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Microscopic description of multinucleon transfer reactions with relativistic TDDFT: mass and spin distributions

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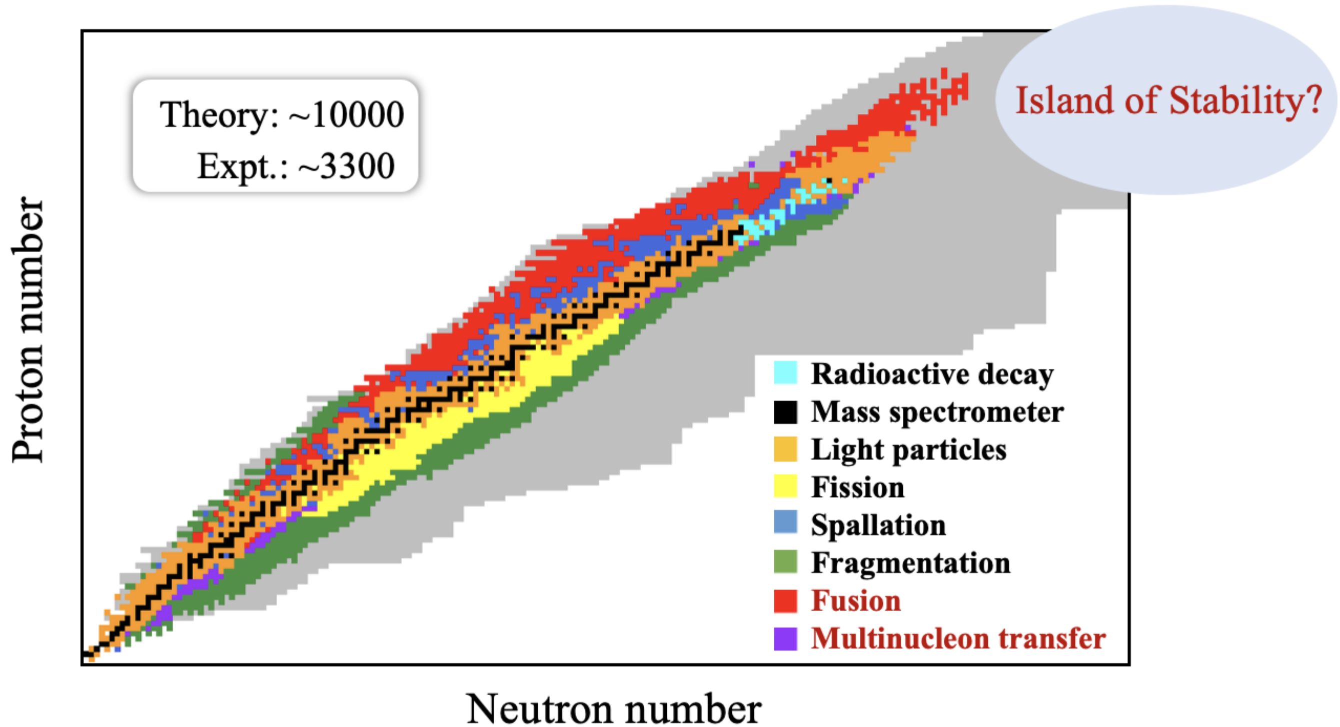
Contents

Heavy-ion reactions

- Heavy-ion reactions, induced by ions heavier than α particles, are one of the important methods for synthesizing new nuclides.



Thoennessen, *The Discovery of Isotopes* (2016)
Xia et al., ADNDT 121, 1 (2018)

- Fusion: synthesizing superheavy nuclei (SHN).
- Multinucleon transfer (MNT) reactions: synthesizing neutron-rich nuclei.

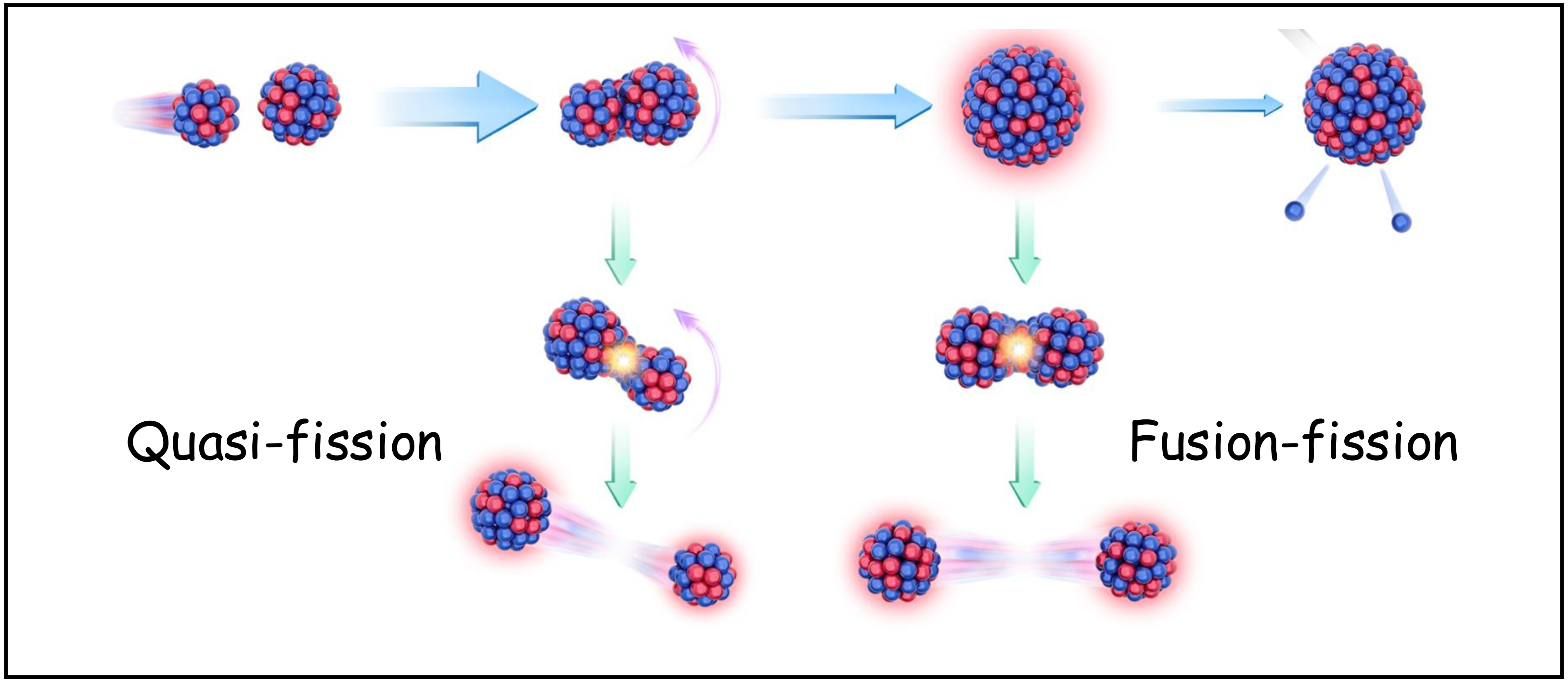
Jiang, **DDZ**, Zhou. Physics 54, 599 (2025)

Fusion: Neutron-deficient superheavy nuclei

- Fusion is the only successful method for synthesizing SHN to date.
- However, the cross sections drop rapidly with increasing Z, hindering the synthesis of new elements.

Münzenberg et al., EPJA 59, 21 (2023)
Oganessian, EPJA 60, 227 (2024)
Zhang et al., NST 36, 204 (2025)

  - ✓ Quasi-fission and fusion-fission are two main competitive processes.

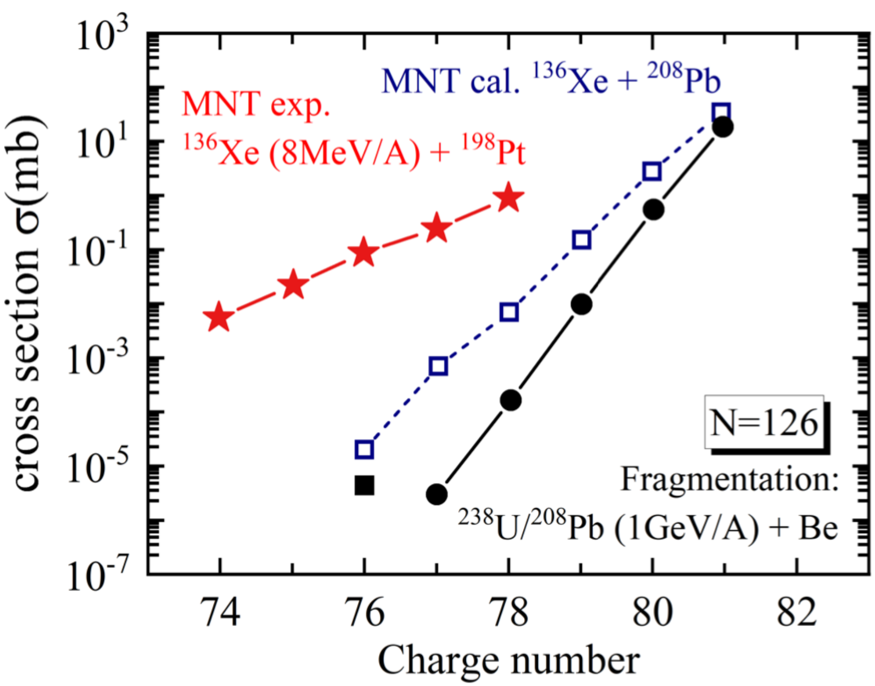


Jiang, **DDZ**, Zhou. Physics 54, 599 (2025)

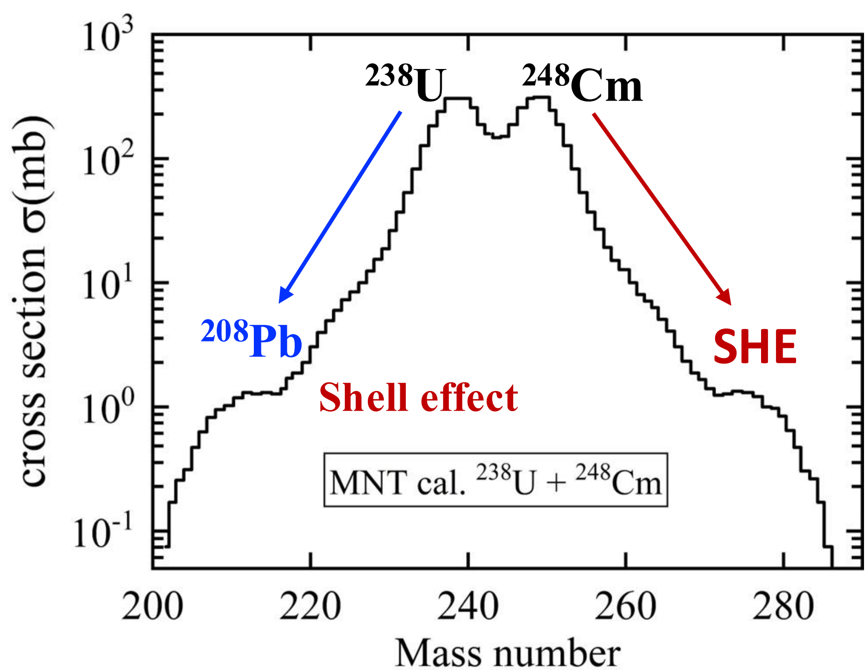
MNT: Neutron-rich nuclei

- Recently, the MNT reaction has been suggested as a possible pathway for the synthesis of neutron-rich heavy and superheavy nuclei
  - ✓ Neutron-rich region around $N = 126$
  - ✓ Possible reaction mechanism

Complex mass and angular distributions!



Zagrebaev and Greiner, PRL 101,122701 (2008)
Watanabe et al., PRL 115,172503 (2015)



Zagrebaev and Greiner, JPG 34, 2265 (2007)
Zagrebaev and Greiner, PRC 87, 034608 (2013)

Theoretical models for MNT reactions

- The multinucleon transfer process is a complex quantum many-body dynamical problem. A broad range of theoretical approaches has been developed:

  - ✓ Coupled channels — Thompson, Comput. Phys. Rep. 7, 167 (1988); Scamps & Hagino, PRC 92, 054614 (2015) …
  - ✓ Dinuclear System Model — Adamian, Antonenko, and Scheid, NPA 618, 176 (1997); Adamian et al., NPA 633, 409 (1998) Adamian et al., PRC 81, 024604 (2010); Feng, PRC 95, 024615 (2017); Zhu et al., JPG 42, 085102 (2015) …
  - ✓ GRAZING Model — Winther, NPA 572, 191 (1994); Yanez and Loveland, PRC 91, 044608 (2015);Wen et al., PRC 99, 034606 (2019) …
  - ✓ Langevin Model — Zagrebaev and Greiner, PRL 101, 122701 (2008); Zagrebaev and Greiner, PRC 78, 034610 (2008) Zhu, PLB 849, 138423 (2024); Dai et al., PRC 109, 024617 (2024) …
  - ✓ (Improved) Quantum Molecular Dynamics — Wang et al., PRC 65, 064608 (2002); Li et al., PRC 93, 014618 (2016); Zhao et al., PRC 92, 024613 (2015) …
  - ✓ Time-Dependent Density Functional Theory (TDDFT) — Simenel, PRL 105, 192701 (2010); Sekizawa and Yabana, PRC 88, 014614 (2013) Zhang et al., PRC 109, 024614 (2024); Li et al., PRC 110, 034611 (2024) Zhang et al., PLB 869, 139828 (2025) …
  - ✓ Stochastic Mean-Field / TDRPA — Simenel, PRL 106, 112502 (2011); Ayik et al., PRC 97, 054618 (2018); Yilmaz et al., PRC 98, 034604 (2018); Sekizawa and Ayik, PRC 102, 014620 (2020); Gao, Sekizawa, and Zhu, PRC 112, 014602 (2025);…
  - ✓ Other approaches

Contents

Relativistic TDDFT

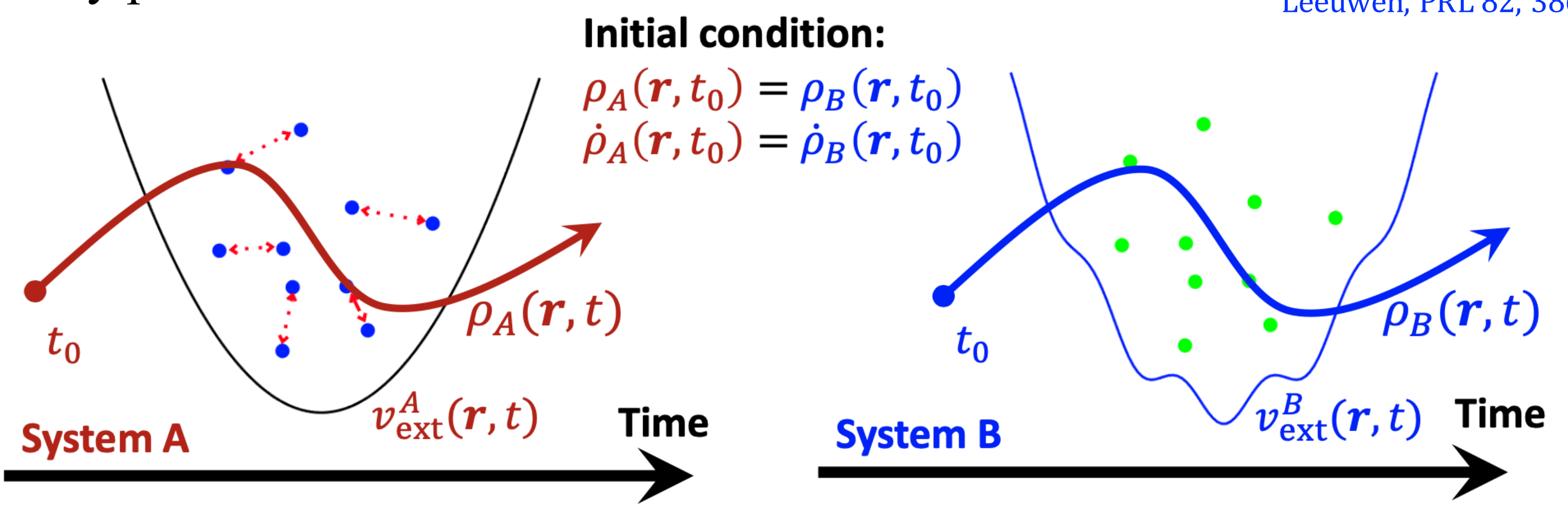
- Relativistic TDDFT has been developed and applied to a series of nuclear dynamical phenomena.

Ren, Zhao, and Meng, PRC 102, 044603 (2020)
Ren, Zhao, and Meng, PLB 801, 135194 (2020)
Ren, Zhao, and Meng, PRC 105, L011301 (2022)
Ren, Zhao, Vretenar, Nikšić, Zhao, Meng, PRC 105, 044313 (2022)
Ren, Vretenar, Nikšić, Zhao, Zhao, Meng, PRL 128, 172501 (2022)

Li, Vretenar, Ren, Nikšić, Zhao, Zhao, Meng, PRC 107, 014303 (2023)
Li, Vretenar, Nikšić, Zhao, Meng, PRC 110, 034302 (2024)
Li, Zhao, Meng, PLB 856, 138877 (2024)
DDZ, Vretenar, Nikšić, Zhao, Meng, PRC 109, 024614 (2024)
DDZ, Li, Vretenar, Nikšić, Ren, Zhao, Meng, PRC 109, 024316 (2024)
DDZ, Vretenar, Nikšić, Zhao, Meng, PLB 869, 139828 (2025)
DDZ, Li, Vretenar, Nikšić, Ren, Zhao, Meng, PRC 114, 014628 (2026)

- **Idea:** Transforming the time-dependent many-body problem to a time-dependent one-body problem.

Runge and Gross, PRL 52, 997(1984)
Leeuwen, PRL 82, 3863(1999)

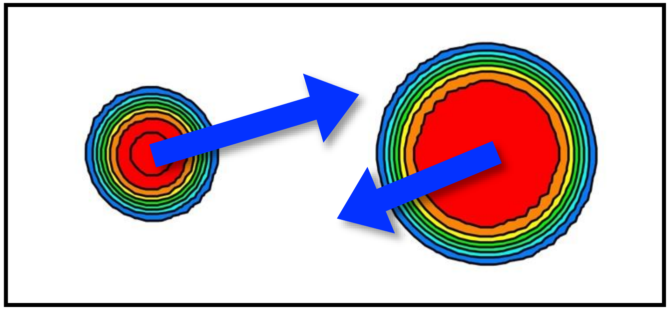


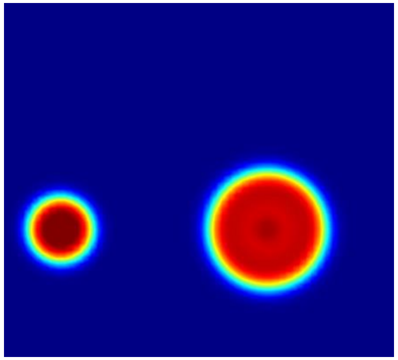
Time-dependent many-body problem **Time-dependent one-body problem**

Figure is taken from Z. X. Ren

Particle number and angular momentum projection

- TDDFT gives the most probable reaction path, and the wavefunction of reaction products typically lacks well-defined quantum numbers (particle number, spin)





- We extended relative TDDFT to include particle number projection and angular momentum projection.

DDZ, Vretenar, Nikšić, Zhao, Meng, PRC 109, 024614 (2024)
DDZ, Vretenar, Nikšić, Zhao, Meng, PLB 869, 139828 (2025)

Particle number projection

Particle number projection operator:

$$\hat{P}_n^V = \frac{1}{2\pi} \int d\theta \, e^{i\theta(n-\hat{N}_V)}.$$

$$P(n) = \langle \Psi | \hat{P}_n^V | \Psi \rangle, \quad P(n) = \frac{\langle \Psi | \hat{P}_n^V \hat{P}_N | \Psi \rangle}{\langle \Psi | \hat{P}_N | \Psi \rangle}.$$

Angular momentum projection

Angular momentum projection operator:

$$\hat{P}_{MK}^S = \frac{2S+1}{16\pi^2} \int d\Omega \left(D_{MK}^S(\Omega) \right)^* \hat{R}(\Omega).$$

$$P(S,K) = \langle \Psi | (\hat{P}_{MK}^S)^+ \hat{P}_{MK}^S | \Psi \rangle = \langle \Psi | \hat{P}_{KK}^S | \Psi \rangle.$$

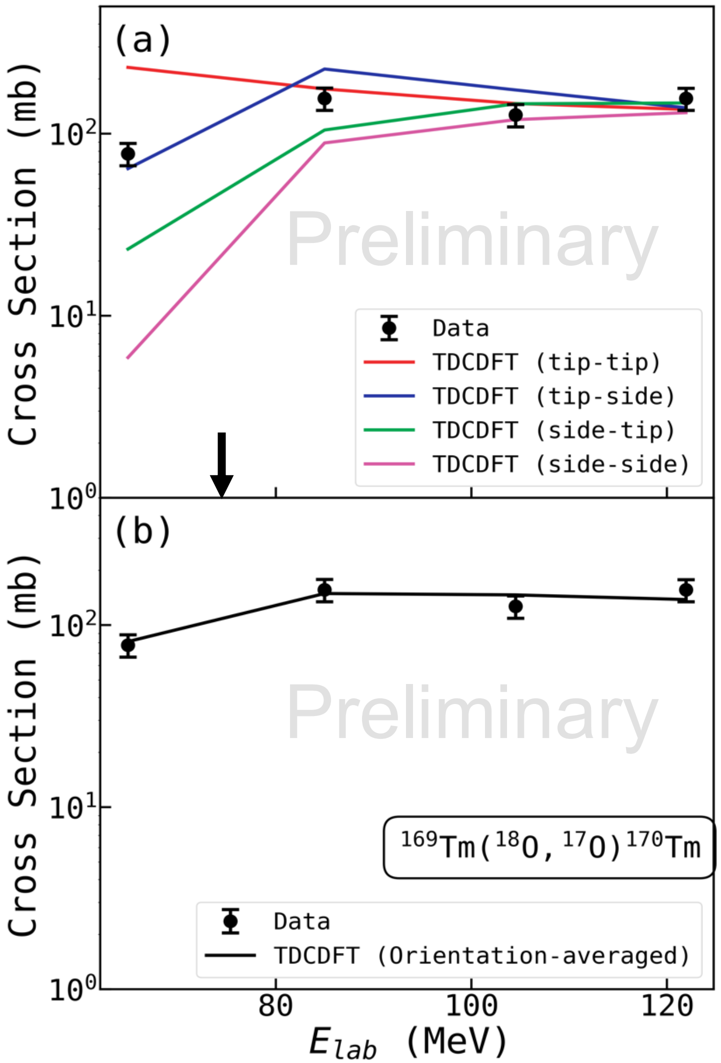
Simenel, PRL 105, 192701 (2010); Sekizawa and Yabana, PRC 88,014614 (2013)

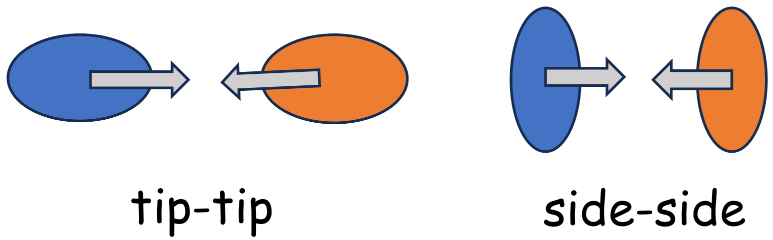
Scamps et al., PRC 108, L061602 (2023)

Contents

Predictions of one-neutron transfer cross-section

- One-neutron transfer cross-section prediction of ^{18}O + ^{169}Tm:





✓ The orientation effects are rather strong below the Coulomb barrier.

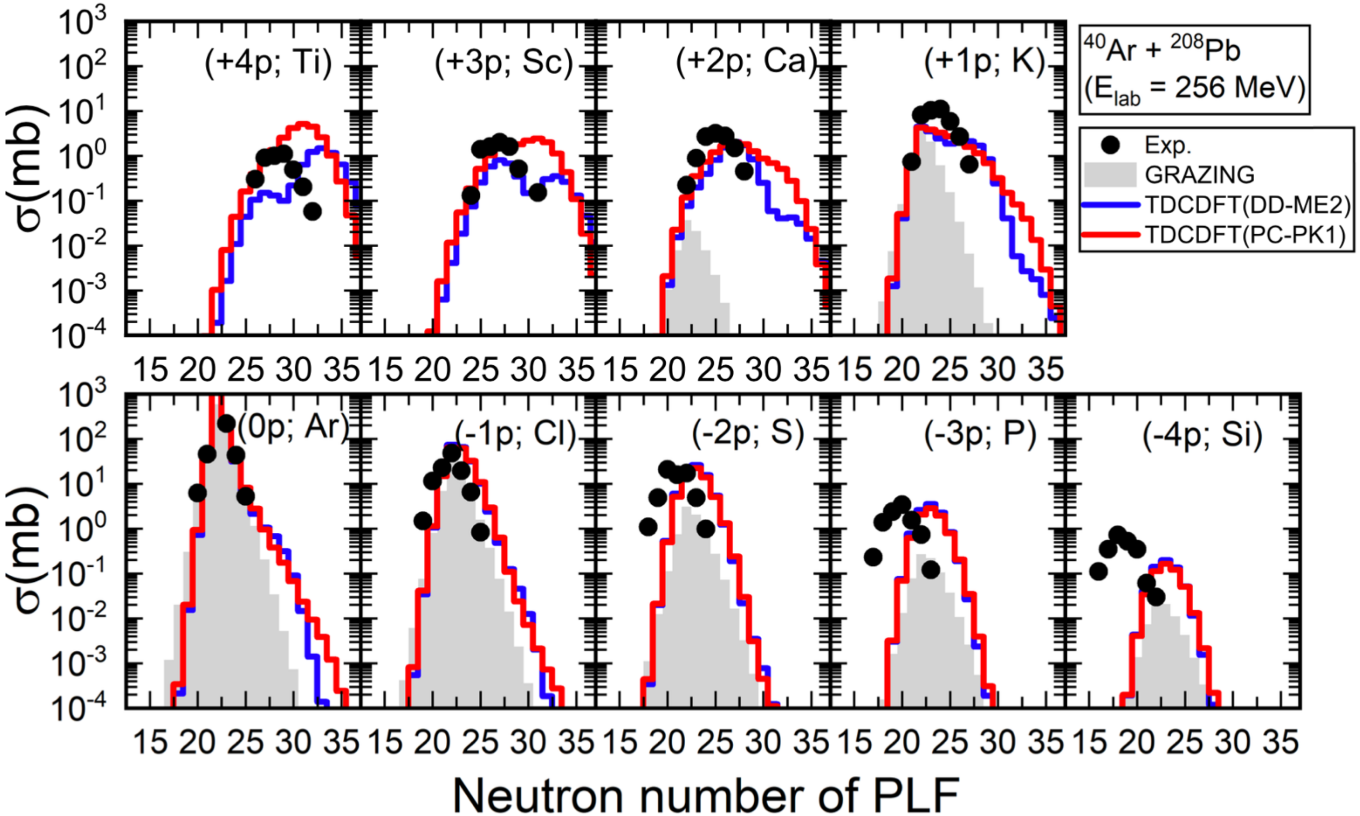
✓ Compared with the data, relativistic TDDFT+GEMINI accurately predicts the one-neutron transfer cross-section.

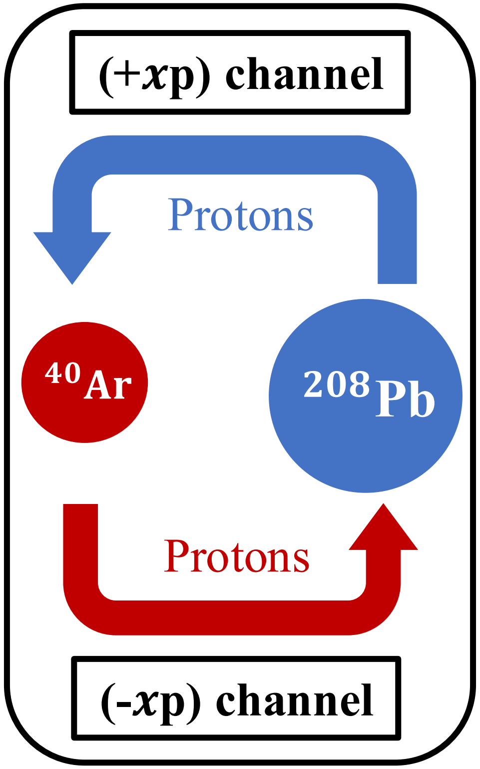
In preparation

Data are measured by G. S. Li's group (Institute of Modern Physics)

Multinucleon transfer cross-sections

- For the MNT reaction ^{40}Ar + ^{208}Pb,





D. D. Zhang, D. Vretenar, T. Nikšić, P. W. Zhao, and J. Meng, Phys. Rev. C 109, 024614 (2024)

- ✓ Relativistic TDDFT gives a reasonable description of the cross-section.
- ✓ The inclusion of the de-excitation process would improve the results.

Ternary quasi-fission in $^{238}U + ^{238}U$ collision

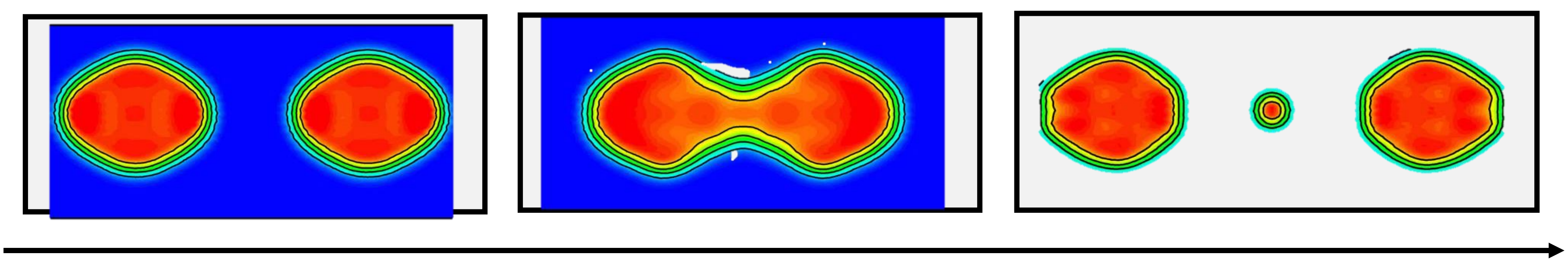
PRL **103,** 042701 (2009) PHYSICAL REVIEW LETTERS week ending 24 JULY 2009

Collision Dynamics of Two ^{238}U Atomic Nuclei

Cédric Golabek
GANIL (IN2P3/CNRS - DSM/CEA), BP 55027, F-14076 Caen Cedex 5, France

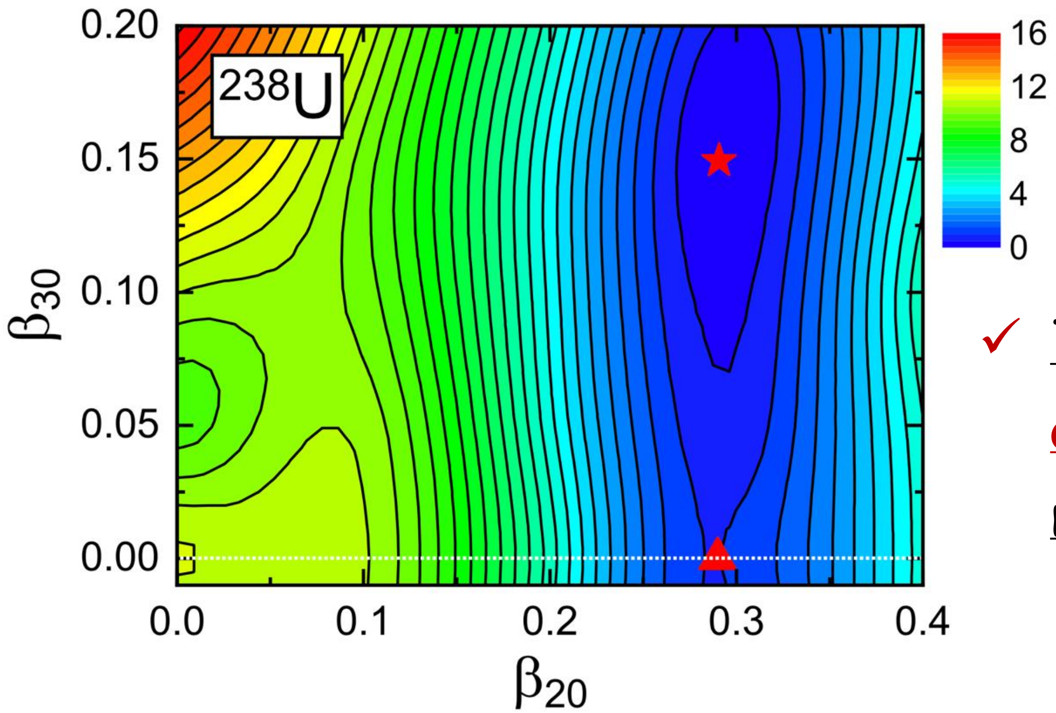
Cédric Simenel
CEA, Centre de Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France
(Received 20 April 2009; revised manuscript received 19 May 2009; published 24 July 2009)

"…Surprisingly, we also observe **ternary fission** due to purely dynamical effects. "



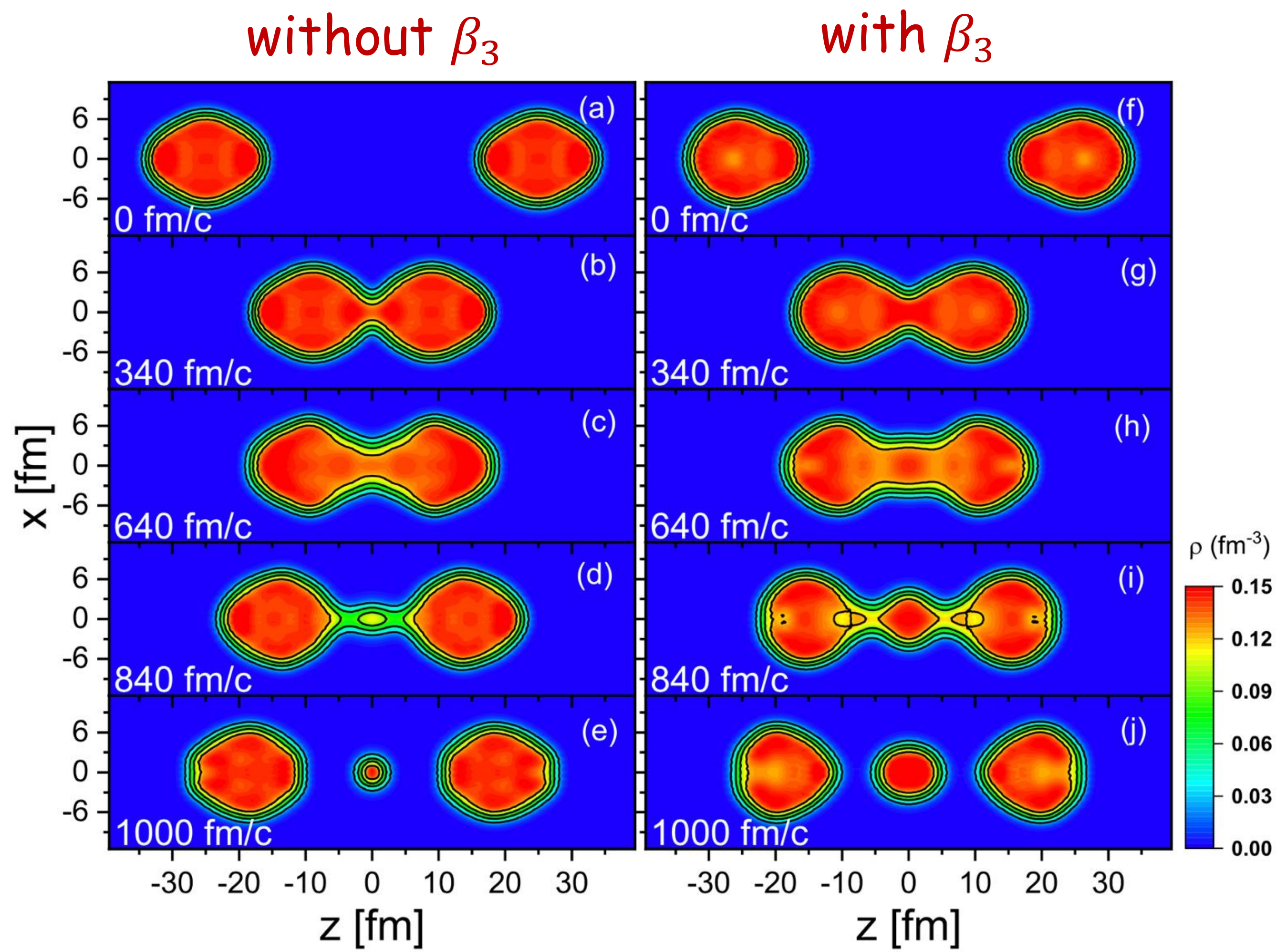
Time evolution

Ternary quasi-fission in collisions of actinide nuclei



✓ The ground state of ^{238}U is **octupole-deformed** in the mean-filed level.

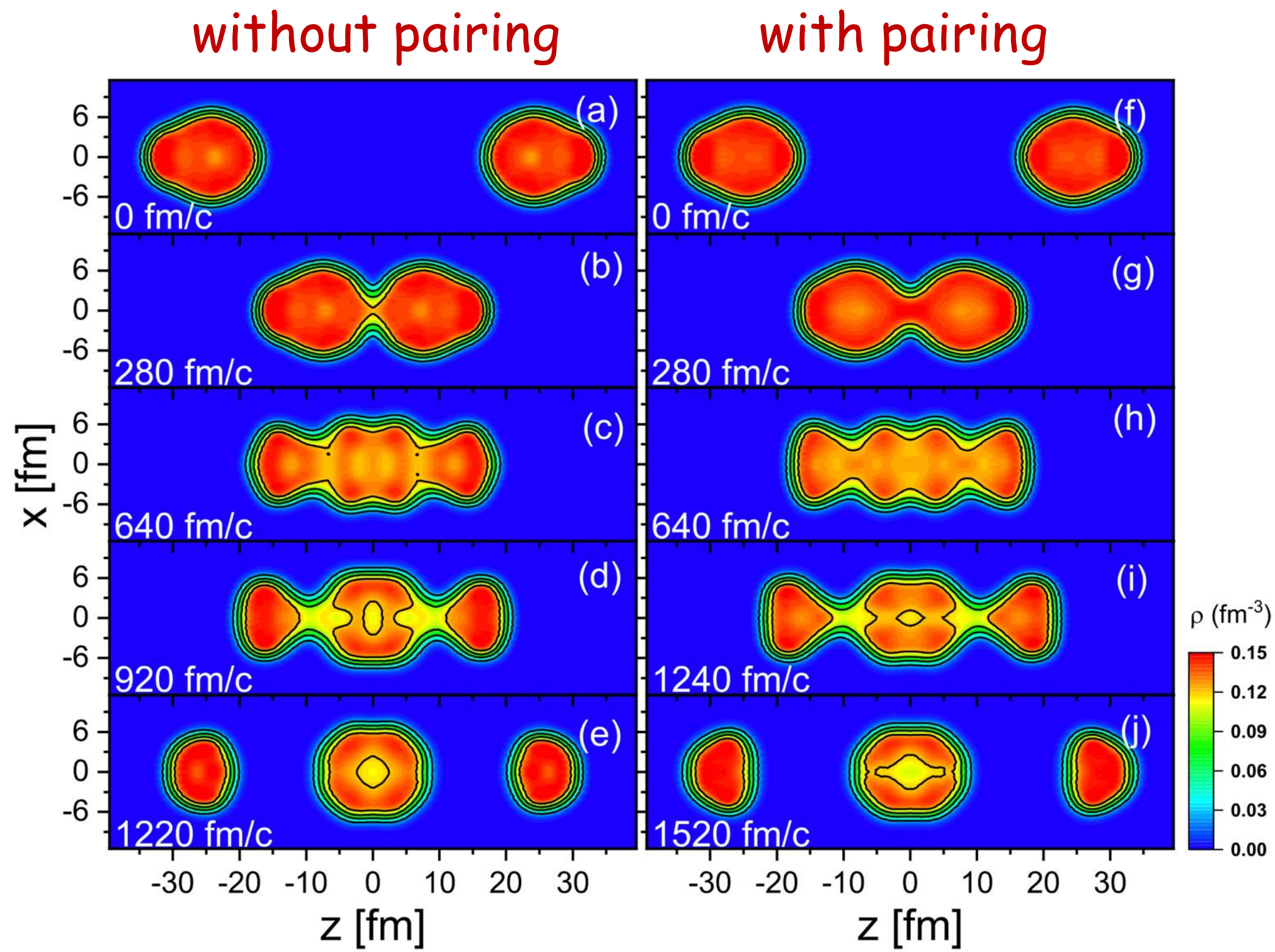
Octupole deformation



✓ The octupole deformation affects the ternary quasi-fission.

D. D. Zhang, B. Li, D. Vretenar, T. Nikšić, Z. X. Ren, P. W. Zhao, and J. Meng, Phys. Rev. C 109, 024316 (2024)

Orientations



✓ Neutron-rich heavy nuclei around uranium are formed in the middle.

D. D. Zhang, B. Li, D. Vretenar, T. Nikšić, Z. X. Ren, P. W. Zhao, and J. Meng, Phys. Rev. C 109, 024316 (2024)

Contents

Fragment intrinsic spins and their correlations

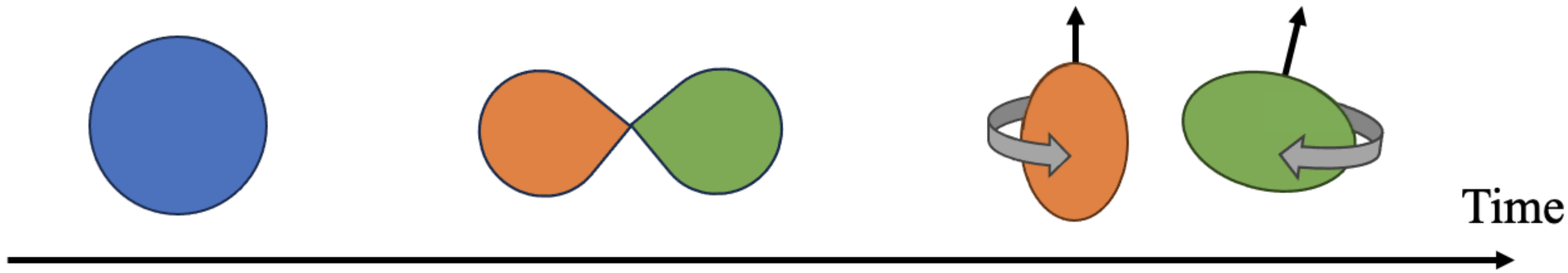
- In a system that consists of two fragments, the conservation of angular momentum requires

$$J = S^L + S^H + \Lambda.$$

S^L, S^H: spins of two fragments. Λ: orbital angular momentum.

- The spontaneous fission of even-even nuclei ($J = 0$) is a typical case.

The generation of spins and their correlations.

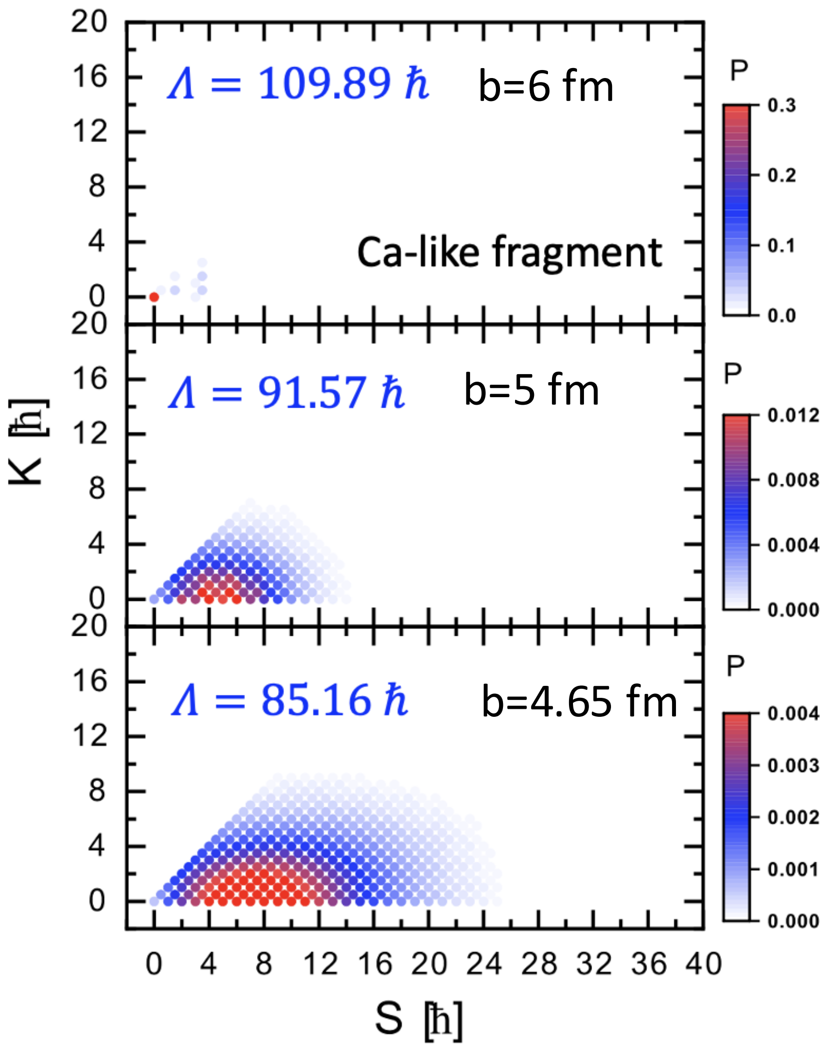


The fragment intrinsic spins and their correlations in fission have attracted broad interest.

Wilson et al., Nature 590, 566 (2021)
Bulgac et al., PRL 126, 142502 (2021); Bulgac et al., PRL 128, 022501 (2022); Scamps et al., PRC 108 L061602 (2023)

- **Lack such investigations in reactions** (more complex and challenging).

Spin distributions in the MNT reactions $^{40}Ca + {}^{208}Pb$



$$J = S^L + S^H + \Lambda.$$

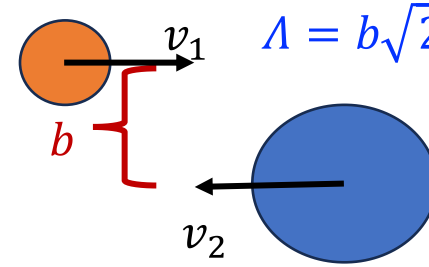
At the beginning, $J = 0 + 0 + \Lambda$

Almost no nucleon transfer

- ✓ The spins are generated.
- ✓ The orbital angular momentum is converted into intrinsic spin.

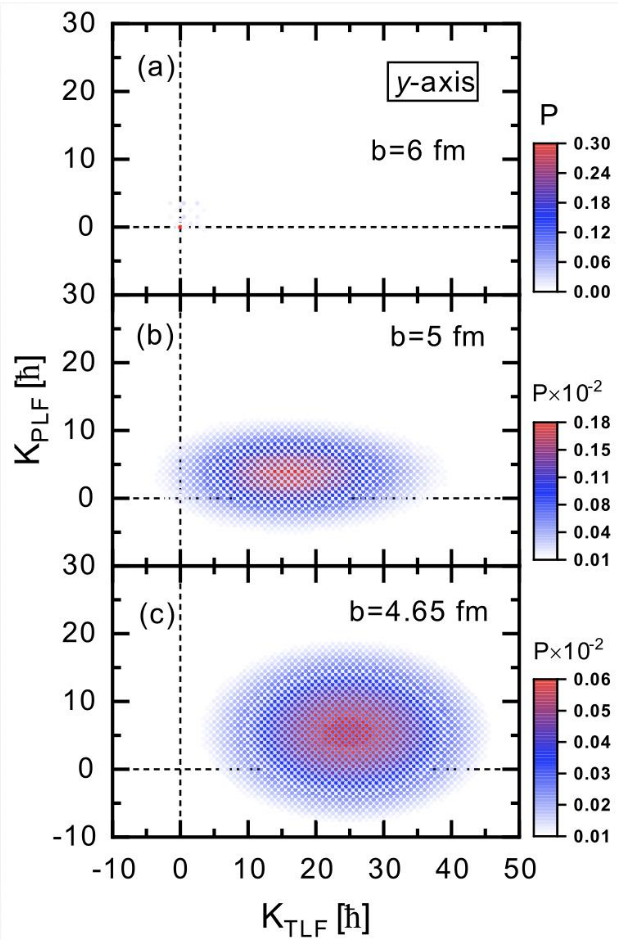
Nucleon transfer

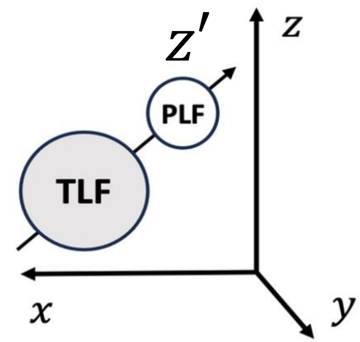
$$\Lambda = b\sqrt{2\mu E_{cm}}$$

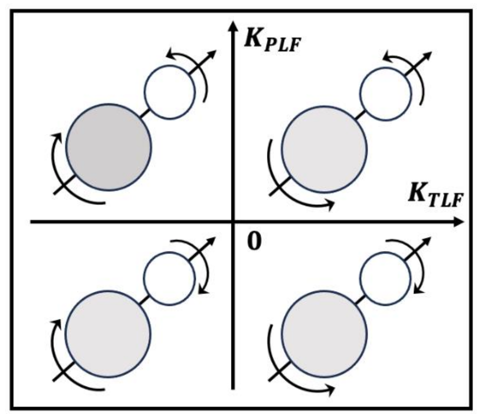


DDZ, Vretenar, Nikšić, Zhao, Meng, PLB 869, 139828 (2025)

The joint spin distribution of two fragments (y-axis)







Joint spin distribution:

$P(K_{\mathrm{PLF}}, K_{\mathrm{TLF}}) = \langle \Psi | \hat{P}_{K_P} \hat{P}_{K_T} | \Psi \rangle.$

$K_{\mathrm{PLF}} K_{\mathrm{TLF}} > 0$, wriggling

$K_{\mathrm{PLF}} K_{\mathrm{TLF}} < 0$, bending

Various collective rotational modes are revealed.

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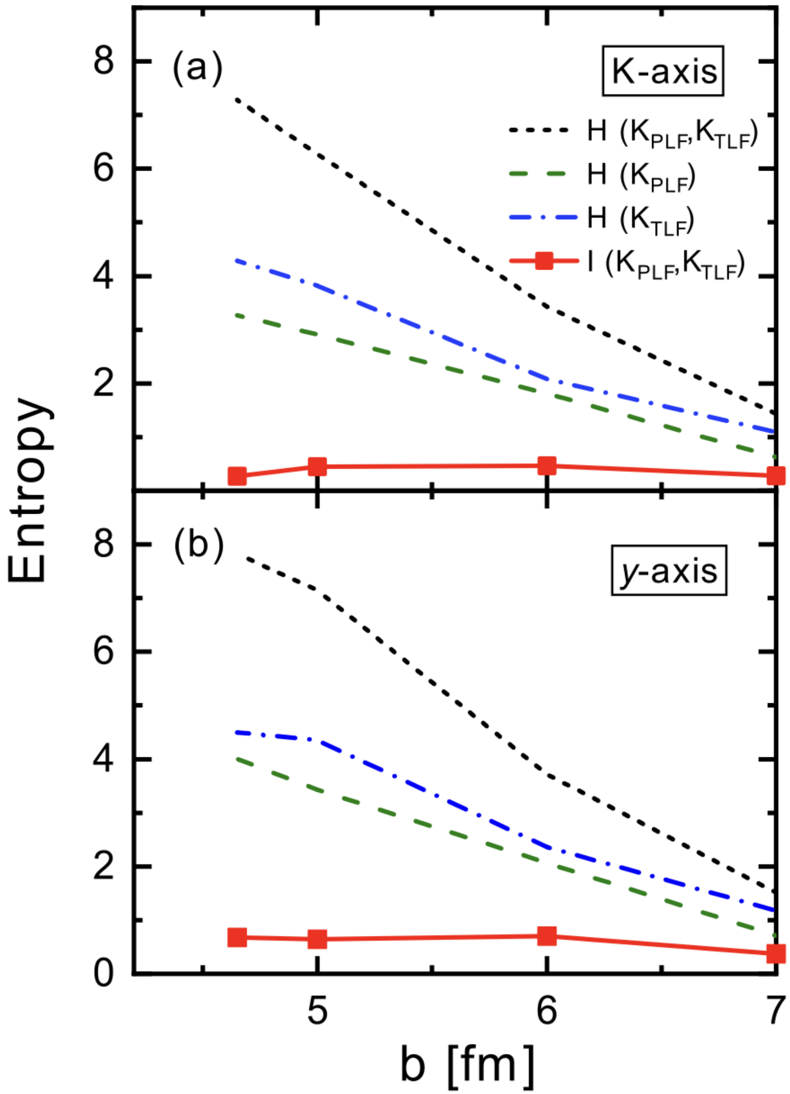
How to quantify the correlations between the two fragments' spins?

The correlations between two fragments



Entanglement Shannon entropy I(A, B)

$$I(A,B) = H(A) + H(B) - H(A,B).$$

$$H(A) = -\sum_{A} P(A)\ln\big(P(A)\big).$$

$$H(A,B) = -\sum_{A,B} P(A,B)\ln\big(P(A,B)\big).$$

The smaller entanglement Shannon entropy indicates fewer correlations.

The spins of the two fragments are correlated, but the correlations are rather weak.

DDZ, Vretenar, Nikšić, Zhao, Meng, PLB 869, 139828 (2025)

Contents

- Introduction
- Relativistic time-dependent density functional theory
- Multinucleon transfer reaction
  - Mass distribution
  - Angular momentum distribution
- Summary and outlook

Summary and outlook

- Relativistic TDDFT is extended to incorporate particle number projection and angular momentum projection, and then applied to the MNT reaction.

  ✓ Mass distribution

  DDZ, Vretenar, Niksic, Zhao, Meng PRC 109, 024614 (2024)
  DDZ, Li, Vretenar, Niksic, Zhao, Meng, PRC 109, 024316 (2024)
  DDZ, Li, Vretenar, Niksic, Zhao, Meng, PRC 114, 014628 (2026)
  Yang, **DDZ**, Vretenar, Li, Niksic, Zhao, Meng, PRC 113, 044626 (2026)

  ✓ Spin distribution

  DDZ, Vretenar, Niksic, Zhao, Meng, PLB 869, 139828 (2025)
  Li, **DDZ**, Vretenar, Niksic, Zhao, Meng, PRL 136, 252502 (2026)

- MNT reaction: What's the candidate reaction condition for the synthesis of new superheavy nuclei and neutron-rich nuclei (U+U, U+Cm, U+Bi, …).

Thanks for your attention!