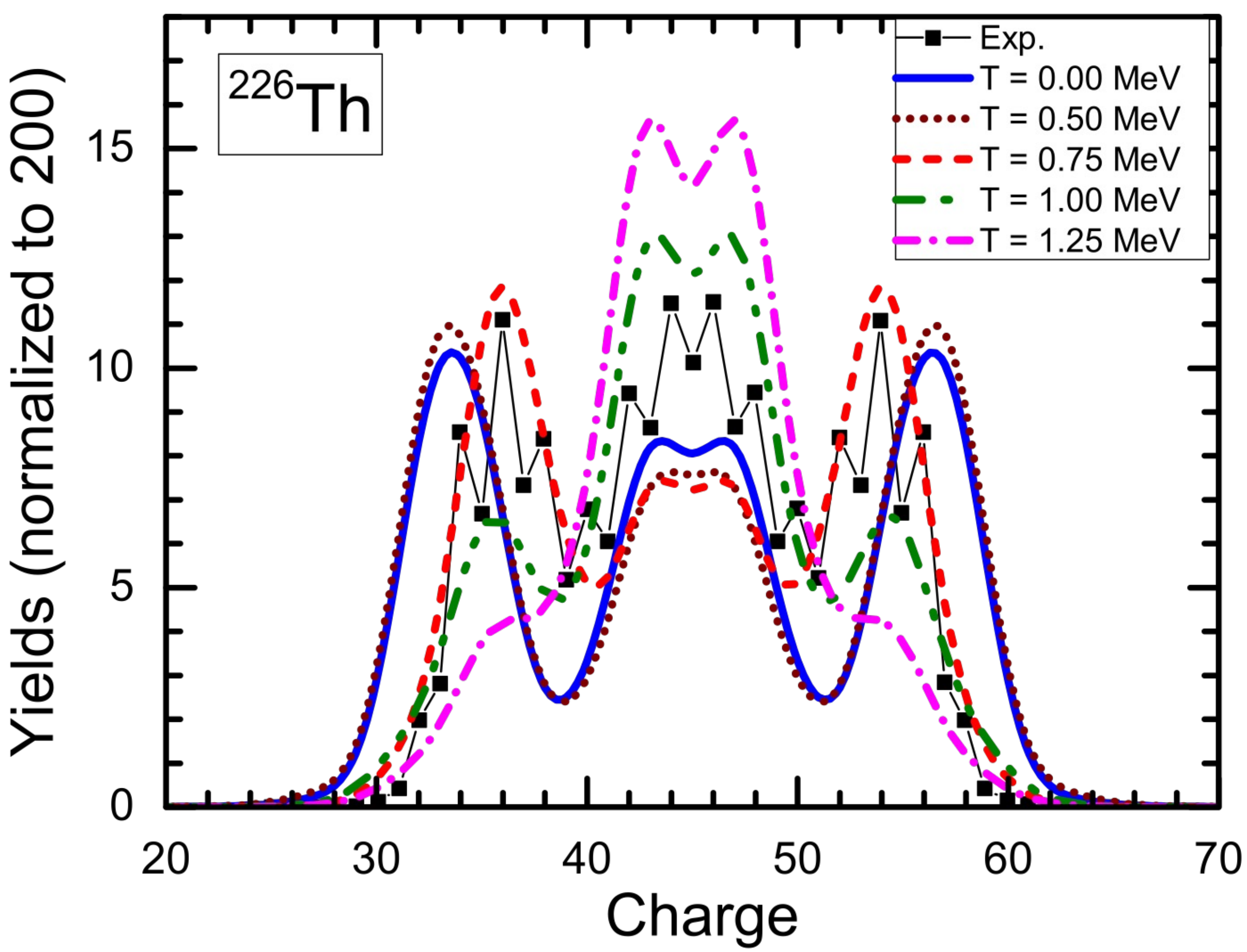


Dynamics of induced fission

Zhao, Nikšić, Vretenar, Zhou

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

Charge yields:



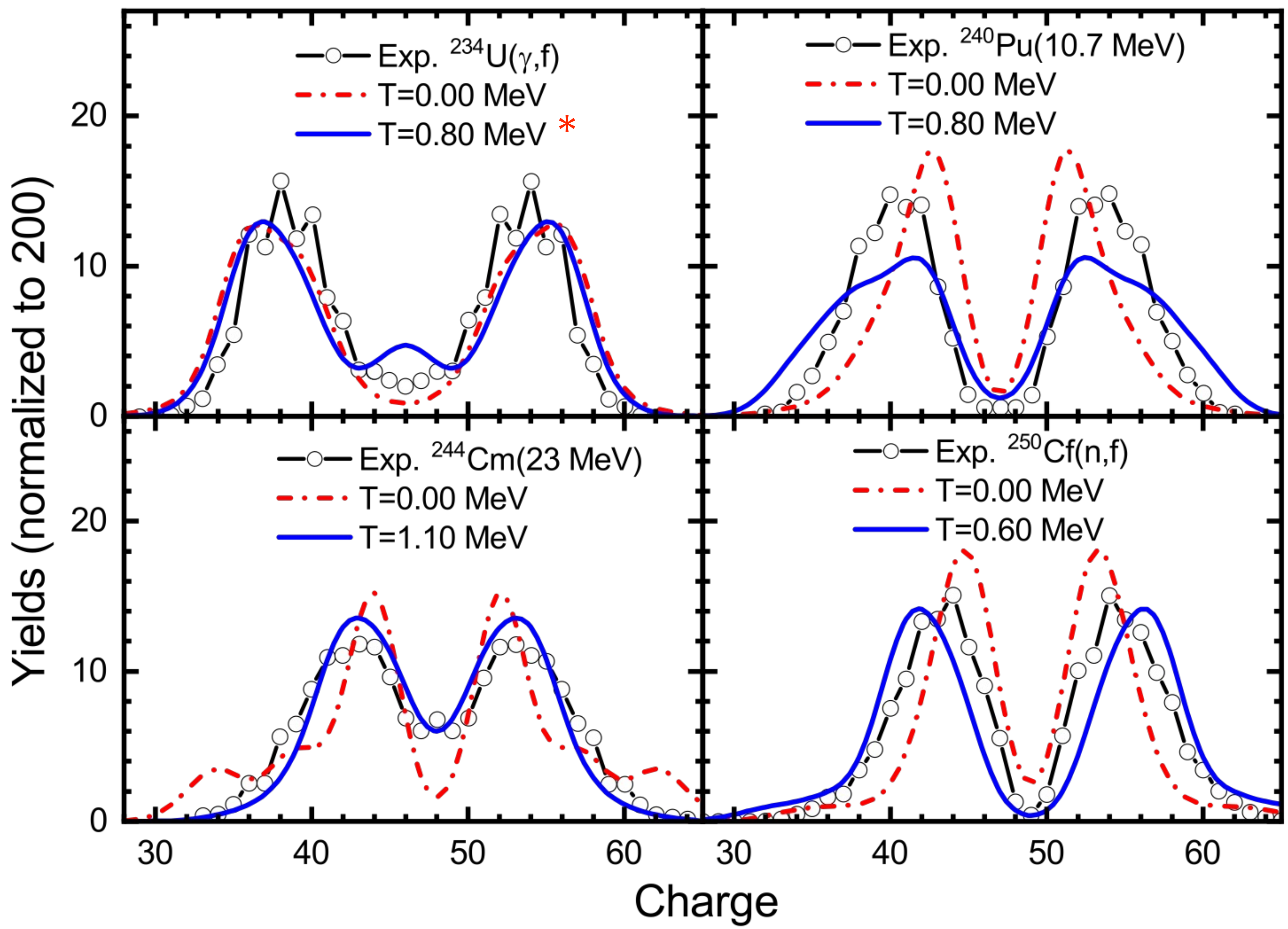
Experimental results ➠ photoinduced fission with photon energies in the interval 8 − 14 MeV, and a peak value Eγ = 11 MeV.

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:

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

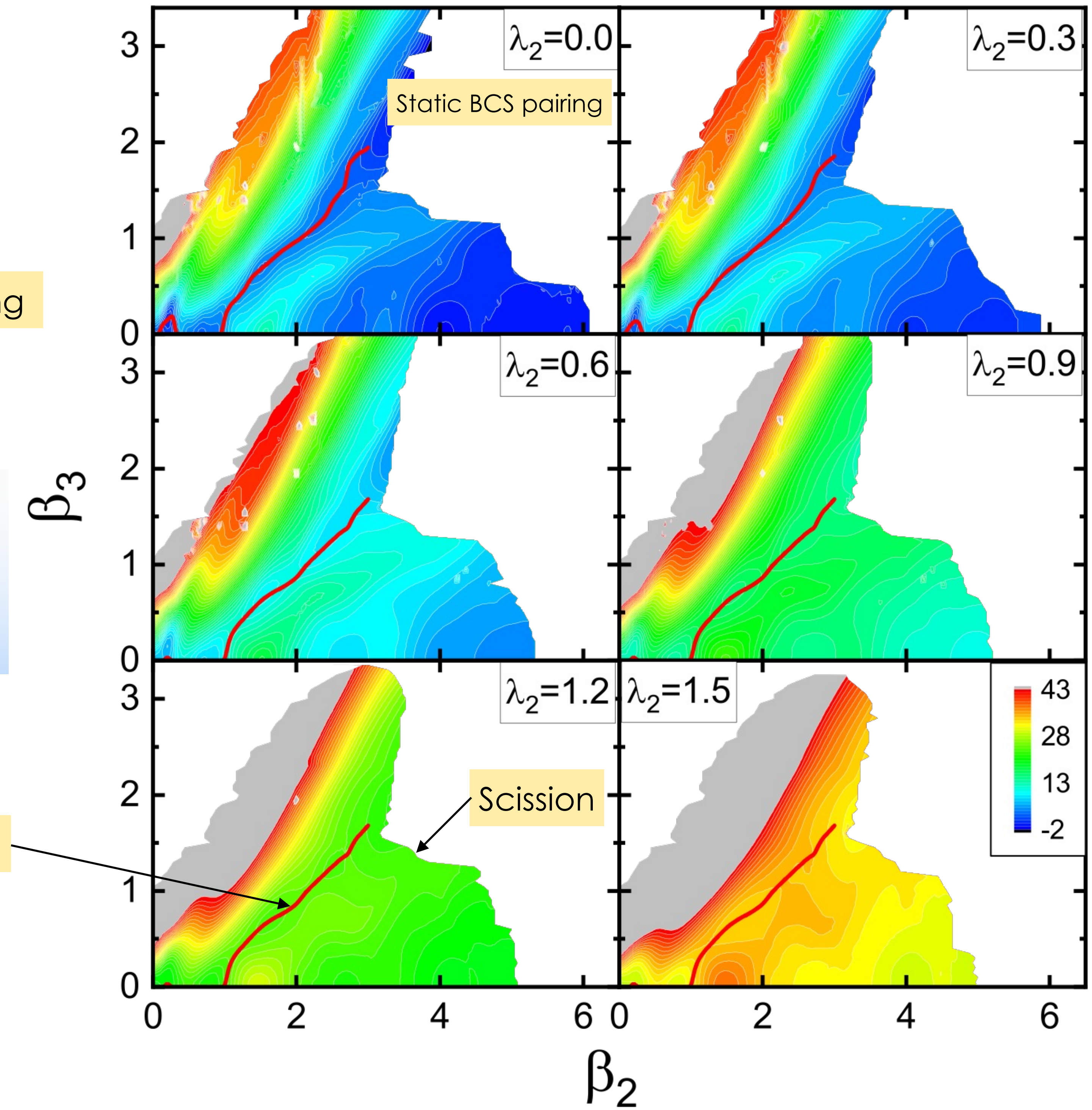
… the Routhian:

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

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.

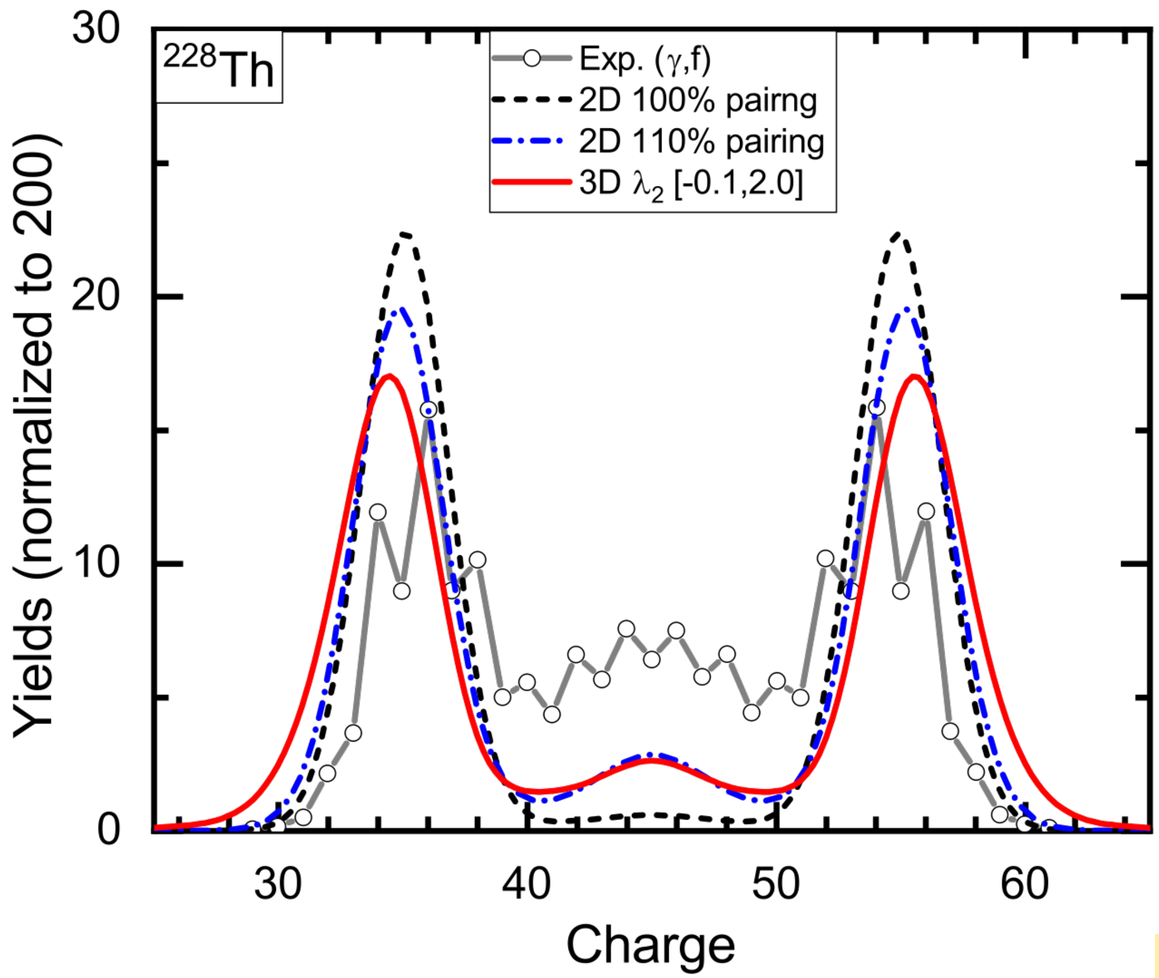
Static fission path of minimum energy

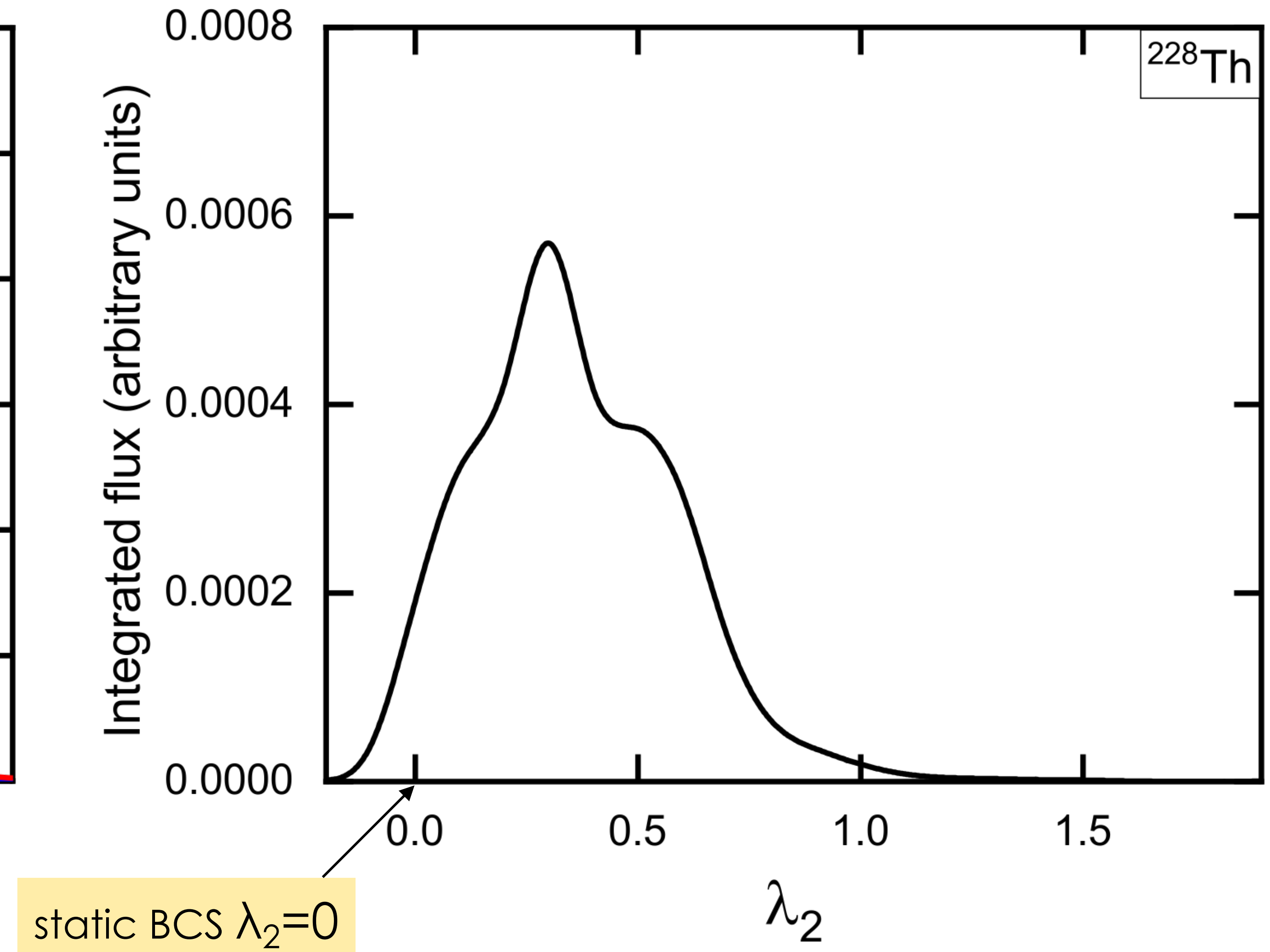


3D TDGCM+GOA calculation

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

q≡{β_2,β_3,λ_2}





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

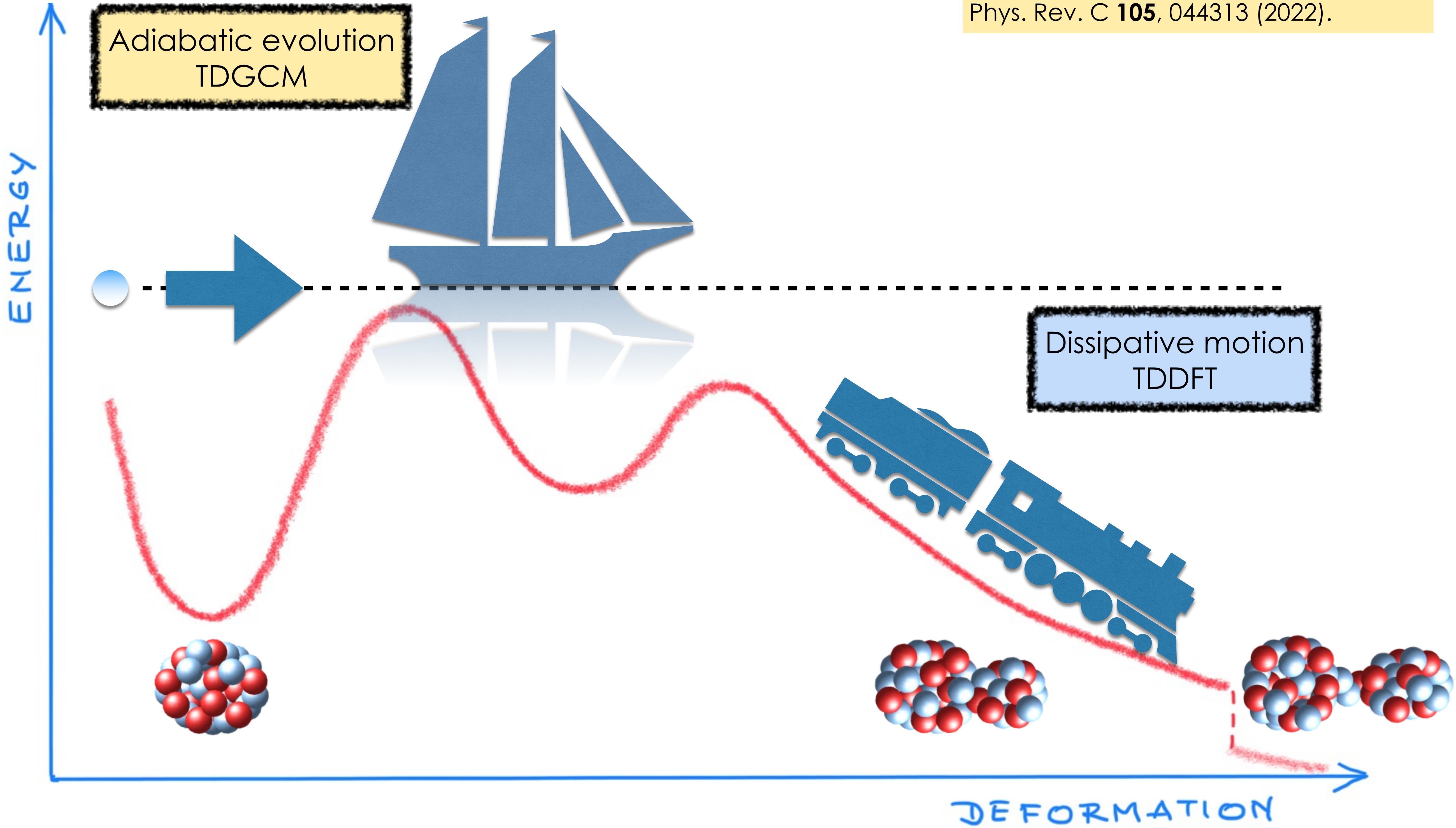
Effect of dynamical pairing on the flux of the probability current through the scission hyper-surface:

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

→ 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)

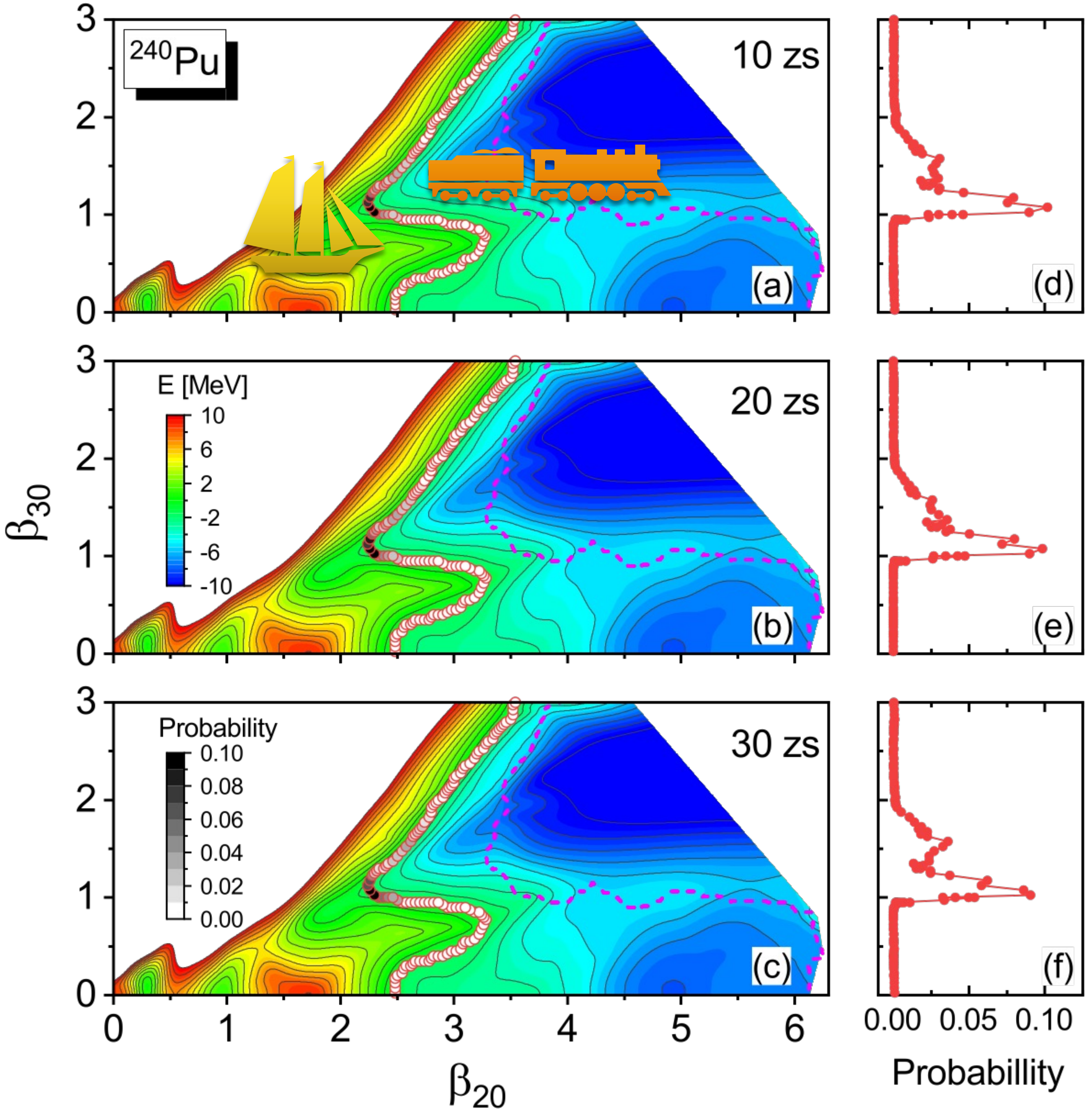
$$i\frac{\partial}{\partial t}\psi_k(\boldsymbol{r},t) = \left[\hat{h}(\boldsymbol{r},t) - \varepsilon_k(t)\right]\psi_k(\boldsymbol{r},t),$$

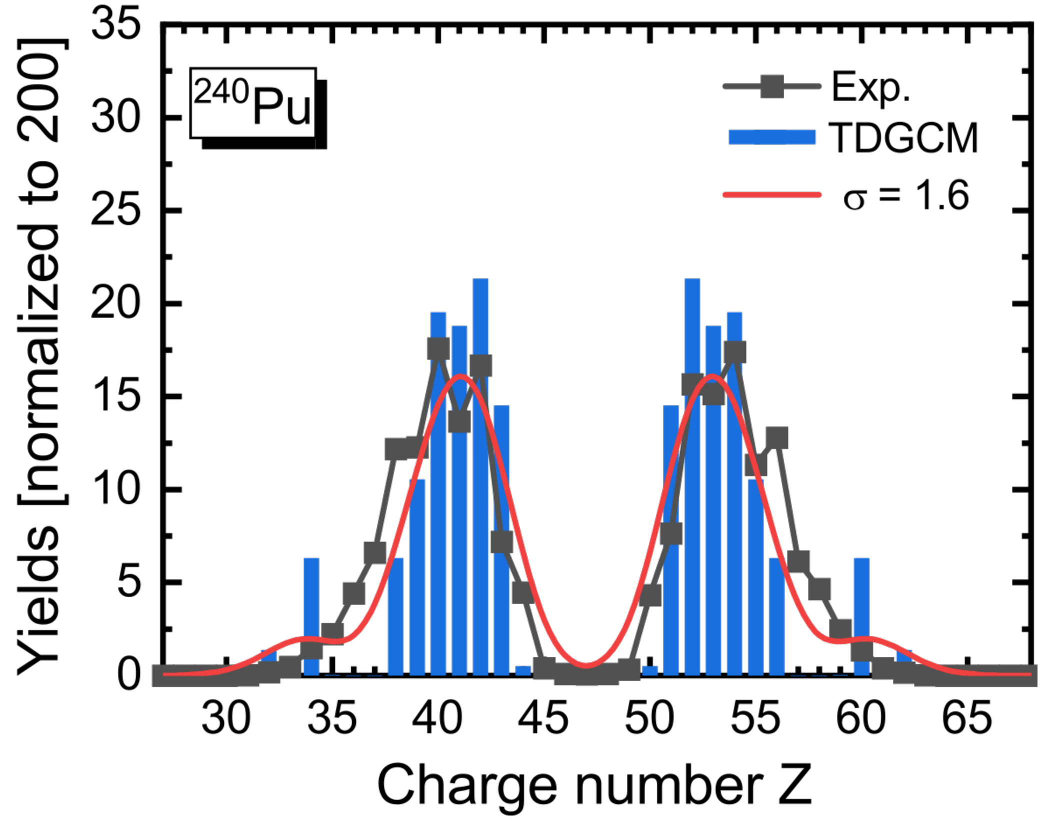
$$i\frac{d}{dt}n_k(t) = n_k(t)\Delta_k^*(t) - n_k^*(t)\Delta_k(t),$$
$$i\frac{d}{dt}\kappa_k(t) = [\varepsilon_k(t) + \varepsilon_{\bar{k}}(t)]\kappa_k(t) + \Delta_k(t)[2n_k(t) - 1].$$

⇒ 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.

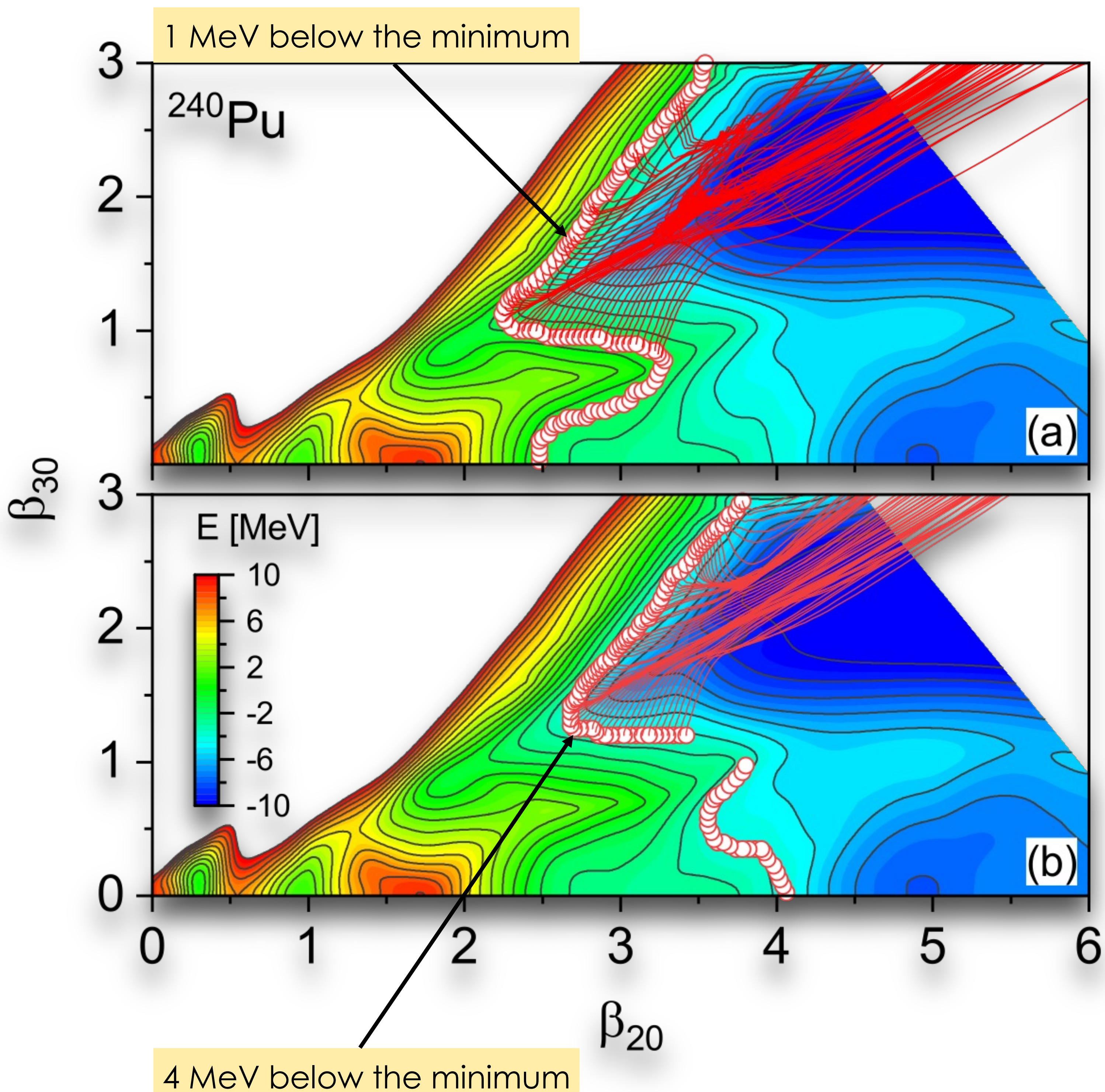
Negele et al. (1978) ➟ use an adiabatic model for the time interval in which the fissioning nucleus evolves from the quasi-stationary initial state to the saddle point, and a non-adiabatic method for the saddle-to-scission and beyond-scission dynamics.

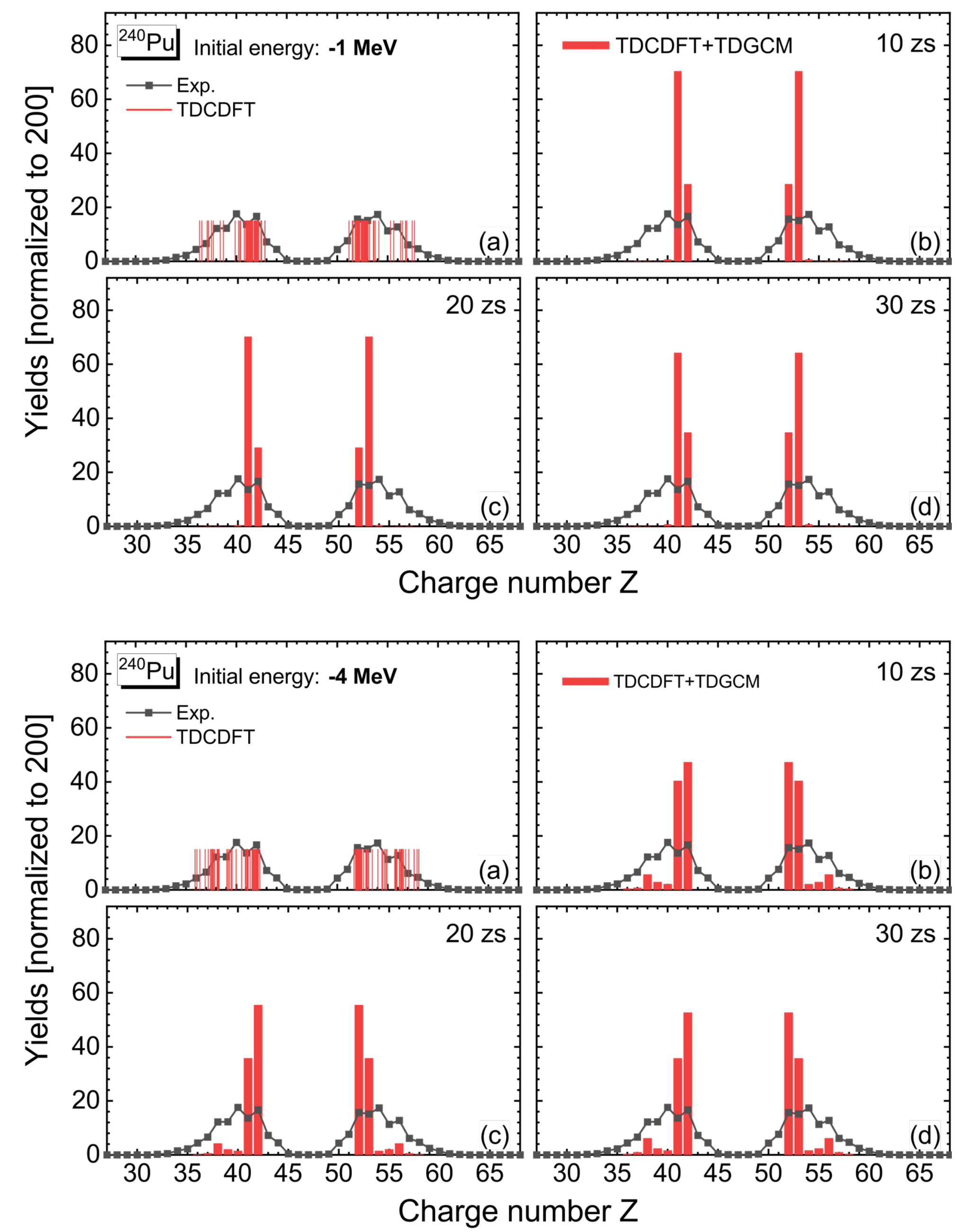




Ren, Zhao, Vretenar, Nikšić, Zhao, Meng
Phys. Rev. C **105**, 044313 (2022).

TDDFT fission trajectories





Total kinetic energies (TKEs) of the fragments

TDGCM+GOA

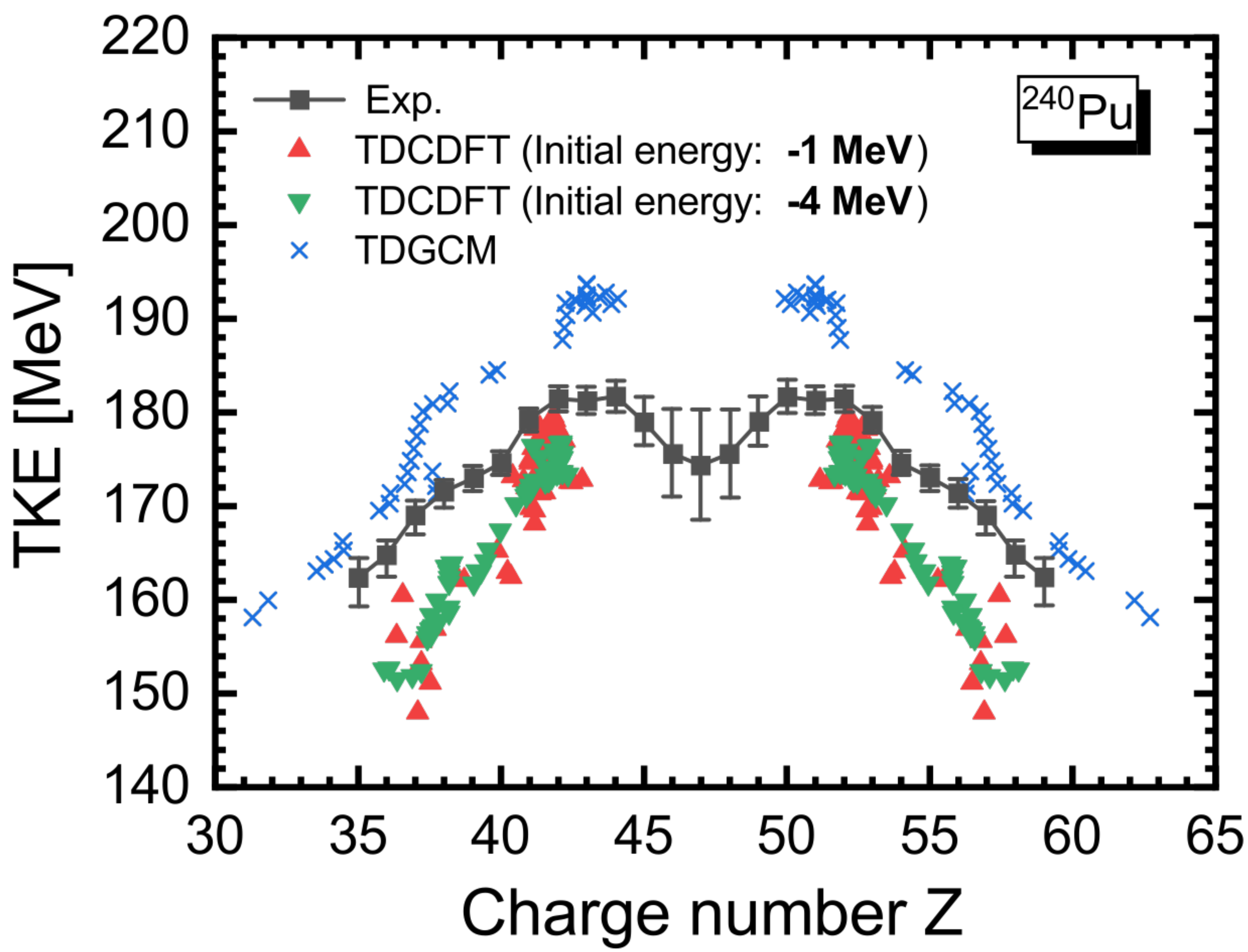
$$E_{\mathrm{TKE}} = \frac{e^2 Z_H Z_L}{d_{\mathrm{ch}}},$$

$\rightarrow$ distance between centers of charge at the point of scission.

TDDFT

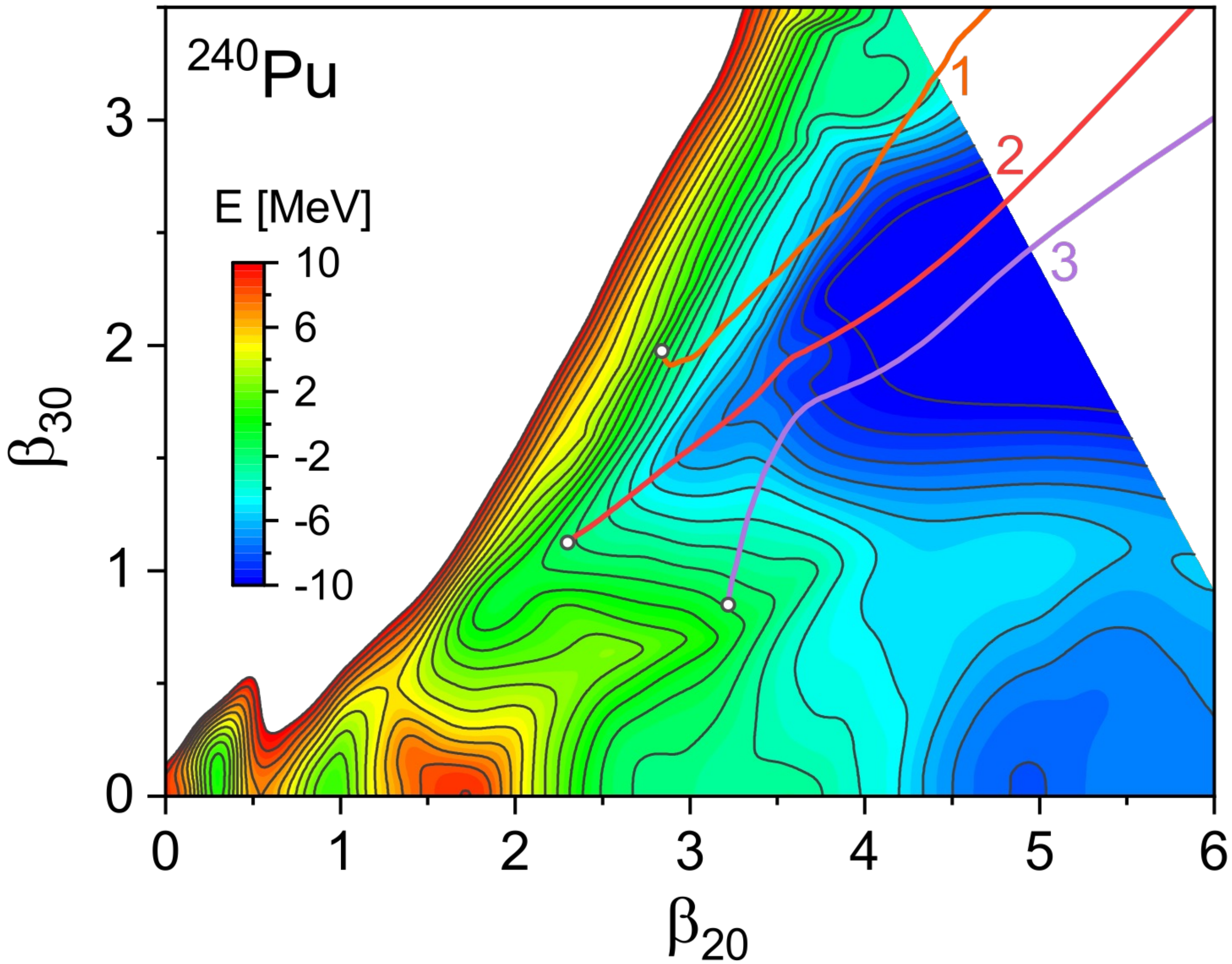
$$E_{\mathrm{TKE}} = \frac{1}{2} m A_{\mathrm{H}} \boldsymbol{v}_{\mathrm{H}}^2 + \frac{1}{2} m A_{\mathrm{L}} \boldsymbol{v}_{\mathrm{L}}^2 + E_{\mathrm{Coul}},$$

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

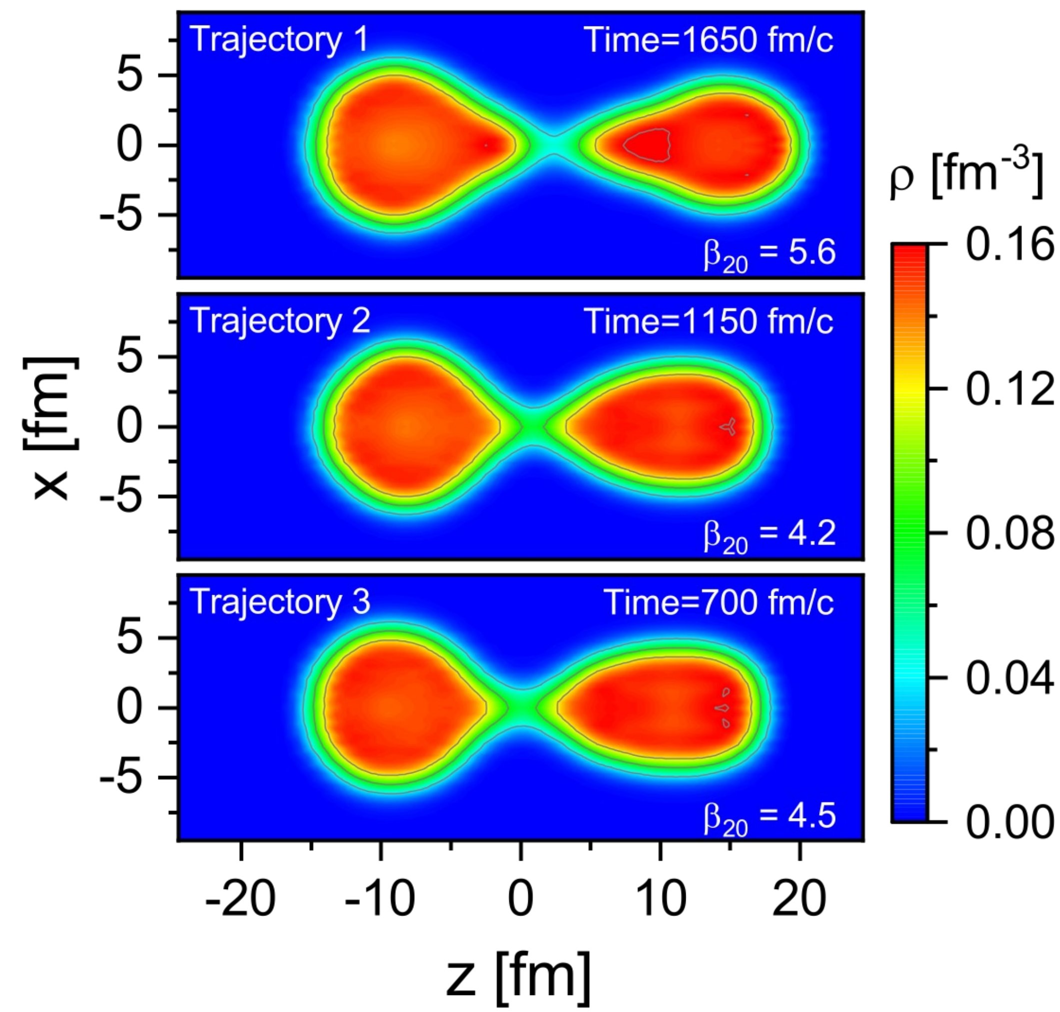


Dynamical synthesis of ^{4}He in the scission phase of nuclear fission

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:

kinetic energy density

density

current density

$\sigma\ (\uparrow \text{ or } \downarrow)$

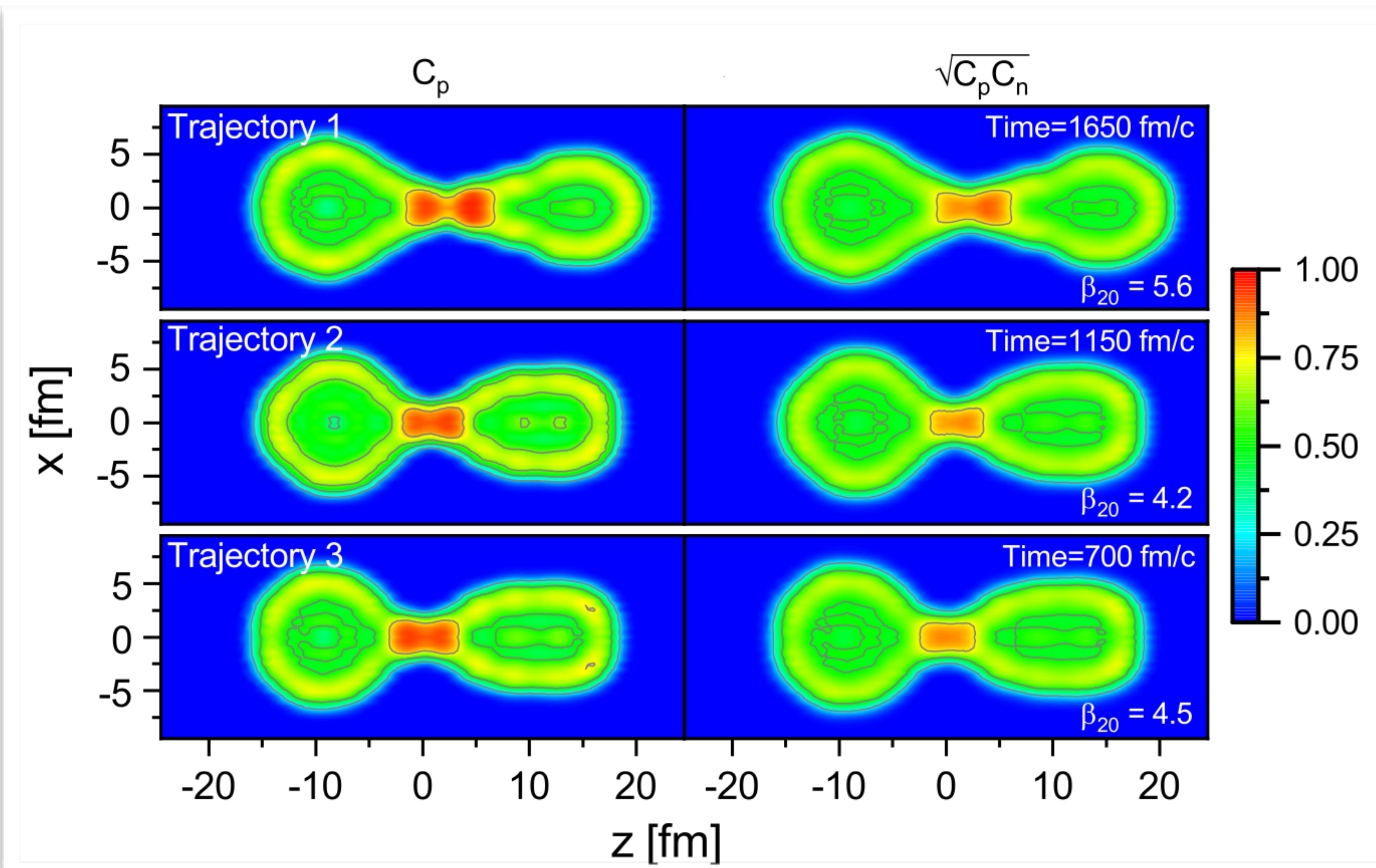
$q\ (n \text{ or } p)$

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

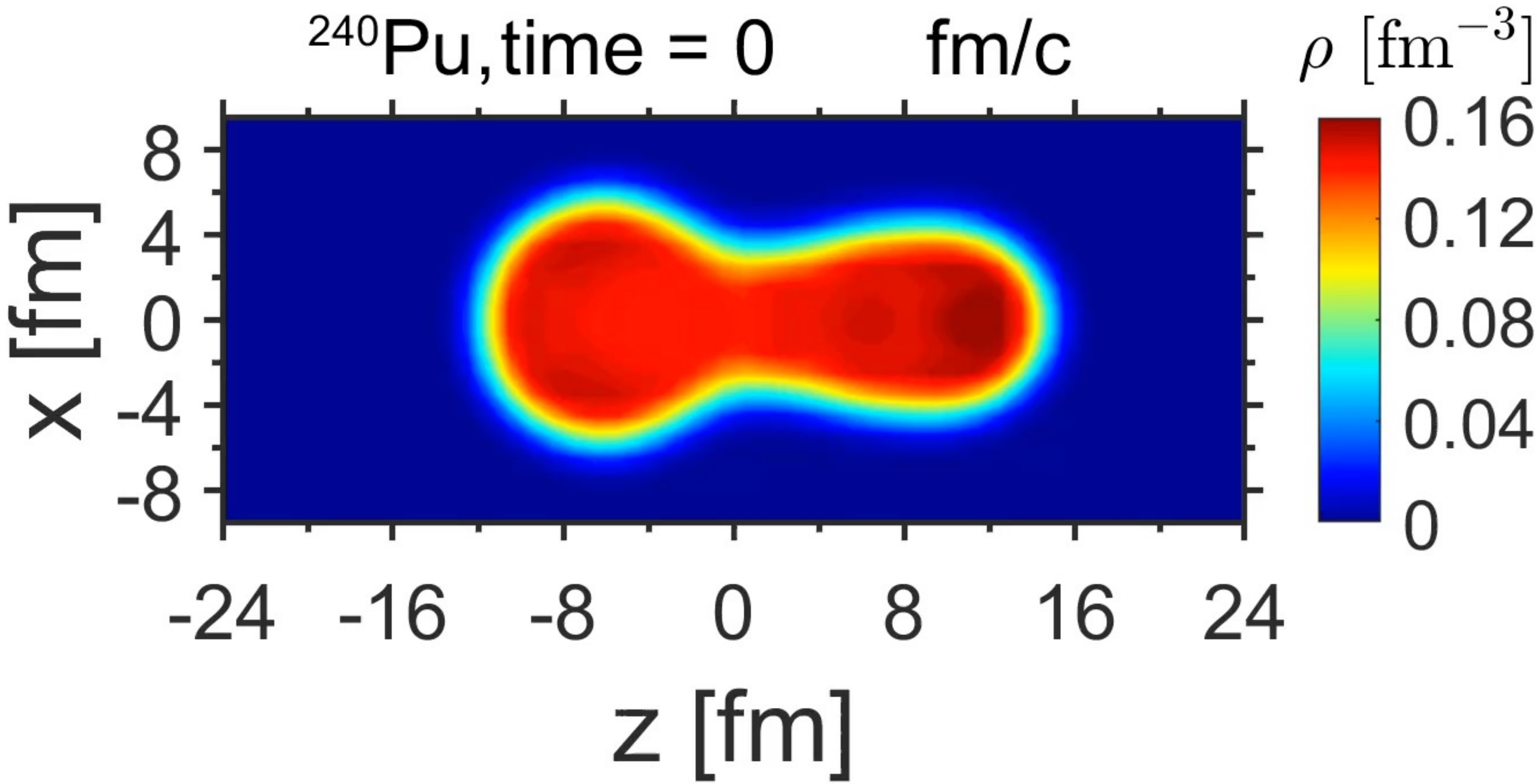
$$\tau^{\mathrm{TF}}_{q\sigma} = \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3}_{q\sigma}$$

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

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

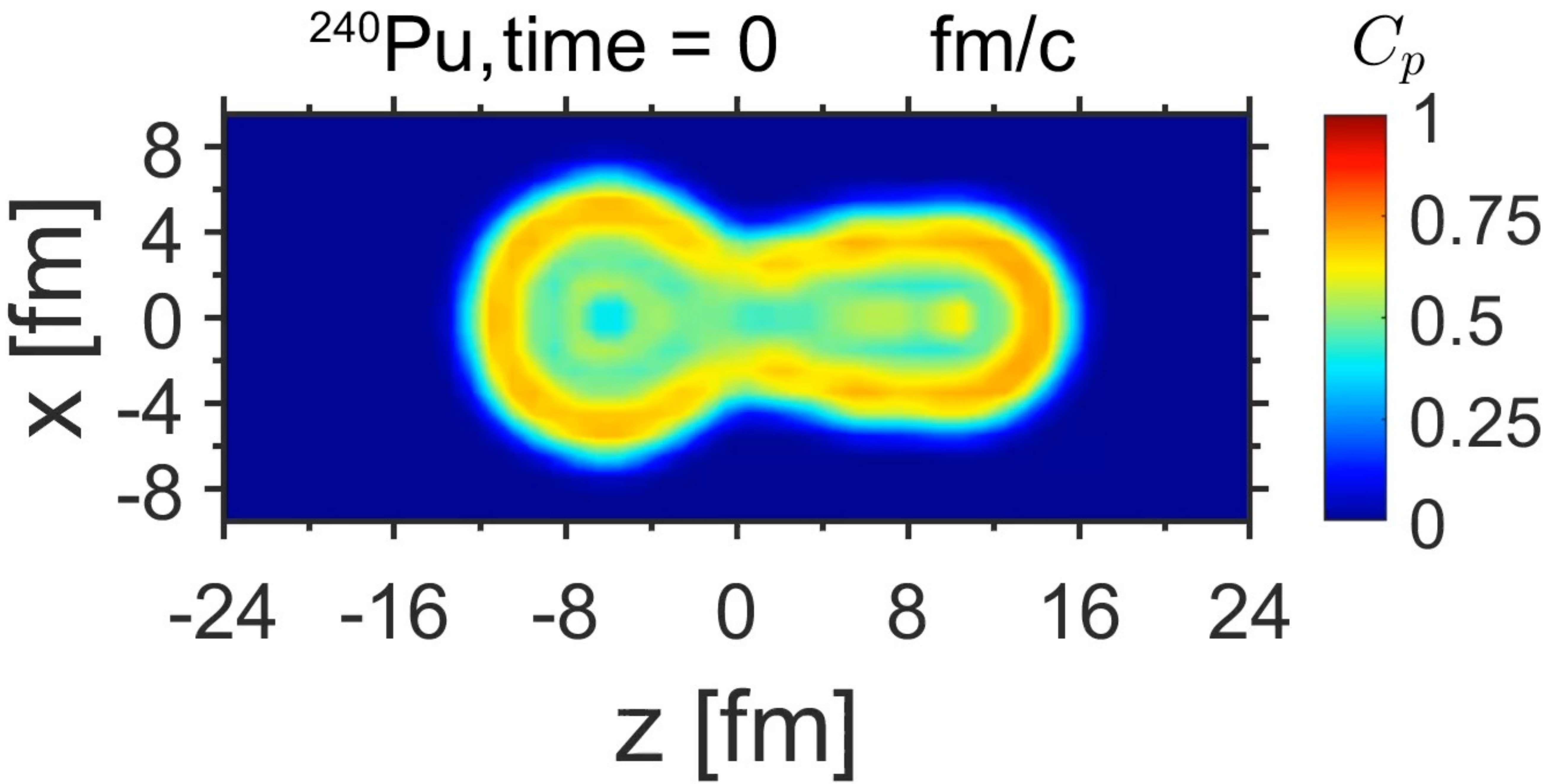


Trajectory 2



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

Trajectory 2

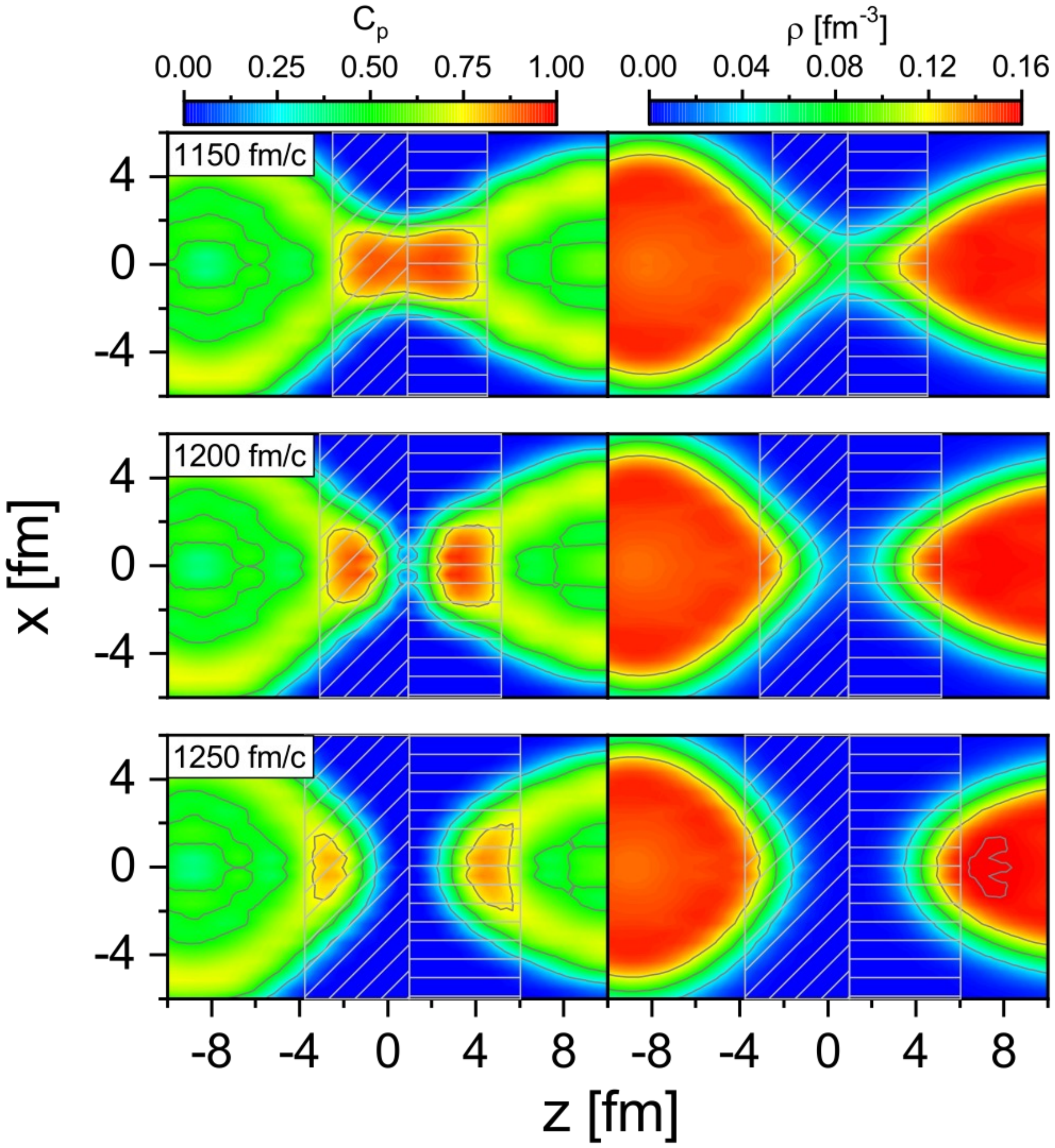


Ren, Vretenar, Nikšić, Zhao, Zhao, Meng, Phys. Rev. Lett. **128**, 172501 (2022).

Trajectory 2

Proton localization

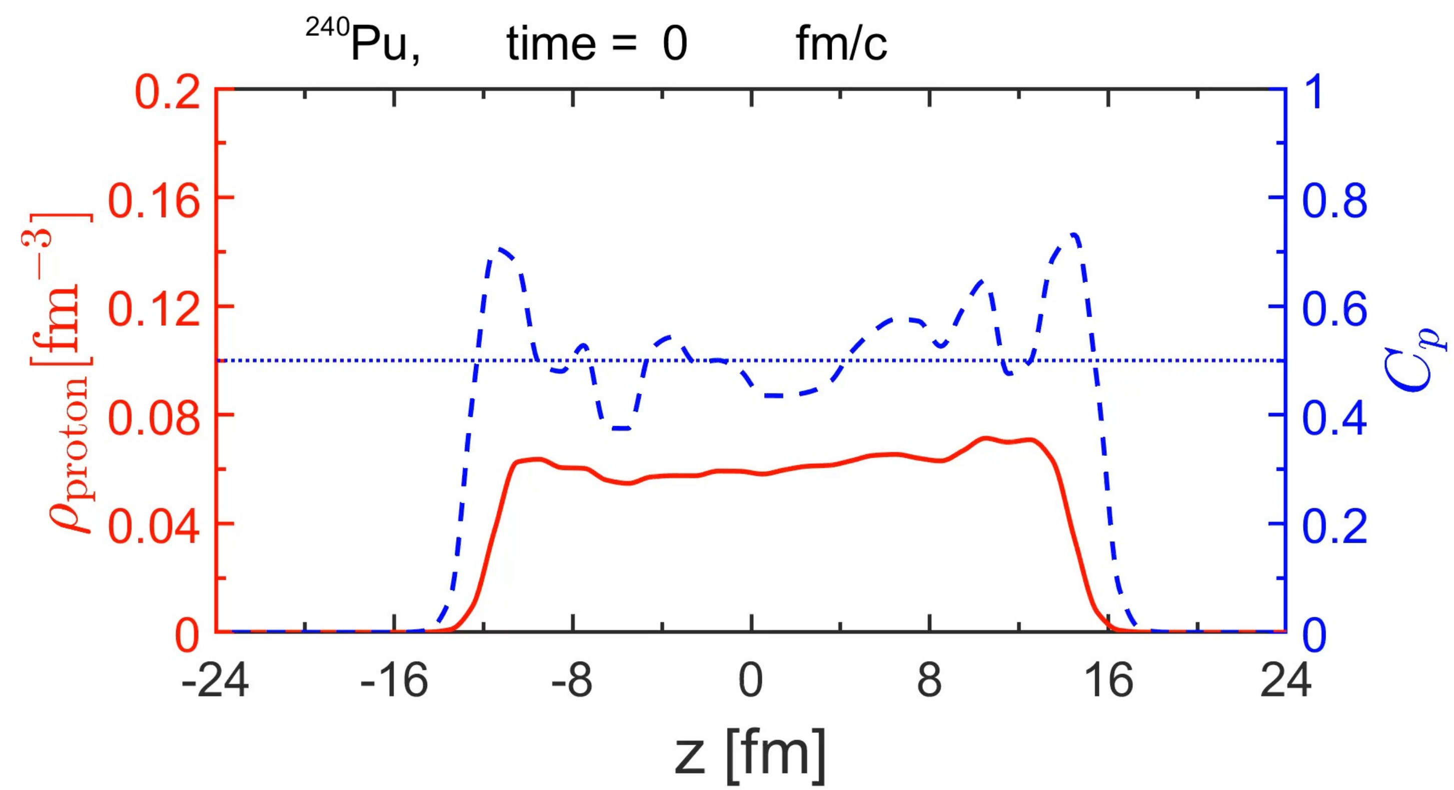
Density



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).

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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https://strukturnifondovi.hr/

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