Induced Nuclear Fission Dynamics

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Microscopic Models

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)

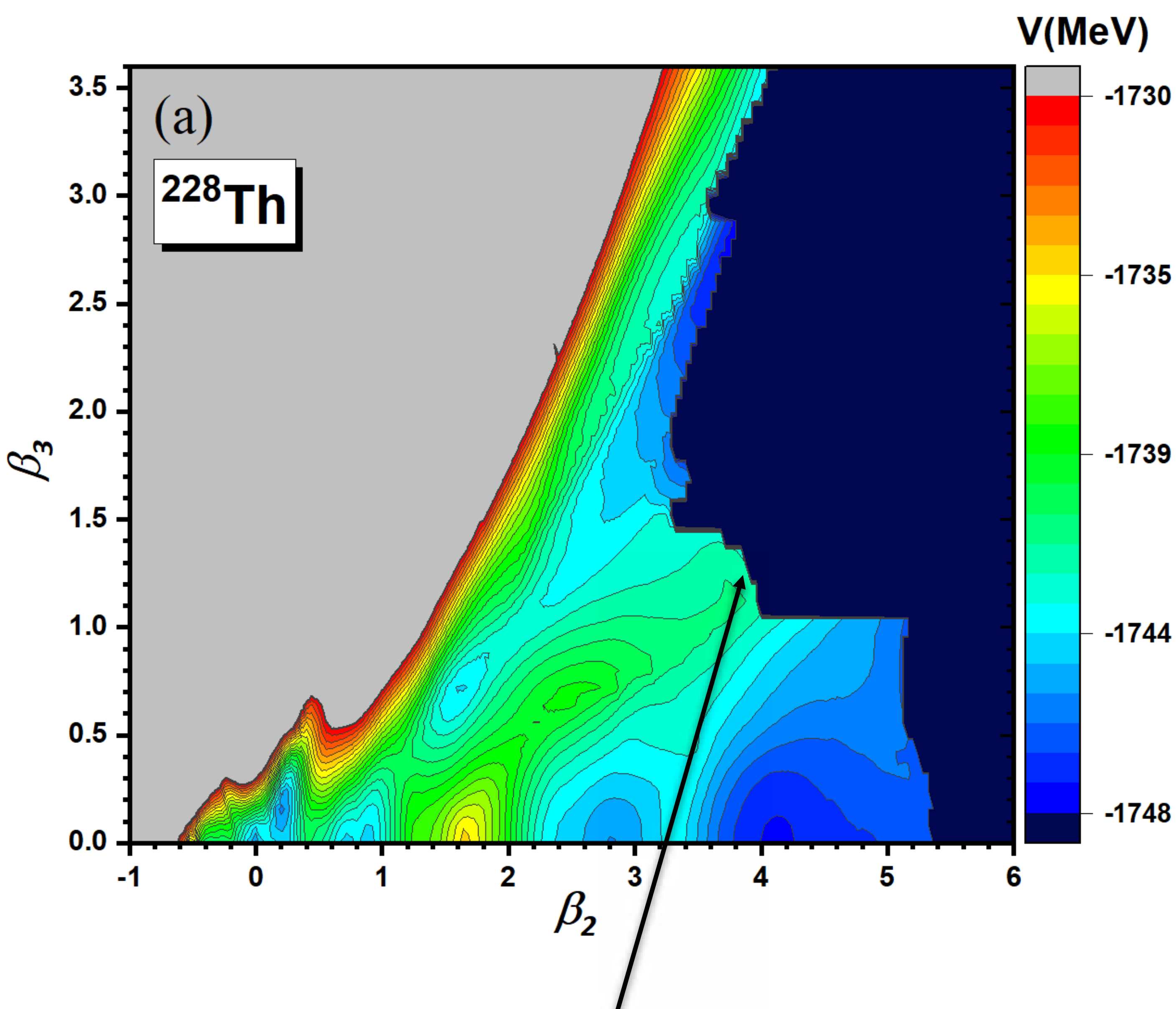
Example

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

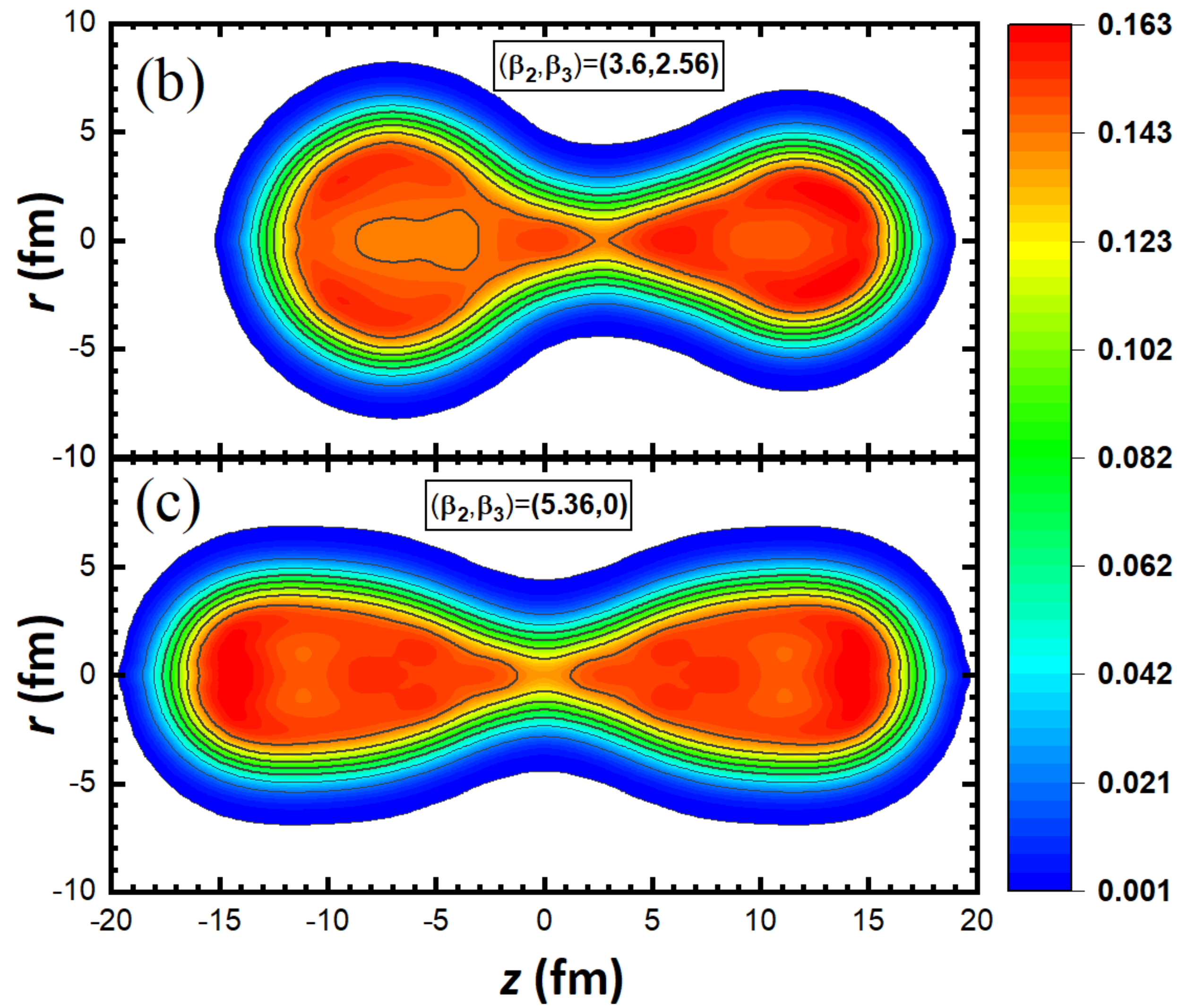
$$i\hbar\frac{\partial}{\partial t}g(\beta_2,\beta_3,t) = \left[-\frac{\hbar^2}{2}\sum_{kl}\frac{\partial}{\partial\beta_k}B_{kl}(\beta_2,\beta_3)\frac{\partial}{\partial\beta_l} + V(\beta_2,\beta_3)\right]g(\beta_2,\beta_3,t)$$

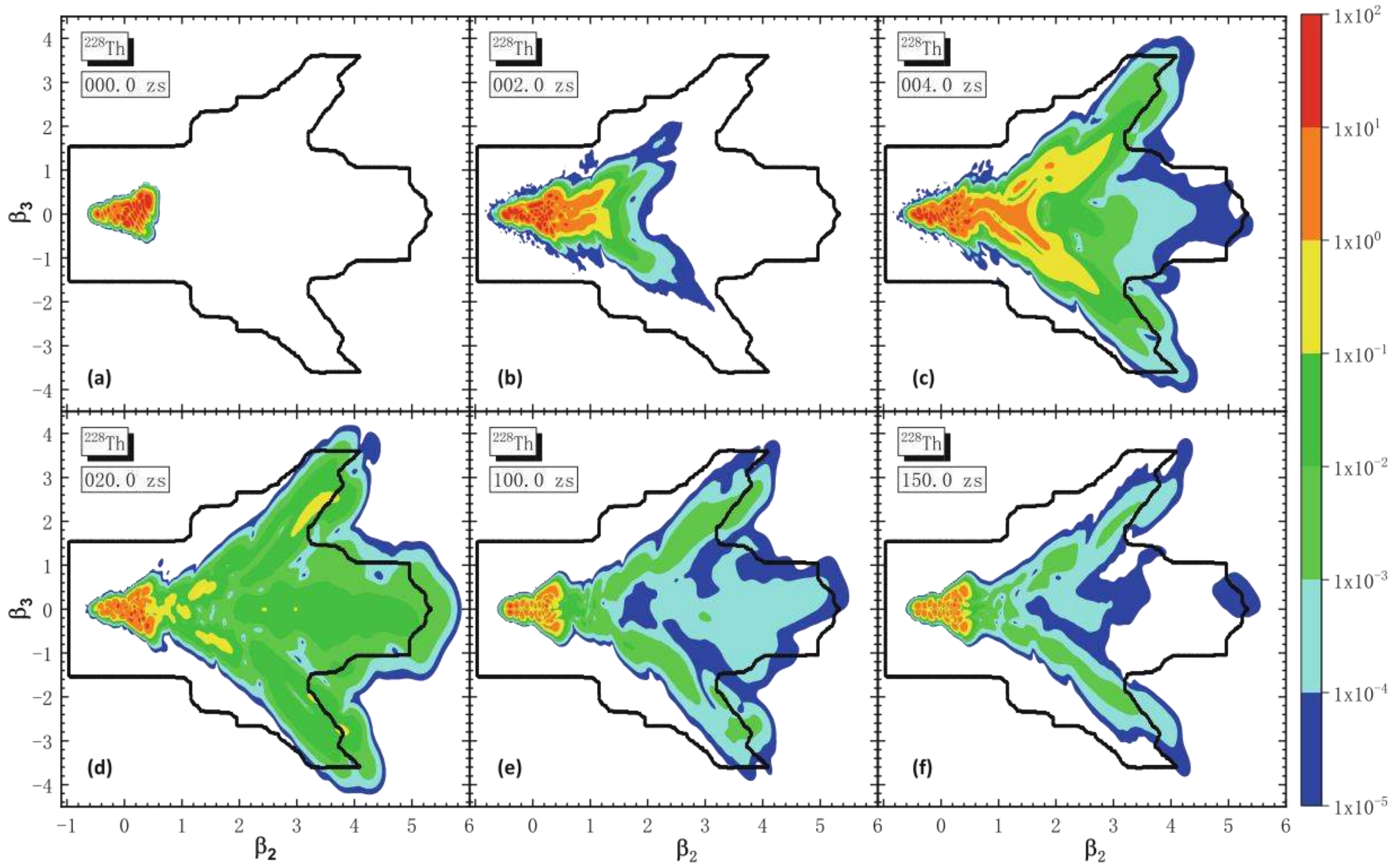
Quadrupole and octupole constrained deformation energy surface of ^{228}Th in the $\beta_2 - \beta_3$ plane.

Density profiles on the scission contour.



Scission contour





Time evolution of the probability density $|g|^2$ in the (β_2, β_3) plane. The solid line corresponds to the scission hypersurface.

…current

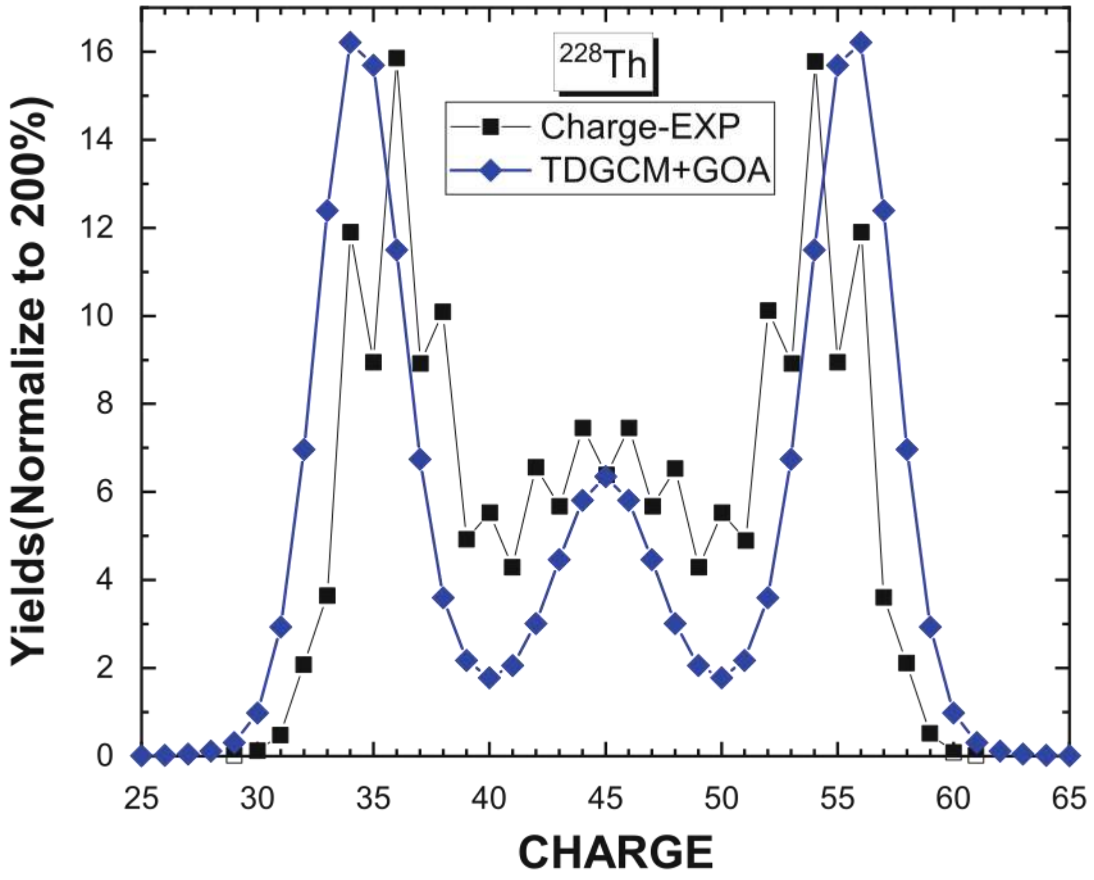
$$J_k(\beta_2, \beta_3, t) = \frac{\hbar}{2i} \sum_{l=2}^{3} B_{kl}(\beta_2, \beta_3)[g^*(\beta_2, \beta_3, t) \frac{\partial g(\beta_2, \beta_3, t)}{\partial \beta_l} - g(\beta_2, \beta_3, t) \frac{\partial g^*(\beta_2, \beta_3, t)}{\partial \beta_l}].$$

…integrated flux

$$F(\xi, t) = \int_{t_0}^{t} dt' \int_{\{\beta_{20}, \beta_{30}\} \in \xi} \boldsymbol{J}(\beta_{20}, \beta_{30}, t') d\boldsymbol{S},$$

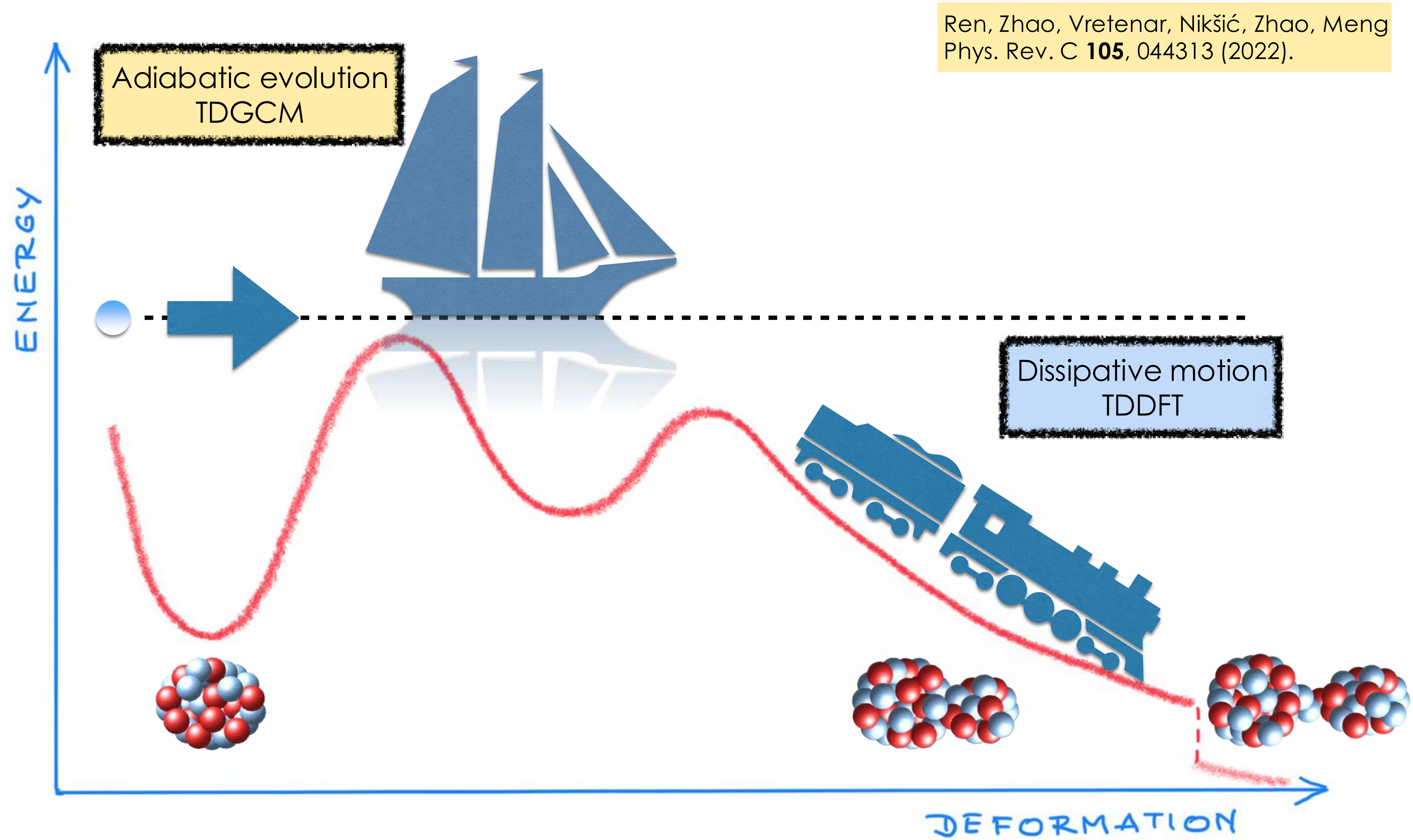
…charge yield

$$Y(Z) \propto \sum_{\xi \in \mathcal{A}} \lim_{t \to \infty} F(\xi, t).$$



Adiabatic evolution and dissipative dynamics

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



Time-dependent density functional theory (TDDFT)

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

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

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

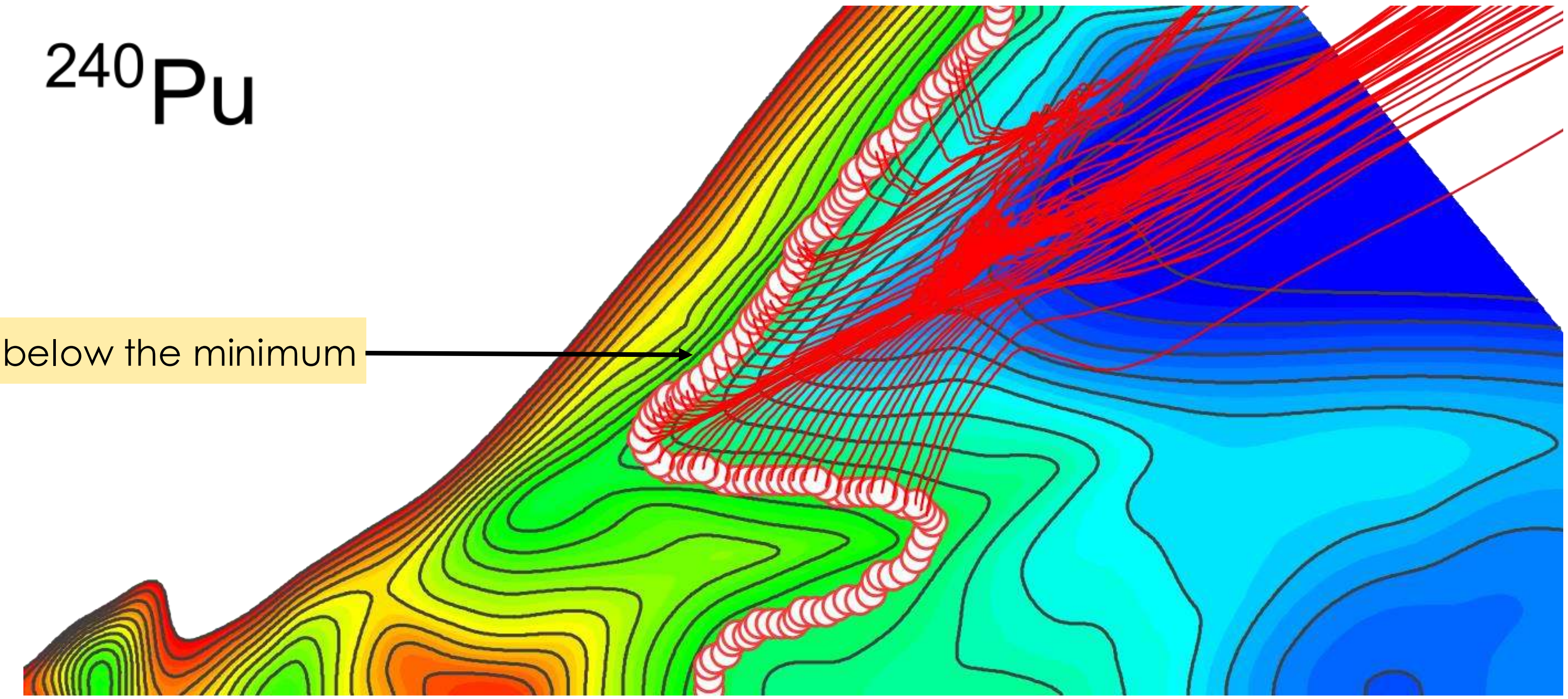
… classical evolution of independent nucleons in mean-field potentials, cannot be applied in classically forbidden regions of the collective space, nor does it take into account quantum fluctuations.

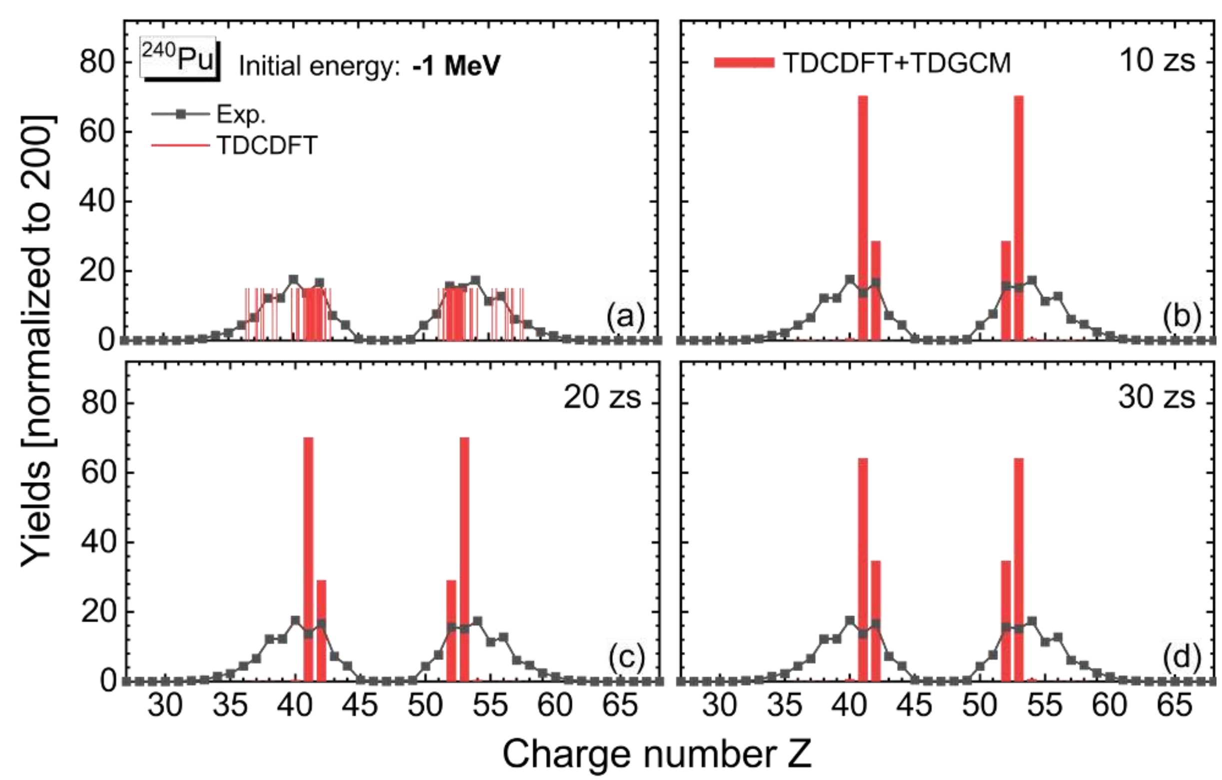
⇒ automatically includes the one-body dissipation mechanism, but can only simulate a single fission event by propagating the nucleons independently.

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.

TDDFT fission trajectories

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





Total kinetic energies (TKEs) of the fragments

TDGCM+GOA

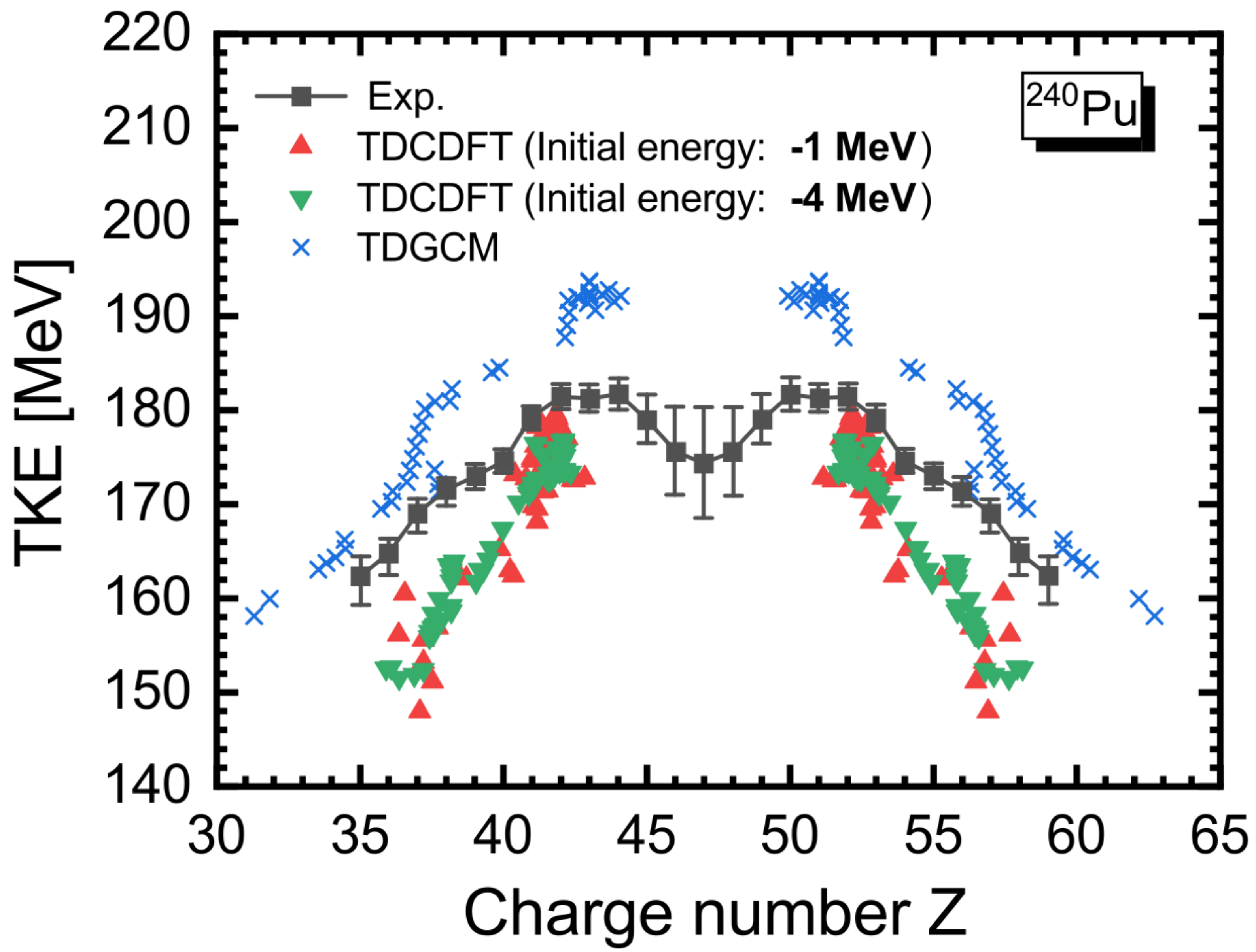
$$E_{\rm TKE} = \frac{e^2 Z_H Z_L}{d_{\rm ch}},$$

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

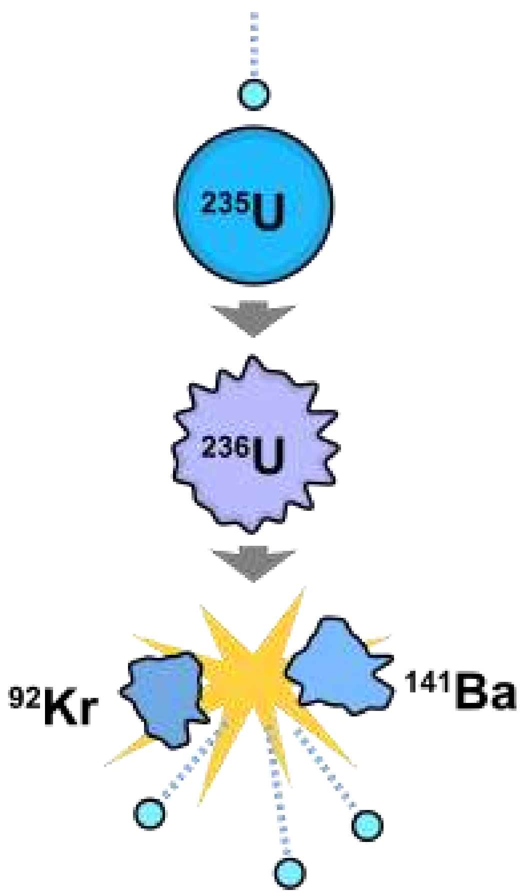
TDDFT

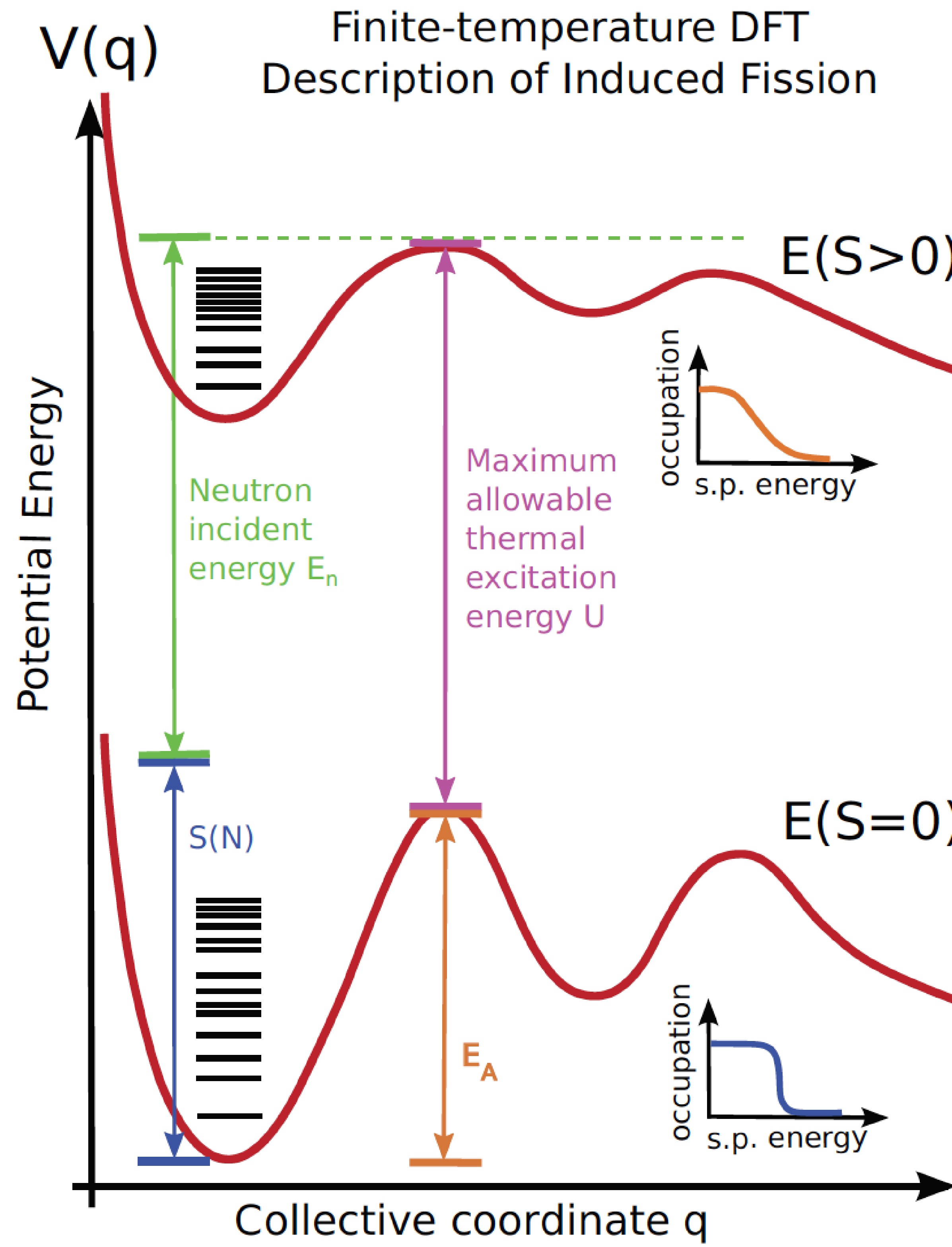
$$E_{\rm TKE} = \frac{1}{2} m A_{\rm H} \boldsymbol{v}_{\rm H}^2 + \frac{1}{2} m A_{\rm L} \boldsymbol{v}_{\rm L}^2 + E_{\rm Coul},$$

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



Induced Fission - Finite Temperature Effects





N. SCHUNCK, D. DUKE, AND H. CARR

PHYSICAL REVIEW C **91**, 034327 (2015)

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

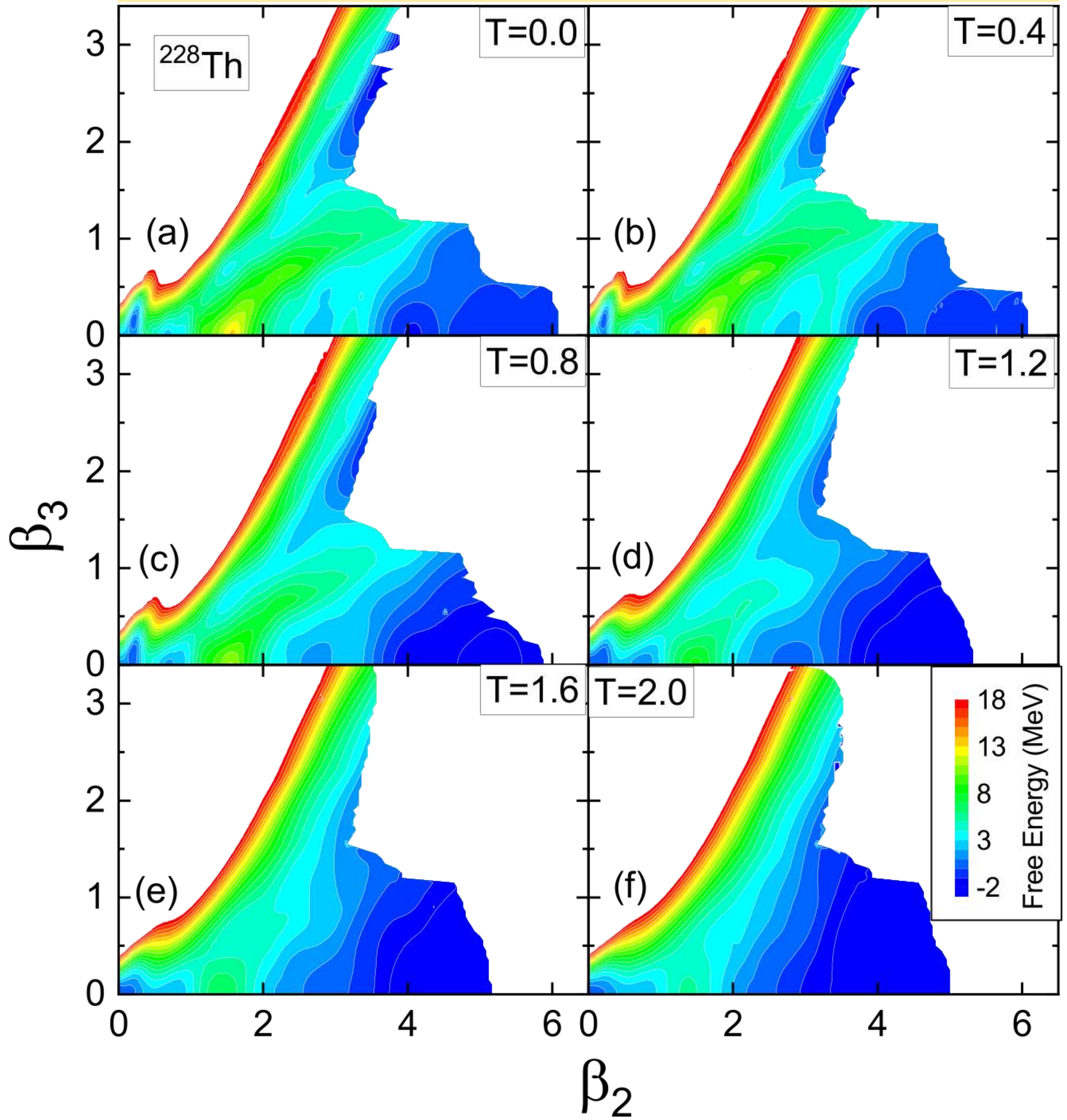
Extended TDGCM

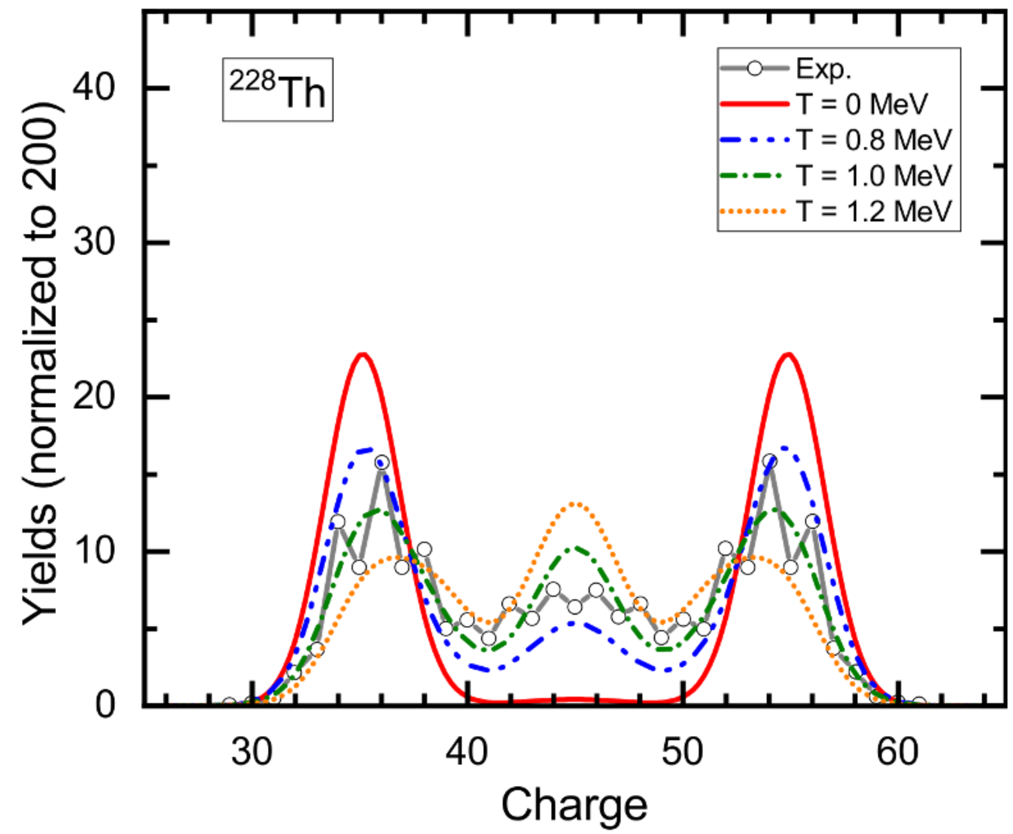
$$i\hbar\partial_t \psi(\boldsymbol{q},T;t) = \left[V(\boldsymbol{q},T) + \boldsymbol{P}\frac{1}{2\mathcal{M}(\boldsymbol{q},T)}\boldsymbol{P}\right]\psi(\boldsymbol{q},T;t) + \frac{i}{2}\int \{\boldsymbol{P},\boldsymbol{\mathcal{O}}(\boldsymbol{q};T,T')\}\,\psi(\boldsymbol{q},T';t)dT',$$

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

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

2D TDGCM+GOA calculation at fixed temperatures T.

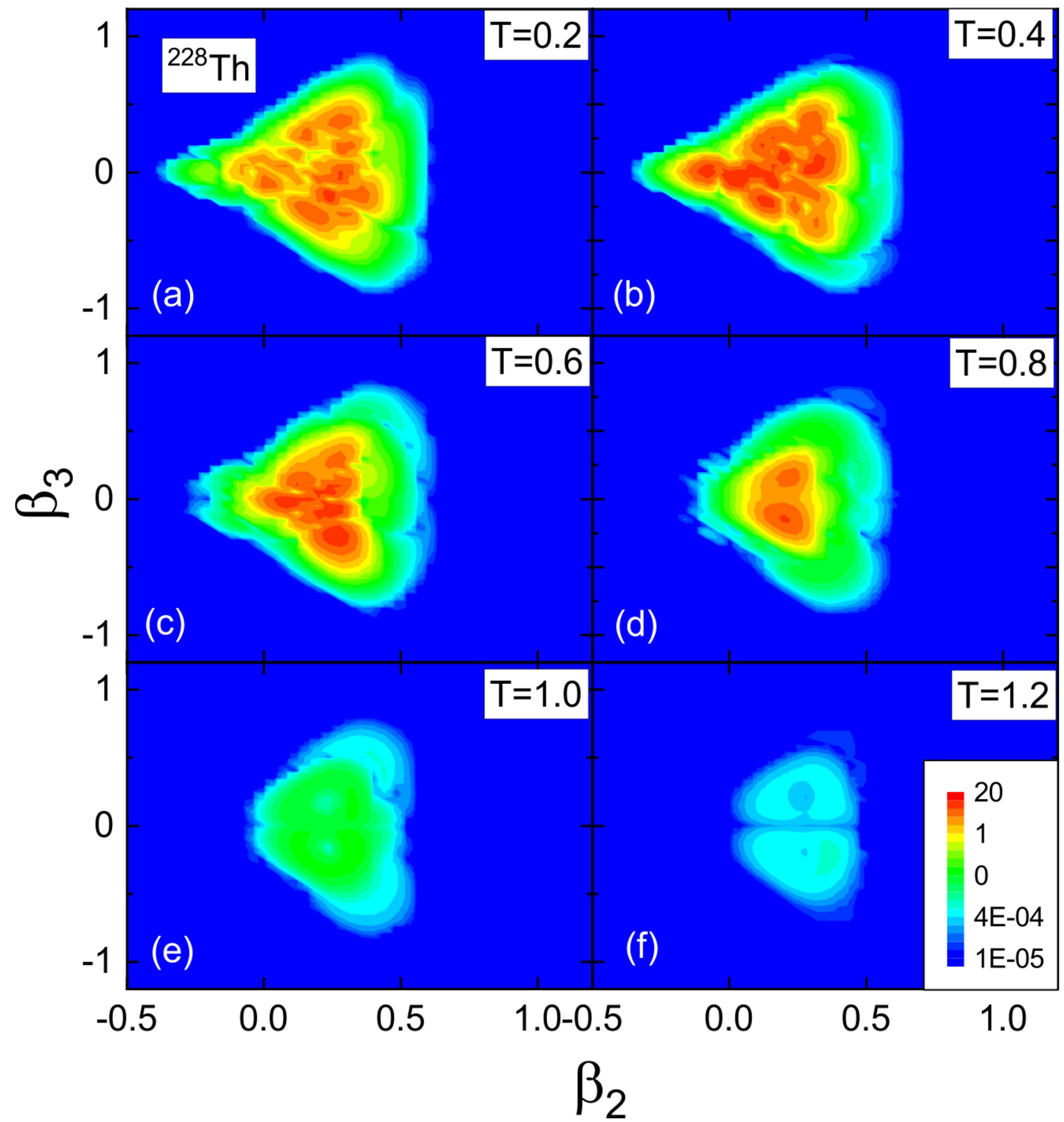




The data for photo-induced fission correspond to photon energies in the interval 8 – 14 MeV, and a peak value of E_γ = 11 MeV.

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:

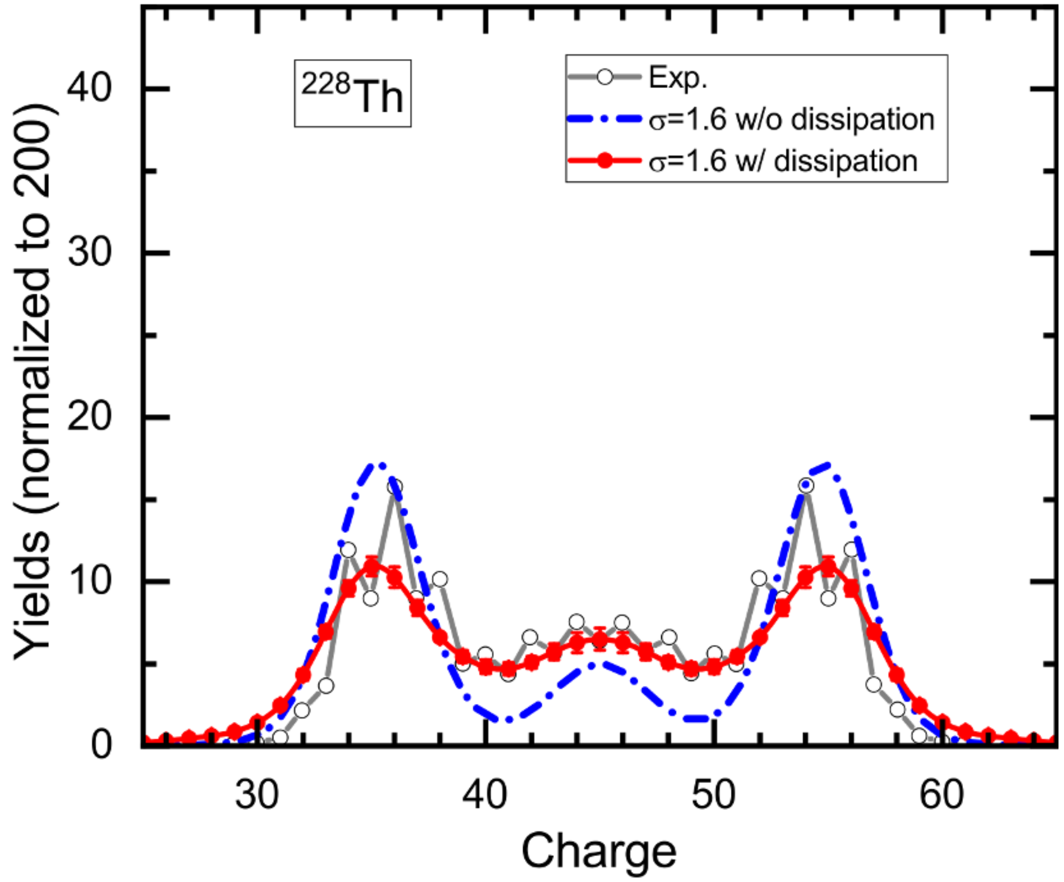
$$V(\boldsymbol{q},T) = \epsilon(T) + F(\boldsymbol{q},T)$$

The dissipation function:

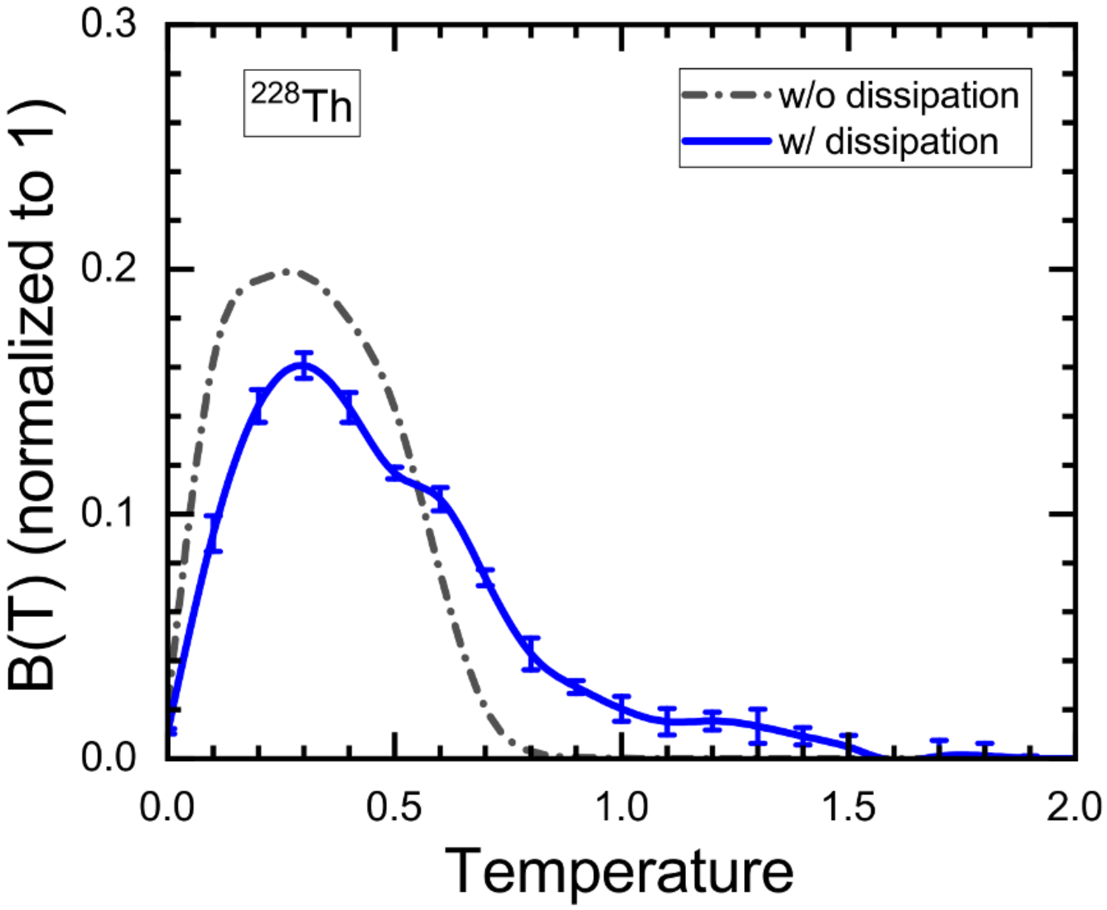
$$\boldsymbol{\eta}(\boldsymbol{q};T,T') = \begin{cases} 0 & \beta_2 < \beta_2^0 \\ \boldsymbol{\eta}(T,T') & \beta_2 \geq \beta_2^0, \end{cases}$$

Gaussian random variables

3D extended TDGCM charge yields.

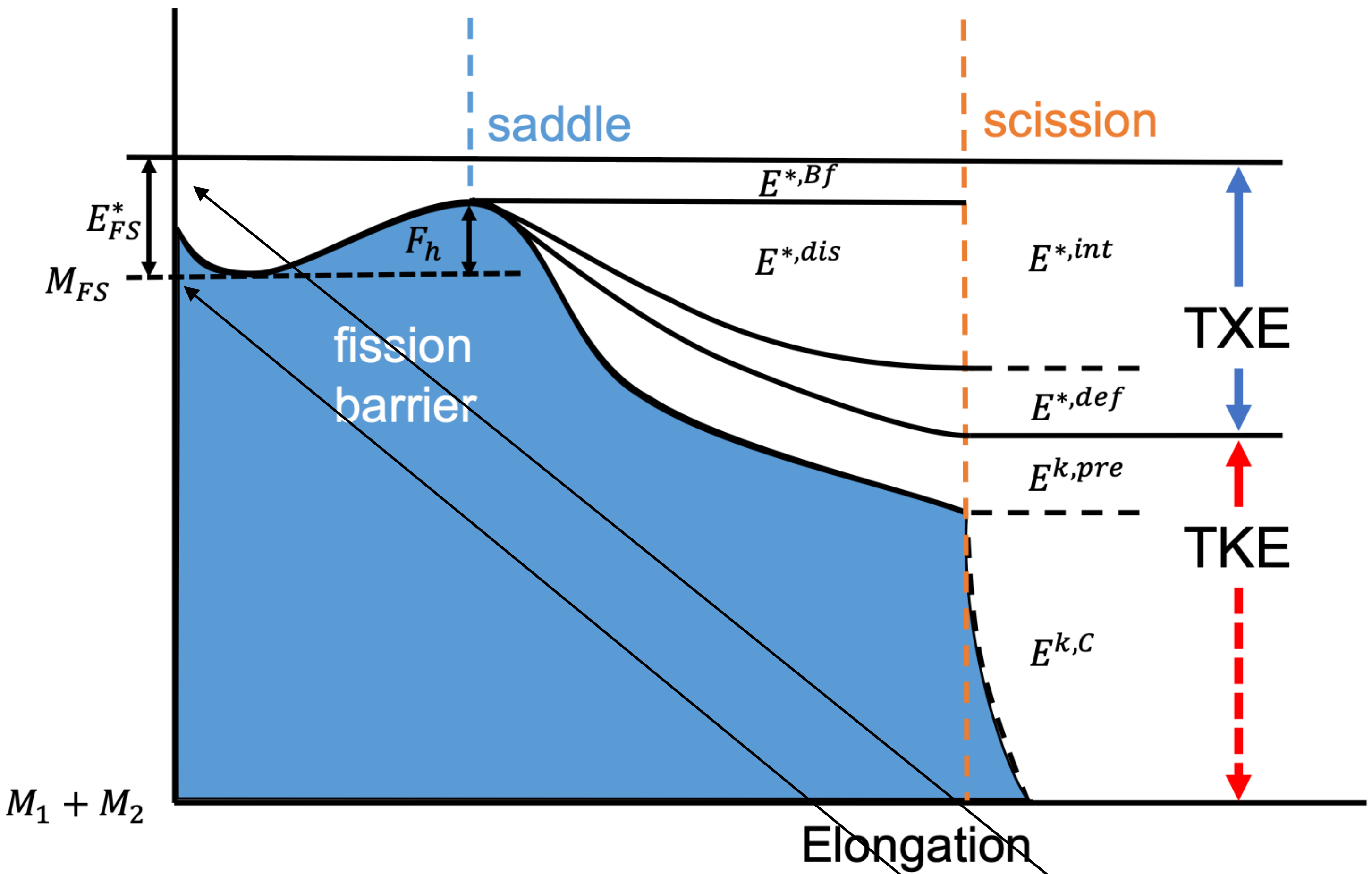


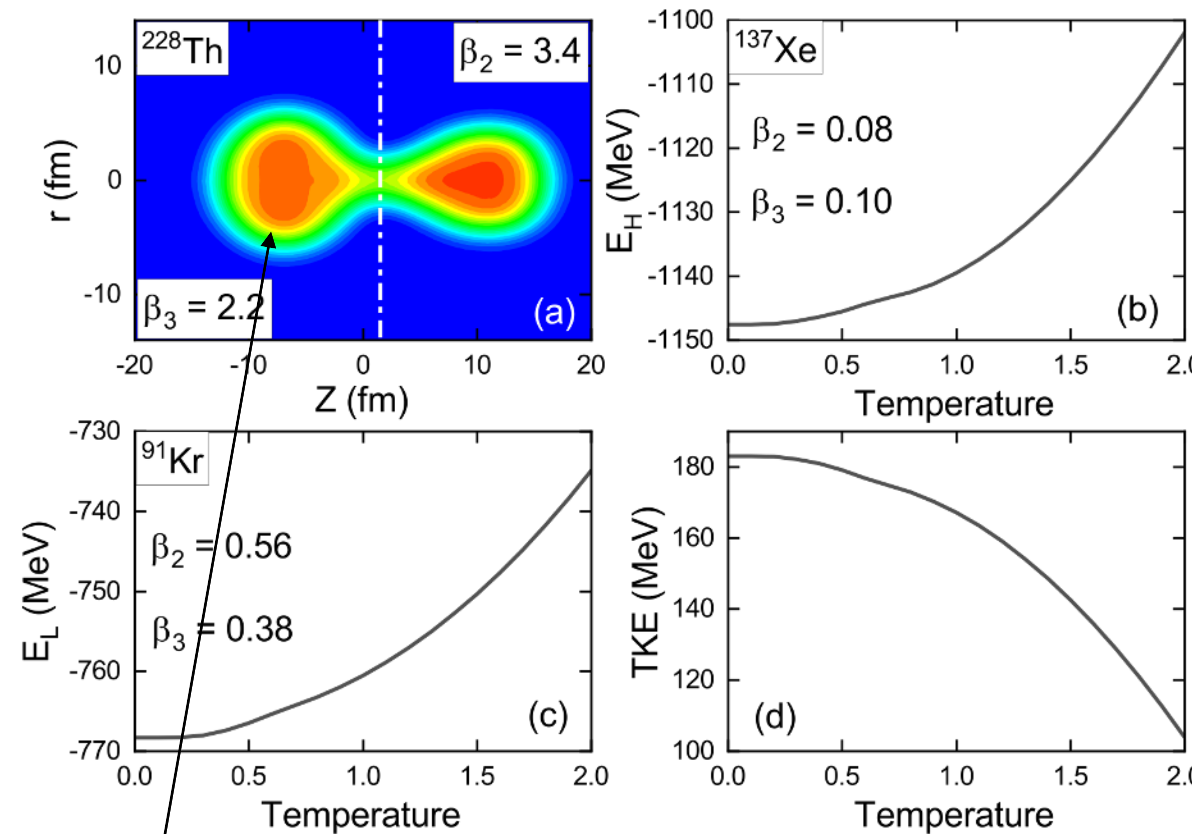
Time-integrated collective flux B(T) through the scission contour, as a function of temperature.



Total Kinetic Energy Distribution

Zhao, Nikšić, Vretenar, arXiv:2210.00460



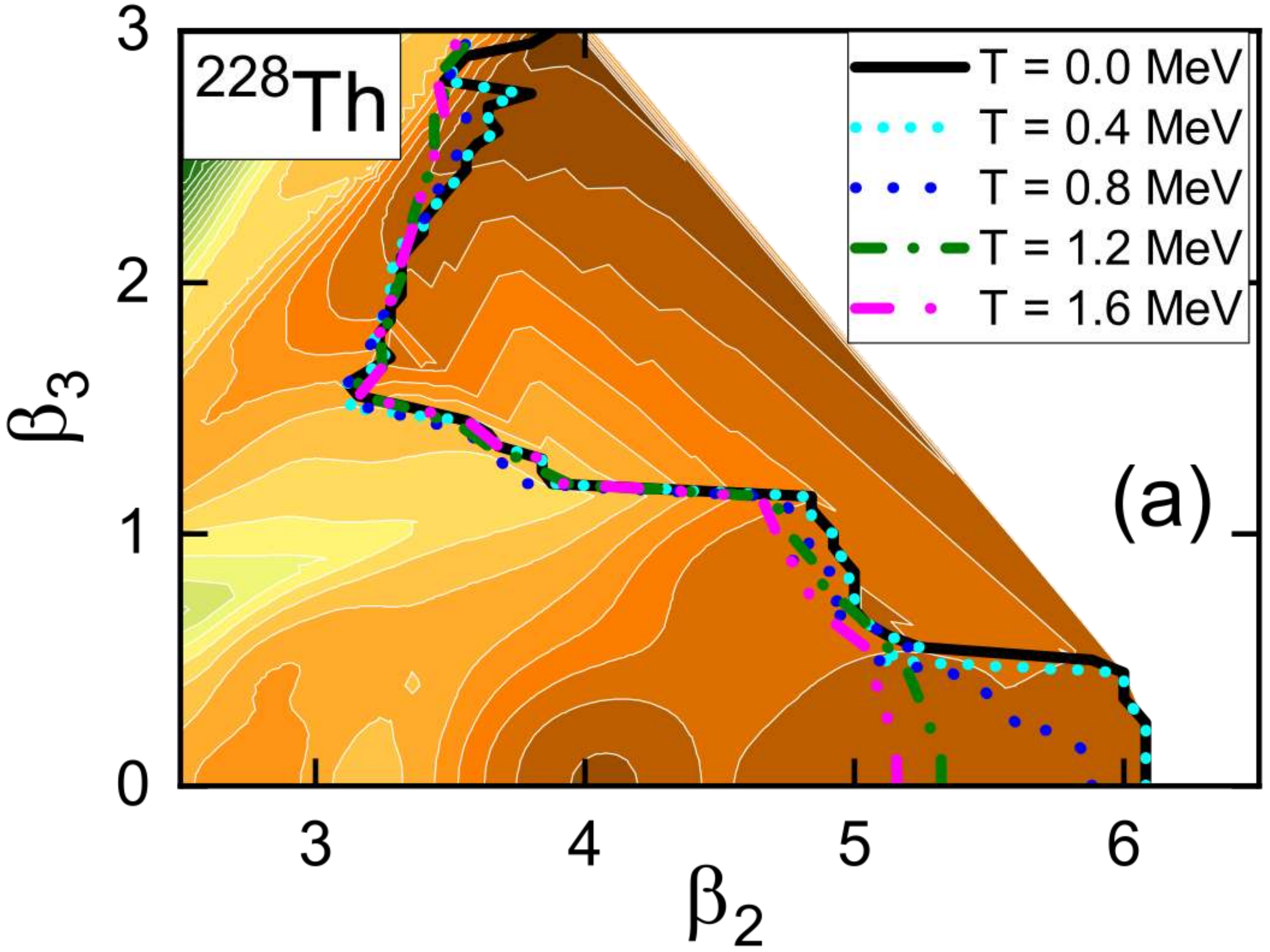


$$\mathrm{TKE}(\xi) = (E_{\mathrm{B}}^{\mathrm{FS}} + E^*_{\mathrm{coll}}) - [E^L(\beta_2^L, \beta_3^L, T) + E^H(\beta_2^H, \beta_3^H, T)]$$

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

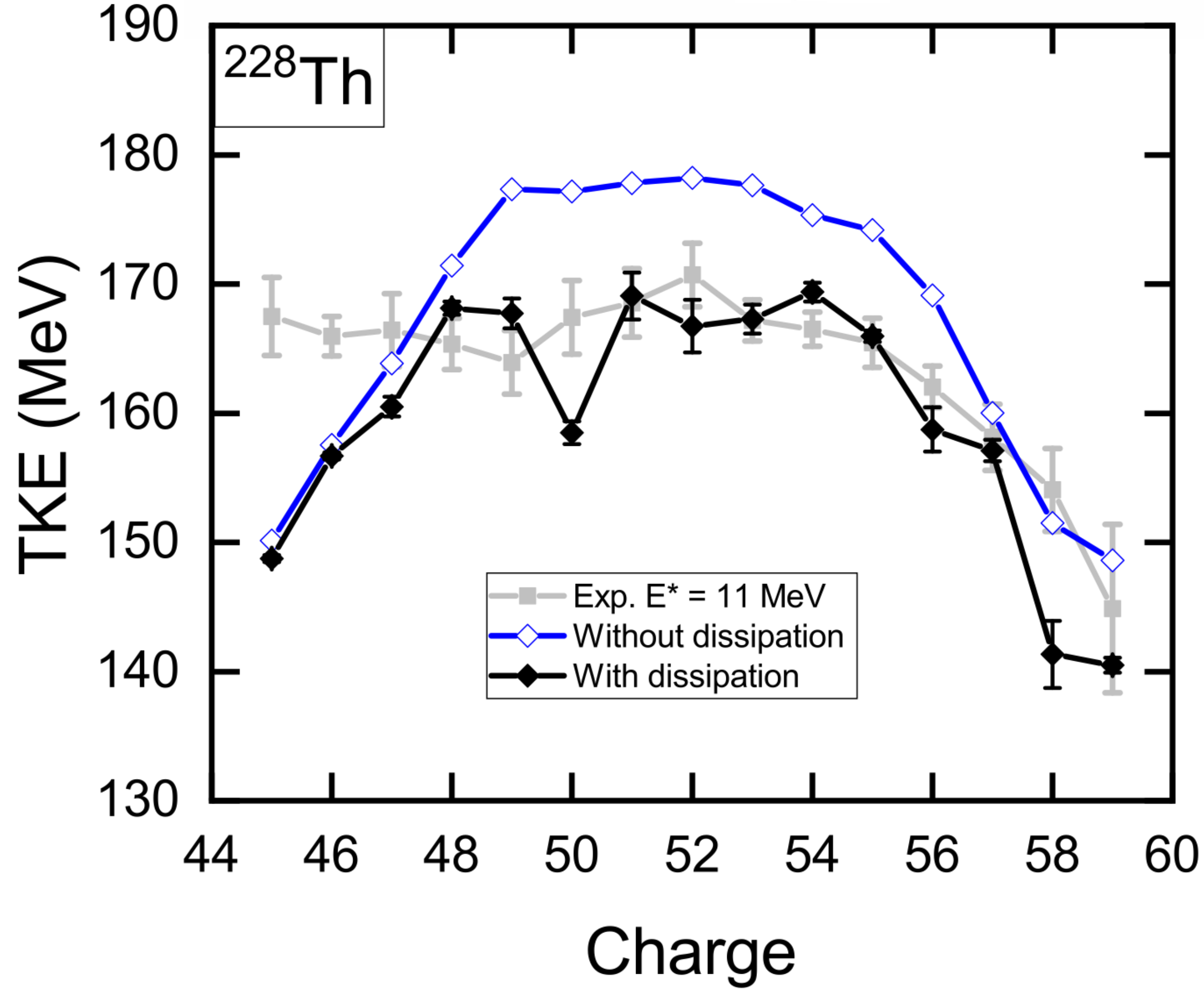
$$F(\xi; t) = \int_{t_0}^{t} dt' \int_{(\boldsymbol{q}, T) \in \xi} \boldsymbol{J}(\boldsymbol{q}, T; t') \cdot d\boldsymbol{S},$$

Scission contours for ^{228}Th in the (β_2, β_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:

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

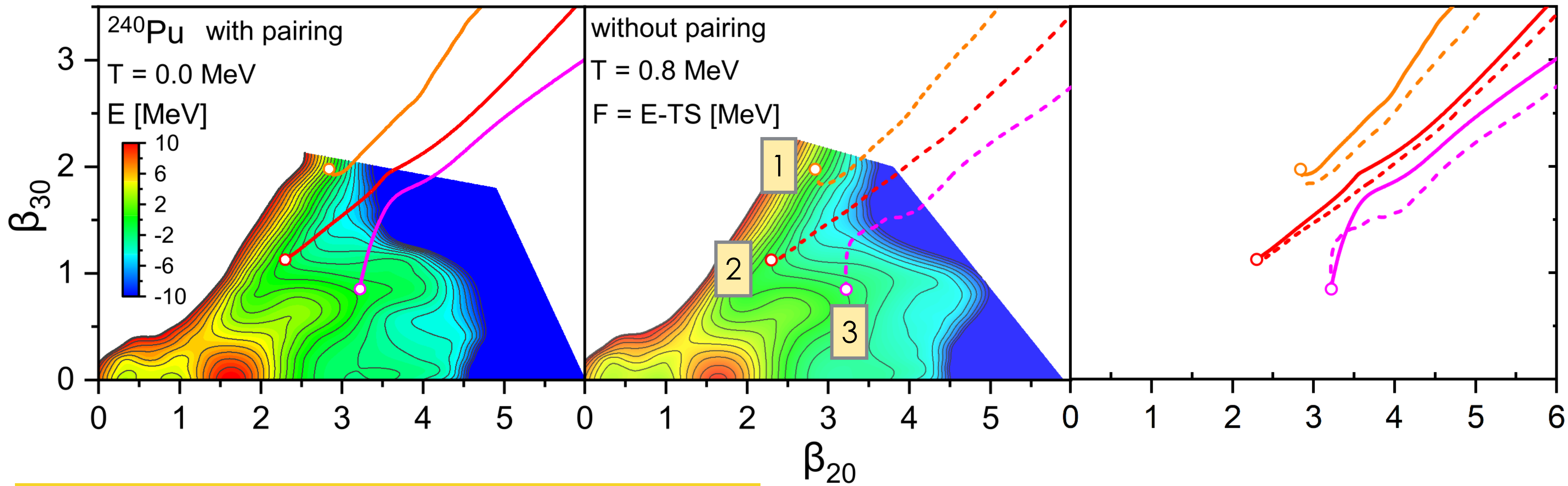


Zhao, Nikšić, Vretenar

Phys. Rev. C **106**, 054609 (2022).

Fission dynamics, dissipation, and clustering at finite temperature

Li, Vretenar, Ren, Nikšić, Zhao, Zhao, Meng, Phys. Rev. C **107**, 014303 (2023).



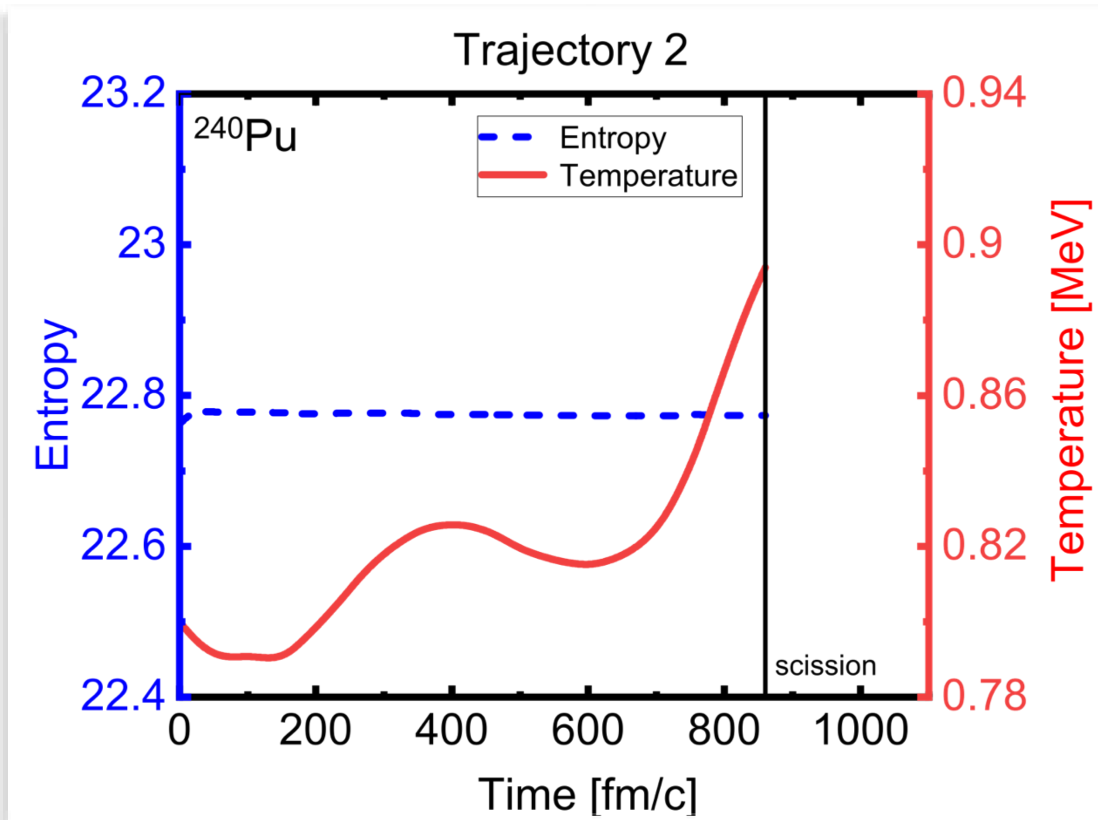
Time-dependent density functional theory (TDDFT)

→ time-dependent thermal occupation factors:

$$f_k(t) = \frac{1}{1 + e^{[\varepsilon_k(t) - \lambda(t)]/k_B T(t)}}$$

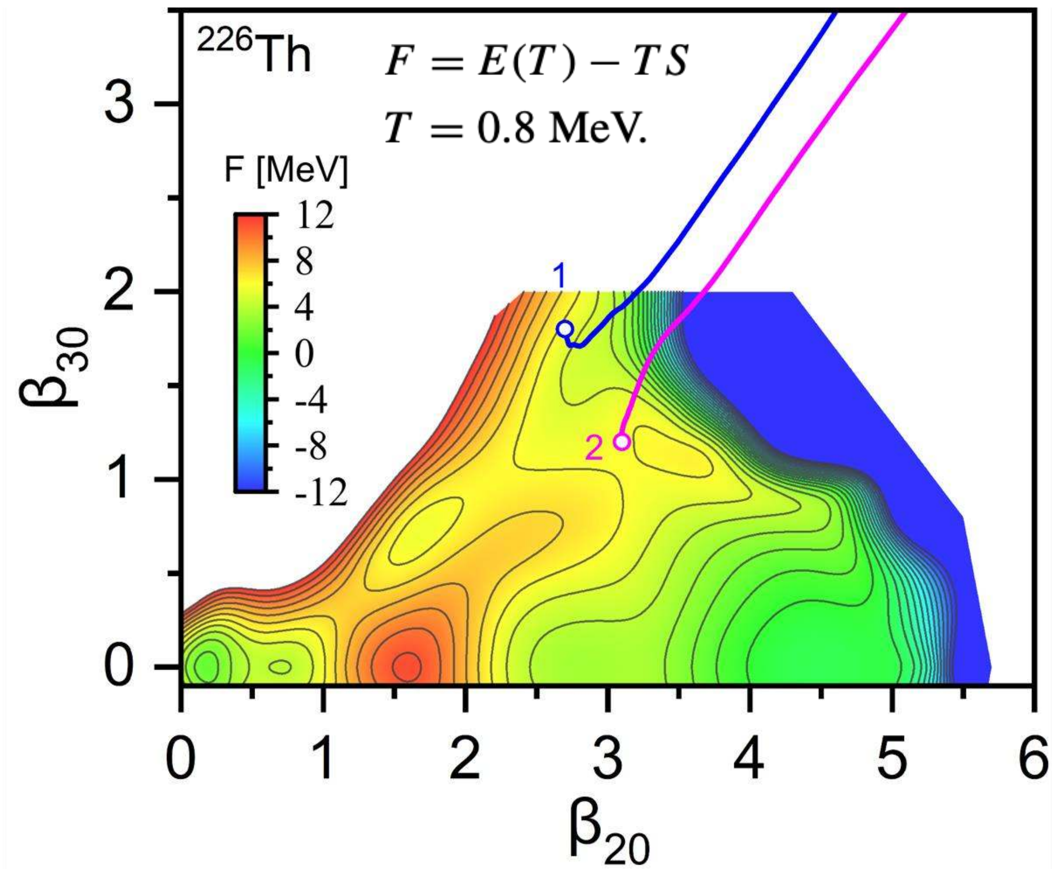
$$\varepsilon_k(t) = \langle \psi_k(\boldsymbol{r}, t) | \hat{h}(\boldsymbol{r}, t) | \psi_k(\boldsymbol{r}, t) \rangle$$

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

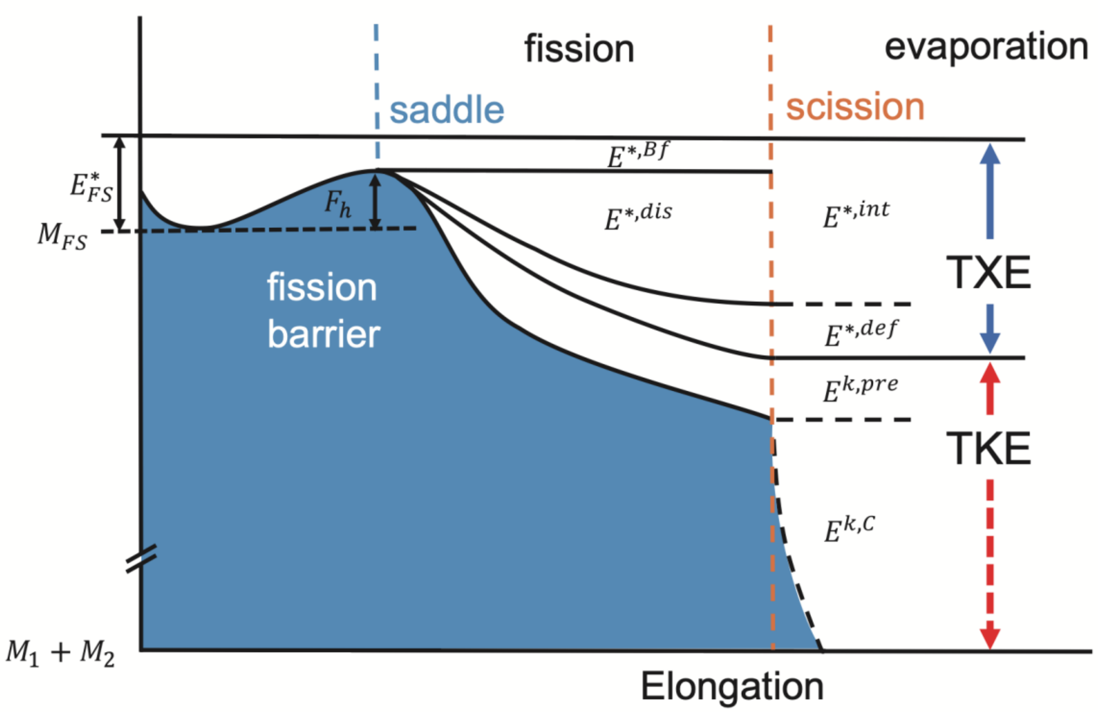


Induced-fission dynamics of ^{226}Th

Li, Vretenar, Nikšić, Zhao, Meng, Phys. Rev. C **110**, 034302 (2024).



Trajectory	1	2
T^{init}	0.80	0.80
E_{init}	−1707.15	−1703.12
E^{*}_{FS}	10.47	10.47
$E^{k,\text{pre}}$	12.19	12.56
$E^{k,C}$	143.60	144.18
$E^{1,T=0}_{\text{g.s.}}(M_1)$	−1155.21	−1131.11
$E^{*,\text{def}}_{1}$	1.82	11.12
$E^{2,T=0}_{\text{g.s.}}(M_2)$	−735.74	−767.06
$E^{*,\text{def}}_{2}$	6.16	5.73
$E^{*,\text{int}}$	20.03	21.47
$E^{*,\text{dis}}$	9.56	11.00
T_{sci}	0.82	0.90



Energy balance:

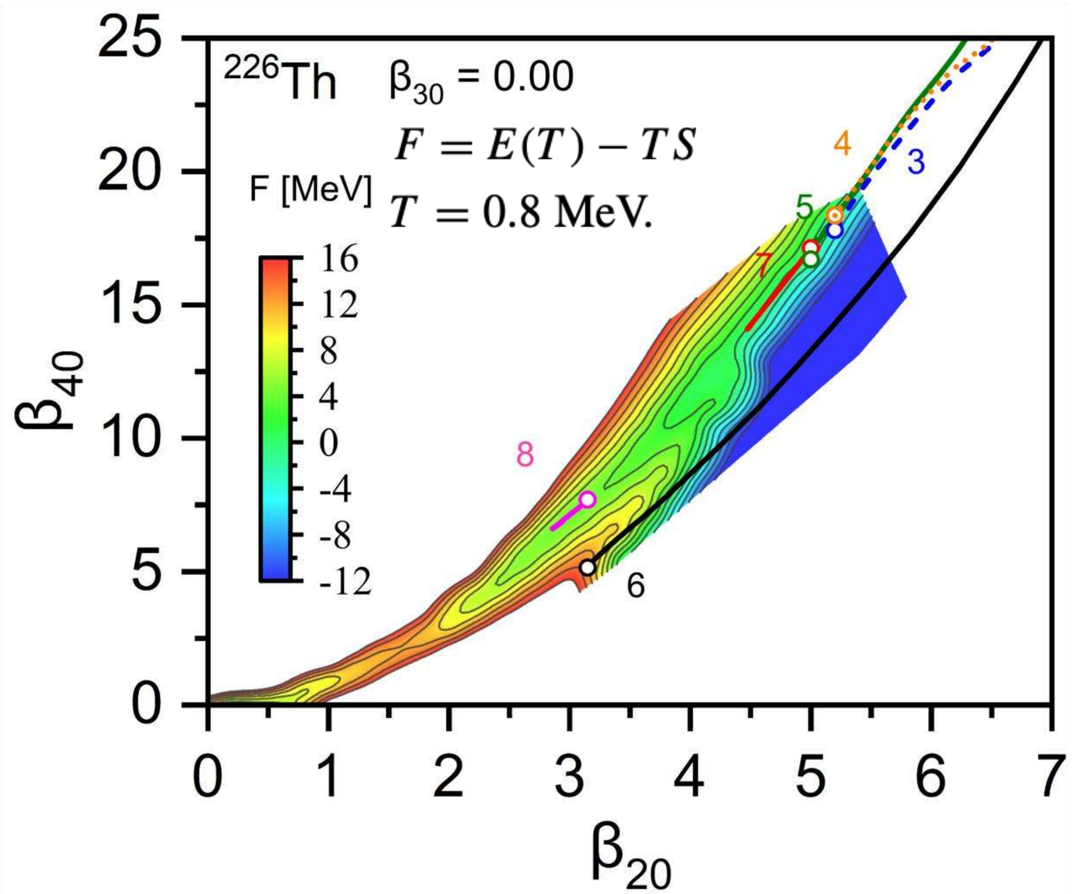
$$E_{\text{init}} = E^{1,T=0}_{\text{g.s.}} + E^{2,T=0}_{\text{g.s.}} + \text{TKE} + \text{TXE}.$$

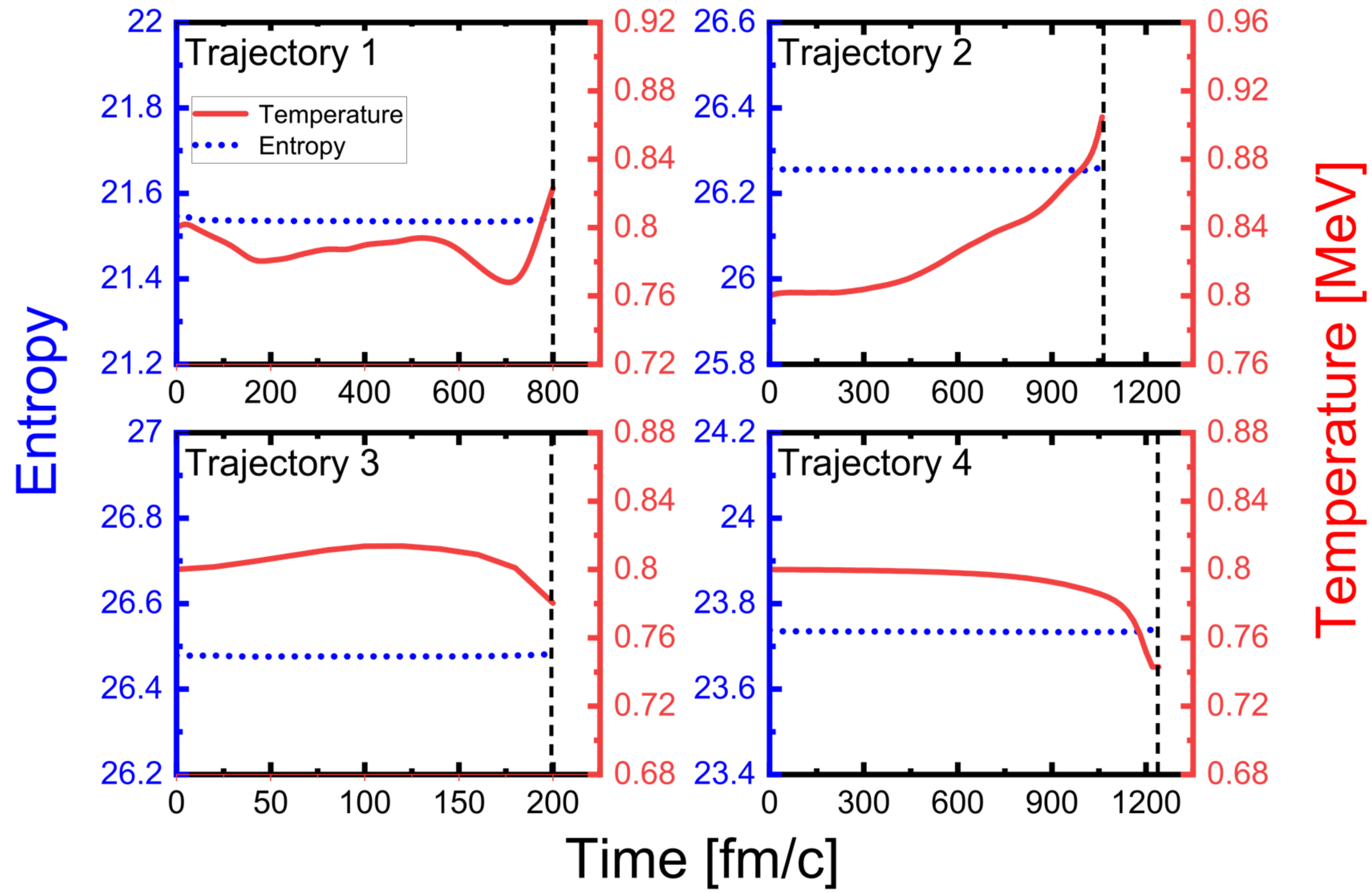
$$E^{k,\text{pre}} = \frac{m}{2}\int \rho(\vec{r}, t_{\text{sci}})\vec{v}^{\,2}(\vec{r}, t_{\text{sci}})d\vec{r},$$

$$\text{TXE} = \sum_{i=1}^{2} E^{*,\text{def}}_{i} + E^{*,\text{int}}$$

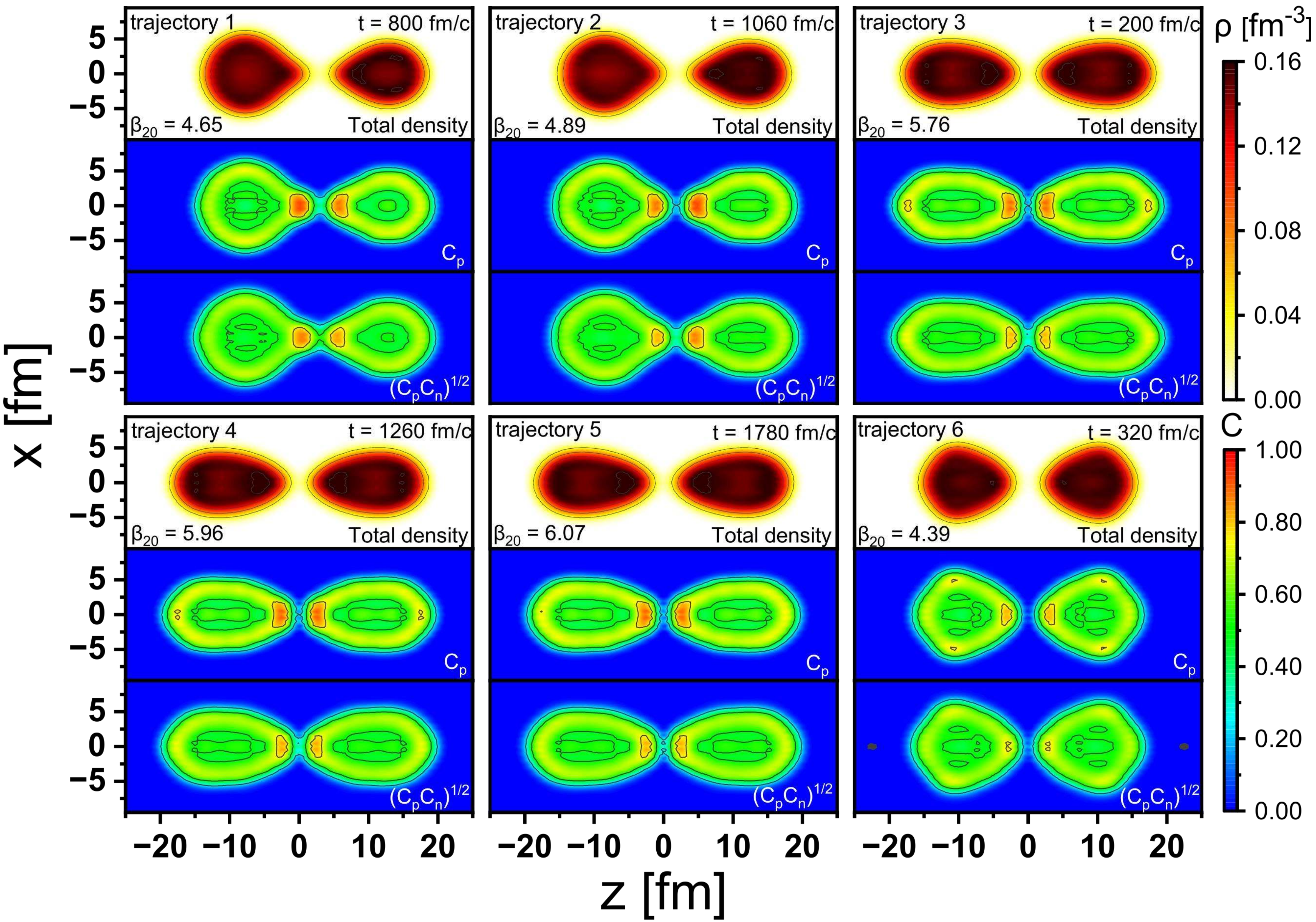
$$E^{*,\text{dis}} = E^{*,\text{int}} - E^{*}_{\text{FS}},$$

Symmetric trajectories





Trajectory	1	2	3	4
T^{init}	0.80	0.80	0.80	0.80
E_{init}	−1707.15	−1703.12	−1708.53	−1711.48
E^{*}_{FS}	10.47	10.47	10.47	10.47
$E^{k,\text{pre}}$	12.19	12.56	6.23	5.57
$E^{k,C}$	143.60	144.18	147.18	144.79
$E^{1,T=0}_{\text{g.s.}}(M_1)$	−1155.21	−1131.11	−946.95	−946.95
$E^{*,\text{def}}_{1}$	1.82	11.12	8.88	9.01
$E^{2,T=0}_{\text{g.s.}}(M_2)$	−735.74	−767.06	−946.95	−946.95
$E^{*,\text{def}}_{2}$	6.16	5.73	8.88	9.01
$E^{*,\text{int}}$	20.03	21.47	14.20	14.04
$E^{*,\text{dis}}$	9.56	11.00	3.73	3.57
T_{sci}	0.82	0.90	0.78	0.74



trajectory 1
t = 800 fm/c
β20 = 4.65
Total density
trajectory 2
t = 1060 fm/c
β20 = 4.89
trajectory 3
t = 200 fm/c
β20 = 5.76
trajectory 4
t = 1260 fm/c
β20 = 5.96
trajectory 5
t = 1780 fm/c
β20 = 6.07
trajectory 6
t = 320 fm/c
β20 = 4.39
Cp
(CpCn)1/2
ρ [fm-3]
C
x [fm]
z [fm]

Entropy of fragments and entanglement at finite temperature

The von Neumann entropy: $$S = -\mathrm{Tr}(\rho \ln \rho),$$

⇒ entropy $S^{(q)}_V$ for neutrons (q= n) or protons (q= p) of a fragment located in the subspace V:

$$S_V^{(q)} = -\mathrm{Tr}\{\boldsymbol{M}_V^{(q)} \ln \boldsymbol{M}_V^{(q)} + [\boldsymbol{I} - \boldsymbol{M}_V^{(q)}] \ln [\boldsymbol{I} - \boldsymbol{M}_V^{(q)}]\}$$
$$= -\sum_{i=1}^{N^{(q)}} \{d_i^{(q)} \ln d_i^{(q)} + [1 - d_i^{(q)}] \ln [1 - d_i^{(q)}]\},$$

$$S_V = S_V^{(n)} + S_V^{(p)}.$$

d_i are the eigenvalues of the overlap matrix $M^{(q)}$: $$[\boldsymbol{M}_V^{(q)}]_{ij} = \sqrt{f_i f_j} \langle \psi_i^{(q)} | \hat{\Theta}_V | \psi_j^{(q)} \rangle, \qquad \Theta_V(\boldsymbol{r}) = \begin{cases} 1 & \text{if } \boldsymbol{r} \in V, \\ 0 & \text{if } \boldsymbol{r} \notin V. \end{cases}$$

The entanglement (mutual information) between the fragments:

$$L = S_V + S_{\bar{V}} - S_{\mathrm{tot}},$$

Nucleus	^{226}Th					
Trajectory	1	2	3	4	5	6
S_{tot}	21.54	26.26	26.48	23.73	24.17	34.61
S_1	14.20	16.55	14.19	12.98	13.33	18.68
S_2	11.52	13.92	14.19	12.98	13.33	18.68
L	4.18	4.21	1.90	2.23	2.49	2.75

Generalized time-dependent generator coordinate method

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

Li, Vretenar, Nikšić, Zhao, Zhao, Meng, Front. Phys. **19**, 44201 (2024).

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:

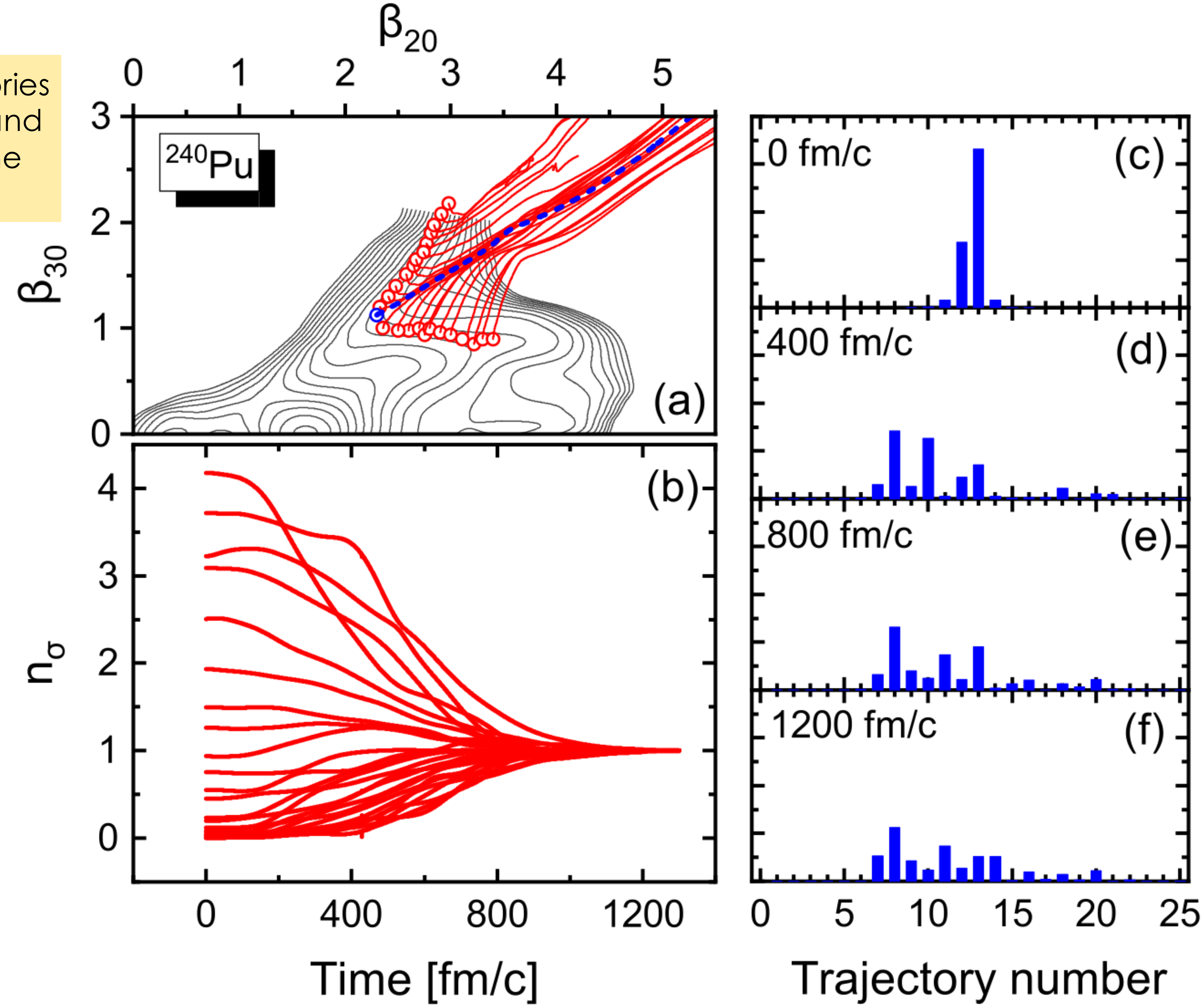
$$\begin{cases} \mathcal{N}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|\Phi_{\boldsymbol{q}}(t)\rangle, \\ \mathcal{H}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|\hat{H}|\Phi_{\boldsymbol{q}}(t)\rangle, \\ \mathcal{H}^{MF}_{\boldsymbol{q}'\boldsymbol{q}}(t)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

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

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

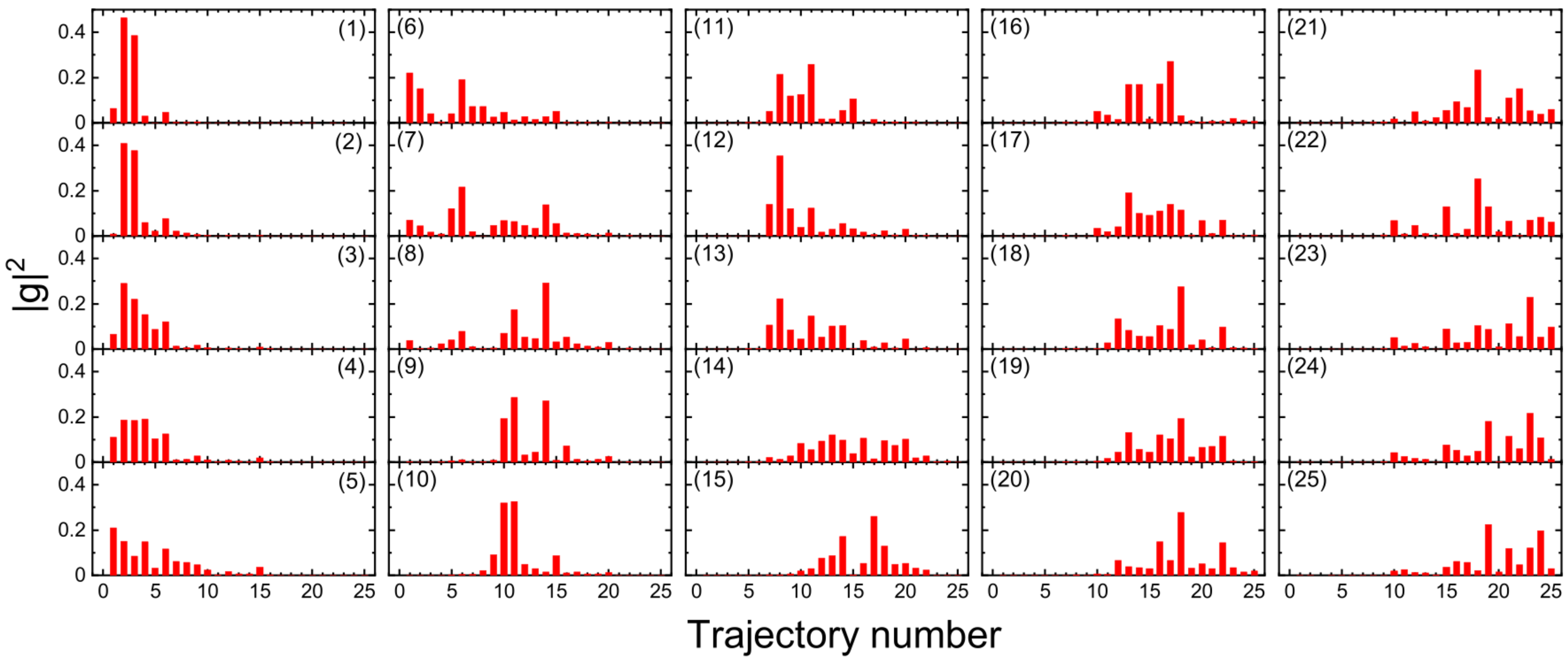
$$i\hbar\dot{g} = \mathcal{N}^{-1/2}(H - H^{MF})\mathcal{N}^{-1/2}g + i\hbar\dot{\mathcal{N}}^{1/2}\mathcal{N}^{-1/2}g.$$

Self-consistent TDDFT fission trajectories that start from the 25 initial points, and are used as a generator basis for the generalized TDGCM.



Time evolution of the eigenvalues of the norm kernel.

Square moduli of the components of the TDGCM collective wave function, that starts from the initial point $(\beta_{20},\beta_{30}) = (2.30,1.13)$ of trajectory number 13.



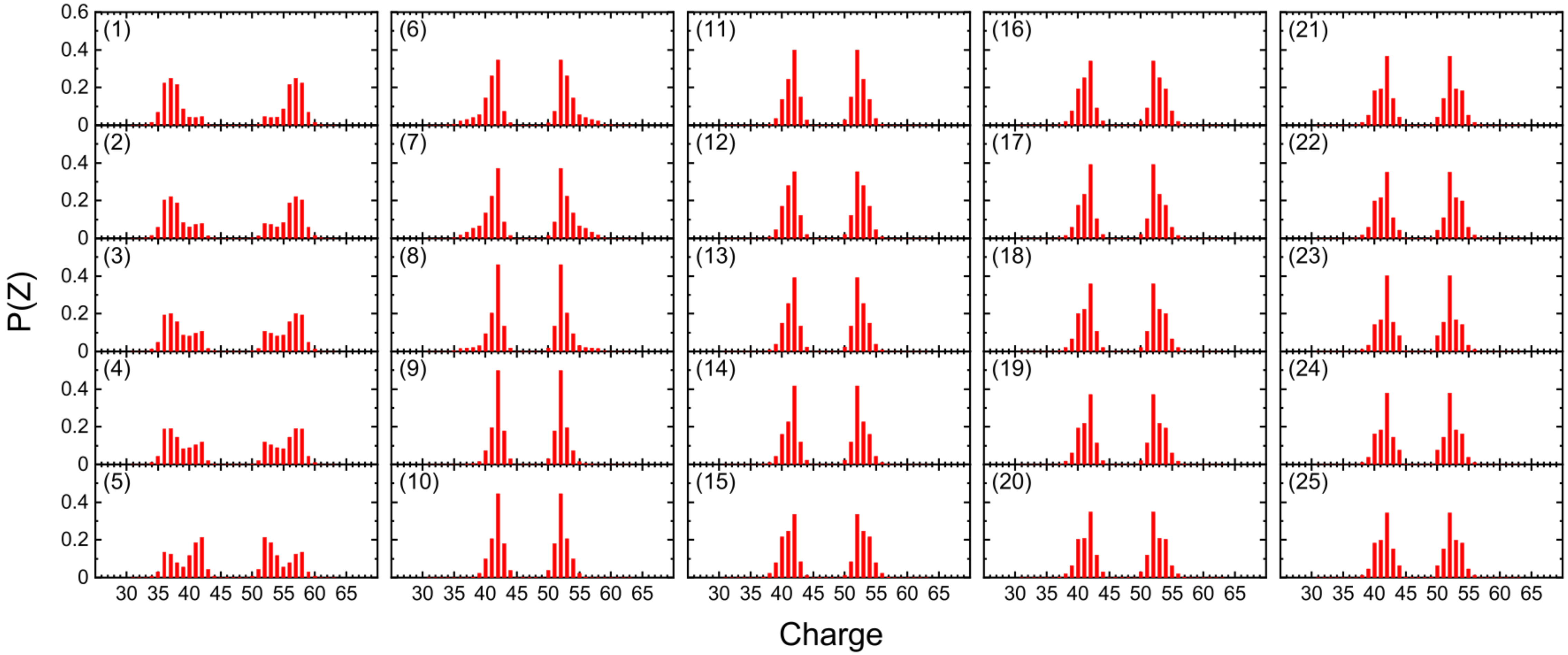
The square moduli of the 25 TDDFT components of the generalized TDGCM collective wave functions $|g|^2$, at time 1300 fm/c. The generalized TDGCM trajectories 1−25 start from the initial points 1−25.

Particle number projection ⇒ charge yields.

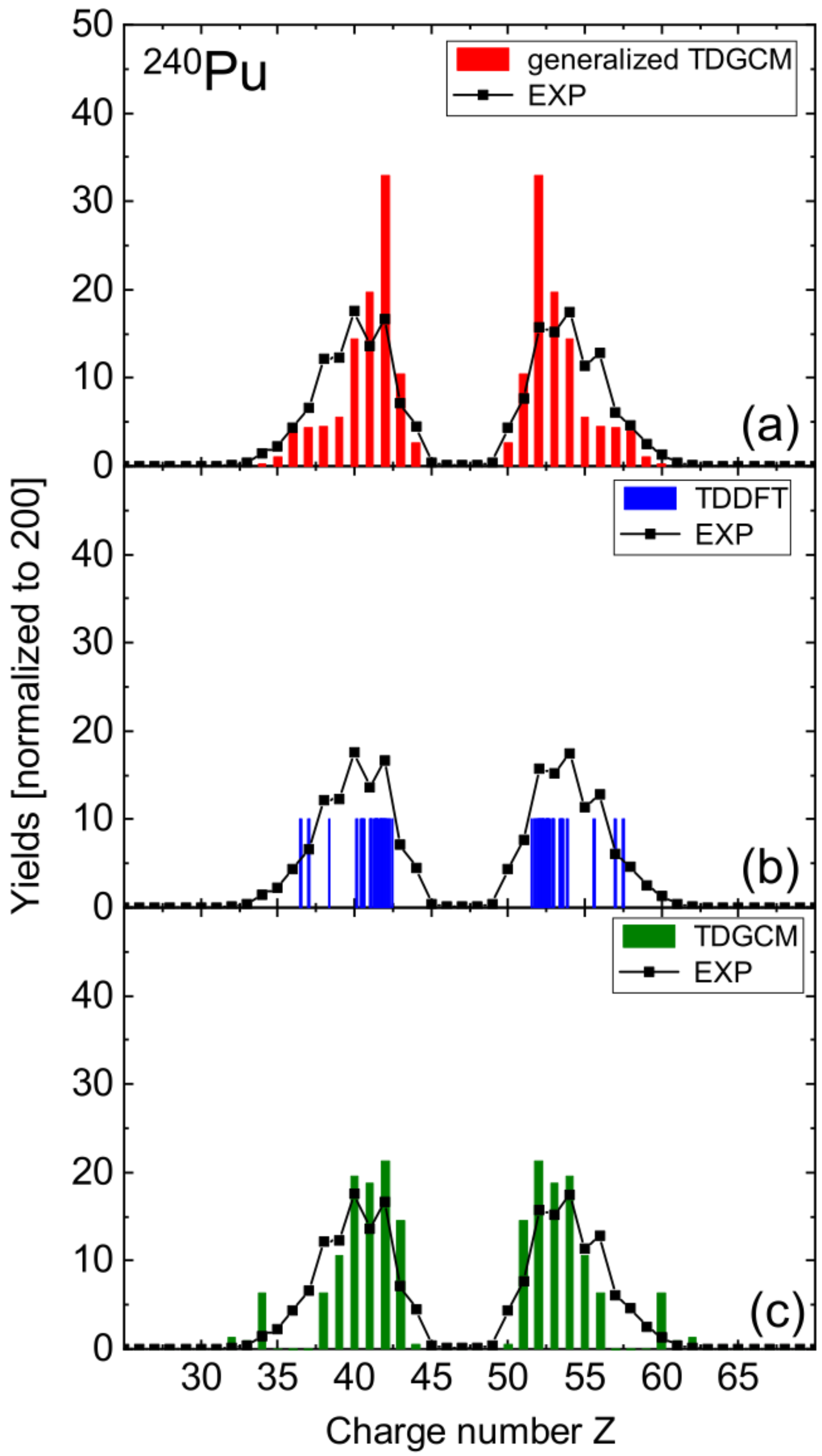
The probability of finding z protons in the subspace V_f that corresponds to one of the fragments, when the total system contains Z protons:

$$P(z|Z,t) = \frac{\langle \Psi(t) \left| \hat{P}_z^{V_f} \hat{P}_Z \right| \Psi(t) \rangle}{\langle \Psi(t) \left| \hat{P}_Z \right| \Psi(t) \rangle} = \frac{\sum_{\boldsymbol{q}\boldsymbol{q}'} f^*_{\boldsymbol{q}'}(t) f_{\boldsymbol{q}}(t) \langle \Phi_{\boldsymbol{q}'}(t) \left| \hat{P}_z^{V_f} \hat{P}_Z \right| \Phi_{\boldsymbol{q}}(t) \rangle}{\sum_{\boldsymbol{q}\boldsymbol{q}'} f^*_{\boldsymbol{q}'}(t) f_{\boldsymbol{q}}(t) \langle \Phi_{\boldsymbol{q}'}(t) \left| \hat{P}_Z \right| \Phi_{\boldsymbol{q}}(t) \rangle},$$

Probability distributions of proton number at time 1300 fm/c. The generalized TDGCM trajectories 1−25 start from the initial points 1−25.



Charge yields for induced fission of ^{240}Pu.



Total kinetic energies of the emerging fragments.