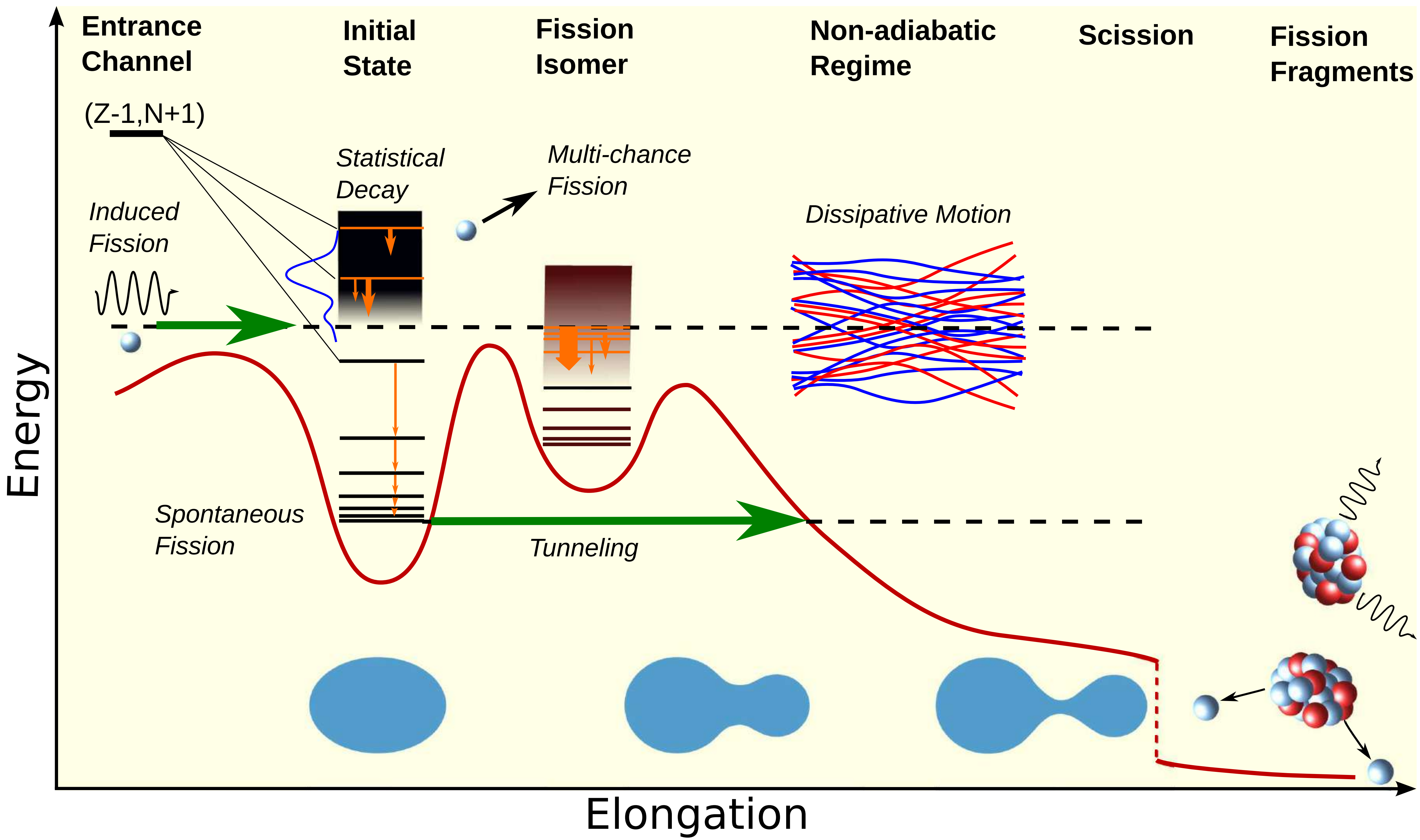
Induced Fission Dynamics

Dario Vretenar
University of Zagreb

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



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

A) 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.

B) 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.

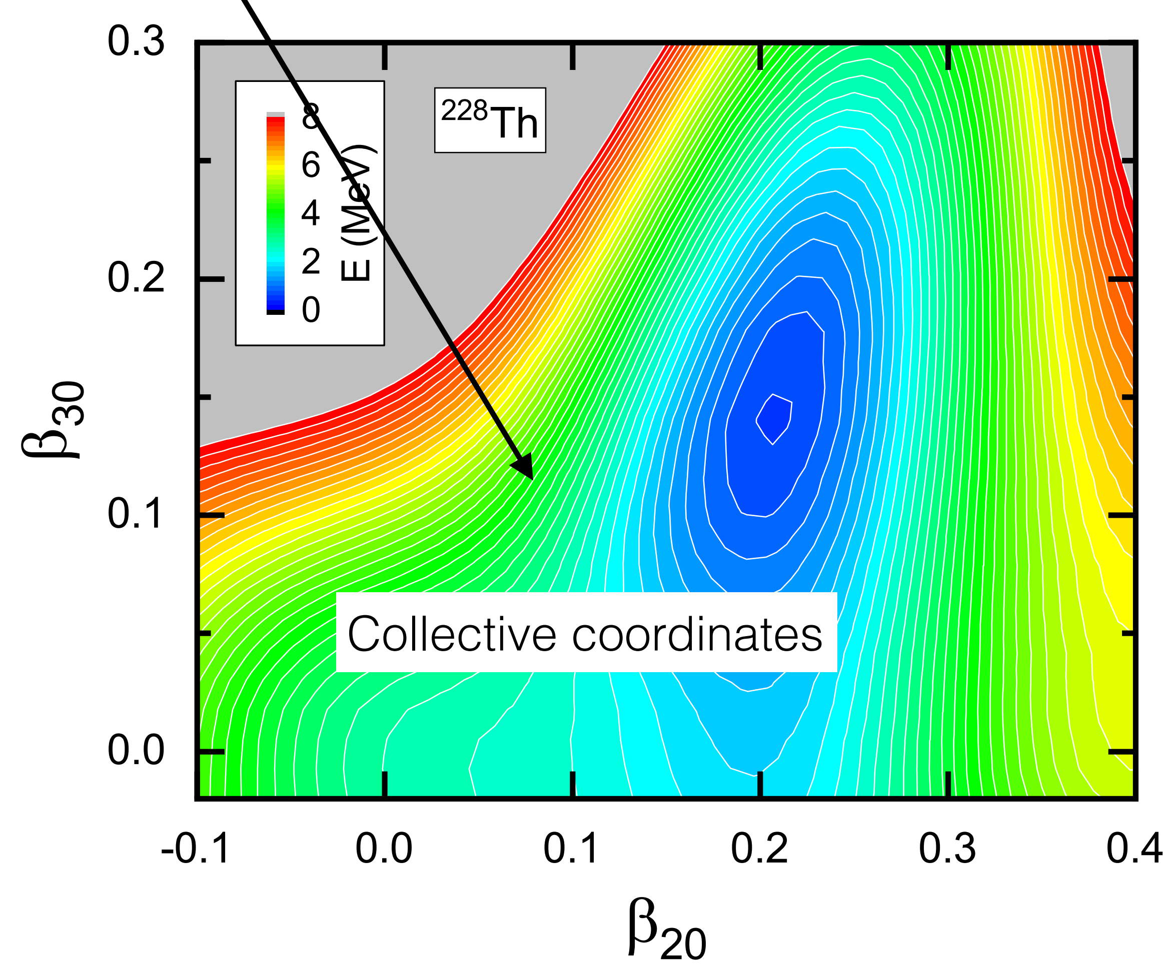
The time-dependent generator coordinate method (TDGCM)

⇒ Griffin-Hill-Wheeler (GHW) ansatz: $|\Psi(t)\rangle = \int_{\boldsymbol{q}\in E} \mathrm{d}\boldsymbol{q}\, |\phi(\boldsymbol{q})\rangle f(\boldsymbol{q}, t).$

GHW equation:

$$\forall \boldsymbol{q}' : \quad \int \mathrm{d}\boldsymbol{q} \Big(\mathcal{H}(\boldsymbol{q}', \boldsymbol{q}) - i\hbar \mathcal{N}(\boldsymbol{q}', \boldsymbol{q}) \frac{\mathrm{d}}{\mathrm{dt}}\Big) f(\boldsymbol{q}, t) = 0.$$

$$\mathcal{H}(\boldsymbol{q}, \boldsymbol{q}') = \langle \phi(\boldsymbol{q}) | \hat{H} | \phi(\boldsymbol{q}') \rangle$$
$$\mathcal{N}(\boldsymbol{q}, \boldsymbol{q}') = \langle \phi(\boldsymbol{q}) | \hat{\mathbb{1}} | \phi(\boldsymbol{q}') \rangle$$



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

➠ time-dependent Schrödinger equation for the collective wave function:

$$i\hbar \dot{g} = \tilde{\mathcal{H}} g.$$

for the collective operator: $\tilde{\mathcal{O}} = \mathcal{N}^{-1/2} \mathcal{O} \mathcal{N}^{-1/2}.$

TDGCM in the Gaussian overlap approximation (TDGCM+GOA)

➠ the overlap between two arbitrary generator states can be approximated by a Gaussian function:

$$\mathcal{N}(\boldsymbol{q},\boldsymbol{q}') \simeq \exp\left[-\frac{1}{2}(\boldsymbol{q}-\boldsymbol{q}')^t G(\bar{\boldsymbol{q}})(\boldsymbol{q}-\boldsymbol{q}')\right],$$

➠ the Hamiltonian kernel can be approximated: $\mathcal{H}(\boldsymbol{q},\boldsymbol{q}') \simeq \mathcal{N}(\boldsymbol{q},\boldsymbol{q}')h(\boldsymbol{q},\boldsymbol{q}'),$

polynomial of degree two in the collective variables

➠ time-dependent Schroedinger-like equation for the collective wave function. The collective Hamiltonian:

$$\tilde{\mathcal{H}}(\boldsymbol{\alpha}) = -\frac{\hbar^2}{2}\nabla_{\boldsymbol{\alpha}} B(\boldsymbol{\alpha})\nabla_{\boldsymbol{\alpha}} + V(\boldsymbol{\alpha}).$$

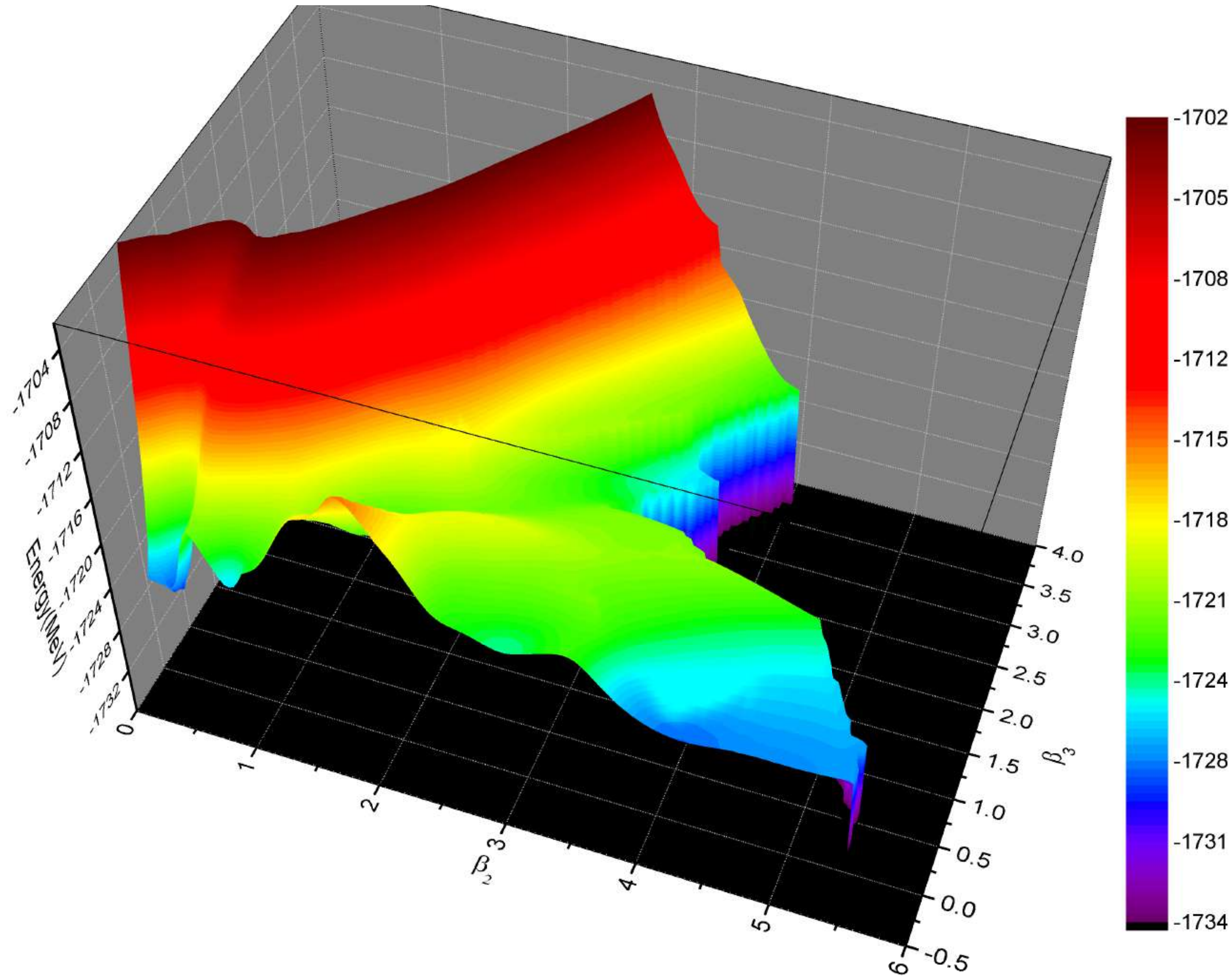
Example Time-dependent Schroedinger-like equation for fission dynamics (axial quadrupole and octupole deformation parameters as collective degrees of freedom):

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

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

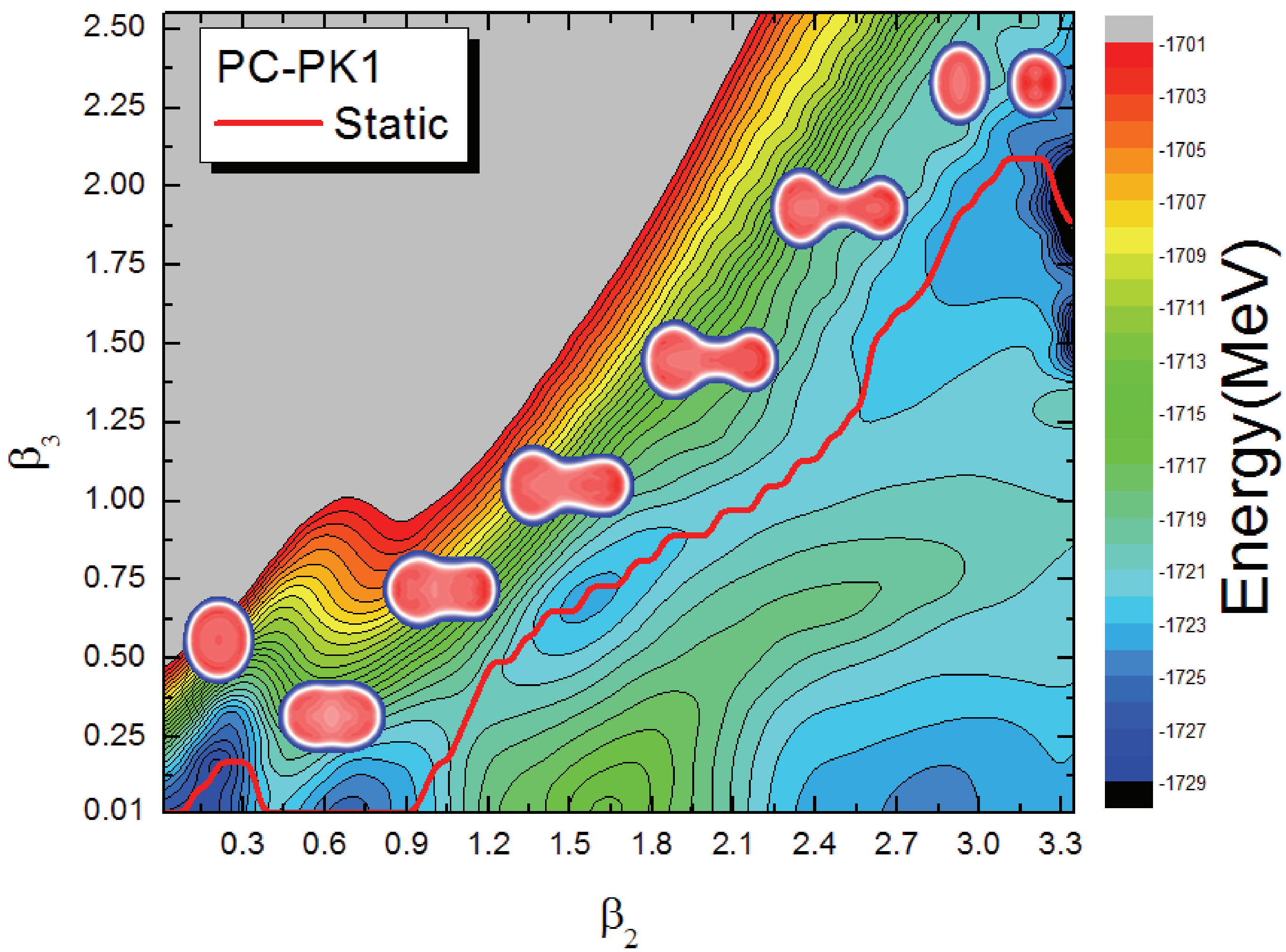
PHYSICAL REVIEW C **96**, 024319 (2017)



→ includes static correlations: deformations & pairing

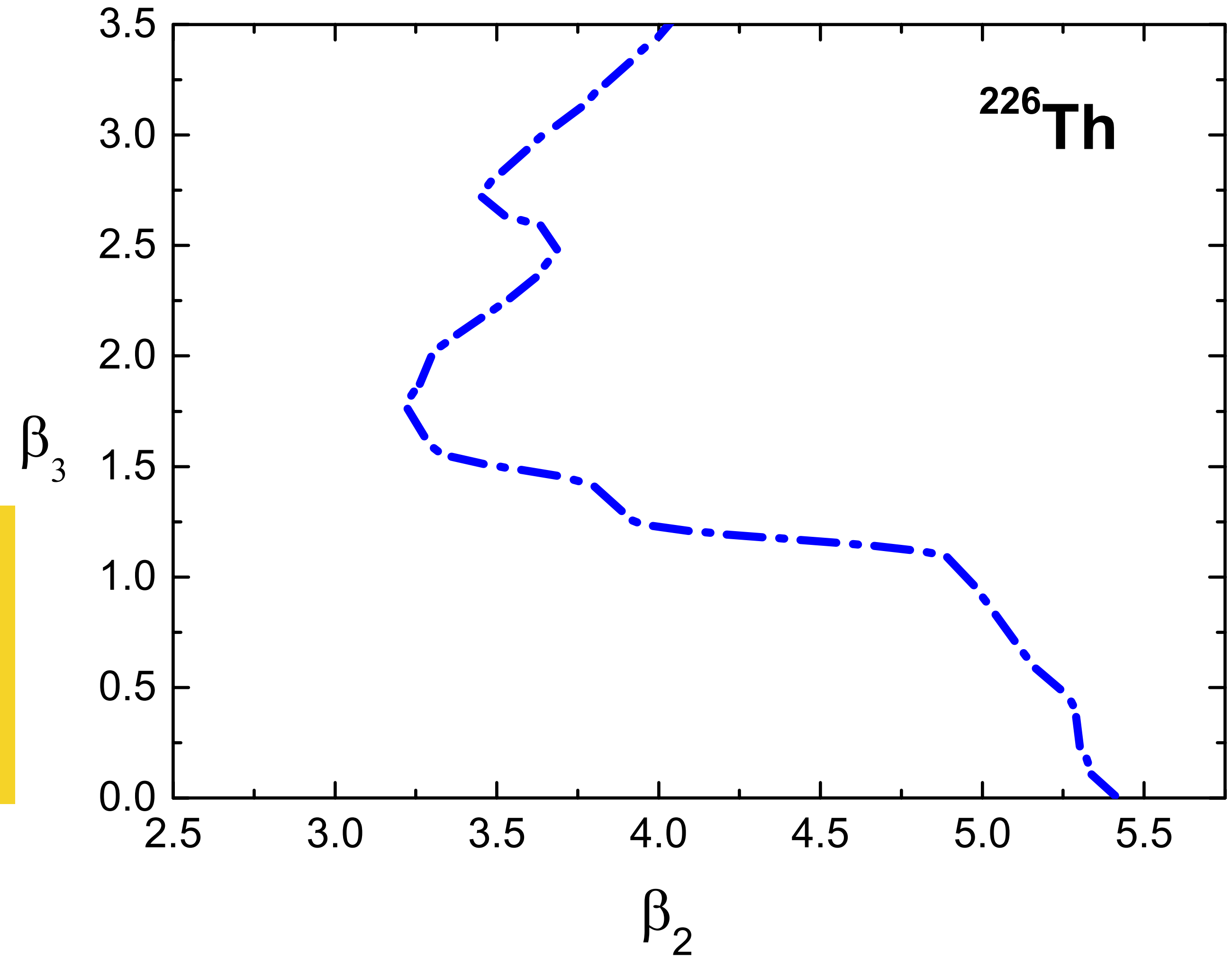
→ does not include dynamic (collective) correlations that arise from symmetry restoration and quantum fluctuations around mean-field minima

PC-PK1 plus δ-force pairing



➠ static fission path

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 collective space is divided into an inner region in which the nucleus is whole, and an external region that contains the two fission fragments. The set of scission configurations defines the hyper-surface that separates the two regions.

⇒ continuity equation for the probability density: $$\frac{\partial}{\partial t}|g(\beta_2, \beta_3, t)|^2 = -\nabla \cdot \mathbf{J}(\beta_2, \beta_3, t)$$

...the probability current:

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

The flux of the probability current through the scission hyper-surface provides a measure of the probability of observing a given pair of fragments at time t.

$$F(\xi, t) = \int_{t=0}^{t} dt \int_{(\beta_2, \beta_3) \in \xi} \mathbf{J}(\beta_2, \beta_3, t) \cdot d\mathbf{S}$$

The yield for the fission fragment with mass A:

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

Collective parameters

The mass tensor associated with $q_2 = \langle Q_2 \rangle$ and $q_3 = \langle Q_3 \rangle$ ➠ perturbative cranking approximation

$$B_{kl}(q_2, q_3) = \frac{2}{\hbar^2} \left[\mathcal{M}_{(1)} \mathcal{M}_{(3)}^{-1} \mathcal{M}_{(1)} \right]_{kl}$$

$$\mathcal{M}_{(n),kl}(q_2, q_3) = \sum_{i,j} \frac{\langle i | \hat{Q}_k | j \rangle \langle j | \hat{Q}_l | i \rangle}{(E_i + E_j)^n} (u_i v_j + v_i u_j)^2$$

Sensitivity of fission dynamics to the pairing strength

… the TDGCM initial state is a Gaussian superposition of quasibound states:

$$g(\boldsymbol{q}, t=0) = \sum_k \exp\left(\frac{(E_k - \bar{E})^2}{2\sigma^2}\right) g_k(\boldsymbol{q})$$

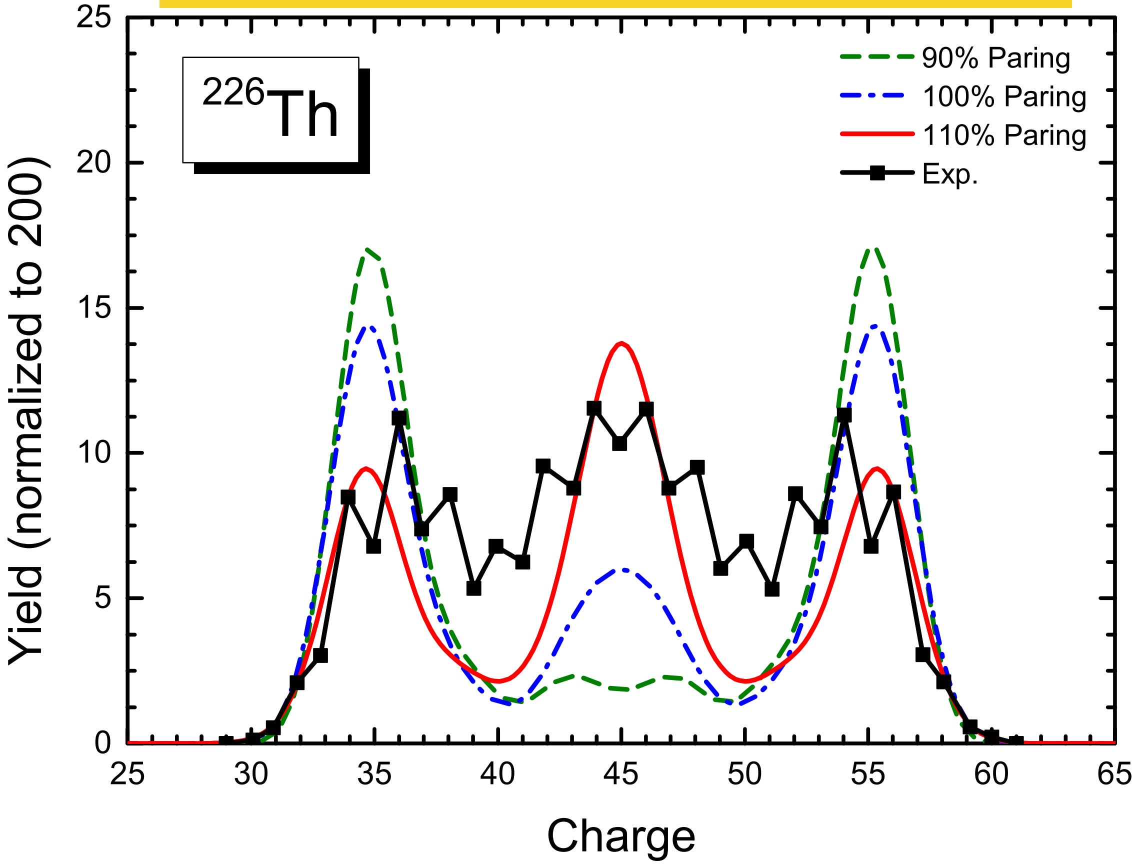
The mean energy is adjusted in such a way that:

$$\langle g(t=0)|\hat{H}_{\rm coll}|g(t=0)\rangle = E^*_{\rm coll.}$$

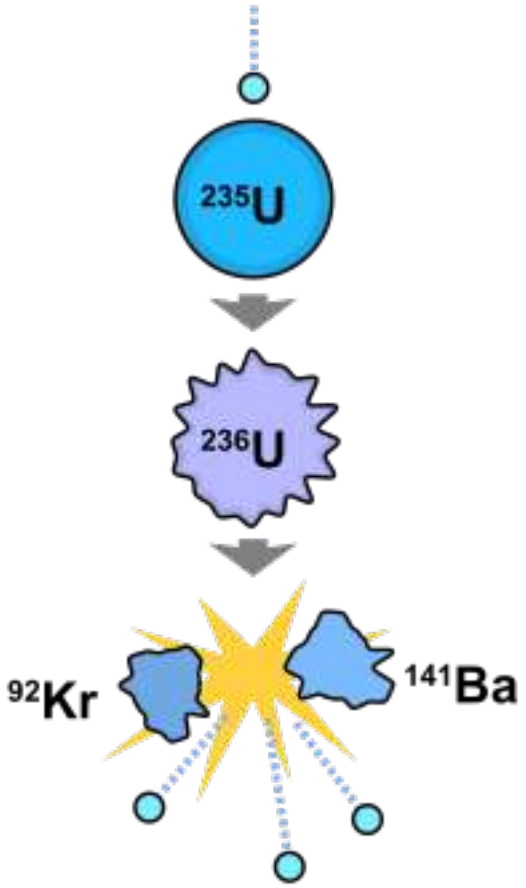
The height of the fission barriers (in MeV) with respect to the corresponding ground-state minima:

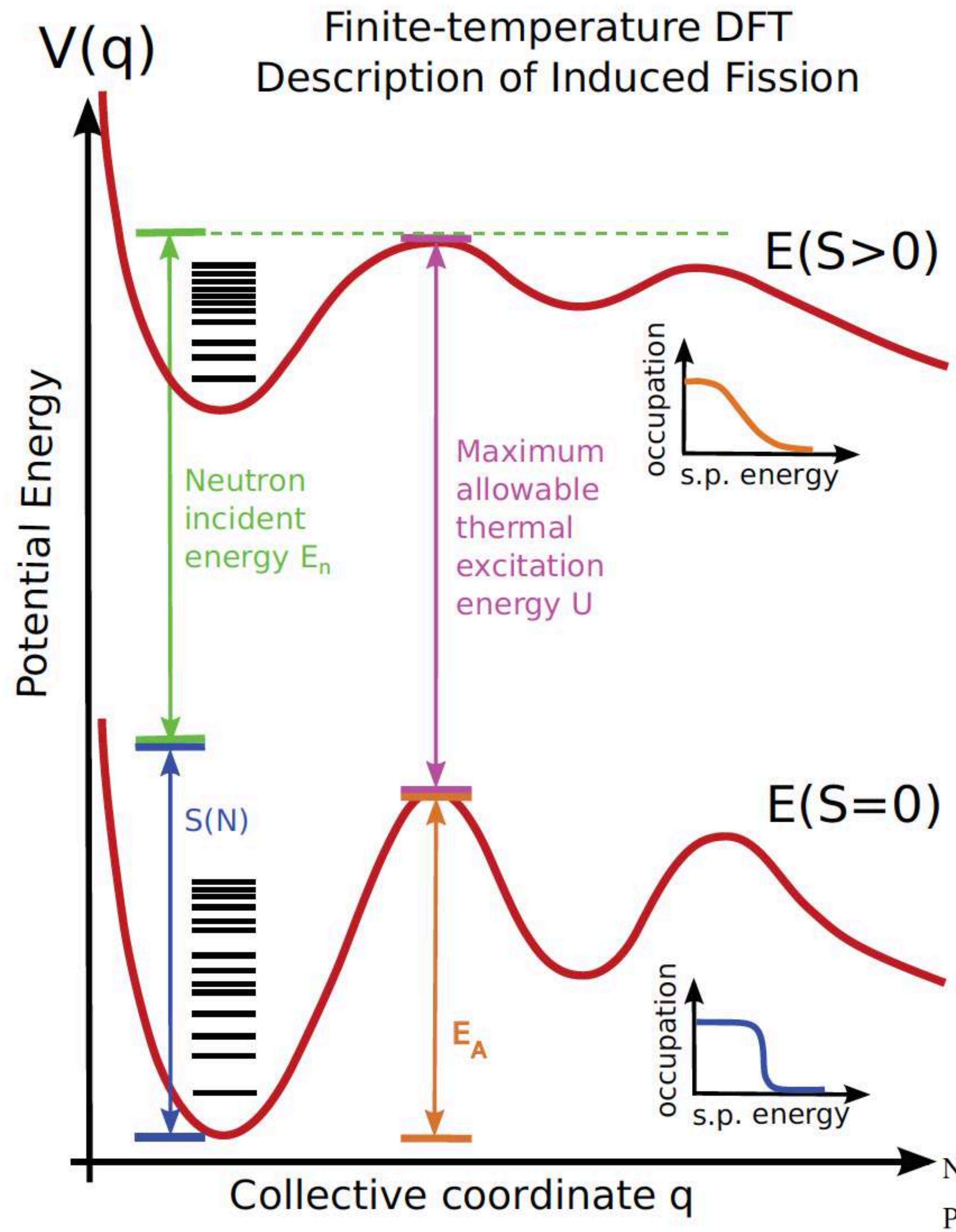
	B_I	$B_{II}^{\rm asy}$	$B_{III}^{\rm asy}$	$B_{II}^{\rm sym}$	$B_{III}^{\rm sym}$
90% pairing	8.23	9.47	7.74	15.64	6.38
100% pairing	7.10	8.58	7.32	14.21	5.72
110% pairing	5.92	7.78	7.09	12.72	5.17

Pre-neutron emission charge yields for photo-induced fission of ^{226}Th.



Induced Fission - Finite Temperature Effects





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

Finite temperature effects:

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

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

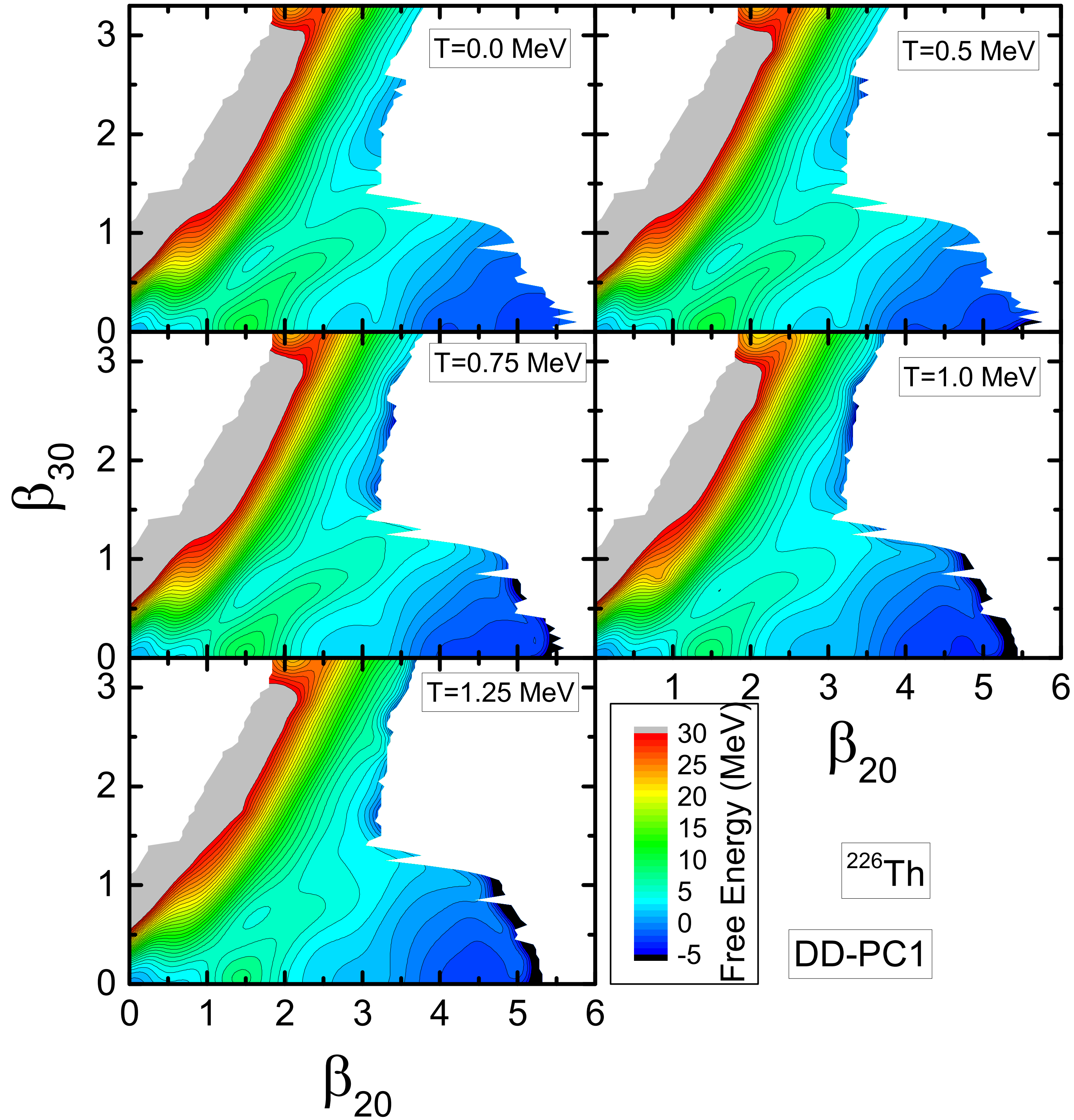
Helmholtz free energy: $F = E(T) - TS$

... 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:

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



$$\rho_V = \sum_k \bar{\psi}_k(\boldsymbol{r})\gamma^0\psi_k(\boldsymbol{r})[v_k^2(1-f_k) + u_k^2 f_k],$$

$$\Delta_k = \frac{1}{2}\sum_{k'>0} V^{pp}_{k\bar{k}k'\bar{k}'} \frac{\Delta_{k'}}{E_{k'}}(1-2f'_k).$$

$$B_{ij}(\boldsymbol{q}) = \mathcal{M}^{-1}(\boldsymbol{q})$$

Perturbative cranking mass tensor: $$\mathcal{M}^{Cp} = \hbar^2 M_{(1)}^{-1} M_{(3)} M_{(1)}^{-1}$$

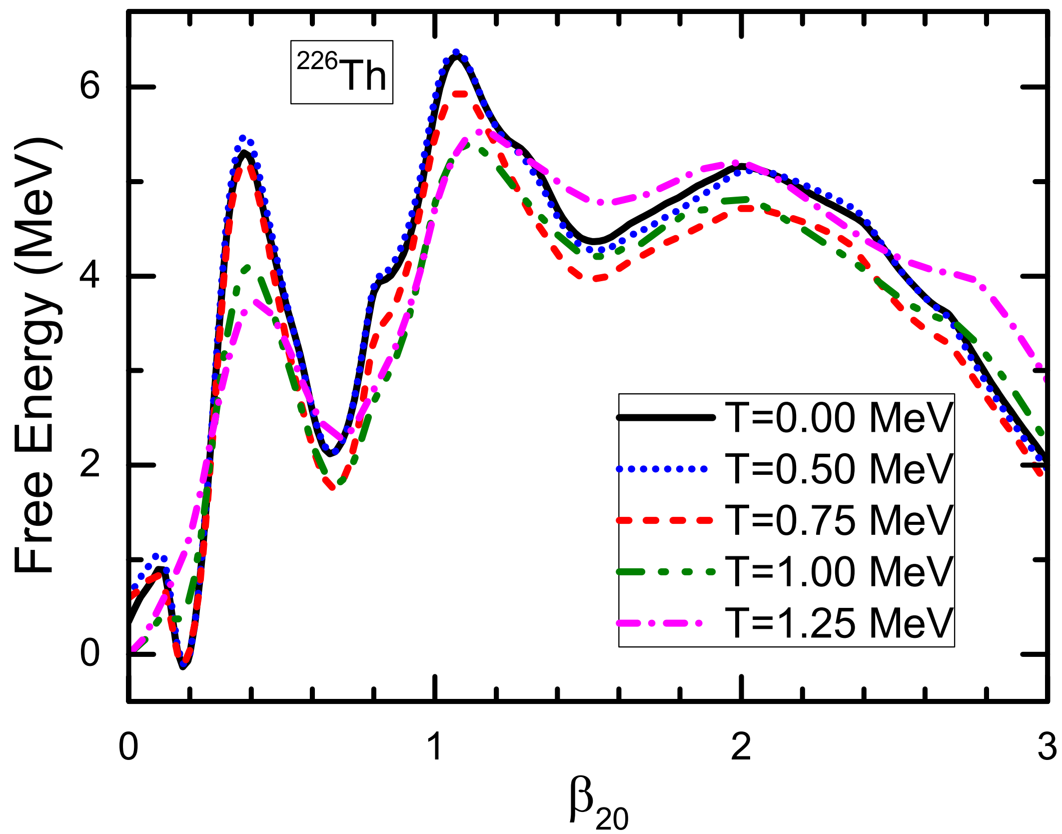
$$[M_{(k)}]_{ij,T} = \frac{1}{2} \sum_{\mu \neq \nu} \langle 0|\hat{Q}_i|\mu\nu\rangle\langle\mu\nu|\hat{Q}_j|0\rangle \left\{ \frac{(u_\mu u_\nu - v_\mu v_\nu)^2}{(E_\mu - E_\nu)^k} \left[\tanh\left(\frac{E_\mu}{2k_B T}\right) - \tanh\left(\frac{E_\nu}{2k_B T}\right)\right]\right\}$$
$$+ \frac{1}{2} \sum_{\mu\nu} \langle 0|\hat{Q}_i|\mu\nu\rangle\langle\mu\nu|\hat{Q}_j|0\rangle \left\{ \frac{(u_\mu v_\nu + u_\nu v_\mu)^2}{(E_\mu + E_\nu)^k} \left[\tanh\left(\frac{E_\mu}{2k_B T}\right) + \tanh\left(\frac{E_\nu}{2k_B T}\right)\right]\right\}$$

… the initial state is a Gaussian superposition of quasibound states:

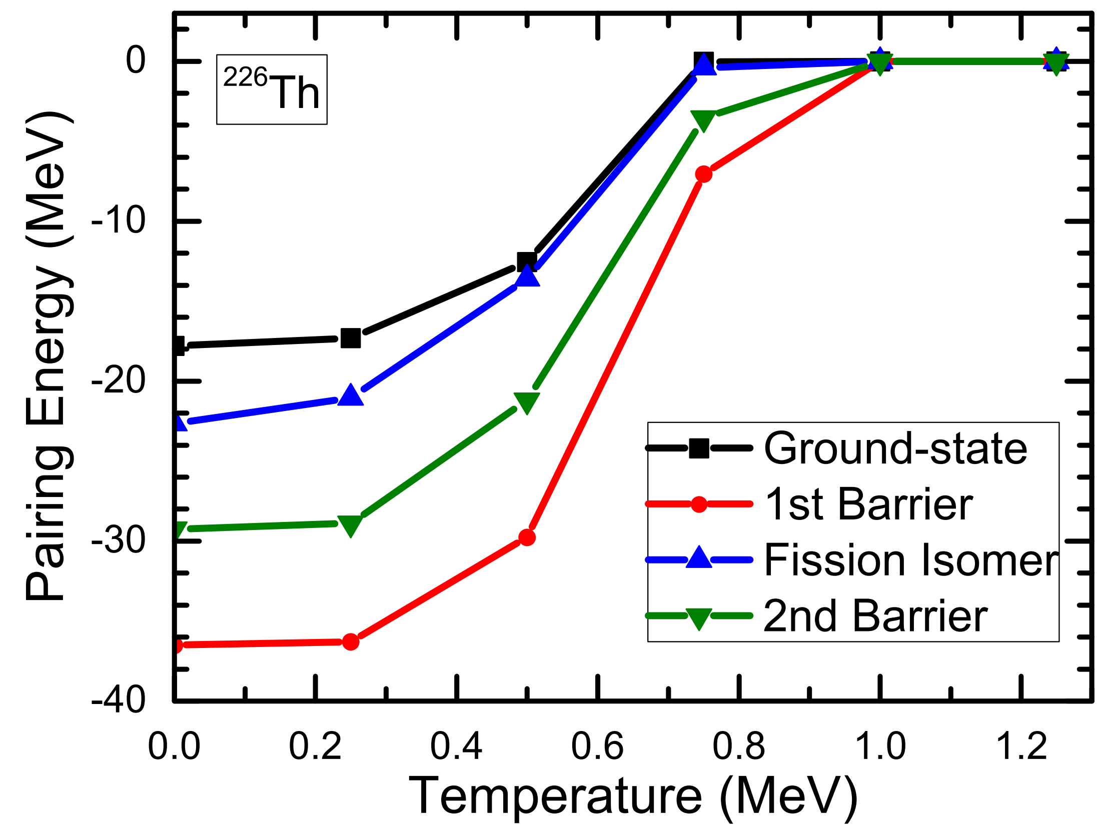
$$g(\boldsymbol{q}, t=0) = \sum_k \exp\left(\frac{(E_k - \bar{E})^2}{2\sigma^2}\right) g_k(\boldsymbol{q})$$

The mean energy is adjusted in such a way that: $\langle g(t=0)|\hat{H}_{\mathrm{coll}}|g(t=0)\rangle = E^*_{\mathrm{coll.}}$

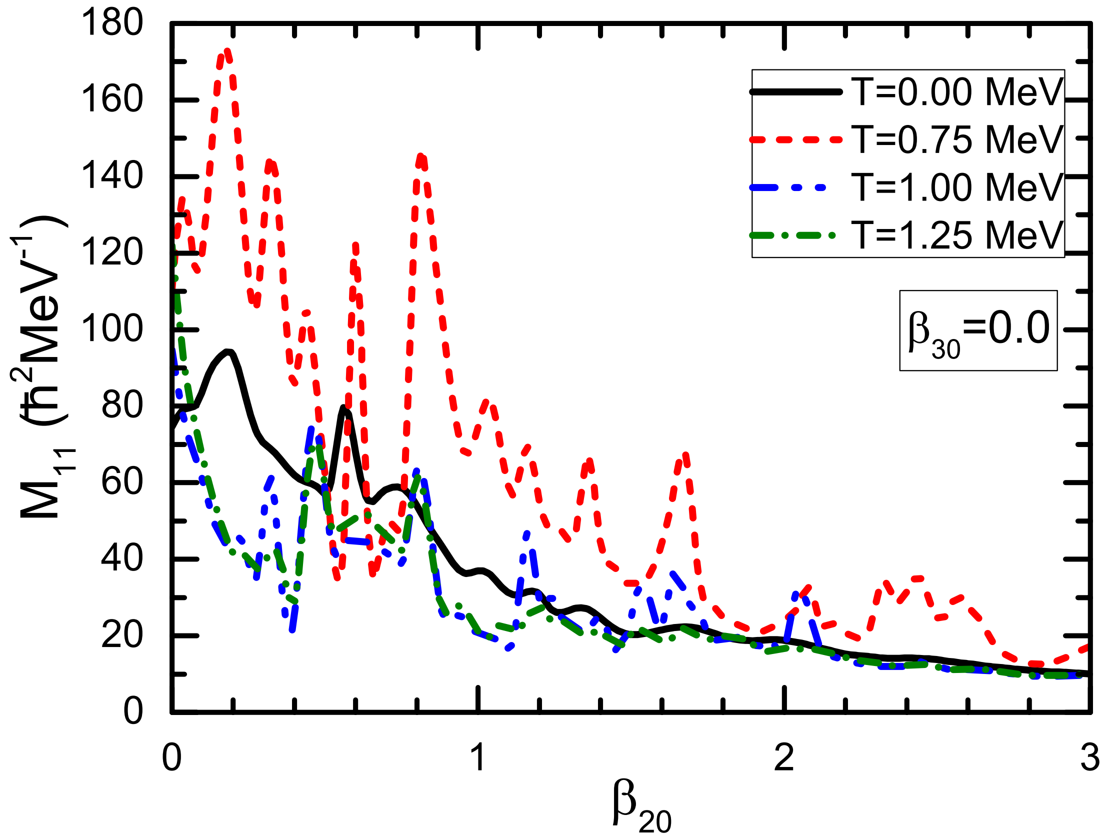
Free energy along the least-energy fission pathway.



Temperature dependence of the pairing energy.



The diagonal components of the mass tensor.

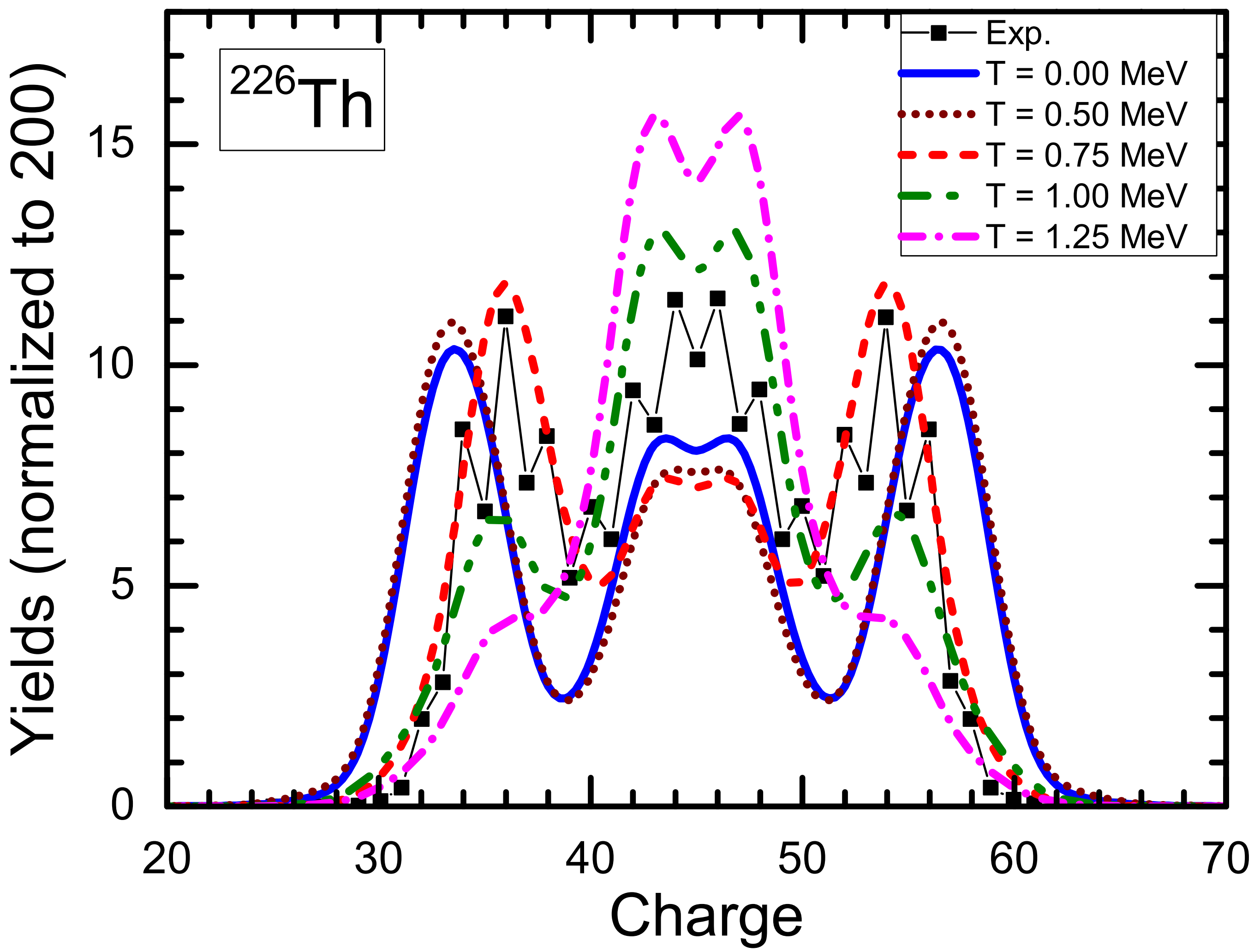


Zhao, Nikšić, Vretenar, Zhou
Phys. Rev. C **99**, 014618 (2019).

Dynamics of induced fission

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

Charge yields:

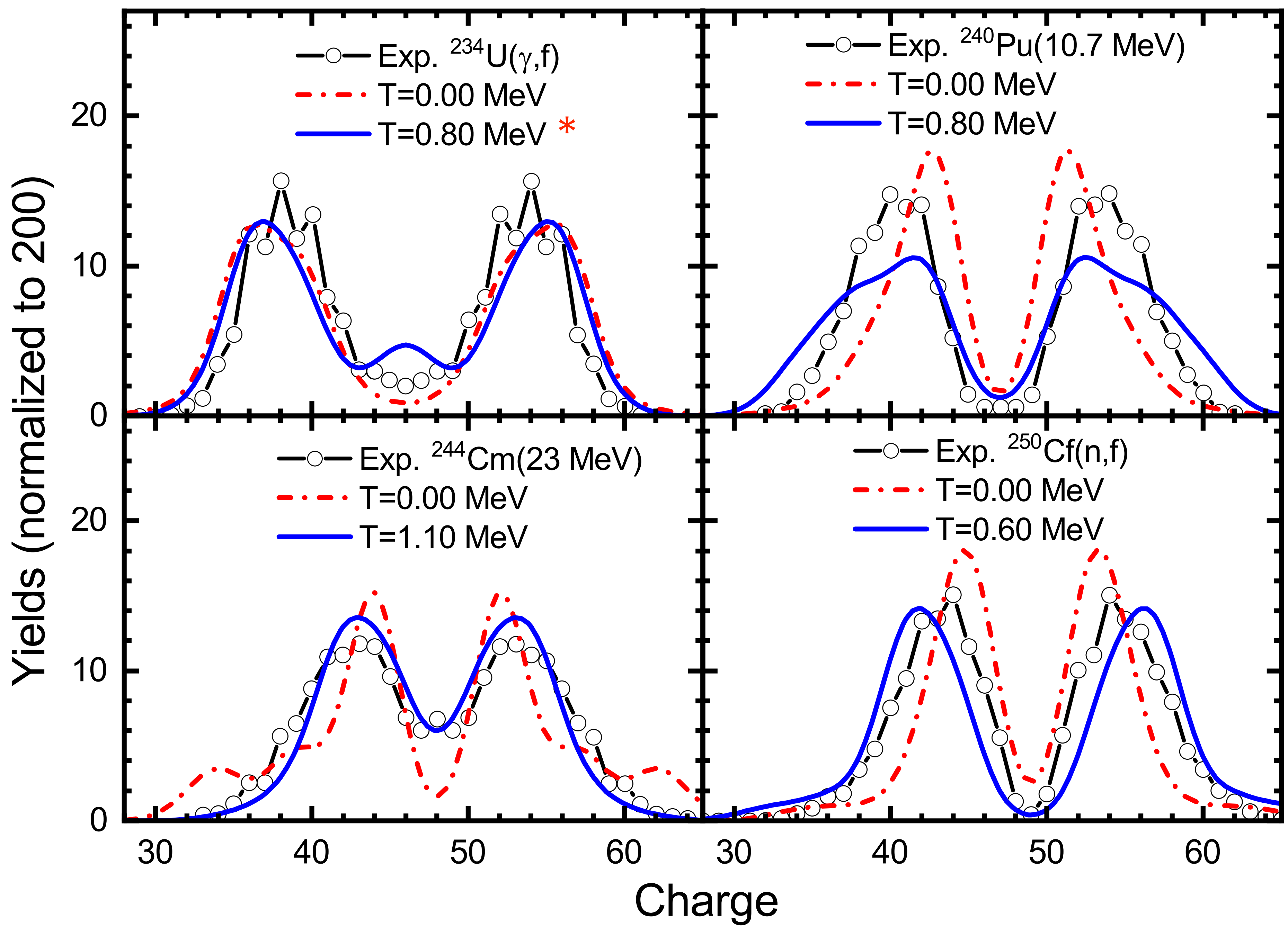


Experimental results ➠ photoinduced fission with photon energies in the interval 8 − 14 MeV, and a peak value Eγ = 11 MeV.

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

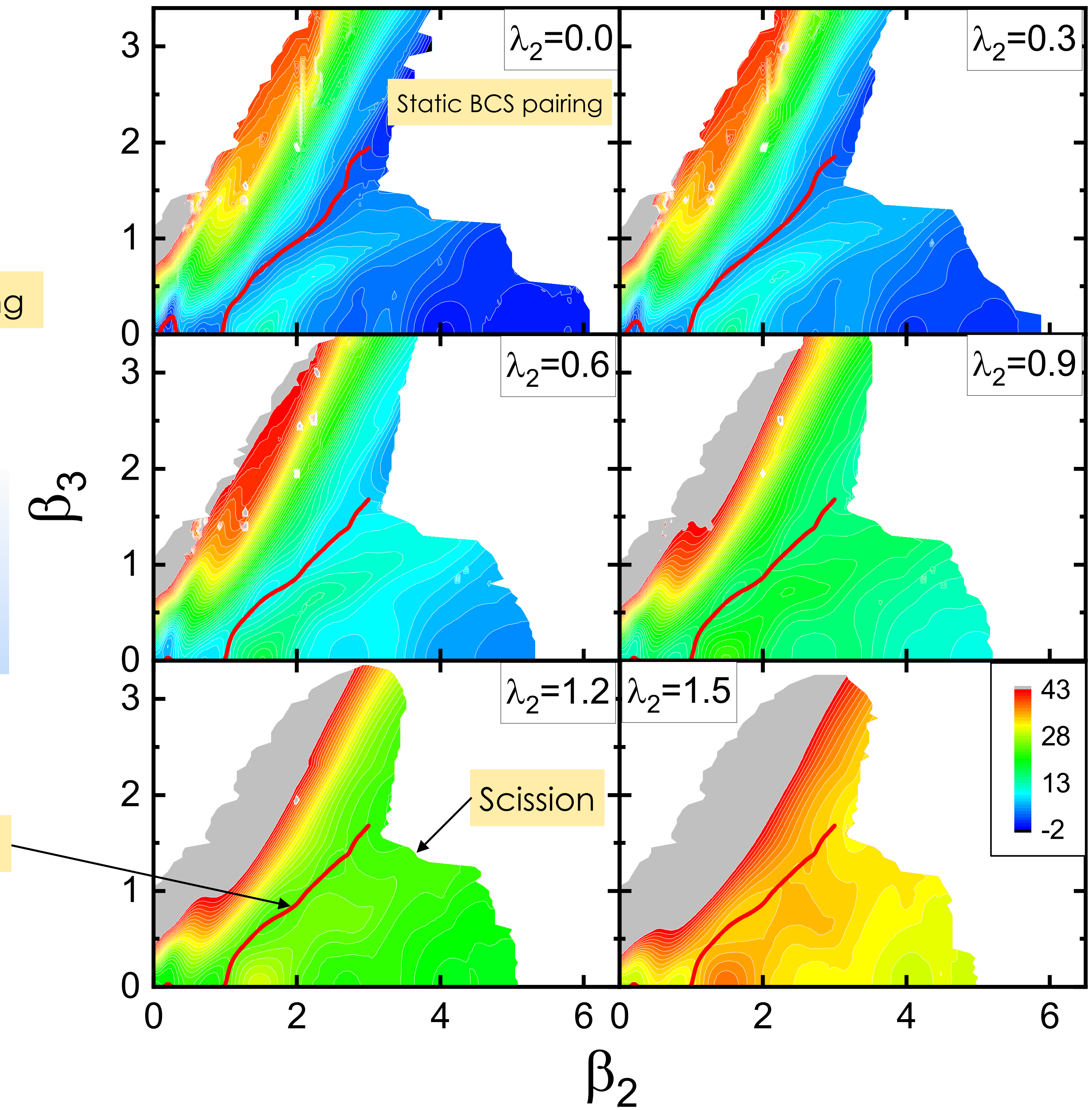
... the Routhian:

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

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.

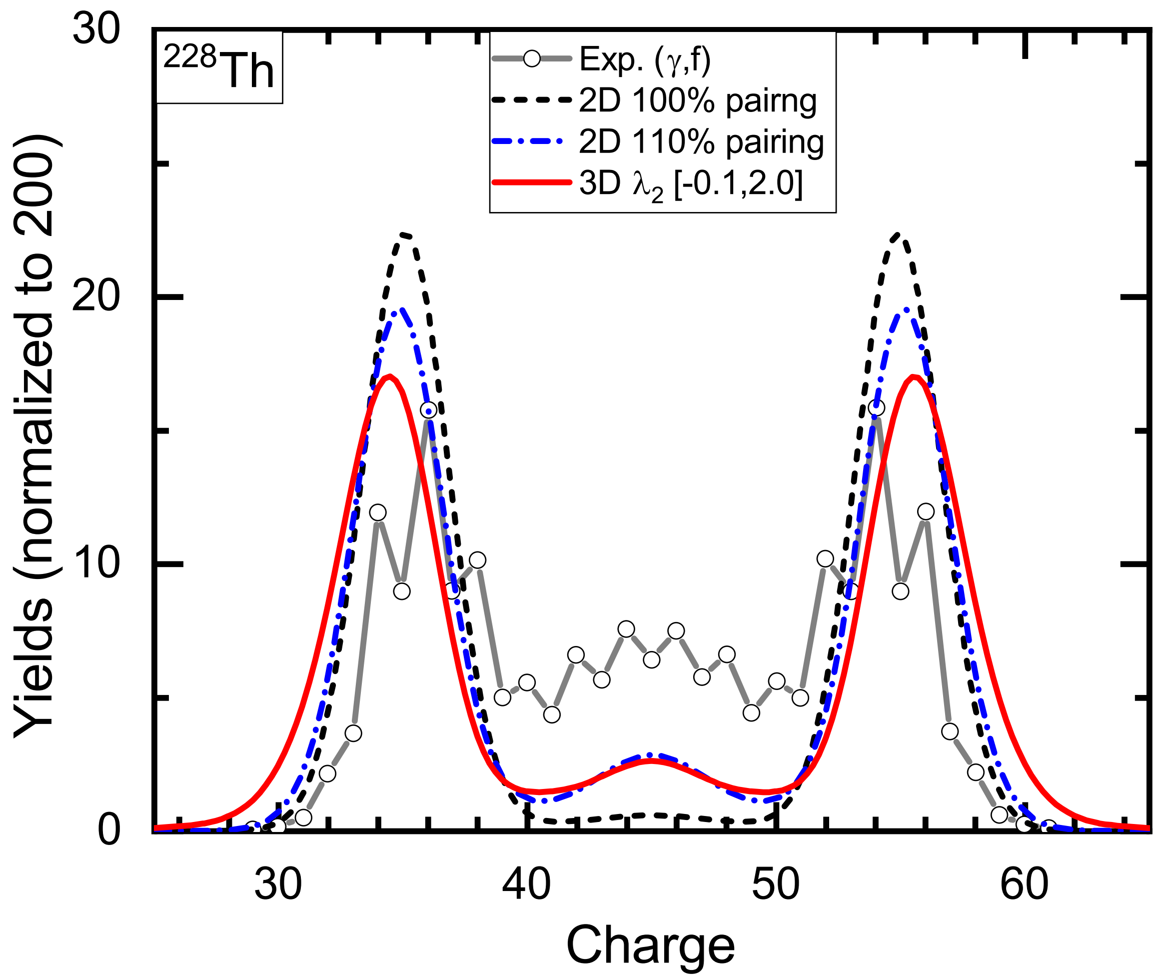
Static fission path of minimum energy

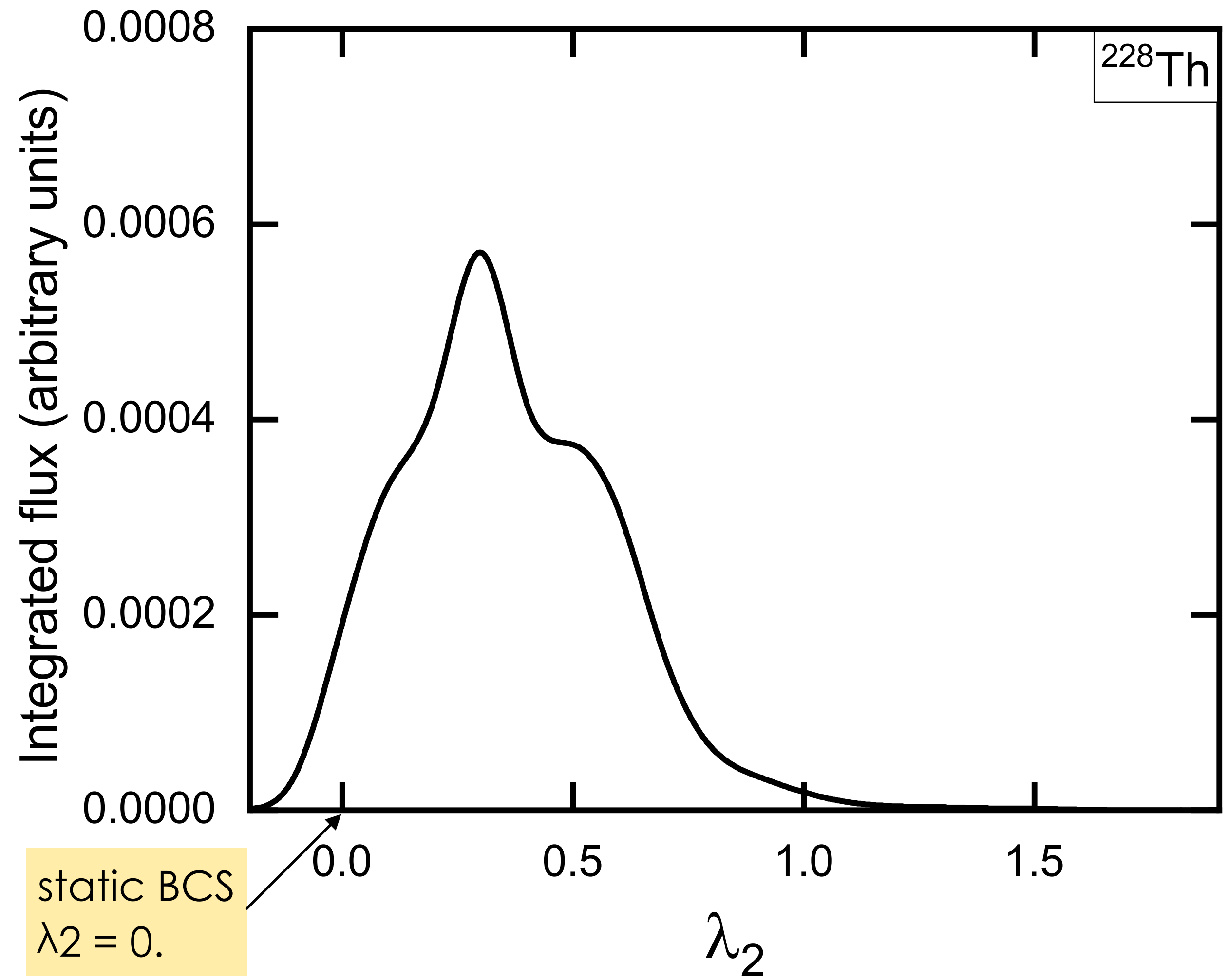


3D TDGCM+GOA calculation

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

q≡{β2,β3,λ2}





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

Comparison to the results obtained in the 2D space of β2 and β3, with static pairing correlations adjusted to empirical ground-state pairing gaps (100% pairing strength), and enhanced (110% pairing strength).

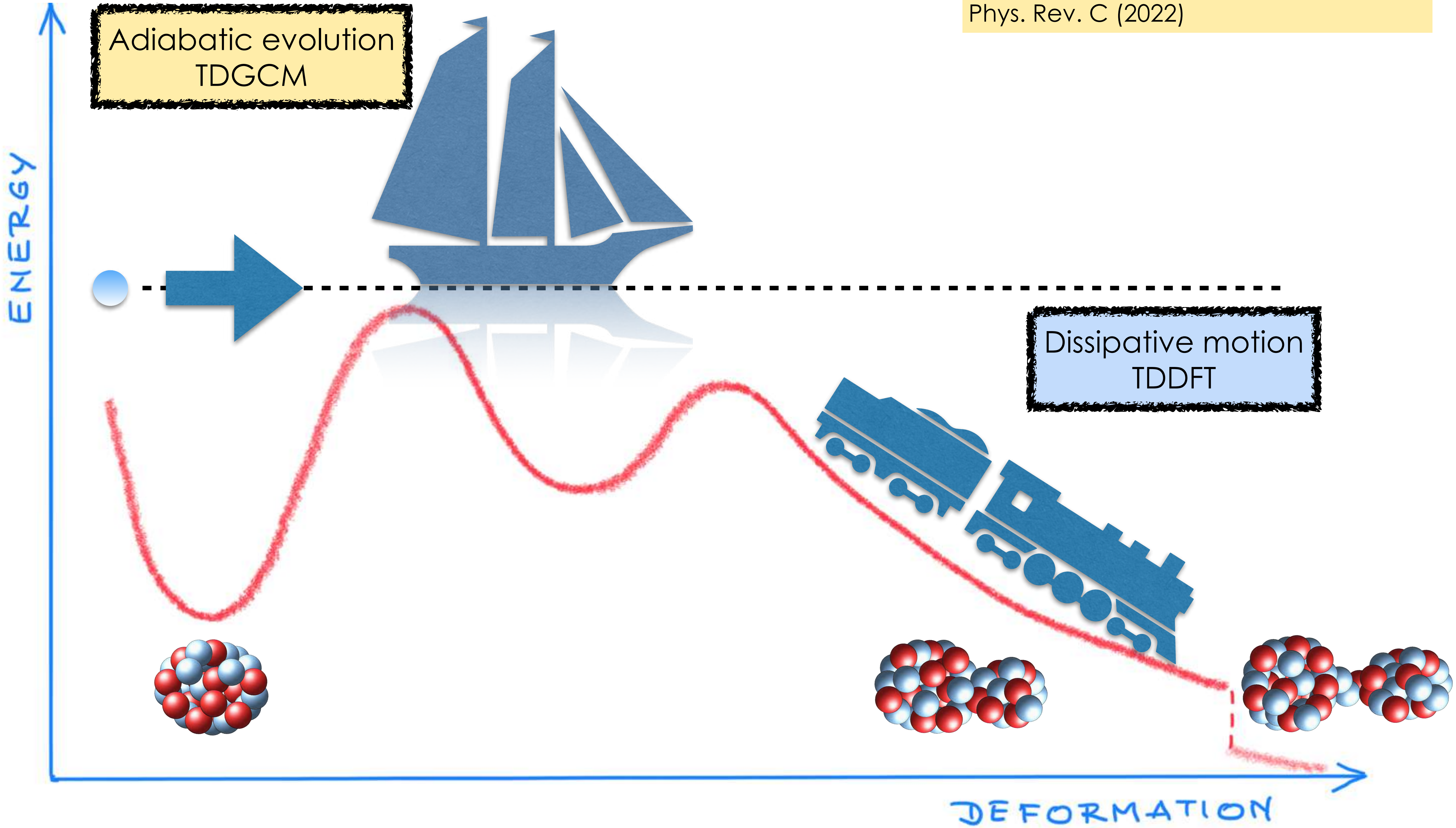
Effect of dynamical pairing on the flux of the probability current through the scission hyper-surface:

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

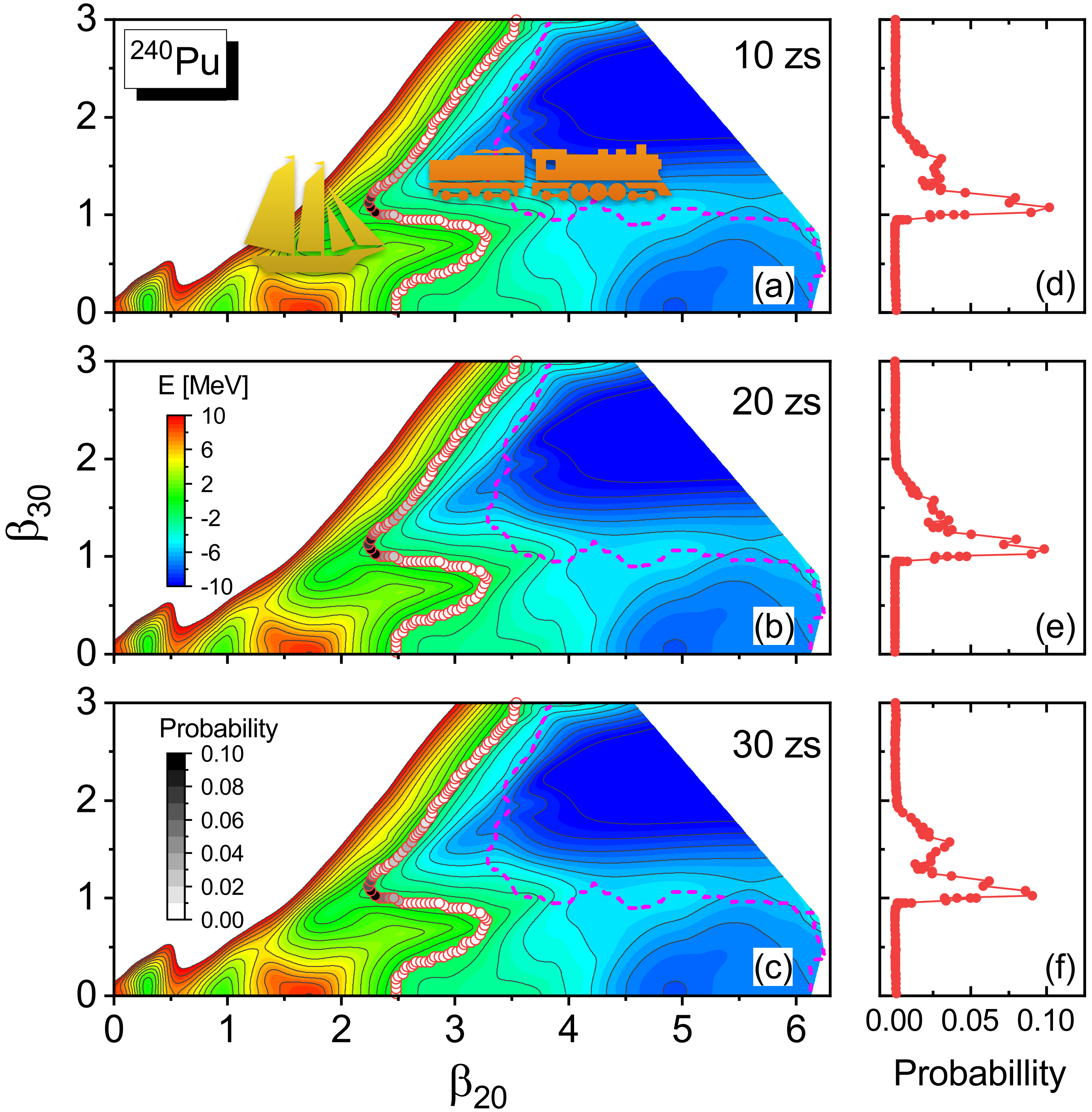
→ time-integrated flux through the scission contour in the (β2, β3) plane, for a given value of the pairing collective coordinate λ2 .

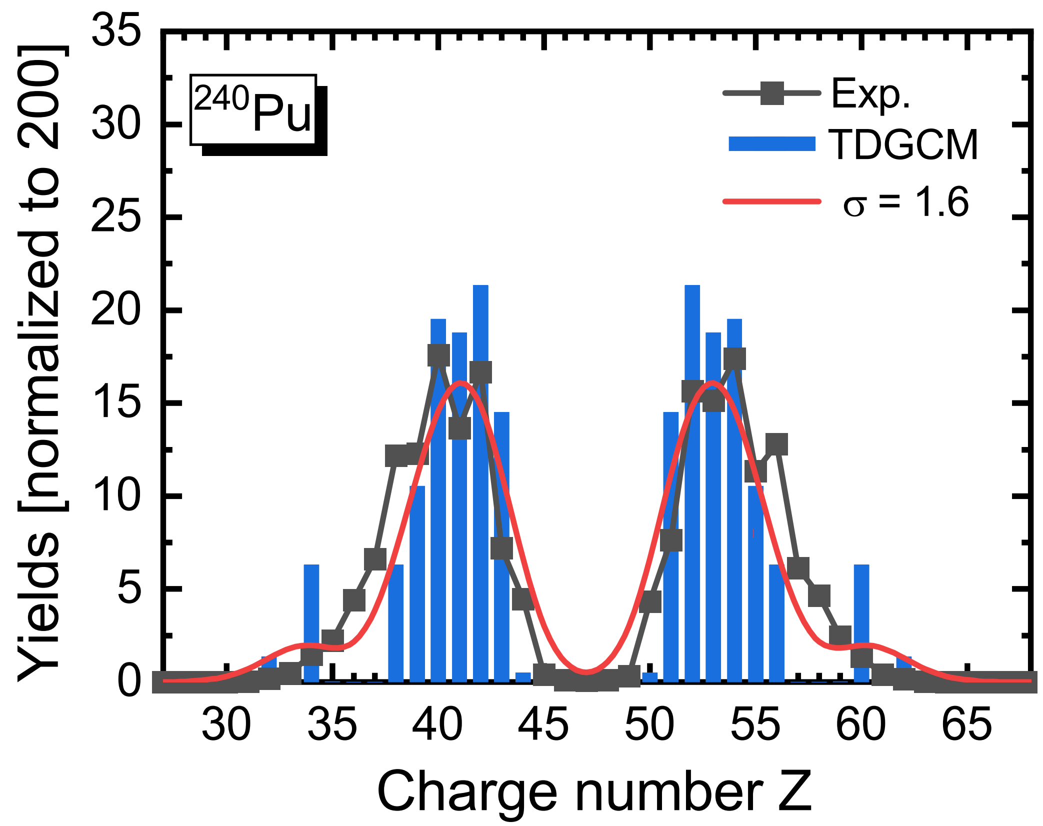
Adiabatic evolution and dissipative dynamics

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



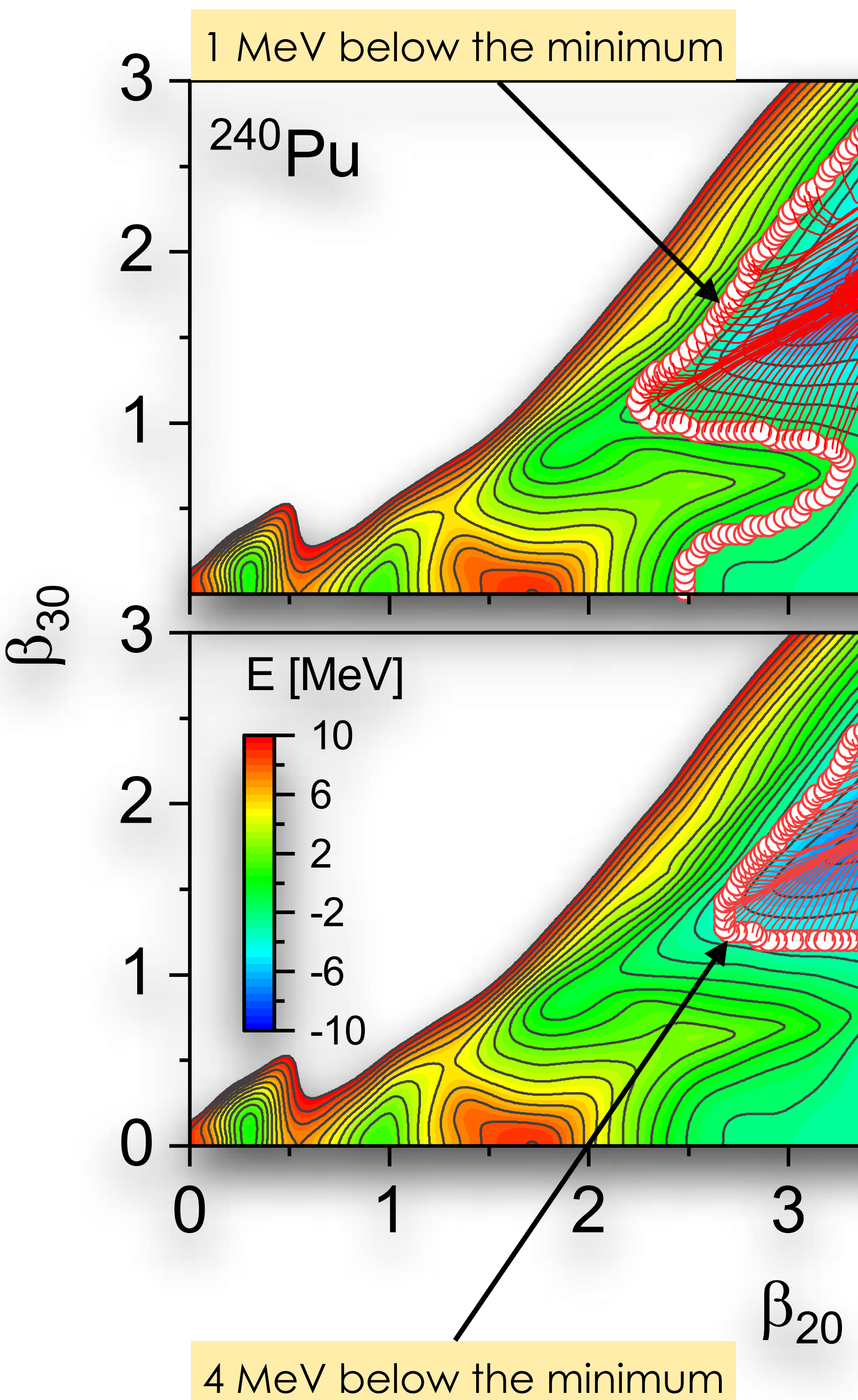
Negele et al. (1978) ➟ use an adiabatic model for the time interval in which the fissioning nucleus evolves from the quasi-stationary initial state to the saddle point, and a non-adiabatic method for the saddle-to-scission and beyond-scission dynamics.

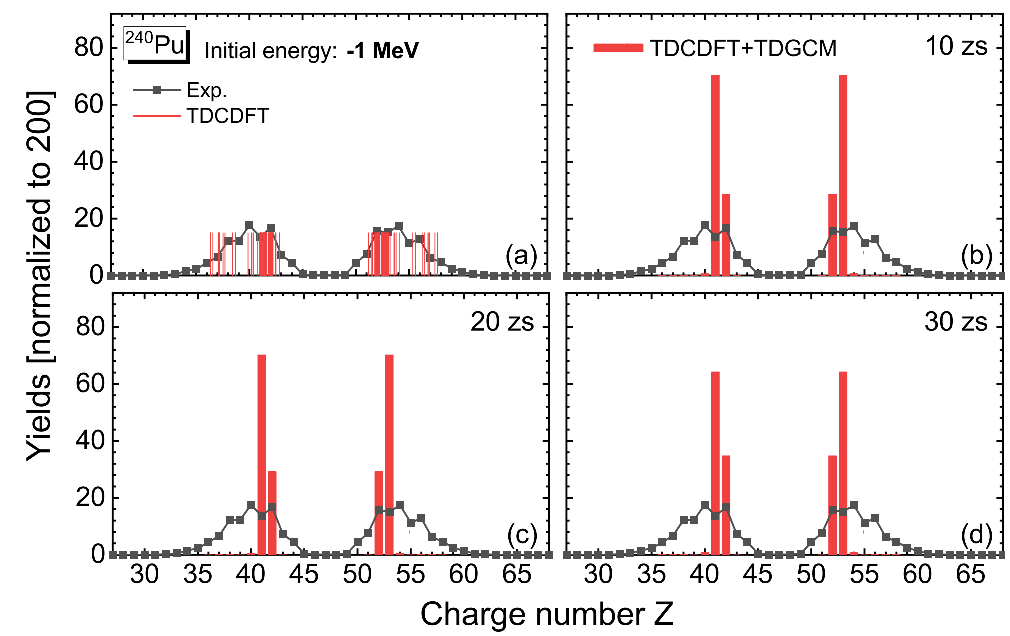


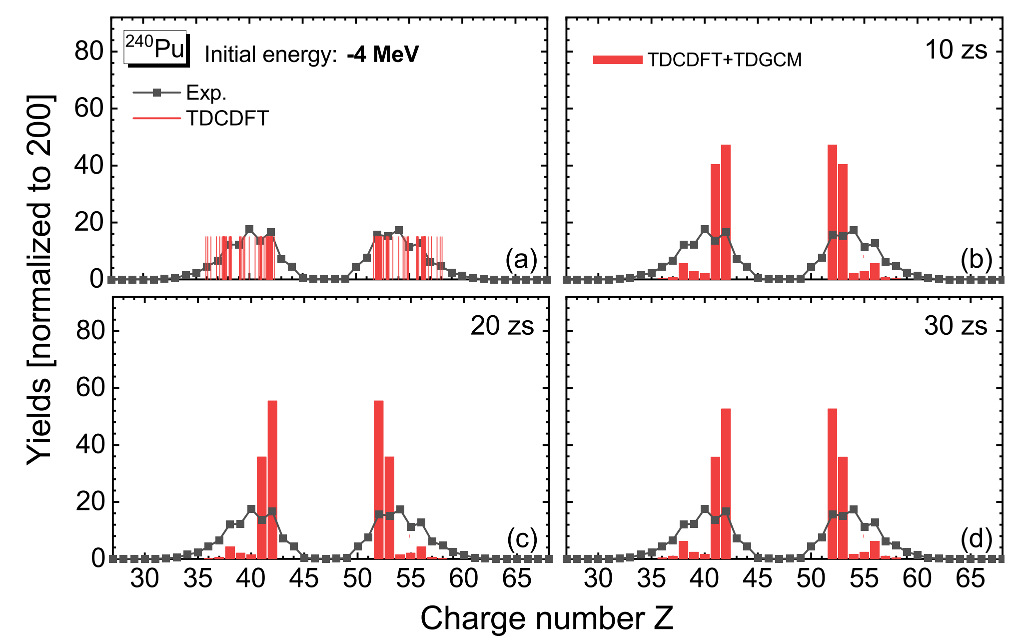


Ren, Zhao, Vretenar, Nikšić, Zhao, Meng, Phys. Rev. C (2022).

TDDFT fission trajectories







Total kinetic energies (TKEs) of the fragments

TDGCM+GOA

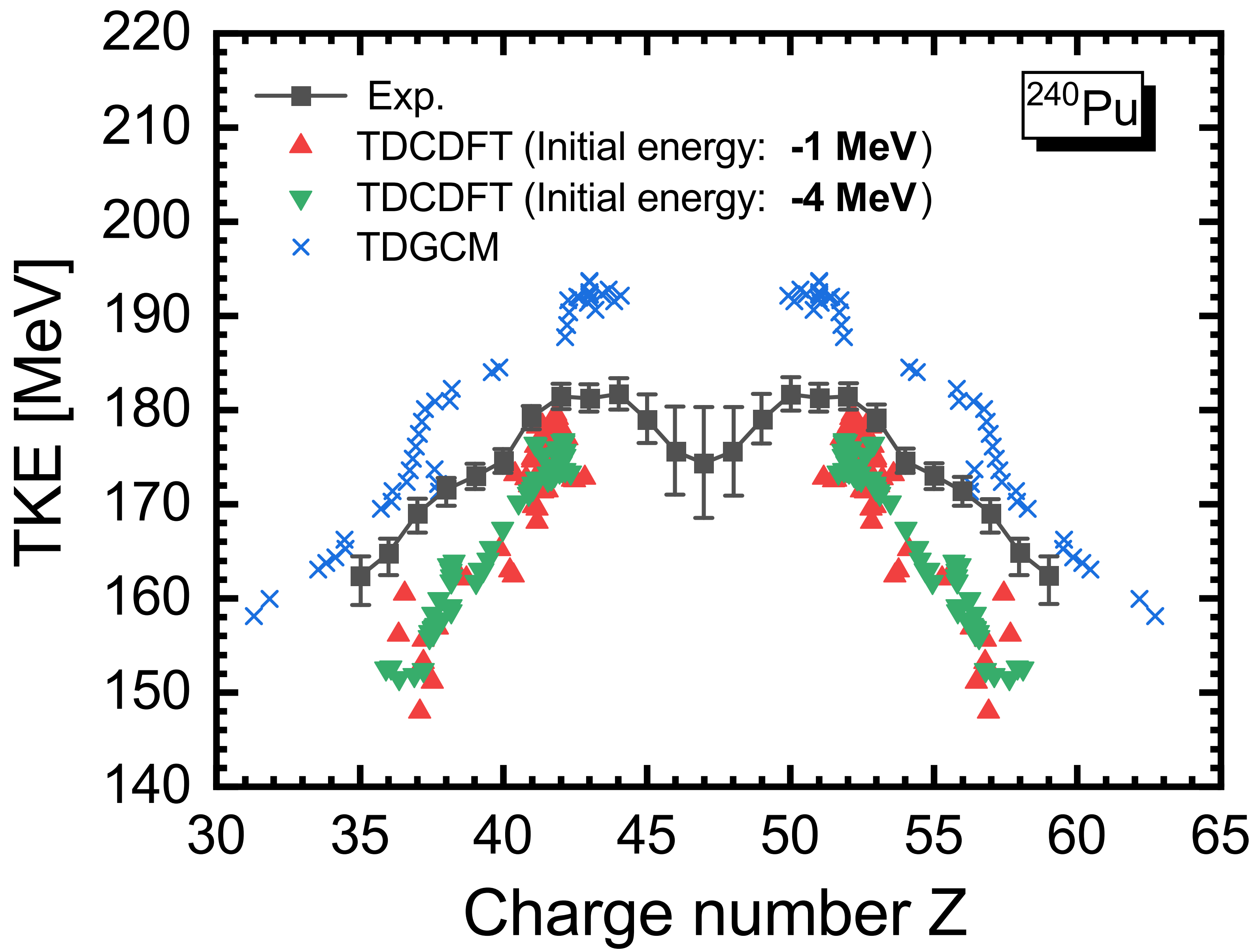
$$E_{\mathrm{TKE}} = \frac{e^2 Z_H Z_L}{d_{\mathrm{ch}}},$$

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

TDDFT

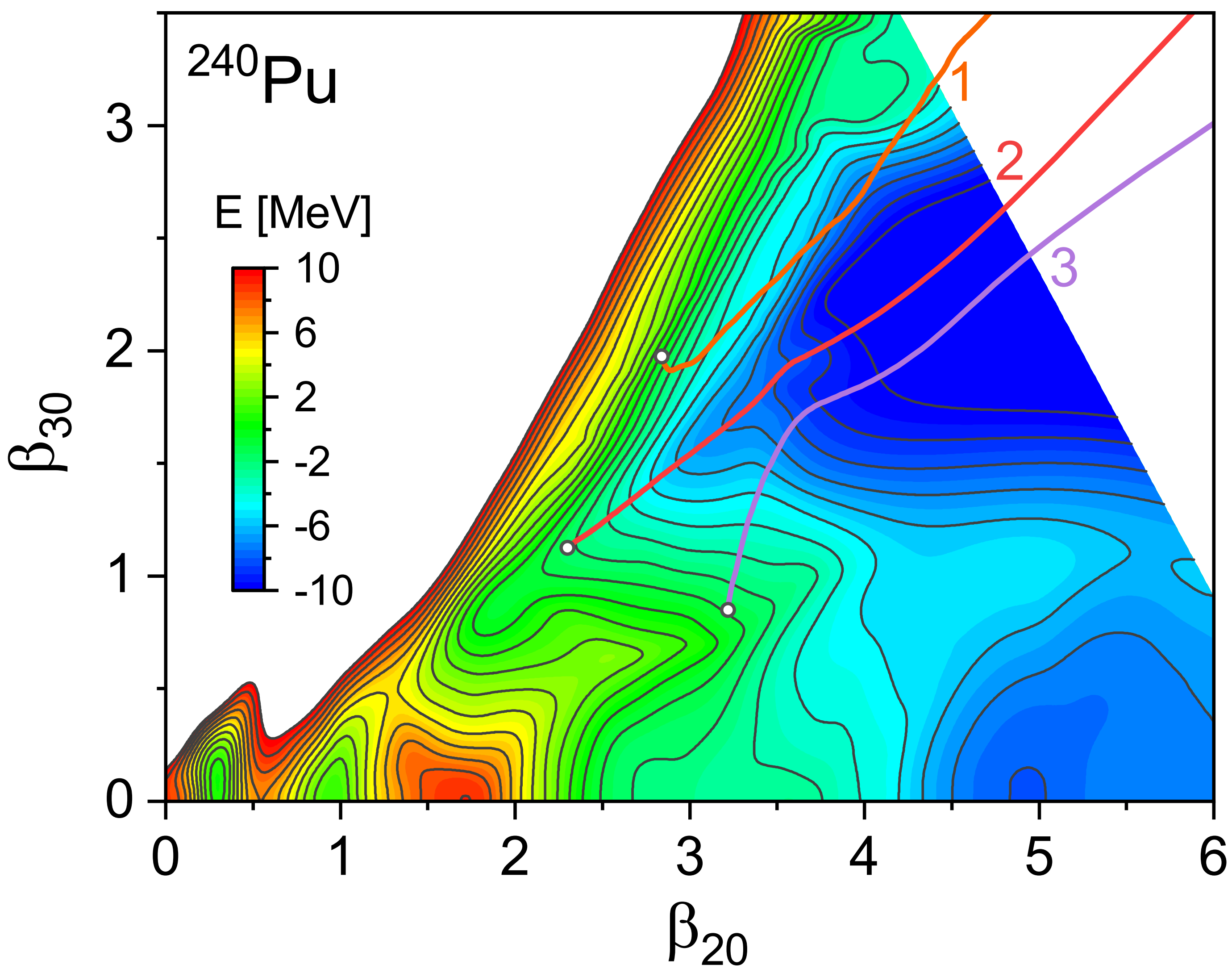
$$E_{\mathrm{TKE}} = \frac{1}{2} m A_{\mathrm{H}} \boldsymbol{v}_{\mathrm{H}}^2 + \frac{1}{2} m A_{\mathrm{L}} \boldsymbol{v}_{\mathrm{L}}^2 + E_{\mathrm{Coul}},$$

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

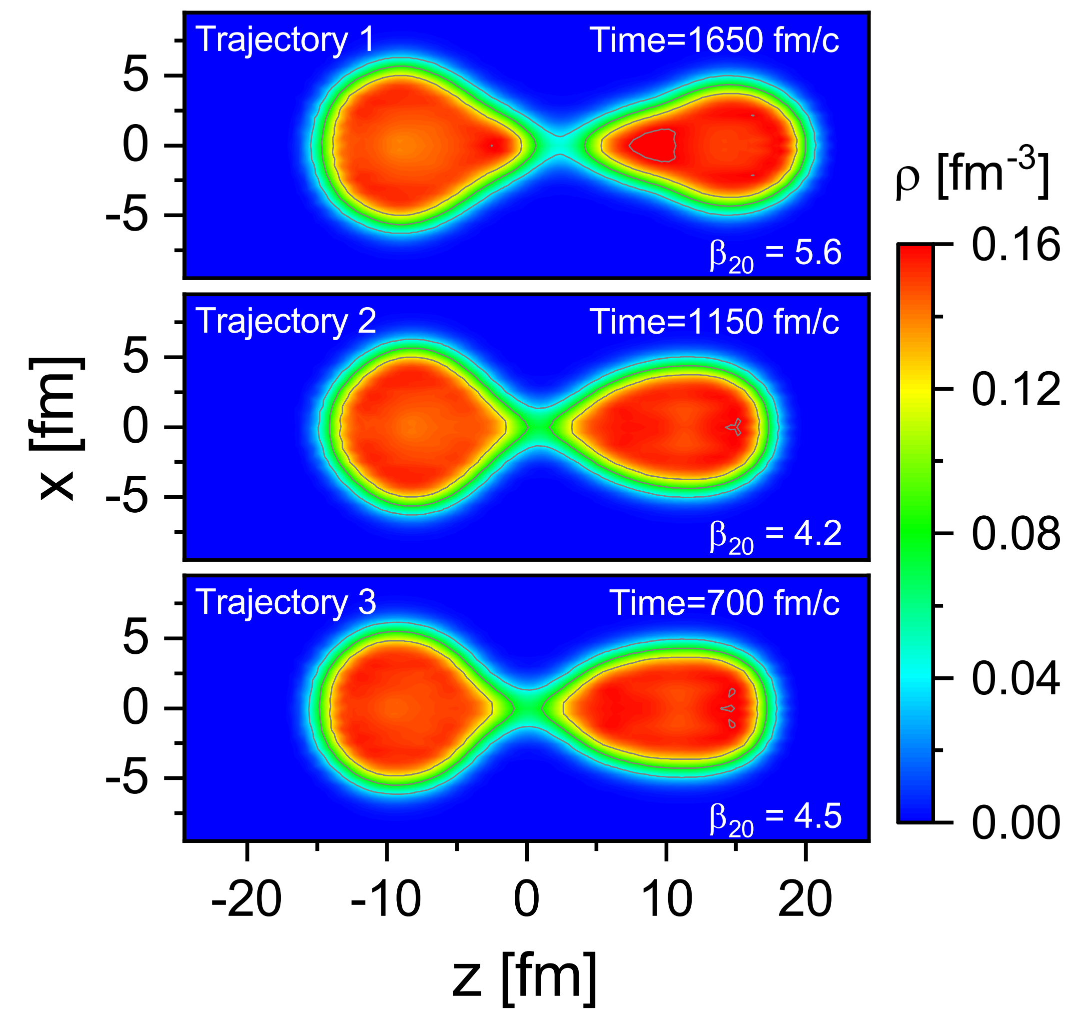


Dynamical synthesis of ^{4}He in the scission phase of nuclear fission

TDDFT fission trajectories



Density profiles at times immediately prior to the scission event.



Ren, Vretenar, Nikšić, Zhao, Zhao, Meng (2022)

Nucleon localization functions:

σ ($\uparrow$ or $\downarrow$)

q (n or p)

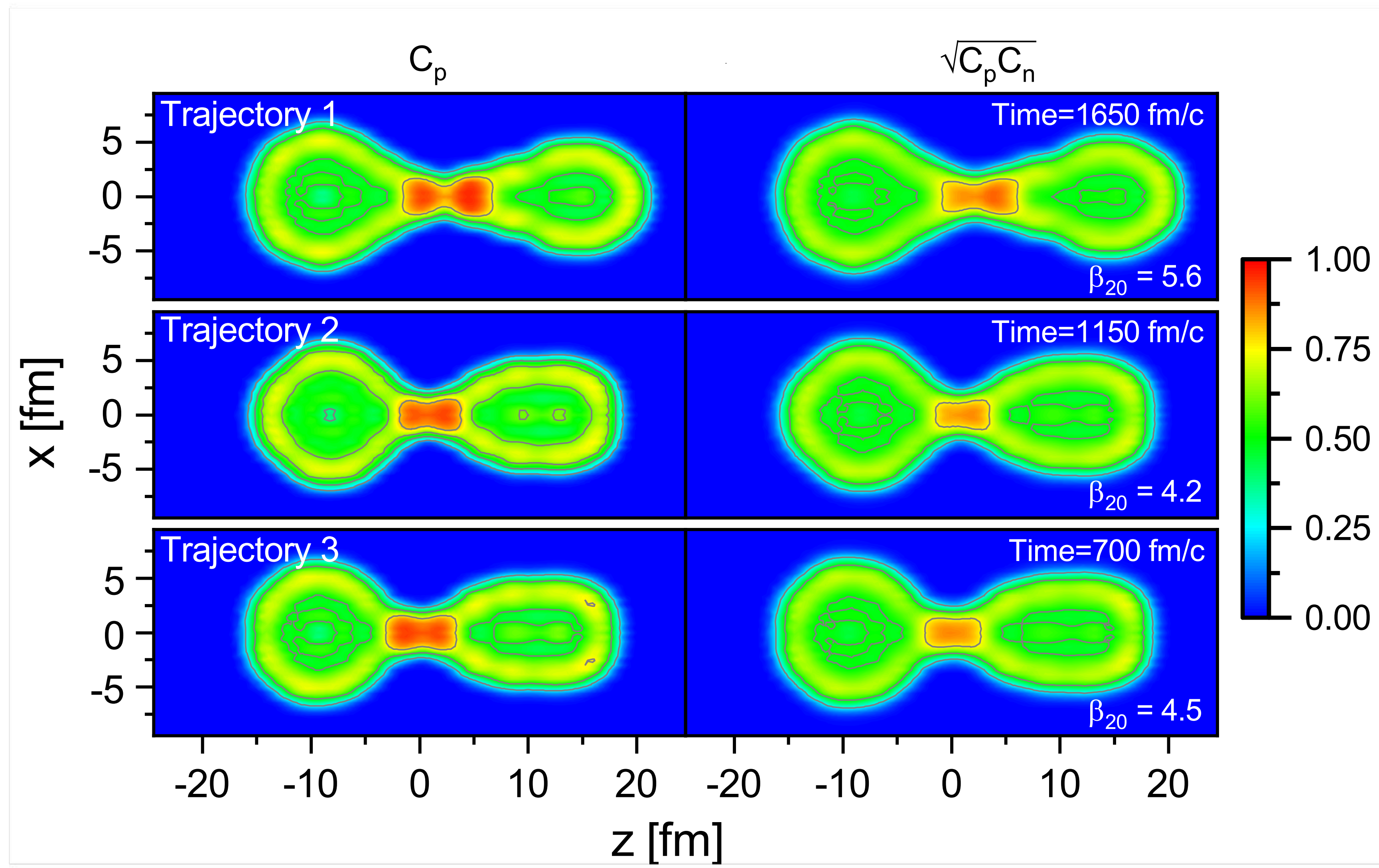
kinetic energy density — density — current density

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

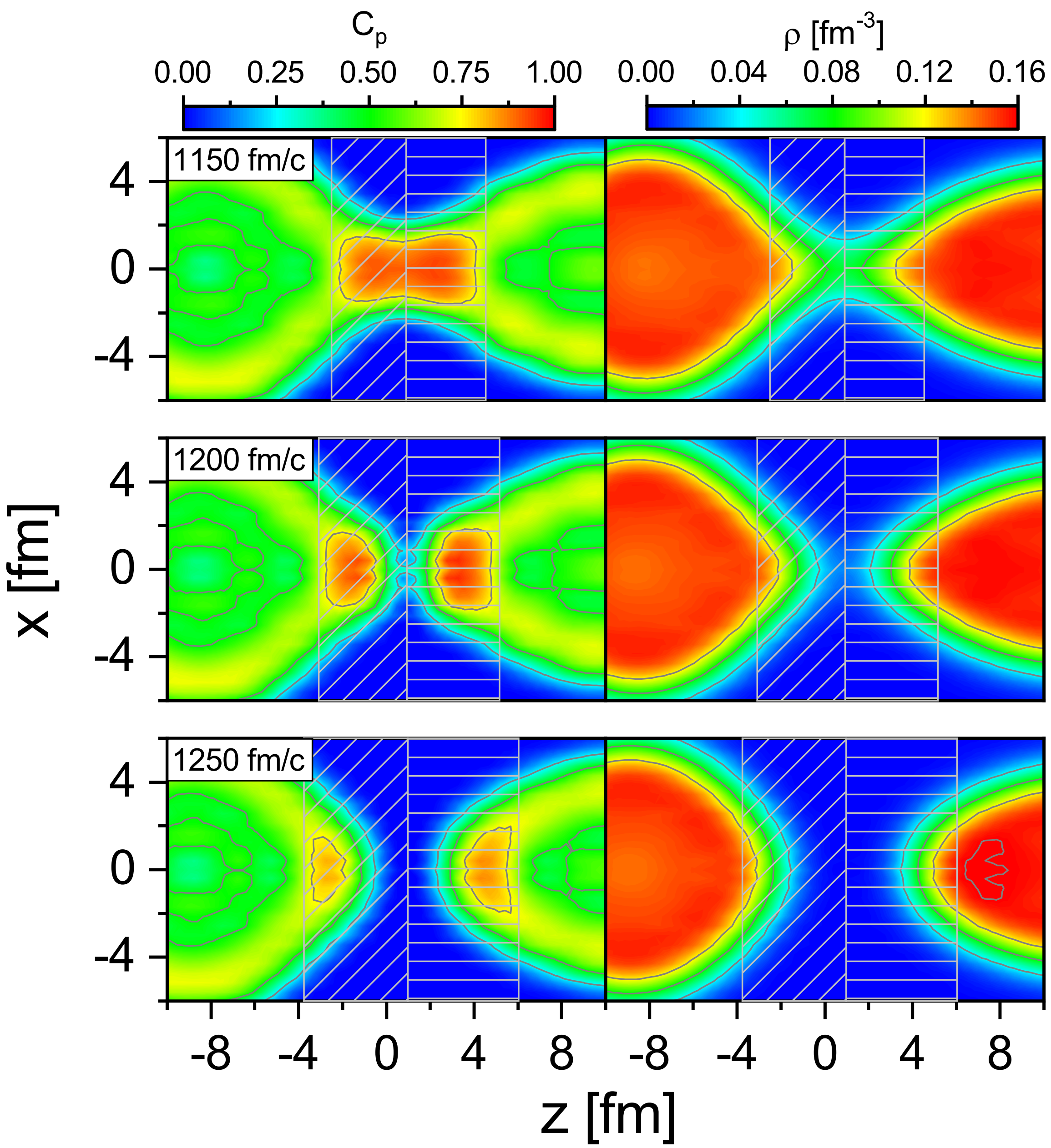
$$\tau_{q\sigma}^{\mathrm{TF}} = \frac{3}{5}(6\pi^2)^{2/3}\rho_{q\sigma}^{5/3}$$

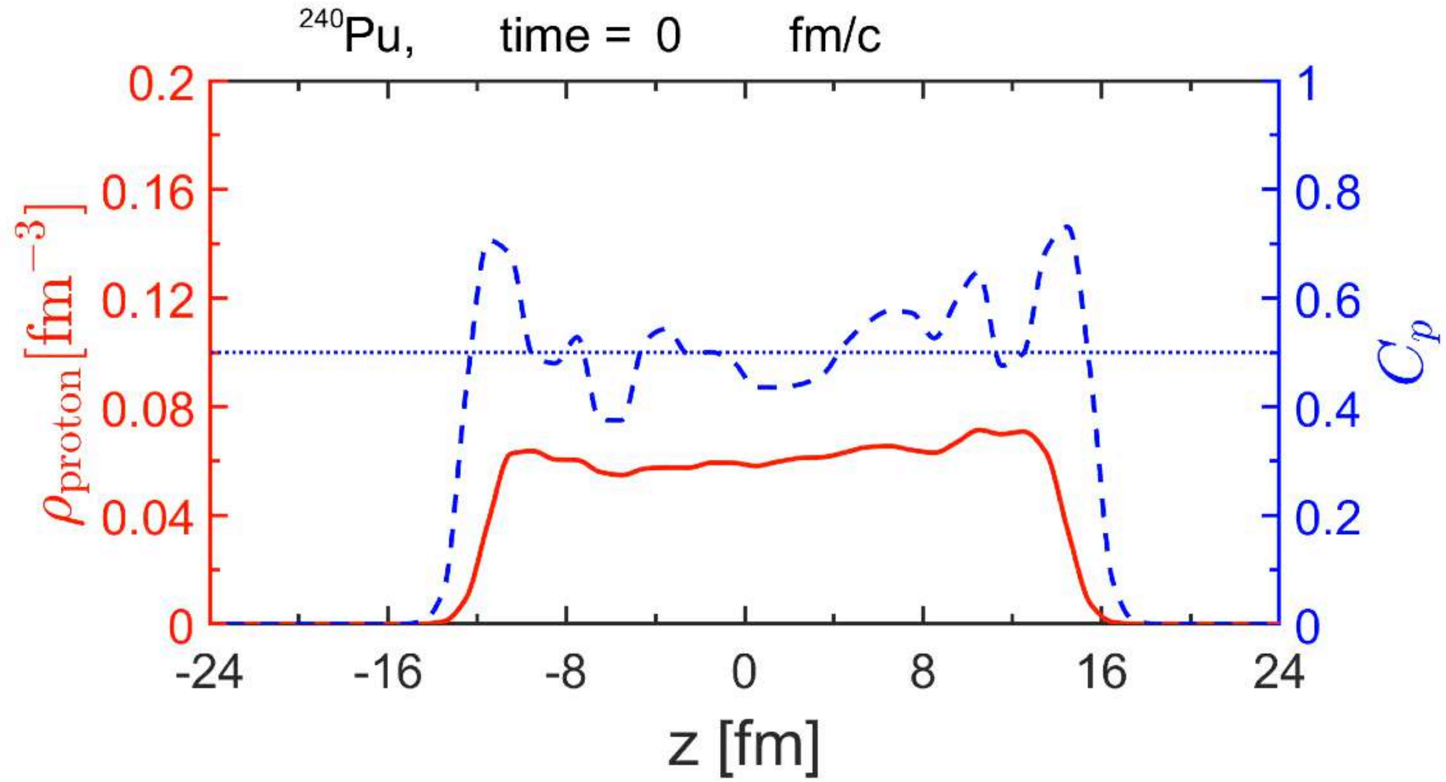
For homogeneous nuclear matter: $C_{q\sigma} = 1/2$

For the 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 (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