北京大學
PEKING UNIVERSITY

Workshop on Fission Dynamics, 2026.05.11

Microscopic Study of Fission Dynamics and Fragment Distributions

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Outline

- Introduction
- Theoretical framework
- Fission fragment distribution
  - Charge yield and total kinetic energy
  - Spin correlation
- Summary and outlook

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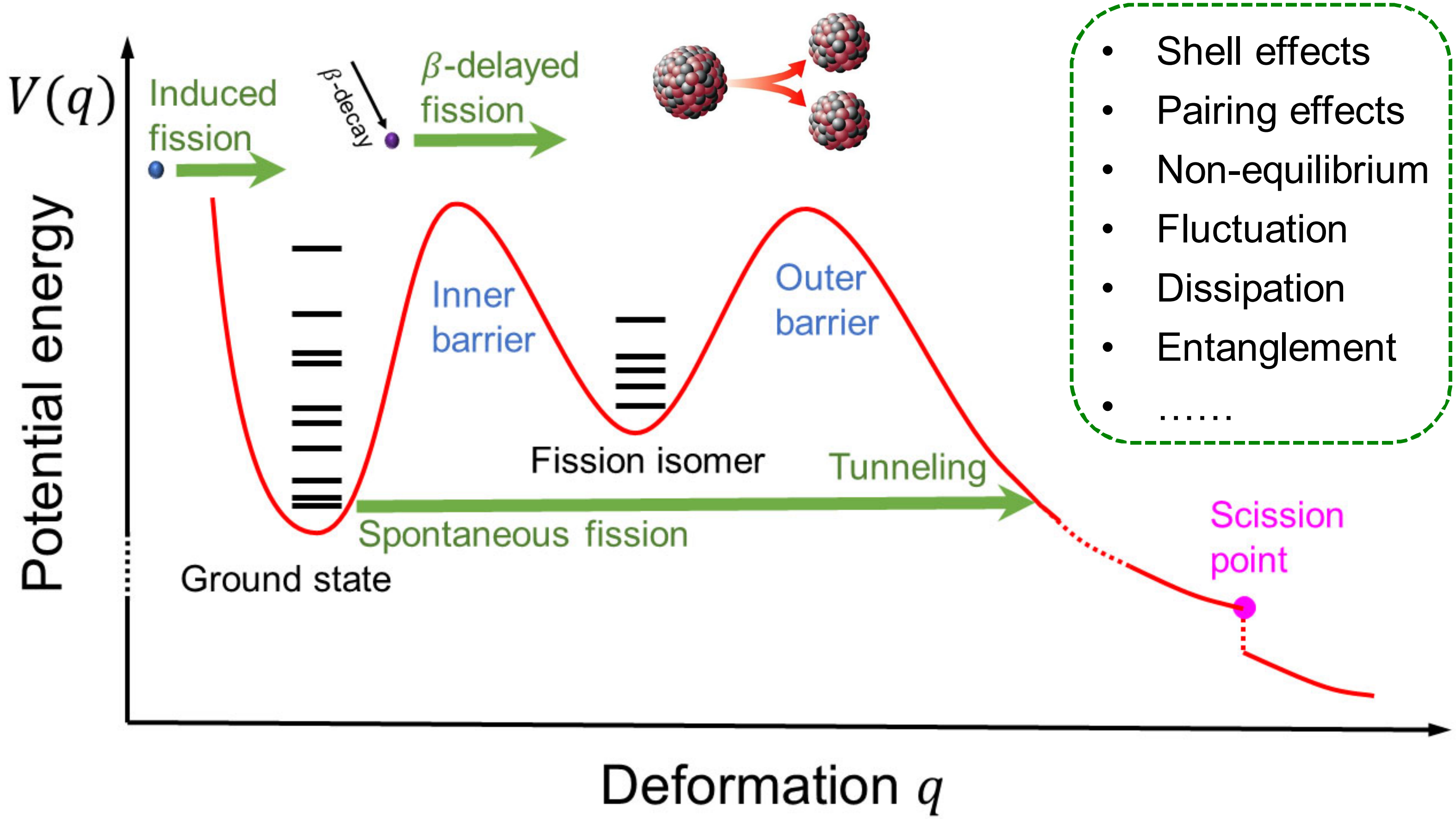
Nuclear fission

- Nuclear fission is a decay process by which a heavy nucleus splits into two or more lighter fragments.
- Nuclear fission is a dynamic process of a complex quantum many-body system and involves many complicated mechanisms.



- Shell effects
- Pairing effects
- Non-equilibrium
- Fluctuation
- Dissipation
- Entanglement
- ……

Fission fragment distribution

- Understanding these physical mechanisms in nuclear fission plays an important role in the prediction of the fragment observable distributions.
- The fragment observable distributions reflect these physical mechanisms and can provide tests for nuclear models.

Mechanism

- Shell effects
- Pairing effects
- Non-equilibrium
- Fluctuation
- Dissipation
- Entanglement
- ……

Affect →

← Reflect

Observable

- Charge yield
- Mass yield
- Kinetic energy
- Spin
- Prompt neutron
- γ-emission
- ……

- Developing a nuclear model that can **simultaneously include these mechanisms** and **accurately predict fragment observable distribution** is one of the long-standing goals of nuclear theory.

Nuclear models for nuclear fission

- Liquid drop model Meitner and Frisch, Nature **143**, 239 (1939); Bohr and Wheeler, PR **56**, 426 (1939).
- Macroscopic-microscopic model Brack, *et al.*, RMP **44**, 320 (1972); Kowal, *et al.*, PRC **82**, 014303 (2010).
- Langevin approach Aritomo, *et al.*, PRC **88,** 044614 (2013); Liu, *et al.*, RPC 111, 024607 (2025).
- FREYA model Randrup and Vogt, PRC **80**, 024601 (2009); Randrup and Vogt, PRL **127**, 062502 (2009).
- Dinuclear model Shneidman, *et al.*, PRC **111**, 064521 (2025).
- Nonequilibrium Green's function approach Uzawa and Hagino, PRC **110**, 014321 (2024).
- Improved quantum molecular dynamics approach Zhao, *et al.*, PLB **839**, 137817 (2023).
- **Density functional theory** Flocard, *et al.*, NPA **203**, 433 (1973); Egido and Robledo, RPL **85**, 1998 (2000).
  - ✓ **Time-dependent density functional theory (TDDFT)**

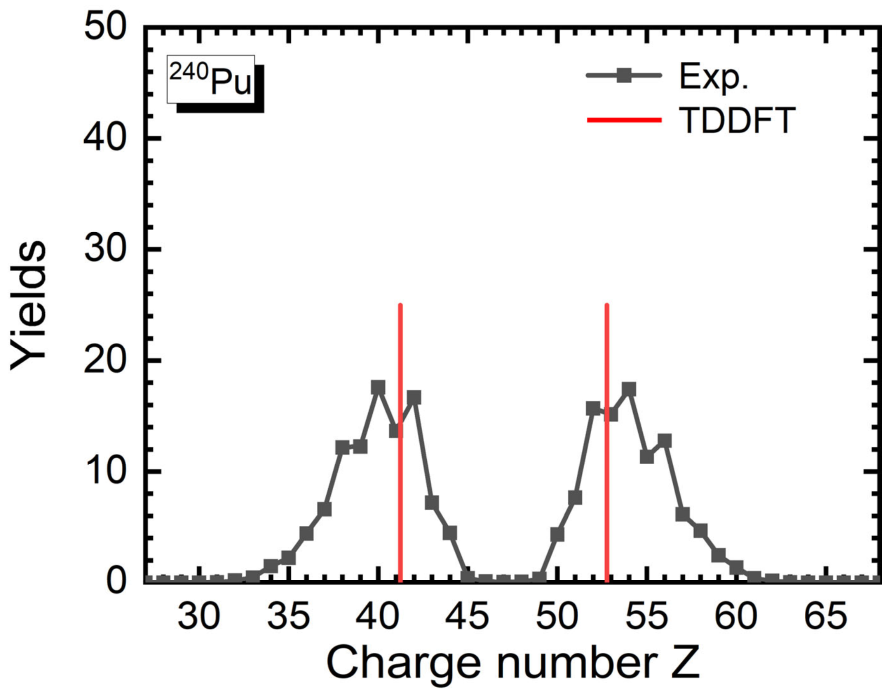
    Simenel and Umar, PRC **89**, 031601(R) (2014); Nakatsukasa, *et al,* RMP **88**, 045004 (2016);
    Bulgac, *et al.*, PRL **116**, 122504 (2016); Ren, *et al.*, PRL **128**, 172501 (2022); Scamps, *et al.*, PRC **108** L061602 (2023)
  - ✓ **Time-dependent generator coordinate method (TDGCM)**

    Goutte, *et al.*, PRC **71**, 024316 (2005); Tao, *et al.*, PRC **96**, 024319 (2017); Zhao, *et al*, PRC **99**, 054613 (2019)
- ……

There remain several open questions in understanding fission mechanisms and predicting fragment distributions.

Classical aspects of TDDFT

- Since TDHF equations emerge as a classical field theory for interacting single-particle fields, the TDDFT approach can neither describe the motion of the system in classically-forbidden regions of the collective space nor **quantum fluctuations**. Bender, *et al*., JPG: NNP **47**, 113002 (2020)

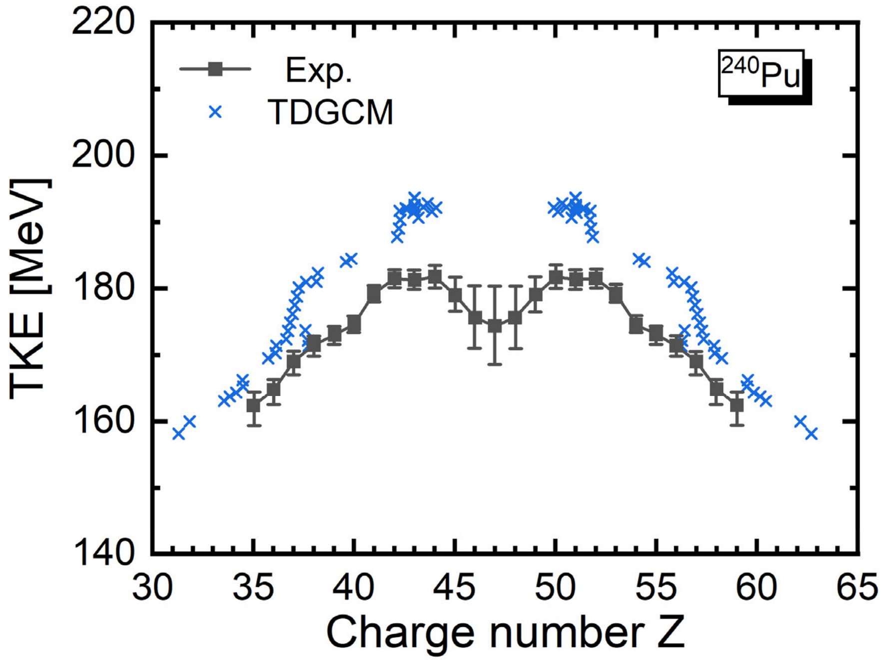


- TDDFT lacks quantum fluctuations of collective degree of freedom, since **underestimates the width of fission fragment yield**.

Adiabatic approximation in TDGCM

- Most implementations of TDGCM assume that the collective motion stays in the adiabatic potential energy surface, since the manifestation of non-adiabaticity, and **a proper description of the transfer of energy from collective motion to internal excitation, cannot be achieved.**

Bender, *et al.*, JPG: NNP **47**, 113002 (2020)

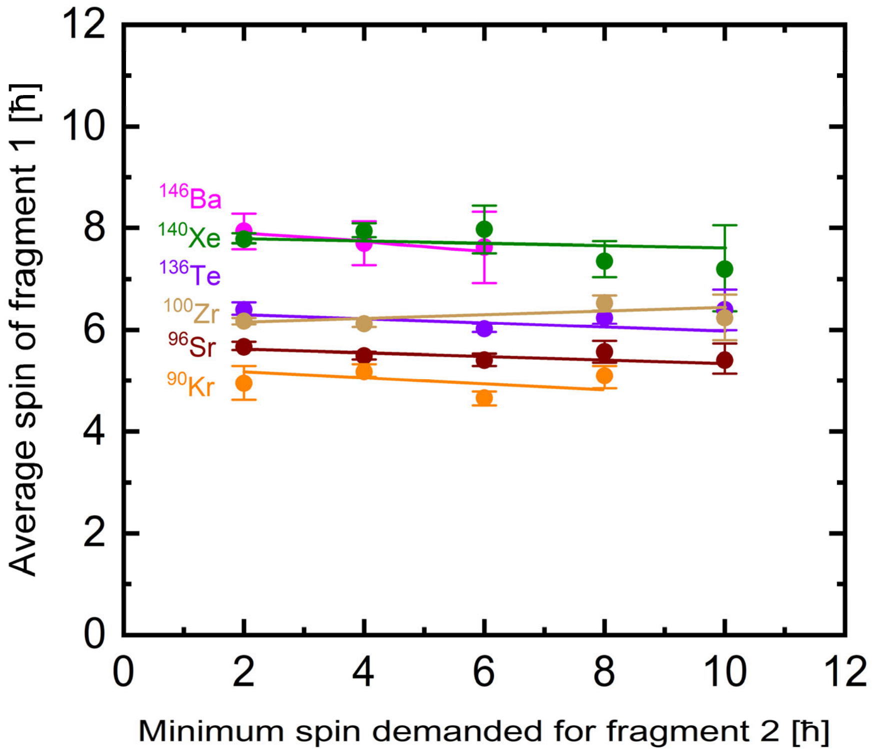


Ren, *et al.*, PRC **105**, 044313 (2022)

- TDGCM lacks dissipative mechanism, since **overestimates the total kinetic energy (TKE) of fission fragment**.

Spin correlation

- Wilson *et al.*'s experiment finds that there is **almost no correlation between the spins of fission fragments**. Wilson, *et al.*, Nature **590**, 566 (2021)



- The fission fragments are generated from a nucleus, which is **a finite complex quantum system with entangled constituents**. What mechanism lead to no correlation between the spins of fragments?

Our work

- We provide some answers to the above open questions based the **relativistic TDDFT.** Ren, Zhao, Meng, PLB **801**, 135194 (2020)

  a) Develop a new method, which simultaneously includes quantum fluctuation and dissipation mechanism in a microscopic framework, and use it to describe charge yield and TKE of fission fragments.

  b) Use relativistic TDDFT to study the spin generation and correlation of fission fragments, and provide a mechanism to explain the disappearance of spin correlations.

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Time-dependent relativistic TDDFT

- In relativistic TDDFT, the nuclear wavefunction is represented as a Slater determinant, and the single-particle wavefunction $\psi_k(\boldsymbol{r},t)$ satisfies **time-dependent Dirac equation**,

$$i\partial_t\psi_k(\boldsymbol{r},t) = \{\alpha\cdot[-i\boldsymbol{\nabla} - \boldsymbol{V}(\boldsymbol{r},t)] + V^0(\boldsymbol{r},t) + \beta[m_N + S(\boldsymbol{r},t)]\}\psi_k(\boldsymbol{r},t),$$

where potential $V^\mu(\boldsymbol{r},t)$ and $S(\boldsymbol{r},t)$ depend on time-dependent densities and currents $\rho_S(\boldsymbol{r},t)$, $j^\mu(\boldsymbol{r},t)$, $j^\mu_{TV}(\boldsymbol{r},t)$,

$$S(\boldsymbol{r},t) = \alpha_S\rho_S + \beta_S\rho_S^2 + \gamma_S\rho_S^3 + \delta_S\Delta\rho_S,$$

$$V^\mu(\boldsymbol{r},t) = \alpha_V j^\mu + \gamma_V(j^\mu j_\mu)j^\mu + \delta_V\Delta j^\mu + \tau_3\alpha_{TV}j^\mu_{TV} + \tau_3\delta_{TV}\Delta j^\mu_{TV} + e\frac{1-\tau_3}{2}A^\mu.$$

Evolution process in relativistic TDDFT

$\cdots \rightarrow \rho(t) \rightarrow \hat{h}_{\mathrm{Dirac}}[\rho(t)] \rightarrow \mathrm{i}\partial_t\psi_k(t) = \hat{h}_{\mathrm{Dirac}}(t)\psi_k(t)$

$\rightarrow \psi_k(t+\delta t) \rightarrow \rho(t+\delta t) \rightarrow \cdots$

Ren, Zhao, Meng, PLB **801**, 135194 (2020)
Ren, Zhao, Meng, PRC **102**, 044603 (2020)

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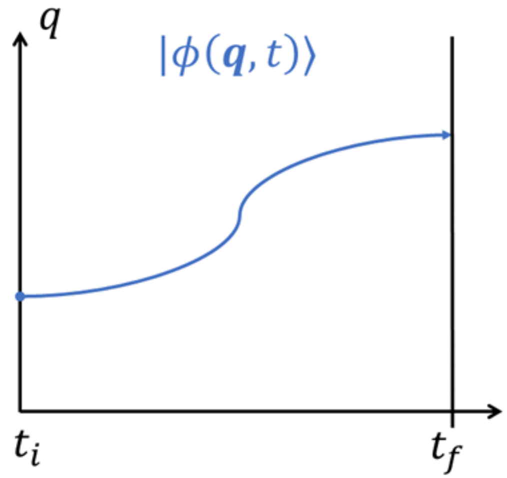
Yield described by TDDFT

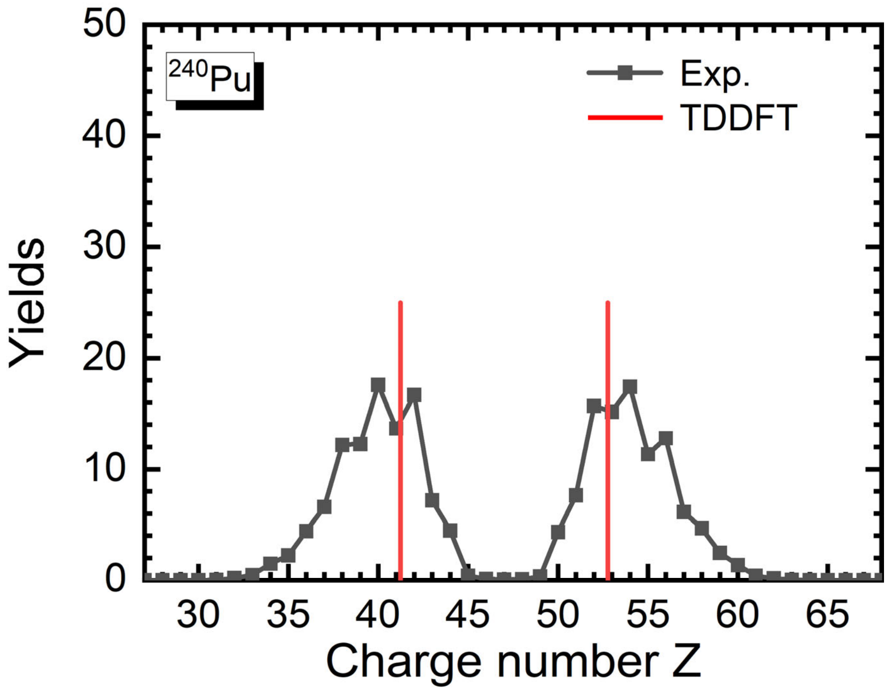
➢ TDDFT represents the nuclear wavefunction as **a Slater determinant** and describes the evolutions of independent nucleons in a mean field.

$$|\Psi(t)\rangle = |\phi(\boldsymbol{q}, t)\rangle$$



$\boldsymbol{q}$: $(\beta_{20}, \beta_{30}, \dots)$

$|\phi(\boldsymbol{q}, t)\rangle$: Slater determinant

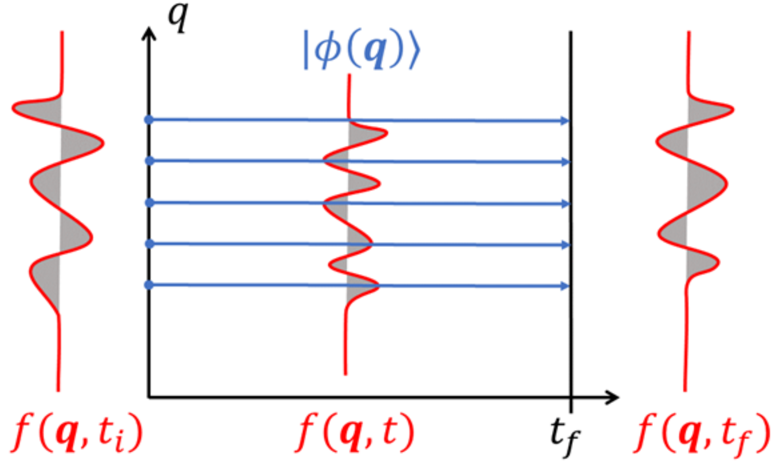


➢ TDDFT lacks the **quantum fluctuations of collective degree of freedom** and is not suitable to describe the yields of fragments.

Yield described by TDGCM

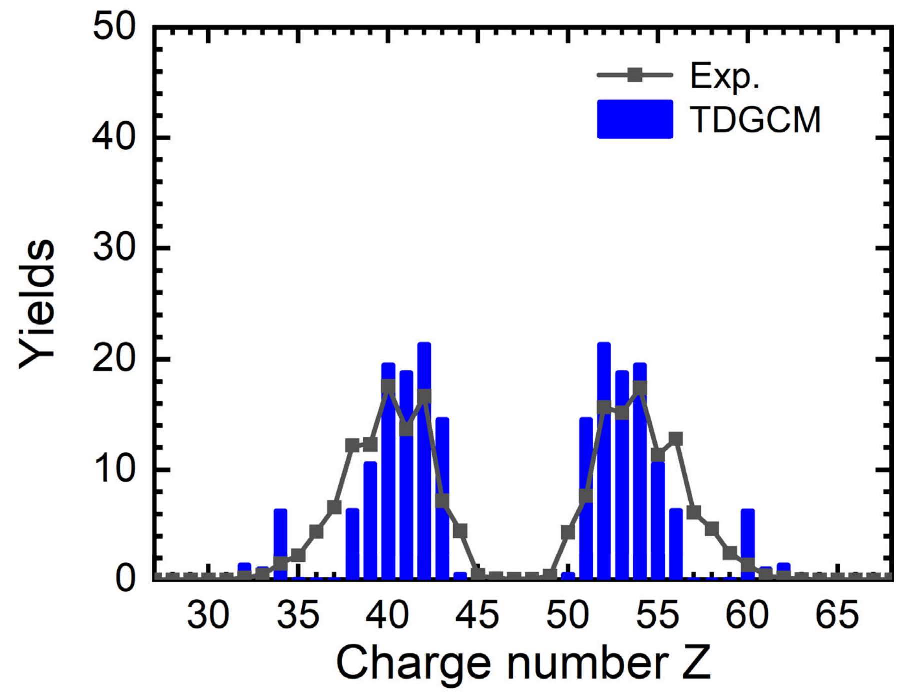
- TDGCM represents the nuclear wavefunction as a superposition of generator states that are functions of collective degree of freedom, and **weight functions evolve with time.**

$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q})\rangle$$



$f(\boldsymbol{q},t)$: weight function

$|\phi(\boldsymbol{q})\rangle$: Slater determinant

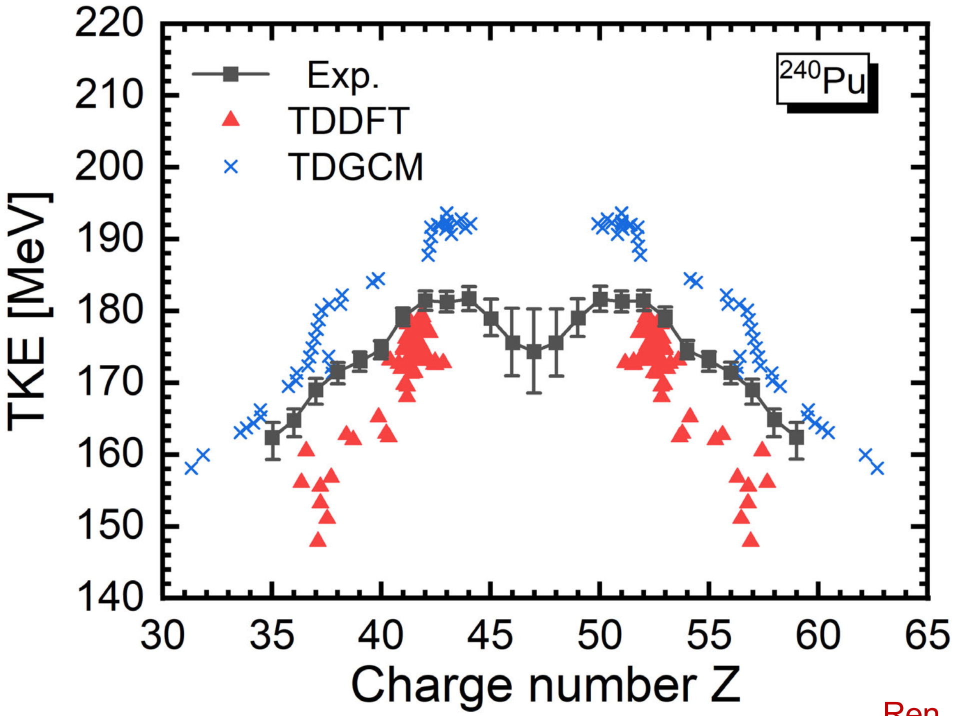


Ren, *et al.*, PRC **105**, 044313 (2022)

- TDGCM includes the **quantum fluctuations of collective degree of freedom** and is more suitable to describe the yields of fragments.

TKE described by TDGCM and TDDFT

- TDGCM lacks **dissipative mechanism** and overestimates the TKE of fission fragments.
- TDDFT includes **one-body dissipative mechanism** and is more suitable to describe the TKE of fission fragments.



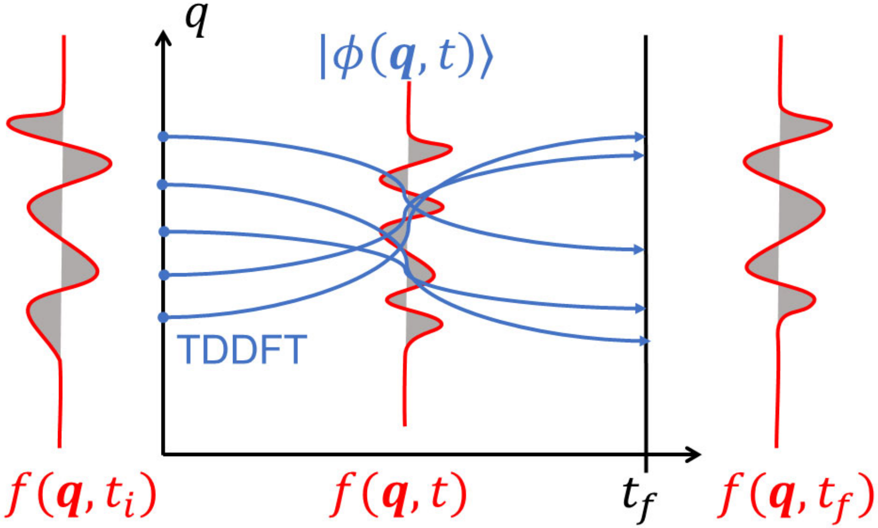
Ren, *et al.*, PRC **105**, 044313 (2022)

- We can combine the respective advantages of TDDFT and TDGCM to describe fission dynamic and predict charge yield and TKE of fragments.

Generalized TDGCM

- **Generalized time-dependent generator coordinate method (gd-TDGCM)** represents the nuclear wavefunction as a superposition of relativistic TDDFT trajectories, and weight functions are evolved by the time-dependent Hill-Wheeler equations.

$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q},t)\rangle$$



BL, Vretenar, Nikšić, Zhao, Meng, PRC **108**, 014321 (2023)
BL, Vretenar, Nikšić, Zhao, Zhao, Meng, FoP **19**, 44201 (2024)
BL, Vretenar, Nikšić, Zhao, Meng, PRC **111**, L051302 (2025)

Weight function (quantum fluctuation):

$$iN\partial_t f = (H - H^{MF})f, \qquad g = N^{1/2} f$$

Regnier and Lacroix, PRC **99**, 064615 (2019)

$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q},t)\rangle$$

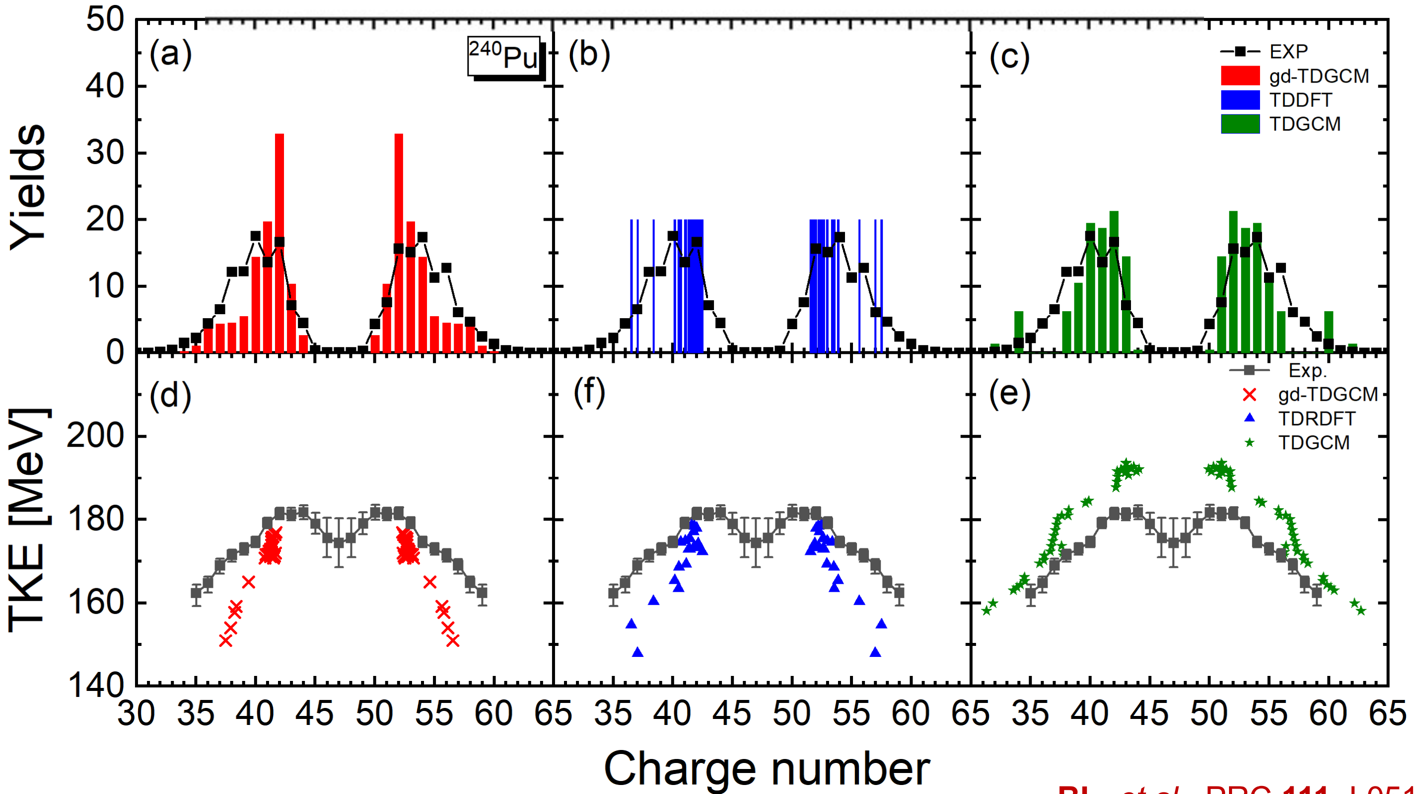
Slater determinant (dissipation):

$$i\frac{\partial}{\partial t}\psi_{k,\boldsymbol{q}}(t) = [h^{\boldsymbol{q}}(t) - \varepsilon_k^{\boldsymbol{q}}]\psi_{k,\boldsymbol{q}}(t)$$

Ren, *et al.*, PRL **128**, 172501 (2022)

See Prof. Nikšić's talk for details

Charge yield and TKE



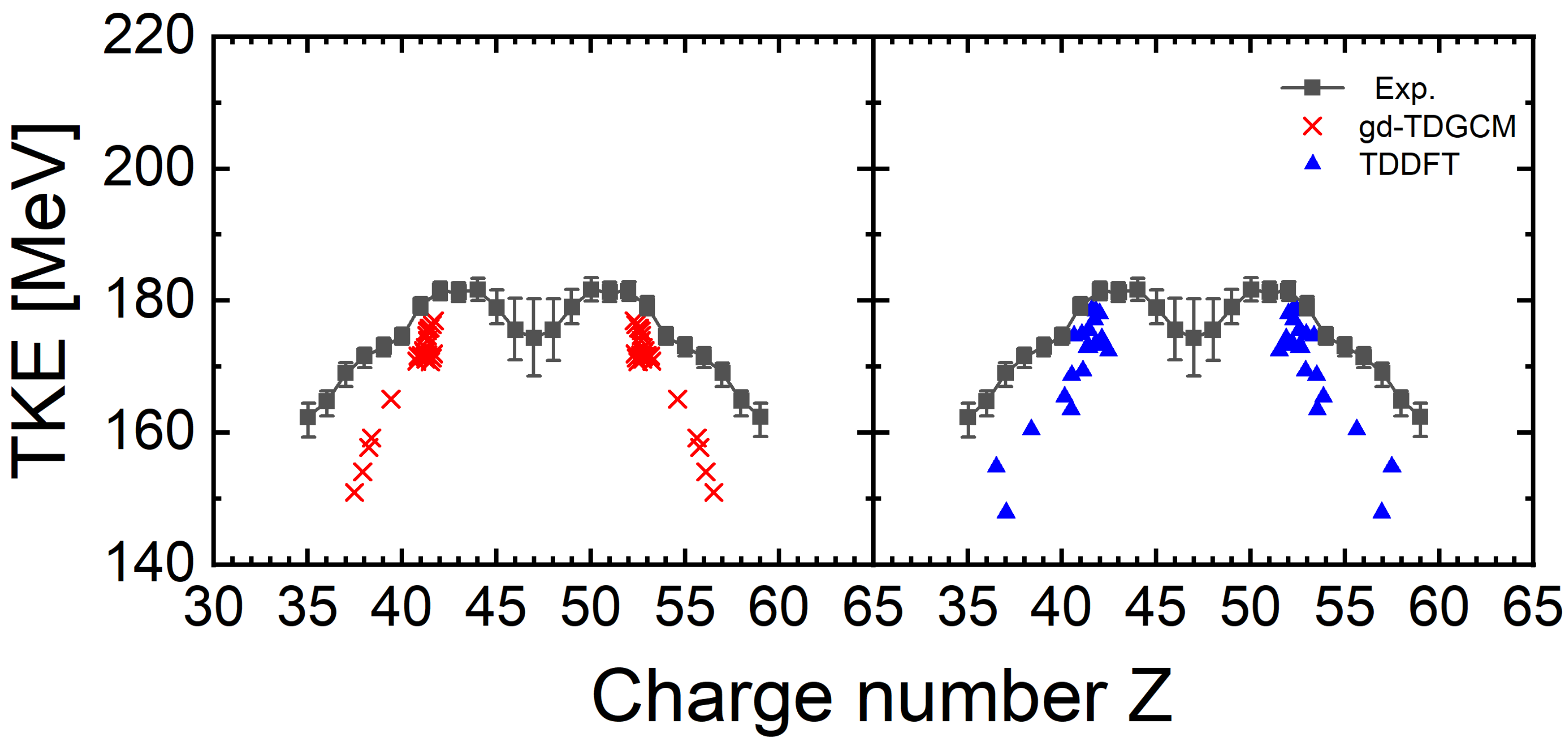
BL, *et al.*, PRC **111**, L051302 (2025)

- ✓ Compared with TDDFT, gd-TDGCM can reproduce the width of charge yield due to including quantum fluctuation of collective degree of freedom.
- ✓ Compared with TDGCM, gd-TDGCM can reproduce the TKE of fission fragment near the peak of charge yield due to including one-body dissipative mechanism.

See Prof. Nikšić's talk for details

Some limitations in the description of TKE

➢ There remain some limitations in the description of TKE within the TDDFT and generalized TDGCM framework.



➢ Limitations:

- ✓ The nucleon number of fission fragment is not integer.
- ✓ Underestimate the TKE of fission fragment at the tail of charge yield.

TKE with integer nucleon number

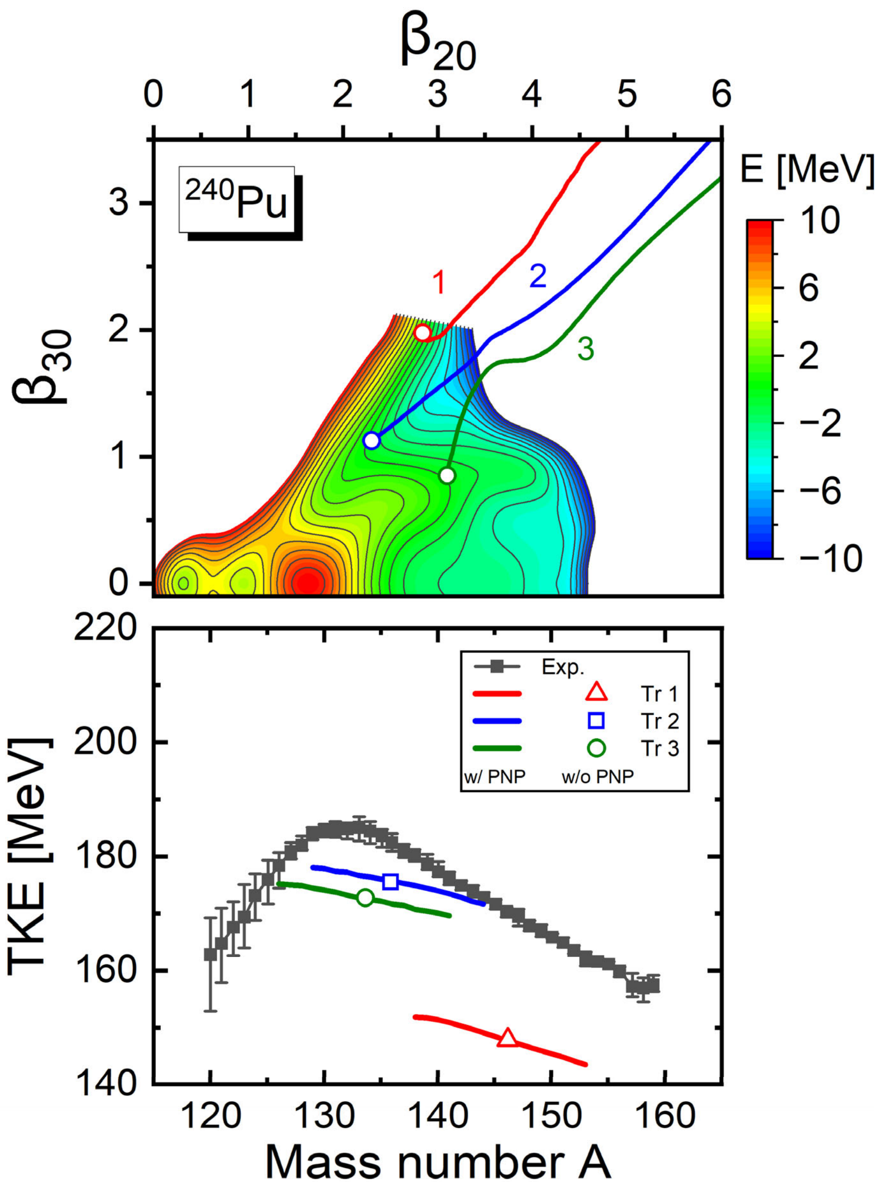
- TKE of fragments with integer nucleon number reads

$$\mathrm{TKE}(N_H, Z_H, N_L, Z_L) = \frac{1}{2} m_H \boldsymbol{v}_H^2 + \frac{1}{2} m_L \boldsymbol{v}_L^2 + E_{\mathrm{coul}}.$$

Kinetic and Coulomb energy are obtained from the projected density and current ($f = H, L$),

$$j^\mu(\boldsymbol{r}, N_f, Z_f) = \frac{\langle \Psi | \bar{\psi}(\boldsymbol{r}) \gamma^\mu \psi(\boldsymbol{r}) \hat{P}_{N_f} \hat{P}_N \hat{P}_{Z_f} \hat{P}_Z | \Psi \rangle}{\langle \Psi | \hat{P}_{N_f} \hat{P}_N \hat{P}_{Z_f} \hat{P}_Z | \Psi \rangle}.$$

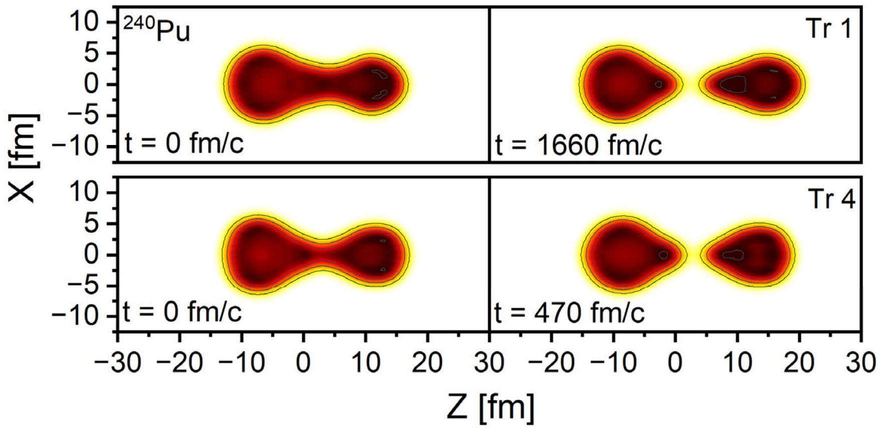
- Particle number projection can widen the TKE distributions of fission fragments.



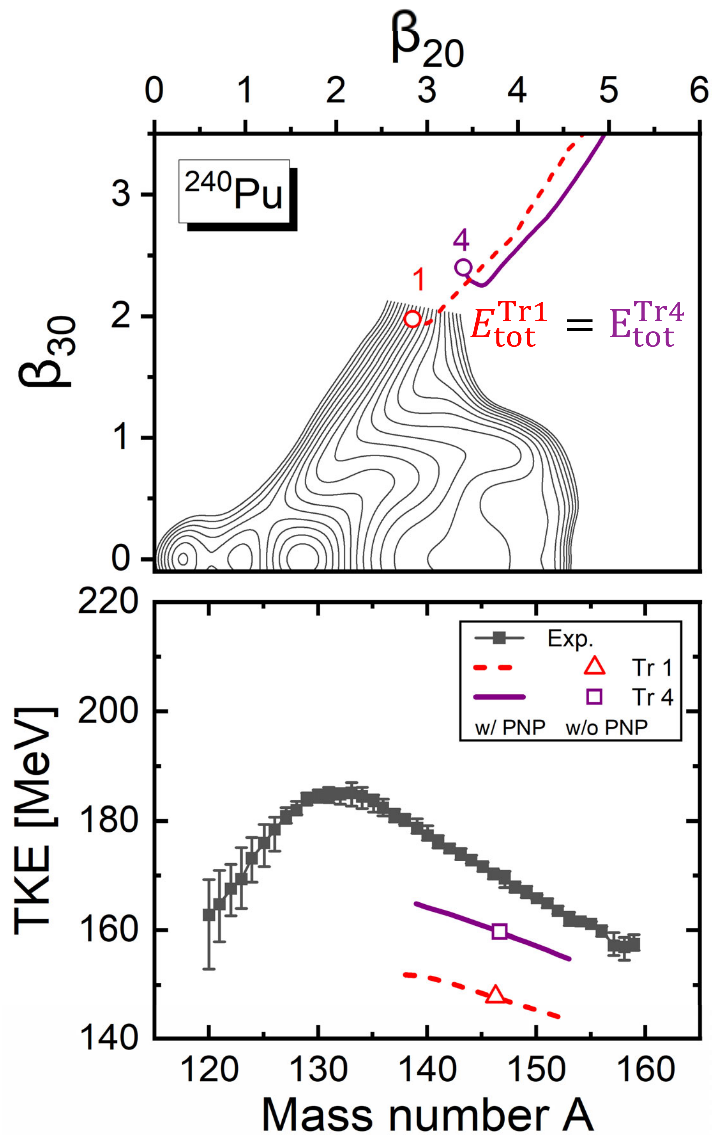
The effects of neck thickness

- The initial configuration with thinner neck is obtained by constraining hexadecapole β_{40} of the nucleus.

Density at initial and scission time

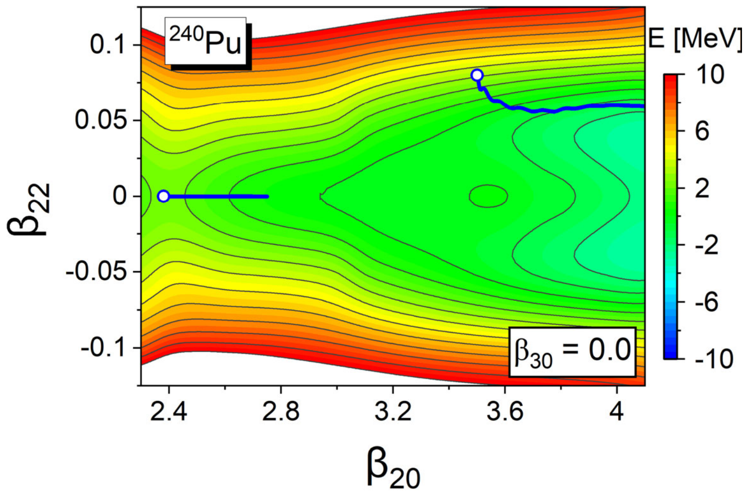


- The TKE of fission fragments in trajectory 4 is higher than that in trajectory 1.



TKE distribution of ^{240}Pu

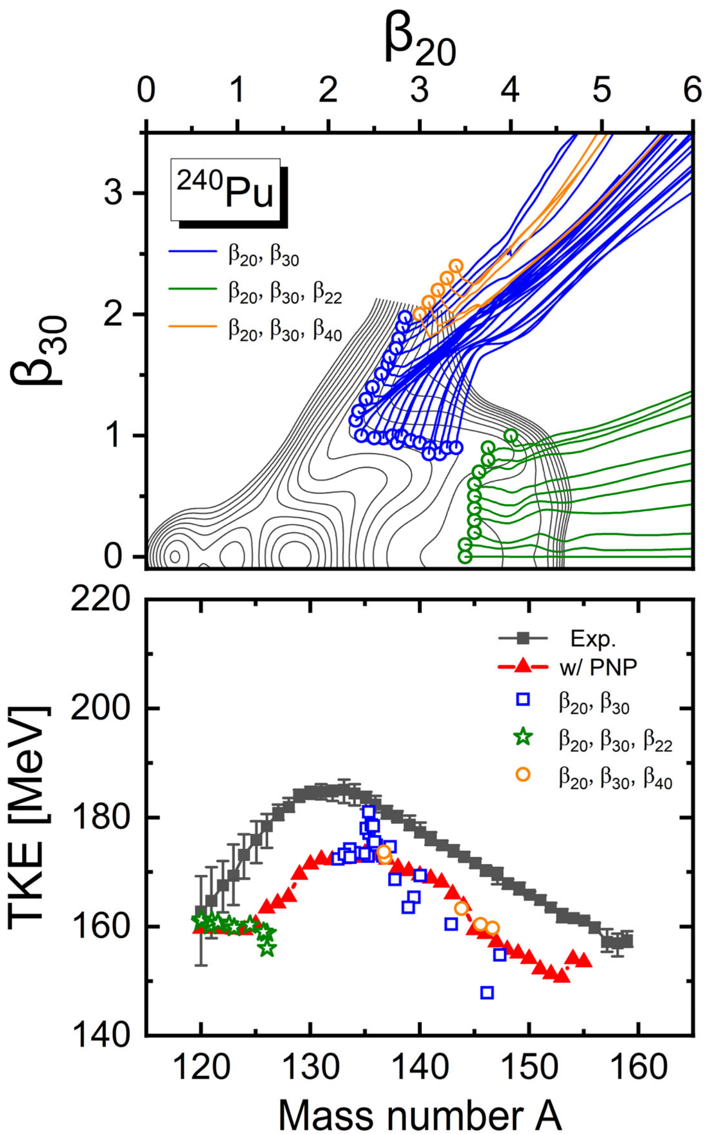
- By introducing triaxial deformation parameter β_{22}, TDDFT can yield mass symmetric fragments



- Total TKE distribution read

$$\mathrm{TKE}(A) = \frac{\sum_q \mathrm{TKE}_q(A)}{\sum_q 1}.$$

The trend of TKE distribution of fission fragments is reproduced.



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Spin correlation

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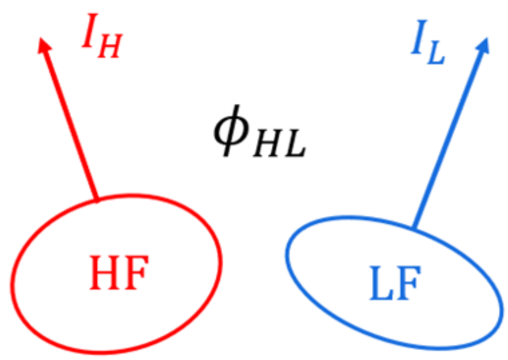
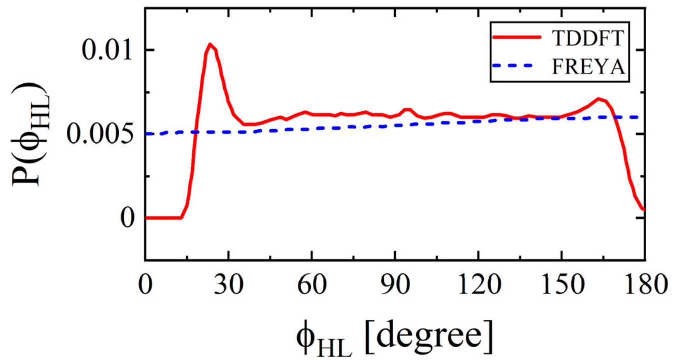
- The theoretical studies on spin correlation:
  1. Spin are produced after scission. Wilson, *et al*., Nature **590**, 566 (2021)
  2. Deexcitation process reduce correlations. Stetcu, et al., PRL **127**, 222502 (2021)
  3. Spin are produced before scission, but the nucleon-exchange mechanism reduces the correlations. Randrup and Vogt, PRL **127**, 062502 (2021).
  4. Spin are produced before scission, and there are some correlations between primary fission fragments. Bulgac, *et al*., PRL **128**, 022501 (2022)
  5. ……

Opening angle





Scamps, *et al*., PRC **108** L061602 (2023)

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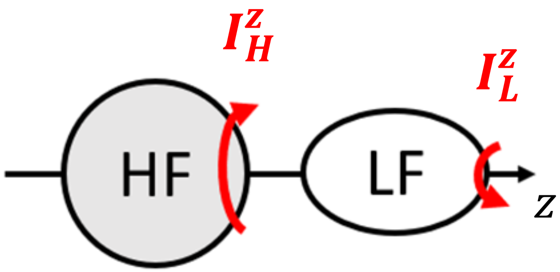

The studies with TDDFT assume that the nucleus is **axial symmetric**, which introduces a constraint on the spins of two fragments,

$$I_{tot}^z = I_H^z + I_L^z = 0.$$

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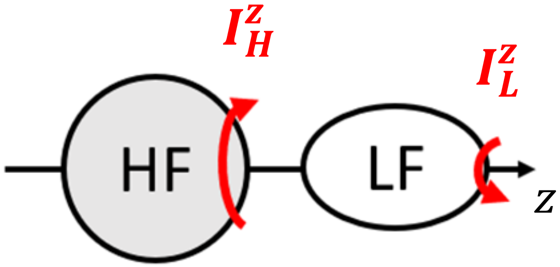


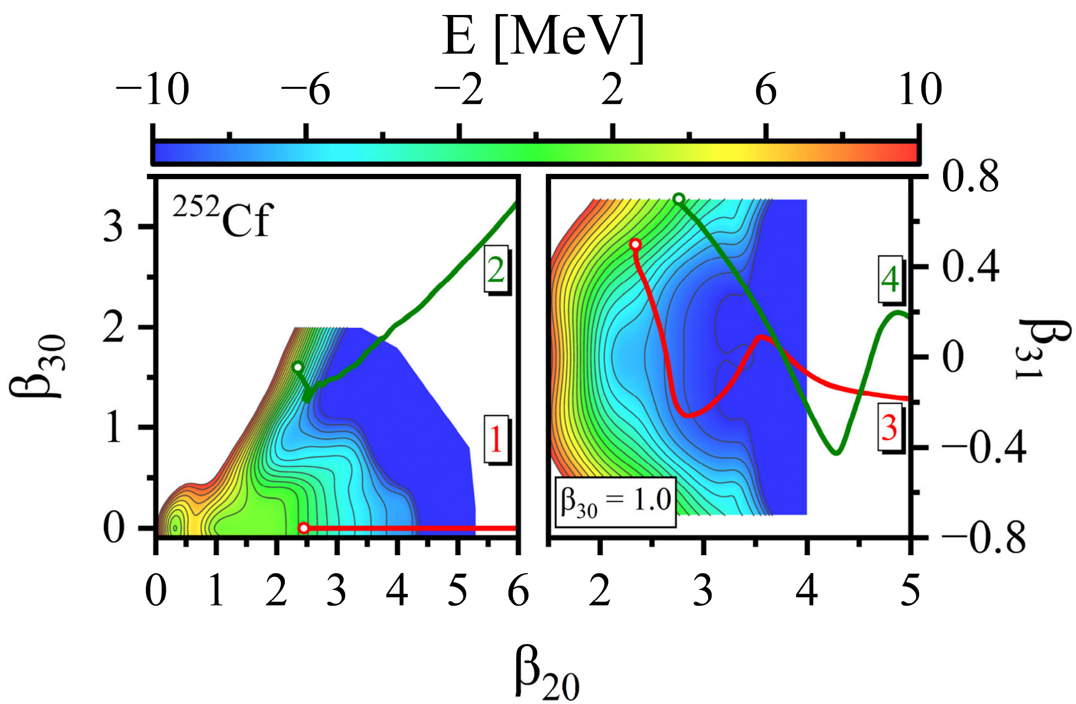
Triaxiality?

The studies with TDDFT assume that the nucleus is **axial symmetric**, which introduces a constraint on the spins of two fragments,

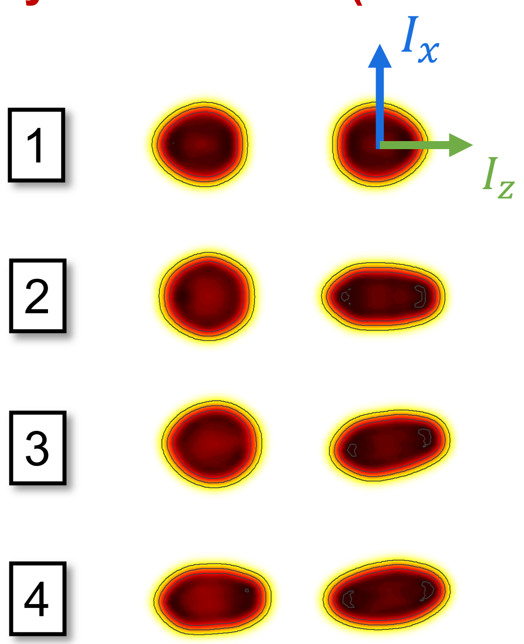
$$I_{tot}^z = I_H^z + I_L^z = 0.$$

TDDFT trajectories for ^{252}Cf

- The initial states of the axial and triaxial TDDFT trajectories are selected beyond the saddle points, and their energies are same as ground state energy of ^{252}Cf.



Density at final time (d = 25 fm)

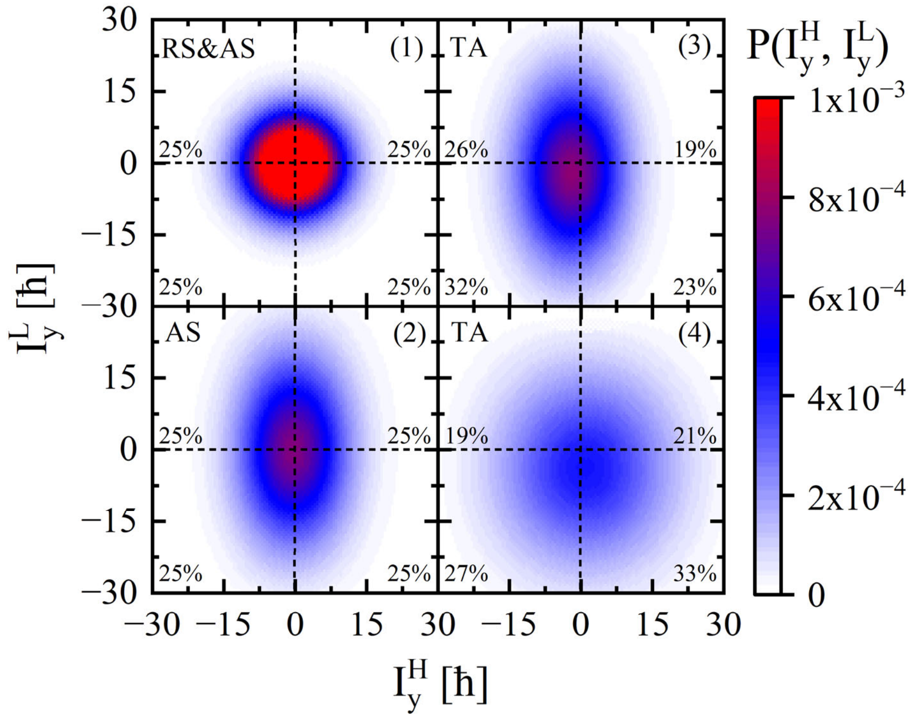


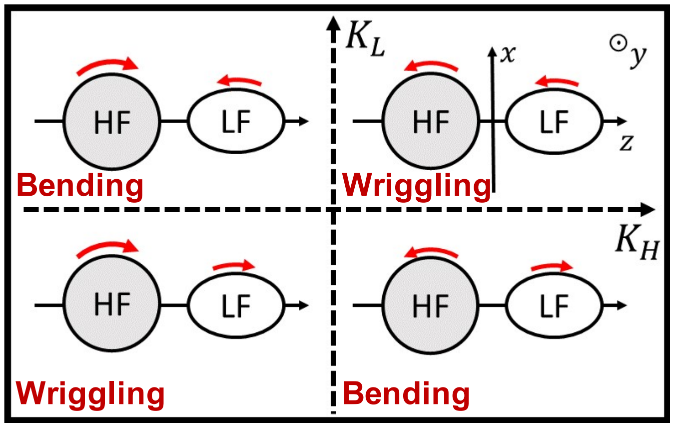
- The spin distribution of fission fragments at final time are obtained by angular momentum projection.

Joint probability distribution $P(I_H^y, I_L^y)$

- The joint probability distribution for the fragment spins along y-axis reads

$$P(I_H^y, I_L^y) = \left\langle \Psi \left| \hat{P}^H_{I_H^y} \hat{P}^L_{I_L^y} \right| \Psi \right\rangle.$$





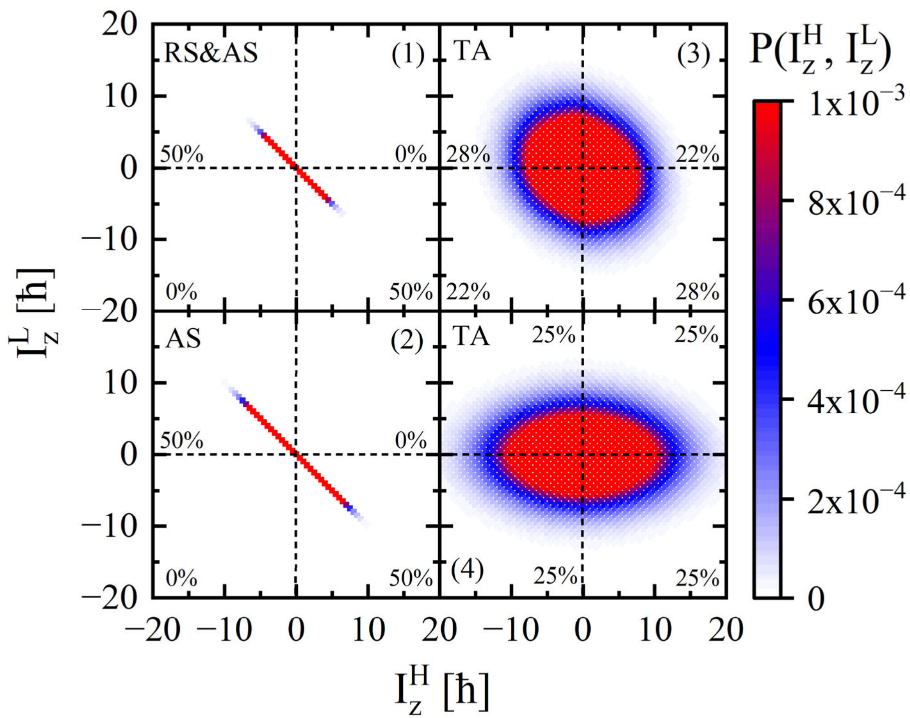
Nix and Swiatecki, Nucl. Phys. **71**, 1 (1965)

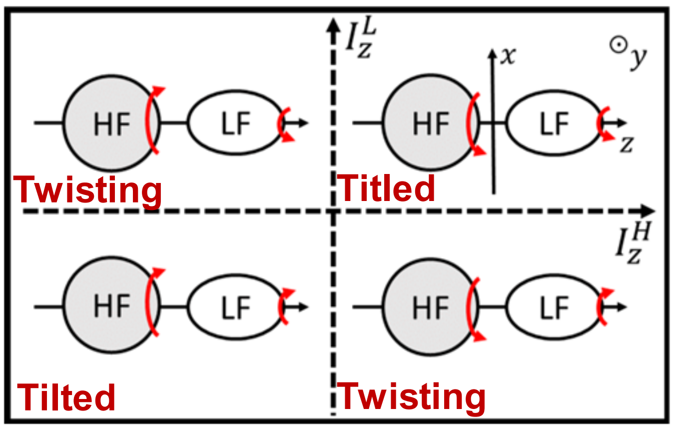
- After including the triaxial degree of freedom, the probabilities of wriggling motion and bending motion are not equal.

Joint probability distribution $P(I_H^Z, I_L^Z)$

- The joint probability distribution for the fragment spins along z-axis reads

$$P(I_H^Z, I_L^Z) = \left\langle \Psi \left| \hat{P}^H_{I_H^Z} \hat{P}^L_{I_L^Z} \right| \Psi \right\rangle.$$





Nix and Swiatecki, Nucl. Phys. **71**, 1 (1965)

- After including the triaxial degree of freedom, the joint probabilities $P(I_H^Z, I_L^Z)$ are not limited to the line $I_H^Z + I_L^Z = 0$, and tilted motion appears.

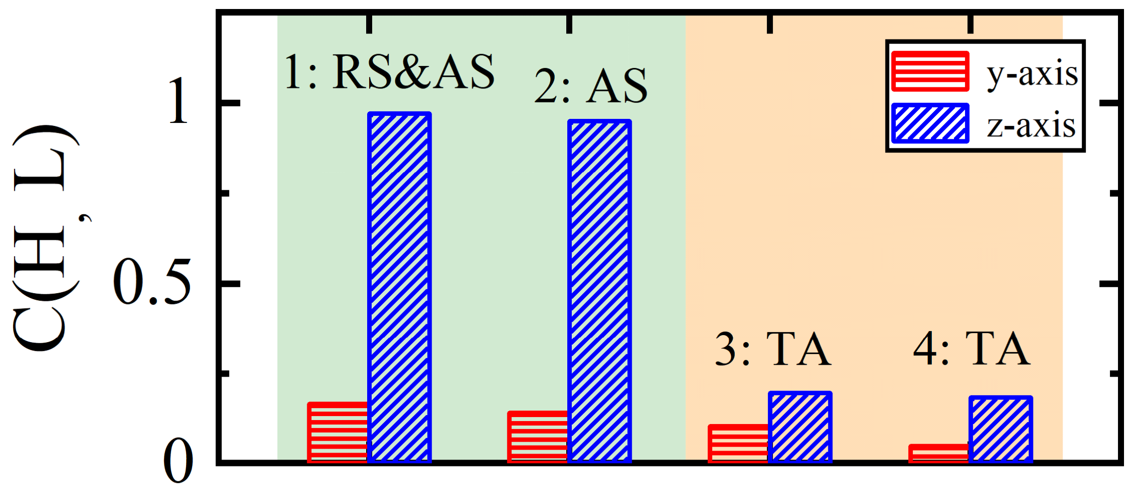
Quantize spin correlation

➢ The spin correlations can be quantized by indicator $C(H^i, L^i)$ $(i = y, z)$,

$$C(H^i, L^i) = \frac{I(H^i, L^i)}{\sqrt{S(H^i)S(L^i)}} = \begin{cases} 0, & \text{not correlated} \\ 1, & \text{fully correlated} \end{cases}.$$

where mutual information $I(H^i, L^i)$ and information entropies $S(H^i)$ and $S(L^i)$ can be obtained from joint probability distribution $P(I_H^i, I_L^i)$.

Ma and Ma, PPNP **99**, 120 (2018)



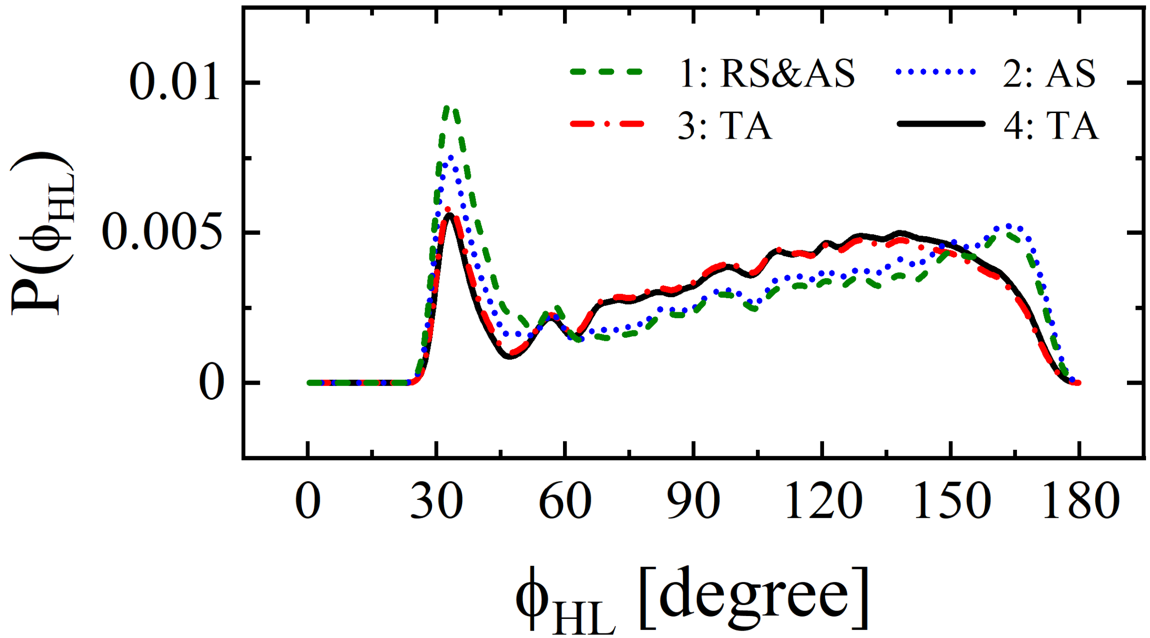
Breaking axial symmetry significantly reduces I_H^z-I_L^z correlations, and slightly reduces I_H^y- I_L^y correlations.

Opening angle

- The probability distributions of opening angle between fragment spins read,

$$P(\phi_{HL}) = P(I_H, I_L, \Lambda) = \sum_{I_H^z I_L^z \Lambda_z} \langle \Psi | \hat{P}^{I_H}_{I_H^z I_H^z} \hat{P}^{I_L}_{I_L^z I_L^z} \hat{P}^{\Lambda}_{\Lambda_z \Lambda_z} | \Psi \rangle$$

Scamps, *et al*., PRC **108** L061602 (2023)



These results underscore the importance of including triaxial degrees of freedom in microscopic models of fission dynamics.

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Summary and outlook

Summary

- Develop a new method, generalized time-dependent generator coordinate method (gd-TDGCM).
  - ✓ Include quantum fluctuation of collective degree and one-body dissipation in a microscopic framework.
  - ✓ Study the effects of mechanism such as quantum fluctuation and dissipation on the charge yield and total kinetic energy of fission fragments.
- Reveal how the triaxiality governs correlation of fragment spins with relativistic time-dependent density functional theory (TDDFT).

Outlook

- Study the effects of quantum fluctuation on the spin generation and correlation of fission fragment based on gd-TDGCM.
- Explore the reason why TDDFT underestimate the TKE of fission fragments.

Acknowledgment

- Supervisor: Pengwei Zhao (赵鹏巍)
- Collaborators: Jie Meng (孟杰), Zhengxue Ren (任政学), Tamara Nikšić, Dario Vretenar, Yiping Wang (王一平), Yaochen Yang (杨曜尘), Dandan Zhang (张丹丹), Jie Zhao (赵杰).
- Conference organizers and participants.

Thank you

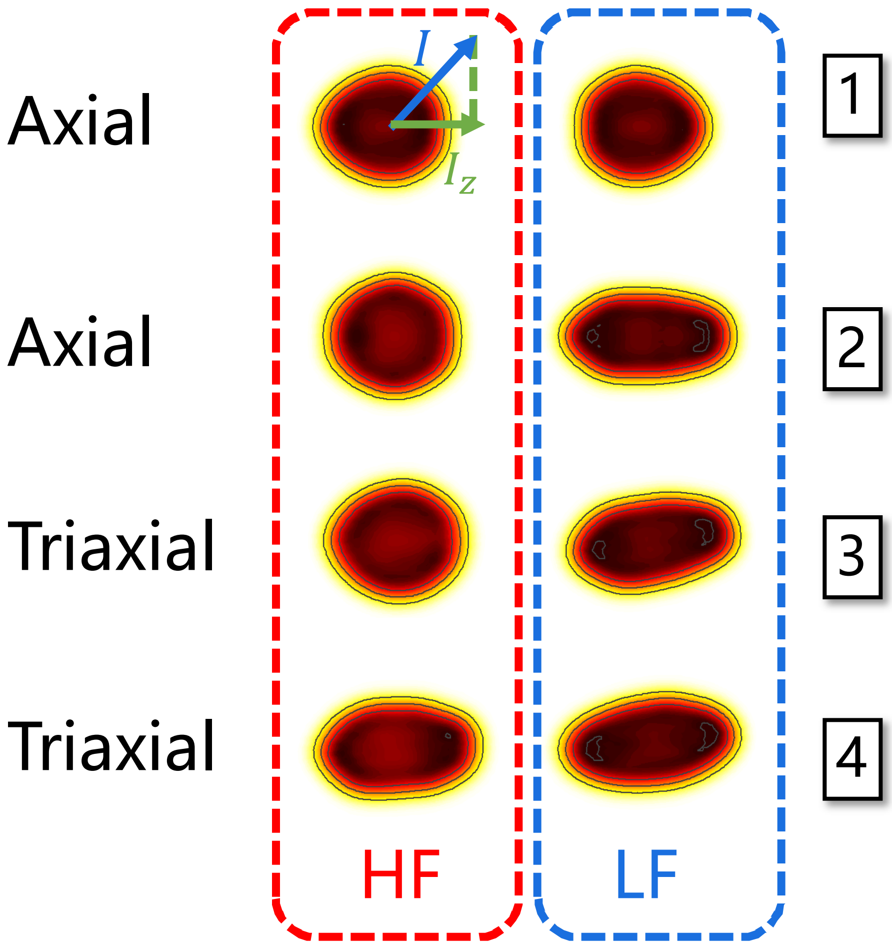
Numerical details for ^{252}Cf

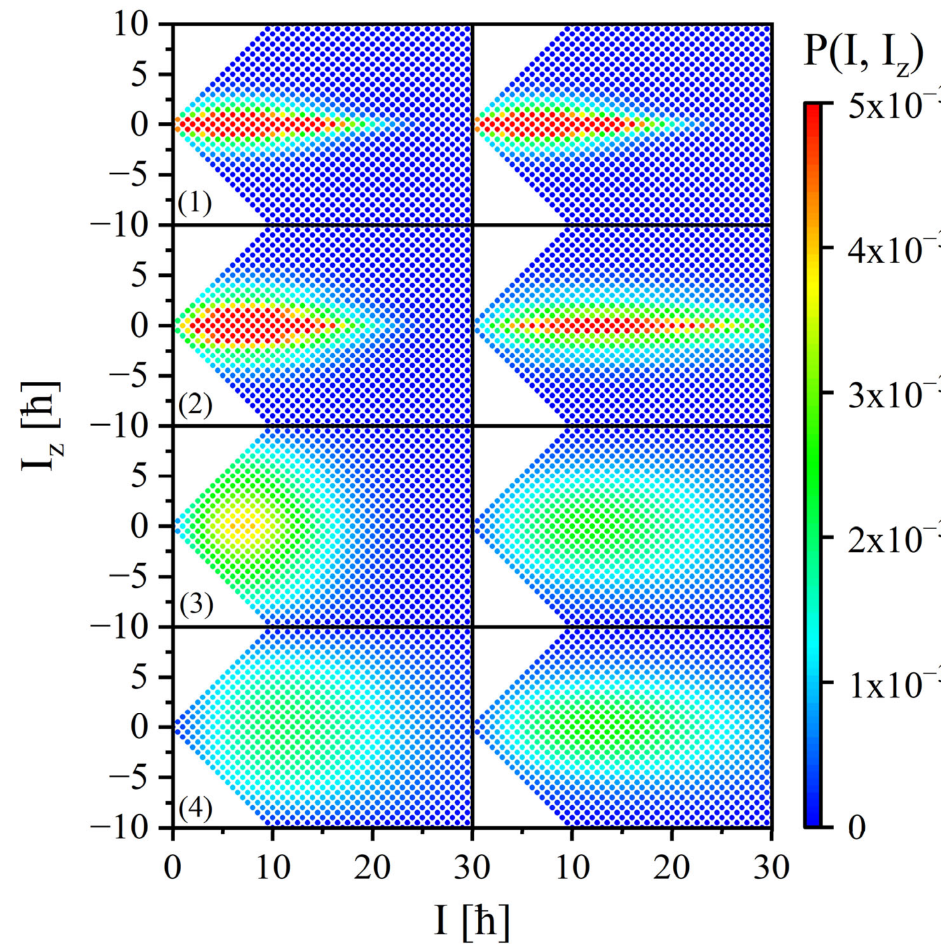
- Nucleus: ^{252}Cf
- Box size: $(L_x, L_y, L_z) = (26,26,60)$ fm
- Step: $(dx, dy, dz) = (1.0,1.0,1.0)$ fm
- Energy density functional: PC-PK1
  Zhao, Li, Yao, Meng, PRC **82**, 054319 (2012)
- Pairing: monopole pairing
- Pairing strength parameters: $G_n = -0.125$ MeV, $G_p = -0.210$MeV

Spin distribution $P^f(I,K)$

$$P^f(I,I_z) = \left\langle \Psi \middle| \hat{P}^{I,f}_{I_z I_z} \middle| \Psi \right\rangle = \int d\Omega \, D^{I,*}_{I_z I_z}(\Omega) \left\langle \Psi \middle| \hat{R}_{V_f}(\Omega) \middle| \Psi \right\rangle$$

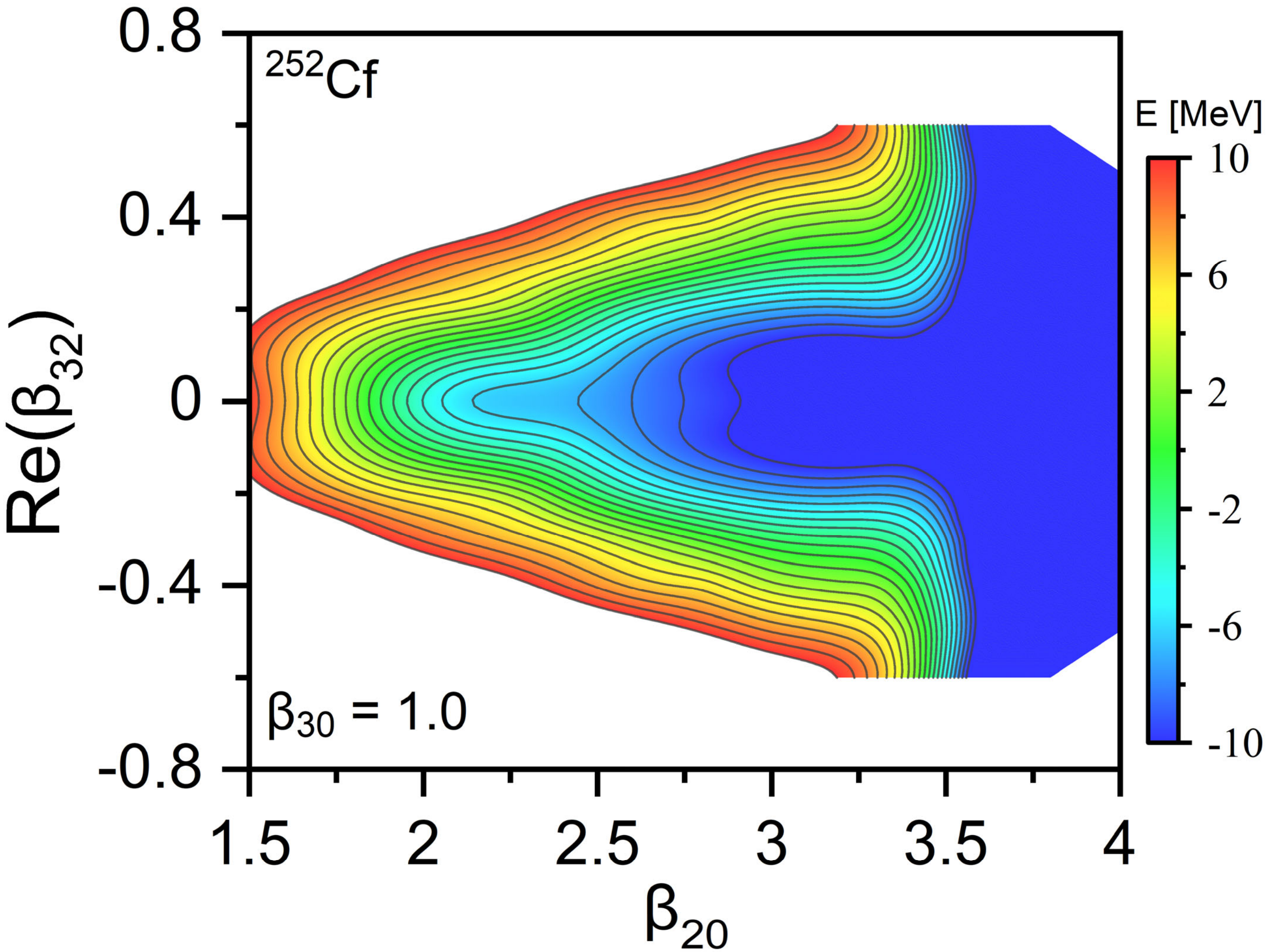
Scamps, et al., PRC **108**, 034616 (2023)





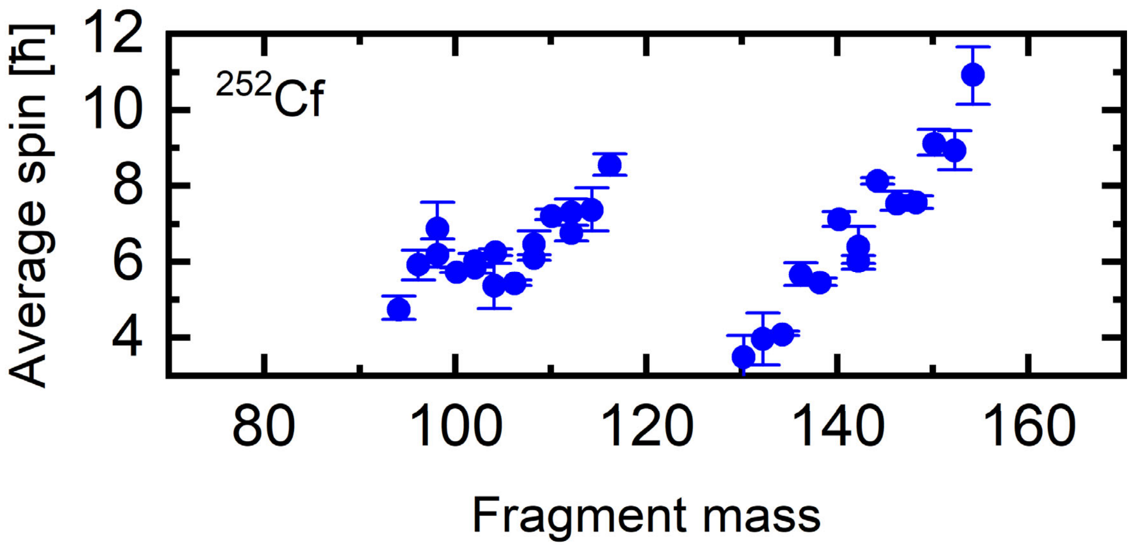
$\beta_{20} - \mathrm{Re}(\beta_{32})$ energy surface

$$\beta_{32} = \frac{4\pi}{3AR_0^3}\int d^3\vec{r}\,\rho(\vec{r})Y_{32}(\theta,\phi)$$



Average spin of fragments

- Wilson et al.'s experiment finds Wilson, *et al.*, Nature **590**, 566 (2021).

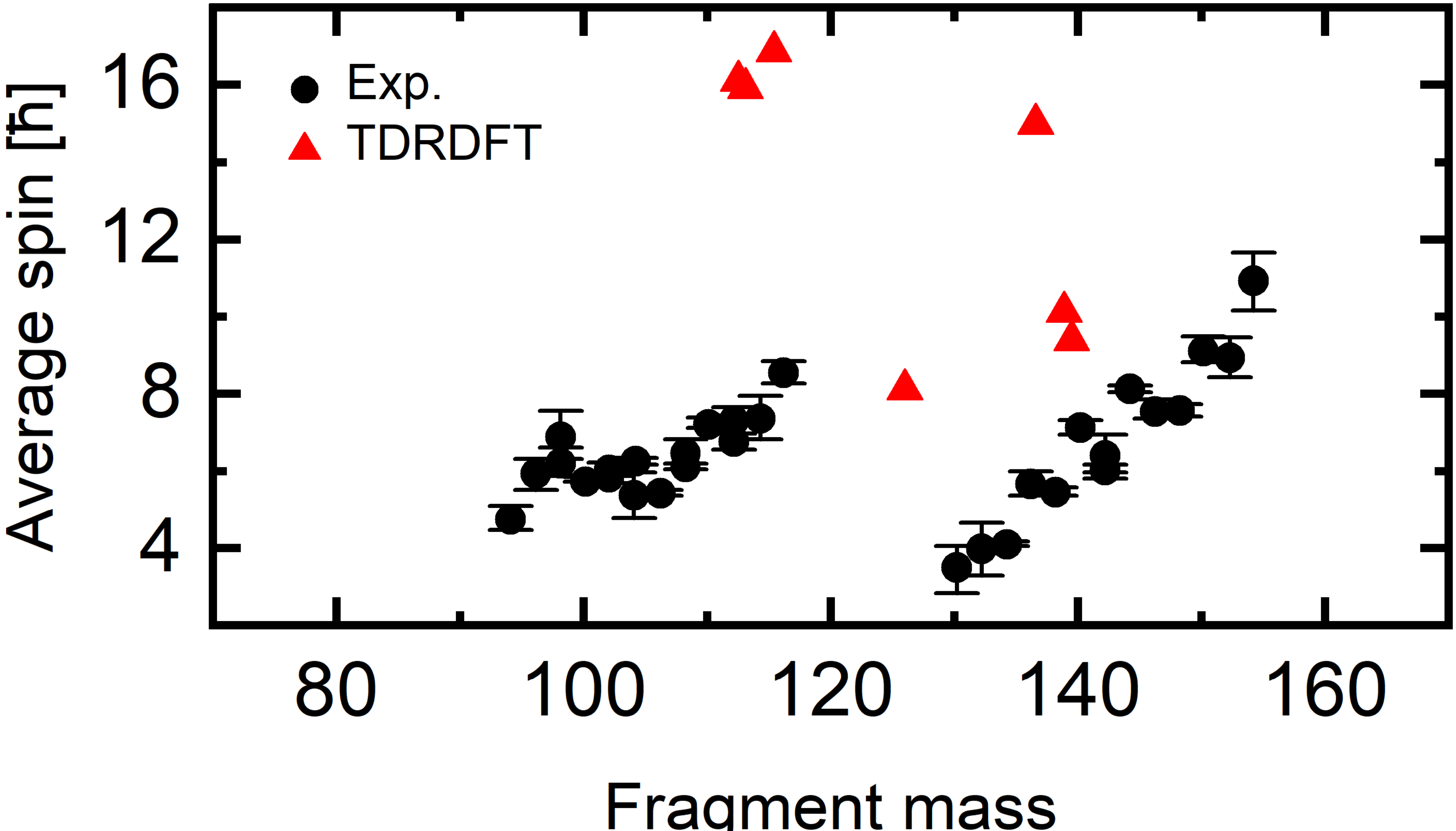


- The fragment mass numbers of four TDRDFT trajectories are

Trajectory	1	2	3	4
M_H	126.0	139.5	138.9	136.6
M_L	126.0	112.5	113.1	115.4

A TDRDFT trajectory only yields one pair of fragments.

Average spin of fragments



Ren, Zhao, Vretenar, Nikšić, Zhao, Meng, PRC **105**, 044313 (2022)

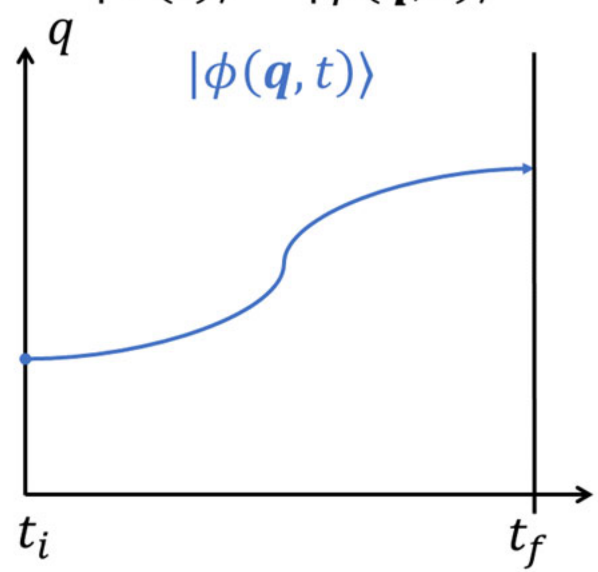
Numerical details for ^{240}Pu

- Nucleus: ^{240}Pu
- Box size: $(L_x, L_y, L_z) = (20,20,60)$ fm
- Step: $(dx, dy, dz) = (1.0,1.0,1.0)$ fm
- Energy density functional: PC-PK1
  Zhao, Li, Yao, Meng, PRC **82**, 054319 (2012)
- Pairing: monopole pairing interaction
- Pairing strength: $G_n = -0.135$ MeV, $G_p = -0.230$ MeV

Yield described by TDRDFT

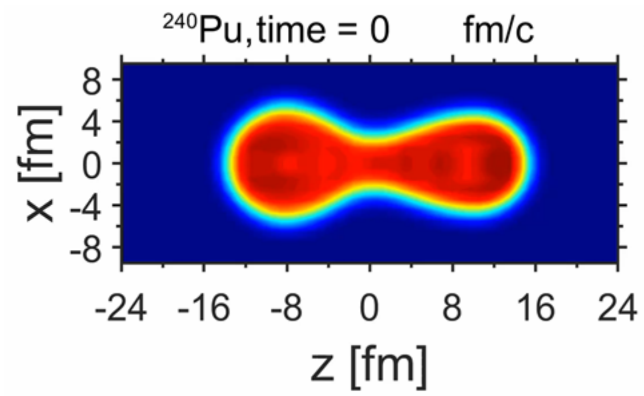
- TDRDFT represents the nuclear wavefunction as **a Slater determinant** and describes the time evolution of independent nucleons in a mean field.
- TDRDFT does not take into account **quantum fluctuations of the collective degree** and is not suitable to describe the yields of fragments.

$$|\Psi(t)\rangle = |\phi(\boldsymbol{q}, t)\rangle$$



$\boldsymbol{q}$: collective degree $(\beta_{20}, \beta_{30}, \ldots)$

$|\phi(\boldsymbol{q}, t)\rangle$: Slater determinant



TDRDFT can only simulate a single fission event.

Ren, Zhao, Vretenar, Nikšić, Zhao, and Meng, PRC **105**, 044313 (2022)

Yield described by TDRDFT

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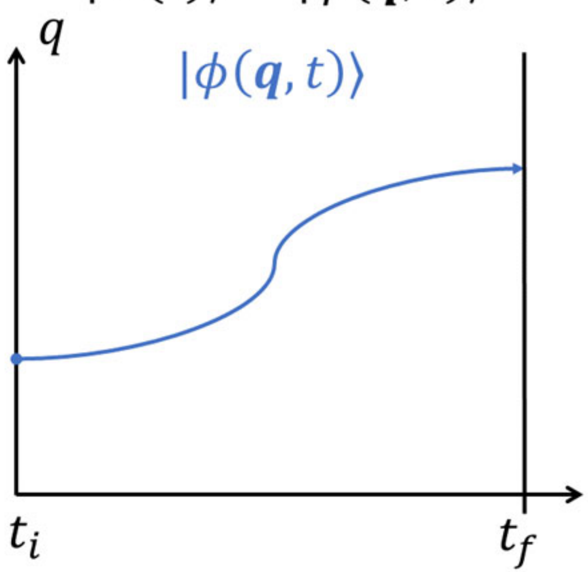
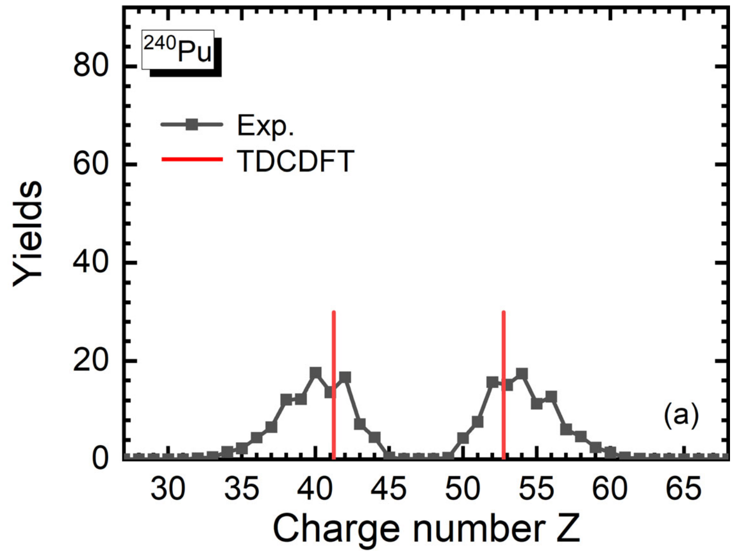


$\boldsymbol{q}$: collective degree $(\beta_{20}, \beta_{30}, \ldots)$

$|\phi(\boldsymbol{q}, t)\rangle$: Slater determinant



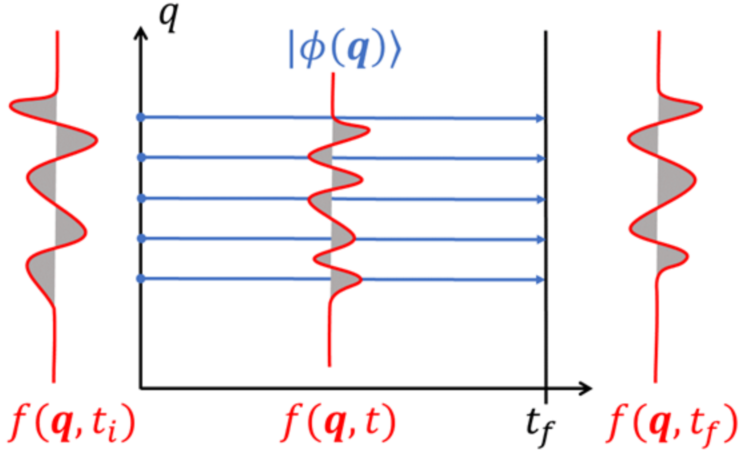
A TDRDFT trajectory only yields one pair of fragments.

Ren, Zhao, Vretenar, Nikšić, Zhao, and Meng, PRC **105**, 044313 (2022)

Yield described by TDGCM

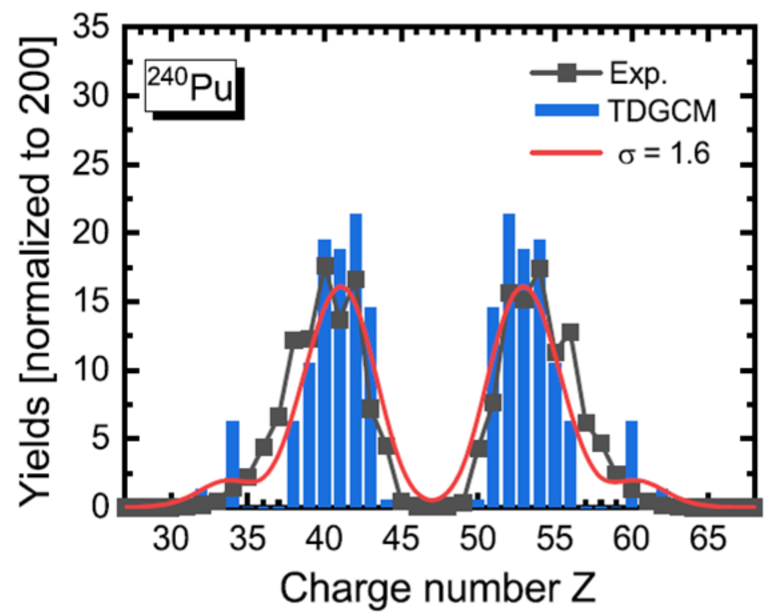
- TDGCM represents the nuclear wavefunction as a superposition of generator states that are functions of collective degree, and **weight functions evolve with time.**
- TDGCM includes **quantum fluctuations of the collective degree** and is more suitable to describe the yields of fragments.

$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q})\rangle$$



$f(\boldsymbol{q},t)$: weight function

$|\phi(\boldsymbol{q})\rangle$: Slater determinant



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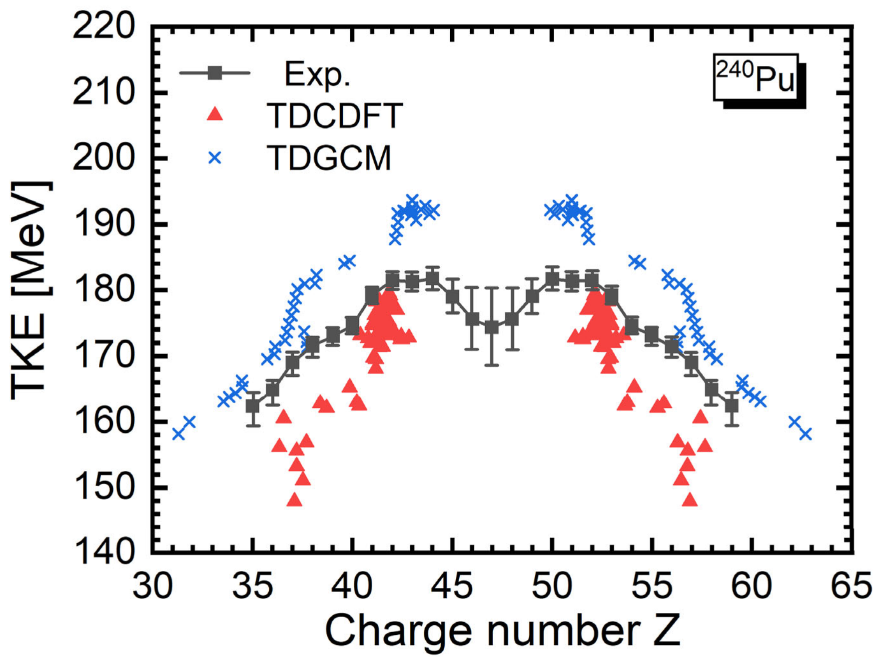
Total kinetic energy (TKE)

- Because of lacking **dissipative mechanism**, TDGCM overestimates the total kinetic energy of fragments.
- Due to including **one-body dissipative mechanism**, TDRDFT is more suitable for describing the total kinetic energy.



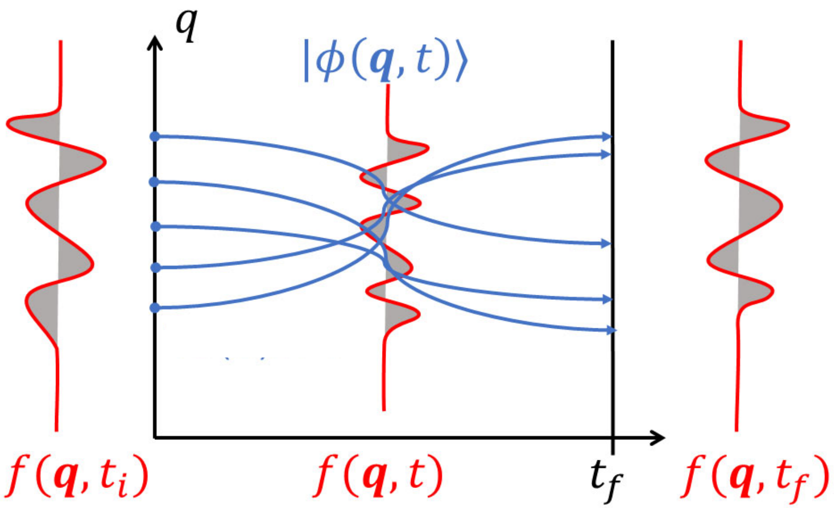
Ren, Zhao, Vretenar, Nikšić, Zhao, Meng, RPC **105**, 044313 (2022)

Can we combine TDRDFT and TDGCM to describe nuclear fission?

New nuclear wavefunction

- To simultaneously include **quantum fluctuations of the collective degree** and **dissipative effects,** one can represent the nuclear wavefunction as a superposition of time-dependent Slater determinants, and the weight functions are also time-dependent.

$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q},t)\rangle$$



Weight function (quantum fluctuation)

$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q},t)\rangle$$

Generator state (dissipative effects)

How do we determine the time-evolution equation of nuclear wavefunction?

Time-dependent variation principle

- Similar with the static equation determined by variation principle, the time-dependent equation can be determined by **time-dependent variation principle.**

$$S = \int \langle \Psi(t) | i\partial_t - \hat{H} | \Psi(t) \rangle \, dt \Rightarrow \delta S = 0$$

TDDFT

$$|\Psi(\boldsymbol{q}, t)\rangle = |\phi(\boldsymbol{q}, t)\rangle$$

$|\phi(\boldsymbol{q}, t)\rangle$: Time-dependent Slater determinant

Time evolution equation

$$S = \int \langle \Psi(t) | i\partial_t - \hat{H} | \Psi(t) \rangle \, dt \,;$$

$$\frac{\delta S}{\delta \psi_k^\dagger} = 0 \Rightarrow i\partial_t \psi_k(t) = \hat{h}(t)\psi_k(t)$$

Simenel, EPJA **48**, 152 (2012)

TDGCM

$$|\Psi(\boldsymbol{q}, t)\rangle = \int f(\boldsymbol{q}, t) |\phi(\boldsymbol{q})\rangle$$

$f(\boldsymbol{q}, t)$: Weight function

$|\phi(\boldsymbol{q})\rangle$: Static Slater determinant

Time evolution equation

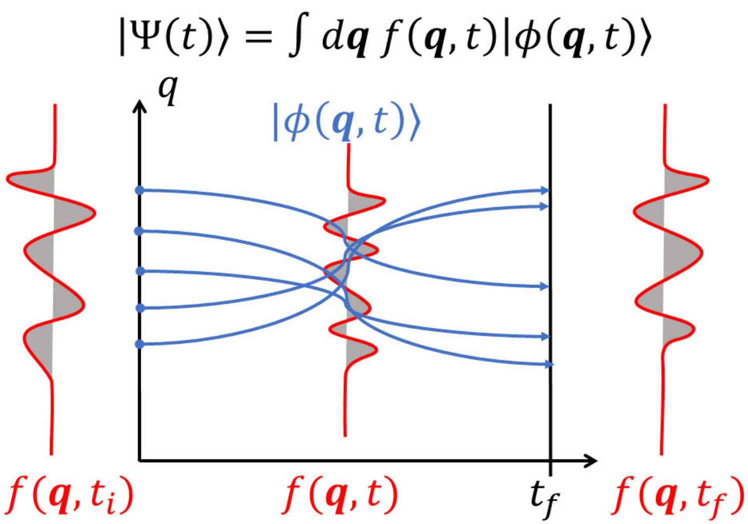
$$S = \int \langle \Psi(t) | i\partial_t - \hat{H} | \Psi(t) \rangle \, dt;$$

$$\frac{\delta S}{\delta f^*} = 0 \Rightarrow iN(t)\partial_t f(t) = H(t) f(t);$$

Schunck and Robledo, PPNP **79**, 116301 (2016)

Time-dependent variation principle

- The time equations for weight functions and generator states can also be determined from the **time-dependent variation principle.**



Weight function

$$S = \int \langle \Psi(t) | i\partial_t - \hat{H} | \Psi(t) \rangle dt; \qquad \frac{\delta S}{\delta f^*} = 0.$$

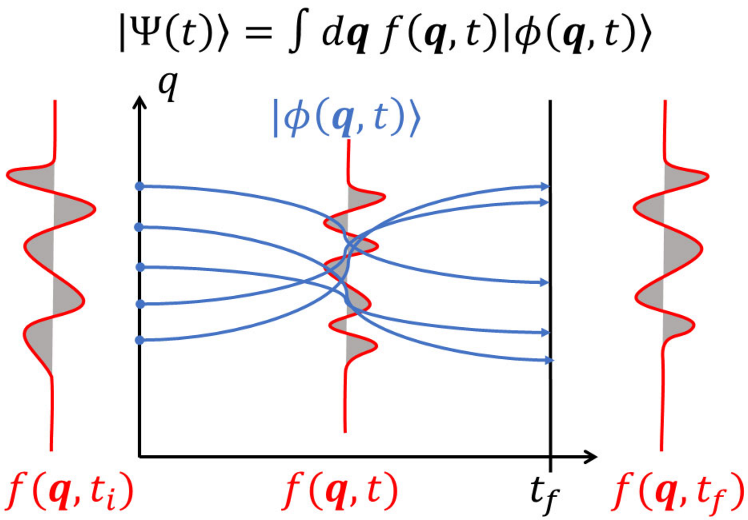
$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q},t)\rangle$$

Generator state

$$S = \int \langle \Psi(t) | i\partial_t - \hat{H} | \Psi(t) \rangle dt; \qquad \frac{\delta S}{\delta \psi^\dagger_{q,k}} = 0.$$

Approximation for action

- The time equations for weight functions and generator states can also be determined from the **time-dependent variation principle.**



Weight function

$$S = \int \langle \Psi(t) | i\partial_t - \hat{H} | \Psi(t) \rangle dt; \qquad \frac{\delta S}{\delta f^*} = 0.$$

$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q},t)\rangle$$

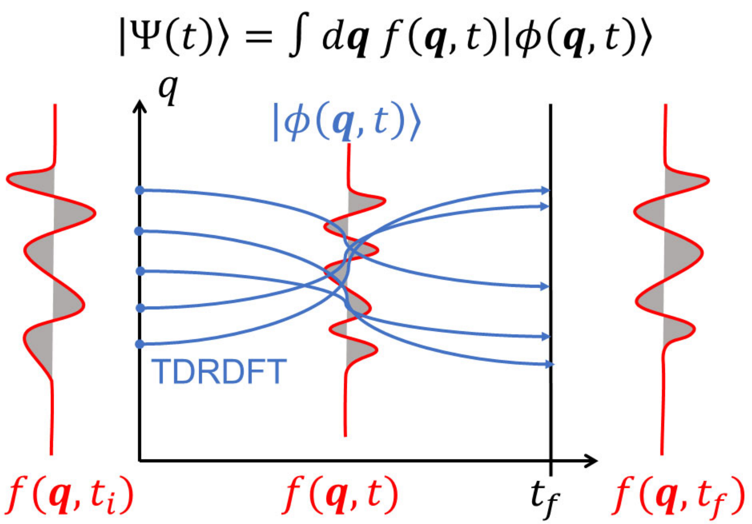
Generator state

$$S \approx \int \sum_{\boldsymbol{q}} |f_{\boldsymbol{q}}|^2 \langle \phi_{\boldsymbol{q}} | i\partial_t - \hat{H} | \phi_{\boldsymbol{q}} \rangle dt; \quad \frac{\delta S}{\delta \psi^\dagger_{\boldsymbol{q},k}} = 0.$$

$S_{\boldsymbol{qq}'} = \int f^*_{\boldsymbol{q}} f_{\boldsymbol{q}'} \langle \phi_{\boldsymbol{q}} | i\partial_t - \hat{H} | \phi_{\boldsymbol{q}'} \rangle dt$ is neglected.

Generalized TDGCM

- **Generalized time-dependent generator coordinate method (TDGCM)** represents the nuclear wavefunction as a superposition of TDRDFT trajectories, and weight functions are evolved by the time-dependent Hill-Wheeler equations.



Weight function: quantum fluctuations

$$iN\partial_t f = (H - H^{MF})f, \qquad g = N^{1/2} f$$

Regnier and Lacroix, PRC **99**, 064615 (2019)D

$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f(\boldsymbol{q},t)|\phi(\boldsymbol{q},t)\rangle$$

TDRDFT trajectory: dissipation

$$i\frac{\partial}{\partial t}\psi_{k,\boldsymbol{q}}(t) = [h^{\boldsymbol{q}}(t) - \varepsilon_k^{\boldsymbol{q}}(t)]\psi_{k,\boldsymbol{q}}(t)$$

Ren, Vretenar, Nikšić, Zhao, Zhao, and Meng, PRL **128**, 172501 (2022)

BL, Vretenar, Nikšić, Zhao, Meng, PRC **108**, 014321 (2023)
BL, Vretenar, Nikšić, Zhao, Zhao, Meng, FoP **19**, 44201 (2024)
BL, Vretenar, Nikšić, Zhao, Meng, PRC **111**, L051302 (2025)

Time evolution of generator states

- The single particle wavefunction $\psi_k^{\boldsymbol{q}}(\boldsymbol{r},t)$ of $|\Phi_{\boldsymbol{q}}(t)\rangle$ in TDRDFT, satisfies

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

where time-dependent single particle Hamiltonian $\hat{h}^{\boldsymbol{q}}(\boldsymbol{r},t)$ is determined by time-dependent densities and currents, and $\varepsilon_k^{\boldsymbol{q}}(t)=\langle\psi_k^{\boldsymbol{q}}(\boldsymbol{r},t)|\hat{h}^{\boldsymbol{q}}(\boldsymbol{r},t)|\psi_k^{\boldsymbol{q}}(\boldsymbol{r},t)\rangle$.

- Ignoring memory effect, the form of $\hat{h}^{\boldsymbol{q}}(\boldsymbol{r},t)$ is same as the static case,

$$\hat{h}^{\boldsymbol{q}}(\boldsymbol{r},t)=\alpha\cdot\left[-i\boldsymbol{\nabla}-\boldsymbol{V}_{\boldsymbol{q}}(\boldsymbol{r},t)\right]+V_{\boldsymbol{q}}^{0}(\boldsymbol{r},t)+\beta\left[m_N+S_{\boldsymbol{q}}(\boldsymbol{r},t)\right],$$

where potential $V_{\boldsymbol{q}}^{\mu}(\boldsymbol{r},t)$ and $S_{\boldsymbol{q}}(\boldsymbol{r},t)$ depend on time-dependent densities and currents $\rho_{S,\boldsymbol{q}}(\boldsymbol{r},t)$, $j_{\boldsymbol{q}}^{\mu}(\boldsymbol{r},t)$, $j_{TV,\boldsymbol{q}}^{\mu}(\boldsymbol{r},t)$,

$$S_{\boldsymbol{q}}(\boldsymbol{r},t)=\alpha_S\rho_{S,\boldsymbol{q}}+\beta_S\rho_{S,\boldsymbol{q}}^2+\gamma_S\rho_{S,\boldsymbol{q}}^3+\delta_S\Delta\rho_{S,\boldsymbol{q}},$$

$$V_q^{\mu}(\boldsymbol{r},t)=\alpha_V j_{\boldsymbol{q}}^{\mu}+\gamma_V\left(j_q^{\mu}j_{\mu,q}\right)j_{\boldsymbol{q}}^{\mu}+\delta_V\Delta j_{\boldsymbol{q}}^{\mu}+\tau_3\alpha_{TV}j_{TV,\boldsymbol{q}}^{\mu}+\tau_3\delta_{TV}\Delta j_{TV,\boldsymbol{q}}^{\mu}+e\frac{1-\tau_3}{2}A_{\boldsymbol{q}}^{\mu}.$$

Ren, Zhao, Meng, Phys. Lett. B **801**, 135194 (2020)
Ren, Vretenar, Nikšić, Zhao, Zhao, Meng, Phys. Rev. Lett. **128**, 172501 (2022)

Time evolution of weight function

- The equation of motion for weight functions is obtained from the time-dependent variational principle, Regnier and Lacroix, PRC **99**, 064615 (2019)

$$iN\partial_t f = (H - H^{MF})f,$$

which reads

$$\sum_q iN_{q'q}(t)\partial_t f_q(t) = \sum_q H_{q'q}(t) f_q(t) - \sum_q H^{MF}_{q'q}(t) f_q(t).$$

The time-dependent kernels are

$$N_{q'q}(t) = \langle \Phi_{q'}(t) | \Phi_q(t) \rangle,$$

$$H_{q'q}(t) = \langle \Phi_{q'}(t) | \hat{H} | \Phi_q(t) \rangle,$$

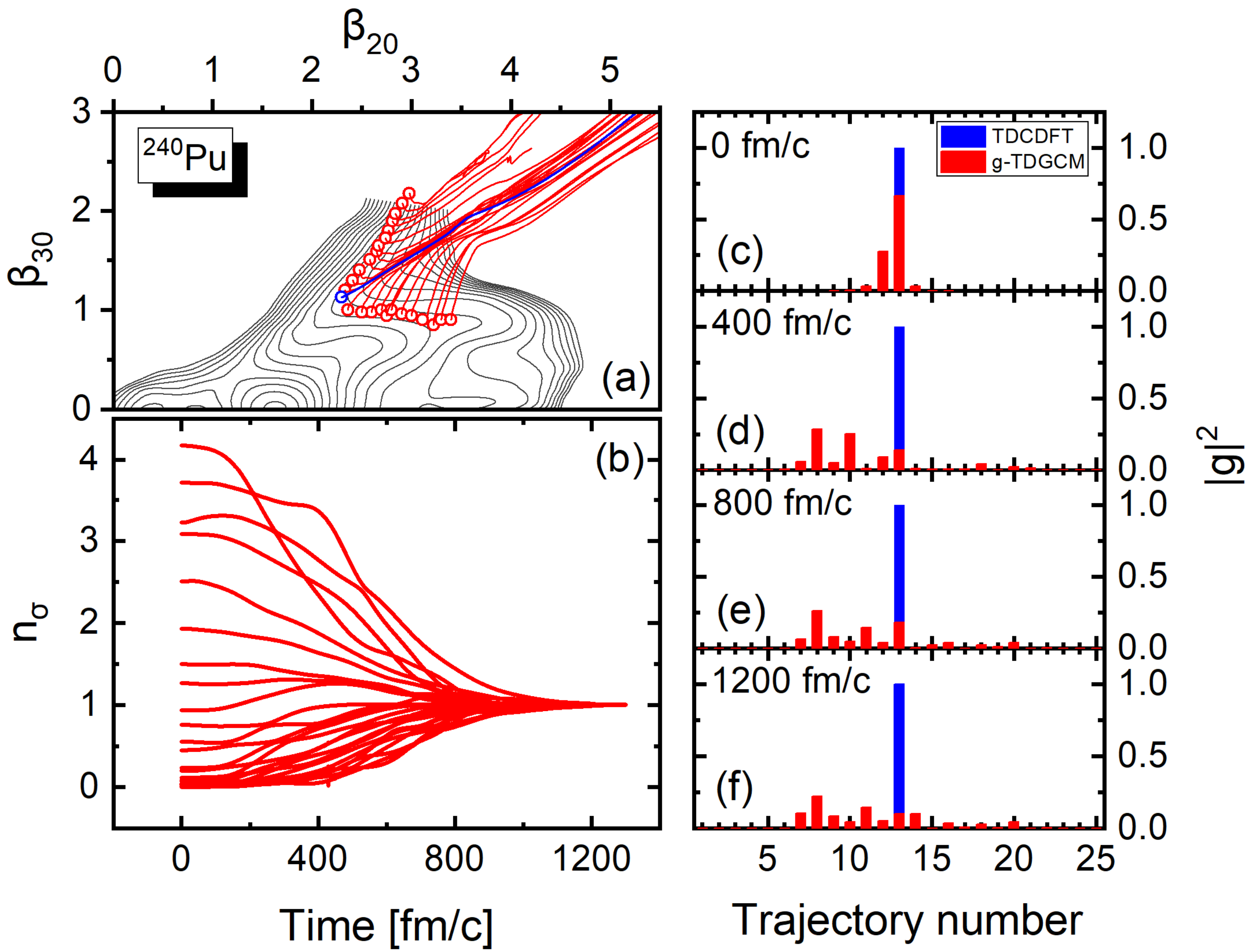
$$H^{MF}_{q'q}(t) = \langle \Phi_{q'}(t) | i\partial_t | \Phi_q(t) \rangle.$$

- The weight function $f_q(t)$ is not the probability amplitude of the nucleus at the collective coordinate $\boldsymbol{q}$. The corresponding probability amplitude $g_q(t)$ is defined by $g = N^{1/2} f$ and satisfies the time evolution equation,

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

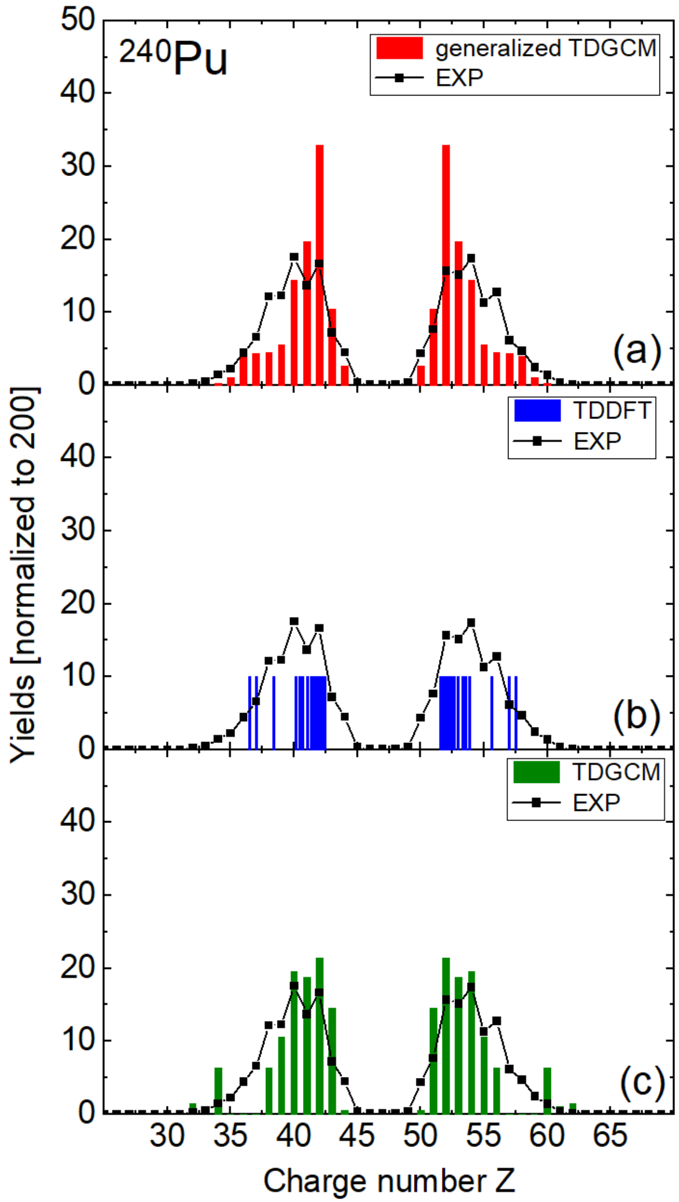
Induced fission of ^{240}Pu

- 25 TDRDFT trajectories are selected as generator states.



BL, Vretenar, Nikšić, Zhao, Meng, PRC **111**, L051302 (2025)

Charge Yields



The proton number distribution of the nuclear wave functions is obtained by **particle number projection method.**

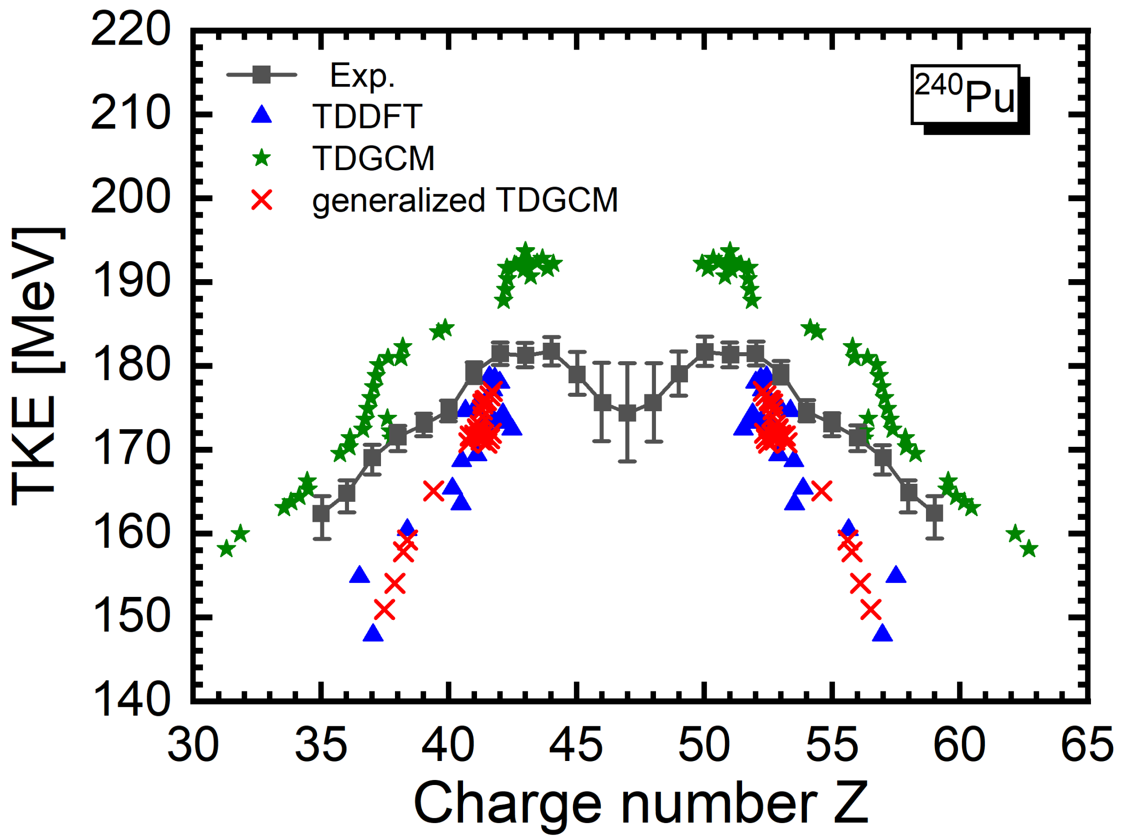
$$P(z|Z) = \frac{\langle\Psi(t)|\hat{P}_Z \hat{P}_z^{V_p}|\Psi(t)\rangle}{\langle\Psi(t)|\hat{P}_Z|\Psi(t)\rangle}$$

Scamps and Lacroix, PRC **87**, 014605 (2013)

✓ Due to the inclusion of **quantum fluctuations in the collective degree**, generalized TDGCM, compared with TDRDFT, can reproduce the yields of fragments better.

BL, Vretenar, Nikšić, Zhao, Meng, PRC **111**, L051302 (2025)

Total kinetic energy (TKE)



✓ Due to the inclusion of the **one-body dissipative mechanism**, generalized TDGCM, compared with TDGCM, can reproduce the total kinetic energy better.

BL, Vretenar, Nikšić, Zhao, Meng, PRC **111**, L051302 (2025)

Relativistic density functional

- Relativistic density functional: point-coupling

$$E_{\text{tot}} = E_{\text{kin}} + E_{\text{int}} + E_{\text{em}}$$

$$= \int d^3\boldsymbol{r} \left\{ \sum_{k=1} n_k \psi_k^\dagger (\boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} + \beta m_N) \psi_k \right.$$

$$+ \frac{1}{2}\alpha_S \rho_S^2 + \frac{1}{3}\beta_S \rho_S^3 + \frac{1}{4}\gamma_S \rho_S^4 + \frac{1}{2}\delta_S \rho_S \Delta \rho_S + \frac{1}{2}\alpha_V j^\mu j_\mu + \frac{1}{4}\gamma_V \left(j^\mu j_\mu\right)^2 + \frac{1}{2}\delta_V j^\mu \Delta j_\mu$$

$$\left. + \frac{1}{2}\alpha_{TV} j_{TV}^\mu (j_{TV})_\mu + \frac{1}{2}\delta_{TV} j_{TV}^\mu \Delta (j_{TV})_\mu + e j_c^\mu A_\mu - \frac{1}{2} A_\mu \Delta A^\mu \right\}$$

- Density and currents：

$$\rho_S = \sum_{k=1} n_k \bar{\psi}_k \psi_k \qquad j^\mu = \sum_{k=1} n_k \bar{\psi}_k \gamma^\mu \psi_k \qquad j_{TV}^\mu = \sum_{k=1} n_k \bar{\psi}_k \gamma^\mu \tau_3 \psi_k$$

(isoscalar-scalar) (isoscalar-vector) (isovector-vector)

Zhao, Li, Yao, Meng, PRC **82**, 054319 (2010)
Relativistic Density Functional for Nuclear Structure, edited by J. Meng, 2016

Solution of TD-KS equation

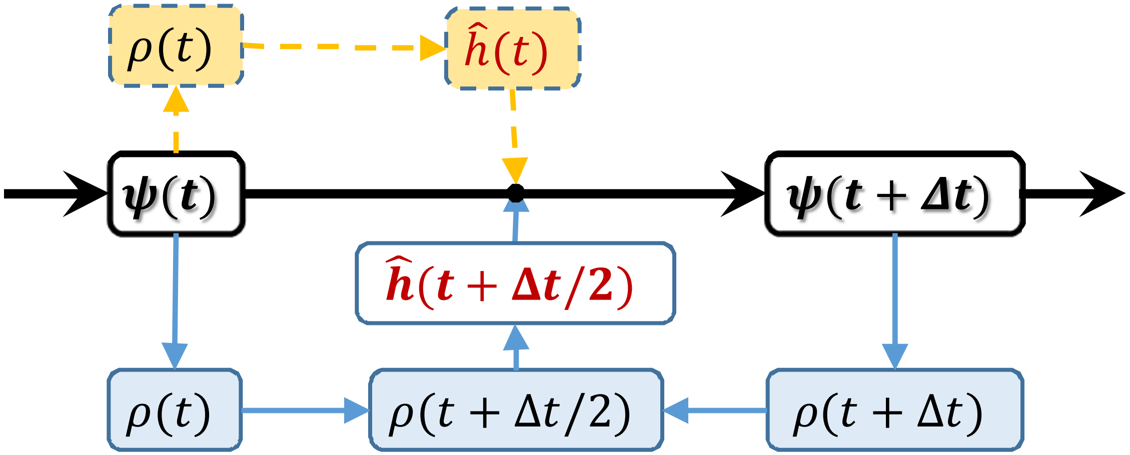
- The formal solution of TD-KS equation is

$$\psi_k(\boldsymbol{r},t) = \hat{\mathcal{T}}\exp\left[-i\int_{t_0}^{t} dt'\,\hat{h}(\boldsymbol{r},t')\right]\psi_k(\boldsymbol{r},t_0),$$

where $\hat{\mathcal{T}}$ is time-ordering operator and $\psi_k(\boldsymbol{r},t_0)$ is the initial wavefunction.

- For the numerical implementation of the formal solution, **the predictor-corrector method** is adopted and the evolution of the single-particle wavefunction from t to $t+\Delta t$ is obtained as Ren, Zhao, Meng, PRC **102**, 044603 (2020)

$$\psi_k(\boldsymbol{r},t+\Delta t) \approx \exp\left[-i\hat{h}(\boldsymbol{r},t+\Delta t/2)\Delta t\right]\psi_k(\boldsymbol{r},t).$$



TKE distribution

- The TKE distribution of fission fragments reads

$$\mathrm{TKE}(N_H, Z_H, N_L, Z_L) = \frac{1}{2} m_H \boldsymbol{v}_H^2 + \frac{1}{2} m_L \boldsymbol{v}_L^2 + E_{\mathrm{coul}},$$

where the mass number and velocity of fragment is

$$A_f = N_f + Z_f, \qquad \boldsymbol{v}_f = \frac{1}{A_f} \int_{V_f} \boldsymbol{j}(\boldsymbol{r_f}, N_f, Z_f) d\boldsymbol{r_f} \quad (f = H, L),$$

and the Coulomb energy between two fission fragments is

$$E_{\mathrm{coul}} = \alpha \int_{V_H} \int_{V_L} \frac{\rho_p(\boldsymbol{r_H}, N_H, Z_H) \rho_p(\boldsymbol{r_L}, N_L, Z_L)}{|\boldsymbol{r_H} - \boldsymbol{r_L}|} d\boldsymbol{r_H}\, d\boldsymbol{r_L}$$

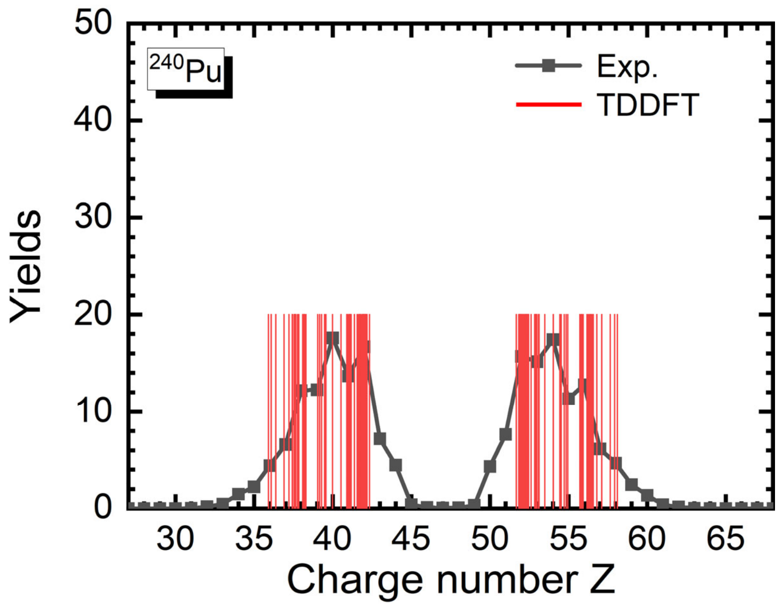
- The projected density and current read [$j^\mu = (\rho, \boldsymbol{j})$]

$$j^\mu(\boldsymbol{r}, N_f, Z_f) = \frac{\left\langle \Psi \left| \bar{\psi}(\boldsymbol{r}) \gamma^\mu \psi(\boldsymbol{r}) \hat{P}_n^{V_f} \hat{P}_N \hat{P}_Z^{V_f} \hat{P}_Z \right| \Psi \right\rangle}{\left\langle \Psi \left| \hat{P}_n^{V_f} \hat{P}_N \hat{P}_Z^{V_f} \hat{P}_Z \right| \Psi \right\rangle}.$$

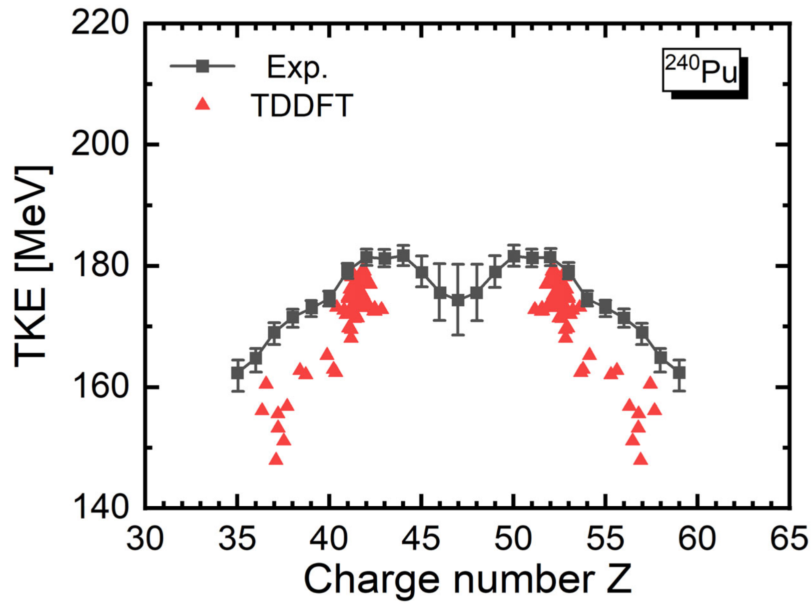
Modern theory extension

- ➢ The review "*Future of nuclear fission theory*" summarise the main recommendations of this report that reflect challenges facing nuclear fission theory

Yields described by TDDFT



TKE described by TDDFT



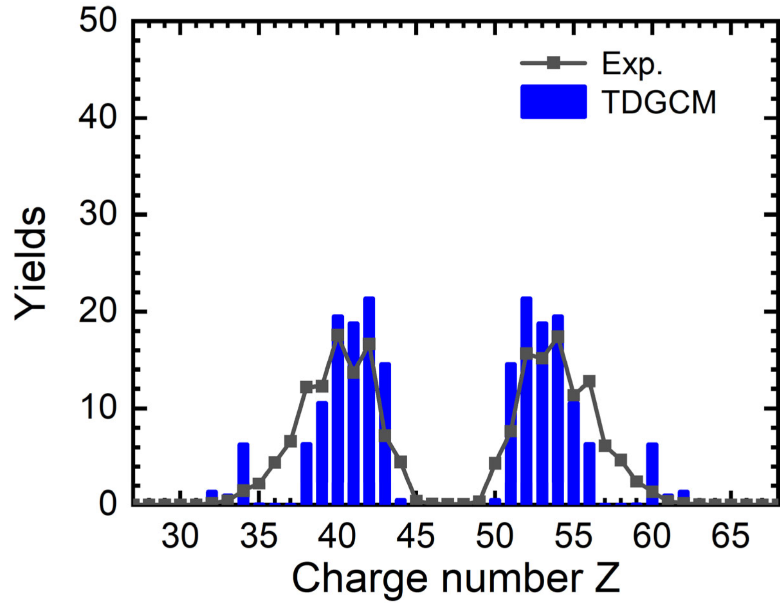
Ren, *et al*., PRC **105**, 044313 (2022)

TDDFT underestimates the width of fission fragment yield.

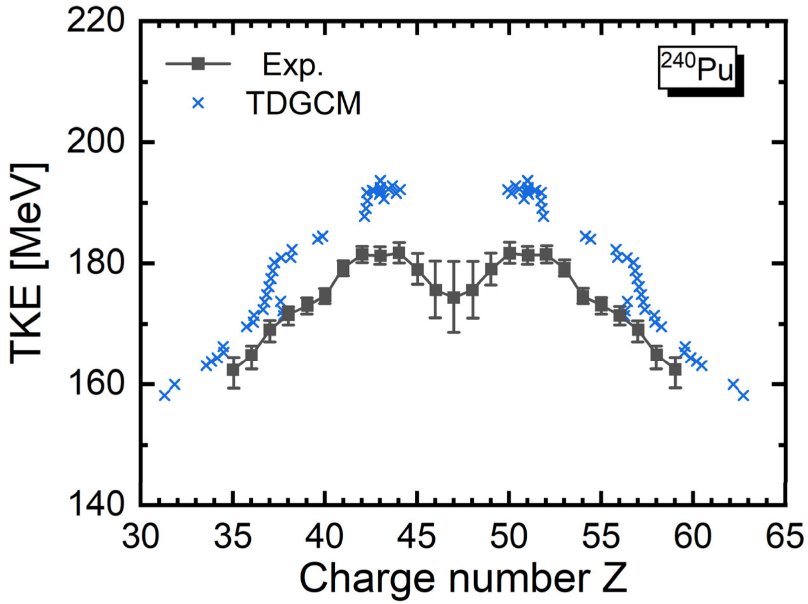
Yield and TKE in a microscopic framework

- How to describe the **charge (mass) yield** and **total kinetic energy (TKE)** of fission fragments in **a microscopic framework**?

Yields described by TDGCM



TKE described by TDGCM



Ren, *et al.*, PRC **105**, 044313 (2022)

TDGCM overestimates the TKE of fission fragment.