北京大学
PEKING UNIVERSITY

The 29th International Nuclear Physics Conference
(INPC2025)

May 25-30, 2025, DCC, Daejeon, Korea

Nuclear Structure and Dynamics in Relativistic Density Functional Theory

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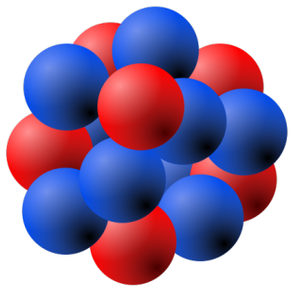
Outline

- Relativistic density functional theory on 3D lattice
- High-order deformation in transfermium nuclei
- Shell Model Like Approach for neutron-proton paring
- ReCD method for nuclear structure and decay properties
- Time-dependent relativistic DFT for nuclear dynamics
- Summary

Relativistic nuclear many-body problem



Schrödinger Equation

$$H|\psi\rangle = (T+V)|\psi\rangle$$

Relativistic QFT

$$L = L_N + L_\sigma + L_\omega + L_{\rm int}$$

Walecka, Ann. Phys., 83, 491 (1974)

Mean-field approximation

1. Mean-field approximation works surprisingly good !
2. Large mean fields *S ≈ -400 MeV, V ≈ 350 MeV*
3. Large spin-orbit splitting *predicts nuclear shell model, no adjustments to spin-orbit force*
4. Relativistic saturation *non-relativistic calculations lead to a collapse*

A Theory of Highly Condensed Matter*

J. D. Walecka

Institute of Theoretical Physics, Department of Physics, Stanford University, Stanford, California 94305

A covariant formulation provides an efficient and comprehensive explanation of observed bulk and single-particle systematics.

Density functional theory

The many-body problem is mapped onto a one-body problem

Hohenberg-Kohn Theorem

The exact ground-state energy of a quantum mechanical many-body system is a universal functional of the local density.

$$E[\rho] = T[\rho] + U[\rho] + \int V(\mathbf{r})\rho(\mathbf{r})\,\mathrm{d}^3\mathbf{r}$$

Kohn-Sham DFT

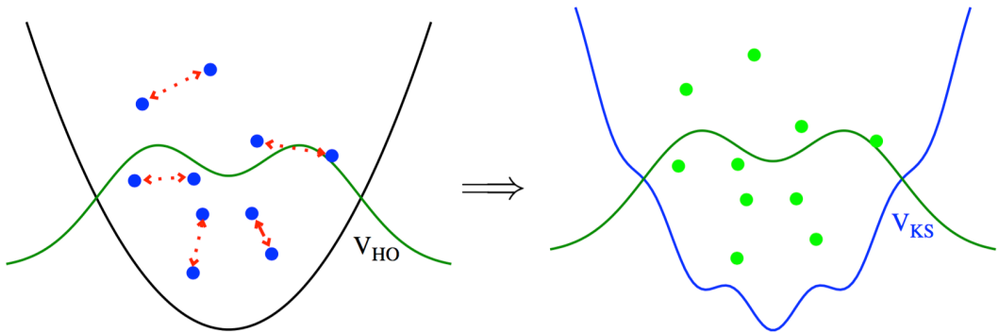


Figure from Drut PPNP 2010

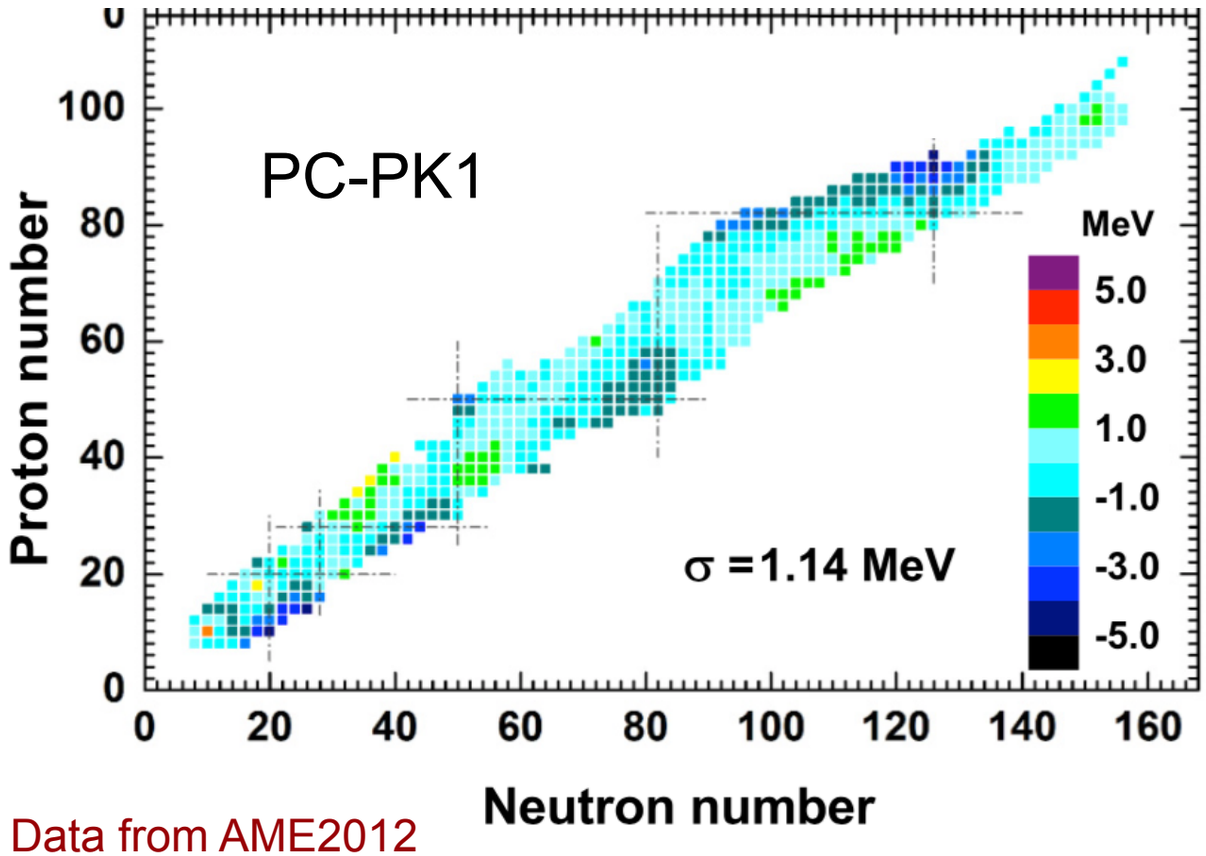
$$T[\rho] \doteq \sum_{i=1}^{N} \left\langle \varphi_i \left| -\frac{\hbar^2}{2m}\nabla^2 \right| \varphi_i \right\rangle$$

$$E[\rho] \Rightarrow \hat{h} = \frac{\delta E}{\delta \rho} \Rightarrow \hat{h}\varphi_i = \varepsilon_i \varphi_i \Rightarrow \rho = \sum_{i=1}^{A} |\varphi_i|^2$$

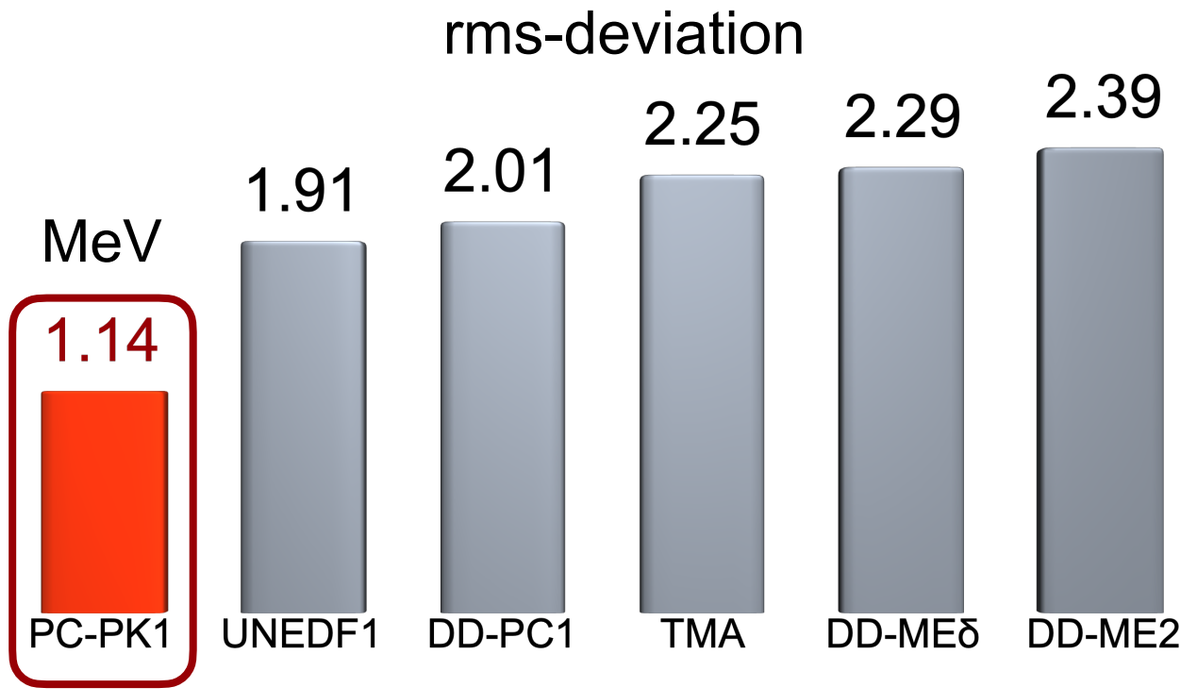
The practical usefulness of the Kohn-Sham theory depends entirely on whether an **Accurate Energy Density Functional** can be found!

Covariant density functional： PC-PK1

Mass Differences: M_{cal} - M_{exp}



Data from AME2012



PWZ, Li, Yao, Meng, PRC 82, 054319 (2010)

Lu, Li, Li, Yao, Meng, PRC 91, 027304 (2015)

http://nuclearmap.jcnp.org

Yang, Wang, PWZ, Li, PRC 104, 054312 (2021)

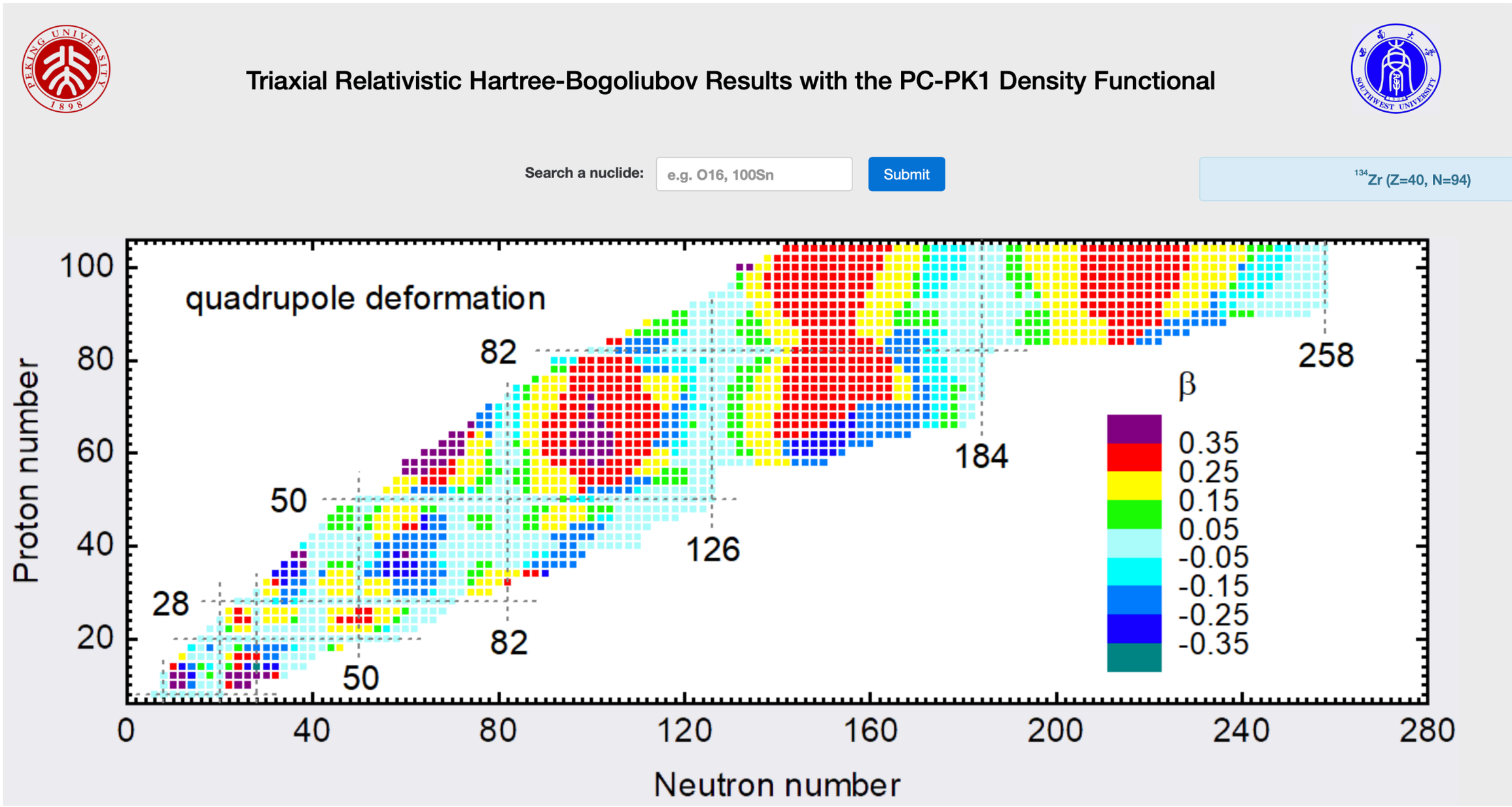
Yang, PWZ, Li, PRC 107, 024308 (2023)

Among the best density-functional description for nuclear masses!

How many nuclei are bound?

http://nuclearmap.jcnp.org/index.html

Triaxial RHB + 5DCH



Yang, Wang, PWZ, Li, Phys. Rev. C 104, 054312 (2021)

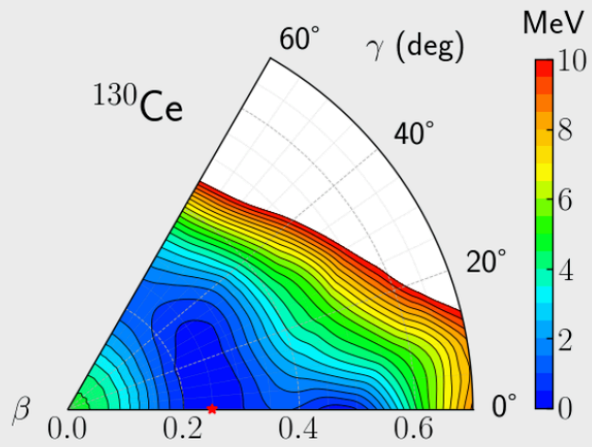
Yang, PWZ, Li, Phys. Rev. C 107, 024308 (2023)

How many nuclei are bound?

http://nuclearmap.jcnp.org/index.html

Triaxial RHB + 5DCH

Results for Cerium 130 (Z=58, N=72)



Potential energy surface calculated by RHB theory with PC-PK1 density functional. All energies are normalized with respect to the binding energy of the absolute minimum. The contours join points on the surface with the same energy, and the energy difference between adjacent contours is 0.5 MeV.

Ground-state properties

Spectroscopy (coming soon)

E_{RHB} = -1079.46 MeV

E_{5DCH} = -1083.50 MeV

E_{exp} = -1083.32 MeV

β = 0.25

γ = 0°

To know the meaning of a quantity, please **hold the mouse still** on it.

Select a nuclide

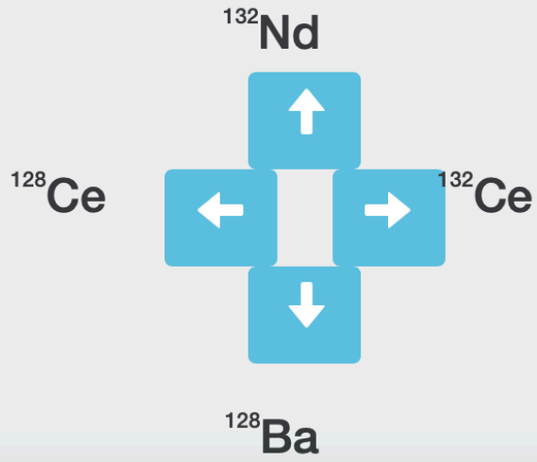
Proton number

0

Neutron number

0

Submit



Yang, Wang, PWZ, Li, Phys. Rev. C 104, 054312 (2021)

Yang, PWZ, Li, Phys. Rev. C 107, 024308 (2023)

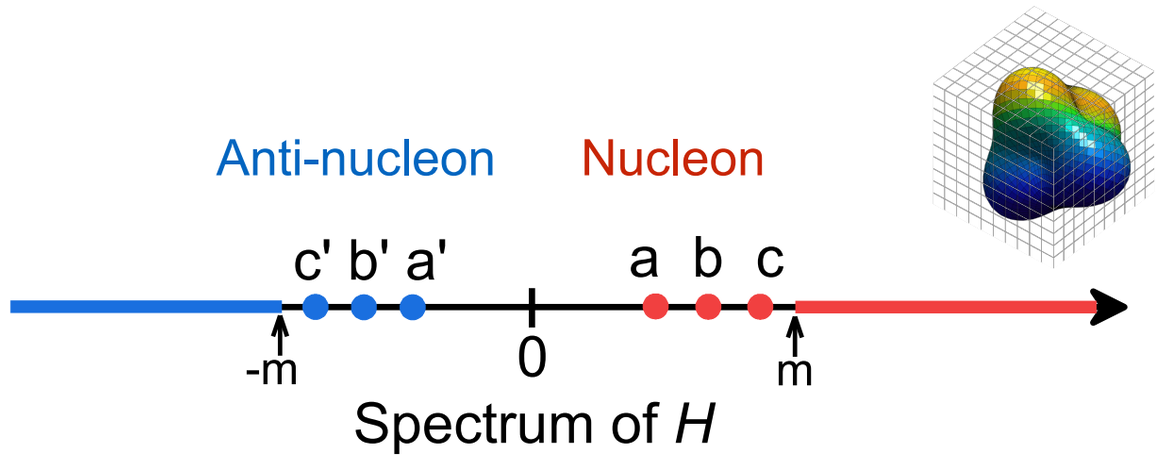
Lattice RDFT

✓ No spatial symmetry restriction

✓ A long-term challenge due to

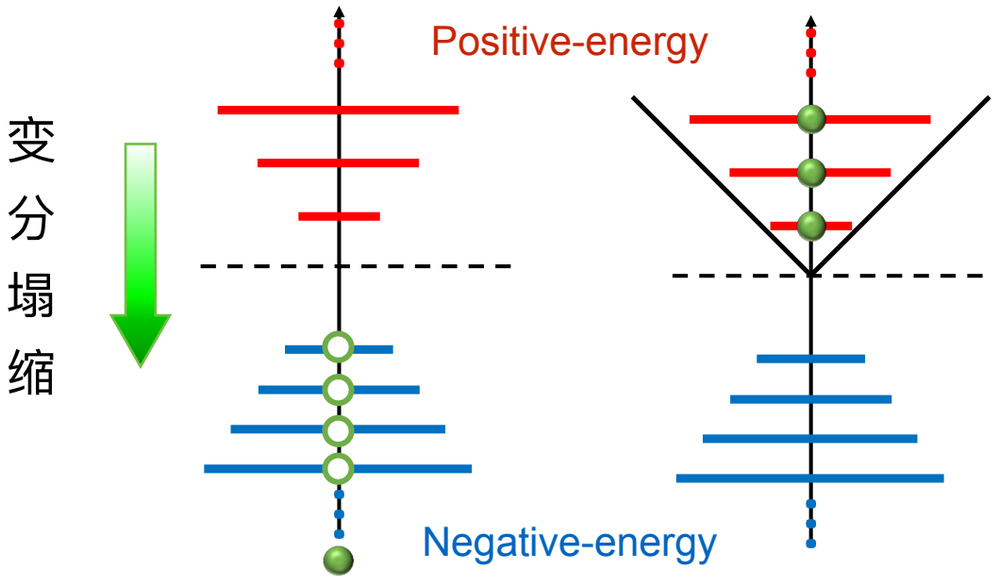
a) variational collapse problem

b) fermion doubling problem



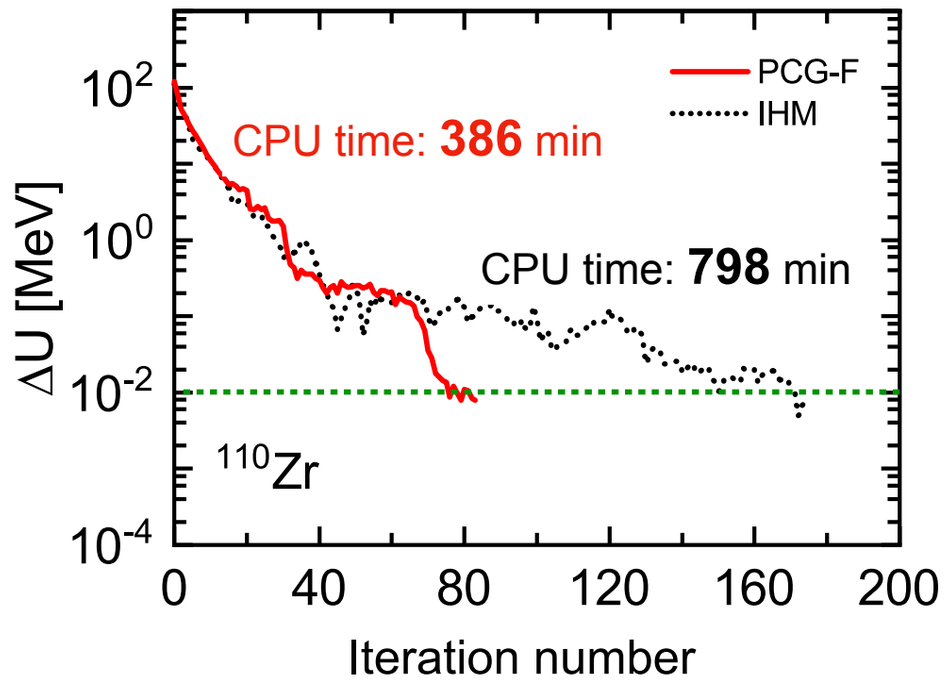
Hagino and Tanimura, PRC 82, 057301 (2010)

PCG-F Method



Li, Ren, **PWZ**, PRC 102, 044307 (2020)

PCG-F saves **~52%** of the CPU time



Xu, Li, Ren, **PWZ**, PRC 109, 014311 (2024)

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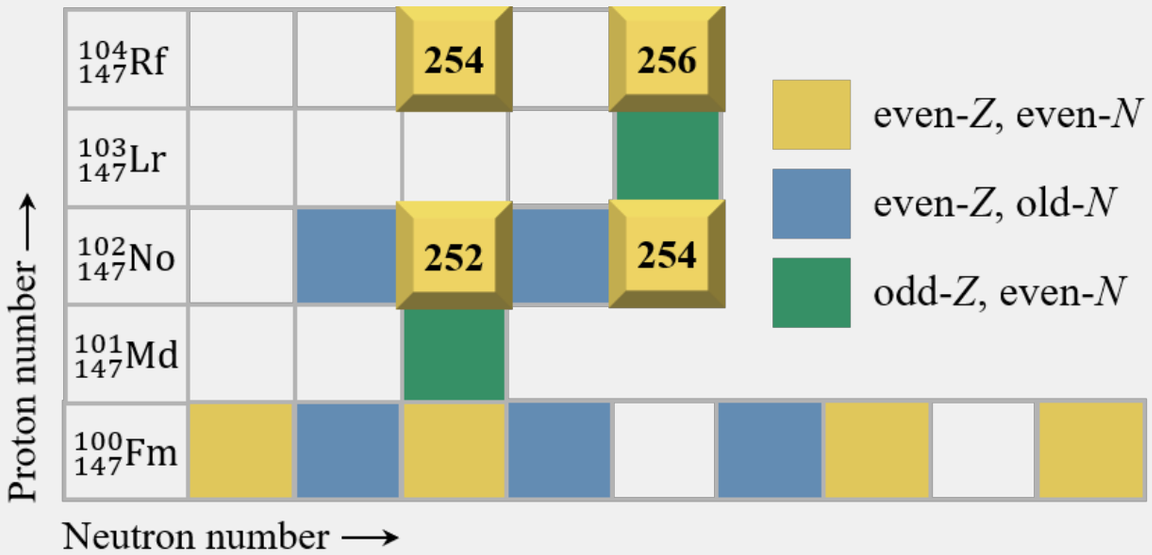
Rotating transfermium nuclei

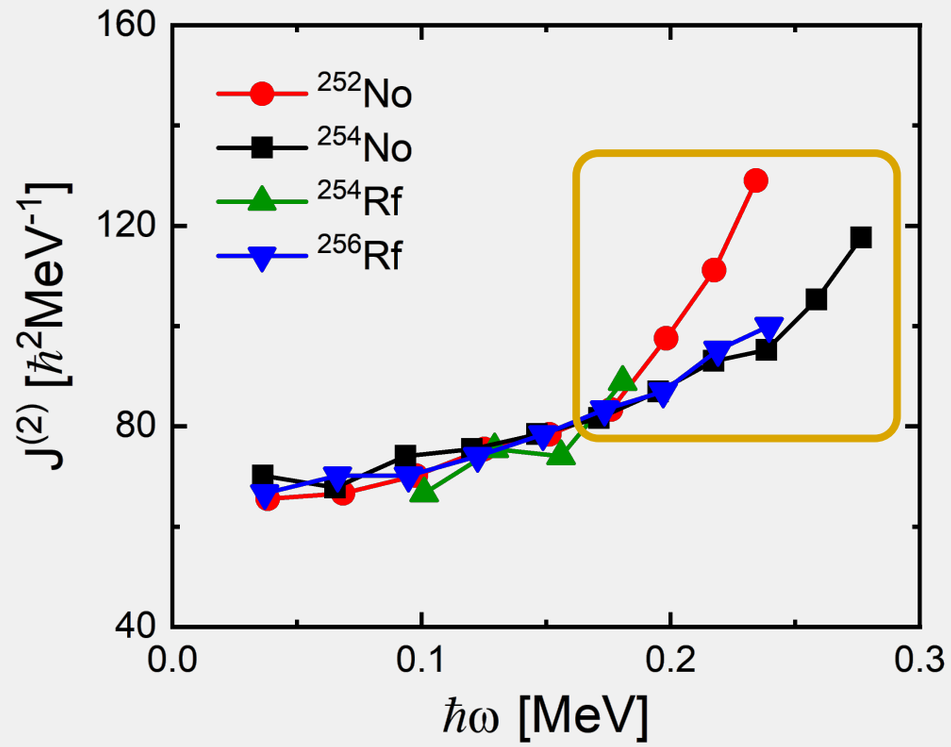
- **Transfermium nuclei** are the heaviest ones, whose rotational spectra have been measured experimentally; important for the location of the **“island of stability”**.

Herzberg, Greenlees, Prog. Part. Nucl. Phys. 61, 674 (2008); Ackermann, Theisen, Phys. Scr. 92, 083002 (2017)

ANL、FLNR、GANIL、GSI、JAEA、JYFL ...



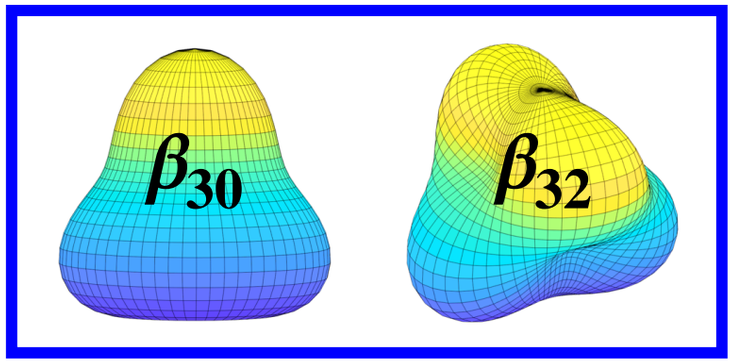
PRL 82, 509 (1999) PRL 85, 1198 (2000) PRL 89, 202501 (2002)
PRL 95, 102502 (2005) PRL 95, 032501 (2005)
PRL 97, 082502 (2006) PRL 98, 132503 (2007)
PRL 102, 212501 (2009) PRL 109, 102501 (2012)
...

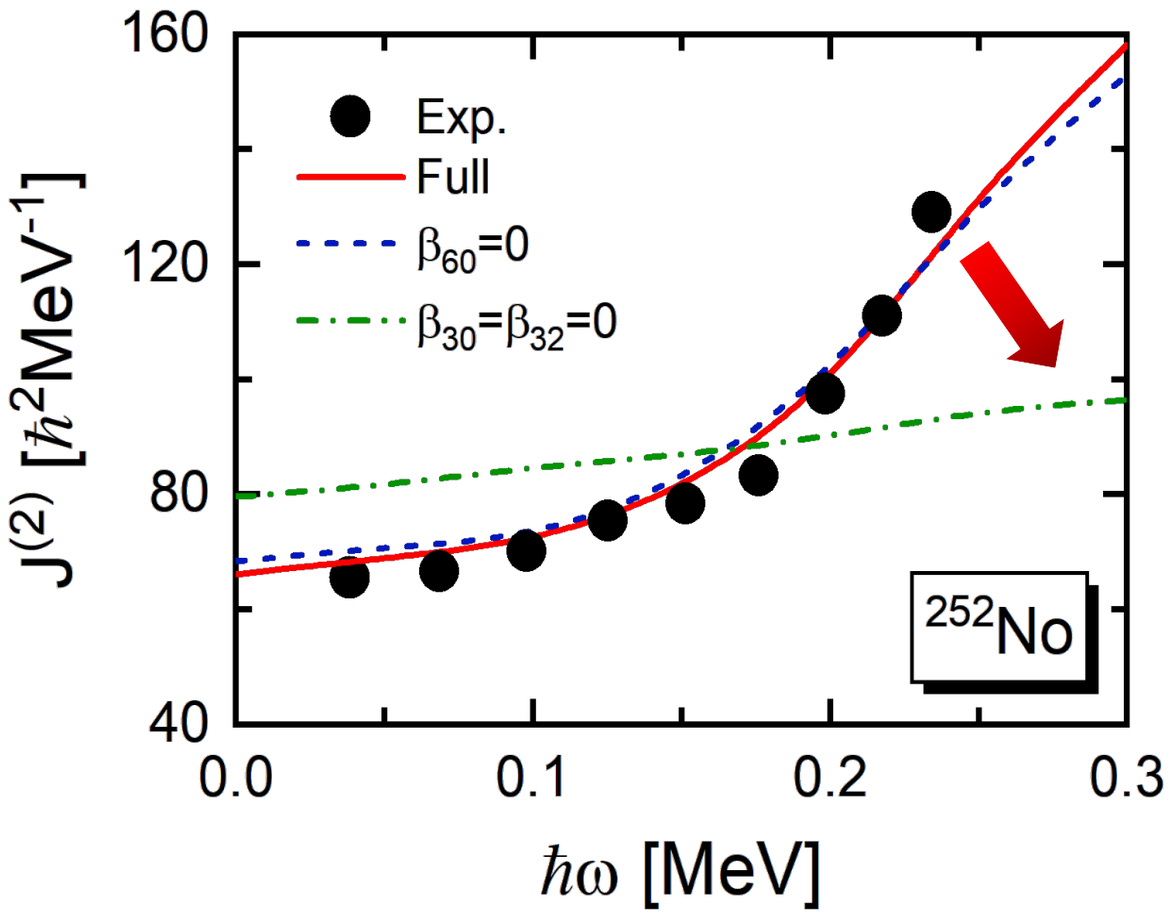


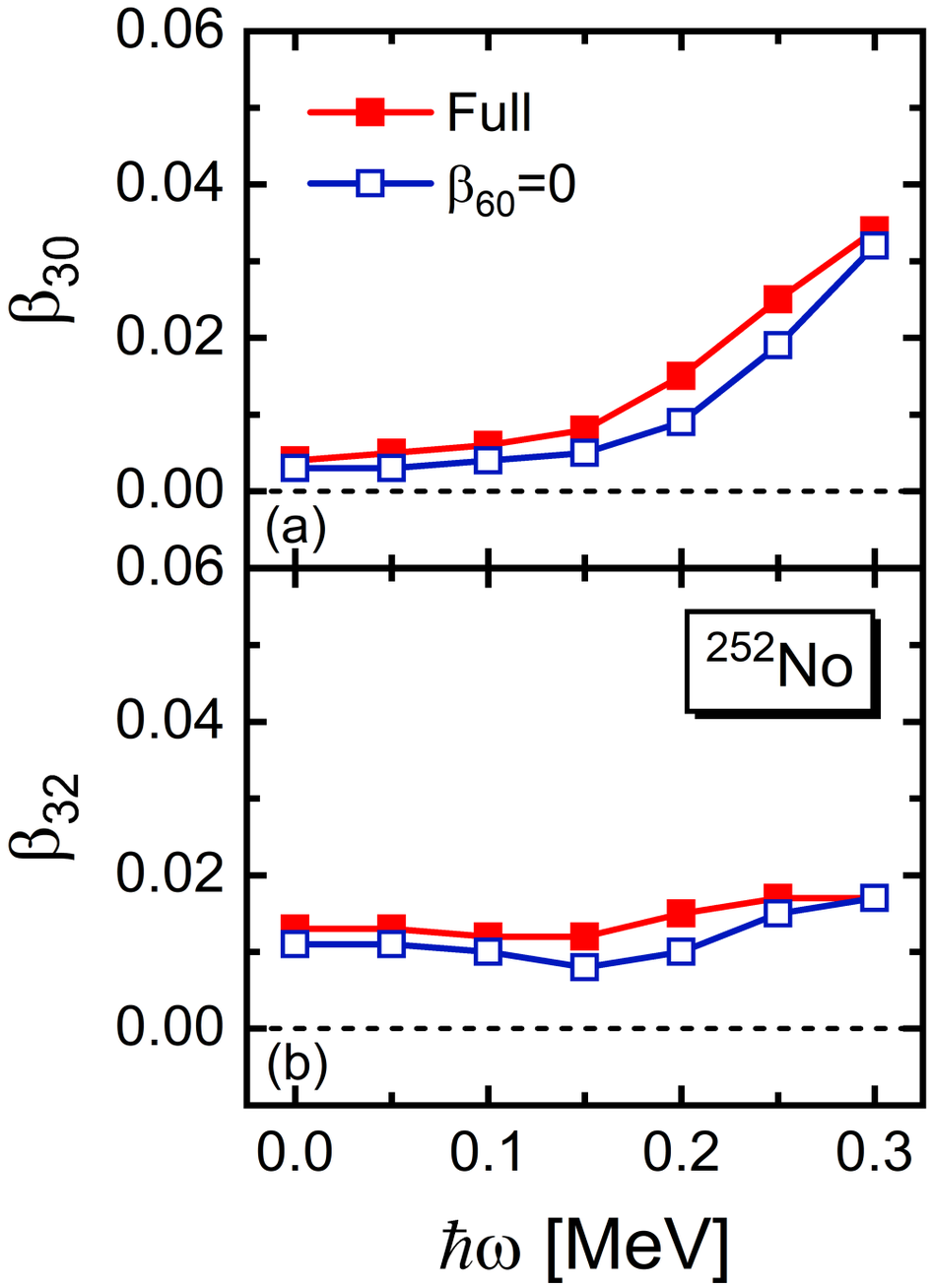
PRL 82, 509 (1999) PRL 109, 102501 (2012)
PRC 65, 014303 (2001) PRC 107, L061302 (2023)

The physical mechanism of the abnormal behavior in ^{252}No and ^{254}No?

High-order deformation in ^{252}No



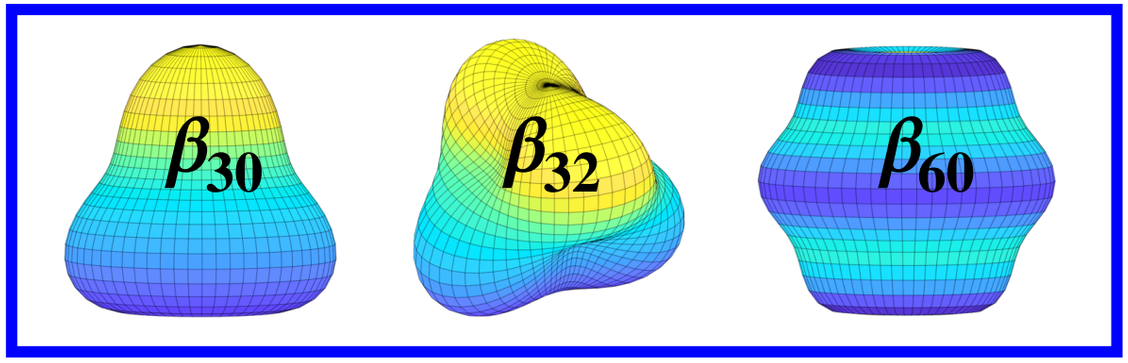


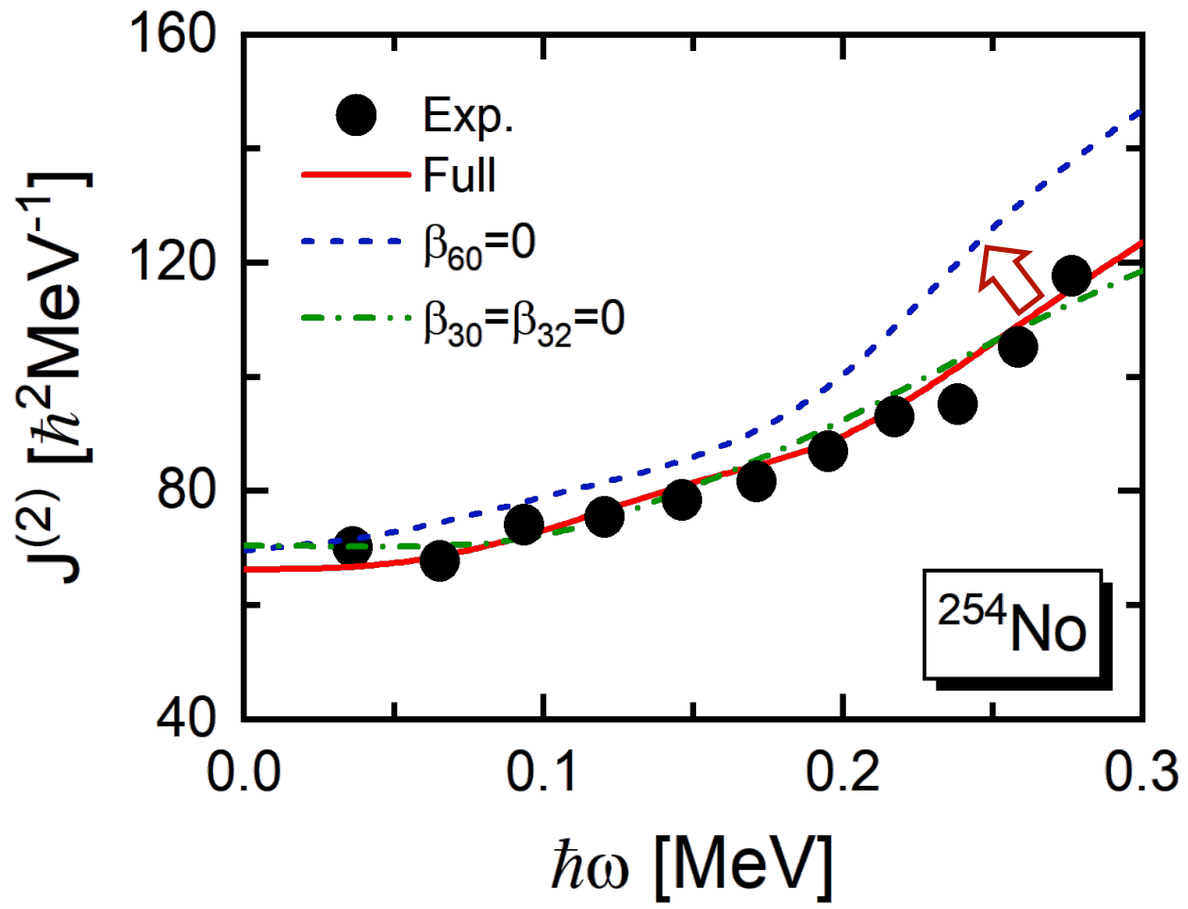


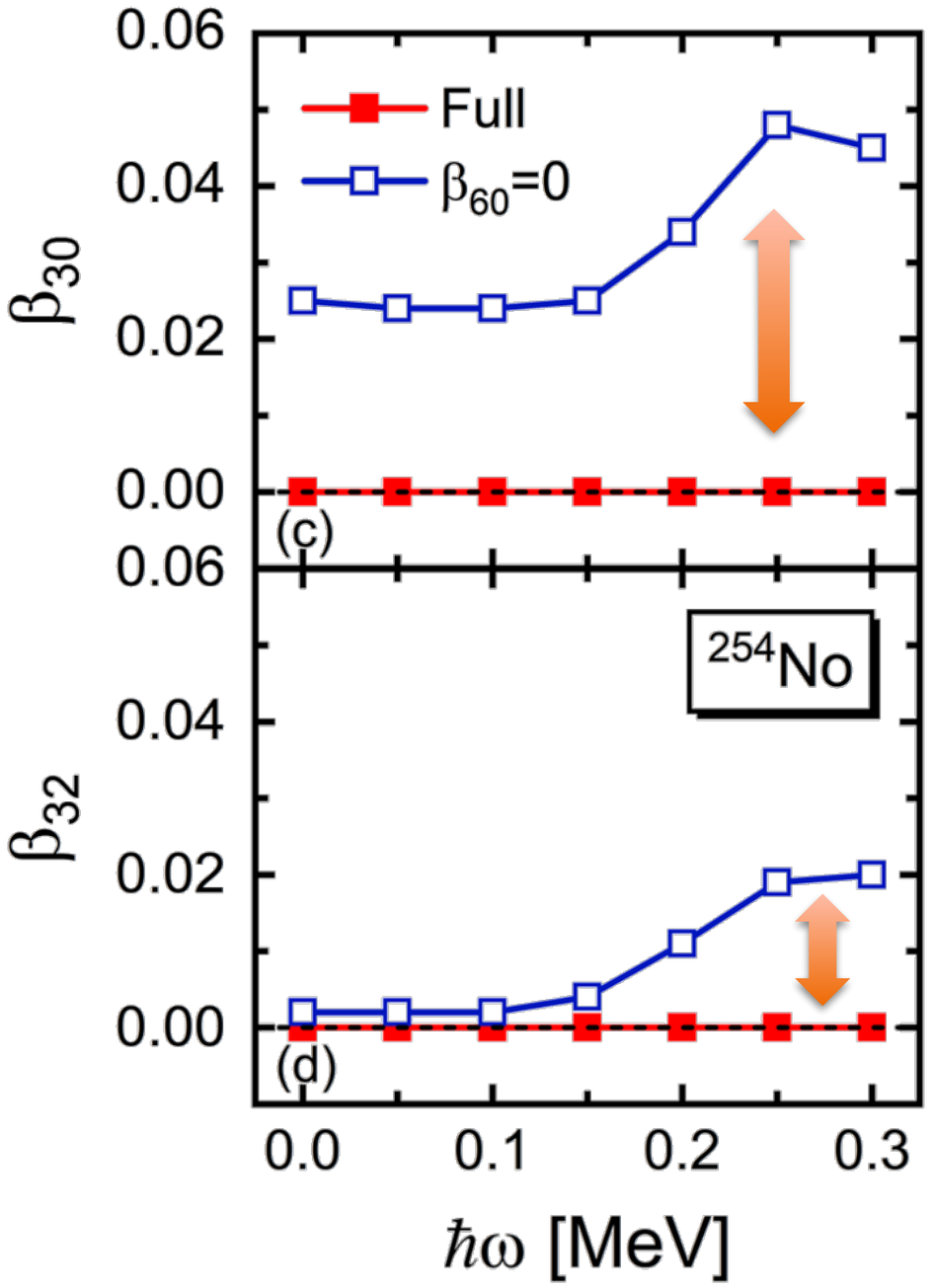
Xu, Wang, Wang, Ring, **PWZ**, PRL 133, 022501 (2024)

Octupole deformation is responsible for the upbending in ^{252}No.

High-order deformation in ^{254}No







Xu, Wang, Wang, Ring, **PWZ**, PRL 133, 022501 (2024)

Octupole and β_{60} deformations are coupled with each other in ^{254}No.

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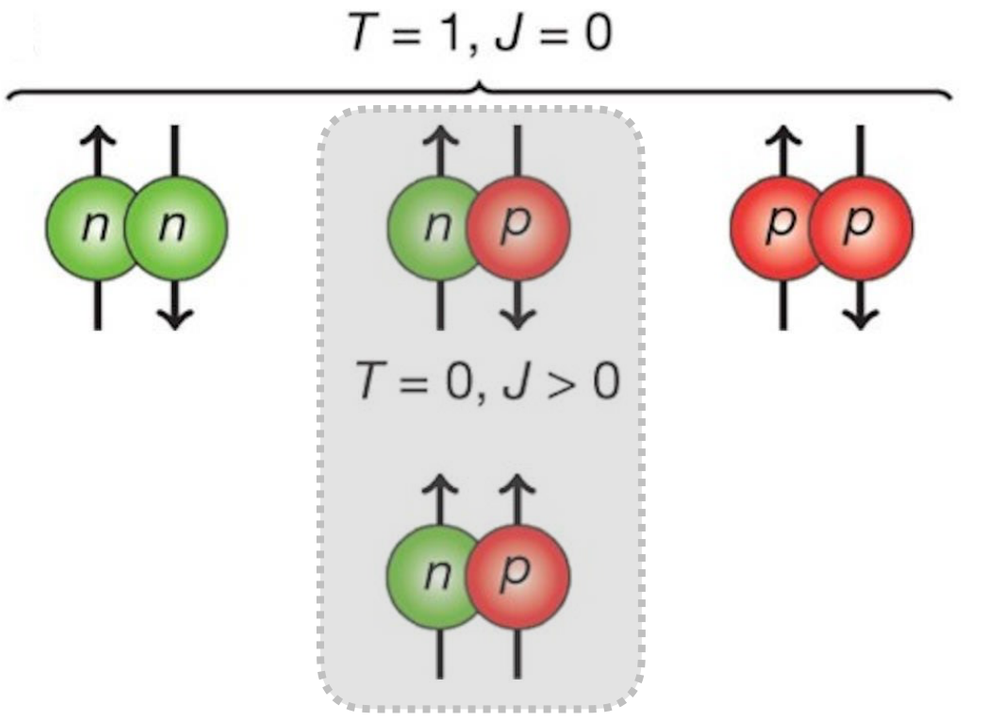
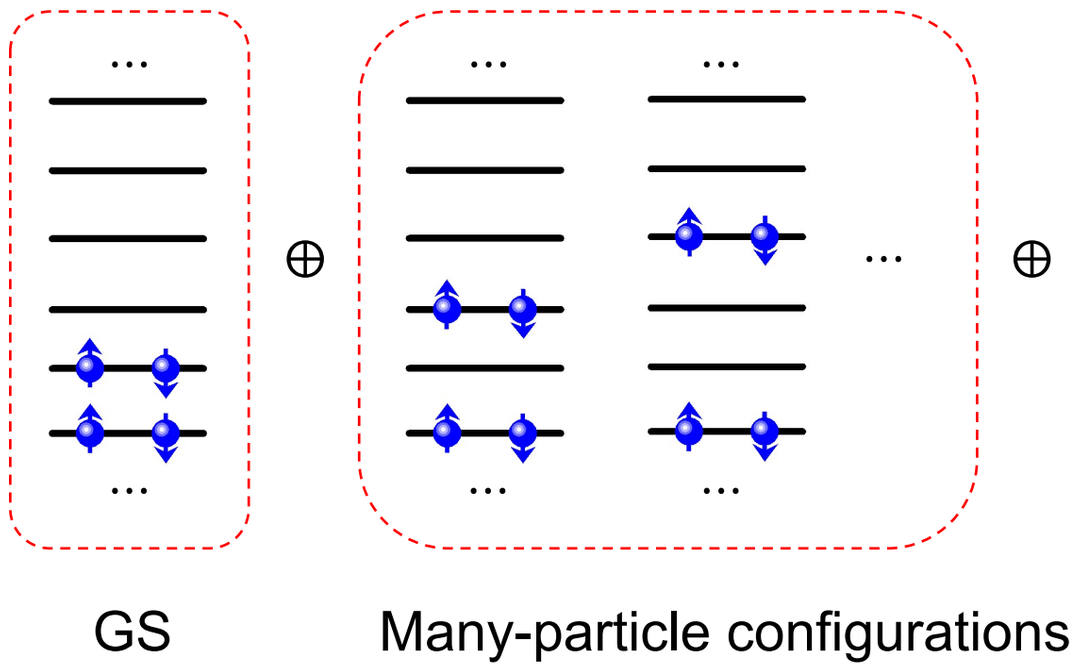
Pairing correlations in nuclei

- **Pairing correlations** are widely observed, particularly between NN and PP pairs.
- Experimental identification of **neutron–proton pairing** remains an open challenge.
- BCS/Bogoliubov method: variational quasiparticle vacuum, **particle number violation**
- Shell-model like approach (SLAP): configuration mixing, **particle number conservation**



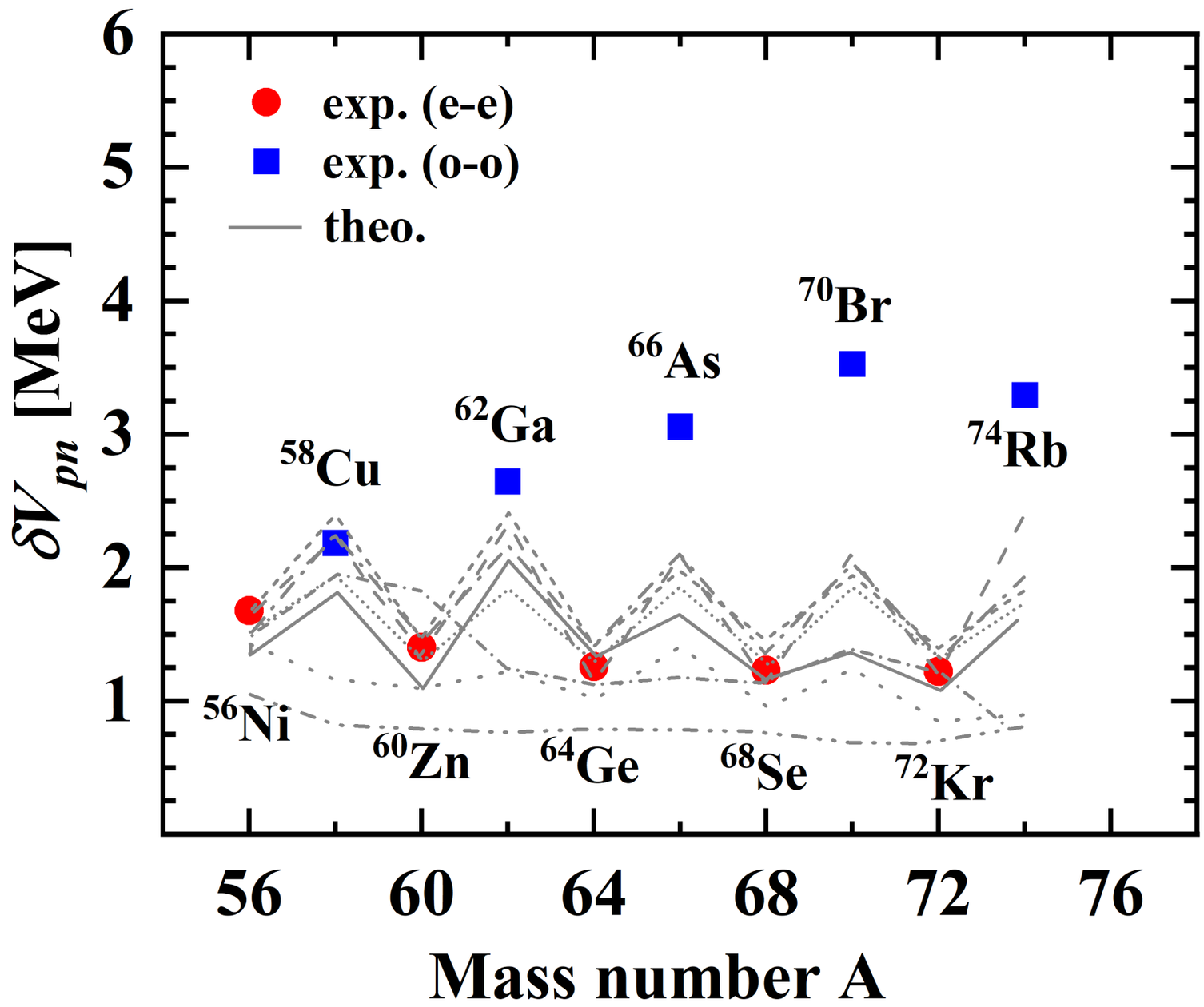


Wang, Wang, Xu, **PWZ**, Meng, PRL 132, 232501 (2024)

RDFT+SLAP: NN, PP, and NP pairing are treated simultaneously, microscopically, and self-consistently.

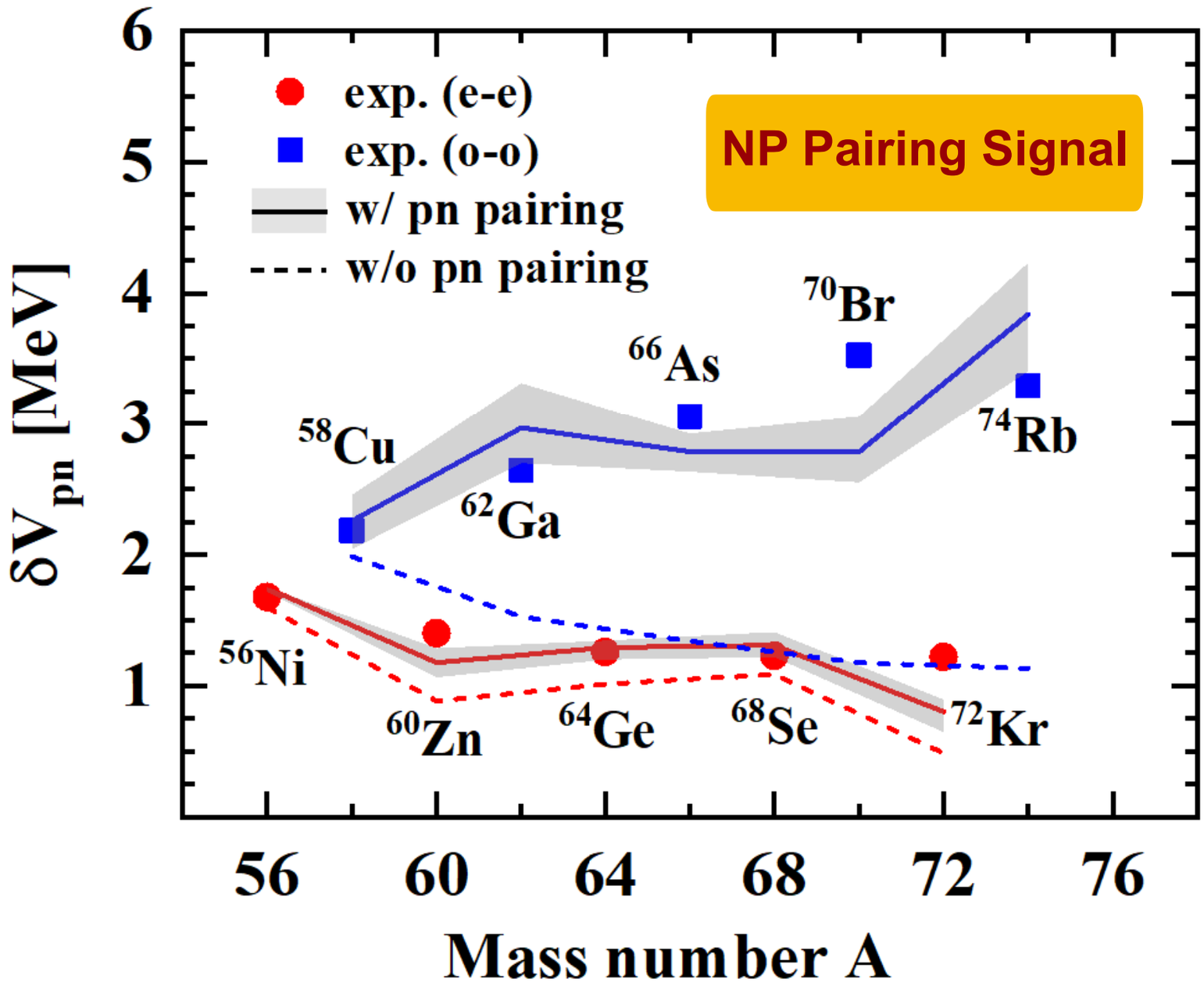
New mass measurement of upper fp-shell nuclei

This bifurcation in the double binding energy differences δV_{pn} cannot be reproduced by existing mass models.



Exp: M. Wang et al., PRL 130, 192501 (2023)

New mass measurement of upper fp-shell nuclei

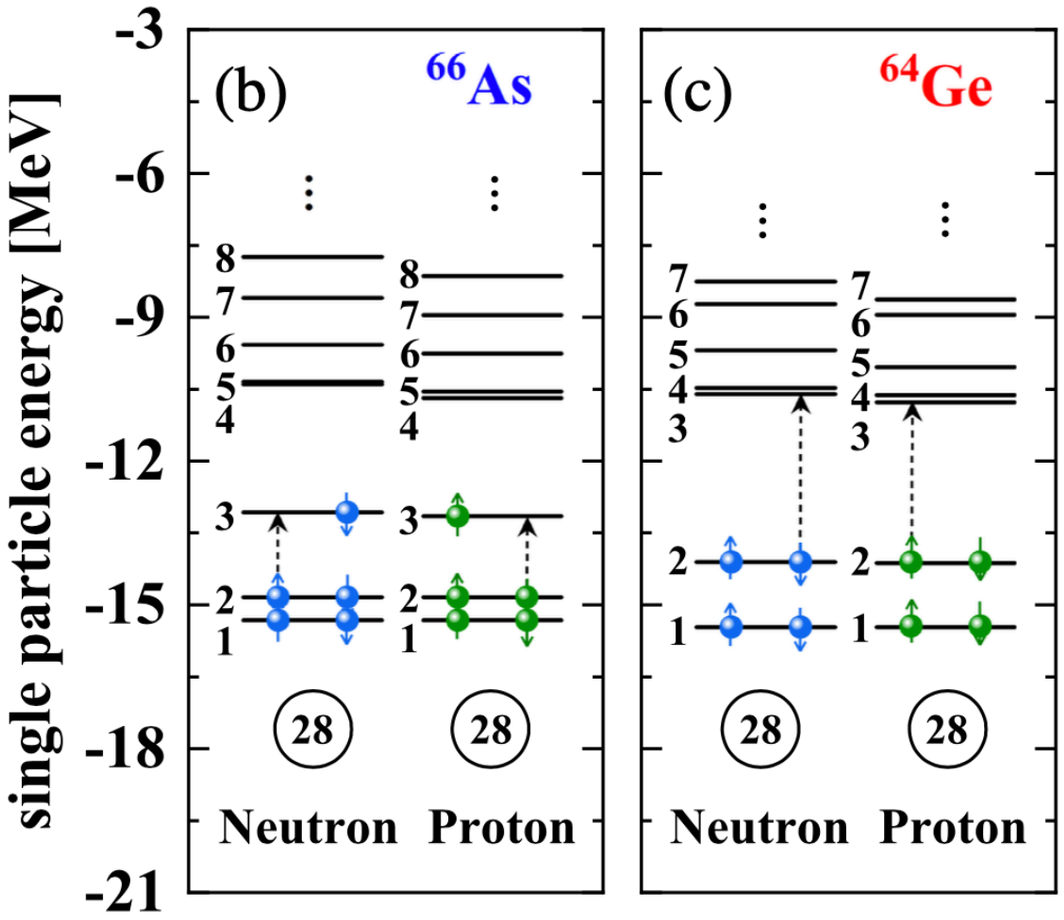


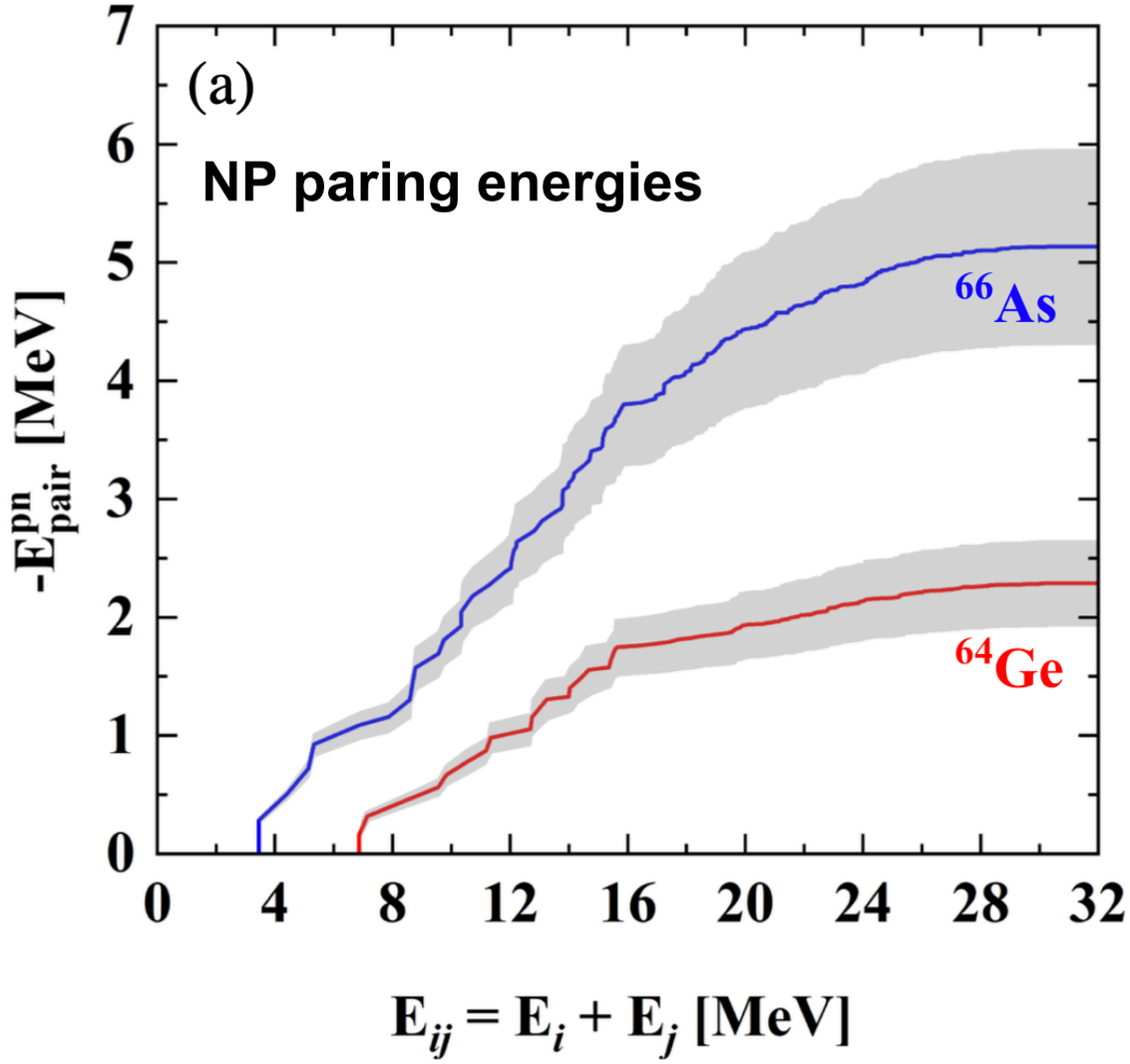
Exp: M. Wang et al., PRL 130, 192501 (2023)

Wang, Wang, Xu, **PWZ**, Meng, PRL 132, 232501 (2024)

NP pairing: odd-odd vs even-even

NP pairing is stronger in odd-odd nuclei than in the even-even ones.





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The ReCD Method

Relativistic **C**onfiguration-interaction **D**ensity functional theory (ReCD)

a theory combining the advantages from both Shell model and DFT

1. **Covariant Density Functional Theory**
   a minimum of the energy surface
2. **Configuration space**
   multi-quasiparticle states
3. **Angular momentum projection**
   rotational symmetry restoration
4. **Shell model calculation**
   configuration mixing / interaction from CDFT

Energy Density Functional

good angular momentum;
from low- to high- spin;

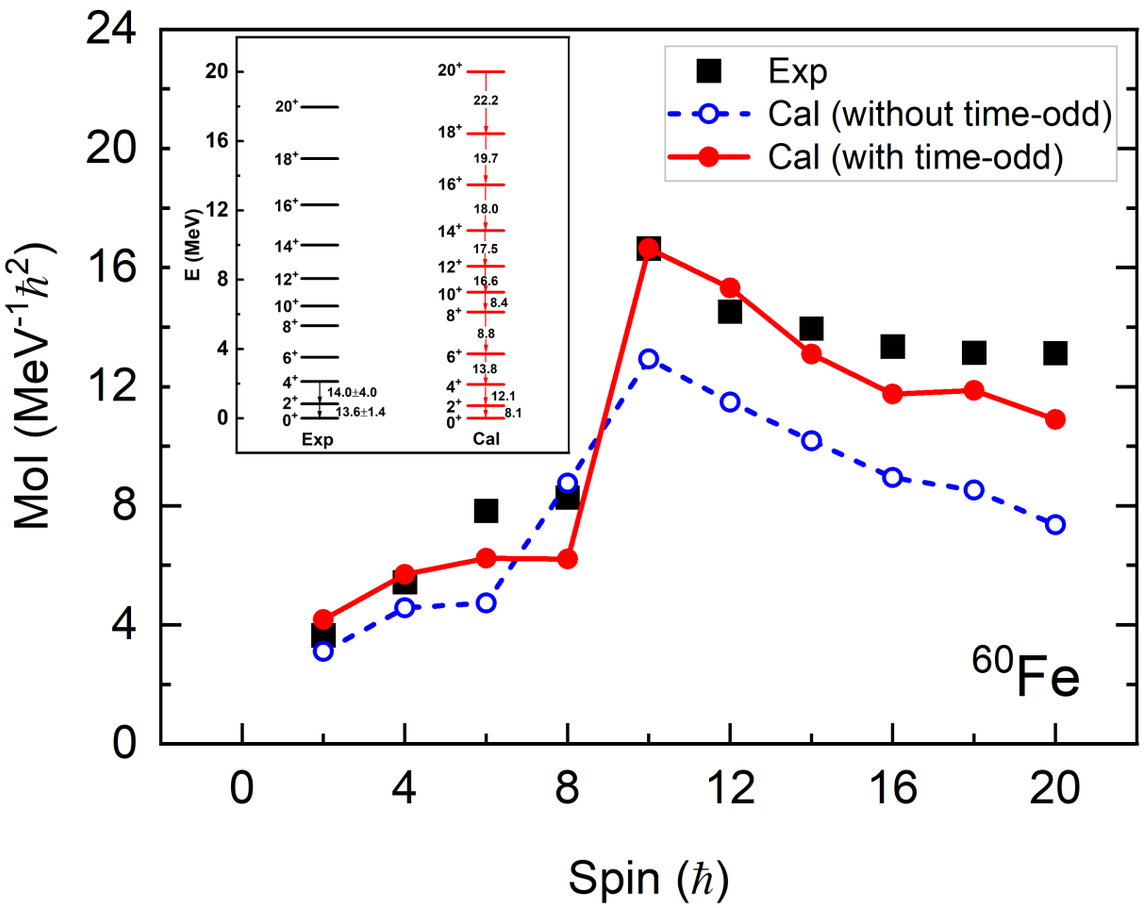
Nuclear Spectroscopy

PWZ, Ring, Meng, PRC 94 (2016) 041301(R)

to provide a global study of nuclear structure and decay properties with no parameters beyond a well-established density functional.

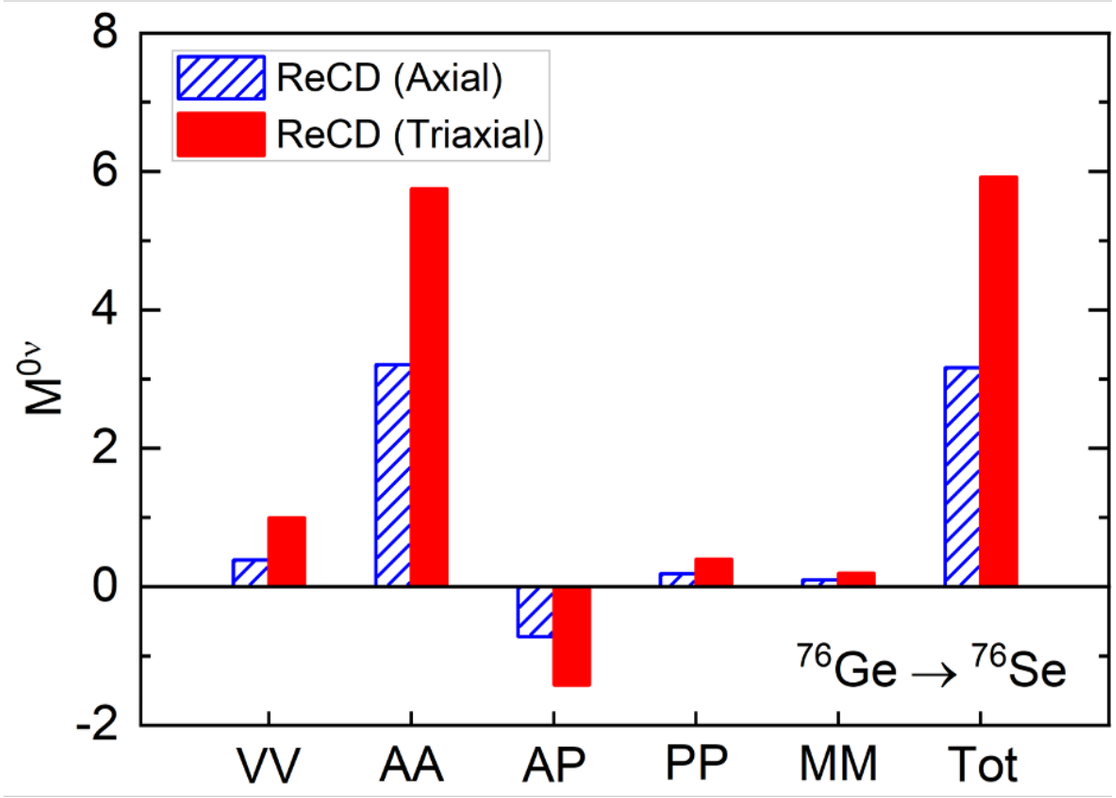
Applications of the ReCD method

Kinetic moment of inertia



Wang, PWZ, Meng, PRC 105 (2022) 054311

Neutrinoless double beta-decay



Wang, PWZ, Meng, Science Bulletin 59 (2024) 2017-2020

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Time-dependent RDFT

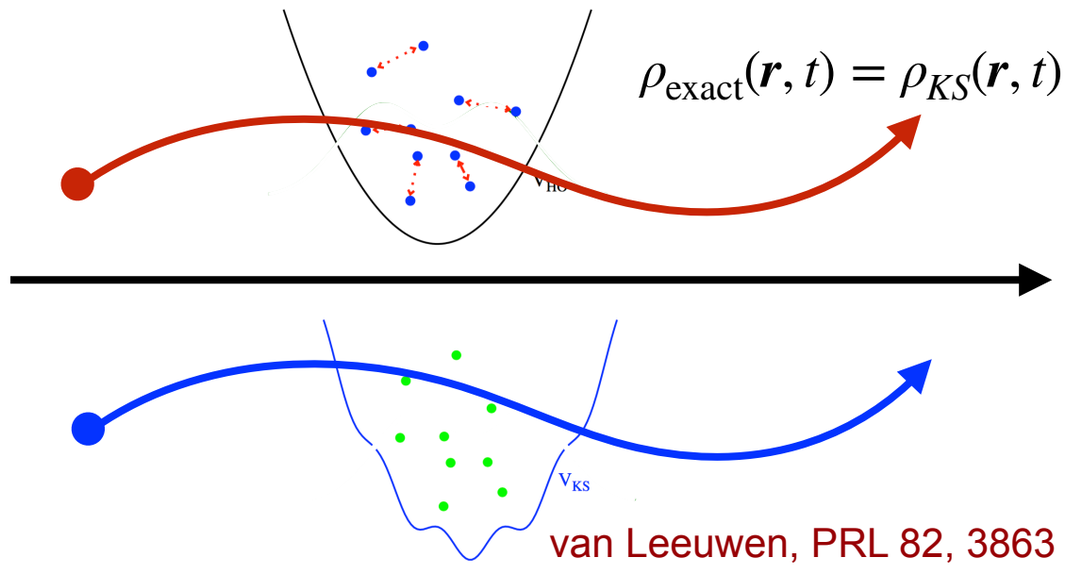
The many-body problem is mapped onto a one-body problem!

Runge-Gross Theorem

There is a unique mapping between the time dependent external potential and the density, for many body systems evolving from a given initial state.

Runge and Gross, PRL 52, 997 (1984)

Time-dependent Kohn-Sham DFT



van Leeuwen, PRL 82, 3863 (1999)

Ren, **PWZ**, Meng, PLB 801,135194 (2020)

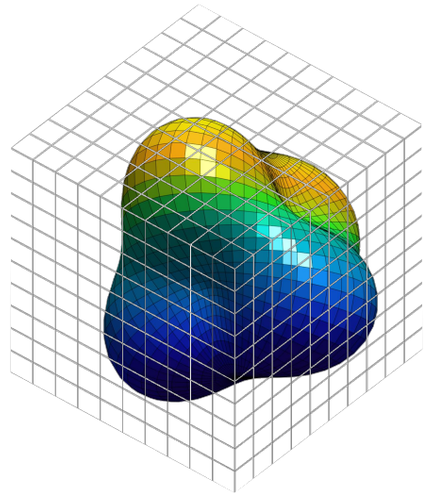
$$i\partial_t \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} m + V + S & \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} & -m + V - S \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}$$

$$\rho(\boldsymbol{r},t) = \sum_i^N f_i^2 + g_i^2$$

$V[\rho](\boldsymbol{r},t)$ No memory effects !

Applications of the TD-RDFT

3D Lattice: no spatial symmetry restriction



✓ Applications include:

Linear alpha-chain PRL 115, 022501 (2015) PLB 801,135194 (2020)

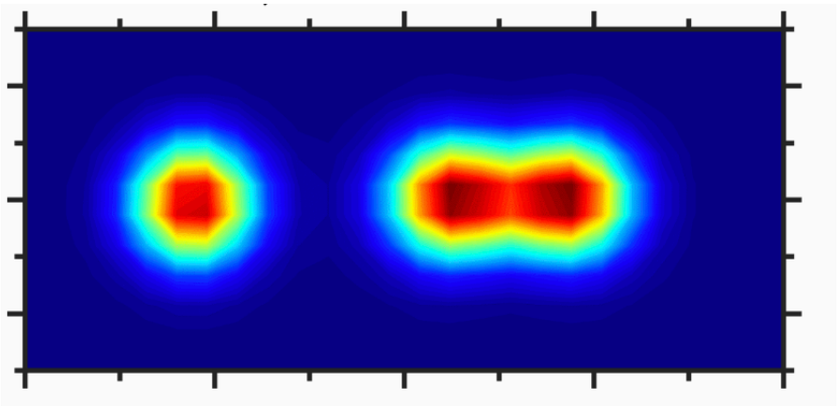
Nuclear fission PRL 128, 172501 (2022) PRC 111, L051302 (2025)

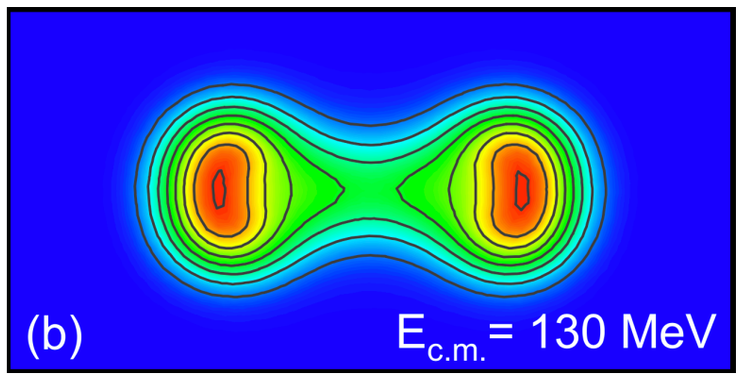
Chiral dynamics PRC 105, L011301 (2022) PLB 856, 138877 (2024)

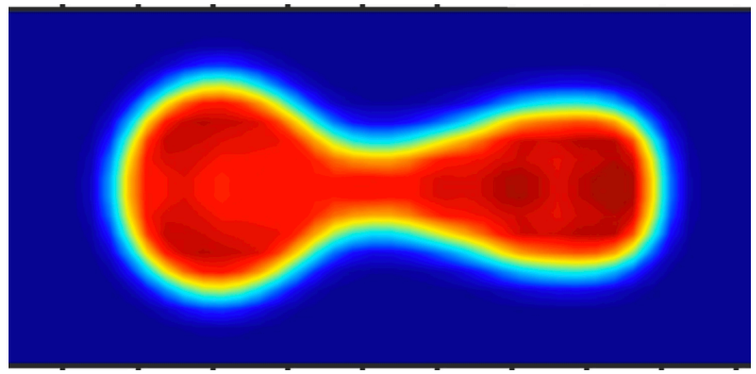
Nuclear reaction PRC 102, 044603 (2020) PRC 109, 024614 (2024) PRC 109, 024316 (2024)

Editors' Suggestion

…





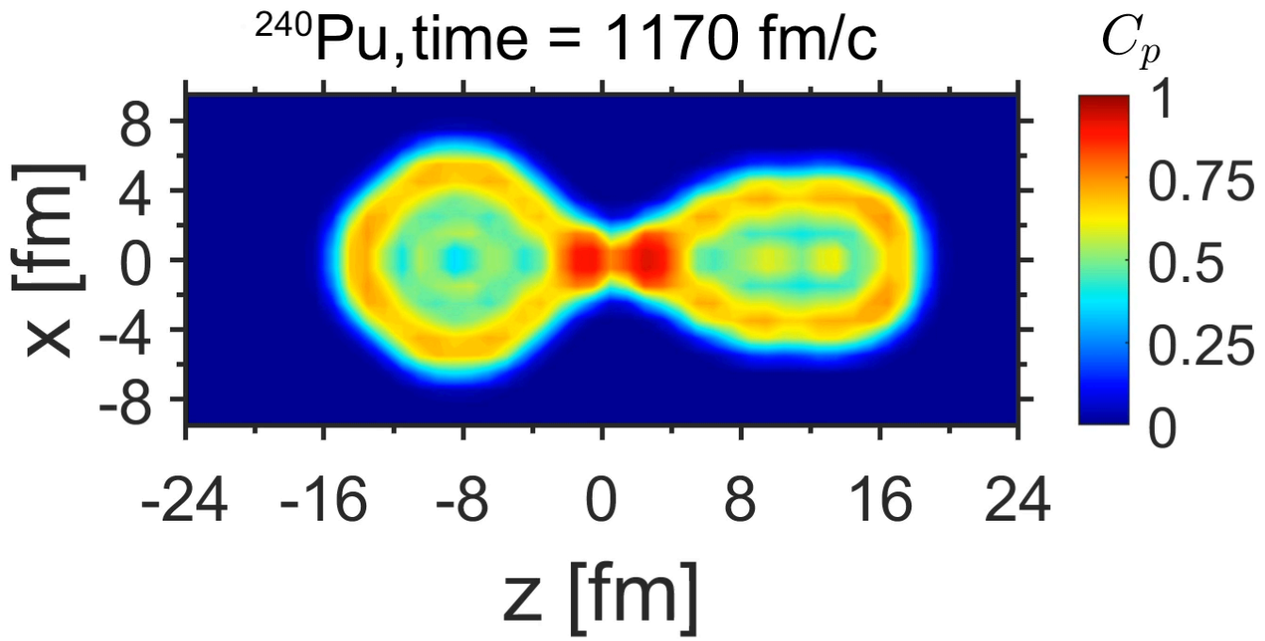


Nuclear fission dynamics

How do heavy nuclei split into two or more fragments?

Scission Mechanism :

- Geometrical definitions
- Nuclear forces / Coul. forces
- Statistical scission-point model
- Random neck rupture model
- Quantum localization method
- ...



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

New mechanism: *neck ruptures between two alpha-like clusters.*

Opens exciting possibilities for a microscopic study of ternary fission.

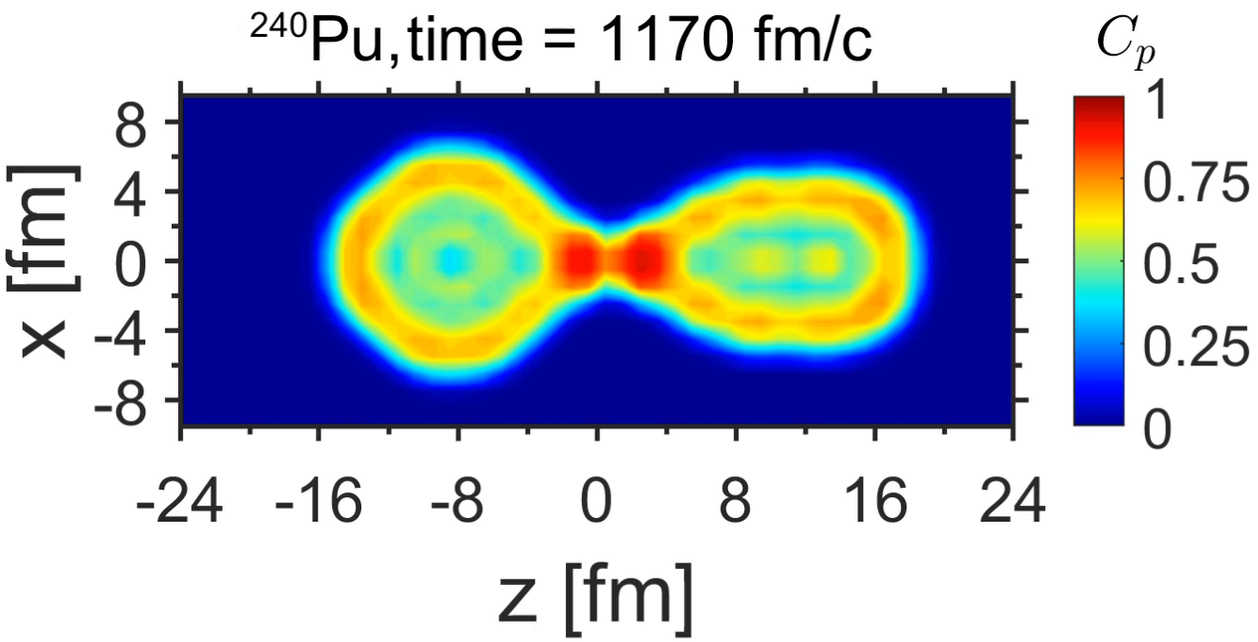
Nuclear fission dynamics

How do heavy nuclei split into two or more fragments?

Scission Mechanism :

- Geometrical definitions
- Nuclear forces / Co…
- Statistical sci… …int model
- Rando… …upture model
- … localization method
- …

Ternary fission NOT explained !



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

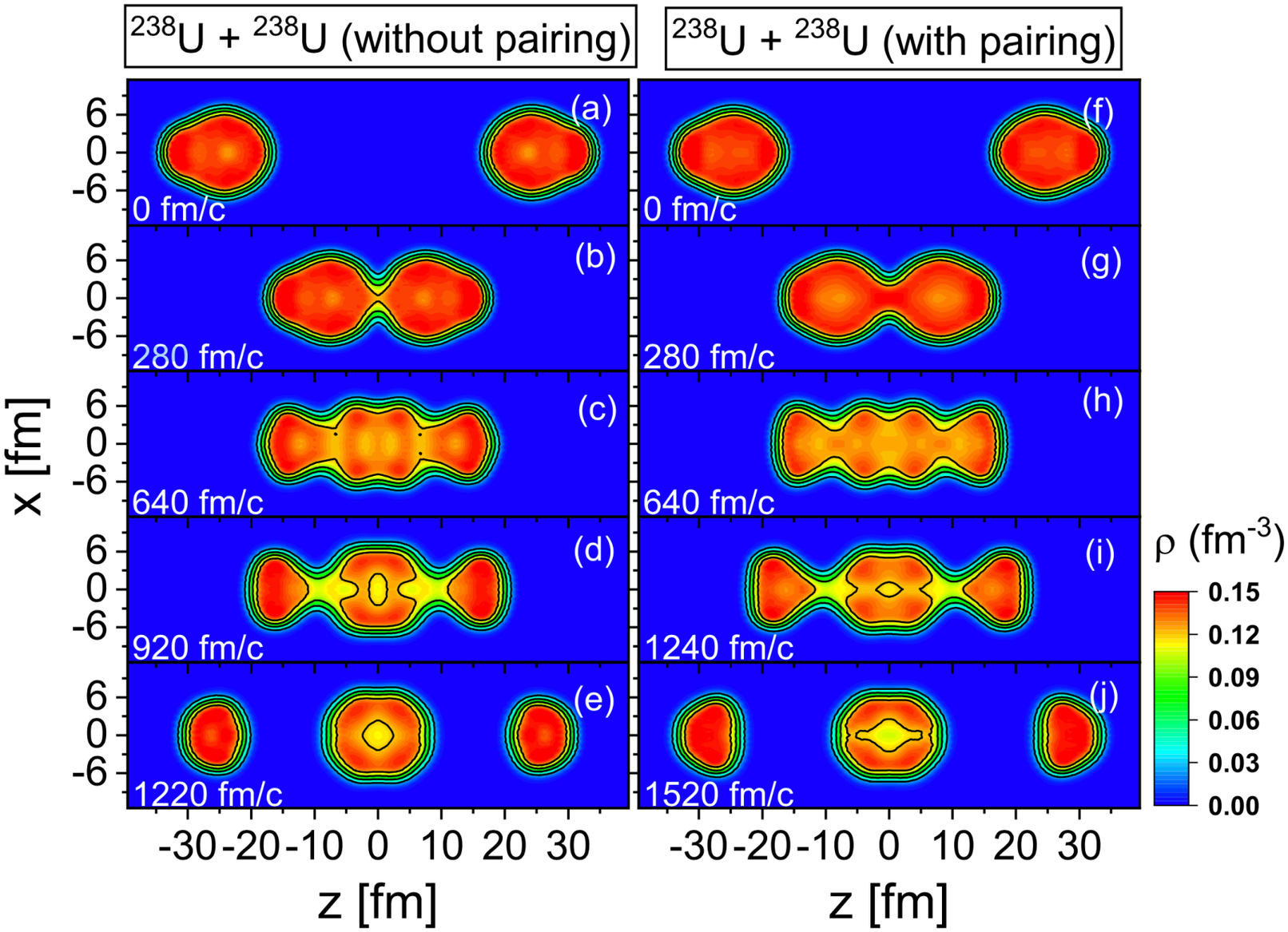
New mechanism: *neck ruptures between two alpha-like clusters.*

Opens exciting possibilities for a microscopic study of ternary fission.

Ternary quasifission

Editors' Suggestion

Zhang, Li, Vretenar, Nikšić , Ren, **PWZ**, Meng, PRC, 109, 024316 (2024)



The formation of very heavy neutron-rich systems; potentially interesting for the synthesis of superheavy elements.

Summary

Relativistic density functional theory (RDFT) has been solved in 3D lattice and extended to its time-dependent version for various nuclear structure and dynamics.

- Nuclear landscape with PC-PK1

  good performance for nuclear global properties

- High-order deformation in transfermium nuclei

  octupole deformation effects

  coupling between the octupole and β_{60} deformation

- Abnormal bifurcation of δVpn: signal of the np pairing correlations

- Nuclear fission dynamics

  new scission mechanism: neck ruptures between two alpha-like clusters

  tail-to-tail collisions of U-238 could form very heavy neutron-rich systems

Thank you.

Collision of two ^{238}U nuclei

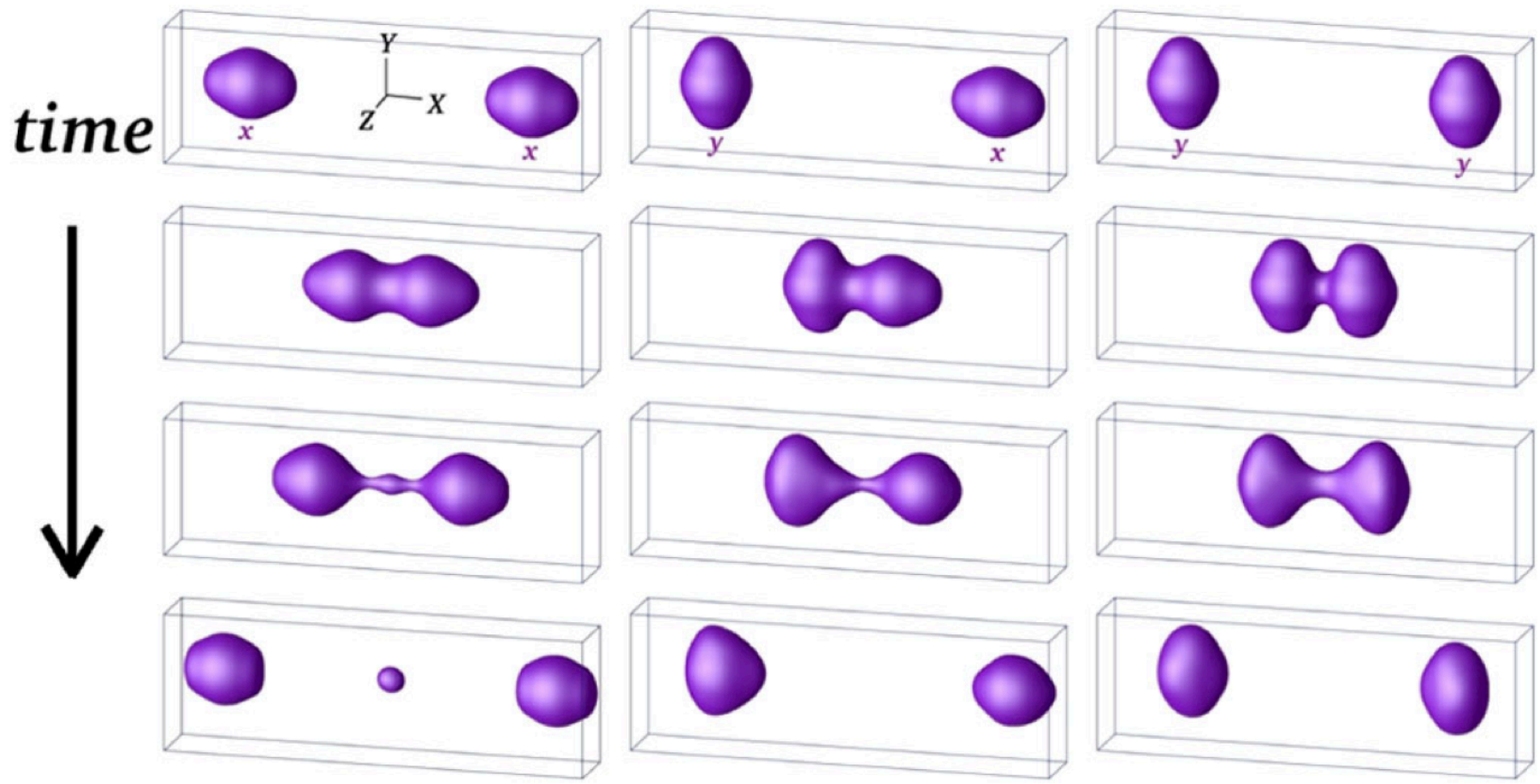
PRL **103,** 042701 (2009) PHYSICAL REVIEW LETTERS week ending 24 JULY 2009

Collision Dynamics of Two ^{238}U Atomic Nuclei

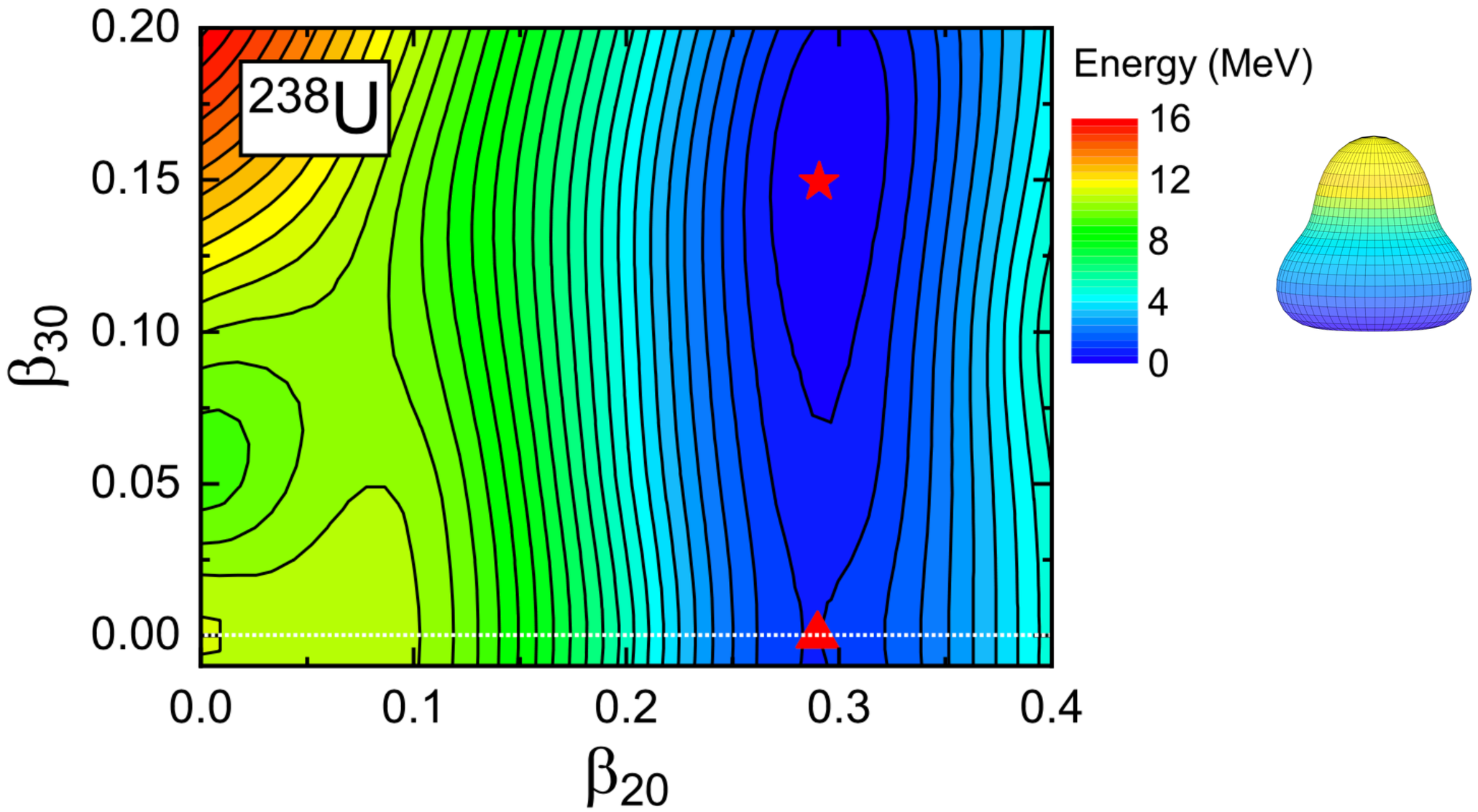
Cédric Golabek
GANIL (IN2P3/CNRS - DSM/CEA), BP 55027, F-14076 Caen Cedex 5, France

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."*



Octupole deformation of ^{238}U



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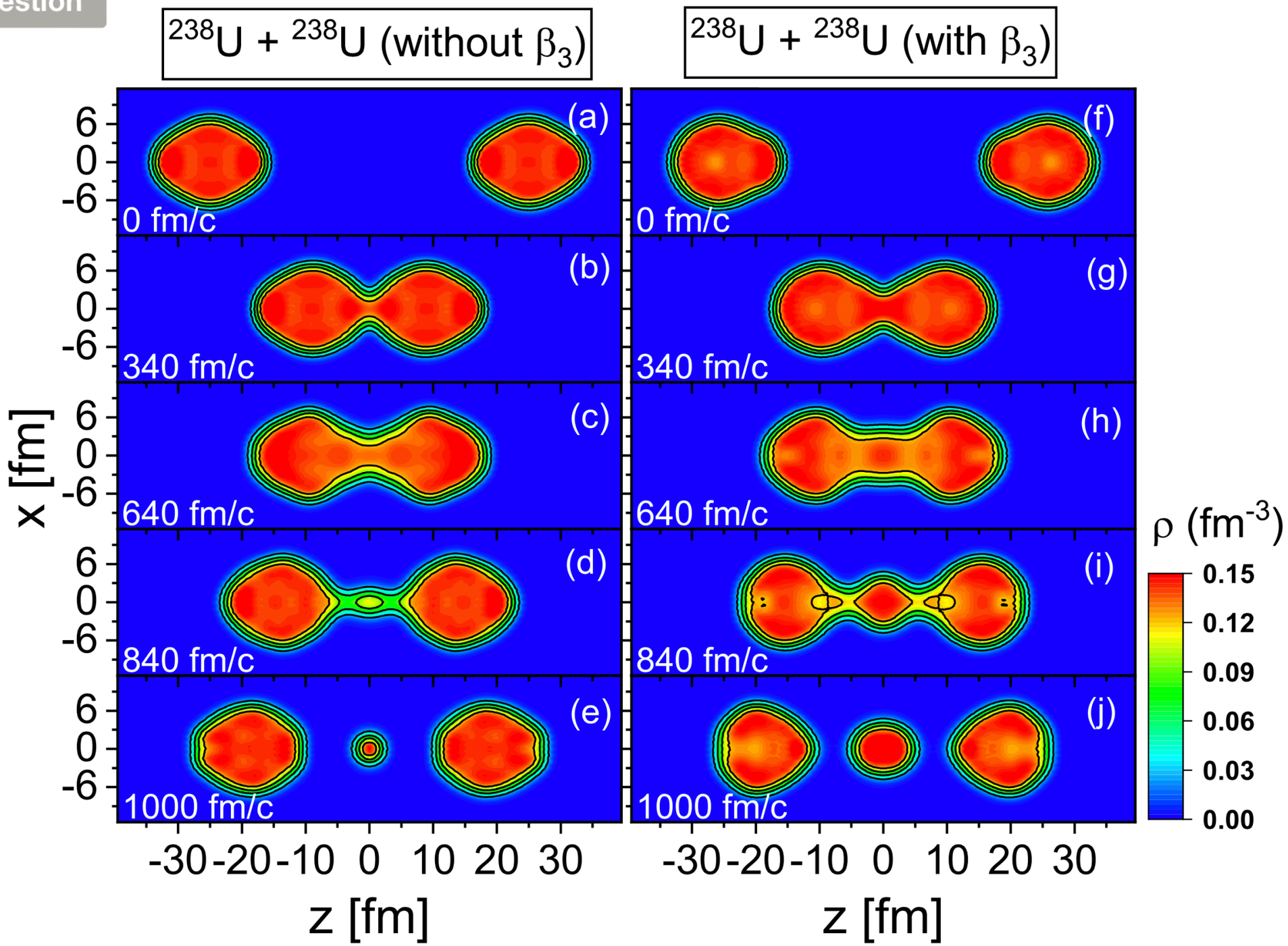
Octupole effects

Editors' Suggestion



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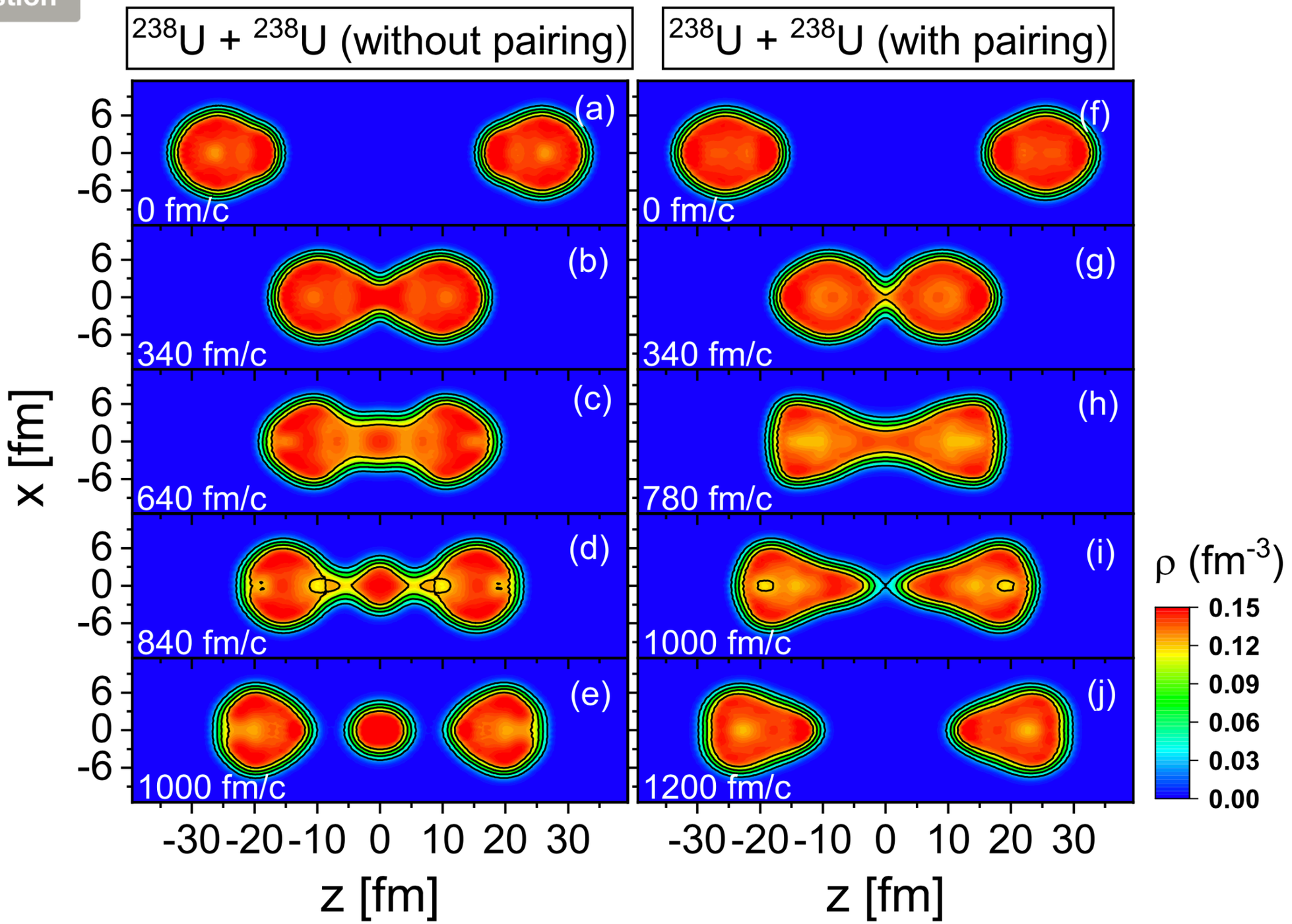
Pairing effects

Editors' Suggestion



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The ReCD Method

Relativistic **C**onfiguration-interaction **D**ensity functional theory (ReCD)

a theory combining the advantages from both Shell model and DFT

RDFT

- ☑ Universal density functionals
  - Symmetry broken
  - Single config. fruitful physics
  - No Configuration mixing
- ☑ Applicable for almost all nuclei
- ☑ No spectroscopic properties

Shell Model

- ☐ Non-universal effective interactions
  - No symmetry broken
  - Single config. little physics
  - Configuration mixing
- ☐ Intractable for deformed heavy nuclei
- ☑ Spectroscopy from multi config.