Microscopic Analysis of Induced Nuclear Fission Dynamics

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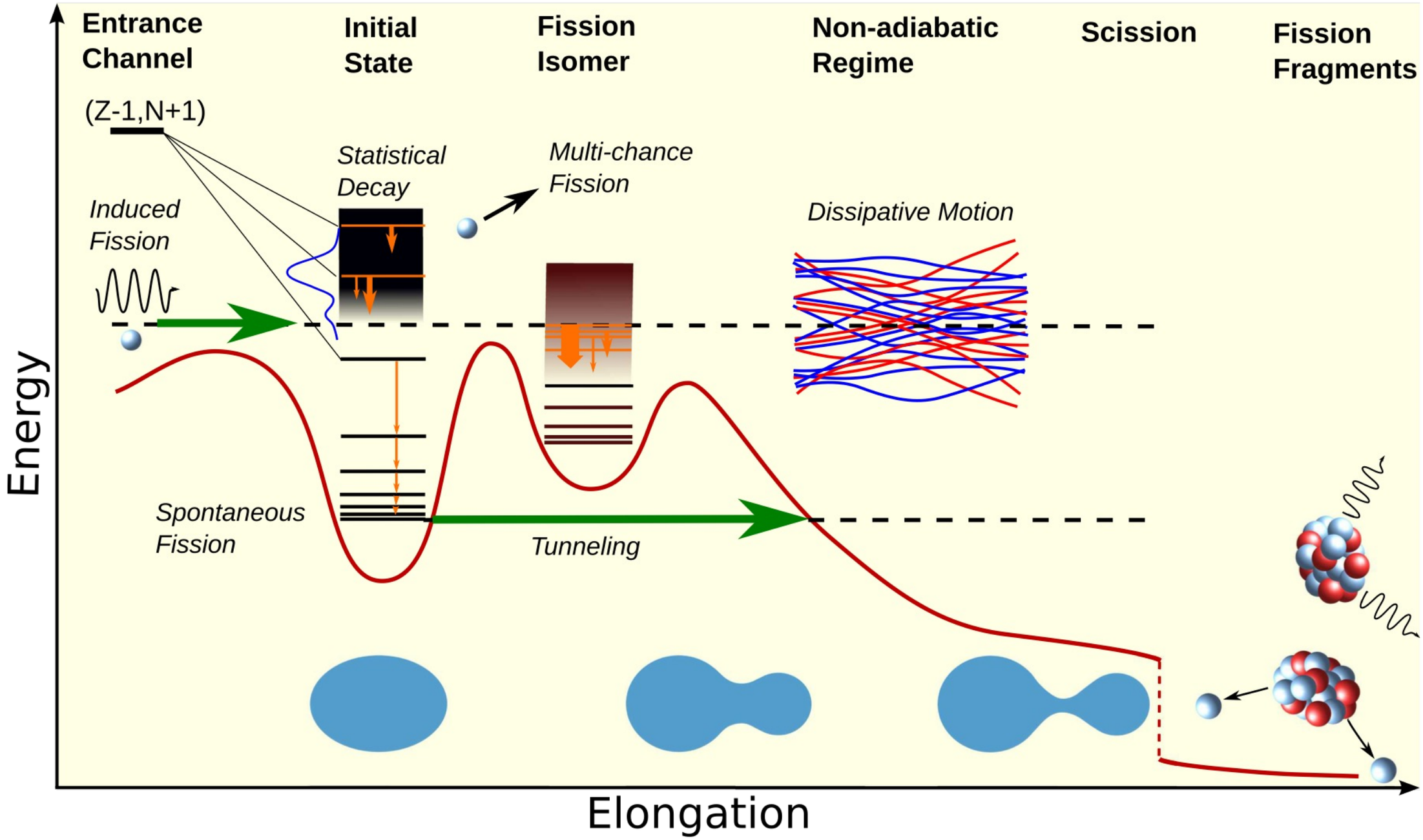
Future of nuclear fission theory

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)

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

⇒ 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

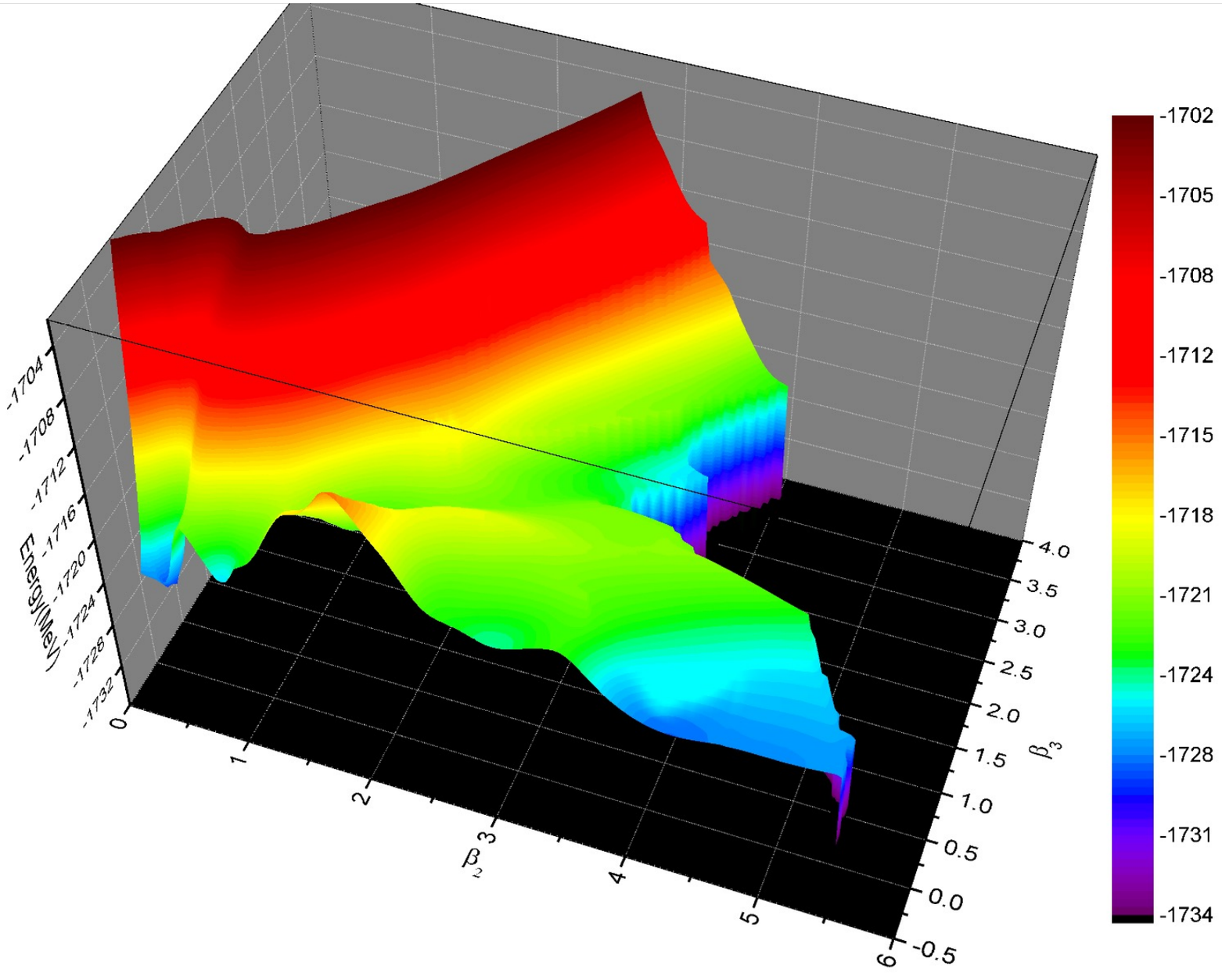
Time-dependent Schroedinger-like equation for fission dynamics (axial quadrupole and octupole deformation parameters as collective degrees of freedom):

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

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

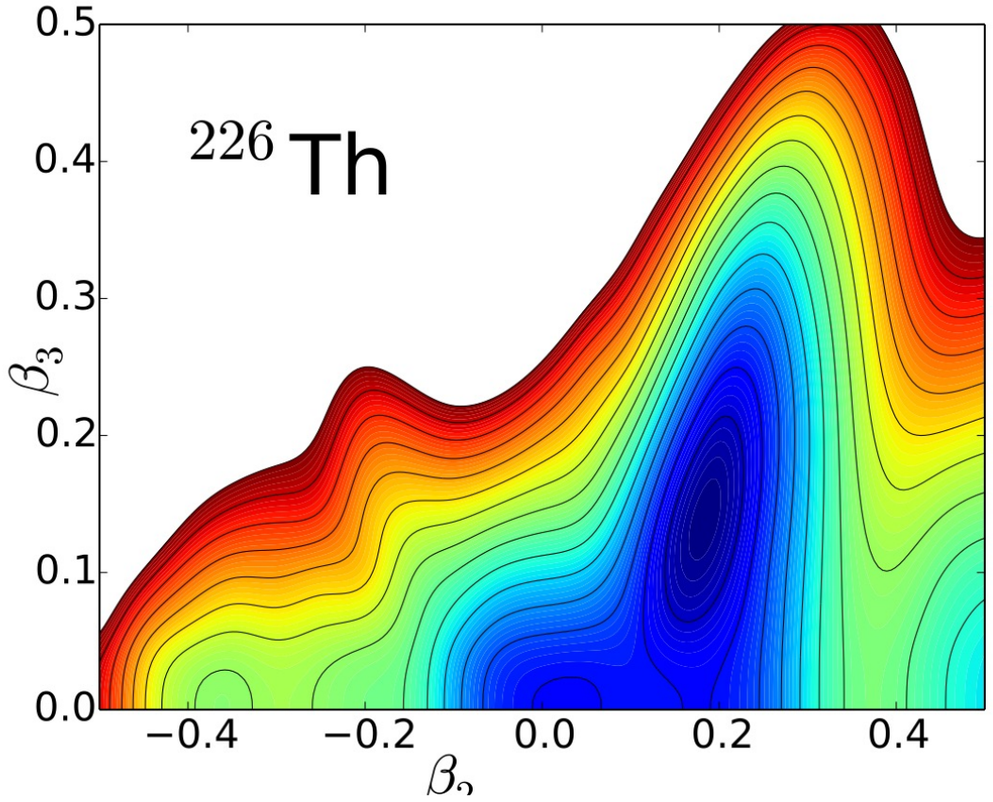
PHYSICAL REVIEW C **96**, 024319 (2017)

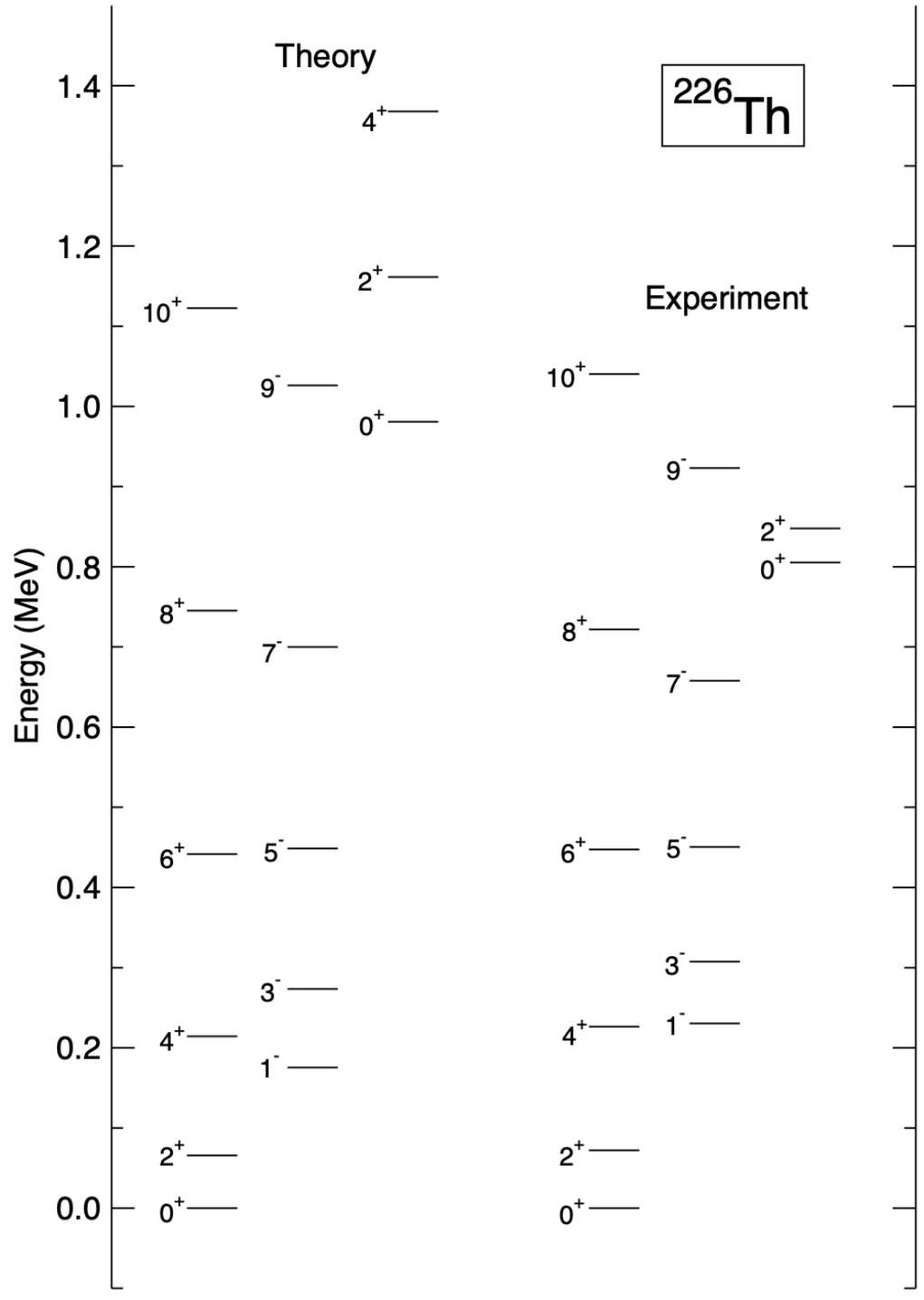


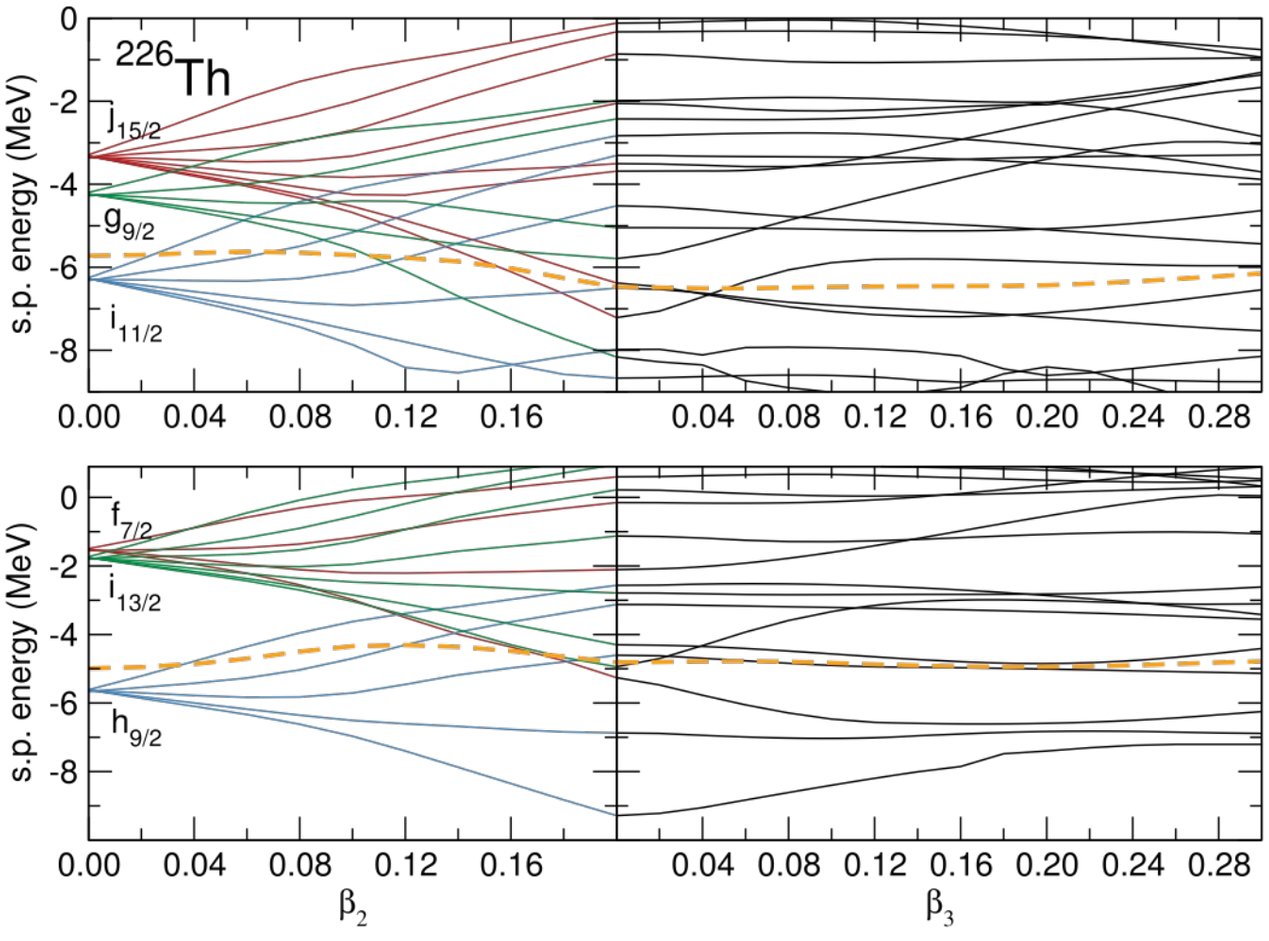
→ includes static correlations: deformations & pairing

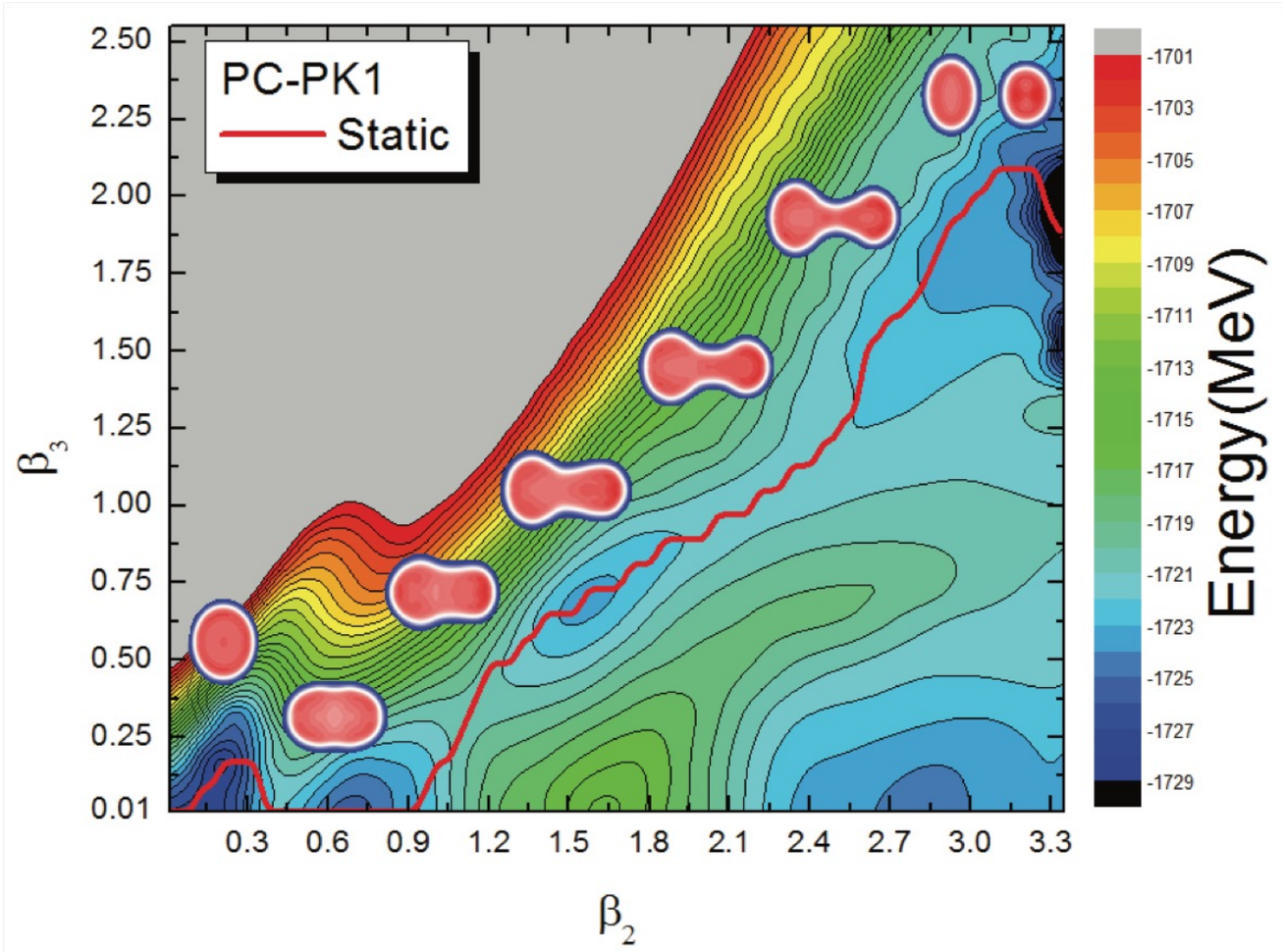
→ does not include dynamic (collective) correlations that arise from symmetry restoration and quantum fluctuations around mean-field minima

PC-PK1 plus δ-force pairing


^{226}Th
β_3
β_2


Theory
^{226}Th
Experiment
Energy (MeV)
4^+
2^+
10^+
9^-
0^+
8^+
7^-
6^+
5^-
3^-
4^+
1^-
2^+
0^+

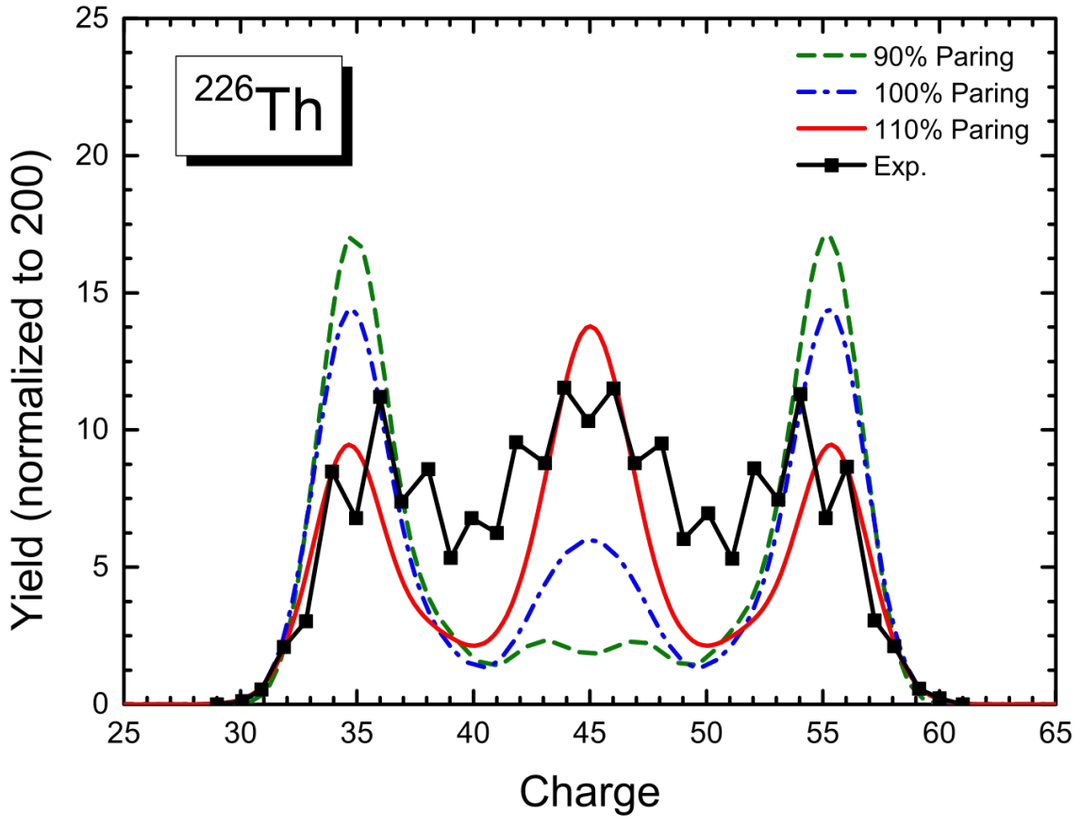

^{226}Th
$j_{15/2}$
$g_{9/2}$
$i_{11/2}$
$f_{7/2}$
$i_{13/2}$
$h_{9/2}$
s.p. energy (MeV)
β_2
β_3



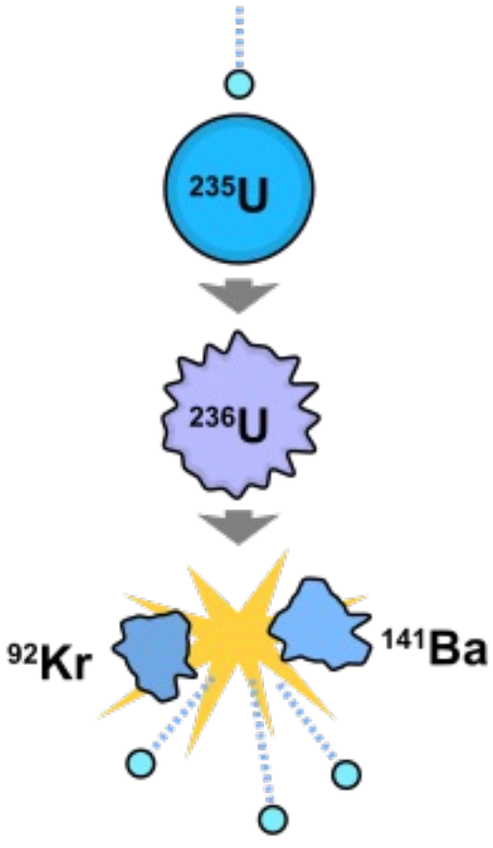
A triple-humped fission barrier is predicted along the static fission path, and the calculated heights are **7.10, 8.58, and 7.32 MeV** from the inner to the outer barrier.

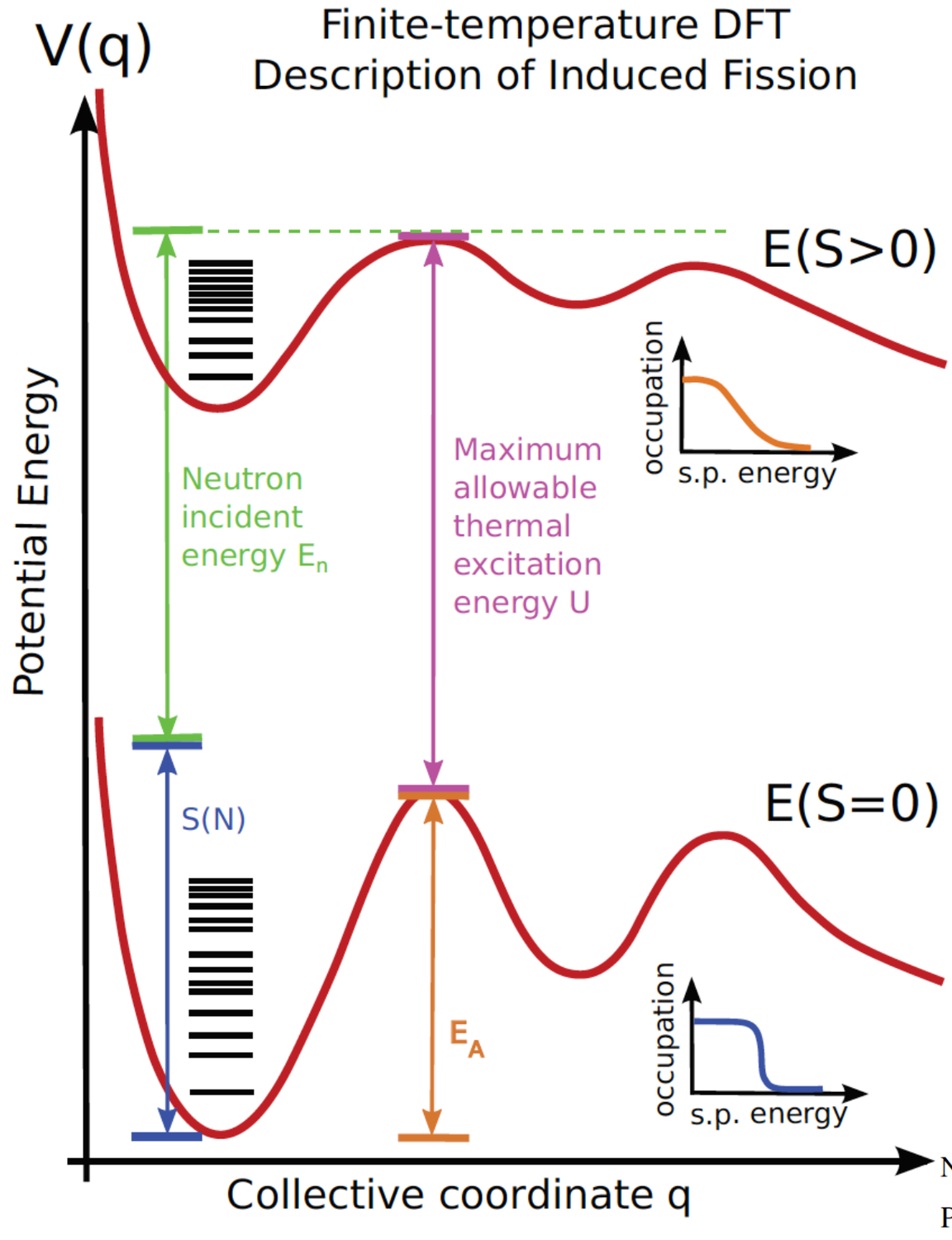
The height of the fission barriers (in MeV) with respect to the corresponding ground-state minima:

	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:

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

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

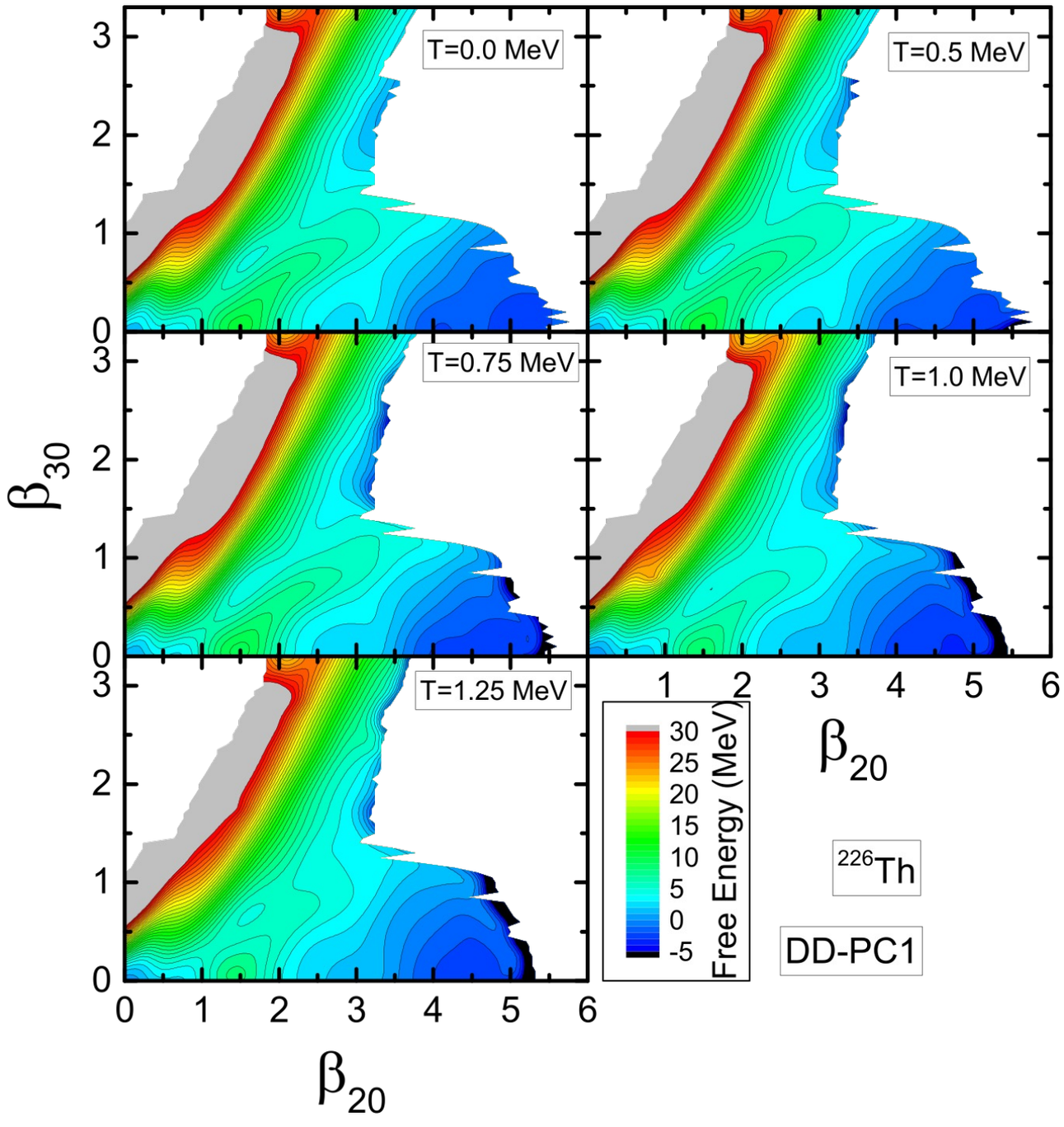
Helmholtz free energy: $F = E(T) - TS$

… 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:

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

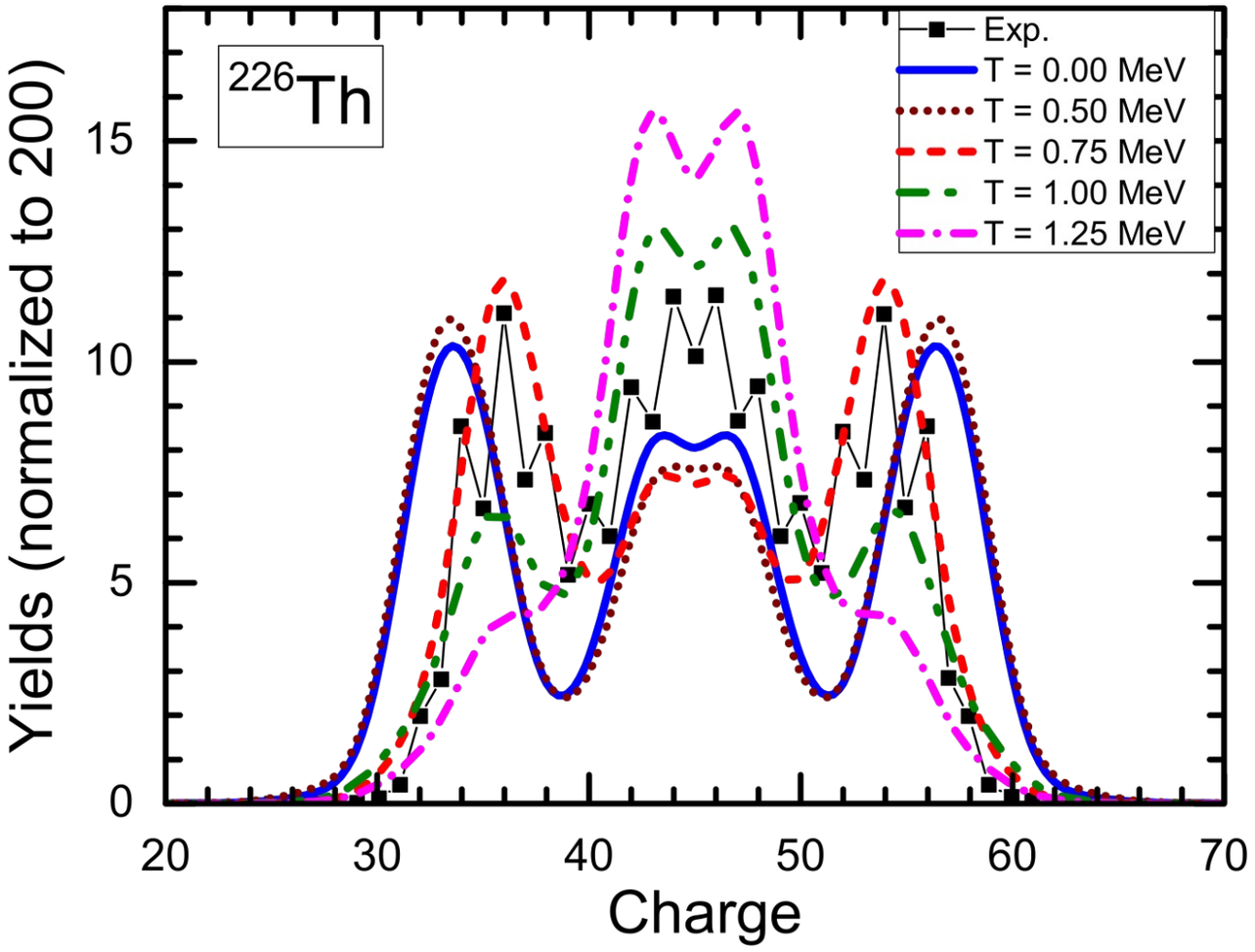


Dynamics of induced fission

Zhao, Nikšić, Vretenar, Zhou

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

Charge yields:



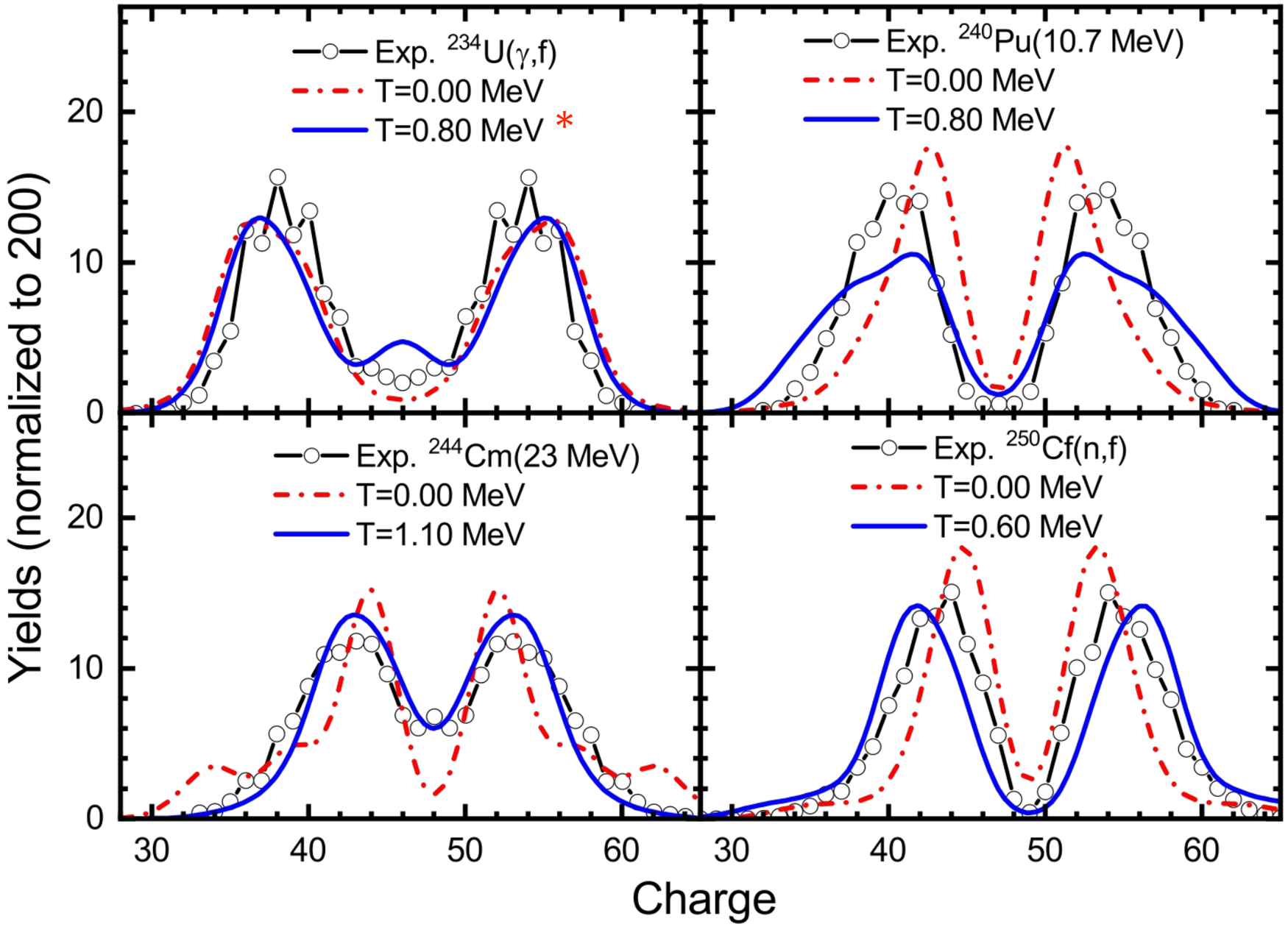
Experimental results ➠ photoinduced fission with photon energies in the interval 8 − 14 MeV, and a peak value Eγ = 11 MeV.

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

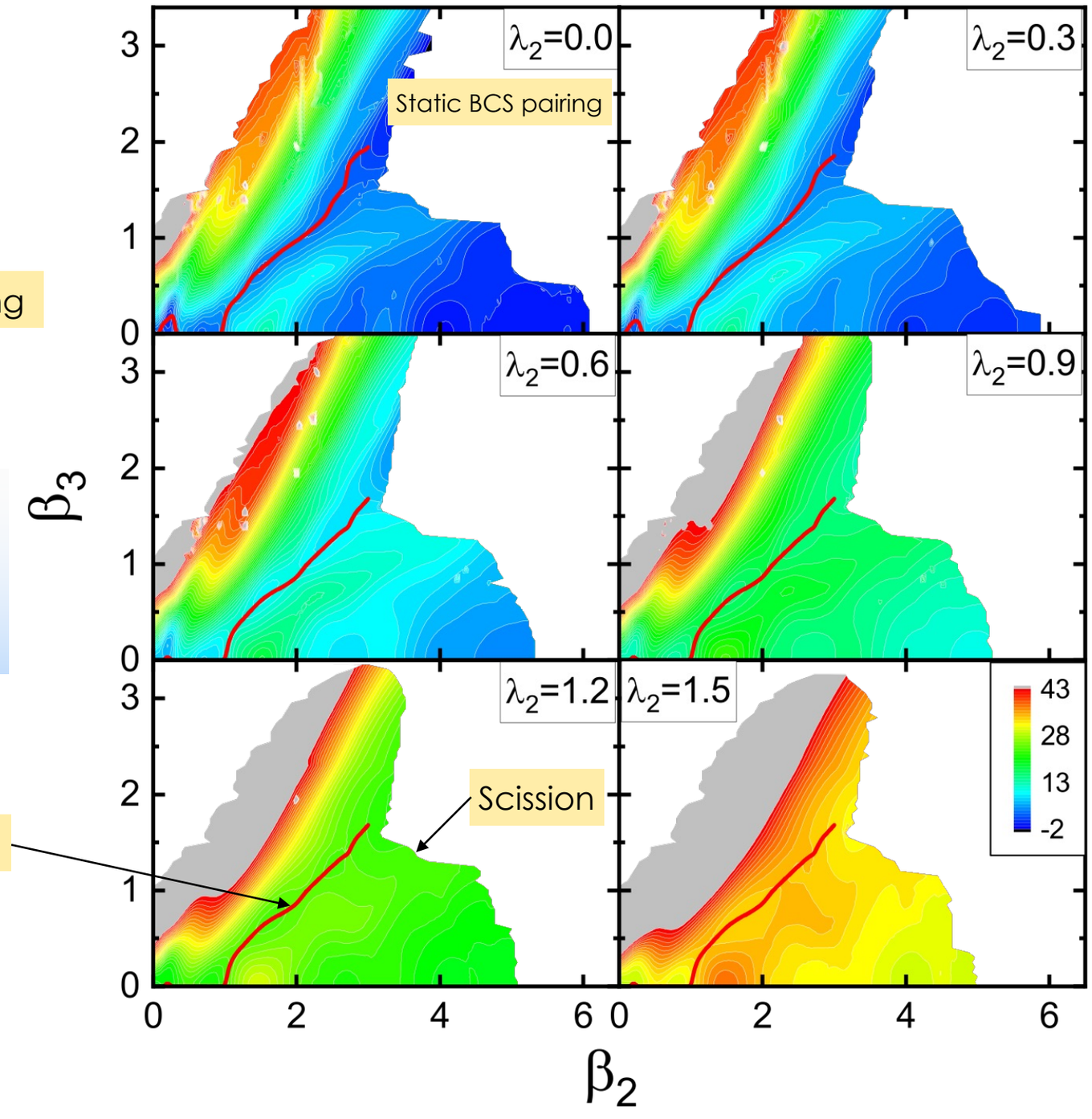
… the Routhian:

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

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.

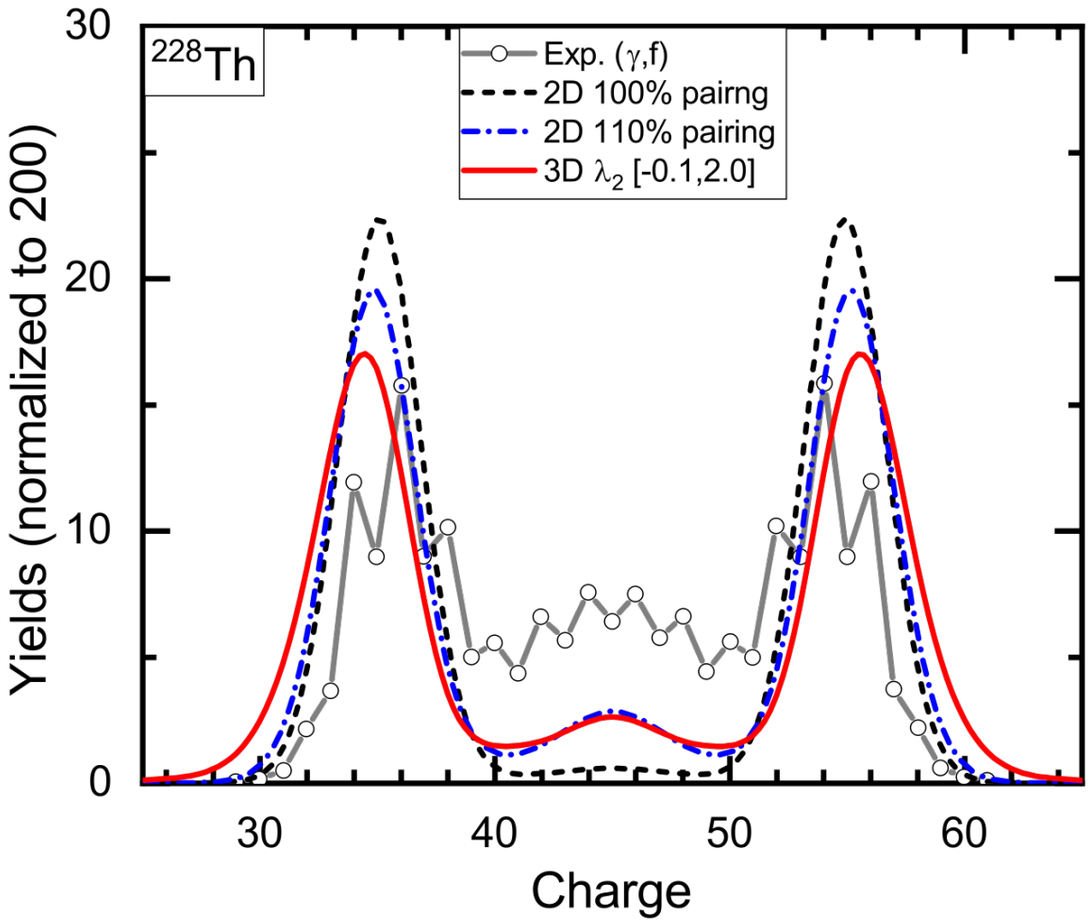
Static fission path of minimum energy



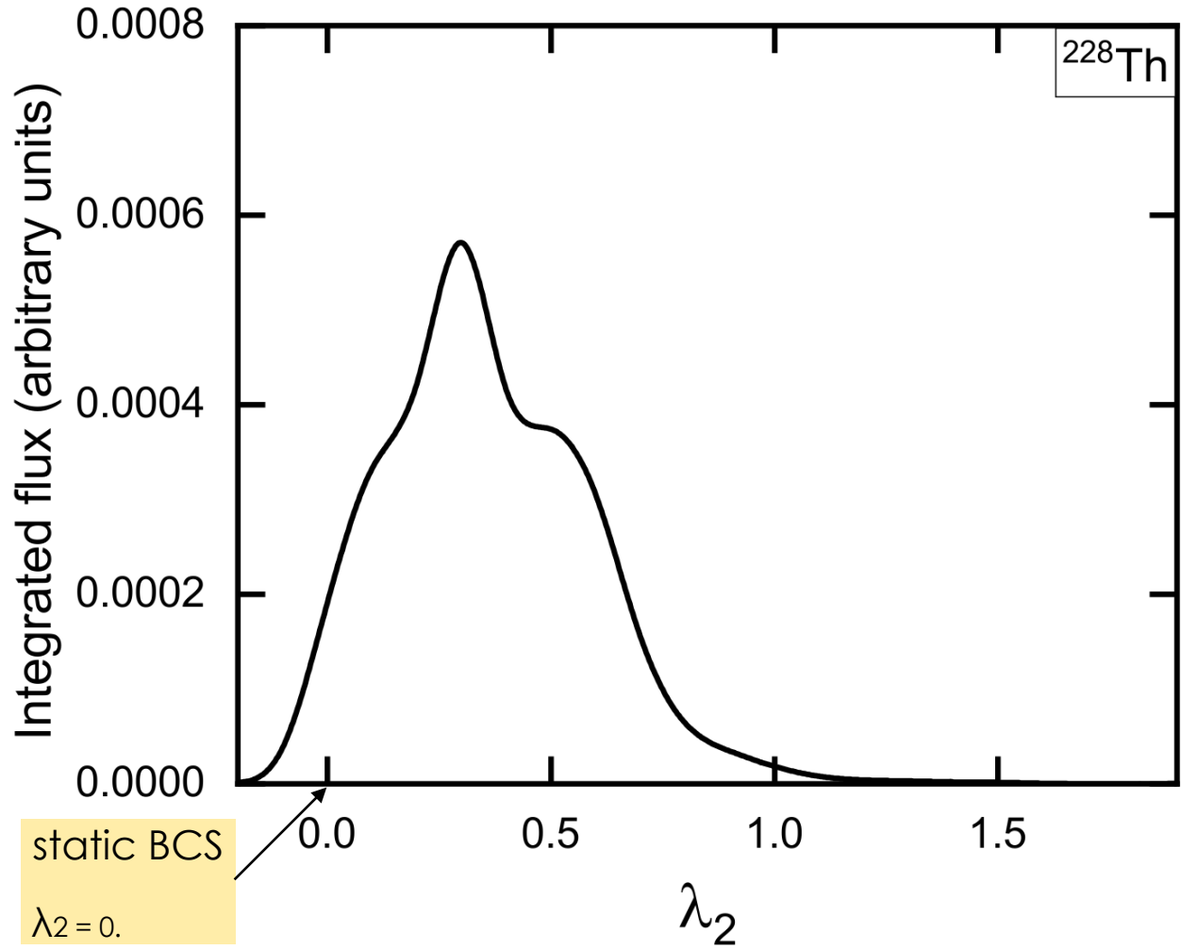
3D TDGCM+GOA calculation

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

q≡{β2,β3,λ2}



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



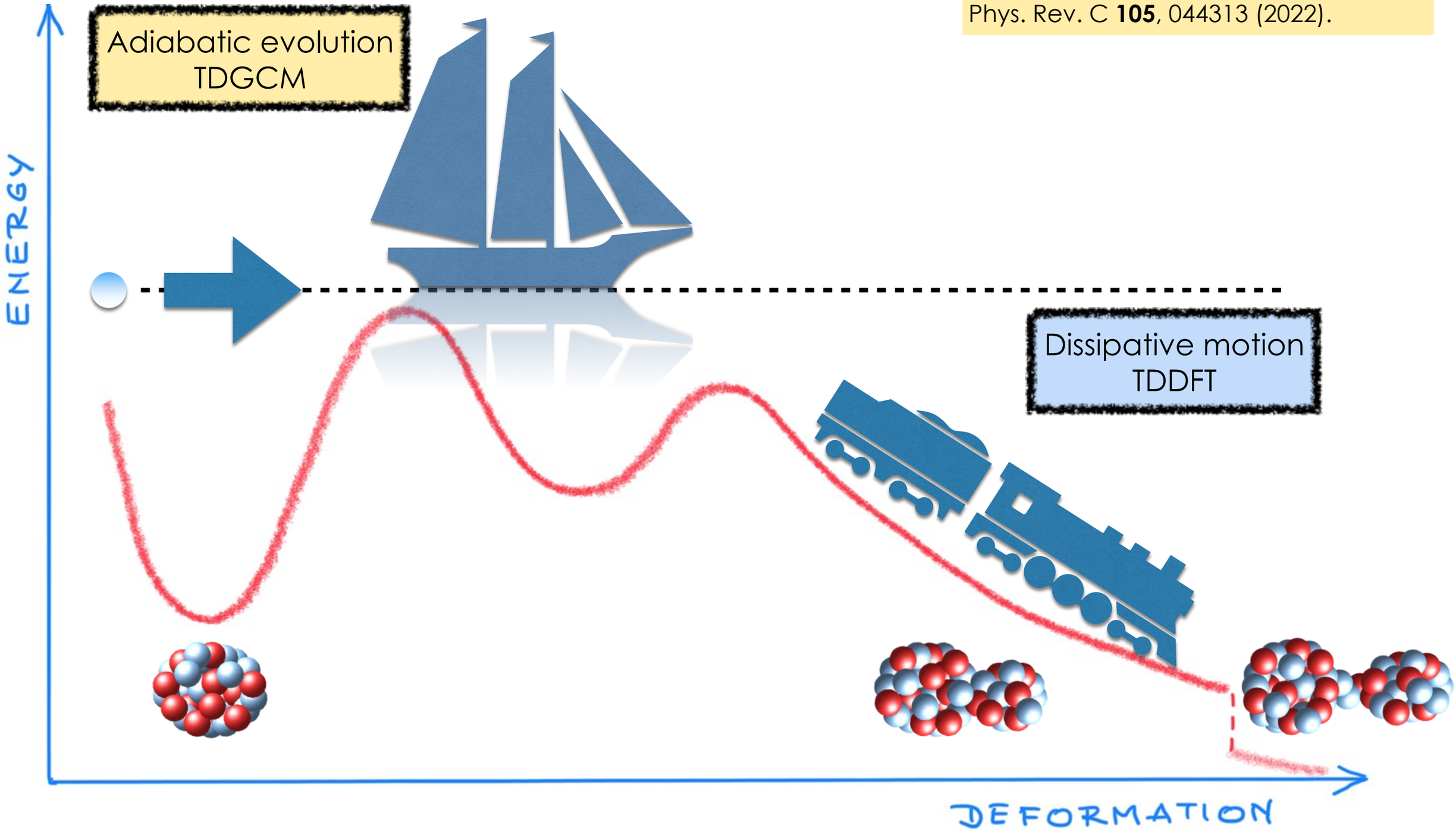
Effect of dynamical pairing on the flux of the probability current through the scission hyper-surface:

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

→ 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)

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

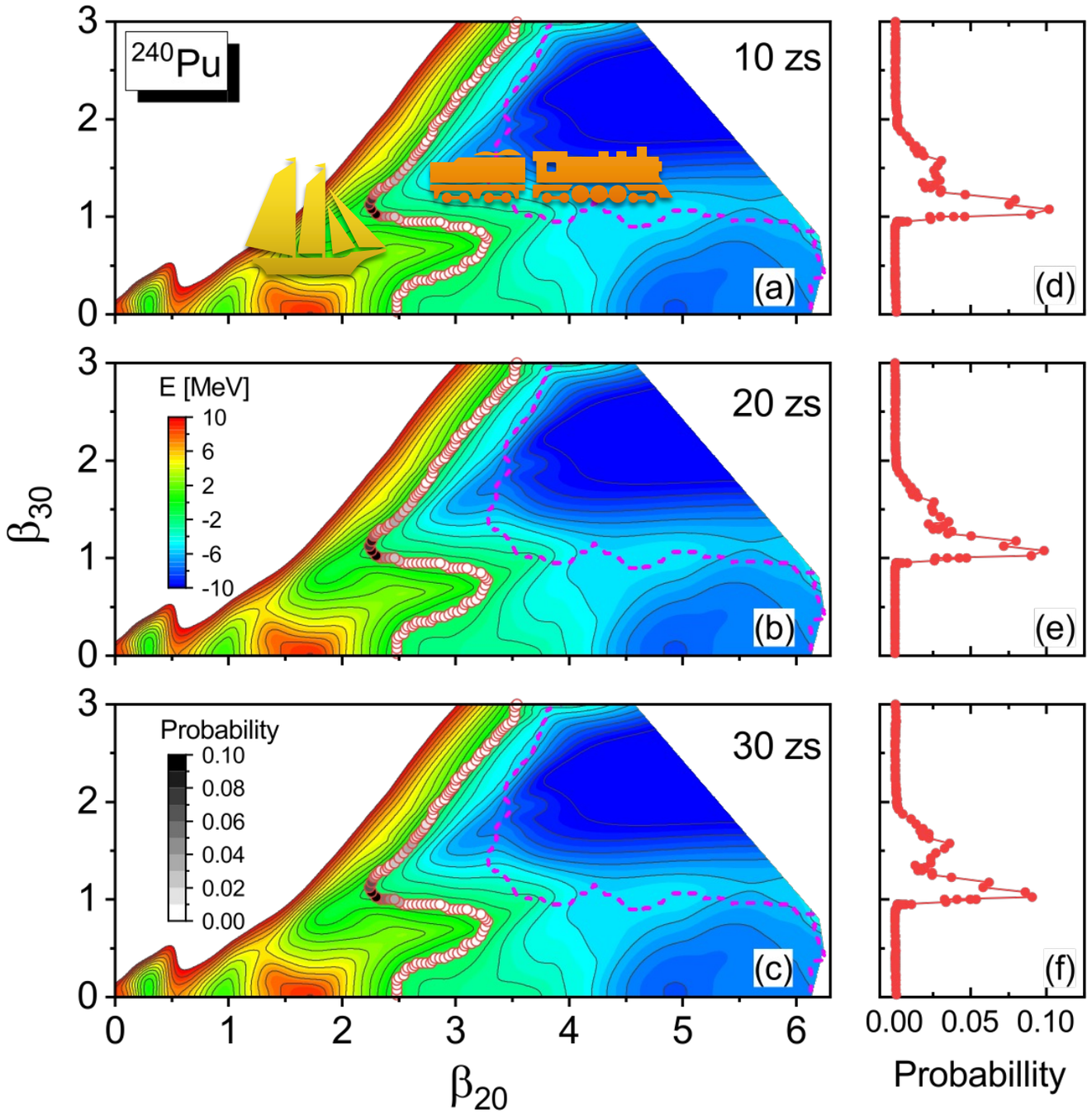
$$i\frac{d}{dt}n_k(t) = n_k(t)\Delta_k^*(t) - n_k^*(t)\Delta_k(t),$$

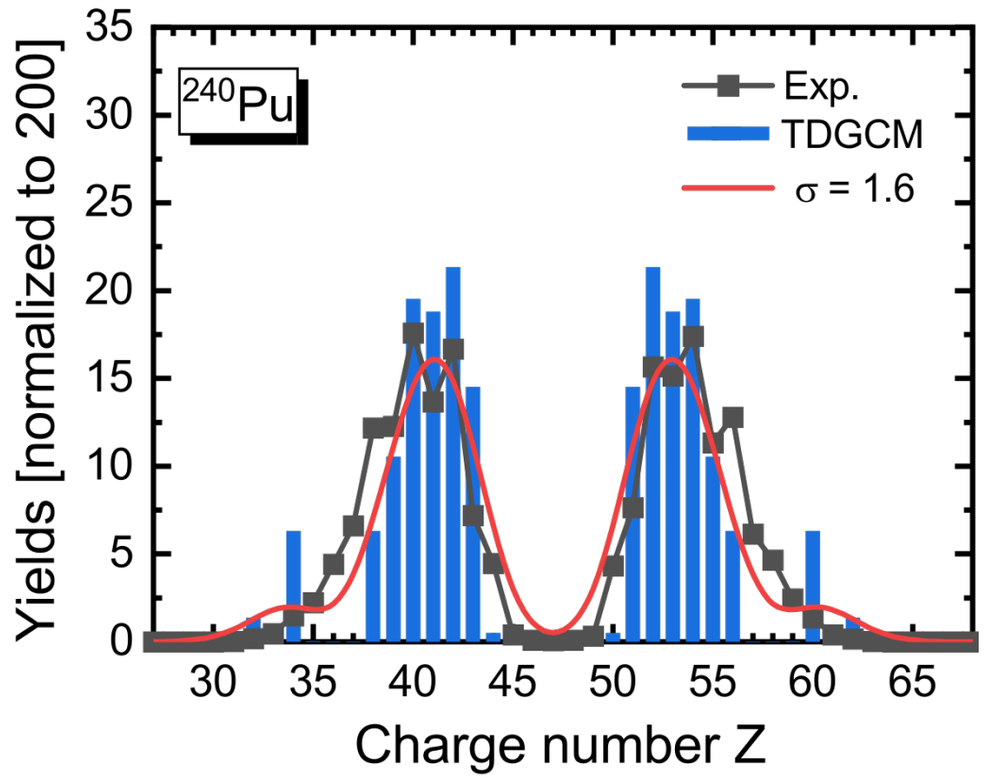
$$i\frac{d}{dt}\kappa_k(t) = [\varepsilon_k(t) + \varepsilon_{\bar{k}}(t)]\kappa_k(t) + \Delta_k(t)[2n_k(t) - 1].$$

⇒ 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.

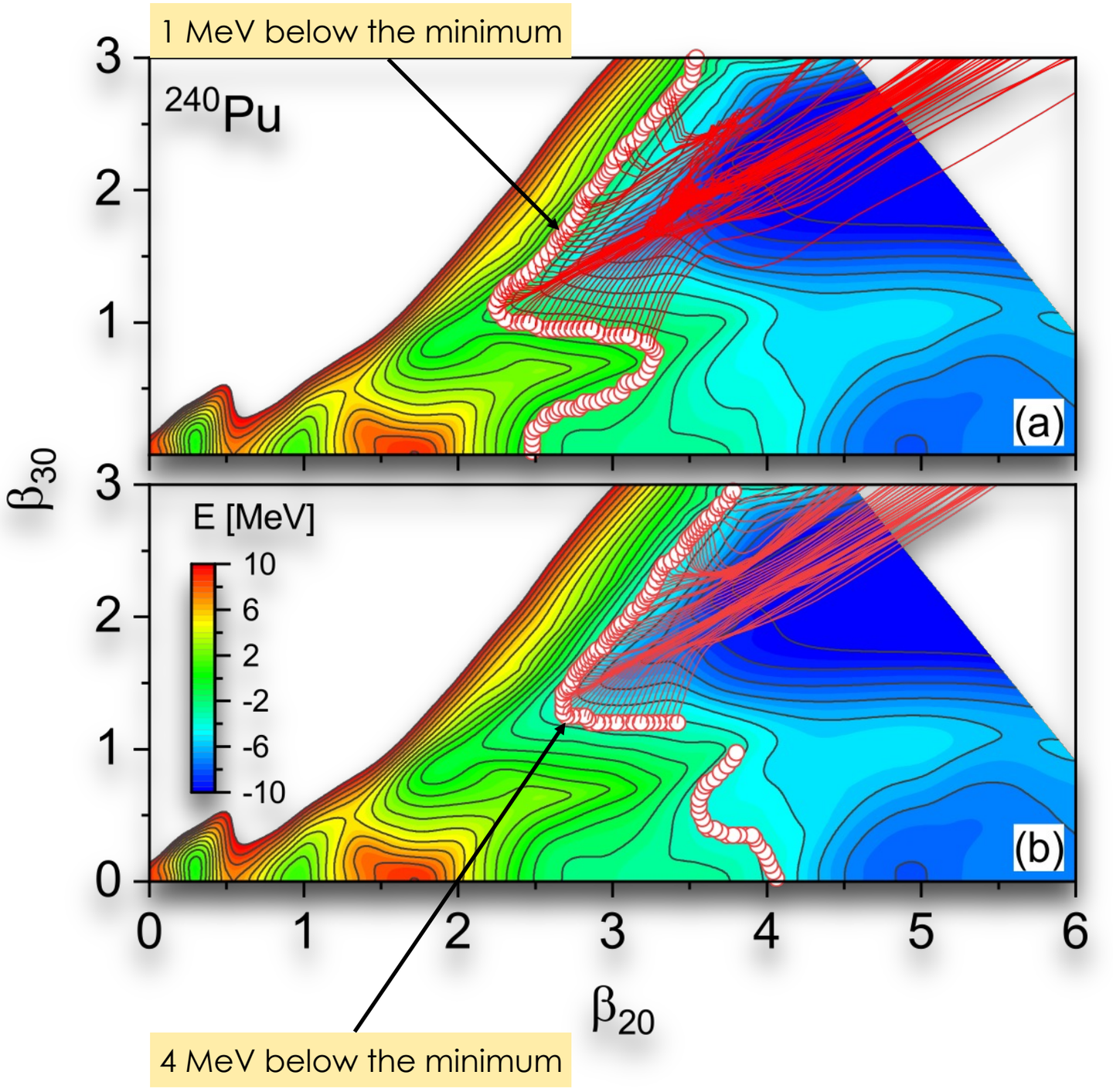
Negele et al. (1978) ➟ use an adiabatic model for the time interval in which the fissioning nucleus evolves from the quasi-stationary initial state to the saddle point, and a non-adiabatic method for the saddle-to-scission and beyond-scission dynamics.

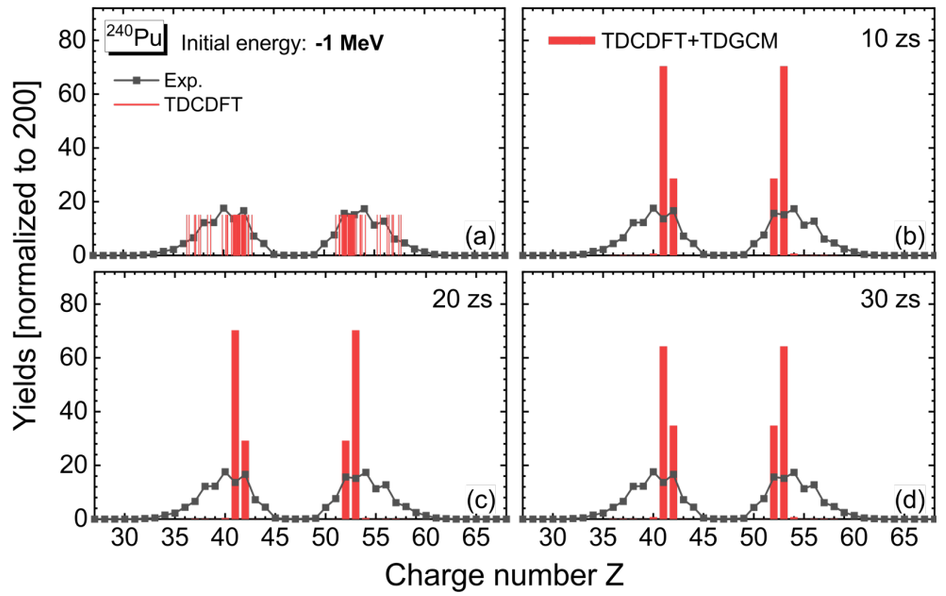


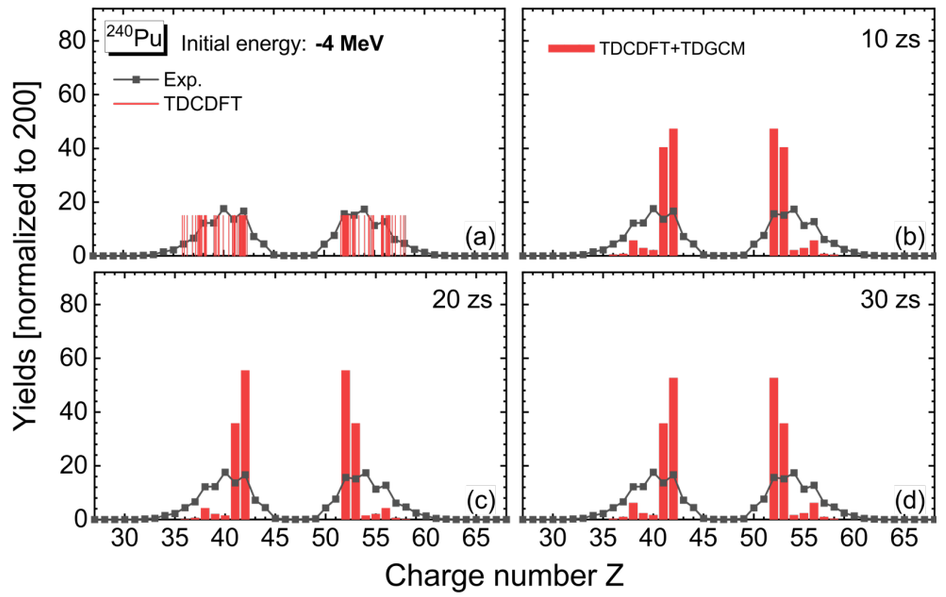


Ren, Zhao, Vretenar, Nikšić, Zhao, Meng
Phys. Rev. C **105**, 044313 (2022).

TDDFT fission trajectories







Total kinetic energies (TKEs) of the fragments

TDGCM+GOA

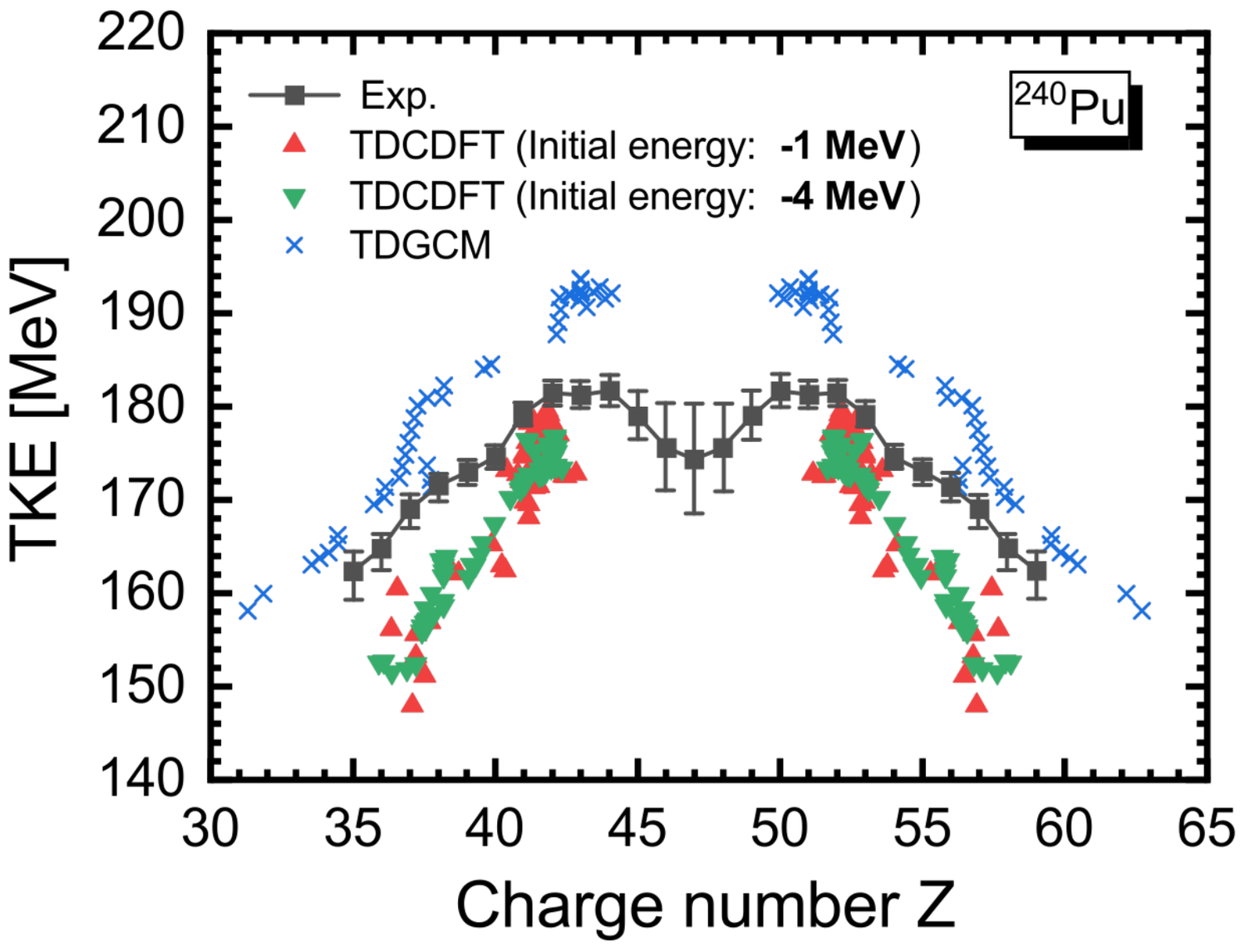
$$E_{\mathrm{TKE}} = \frac{e^2 Z_H Z_L}{d_{\mathrm{ch}}},$$

$\rightarrow$ 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)



Extended TDGCM - dissipation effects

Zhao, Nikšić, Vretenar

Phys. Rev. C **105**, 054604 (2022).

Extended TDGCM many-body wave function: $|\Phi(t)\rangle = \sum_n \int d\boldsymbol{q} f_n(\boldsymbol{q}, t) \, |n\boldsymbol{q}\rangle$

… excited states at each value of the collective coordinate **q**

⇒ the matrix integral Hill-Wheeler equation:

$$\sum_{n'} \int d\boldsymbol{q}' \left\{ \mathcal{H}_{nn'}(\boldsymbol{q}, \boldsymbol{q}') f_{n'}(\boldsymbol{q}', t) - \mathcal{N}_{nn'}(\boldsymbol{q}, \boldsymbol{q}') \left[i\hbar \partial_t f_{n'}(\boldsymbol{q}', t) \right] \right\} = 0$$

… the level density for each value of **q** is high even at low excitation energies ⇒ the discrete label *n* can be separ

$$\sum_{\lambda, \text{ fixed } \epsilon} = \rho(\boldsymbol{q}, \epsilon) d\epsilon,$$

statistical collective wave function

$$i\hbar \frac{\partial}{\partial t} \psi(\boldsymbol{q}, \epsilon; t) = \int d\boldsymbol{q}' h(\boldsymbol{q}, \boldsymbol{q}'; \epsilon, \epsilon) \psi(\boldsymbol{q}', \epsilon; t) + \sum_{\lambda' \neq \lambda} \int \int d\boldsymbol{q}' d\epsilon' h(\boldsymbol{q}, \boldsymbol{q}'; \epsilon, \epsilon') \psi(\boldsymbol{q}', \epsilon'; t),$$

… expansion of the Hamiltonian kernel in a power series in collective momenta: $\boldsymbol{P} = -i\hbar(\partial/\partial \boldsymbol{q})$,

$$i\hbar\partial_t\psi(\boldsymbol{q},\epsilon;t) = \left[V(\boldsymbol{q},\epsilon) + \boldsymbol{P}\frac{1}{2\mathcal{M}(\boldsymbol{q},\epsilon)}\boldsymbol{P}\right]\psi(\boldsymbol{q},\epsilon;t) + \frac{i}{2}\int\{\boldsymbol{P},\boldsymbol{\eta}(\boldsymbol{q};\epsilon,\epsilon')\}\,\psi(\boldsymbol{q},\epsilon';t)d\epsilon'.$$

…dissipation function: $\boldsymbol{\eta}(\boldsymbol{q};\epsilon,\epsilon') = h^{(1)}(\boldsymbol{q};\epsilon,\epsilon')/\hbar$

… excitation energy → nuclear temperature $\eta(\boldsymbol{q};T,T') \equiv \eta(\boldsymbol{q};\epsilon(T),\epsilon(T'))$

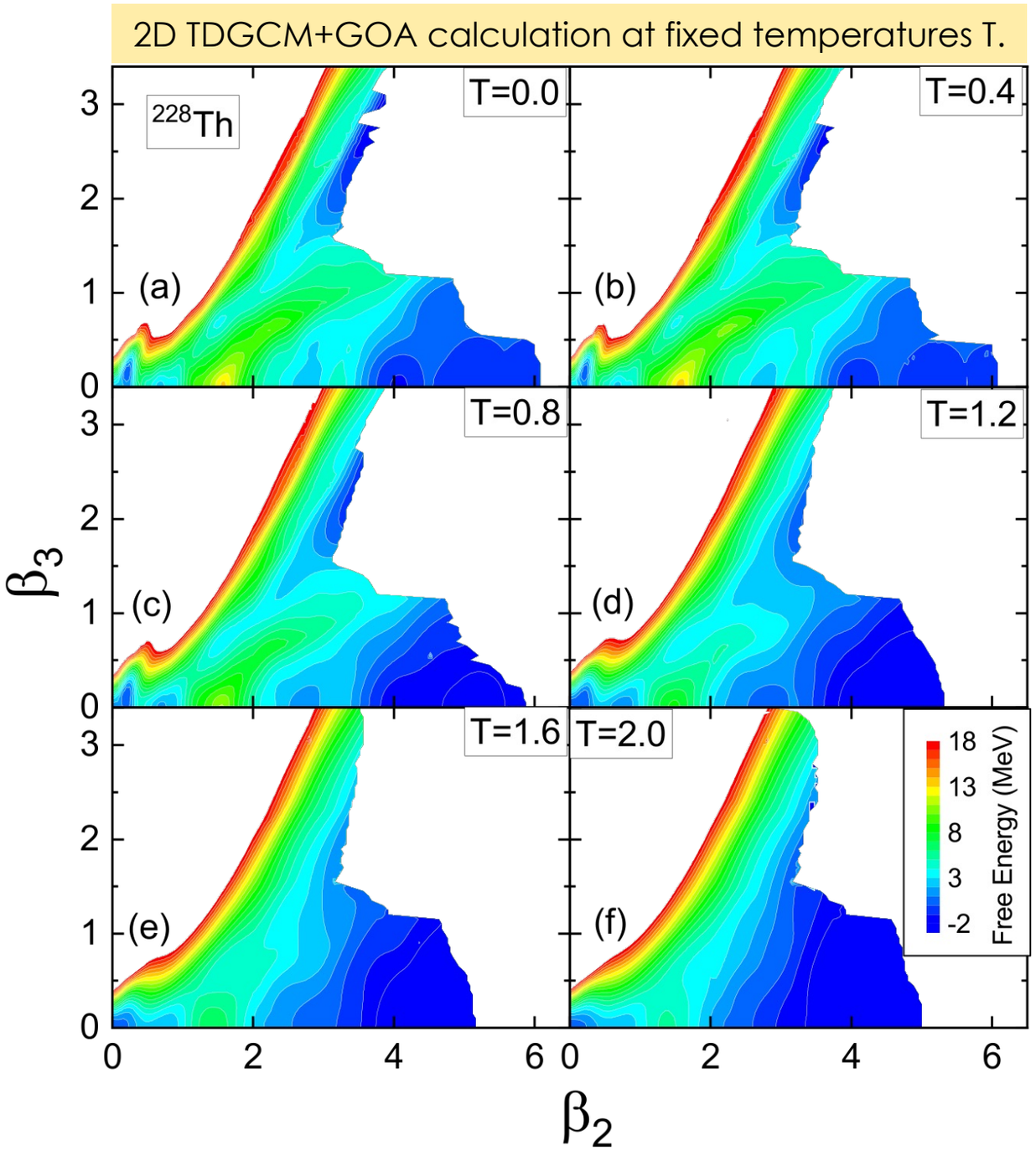
Extended TDGCM

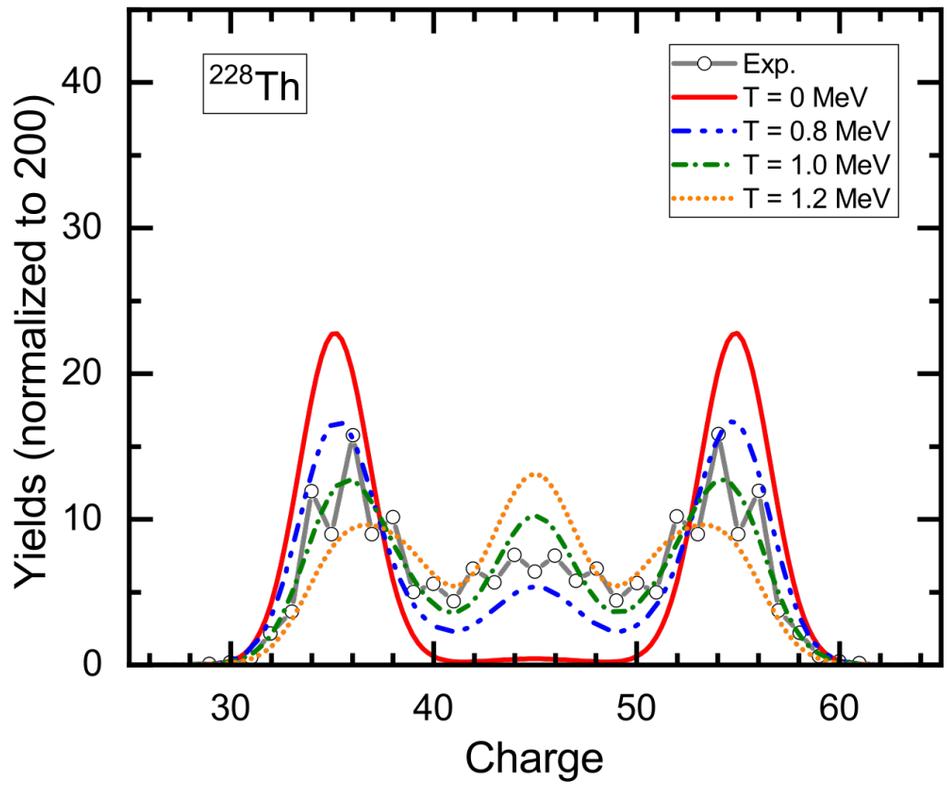
$$i\hbar\partial_t\psi(\boldsymbol{q},T;t) = \left[V(\boldsymbol{q},T) + \boldsymbol{P}\frac{1}{2\mathcal{M}(\boldsymbol{q},T)}\boldsymbol{P}\right]\psi(\boldsymbol{q},T;t) + \frac{i}{2}\int\{\boldsymbol{P},\boldsymbol{\mathcal{O}}(\boldsymbol{q};T,T')\}\,\psi(\boldsymbol{q},T';t)dT',$$

$$\boldsymbol{\mathcal{O}}(\boldsymbol{q};T,T') = \boldsymbol{\eta}(\boldsymbol{q};T,T')d\epsilon(T)/dT.$$

ILLUSTRATIVE CALCULATION: INDUCED FISSION DYNAMICS OF ^{228}Th

2D TDGCM+GOA calculation at fixed temperatures T.

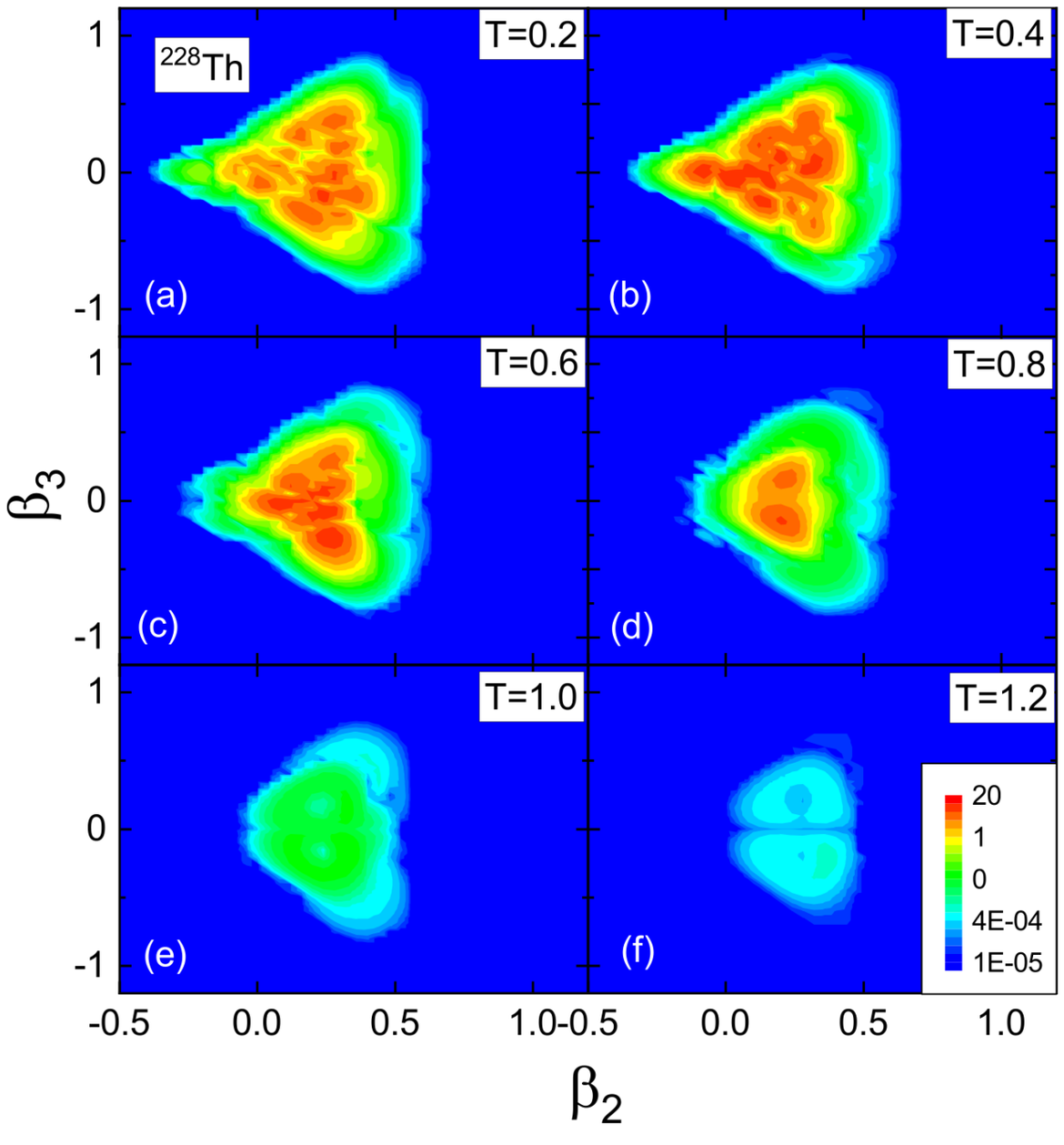




The data for photo-induced fission correspond to photon energies in the interval 8 − 14 MeV, and a peak value of E_γ = 11 MeV.

3D calculation of fission dynamics of ^{228}Th in the space of axial shape variables (β_2, β_3) and temperature T

2D projections on the (β_2, β_3) plane of the probability distribution of the initial wave packet, at different T. The excitation energy of the initial state is $E^* = 11$ MeV.



The collective potential:

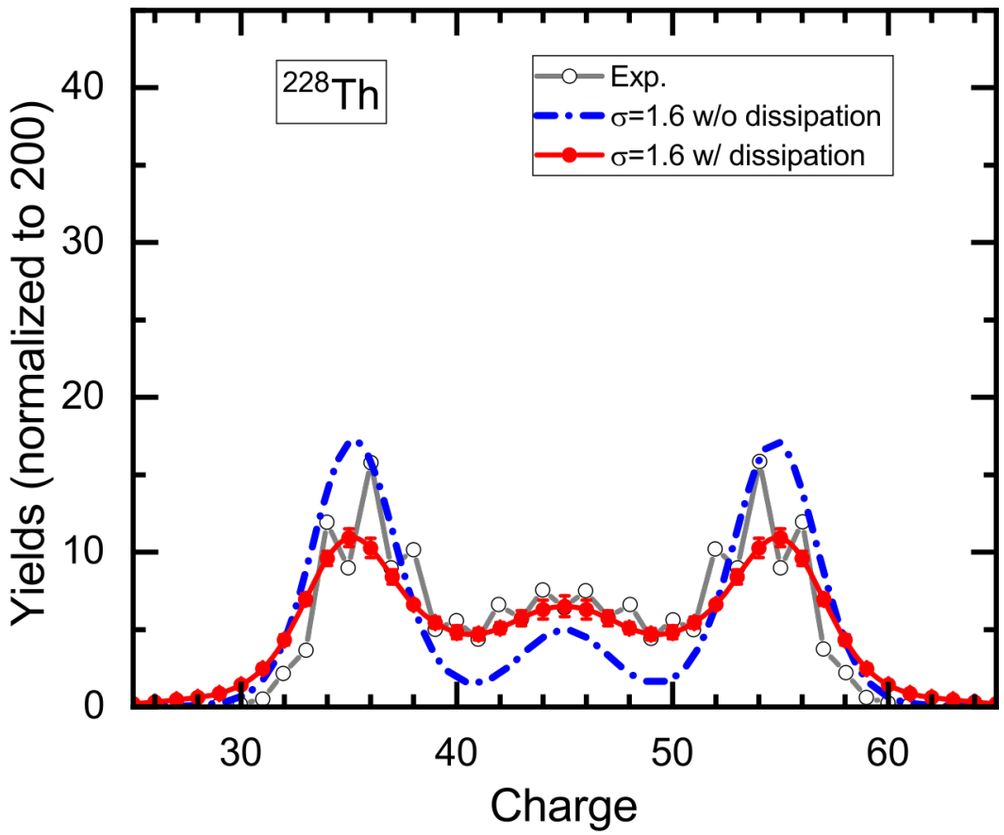
$$V(\boldsymbol{q}, T) = \epsilon(T) + F(\boldsymbol{q}, T)$$

The dissipation function:

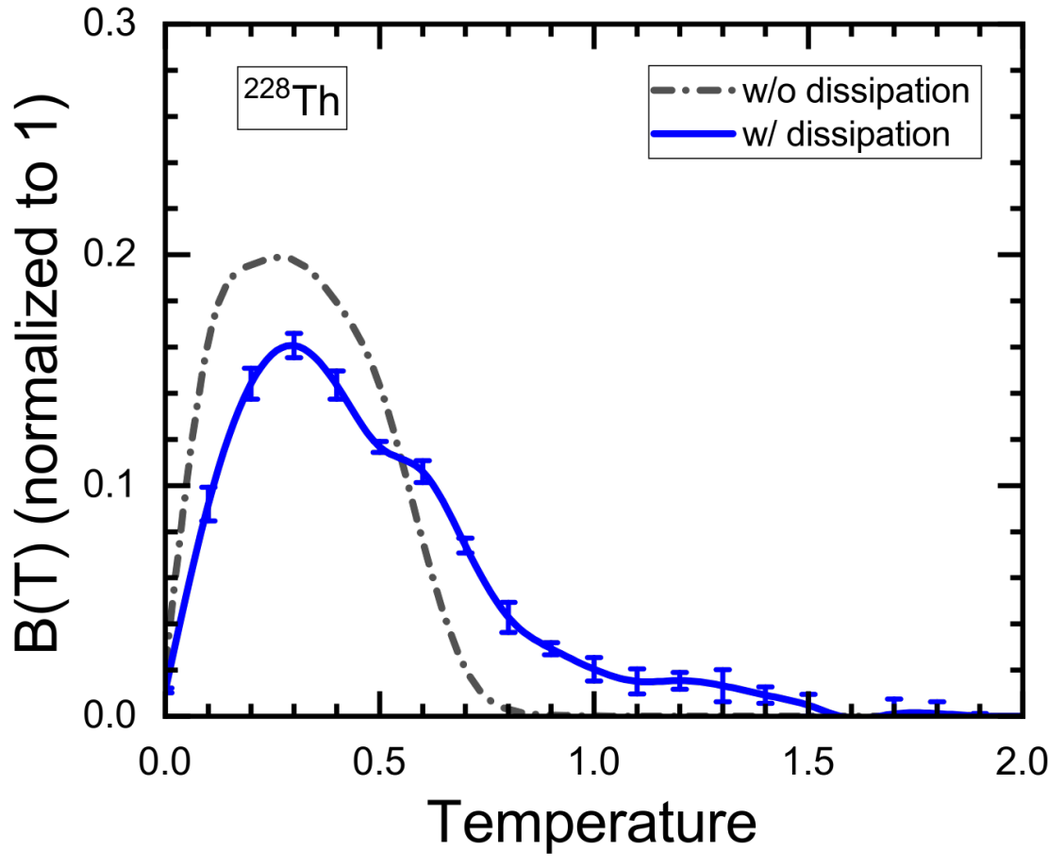
$$\boldsymbol{\eta}(\boldsymbol{q}; T, T') = \begin{cases} 0 & \beta_2 < \beta_2^0 \\ \boldsymbol{\eta}(T, T') & \beta_2 \geq \beta_2^0, \end{cases}$$

Gaussian random variables

3D extended TDGCM charge yields.

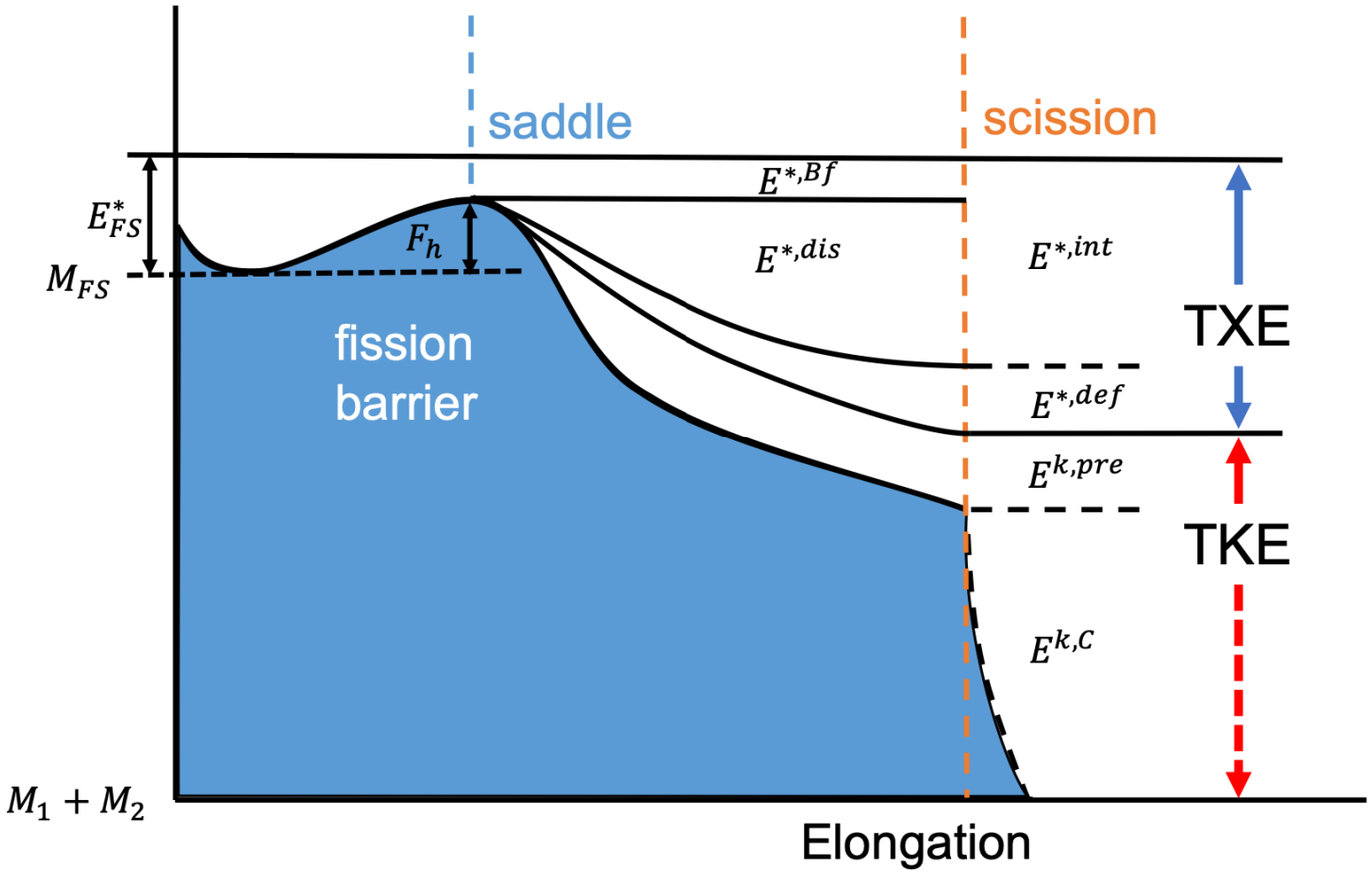


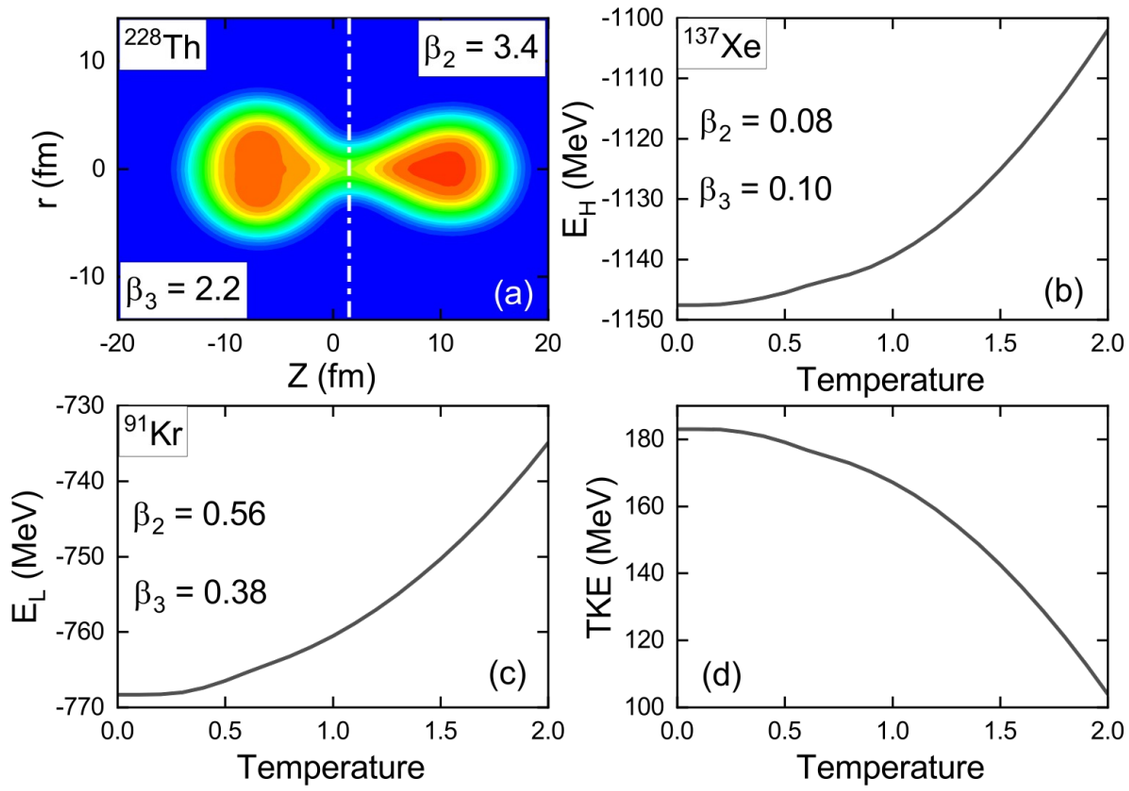
Time-integrated collective flux B(T) through the scission contour, as a function of temperature.



Total Kinetic Energy Distribution

Zhao, Nikšić, Vretenar, arXiv:2210.00460





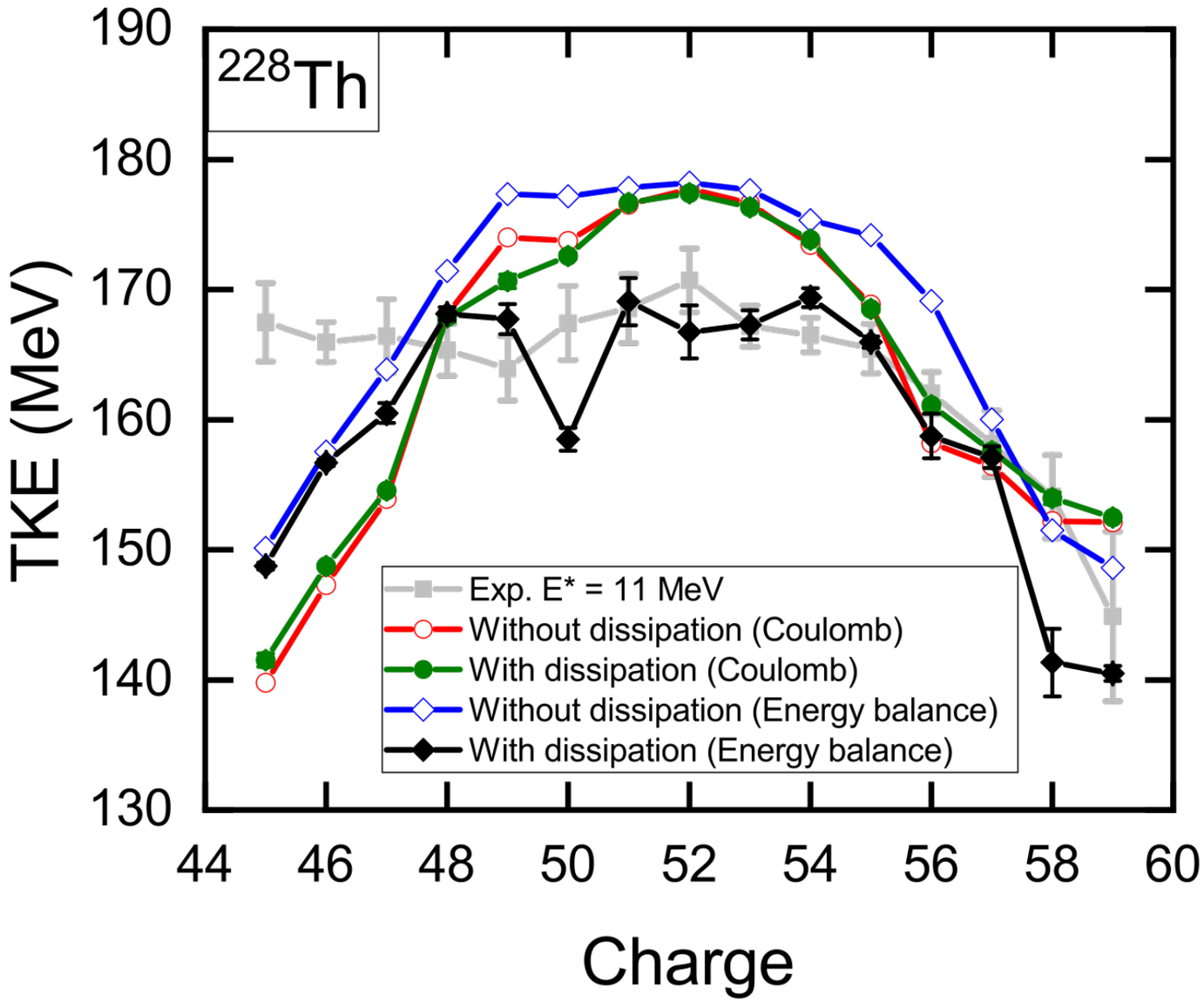
$$\mathrm{TKE}(\xi) = (E_{\mathrm{B}}^{\mathrm{FS}} + E_{\mathrm{coll}}^{*}) - \left[E^{L}(\beta_2^{L}, \beta_3^{L}, T) + E^{H}(\beta_2^{H}, \beta_3^{H}, T)\right]$$

The integrated flux F (ξ; t) for a given scission surface element ξ is defined:

$$F(\xi; t) = \int_{t_0}^{t} dt' \int_{(\boldsymbol{q},T)\in\xi} \boldsymbol{J}(\boldsymbol{q}, T; t') \cdot d\boldsymbol{S},$$

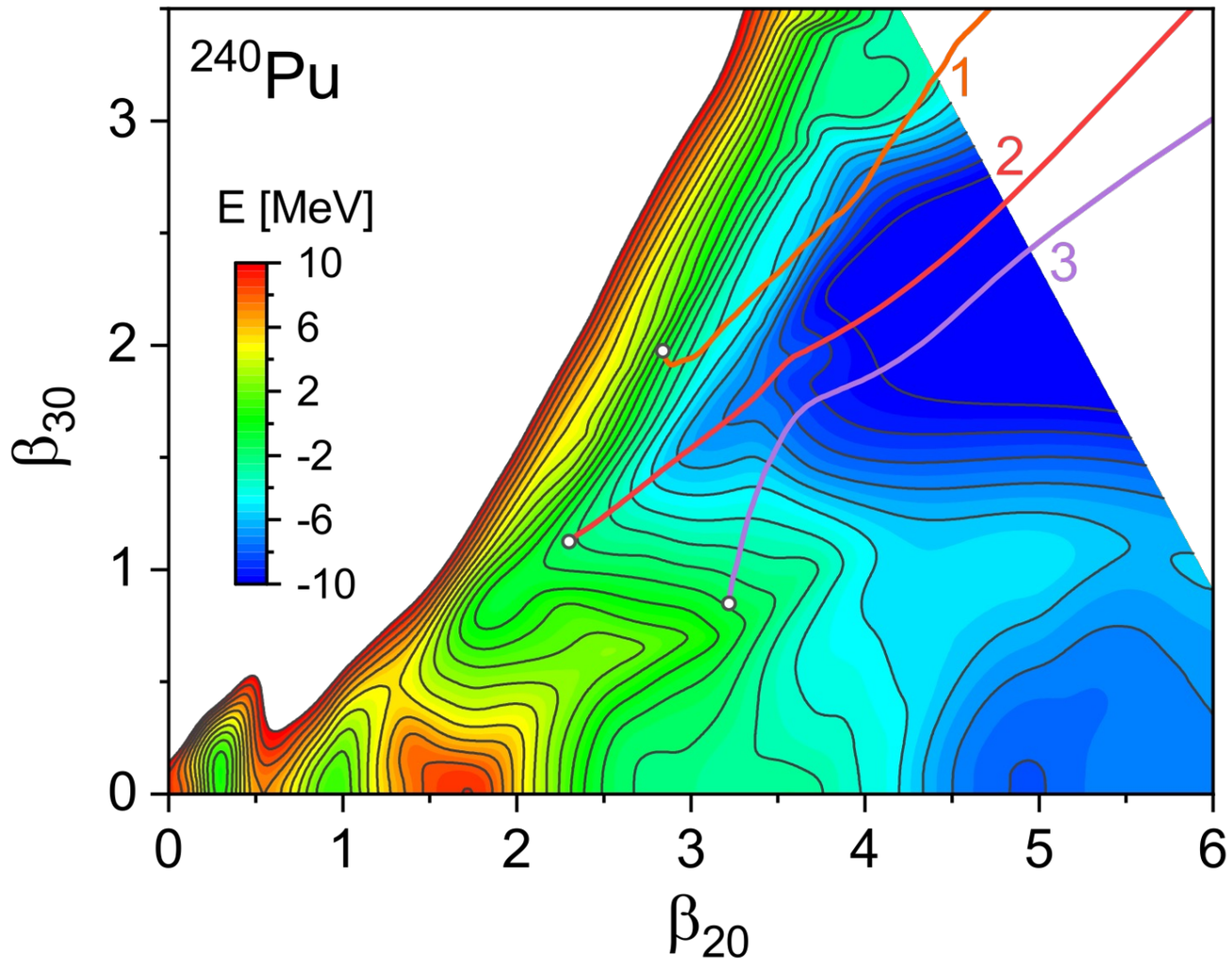
The TKE for the fission fragment with mass A is defined by:

$$\mathrm{TKE(A)} = \lim_{t\to\infty} \frac{\sum_{\xi\in\mathcal{A}} \mathrm{F}(\xi;t)\mathrm{TKE}(\xi)}{\sum_{\xi\in\mathcal{A}} \mathrm{F}(\xi;t)}.$$

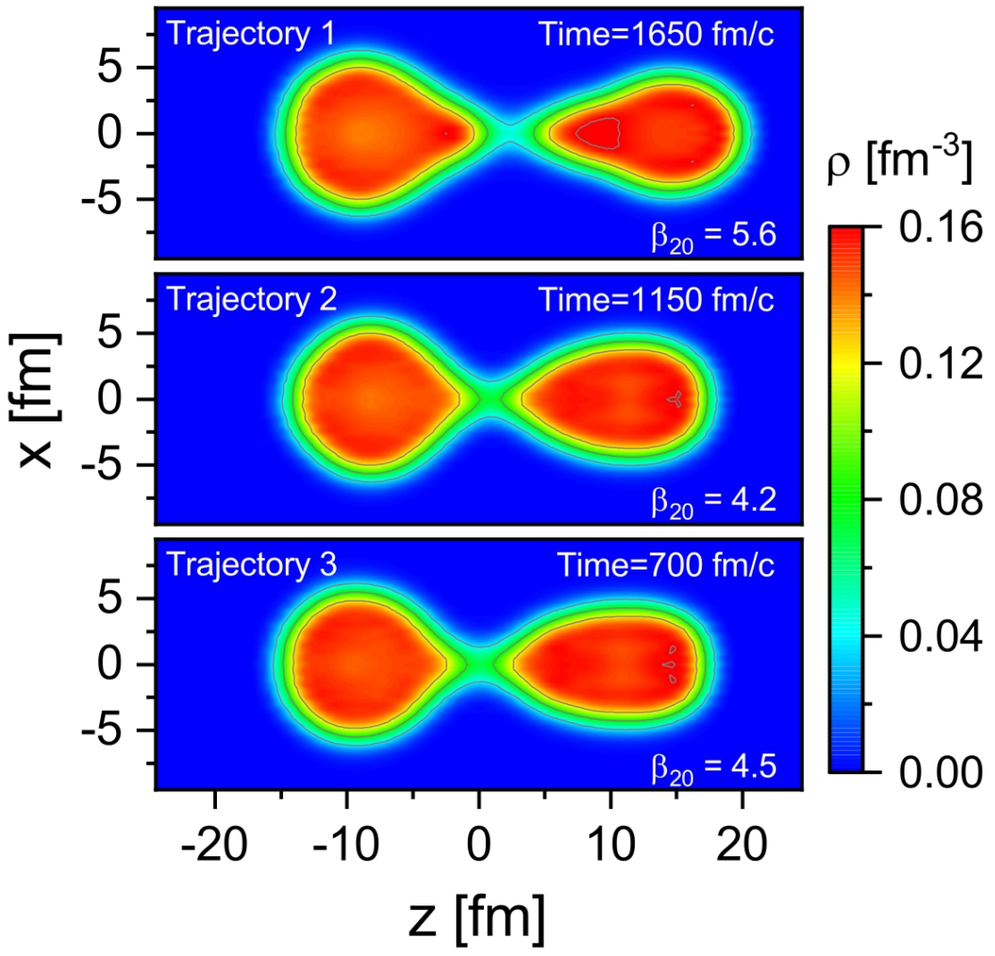


Dynamical synthesis of ^{4}He in the scission phase of nuclear fission

TDDFT fission trajectories



Density profiles at times immediately prior to the scission event.



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Nucleon localization functions:

kinetic energy density — density — current density

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

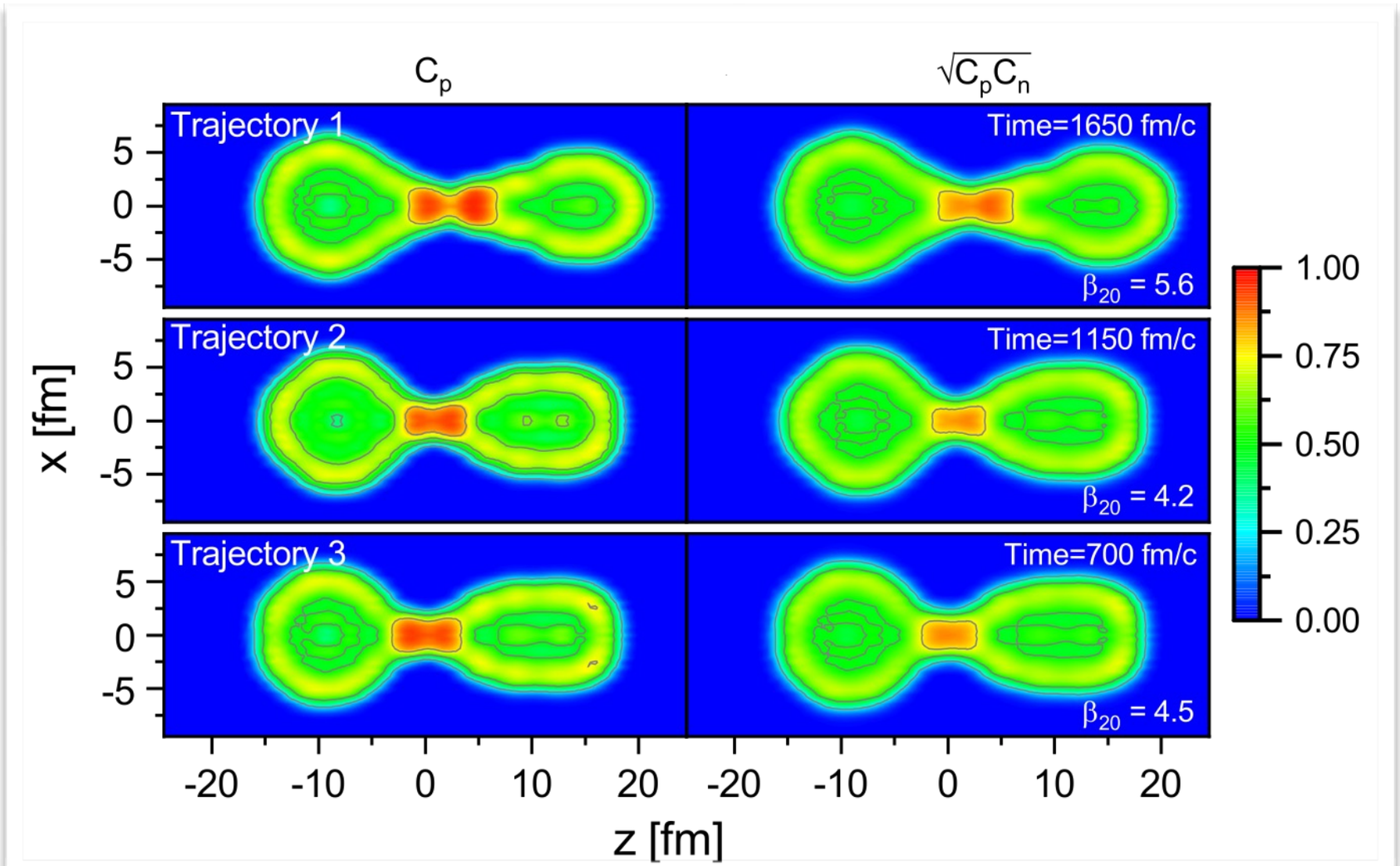
σ ($\uparrow$ or $\downarrow$)

q (n or p)

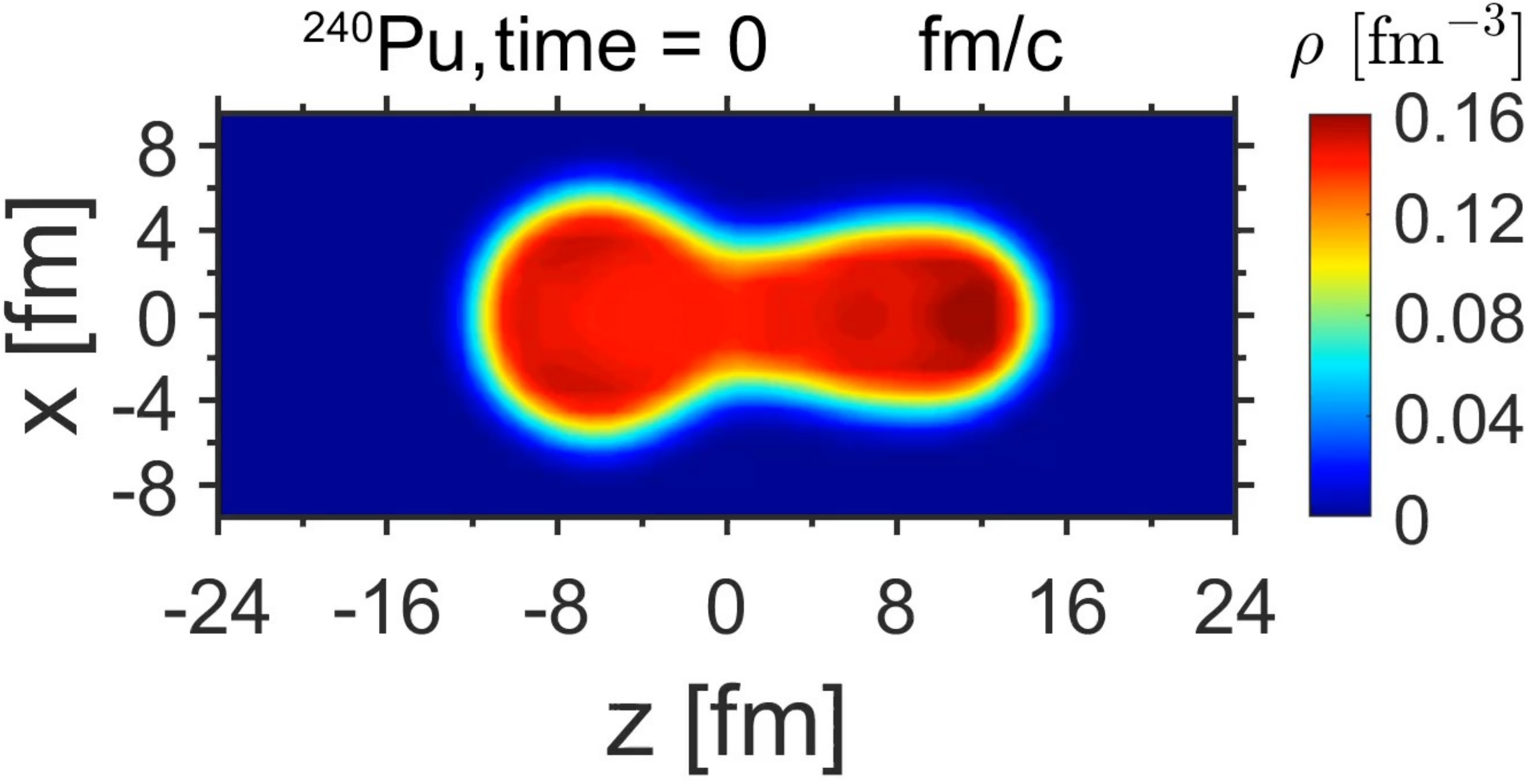
$$\tau^{\mathrm{TF}}_{q\sigma} = \tfrac{3}{5}(6\pi^2)^{2/3}\rho^{5/3}_{q\sigma}$$

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



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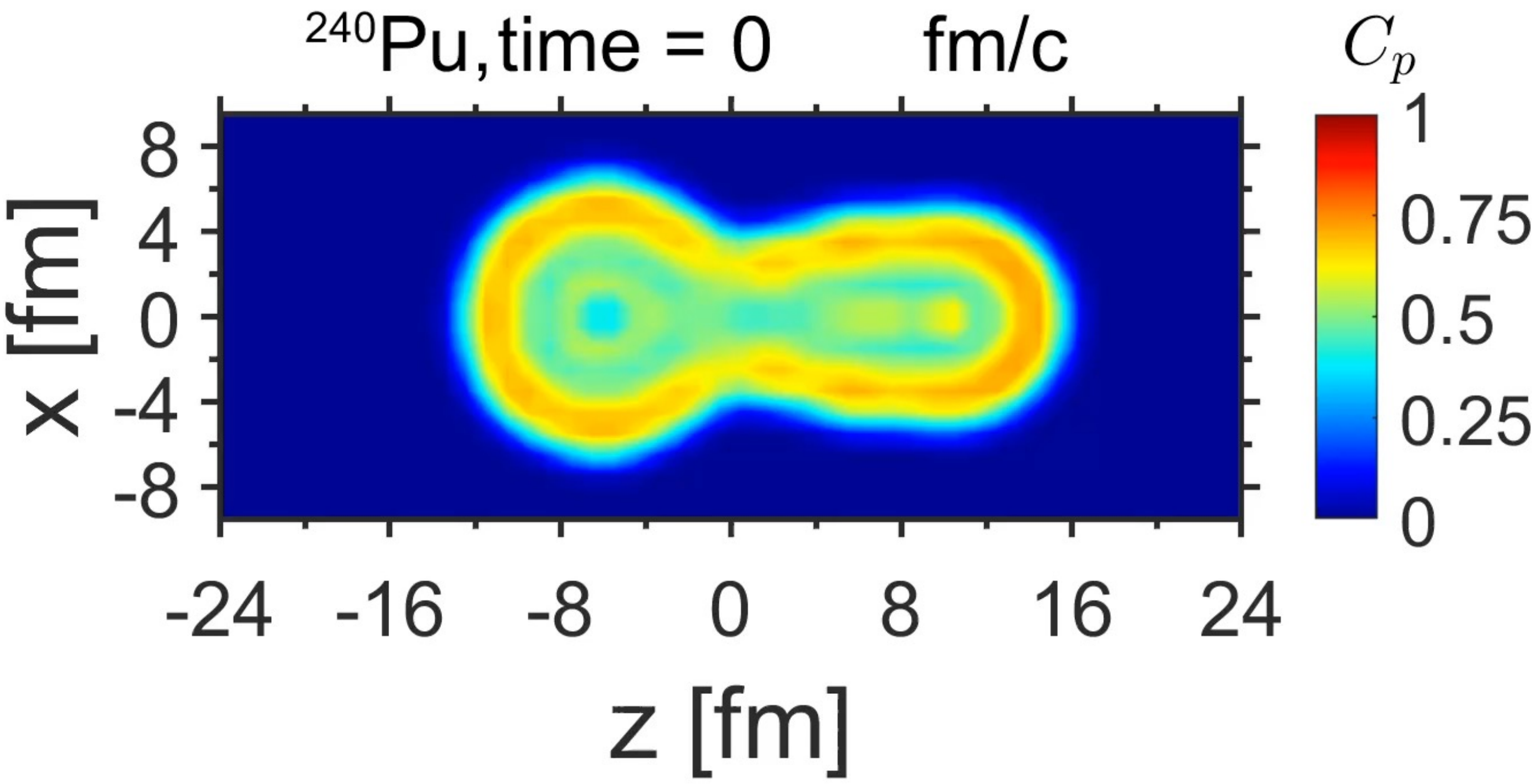
Trajectory 2



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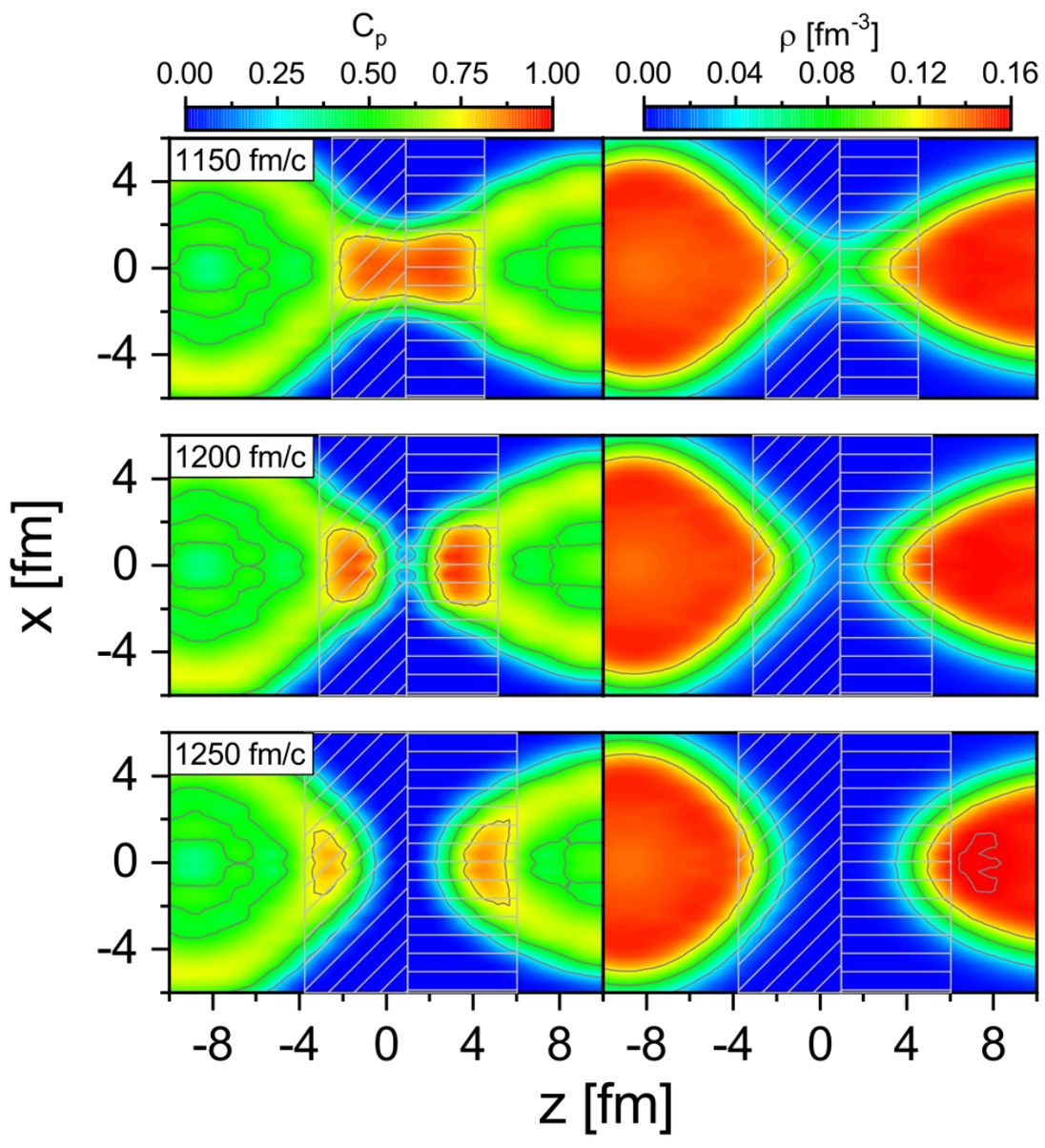
Trajectory 2

Proton localization

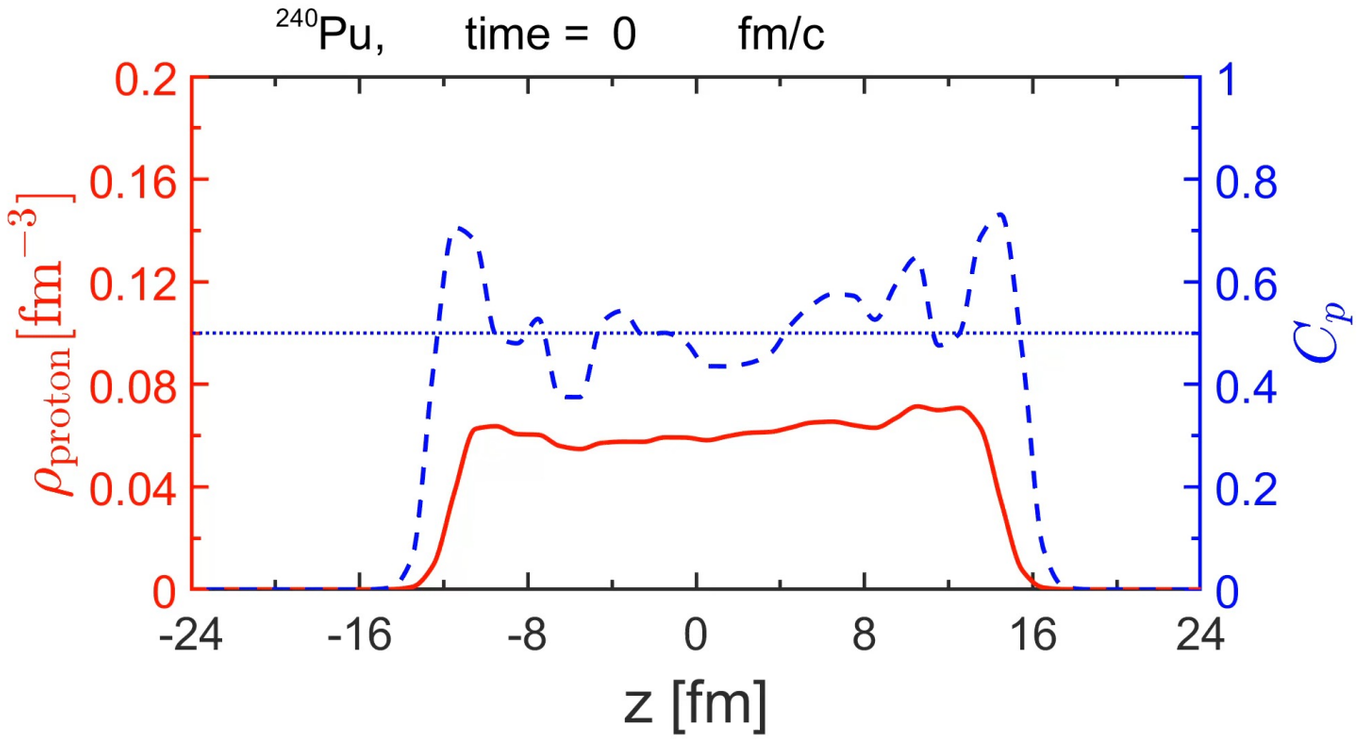
Density



When are these light clusters formed?

What is their structure?

What is their role in the scission mechanism?



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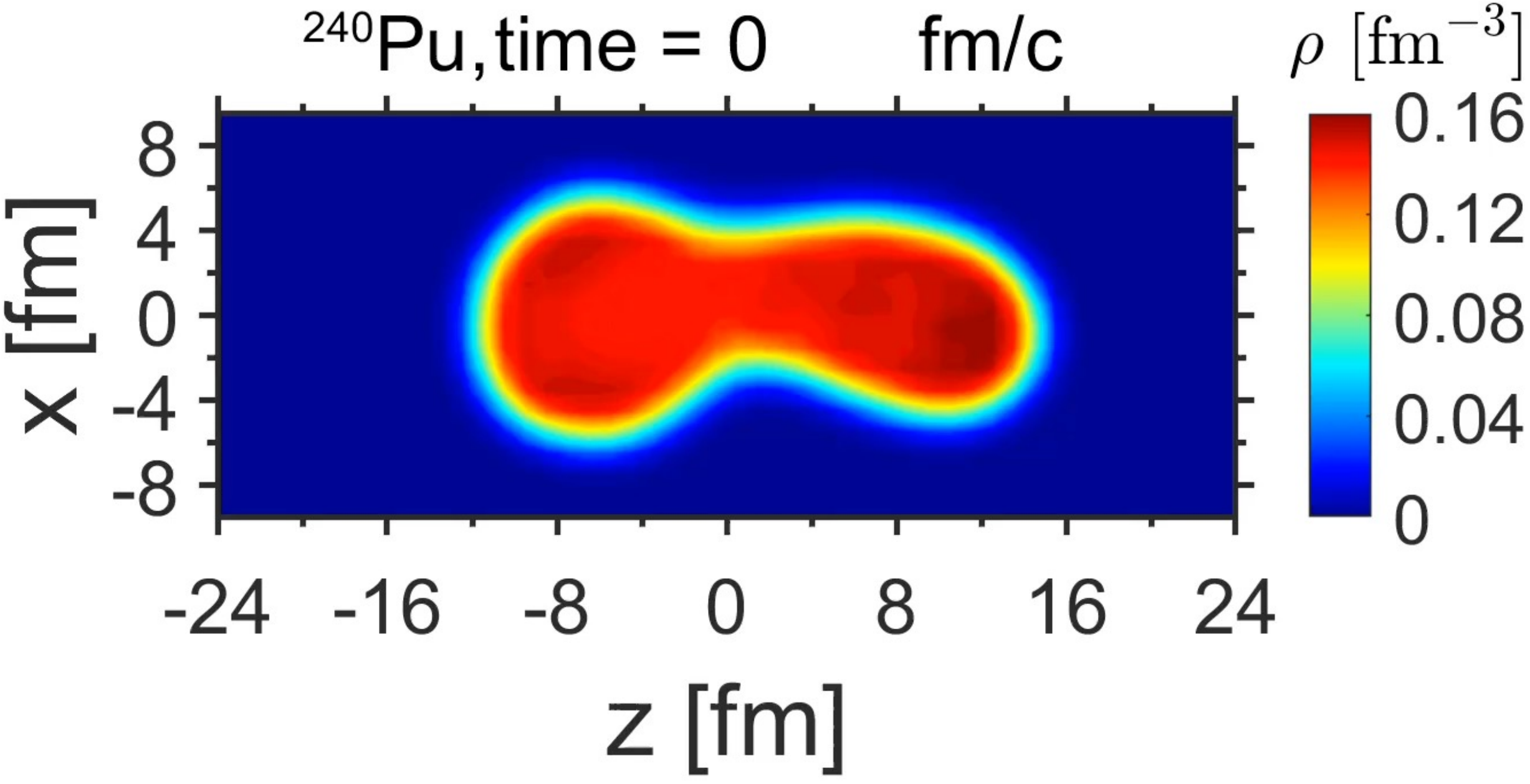
Trajectory 2
Broken axial symmetry



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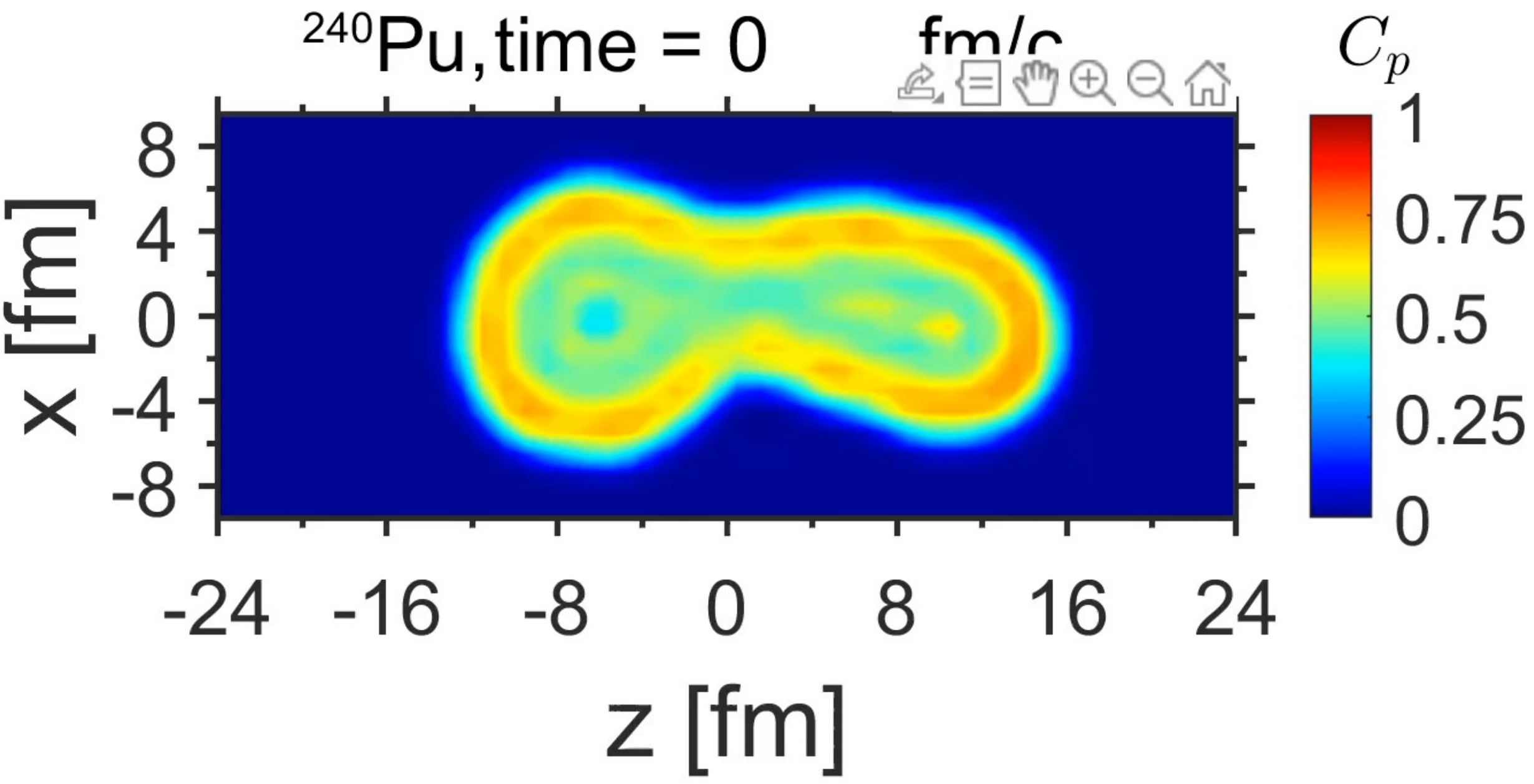
Trajectory 2
Broken axial symmetry



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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:
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