Workshop on fission dynamics 2026
Chongqing, 11-15 May 2026

Microscopic Models of Induced Fission Dynamics

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Outline

Extended temperature-dependent TDGCM

- Finite temperature time-dependent generator coordinate method
- Formalism of the extended temperature-depdendent TDGCM based on the quantum theory of dissipation for collective motion (Kerman & Kooning, 1974)
- Illustrative calculation: induced fission of 228Th

Generalized TDGCM

- Implementation of the generalized time-dependent generator coordinate method
- Both the weight functions and the generator states are time-dependent
- Illustrative calculation: induced fission of 240Pu

Work done in collaboration with:

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- J. Meng, P.W. Zhao, Z.X. Ren, B. Li (PKU, Beijing)
- Z.P. Li (Southwest University, Chongqing)
- J. Zhao (Center for circuits and systems, Shenzshen)

TDGCM - introduction

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)

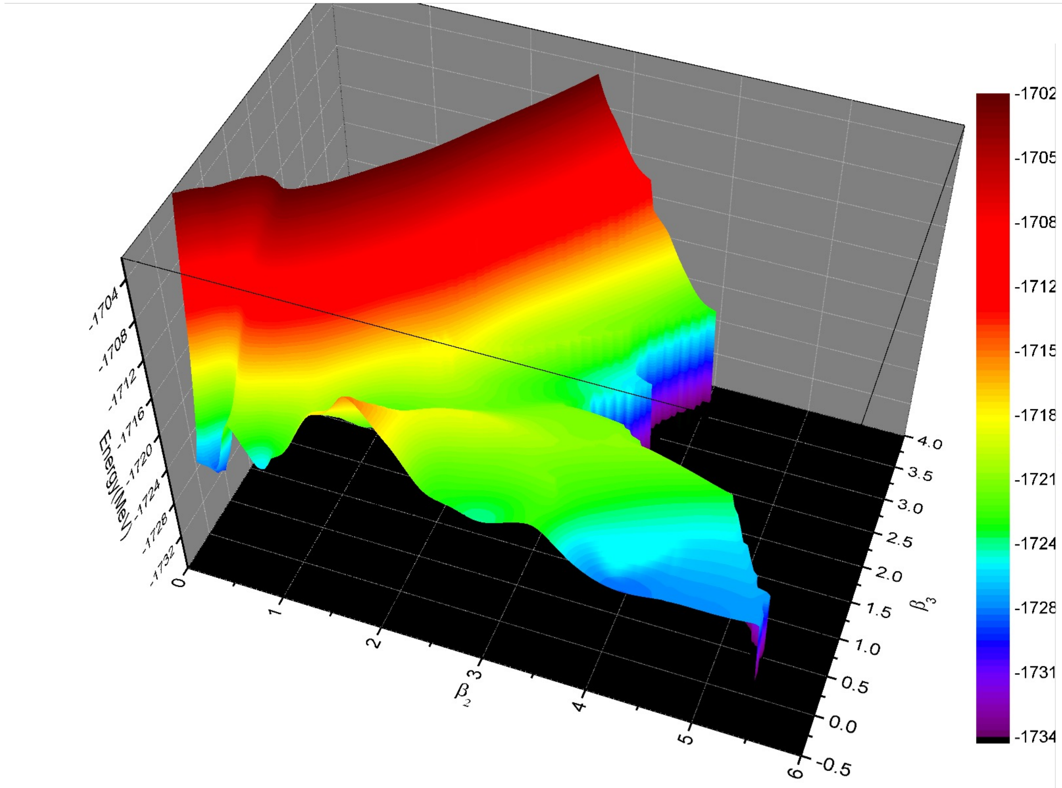
Time-dependent Schroedinger-like equation for fission dynamics (axial quadrupole and octupole deformation parameters as collective degrees of freedom):

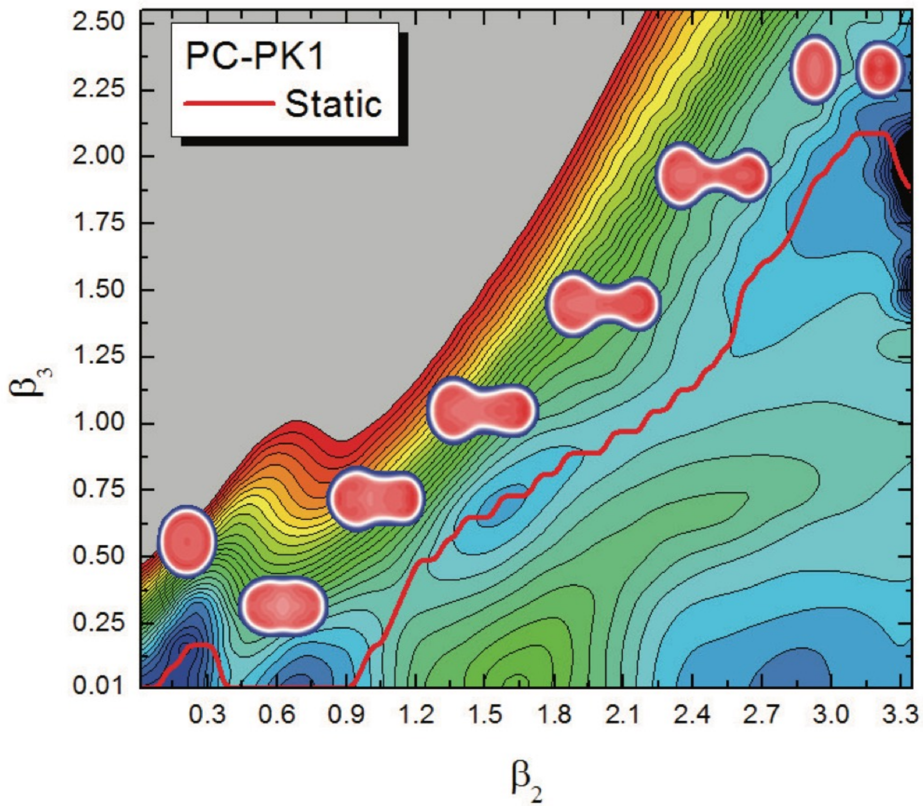
$$i\hbar\frac{\partial}{\partial t}g(\beta_2,\beta_3,t) = \left[-\frac{\hbar^2}{2}\sum_{kl}\frac{\partial}{\partial\beta_k}B_{kl}(\beta_2,\beta_3)\frac{\partial}{\partial\beta_l} + V(\beta_2,\beta_3)\right]g(\beta_2,\beta_3,t)$$

Quadrupole and octupole constrained deformation energy surface of ^{226}Th in the $\beta_2 - \beta_3$ plane.

Tao, Zhao, Li, Nikšić, Vretenar,

Phys. Rev. C **96**, 024319 (2017).





TDGCM - 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:

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

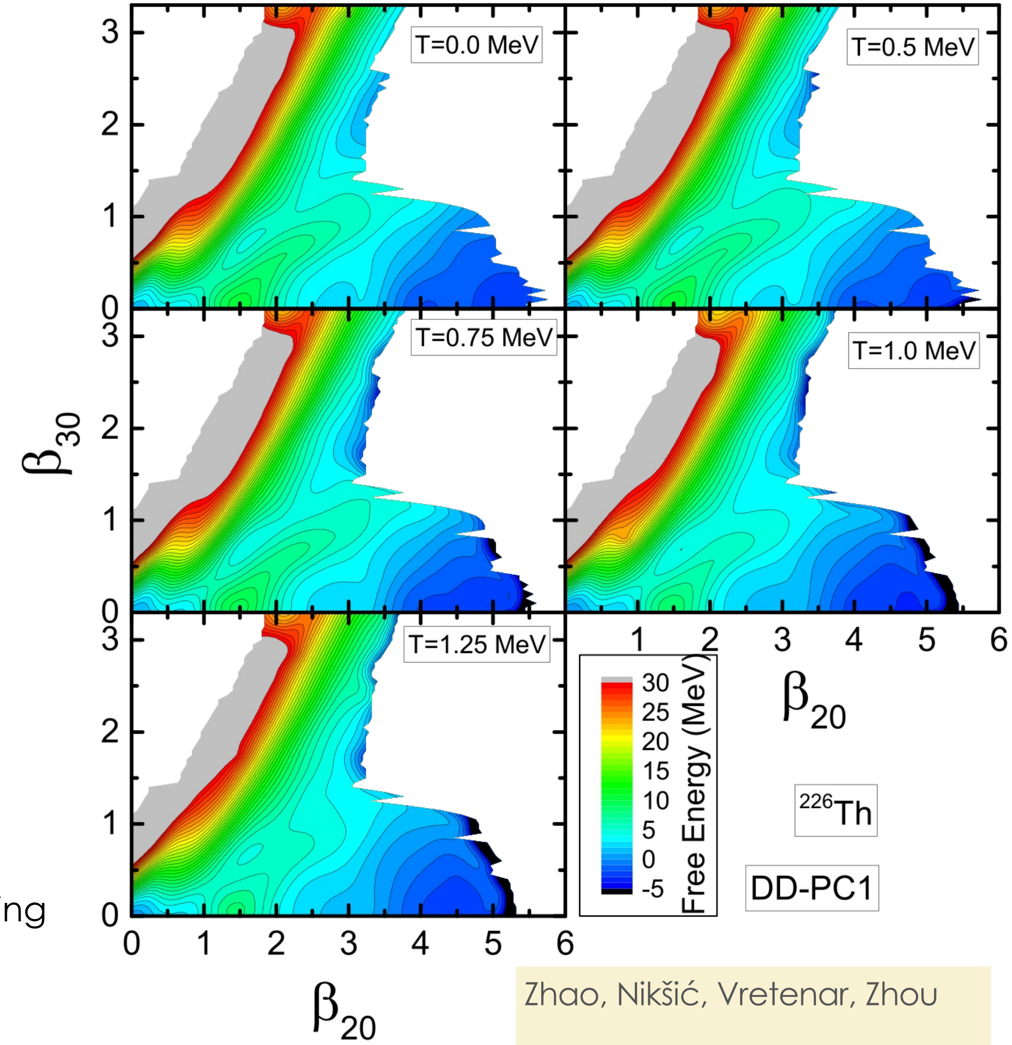
... thermal occupation probabilities:

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

Mass tensor → finite temperature perturbative cranking approximation

$$\mathcal{M}^{Cp} = \hbar^2 M_{(1)}^{-1}M_{(3)}M_{(1)}^{-1}$$

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



Zhao, Nikšić, Vretenar, Zhou

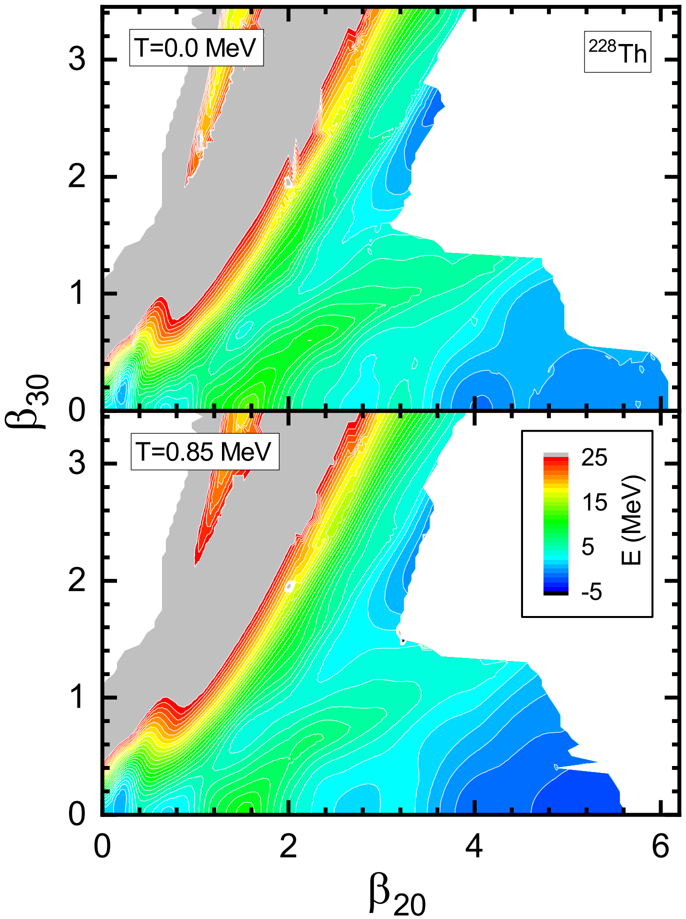
Phys. Rev. C **99**, 014618 (2019).

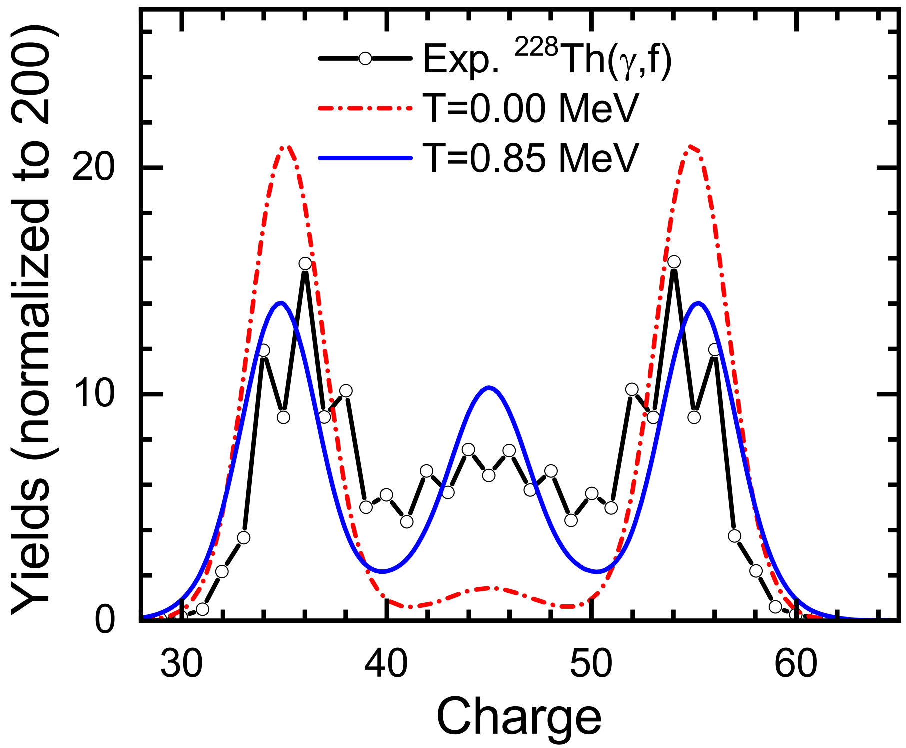
TDGCM - finite temperature effects

Approximation: the compound nucleus is in a state of thermal equilibrium at a temperature that corresponds to the internal excitation energy.

Zhao, Xiang, Li, Nikšić, Vretenar, Zhou

Phys. Rev. C **99**, 054613 (2019).





Charge yields for photoinduced fission of ^{228}Th. T=0.85 MeV corresponds to the intrinsic excitation energy $E^*_{int} \approx 11$ MeV (peak value of the photon energy distribution).

Extended TDGCM – dissipation effects

Kerman, Koonin, Phys. Scr. 10, 118 (1974)

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:

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

$\langle n\boldsymbol{q}|\hat{H}|n'\boldsymbol{q}'\rangle$ (→ $\mathcal{H}_{nn'}$)

$\langle n\boldsymbol{q}|n'\boldsymbol{q}'\rangle$ (→ $\mathcal{N}_{nn'}$)

⇒ another set of functions is defined:

$$g_n(\boldsymbol{q},t) = \sum_{n'} \int d\boldsymbol{q}' \mathcal{N}^{1/2}_{nn'}(\boldsymbol{q},\boldsymbol{q}') f_{n'}(\boldsymbol{q}',t)$$

⇒ Hill-Wheeler equation is re-expressed:

$$i\hbar\partial_t g_n(\boldsymbol{q},t) = \sum_{n'} \int d\boldsymbol{q}' H_{nn'}(\boldsymbol{q},\boldsymbol{q}') g_{n'}(\boldsymbol{q}',t)$$

$$H_{nn'}(\boldsymbol{q},\boldsymbol{q}') = \sum_{n_1 n_2} \int d\boldsymbol{q}_1 d\boldsymbol{q}_2 \mathcal{N}^{-1/2}_{nn_1}(\boldsymbol{q},\boldsymbol{q}_1) \times \mathcal{H}_{n_1 n_2}(\boldsymbol{q}_1,\boldsymbol{q}_2) \mathcal{N}^{-1/2}_{n_2 n'}(\boldsymbol{q}_2,\boldsymbol{q}')$$

Extended TDGCM - dissipation effects

… 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:

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

⇒ substitution:

$$g_n(\boldsymbol{q},t) \rightarrow g_\lambda(\boldsymbol{q},\epsilon;t),$$

$$H_{nn'}(\boldsymbol{q},\boldsymbol{q}') \rightarrow H_{\lambda\lambda'}(\boldsymbol{q},\boldsymbol{q}';\epsilon,\epsilon')$$

⇒statistical wave function is defined as average on λ:

statistical collective wave function

$$\overline{g_\lambda(\boldsymbol{q},\epsilon;t)} = \frac{\psi(\boldsymbol{q},\epsilon;t)}{\sqrt{\rho(\boldsymbol{q},\epsilon)}}$$

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

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

$$h(\boldsymbol{q},\boldsymbol{q}';\epsilon,\epsilon) = \frac{1}{\sqrt{\rho(\boldsymbol{q},\epsilon)}}\sum_\lambda H_{\lambda\lambda}(\boldsymbol{q},\boldsymbol{q}';\epsilon,\epsilon)\frac{1}{\sqrt{\rho(\boldsymbol{q}',\epsilon)}}$$

$$h(\boldsymbol{q},\boldsymbol{q}';\epsilon,\epsilon') = \frac{1}{\sqrt{\rho(\boldsymbol{q},\epsilon)}}\sum_{\lambda,\lambda'\neq\lambda} H_{\lambda\lambda'}(\boldsymbol{q},\boldsymbol{q}';\epsilon,\epsilon')\frac{1}{\sqrt{\rho(\boldsymbol{q}',\epsilon')}}$$

Extended TDGCM - dissipation effects

- Hamiltonian overlap kernel decreases rapidly with increasing **q-q'**
- expansion in a power series in collective momenta
- excitation energy → nuclear temperature $\epsilon(T)$

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

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

Disipation term

- Couples excitation energies via a phenomenological stochastic ansatz
- Matrix elements $\eta(T,T')$ are modeled as Gaussian random variables scaled by intrinsic nuclear level densities

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

β_2^0 - cutoff value beyond the second fission barrier

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

Internal excitation energy -> difference between the B.E. of the equilibrium minimum at temperature T and at T=0

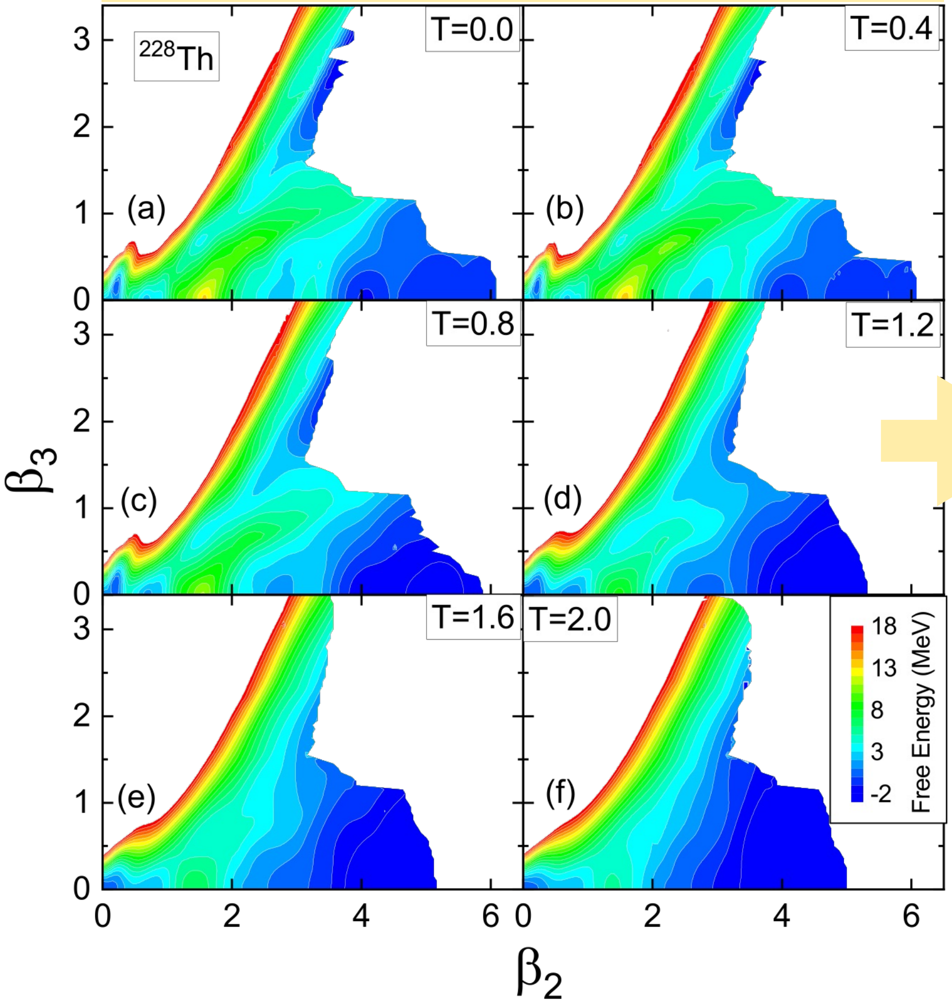
Helmholtz free energy normalized to the value at the equilibrium minimum at temperature T

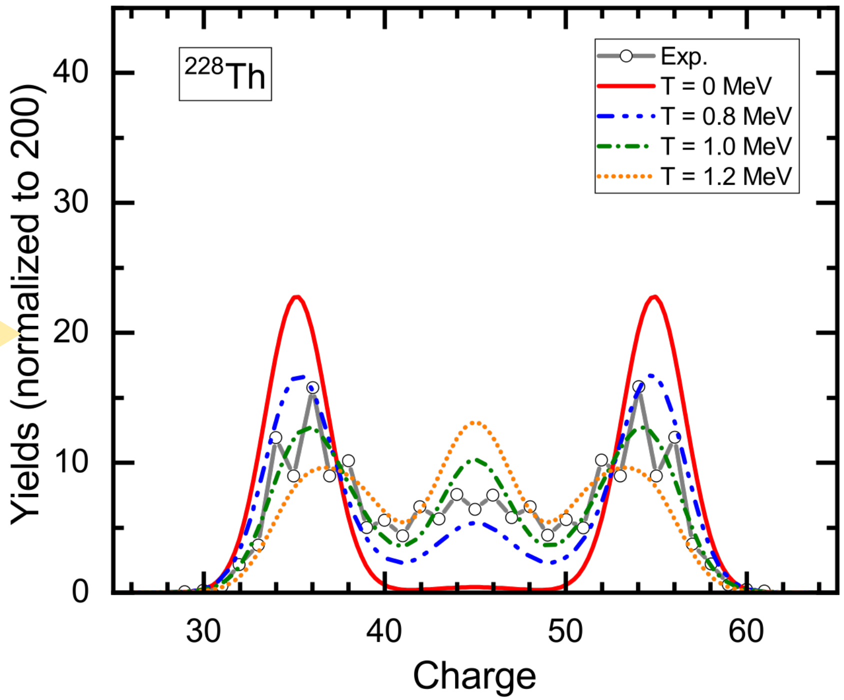
Inertia tensor -> finite temperature perturbative cranking approximation

Extended TDGCM - dissipation effects

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

2D TDGCM+GOA calculation at fixed temperatures T.





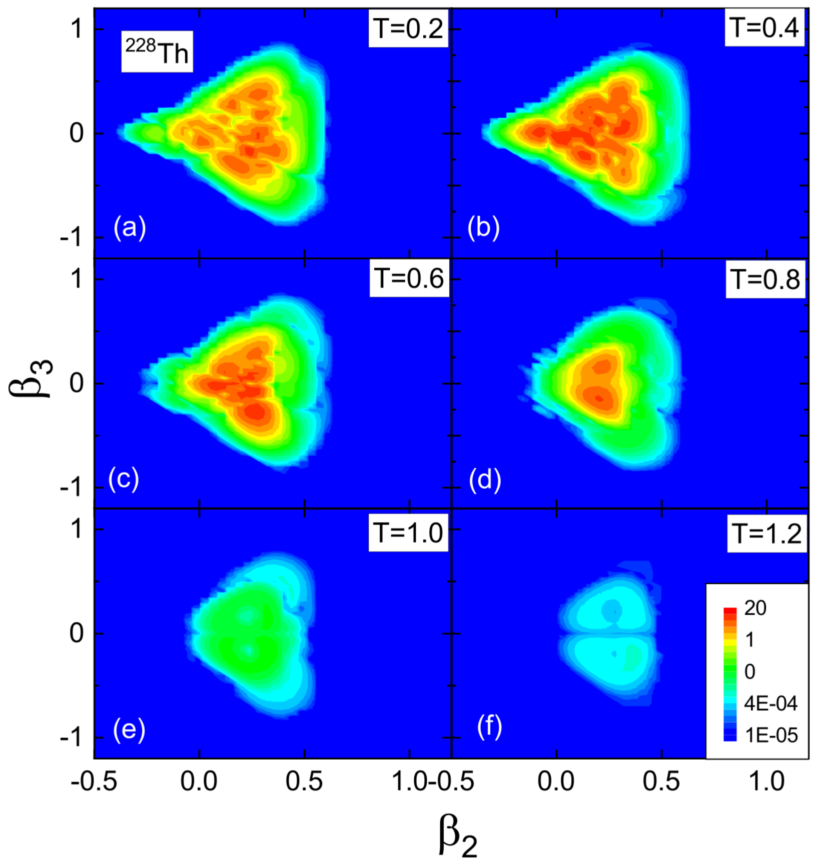
The data for photo-induced fission correspond to photon energies in the interval 8 – 14 MeV, and a peak value of E_γ = 11 MeV.

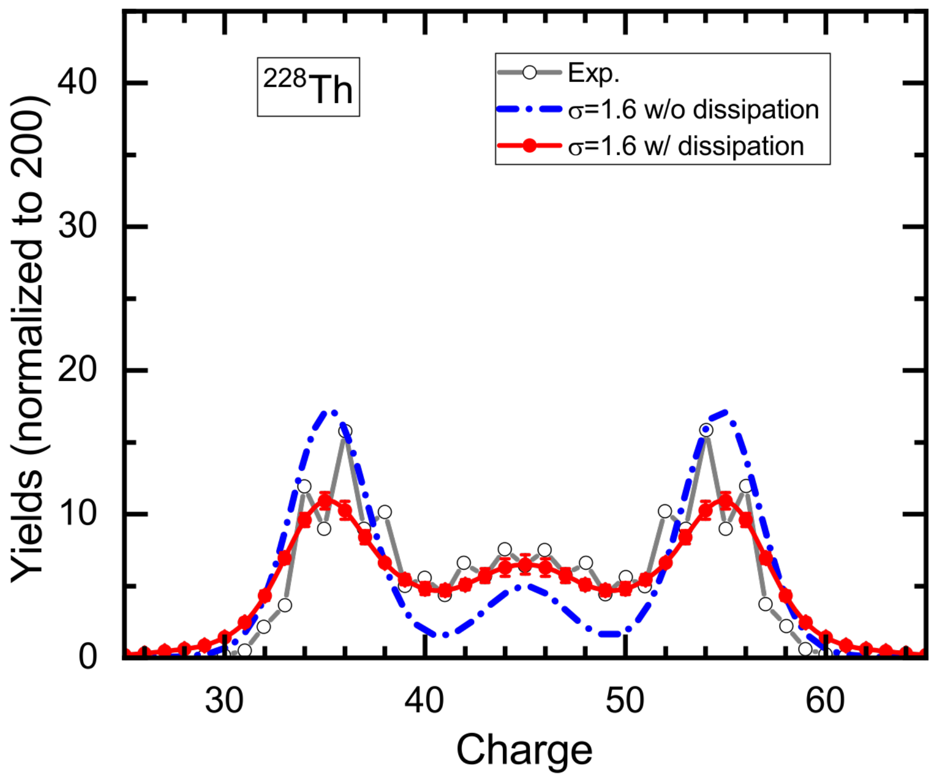
Extended TDGCM - dissipation effects

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.

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

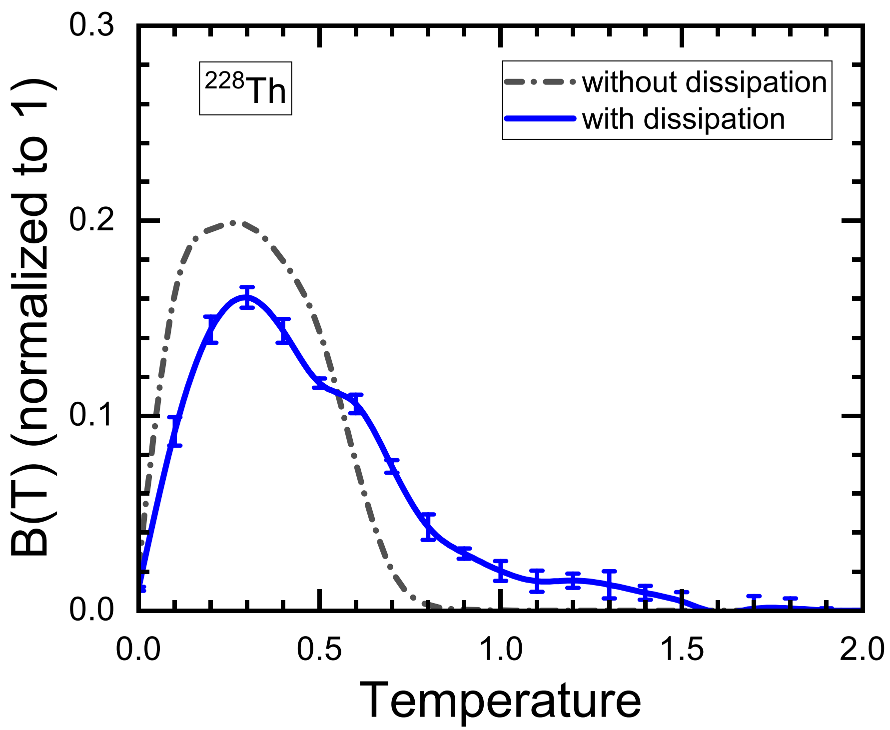




Extended TDGCM - dissipation effects

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

Collective flux B(T) through the scission contour as a function of temperature



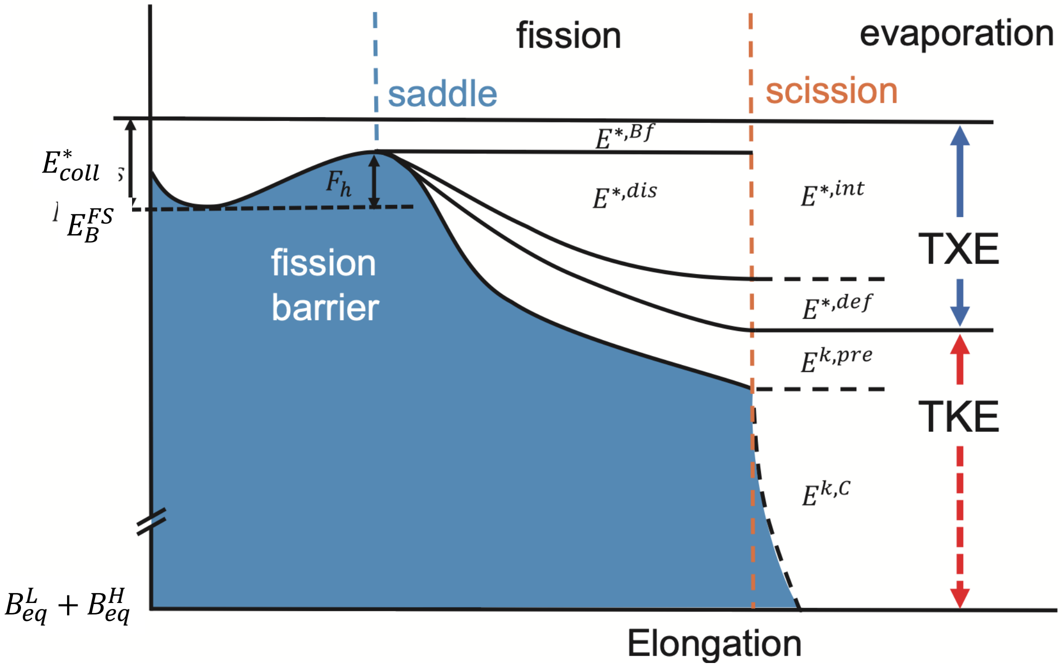
The integrated flux F (ξ; t) for a given scission surface element ξ: $F(\xi;t) = \int_{t_0}^{t} dt' \int_{(\boldsymbol{q},T)\in\xi} \boldsymbol{J}(\boldsymbol{q},T;t') \cdot d\boldsymbol{S},$

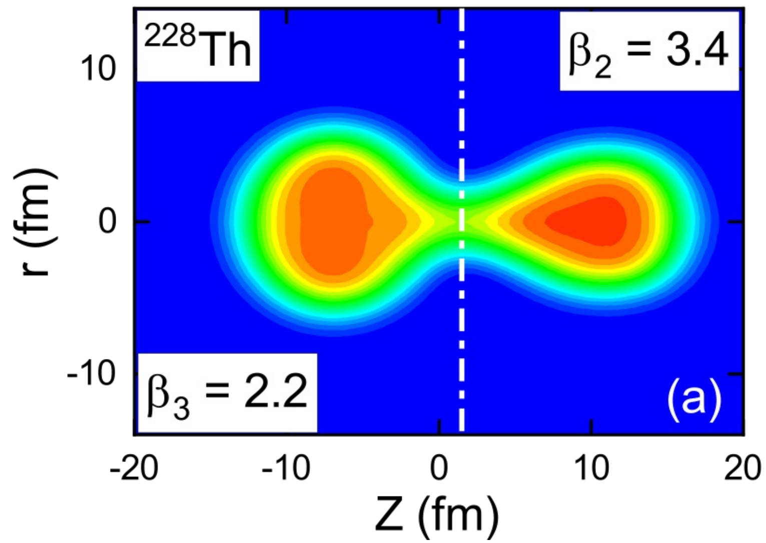
The integrated flux for a given temperature: $B(T) \propto \sum_{\xi \in \mathcal{B}} \lim_{t\to\infty} F(\xi;t)$

Elements on the scission contour with a given temperature T

Total Kinetic Energy Distribution

M. Caamano and F. Farget, Phys. Lett. B 770, 72 (2017)





Energy balance at scission:

$$E_B^{FS} + E^*_{coll} = B^L_{eq} + B^H_{eq} + \text{TKE} + \text{TXE}$$

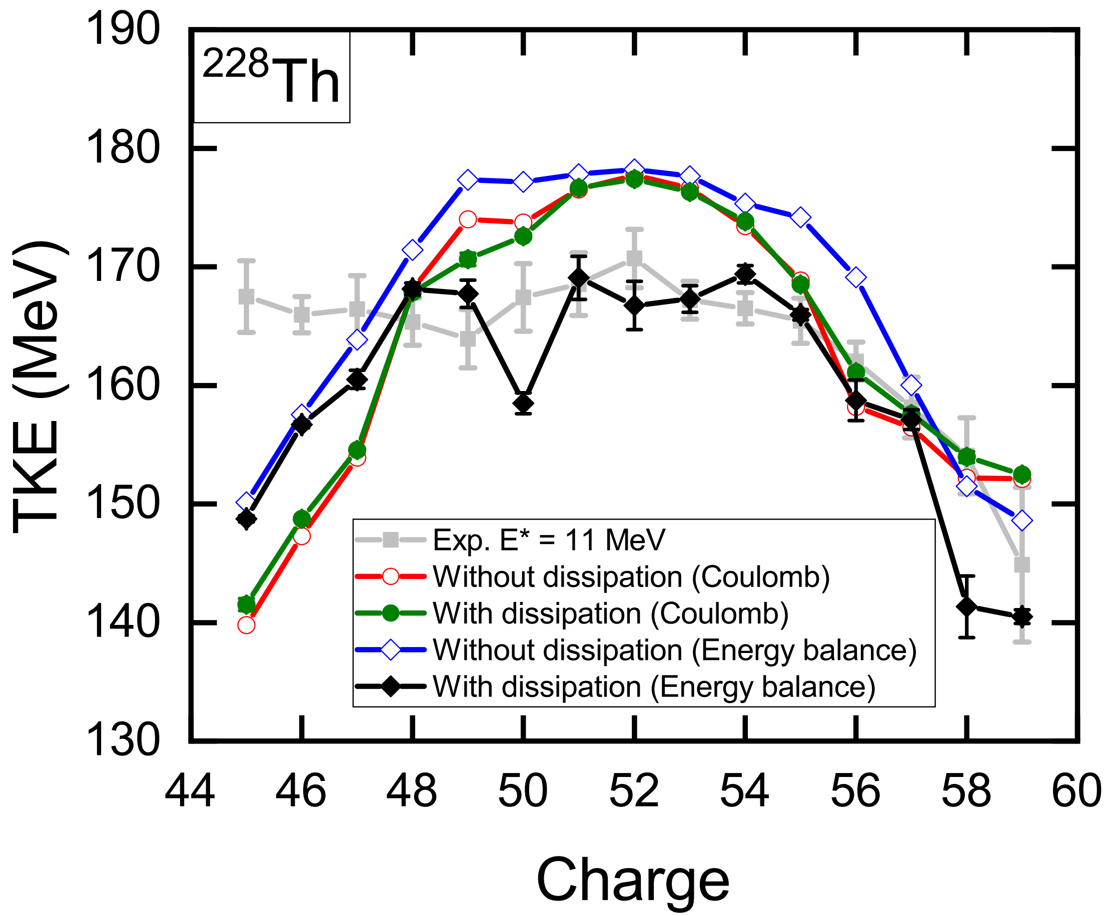
$$\text{TKE}(\xi) = (E_B^{FS} + E^*_{coll}) - \left[E^L(\beta_2^L, \beta_3^L, T) + E^H(\beta_2^H, \beta_3^H, T)\right]$$

Coulomb repulsion for a pair of fission fragments: $E_{\text{Coul}} = \dfrac{e^2 Z_H Z_L}{d_{\text{ch}}}$

Total Kinetic Energy Distribution

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

The TKE for the fission fragment with mass A is defined by: $\mathrm{TKE}(A) = \lim_{t\to\infty} \frac{\sum_{\xi\in\mathcal{A}} F(\xi;t)\mathrm{TKE}(\xi)}{\sum_{\xi\in\mathcal{A}} F(\xi;t)}$



Generalized TDGCM

B. Li, D. Vretenar, T. Nikšić, P.W. Zhao, J. Meng, Phys. Rev. C **108**, 014321 (2023).
B. Li, D. Vretenar, T. Nikšić, J. Zhao, P.W. Zhao, J. Meng, Front. Phys. **19**, 44201 (2024).
B. Li, D. Vretenar, T. Nikšić, P.W. Zhao, J. Meng, Phys. Rev. C **111**, L051302 (2025).

The Griffin-Hill/Wheeler ansatz for the TDGCM nuclear wave function (discretized generator coordinates are mass multipole moments β_{20} and β_{30}): $|\Psi(t)\rangle = \sum_{\boldsymbol{q}} f_{\boldsymbol{q}}(t)|\Phi_{\boldsymbol{q}}(t)\rangle,$

The nuclear wave function is the solution of the time-dependent equation:

$$\mathrm{i}\hbar\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle \longrightarrow \sum_{\boldsymbol{q}} \mathrm{i}\hbar\mathcal{N}_{\boldsymbol{q}'\boldsymbol{q}}(t)\partial_t f_{\boldsymbol{q}}(t) + \sum_{q} \mathcal{H}^{MF}_{\boldsymbol{q}'\boldsymbol{q}}(t) f_{\boldsymbol{q}}(t) = \sum_{q} \mathcal{H}_{\boldsymbol{q}'\boldsymbol{q}}(t) f_{\boldsymbol{q}}(t)$$

The time-dependent kernels:

$$\mathcal{N}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|\Phi_{\boldsymbol{q}}(t)\rangle,$$

$$\mathcal{H}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|\hat{H}|\Phi_{\boldsymbol{q}}(t)\rangle,$$

$$\mathcal{H}^{MF}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|i\hbar\partial_t|\Phi_{\boldsymbol{q}}(t)\rangle$$

Transformation parameters between the canonical and quasiparticle basis

Quasiparticle vacuum:

$$|\Phi_{\boldsymbol{q}}(t)\rangle = \prod_{k>0}[\mu_{\boldsymbol{q},k}(t) + \nu_{\boldsymbol{q},k}(t)c^\dagger_{\boldsymbol{q},k}(t)c^\dagger_{\boldsymbol{q},\bar{k}}(t)]|-\rangle$$

Creation operator associated with the canonical state $\phi^{\boldsymbol{q}}_k(\boldsymbol{r},t)$

Generalized TDGCM

The time evolution of the quasiparticle vacuum is modeled by the time-dependent covariant DFT+ the time-dependent BCS approximation

$$\hat{h}^{\boldsymbol{q}}(\boldsymbol{r},t) = \boldsymbol{\alpha}\cdot(\hat{\boldsymbol{p}} - \boldsymbol{V}_{\boldsymbol{q}}) + V^0_{\boldsymbol{q}} + \beta(m_N + S_{\boldsymbol{q}})$$

$$i\frac{\partial}{\partial t}\phi^{\boldsymbol{q}}_k(\boldsymbol{r},t) = [\hat{h}^{\boldsymbol{q}}(\boldsymbol{r},t) - \varepsilon^{\boldsymbol{q}}_k(t)]\phi^{\boldsymbol{q}}_k(\boldsymbol{r},t)$$

$$\varepsilon^{\boldsymbol{q}}_k(t) = \langle\psi^{\boldsymbol{q}}_k|\hat{h}^{\boldsymbol{q}}|\psi^{\boldsymbol{q}}_k\rangle$$

The time evolution of the occupation probability ($n_{q,k}(t) = |\nu_{q,k}(t)|^2$) and pairing tensor ($\kappa_{q,k}(t) = \mu^*_{q,k}(t)\nu_{q,k}(t)$)

$$i\frac{d}{dt}n_{\boldsymbol{q},k}(t) = \kappa_{\boldsymbol{q},k}(t)\Delta^*_{\boldsymbol{q},k}(t) - \kappa^*_{\boldsymbol{q},k}(t)\Delta_{\boldsymbol{q},k}(t),$$

$$i\frac{d}{dt}\kappa_{\boldsymbol{q},k}(t) = [\varepsilon^{\boldsymbol{q}}_k(t) + \varepsilon^{\boldsymbol{q}}_{\bar{k}}(t)]\kappa_{\boldsymbol{q},k}(t) + \Delta_{\boldsymbol{q},k}(t)[2n_{\boldsymbol{q},k}(t) - 1]$$

Pairing tensor -> monopole pairing with cut-off function for the pairing window

$$\Delta_{\boldsymbol{q},k}(t) = \left[G\sum_{k'>0} f(\varepsilon^{\boldsymbol{q}}_{k'})\kappa_{\boldsymbol{q},k'}\right] f(\varepsilon^{\boldsymbol{q}}_k)$$

Generalized TDGCM

Collective wave function $g = \mathcal{N}^{1/2} f$

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

Observables

$$\mathcal{O}_{\boldsymbol{q'q}} = \langle\Phi_{q'}(t)|\hat{O}|\Phi_q(t)\rangle \longrightarrow \mathcal{O}^c = \mathcal{N}^{-1/2}\mathcal{O}\mathcal{N}^{-1/2}$$

$$\longrightarrow \langle\Psi(t)|\hat{O}|\Psi(t)\rangle = f^\dagger\mathcal{O}f = g^\dagger\mathcal{O}^c g$$

Particle number projection

Probability of finding z protons in the subspace V_f corresponding to one of the fragments (total number of protons is Z)

$$P(z|Z,t) = \frac{\langle\Psi(t)\big|\hat{P}_z^{V_f}\hat{P}_Z\big|\Psi(t)\rangle}{\langle\Psi(t)\big|\hat{P}_Z\big|\Psi(t)\rangle}$$

$$= \frac{\sum_{\boldsymbol{qq'}} f^*_{\boldsymbol{q'}}(t)f_{\boldsymbol{q}}(t)\langle\Phi_{\boldsymbol{q'}}(t)\big|\hat{P}_z^{V_f}\hat{P}_Z\big|\Phi_{\boldsymbol{q}}(t)\rangle}{\sum_{\boldsymbol{qq'}} f^*_{\boldsymbol{q'}}(t)f_{\boldsymbol{q}}(t)\langle\Phi_{\boldsymbol{q'}}(t)\big|\hat{P}_Z\big|\Phi_{\boldsymbol{q}}(t)\rangle}$$

Generalized TDGCM

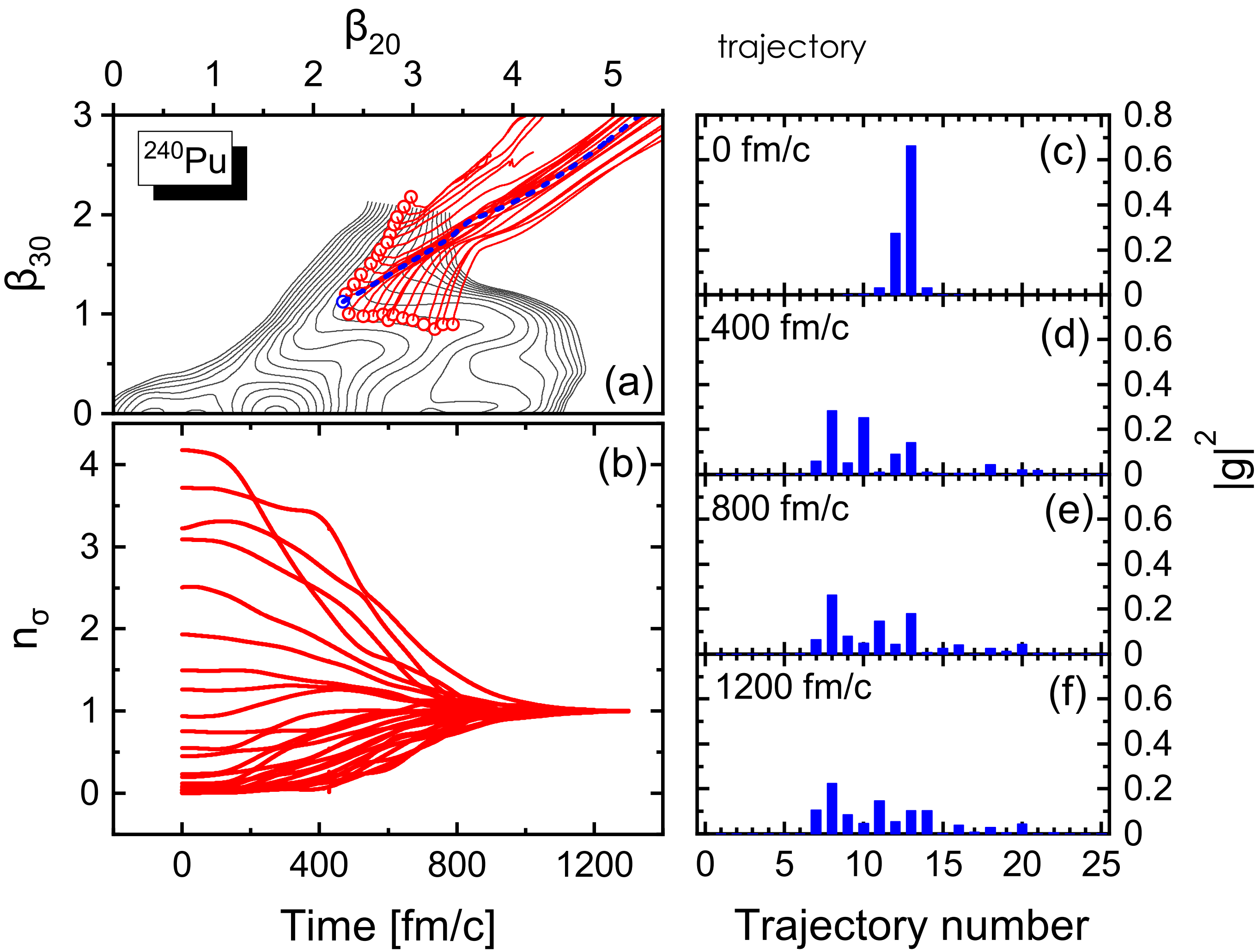
25 different TDDFT trajectories that start beyond the outer barrier

components of the collective wave function for the blue trajectory

Blue trajectory:

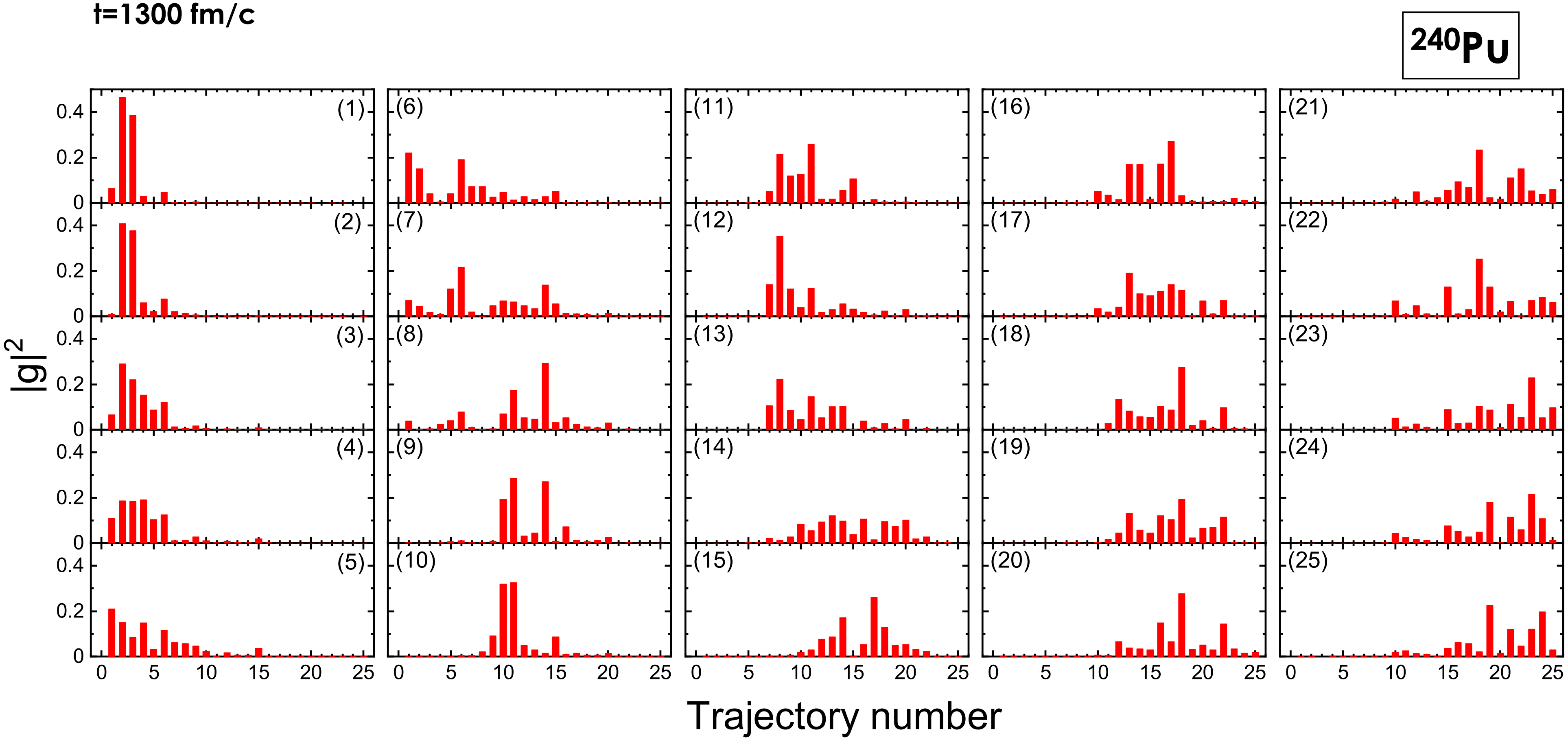
$$(\beta_{20}, \beta_{30}) = (2.30, 1.13)$$

Time evolution of the eigenvalues of the norm kernel



Generalized TDGCM

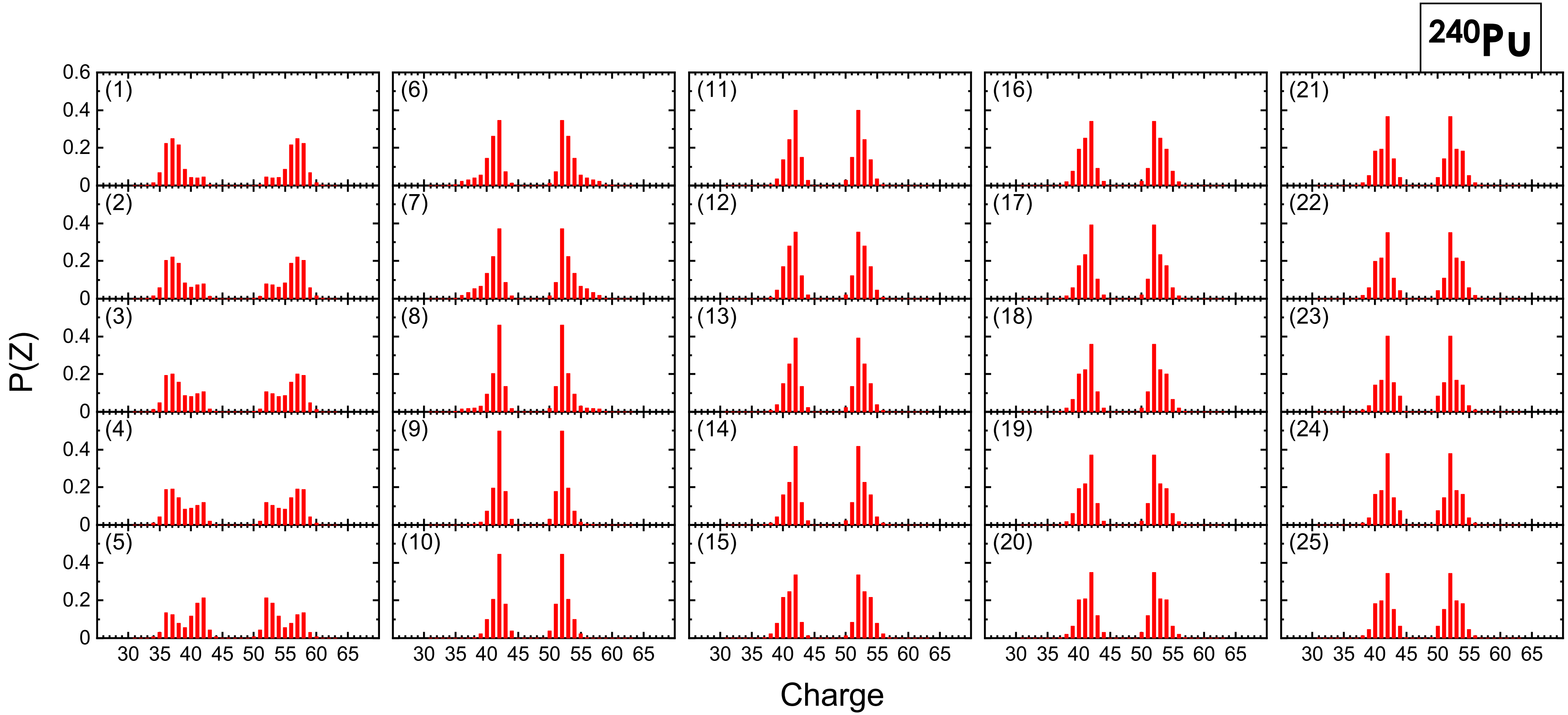
Components of the collective wave functions for 25 generalized TDGCM trajectories (each trajectory starts from different initial point)



Generalized TDGCM

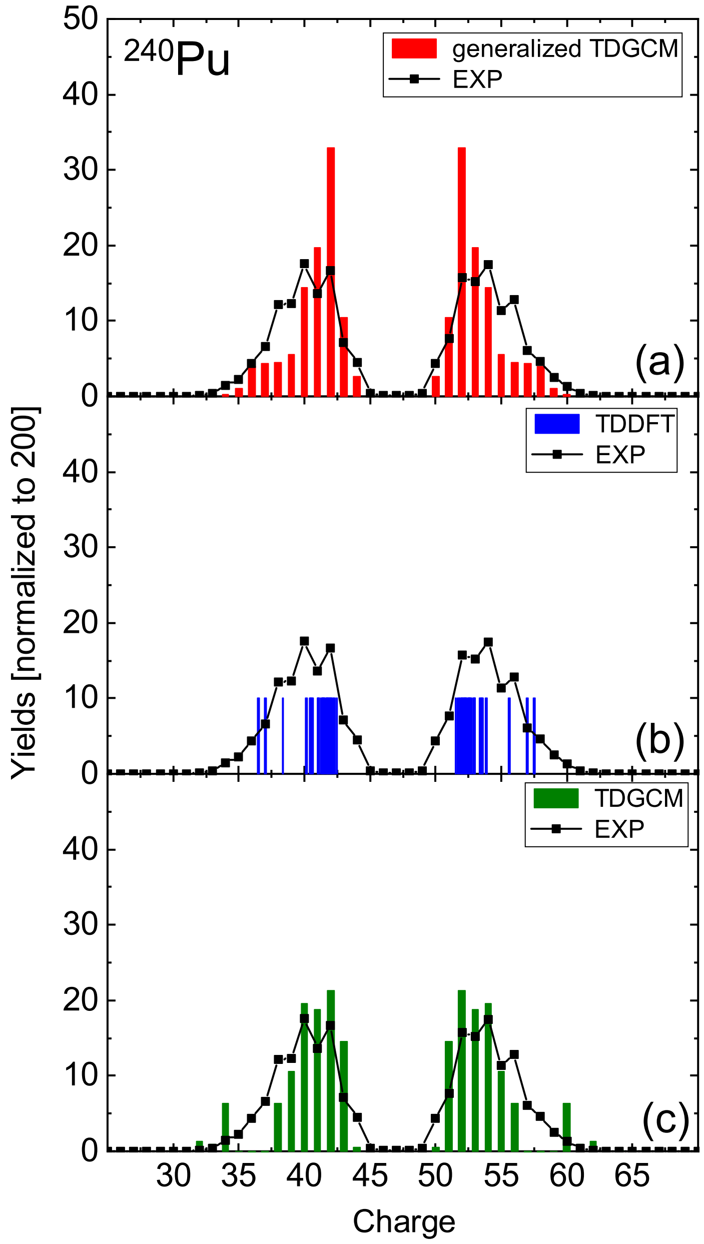
Probability distributions of proton number for 25 generalized TDGCM trajectories (each trajectory starts from different initial point)

t=1300 fm/c

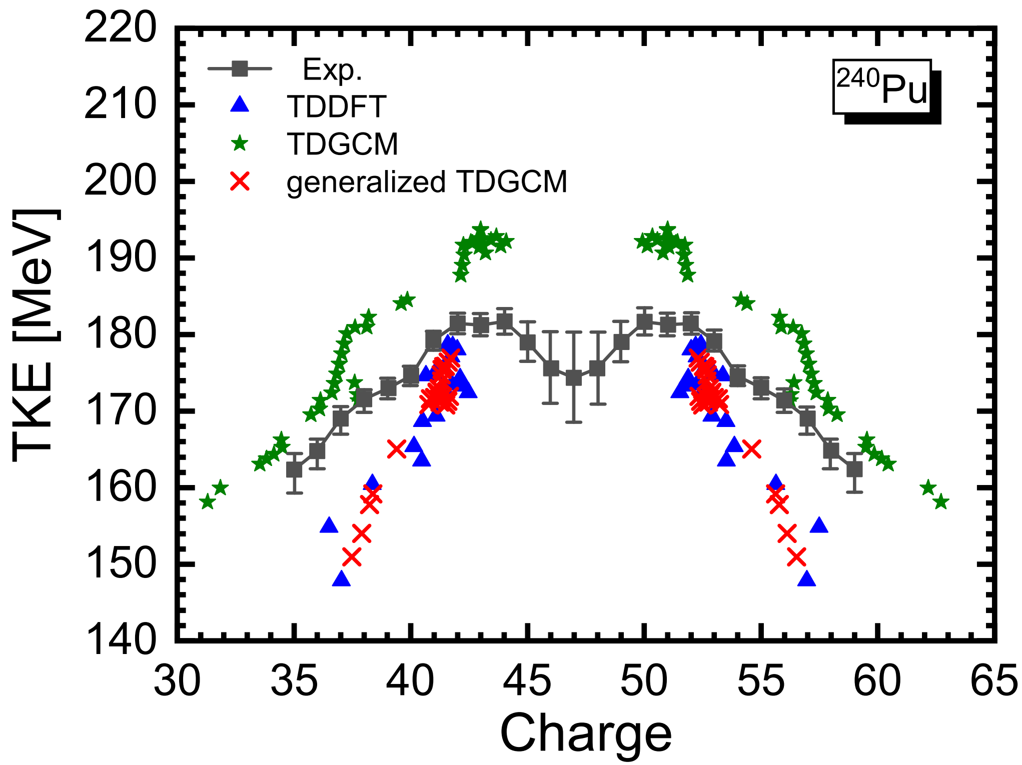


Generalized TDGCM

Charge yields for induced fission of ^{240}Pu



Total kinetic energies of the emerging fragments for induced fission of ^{240}Pu



Summary

- Starting from a quantum theory of dissipation for nuclear collective motion (Kerman & Koonin, 1974) we have extended the temperature-dependent TDGCM for induced fission dynamics, to allow for dissipation effects
- We have developed a method to calculate the corresponding distribution of total kinetic energies as a function of charge and mass of fission fragments

- An extension of time-dependent density functional theory, based on the time-dependent generator coordinate method, has been applied to nuclear fission dynamics
- Time-dependent generator states provide more realistic description of the saddle-to-fission phase of induced fission process
- Simultaneously Includes both the one-body dissipation mechanism and quantum fluctuations

This work was supported by the QuantiXLie Centre of Excellence, a project co-financed by the Croatian Government and European Union through the European Regional Development Fund - the Competitiveness and Cohesion Operational Program
(Grant KK.01.1.1.01.0004).

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Supported by the Croatian Science Foundation under the project Dynamics of complex femtosystems (IP-2025-02-4214).