Microscopic Analysis of Induced Nuclear Fission Dynamics

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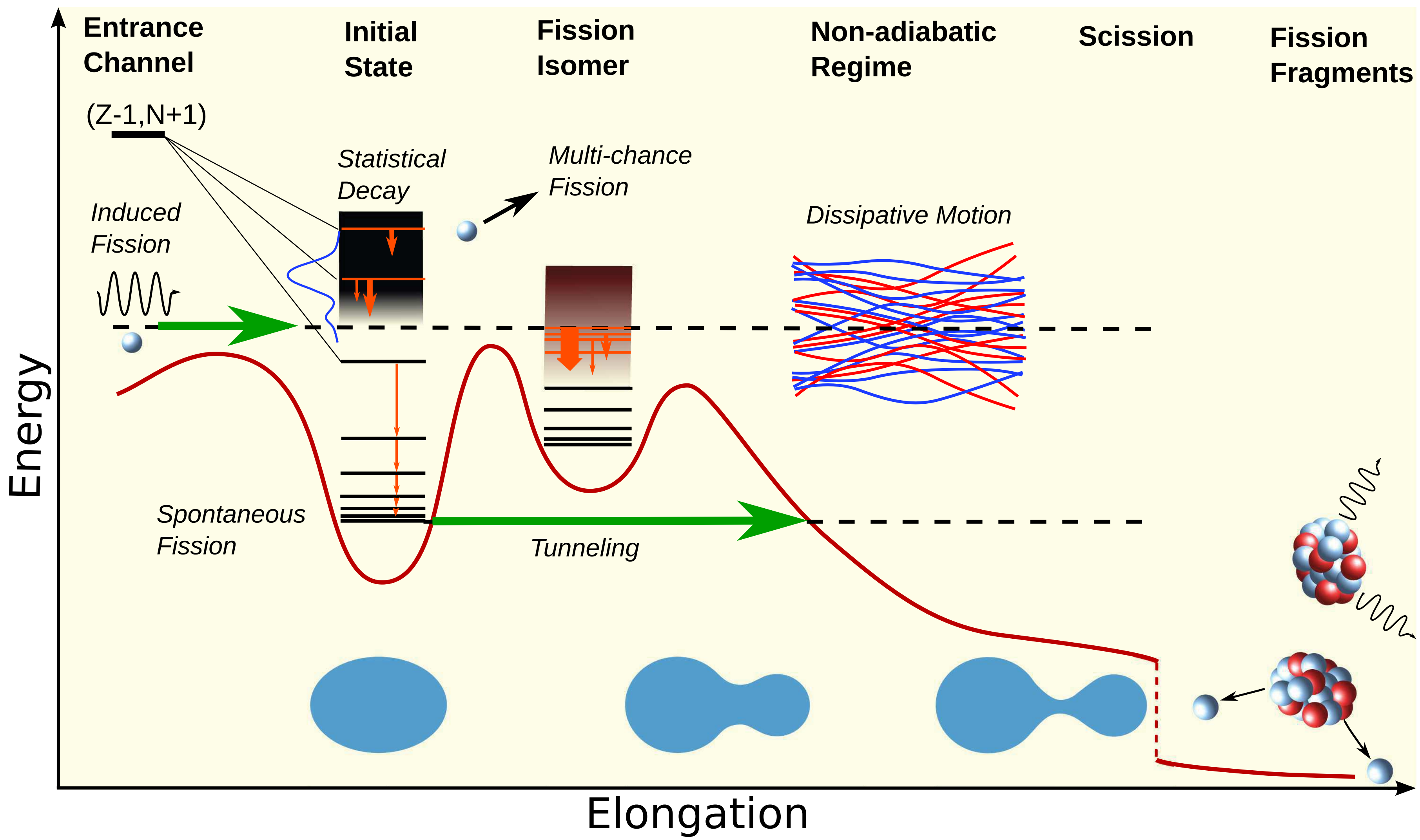

Entrance Channel
Initial State
Fission Isomer
Non-adiabatic Regime
Scission
Fission Fragments
(Z-1,N+1)
Statistical Decay
Multi-chance Fission
Induced Fission
Dissipative Motion
Spontaneous Fission
Tunneling
Energy
Elongation

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

The time-dependent generator coordinate method (TDGCM)

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

⇒ 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

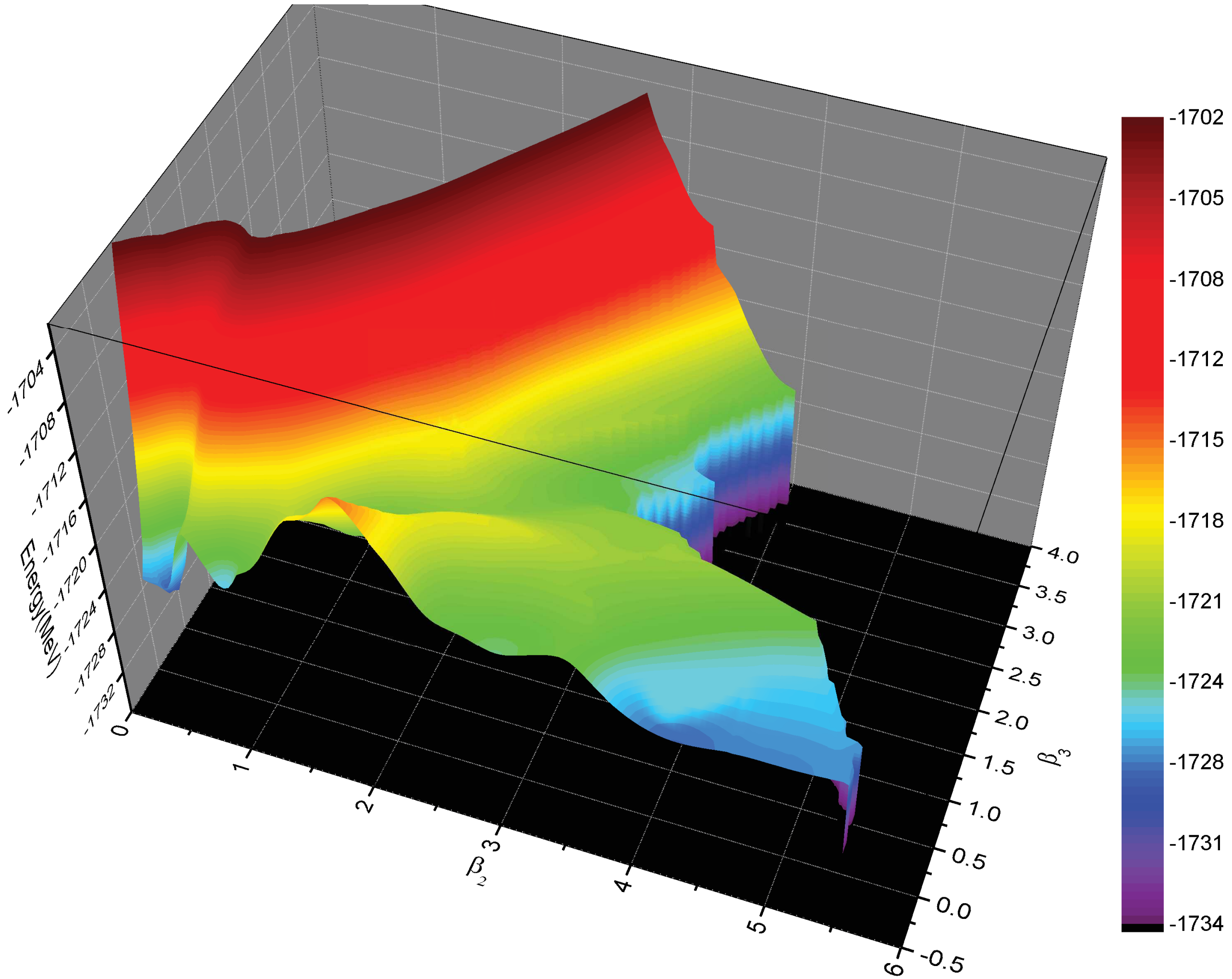
Time-dependent Schroedinger-like equation for fission dynamics (axial quadrupole and octupole deformation parameters as collective degrees of freedom):

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

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

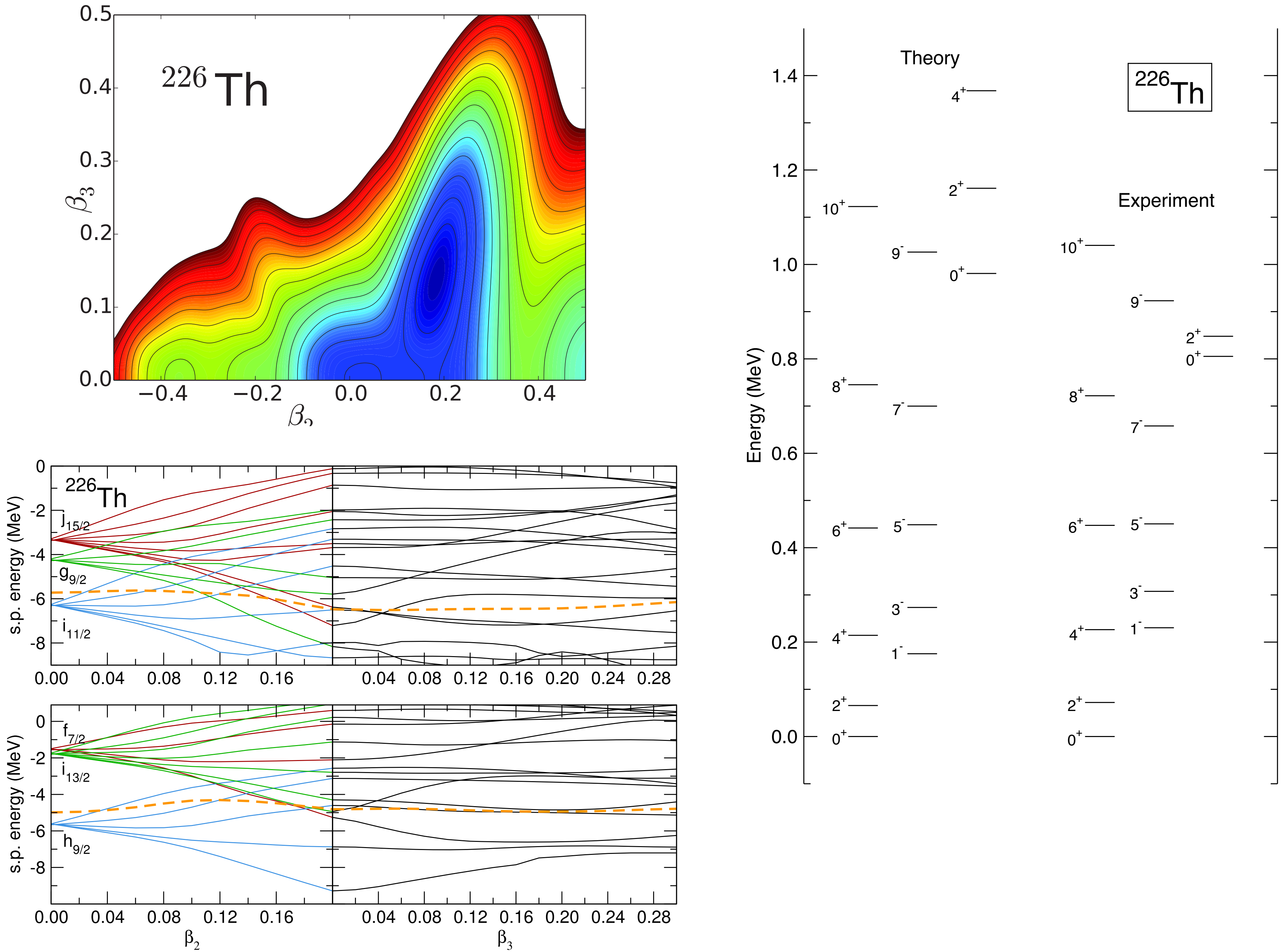
PHYSICAL REVIEW C **96**, 024319 (2017)



→ 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



226Th
β3
β2
0.5
0.4
0.3
0.2
0.1
0.0
−0.4
−0.2
0.0
0.2
0.4
226Th
j15/2
g9/2
i11/2
s.p. energy (MeV)
0
-2
-4
-6
-8
0.00
0.04
0.08
0.12
0.16
0.20
0.24
0.28
f7/2
i13/2
h9/2
s.p. energy (MeV)
β2
β3
Theory
Experiment
226Th
Energy (MeV)
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
10+
8+
6+
4+
2+
0+
9-
7-
5-
3-
1-
4+
2+
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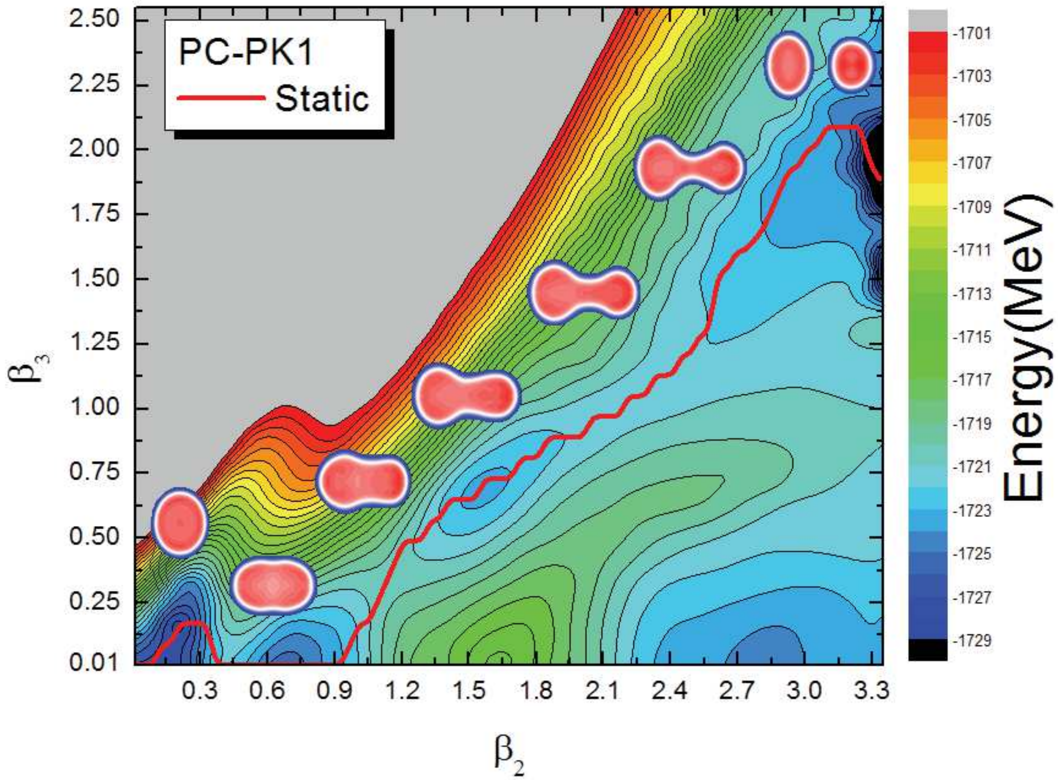
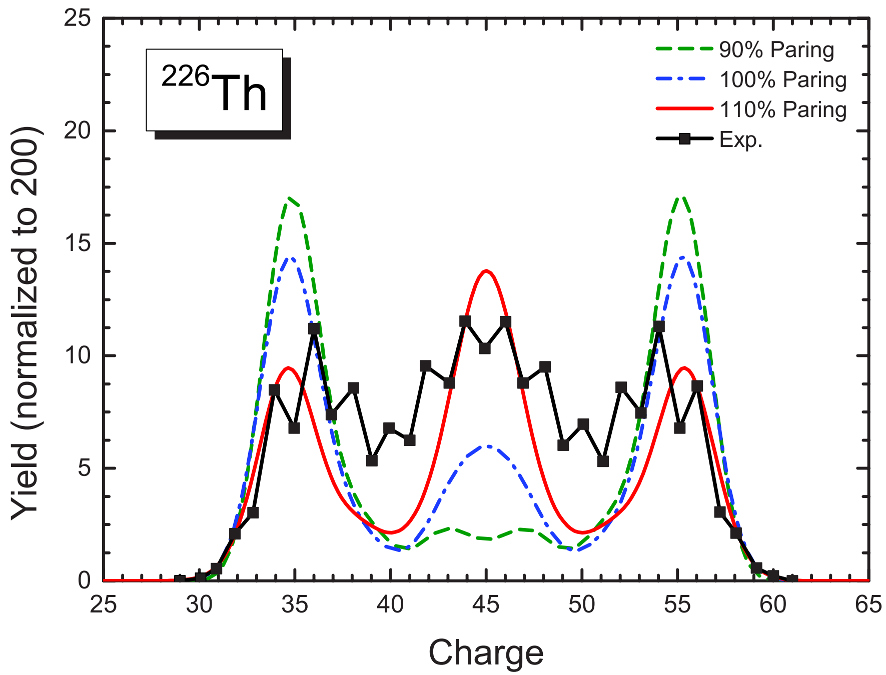
5-
3-
1-
2+
0+



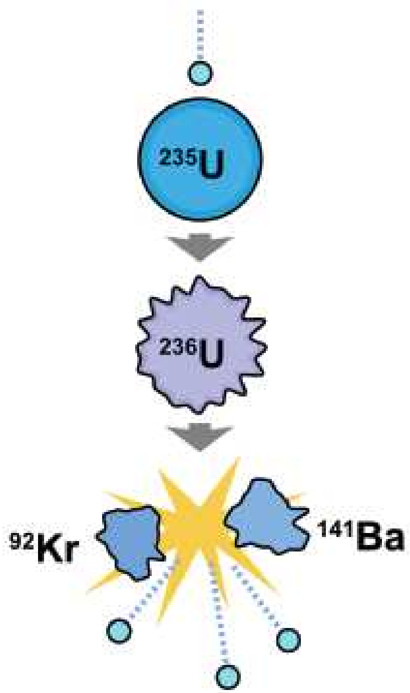
A triple-humped fission barrier is predicted along the static fission path, and the calculated heights are **7.10, 8.58, and 7.32 MeV** from the inner to the outer barrier.

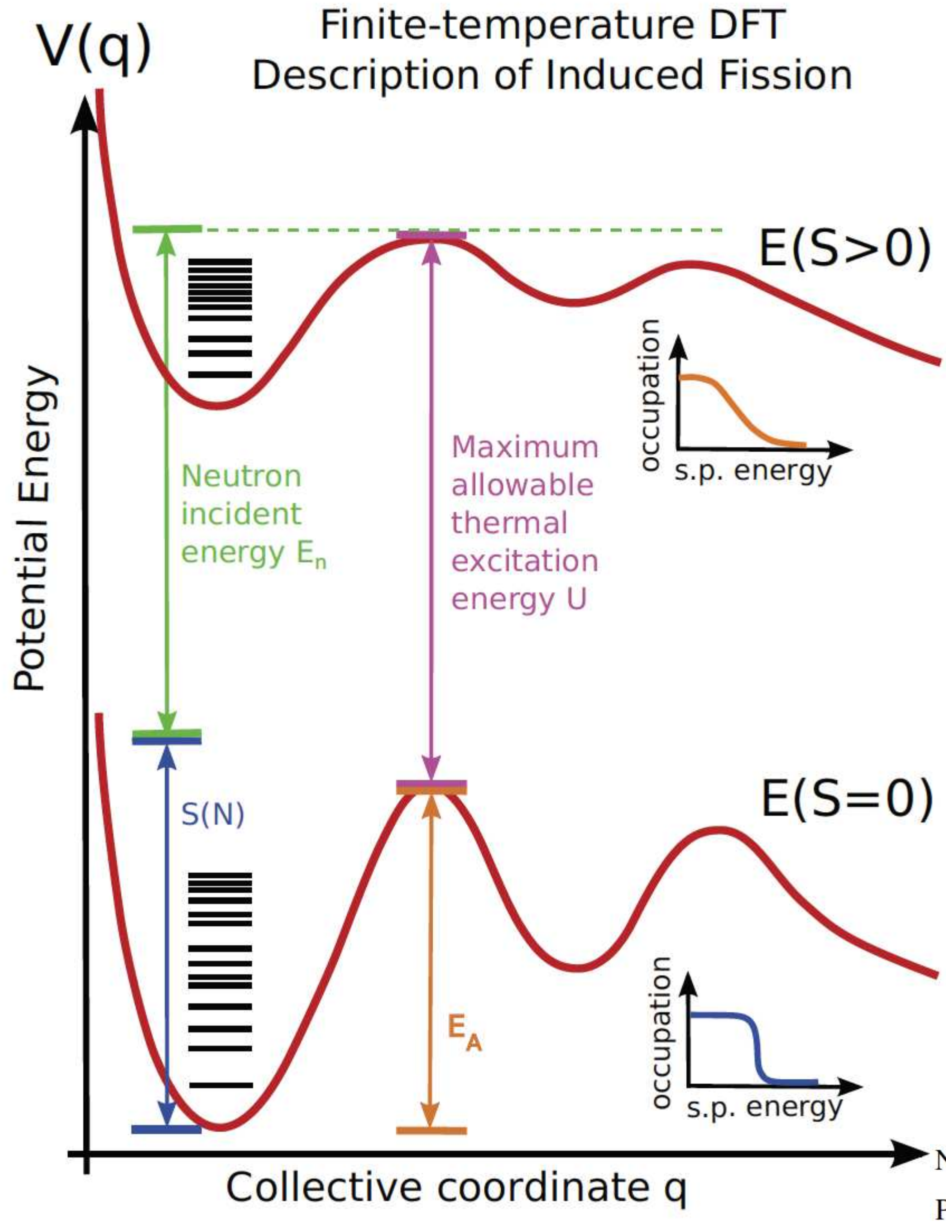
The height of the fission barriers (in MeV) with respect to the corresponding ground-state minima:

	B_I	$B_{II}^{\rm asy}$	$B_{III}^{\rm asy}$	$B_{II}^{\rm sym}$	$B_{III}^{\rm sym}$
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:

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

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

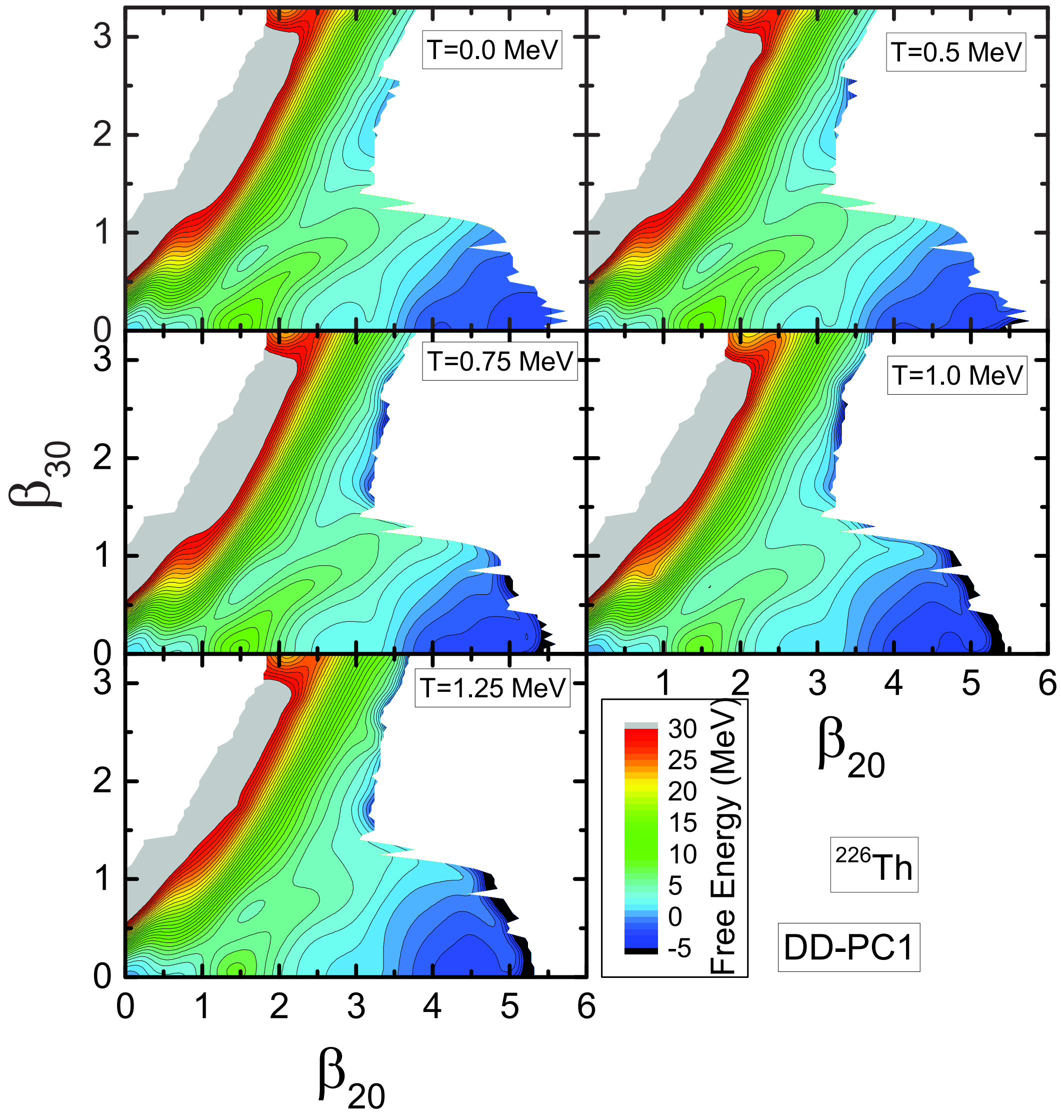
Helmholtz free energy: $F = E(T) - TS$

… 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:

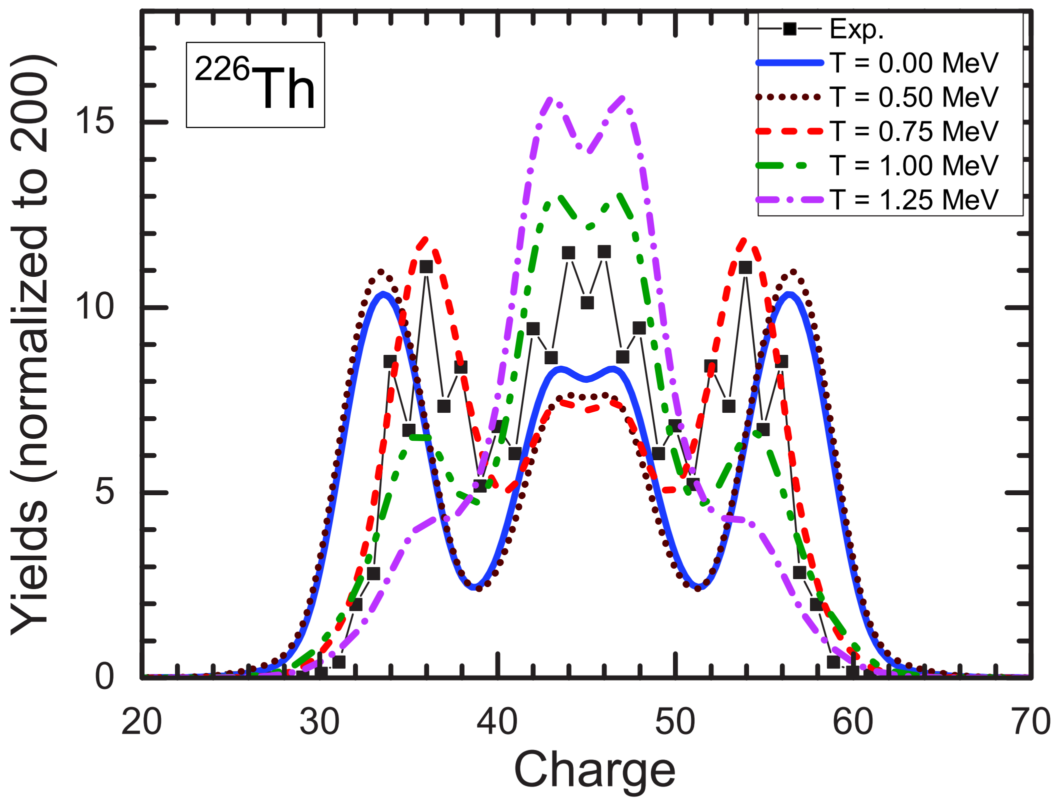
$$f_k = \frac{1}{1+e^{\beta E_k}}$$



Dynamics of induced fission

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

Charge yields:

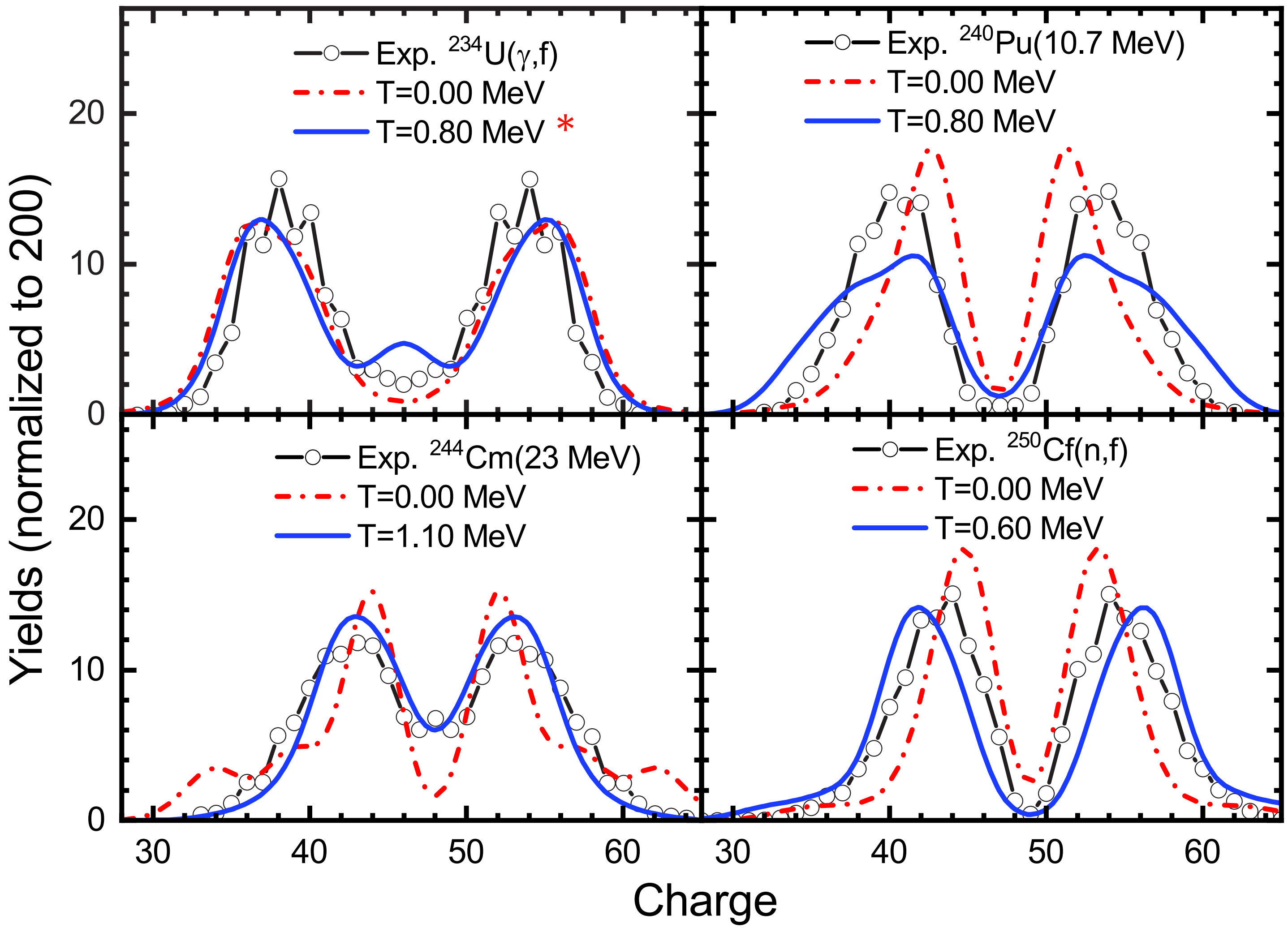


Experimental results ➠ photoinduced fission with photon energies in the interval 8 – 14 MeV, and a peak value Eγ = 11 MeV.

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

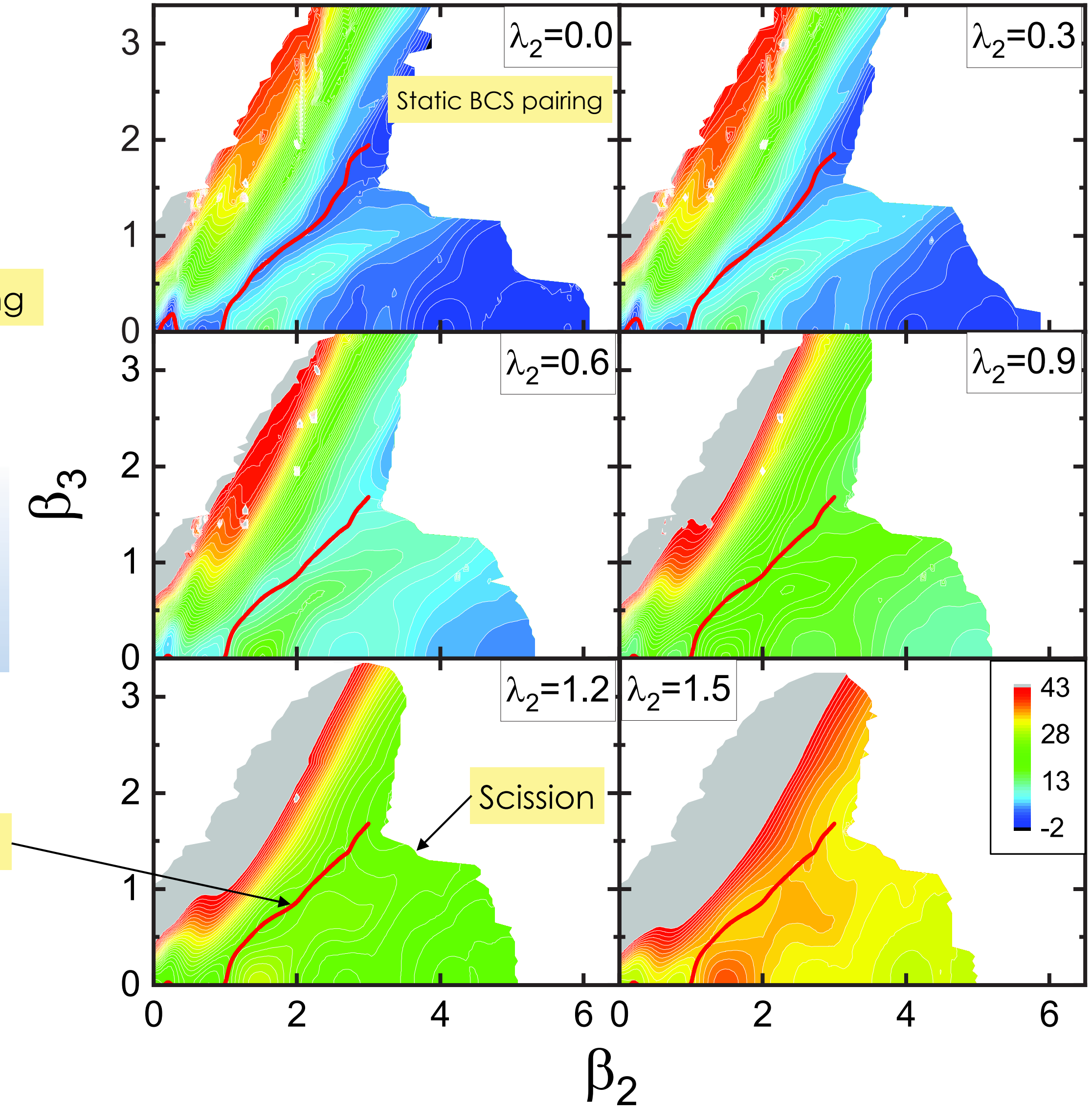
... the Routhian:

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

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.

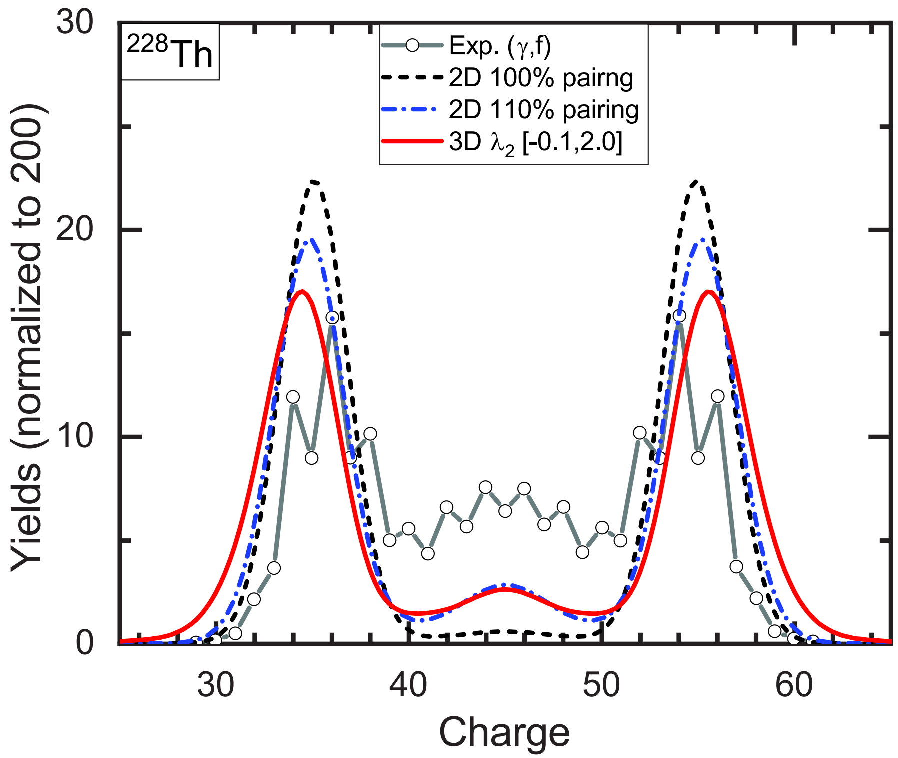
Static fission path of minimum energy

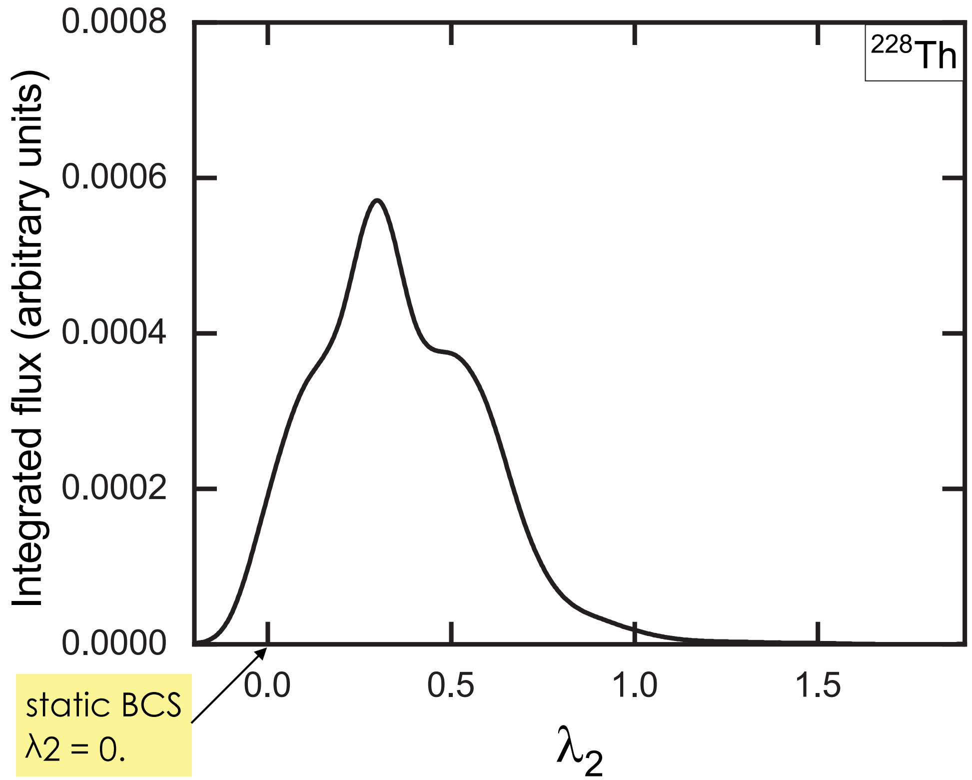


3D TDGCM+GOA calculation

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

q≡{β2,β3,λ2}





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

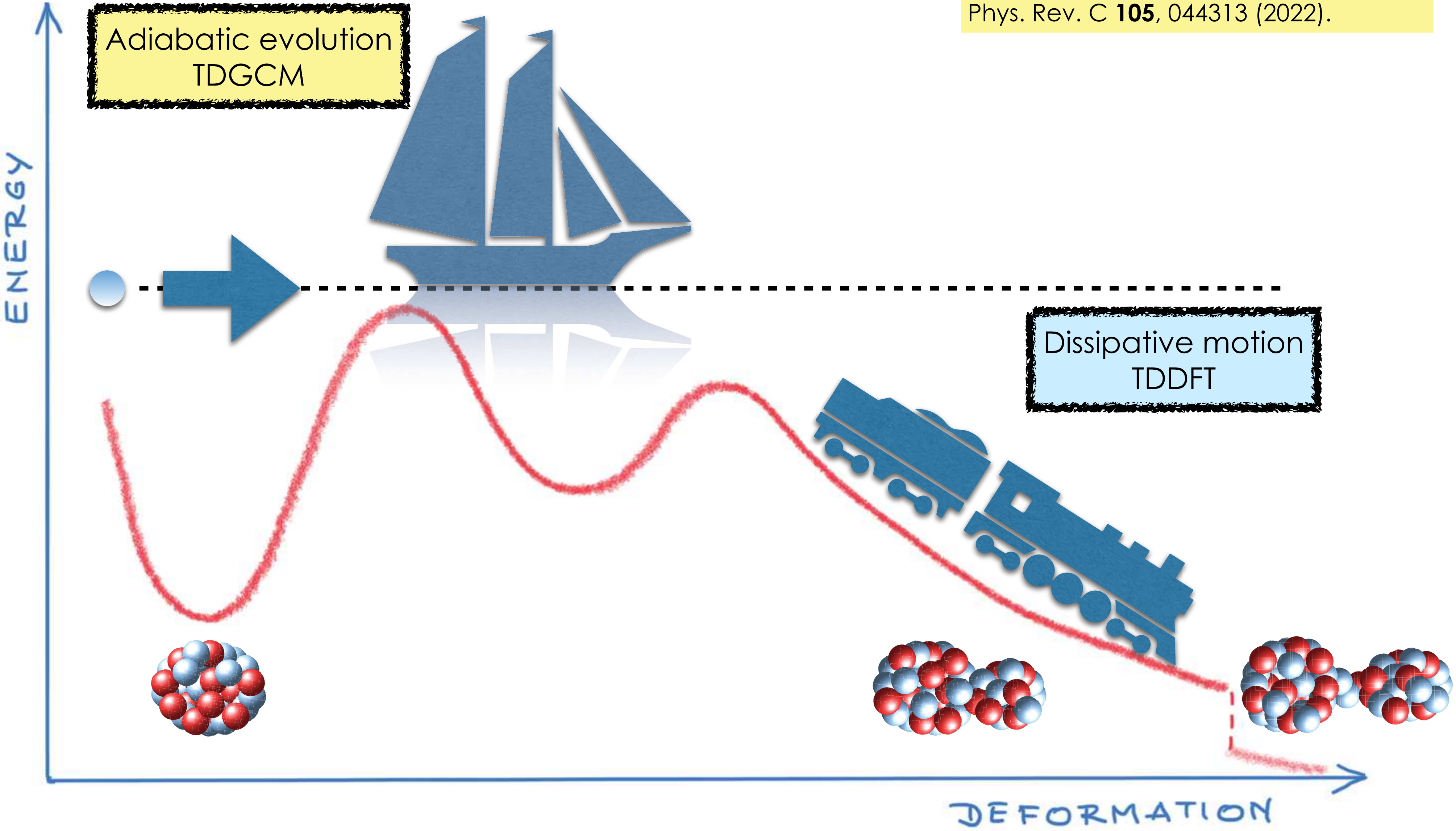
Effect of dynamical pairing on the flux of the probability current through the scission hyper-surface:

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

→ 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)

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

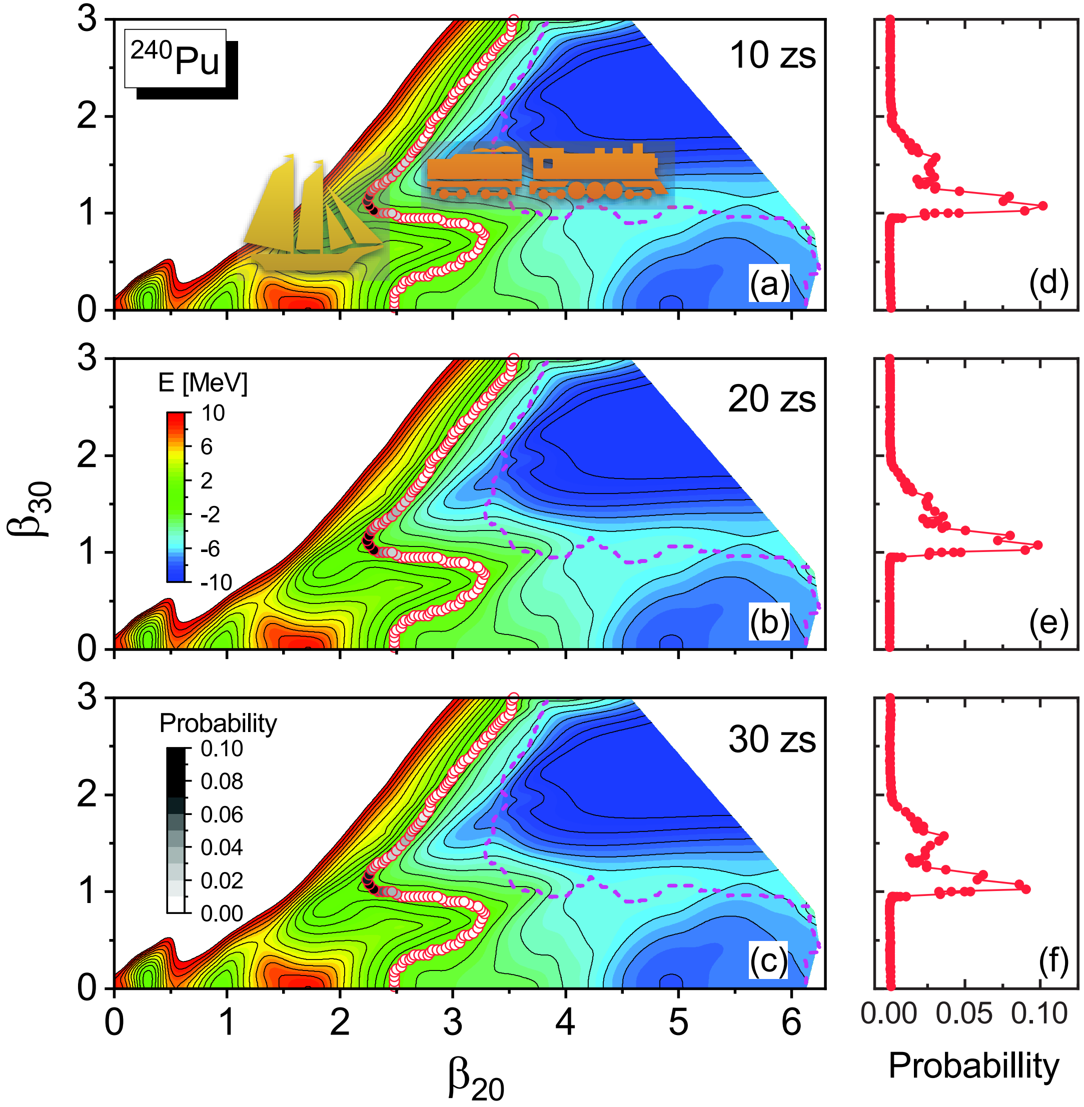
⇒ classical evolution of independent nucleons in mean-field potentials, cannot be applied in classically forbidden regions of the collective space, nor does it take into account quantum fluctuations.

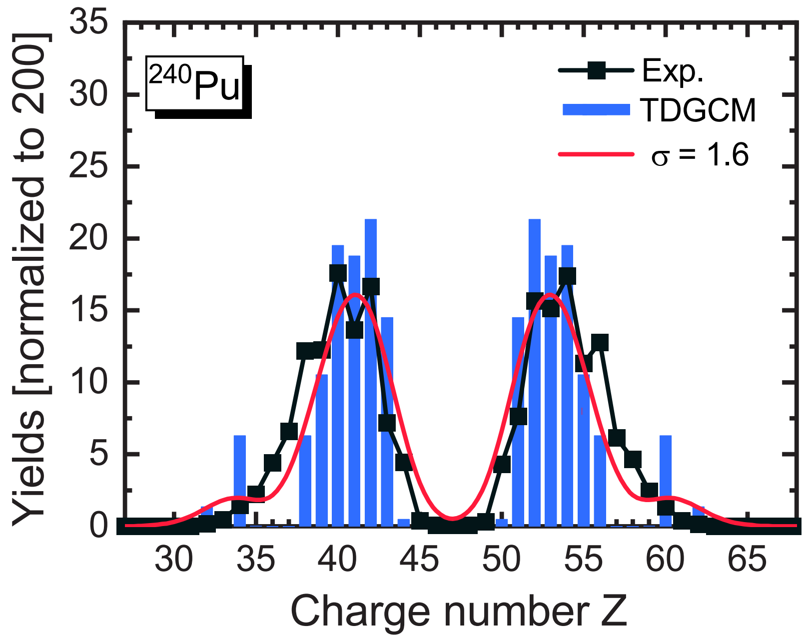
$$i\frac{d}{dt}n_k(t) = n_k(t)\Delta_k^*(t) - n_k^*(t)\Delta_k(t),$$

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

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

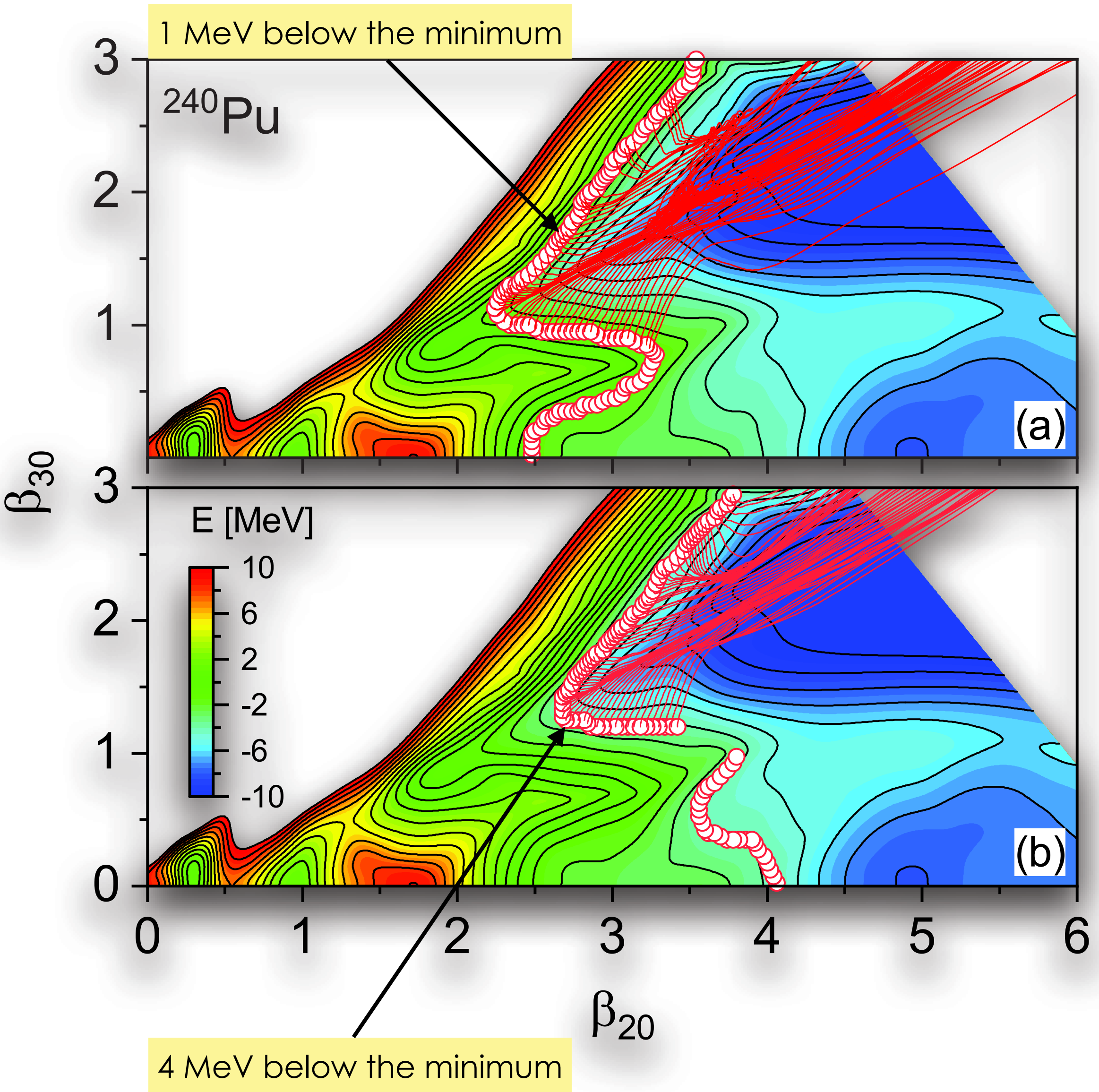
Negele et al. (1978) ➠ use an adiabatic model for the time interval in which the fissioning nucleus evolves from the quasi-stationary initial state to the saddle point, and a non-adiabatic method for the saddle-to-scission and beyond-scission dynamics.

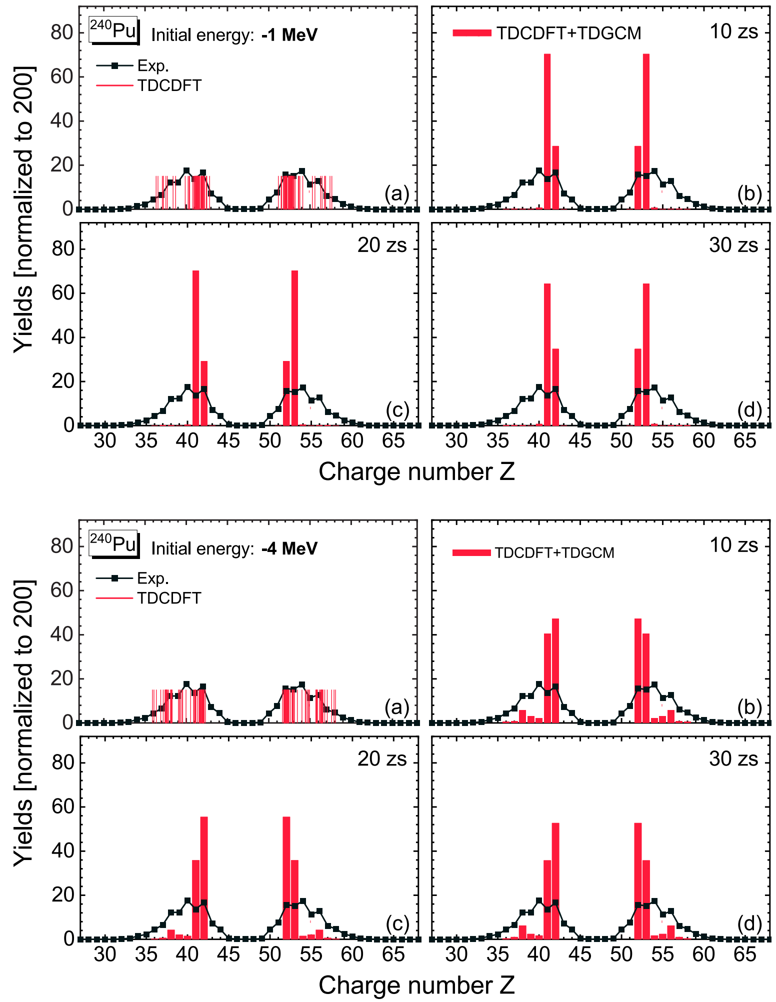




Ren, Zhao, Vretenar, Nikšić, Zhao, Meng
Phys. Rev. C **105**, 044313 (2022).

TDDFT fission trajectories





Total kinetic energies (TKEs) of the fragments

TDGCM+GOA

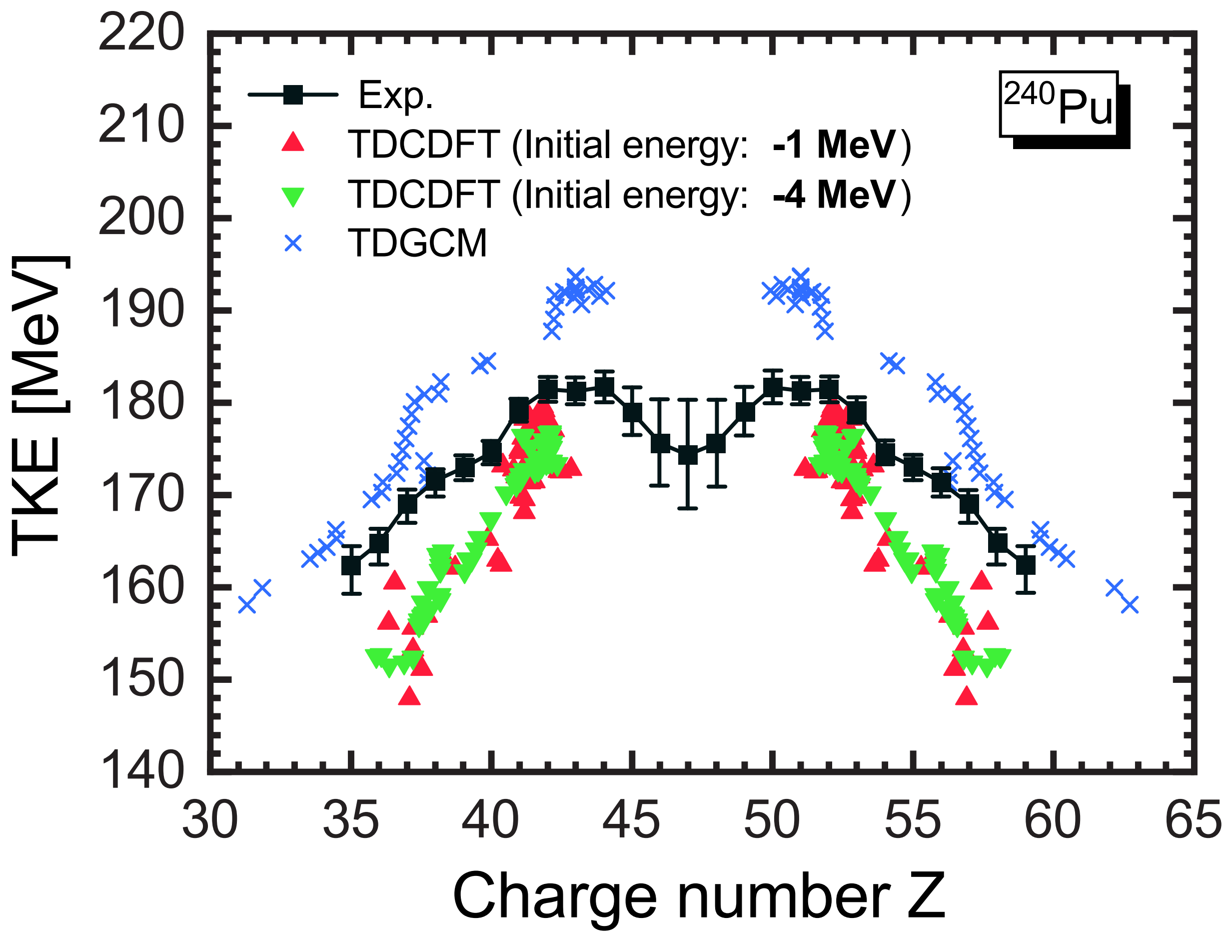
$$E_{\text{TKE}} = \frac{e^2 Z_H Z_L}{d_{\text{ch}}},$$

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

TDDFT

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

(≈ 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:

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

... the level density for each value of **q** is high even at low excitation energies ⇒ the discrete label *n* can be separated into a continuous excitation energy variable ε, and a degeneracy label λ:

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

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 $\eta(\boldsymbol{q};T,T') \equiv \eta(\boldsymbol{q};\epsilon(T),\epsilon(T'))$

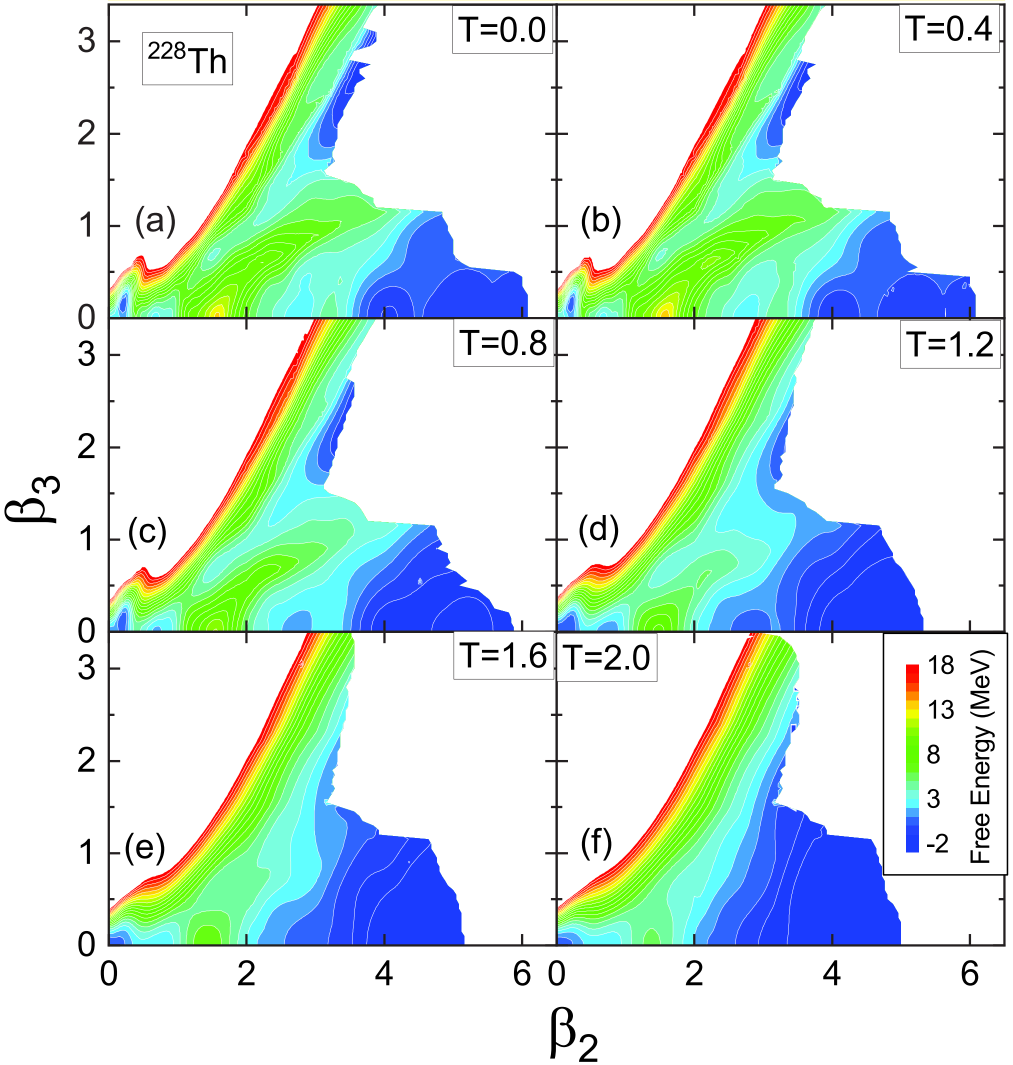
Extended TDGCM

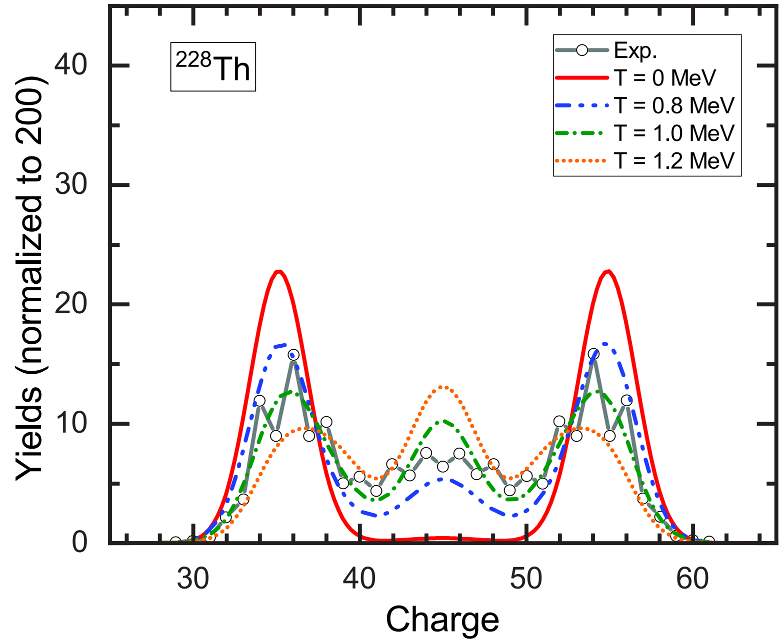
$$i\hbar\partial_t\psi(\boldsymbol{q},T;t) = \left[V(\boldsymbol{q},T) + \boldsymbol{P}\frac{1}{2\mathcal{M}(\boldsymbol{q},T)}\boldsymbol{P}\right]\psi(\boldsymbol{q},T;t) + \frac{i}{2}\int\{\boldsymbol{P},\boldsymbol{\mathcal{O}}(\boldsymbol{q};T,T')\}\,\psi(\boldsymbol{q},T';t)dT',$$

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

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

2D TDGCM+GOA calculation at fixed temperatures T.

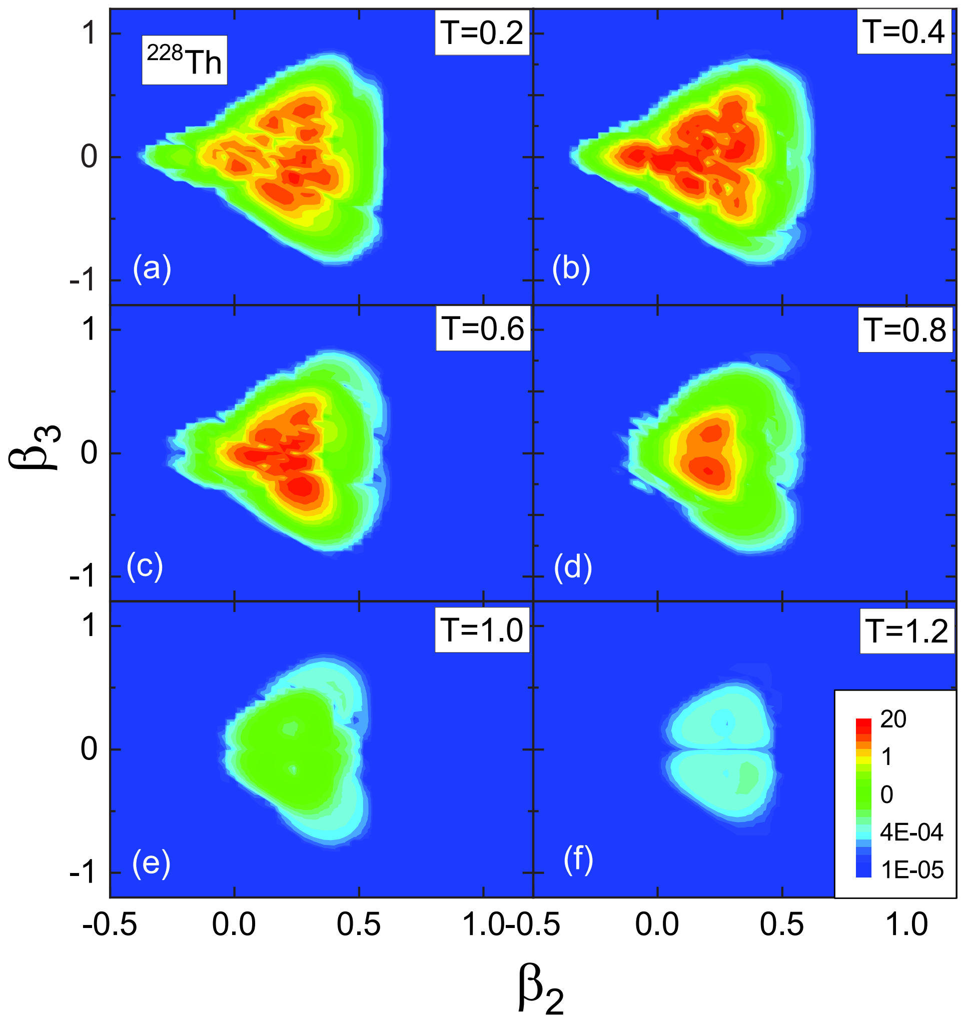




The data for photo-induced fission correspond to photon energies in the interval 8 − 14 MeV, and a peak value of Eγ = 11 MeV.

3D calculation of fission dynamics of ^{228}Th in the space of axial shape variables (β2, β3) and temperature T

2D projections on the (β2, β3) 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:

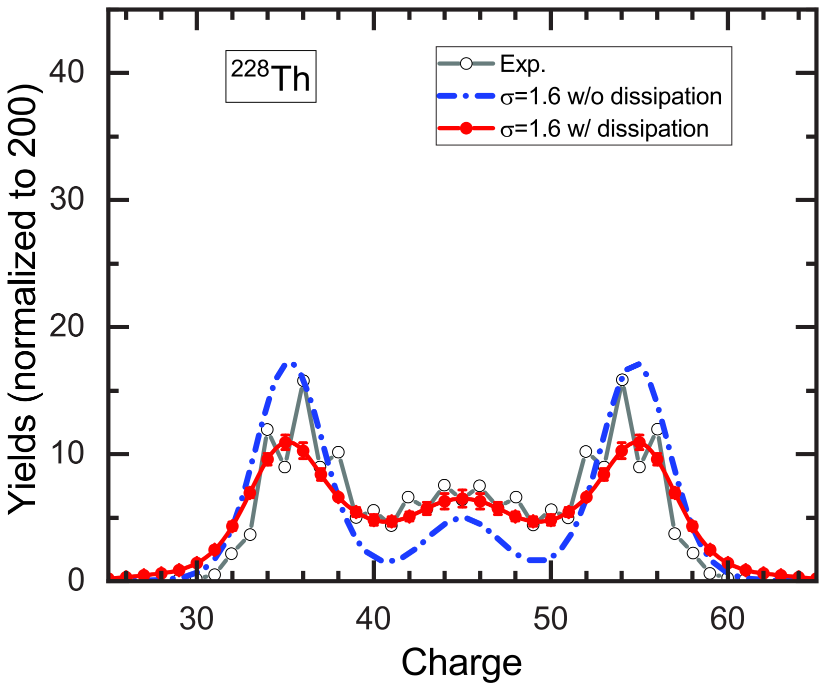
$$V(\boldsymbol{q},T) \;=\; \epsilon(T) + F(\boldsymbol{q},T)$$

The dissipation function:

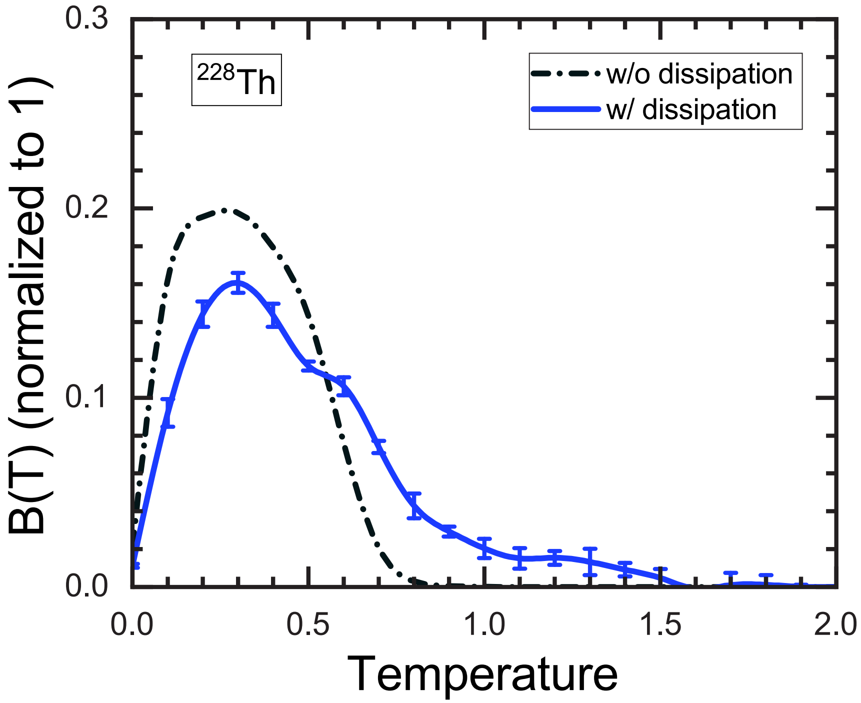
$$\boldsymbol{\eta}(\boldsymbol{q};T,T') = \begin{cases} 0 & \beta_2 < \beta_2^0 \\ \boldsymbol{\eta}(T,T') & \beta_2 \geq \beta_2^0, \end{cases}$$

Gaussian random variables

3D extended TDGCM charge yields.

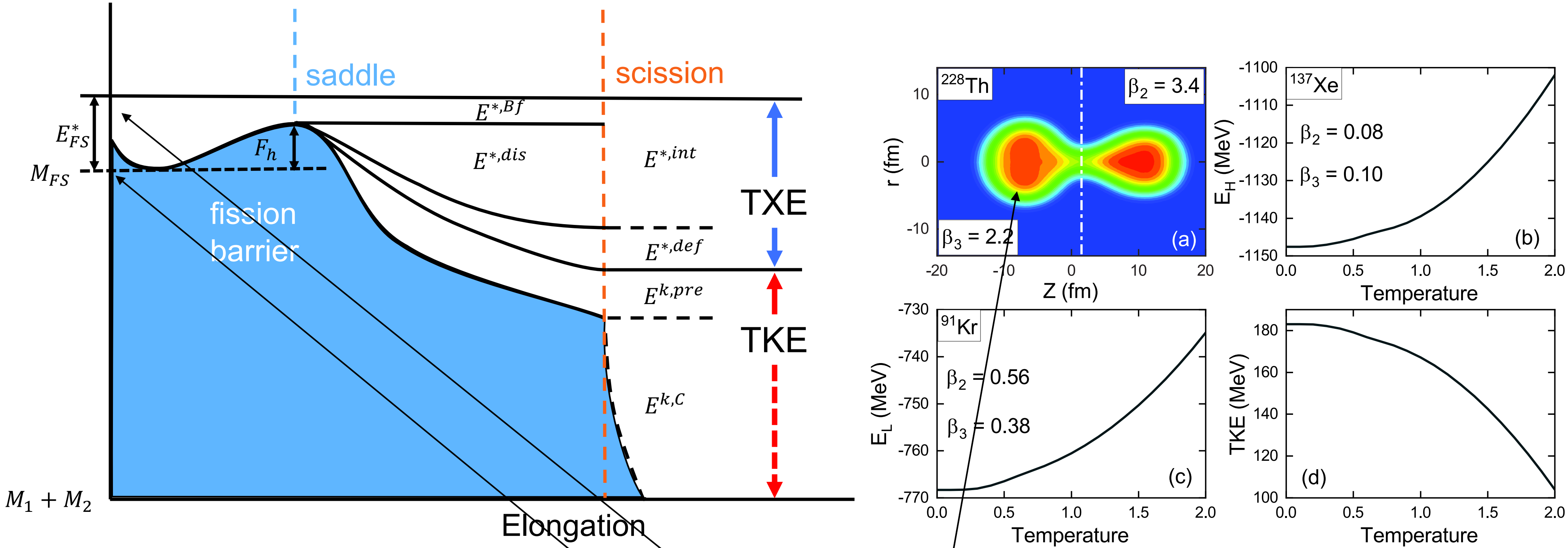


Time-integrated collective flux B(T) through the scission contour, as a function of temperature.



Total Kinetic Energy Distribution

Zhao, Nikšić, Vretenar, arXiv:2210.00460

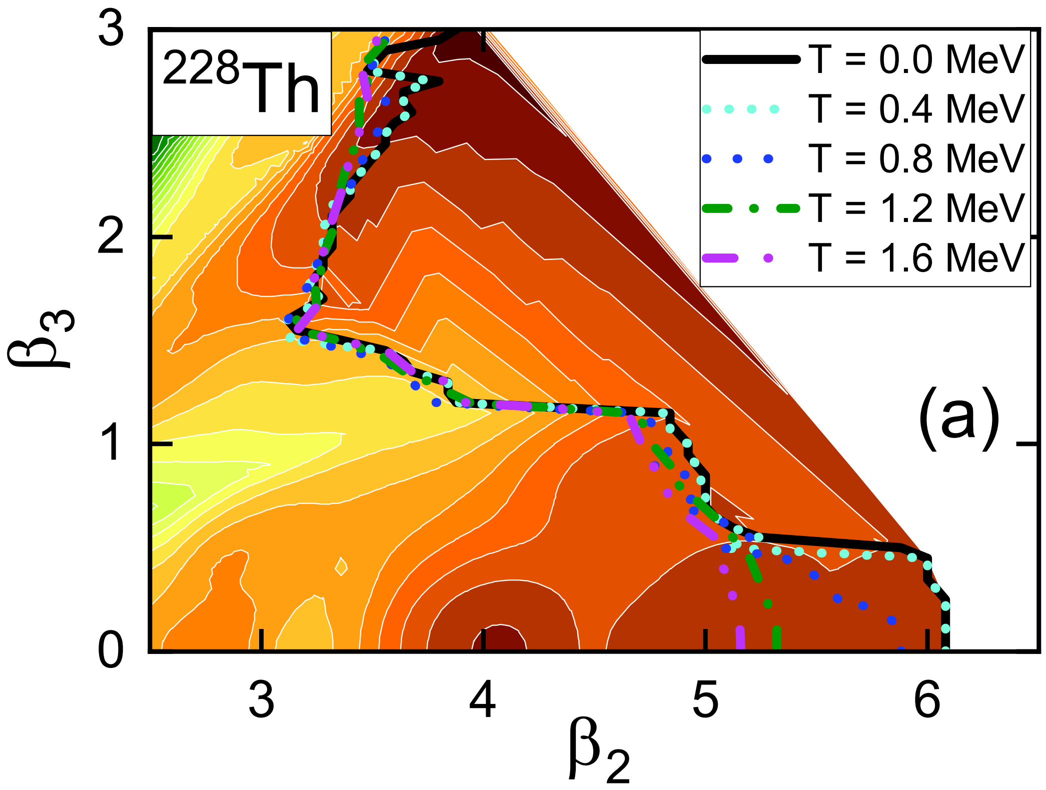


$$\mathrm{TKE}(\xi) = (E_{\mathrm{B}}^{\mathrm{FS}} + E_{\mathrm{coll}}^{*}) - \left[E^L(\beta_2^L, \beta_3^L, T) + E^H(\beta_2^H, \beta_3^H, T)\right]$$

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

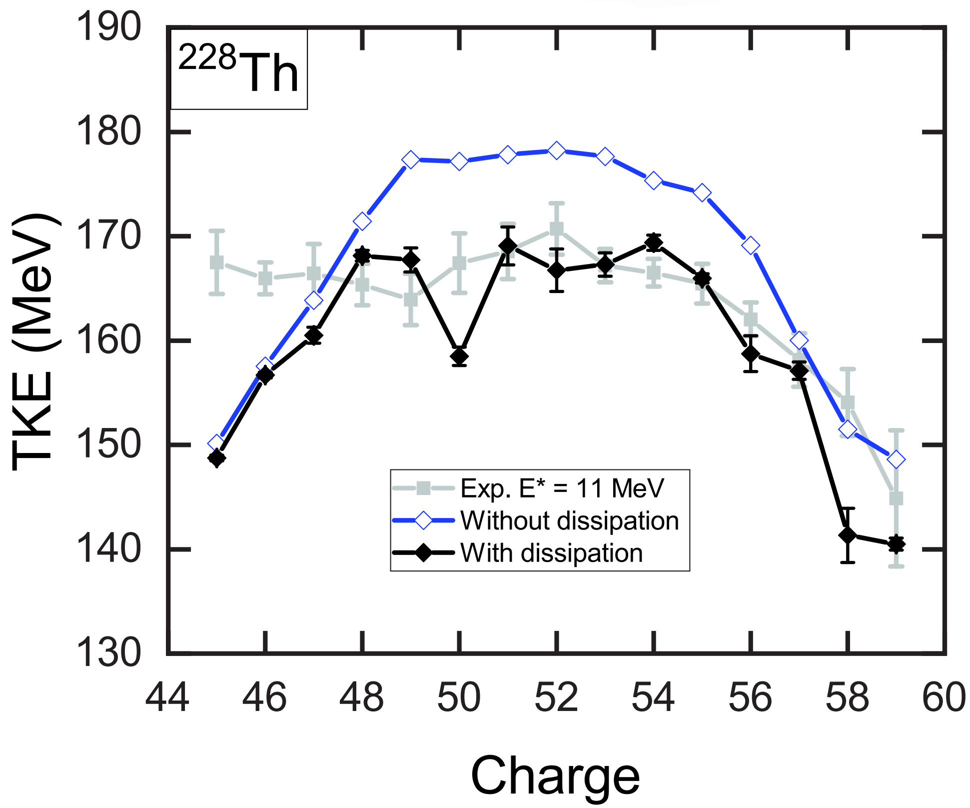
$$F(\xi; t) = \int_{t_0}^{t} dt' \int_{(\boldsymbol{q},T)\in\xi} \boldsymbol{J}(\boldsymbol{q}, T; t') \cdot d\boldsymbol{S},$$

Scission contours for ^{228}Th in the ($\beta 2$, $\beta 3$) deformation plane for several values of the nuclear temperature *T*, plotted on the deformation energy surface calculated at zero temperature.



The TKE for the fission fragment with mass A:

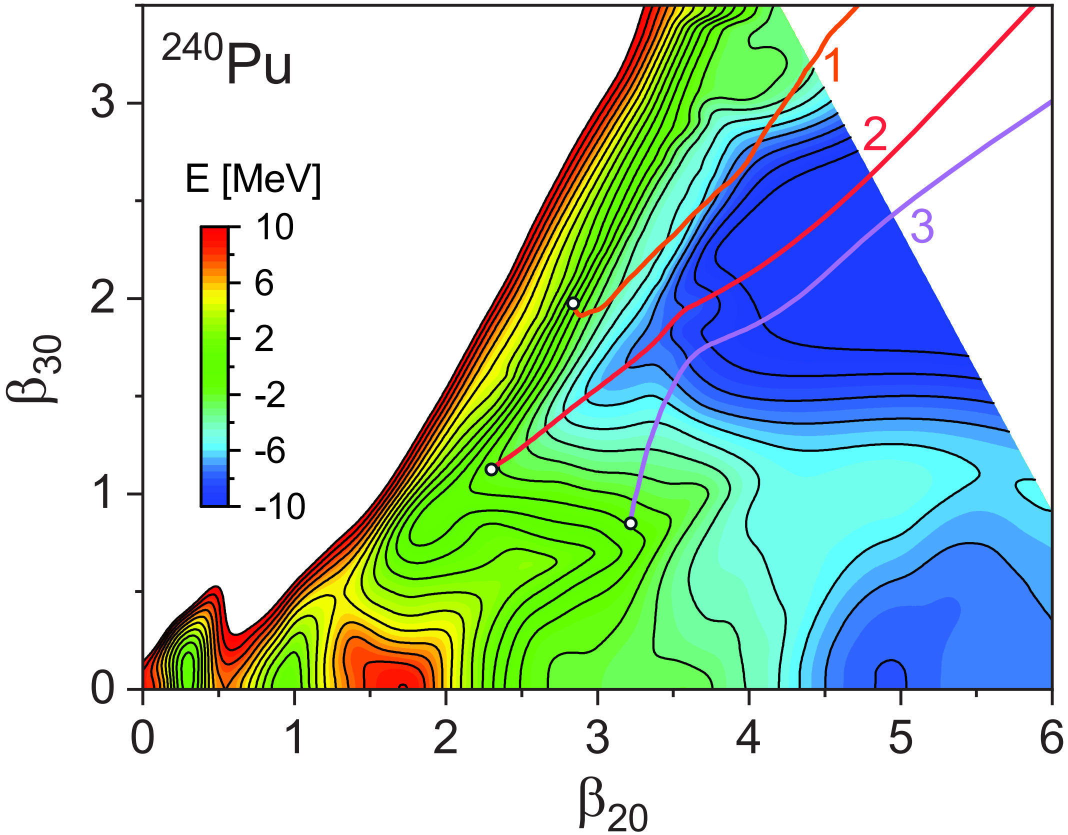
$$\mathrm{TKE(A)} = \lim_{t\to\infty} \frac{\sum_{\xi\in\mathcal{A}} F(\xi;t)\mathrm{TKE}(\xi)}{\sum_{\xi\in\mathcal{A}} F(\xi;t)}.$$



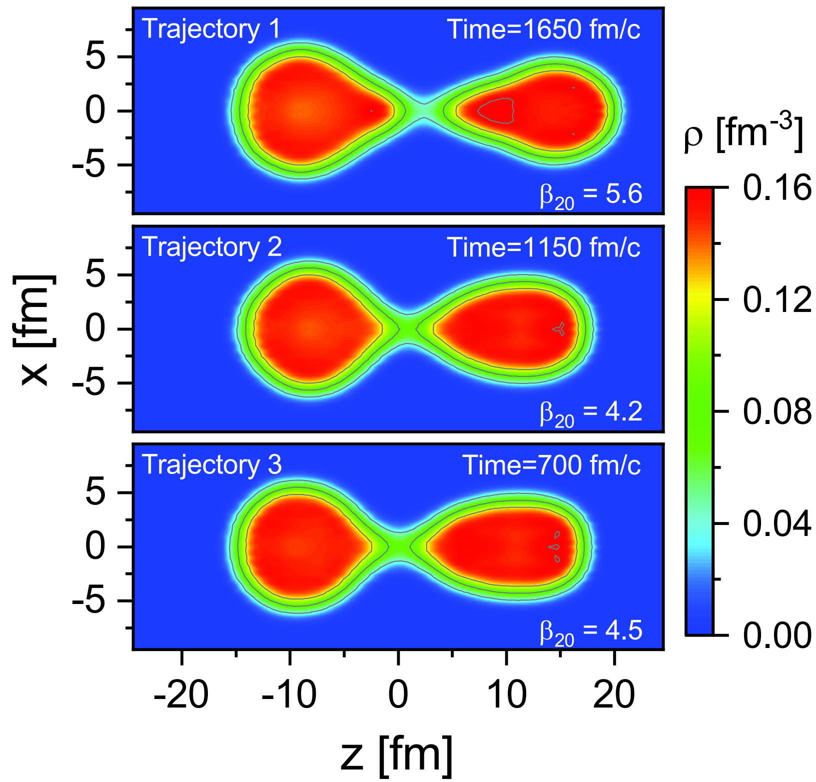
Zhao, Nikšić, Vretenar
Phys. Rev. C **106**, 054609 (2022).

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:

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

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

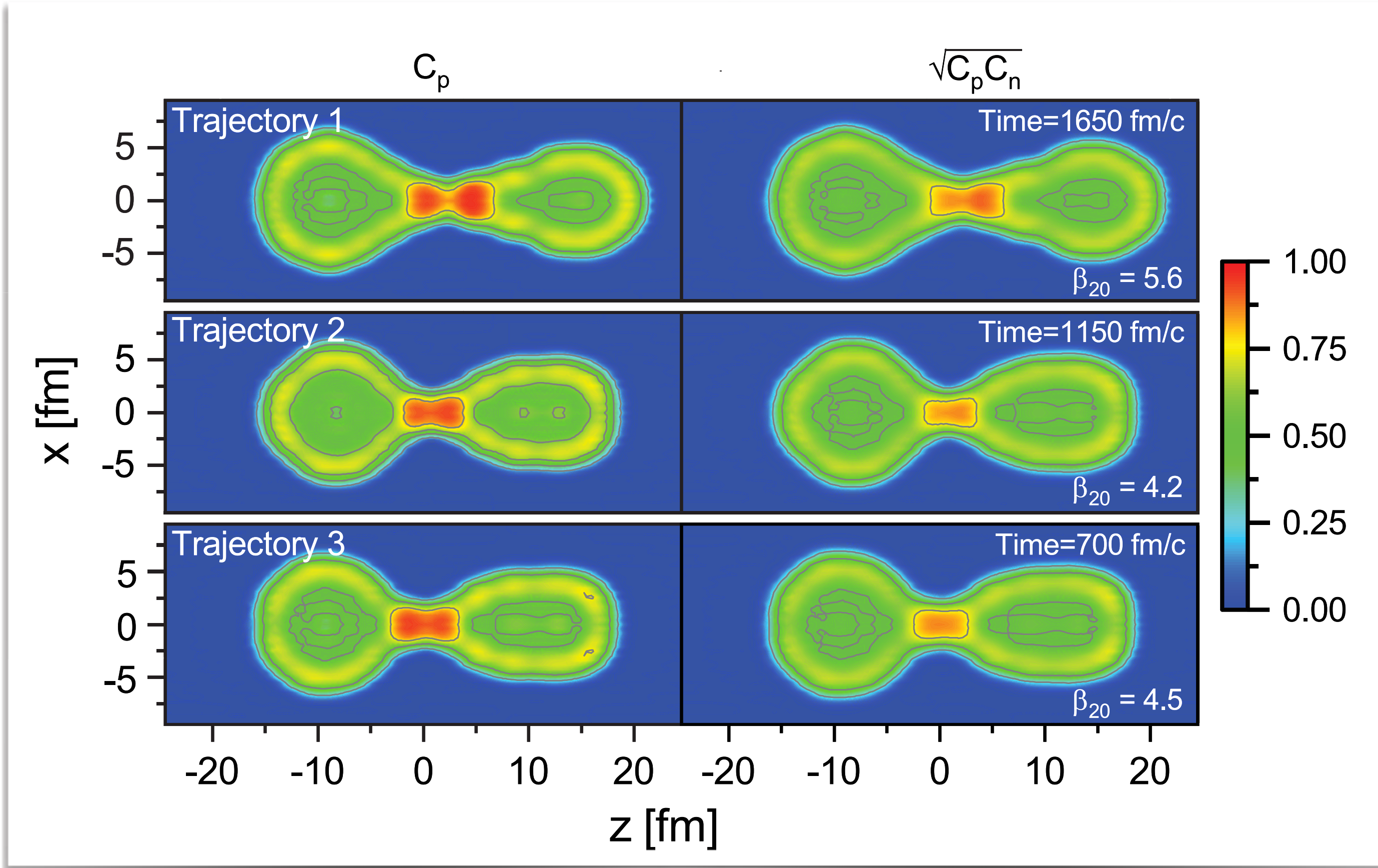
kinetic energy density, density, current density

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

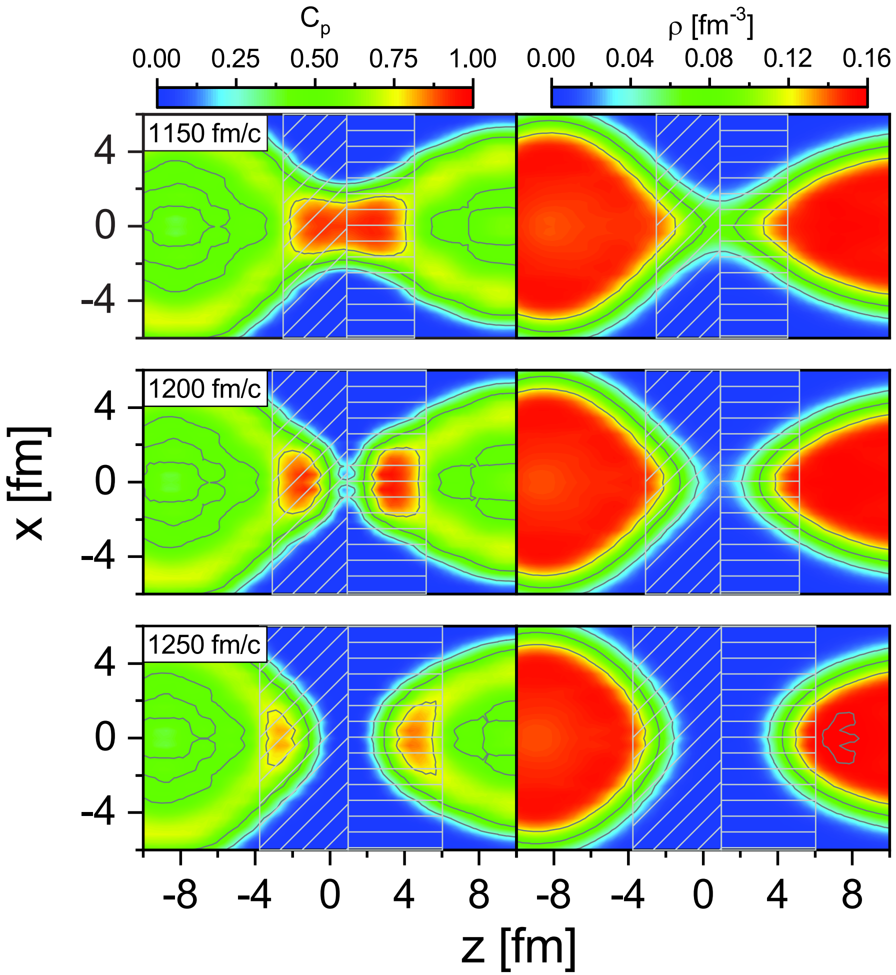
$$\tau^{\mathrm{TF}}_{q\sigma} = \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3}_{q\sigma}$$

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

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



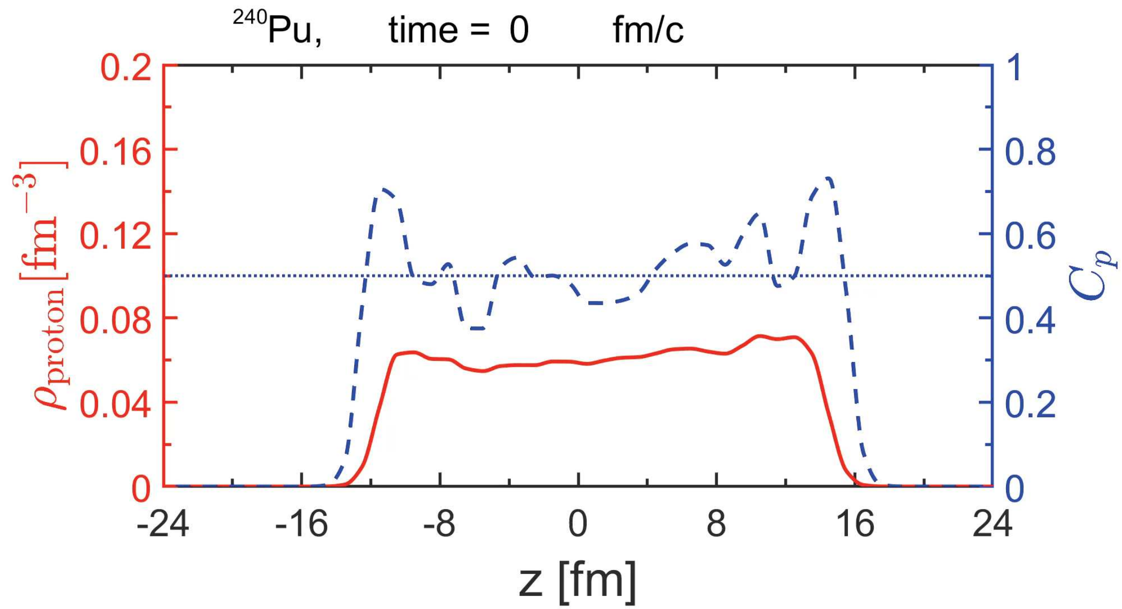
Trajectory 2



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).

Generalized time-dependent generator coordinate method

Li, Vretenar, Nikšić, Zhao, Meng, Phys. Rev. C **108**, 014321 (2023).

The nuclear wave function: $|\Psi(t)\rangle = \sum_{\boldsymbol{q}} f_{\boldsymbol{q}}(t)|\Phi_{\boldsymbol{q}}(t)\rangle$ $\quad\Rightarrow\quad$ $i\hbar\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$

$\Rightarrow$ equation of motion for the weight functions: $\sum_{\boldsymbol{q}} i\hbar\mathcal{N}_{\boldsymbol{q}'\boldsymbol{q}}(t)\partial_t f_{\boldsymbol{q}}(t) + \sum_{q} \mathcal{H}^{MF}_{\boldsymbol{q}'\boldsymbol{q}}(t) f_{\boldsymbol{q}}(t) = \sum_{q} \mathcal{H}_{\boldsymbol{q}'\boldsymbol{q}}(t) f_{\boldsymbol{q}}(t)$

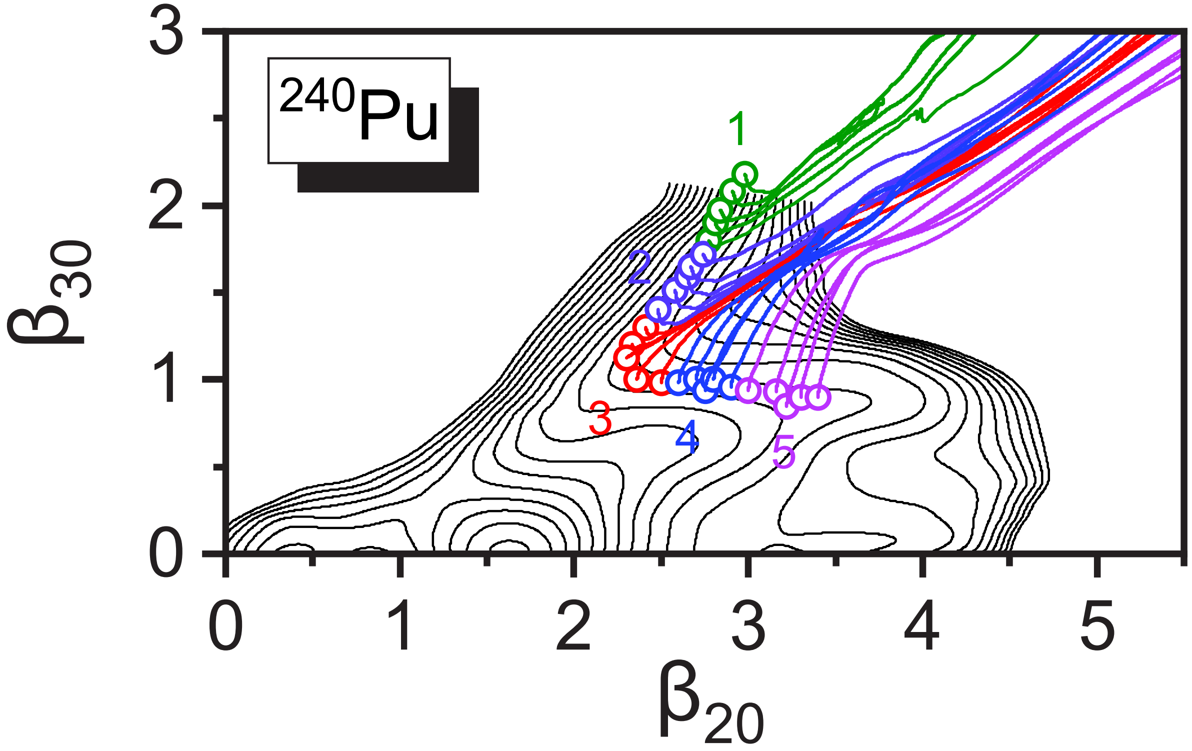
...time-dependent kernels:

$$
\begin{cases}
\mathcal{N}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|\Phi_{\boldsymbol{q}}(t)\rangle, \\
\mathcal{H}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|\hat{H}|\Phi_{\boldsymbol{q}}(t)\rangle, \\
\mathcal{H}^{MF}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|i\hbar\partial_t|\Phi_{\boldsymbol{q}}(t)\rangle,
\end{cases}
$$

The time-dependent generator states are independent TDDFT fission trajectories on the PES.

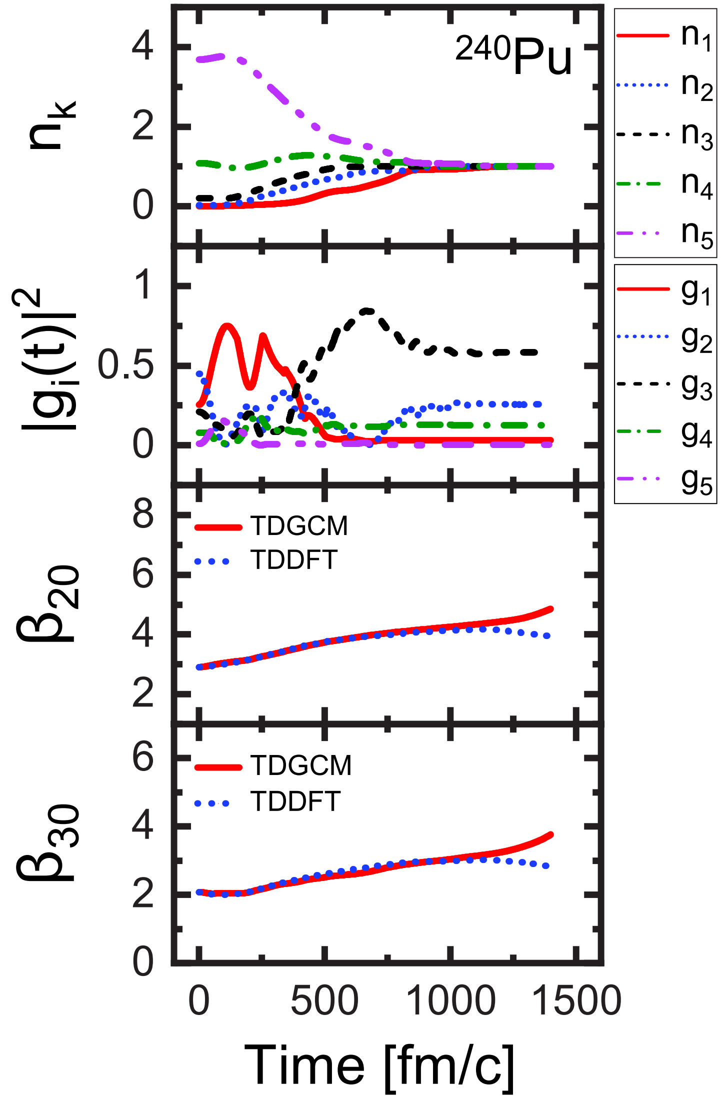
...collective wave function: $g = \mathcal{N}^{1/2} f$

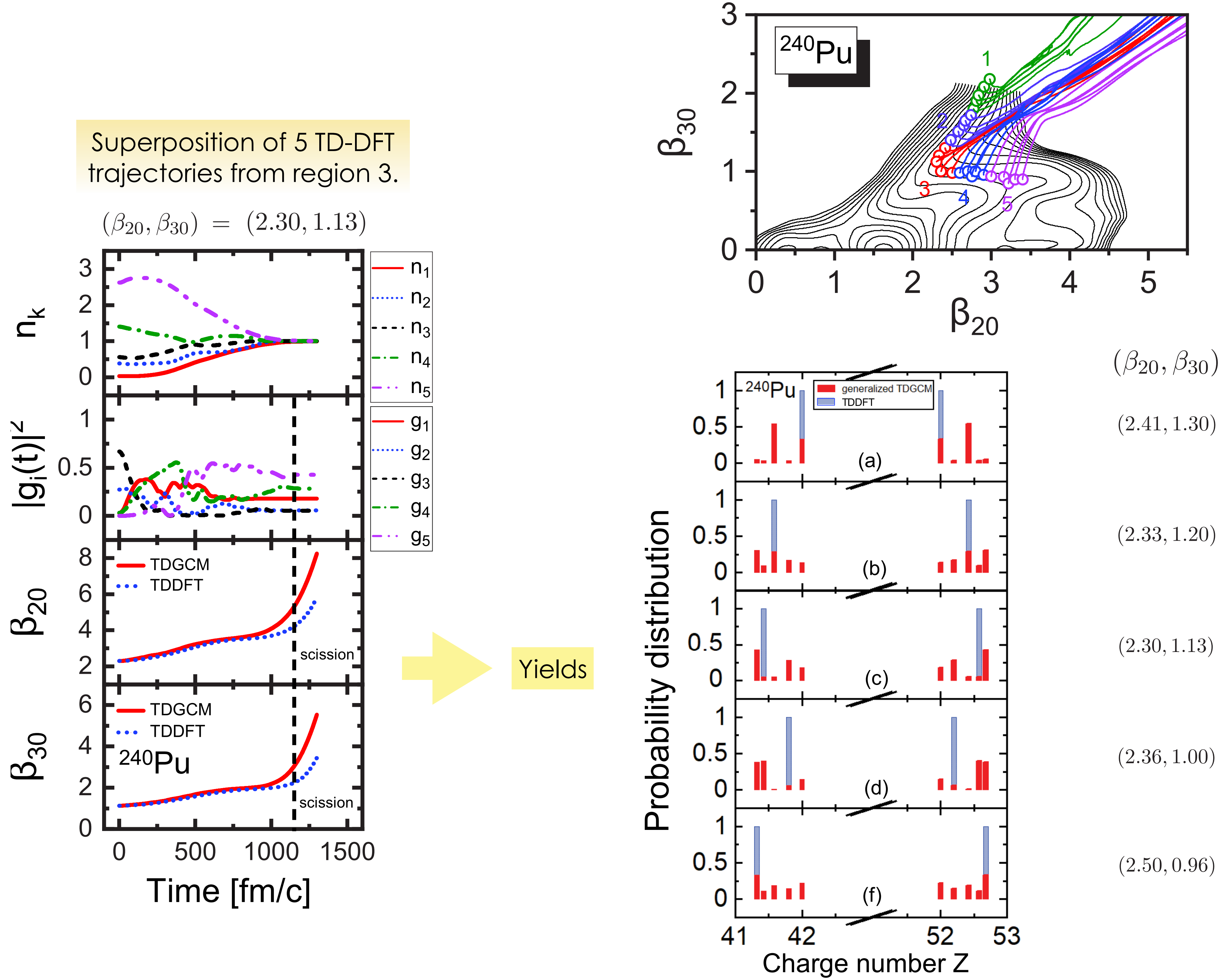
$$
\boxed{i\hbar\dot{g} = \mathcal{N}^{-1/2}(H - H^{MF})\mathcal{N}^{-1/2}g + i\hbar\dot{\mathcal{N}}^{1/2}\mathcal{N}^{-1/2}g.}
$$



The initial point for the generalized GCM evolution is at β_{20} = 2.91 and β_{30} = 2.08.

Superposition of 5 TD-DFT trajectories from region 1.





Superposition of 5 TD-DFT trajectories from region 3.
$(\beta_{20}, \beta_{30}) = (2.30, 1.13)$
n_k
$|g_i(t)|^2$
β_{20}
β_{30}
Time [fm/c]
n_1 n_2 n_3 n_4 n_5
g_1 g_2 g_3 g_4 g_5
TDGCM
TDDFT
scission
^{240}Pu
Yields
β_{30}
β_{20}
(β_{20}, β_{30})
generalized TDGCM
TDDFT
Probability distribution
Charge number Z
(a) $(2.41, 1.30)$
(b) $(2.33, 1.20)$
(c) $(2.30, 1.13)$
(d) $(2.36, 1.00)$
(f) $(2.50, 0.96)$

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