Alpha and alpha cluster in nuclei

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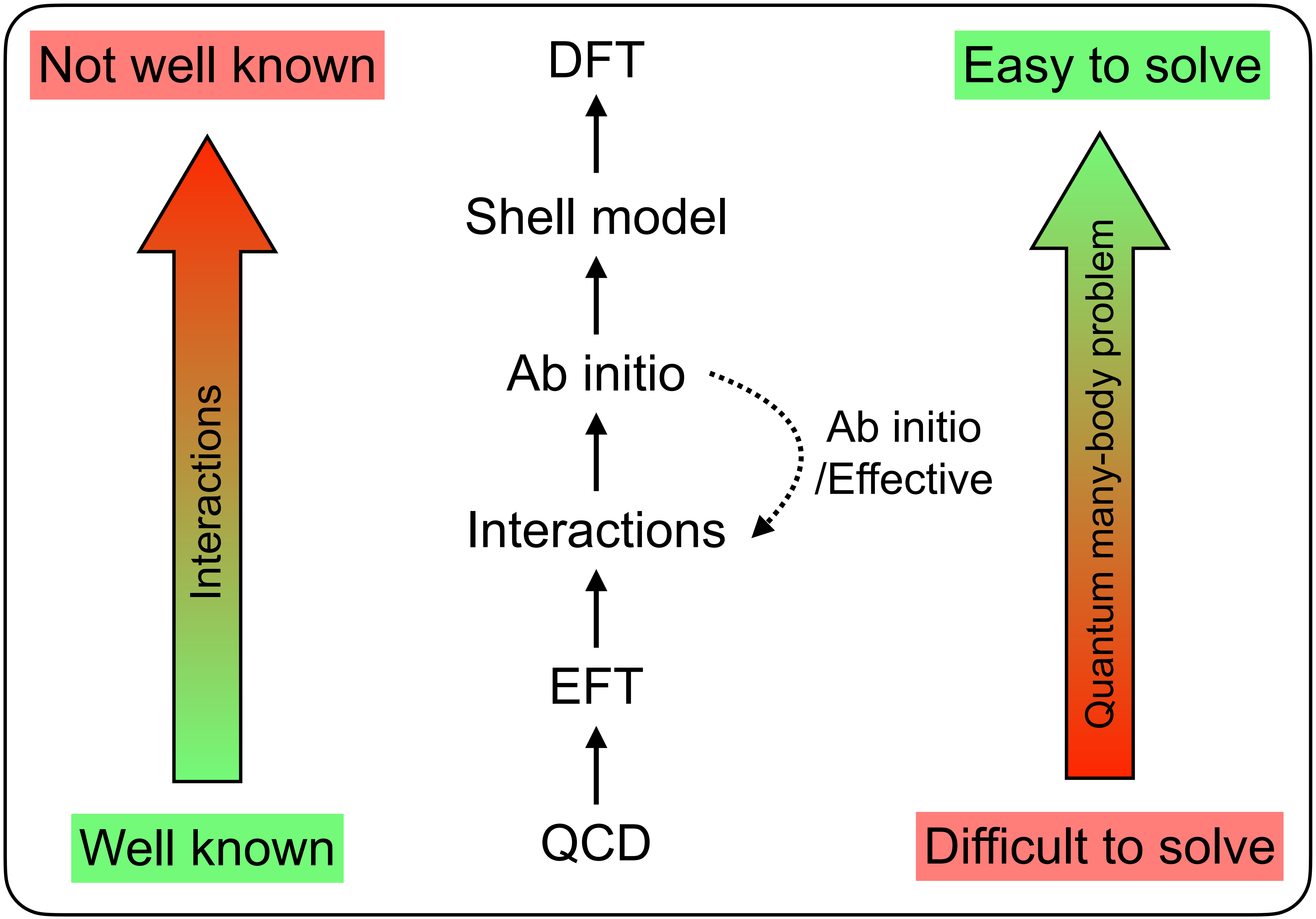
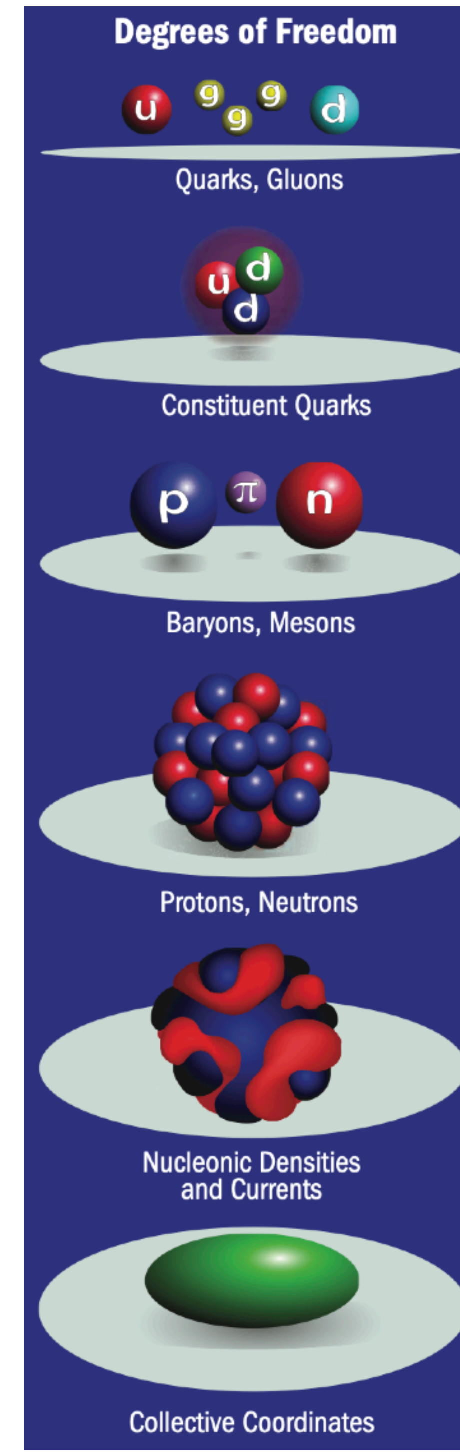
Outline

- A single alpha:
  relativistic variational Monte Carlo
- Alpha clustering nuclei:
  relativistic density functional theory
- Alpha dynamics:
  time-dependent relativistic density functional theory
- Summary

原子核理论

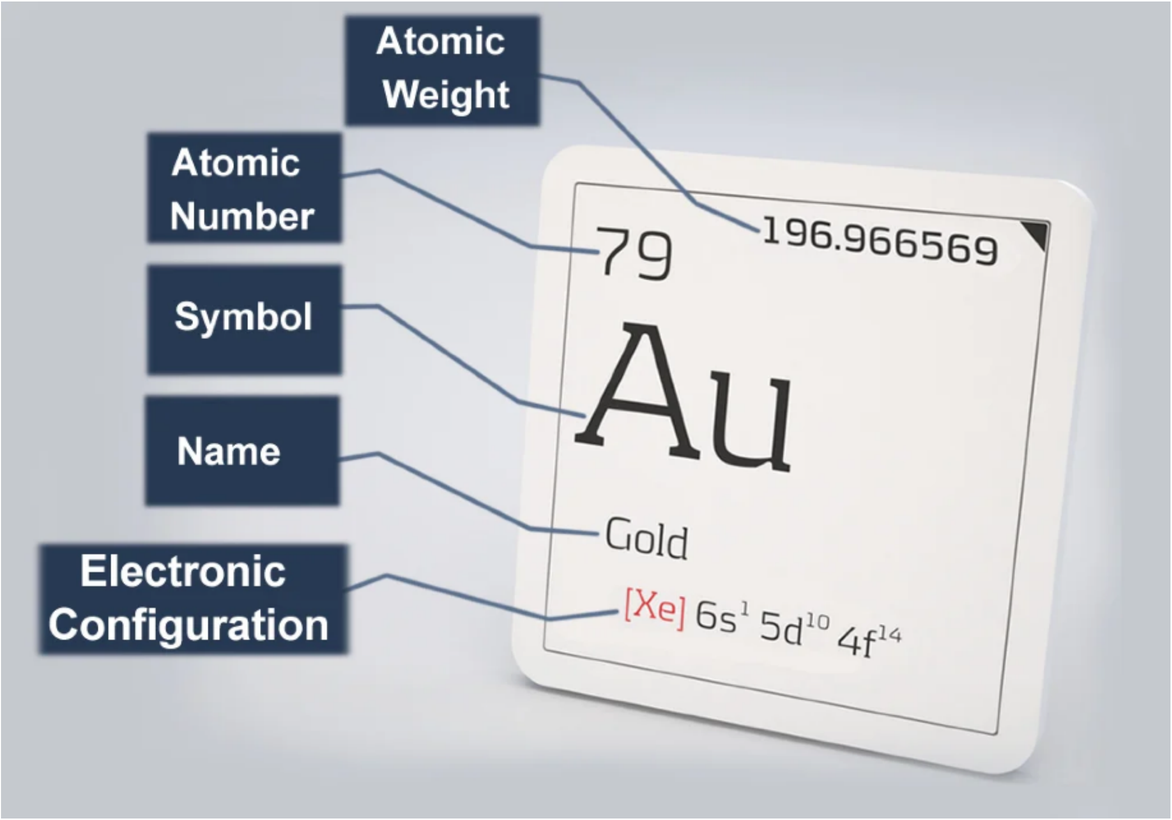
Overarching goal: *understand nuclear properties from a unified theoretical view rooted in the forces among nucleons*.

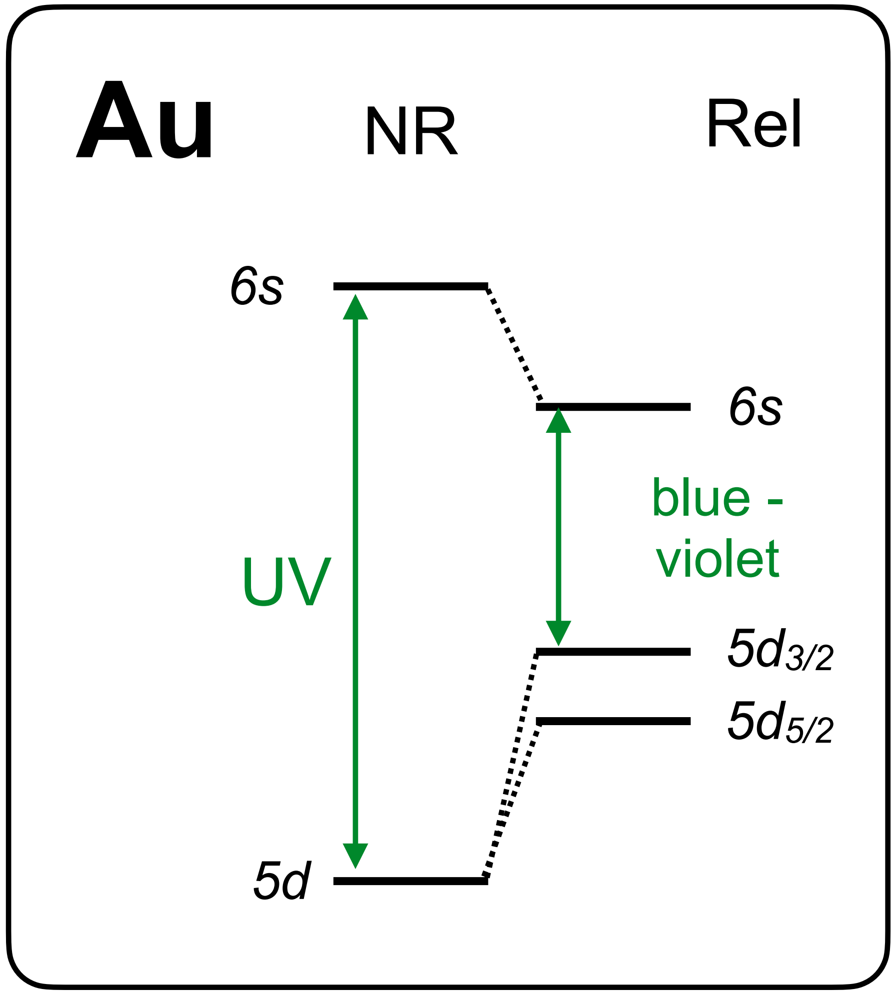




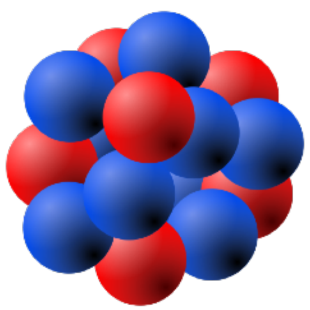
Relativistic Effects: More Common Than You Thought

Why gold is yellow?





Relativistic nuclear many-body problem



Schrödinger Equation

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

Relativistic QFT

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

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

Mean-field approximation

A Theory of Highly Condensed Matter*

J. D. WALECKA

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

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 covariant formulation provides an <u>efficient and comprehensive</u> explanation of observed bulk and single-particle systematics.

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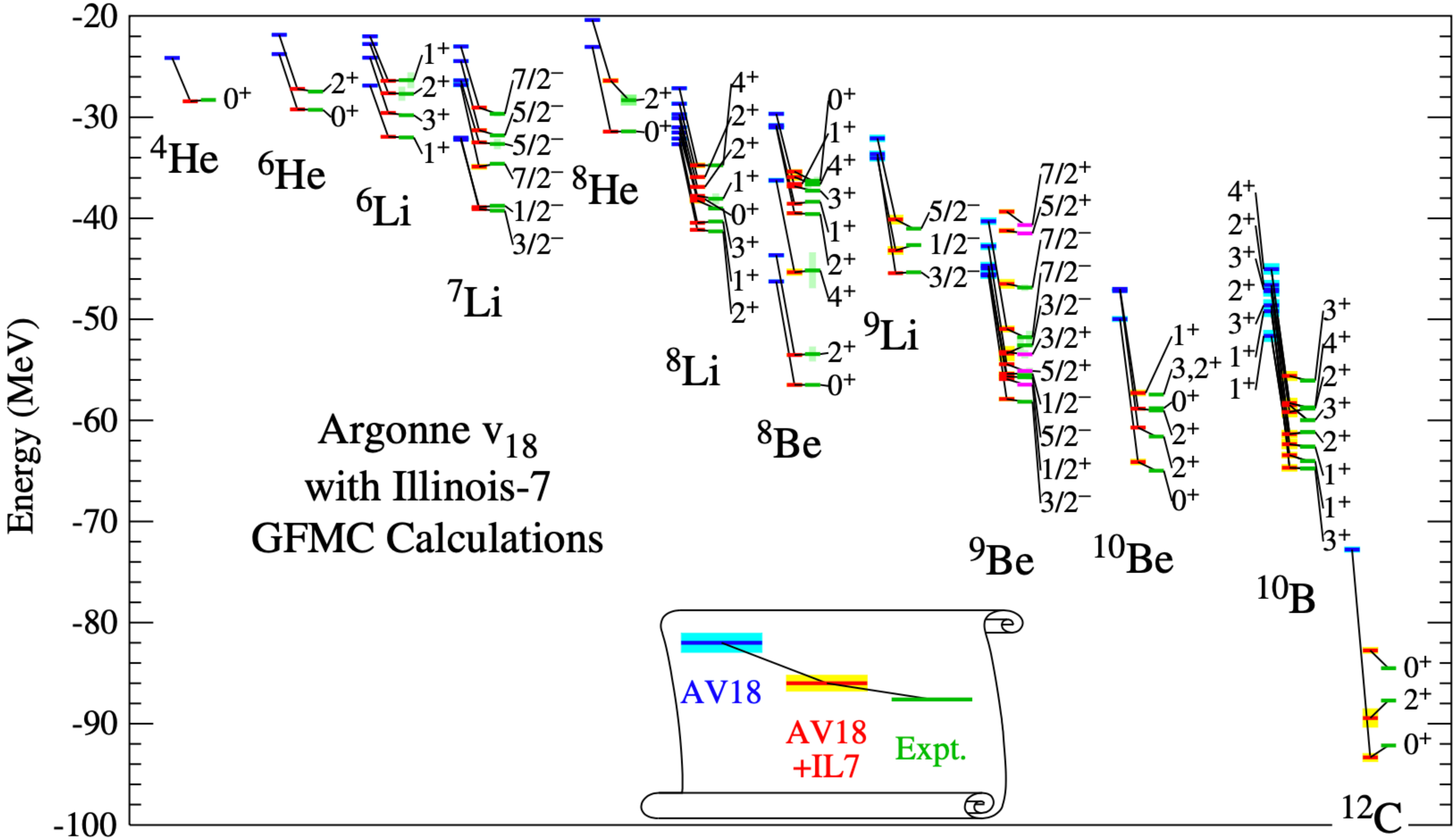
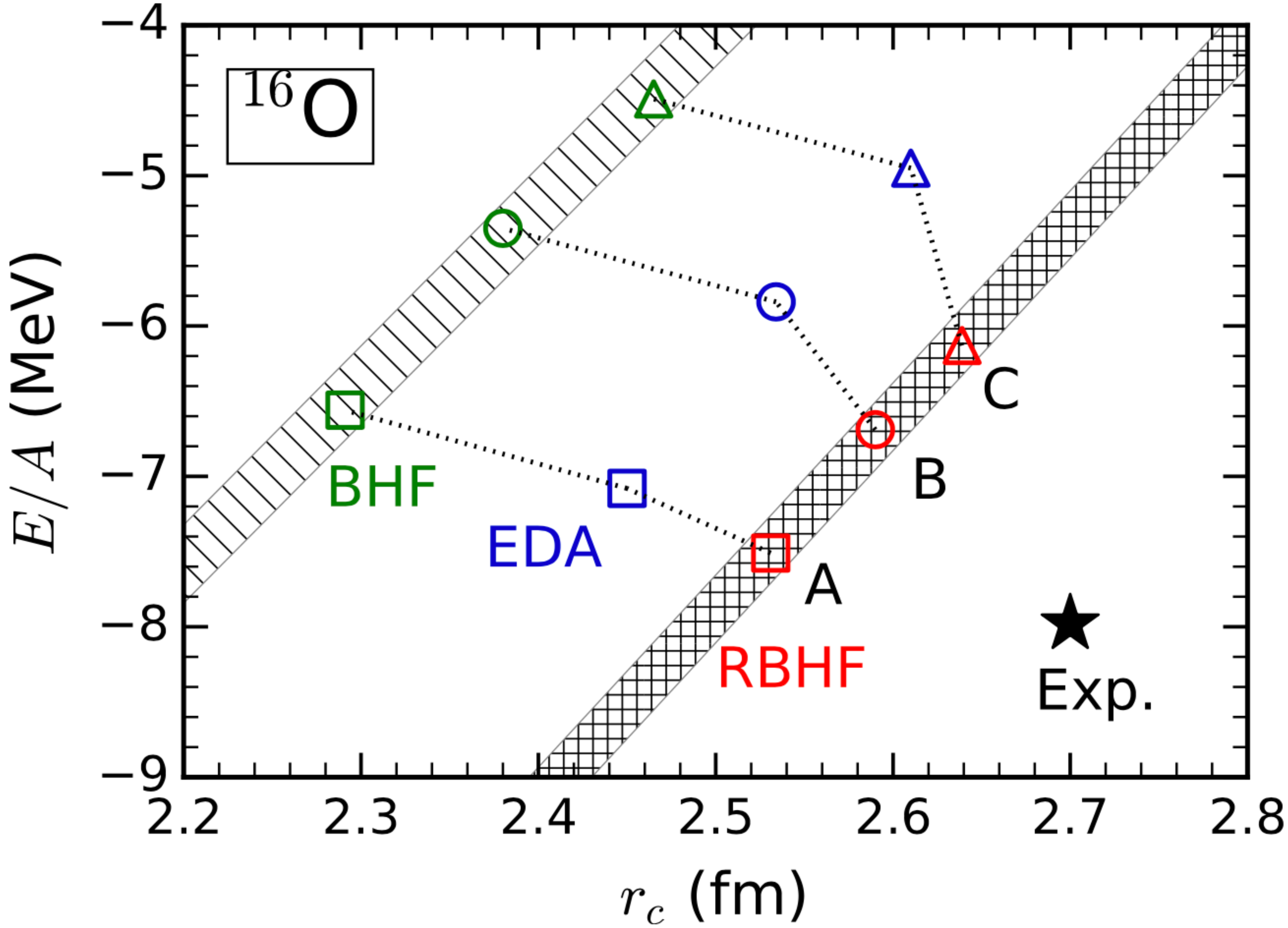
Three-body force is important



Carlson, et al., Rev. Mod. Phys., 2015, 87, 1067-1118

Relativistic effects are important

Relativistic Brueckner Hartree Fock



Shen, et al., Prog. Part. Nucl. Phys., 2019, 109, 103713

A consistent study of relativistic effects and three-body forces

✓ QFT: To include three-body force in RBHF is very difficult !

✓ Relativistic Hamiltonian dynamics via Poincaré group theory !

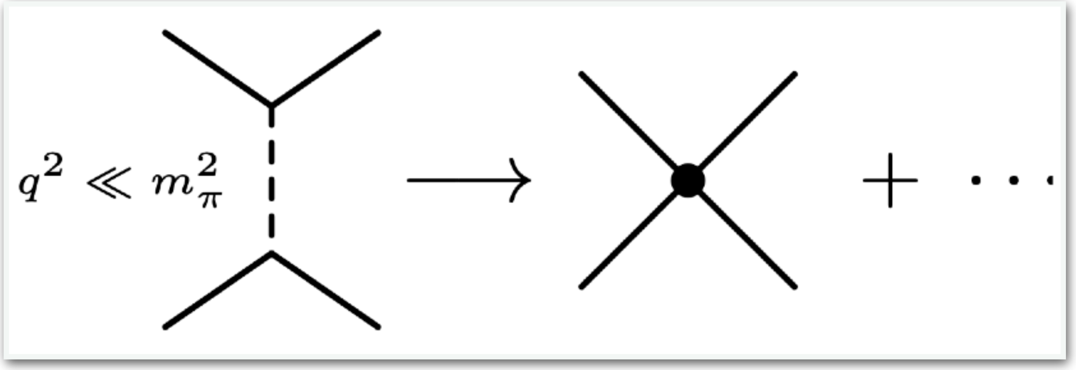
Carlson, Pandharipande, and Schiavilla, Phys. Rev. C 47, 484 (1993)

✓ A relativistic Hamiltonian derived from covariant pionless EFT.

Yang, PWZ, arXiv:2206.13208 [nucl-th]

At leading order

$$\mathscr{L}_{NN}^{(0)} = -\frac{1}{2}\Big[C_S(\bar{\psi}\psi)(\bar{\psi}\psi) + C_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) + C_P(\bar{\psi}\gamma_5\psi)(\bar{\psi}\gamma_5\psi) + C_{AV}(\bar{\psi}\gamma_5\gamma_\mu\psi)(\bar{\psi}\gamma_5\gamma^\mu\psi) + C_T(\bar{\psi}\sigma_{\mu\nu}\psi)(\bar{\psi}\sigma^{\mu\nu}\psi)\Big]$$



$$\hat{H}_{\rm LO} = \sum_{i=1}^{A}\left[(m_N^2 - \nabla_i^2)^{1/2} - m_N\right] + \sum_{i<j}^{A}(C_1 + C_2\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)\left(1 + V_{\rm b} + V_{\rm t}\right)\mathrm{e}^{-\frac{\Lambda^2}{4}\boldsymbol{r}_{ij}^2}$$

relativistic effects

$$V_{\rm b}(\boldsymbol{r}_{ij}) = -\frac{\hat{\boldsymbol{P}}_{ij}^2}{8m_N^2} - \frac{\Lambda^2}{16m_N^2}(\hat{\boldsymbol{P}}_{ij}\cdot\boldsymbol{r}_{ij})^2, \qquad V_{\rm t}(\boldsymbol{r}_{ij}) = -\frac{\Lambda^2}{4m_N^2}\left[\left(3 - \frac{\Lambda^2}{2}\boldsymbol{r}_{ij}^2\right) + 2\mathrm{i}\boldsymbol{r}_{ij}\cdot\hat{\boldsymbol{p}}_{ij} + 4\frac{\hat{\boldsymbol{p}}_{ij}^2}{\Lambda^2}\right]$$

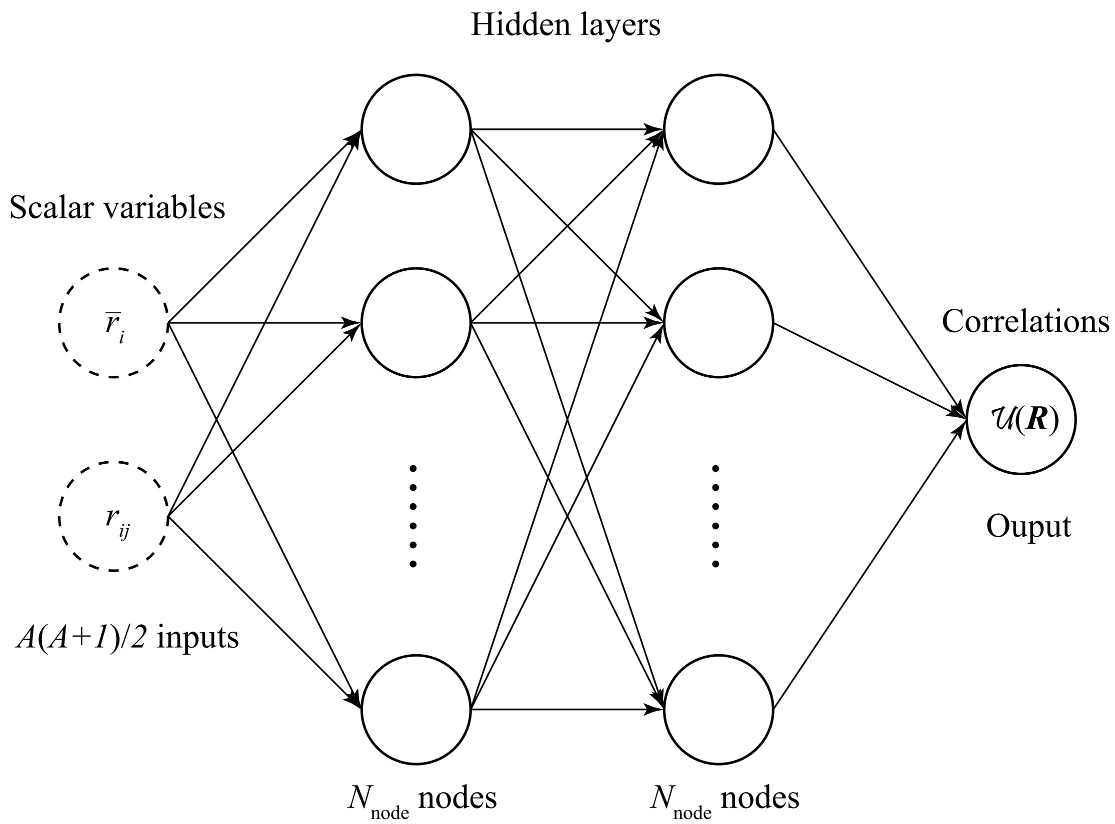
Variational Monte Carlo

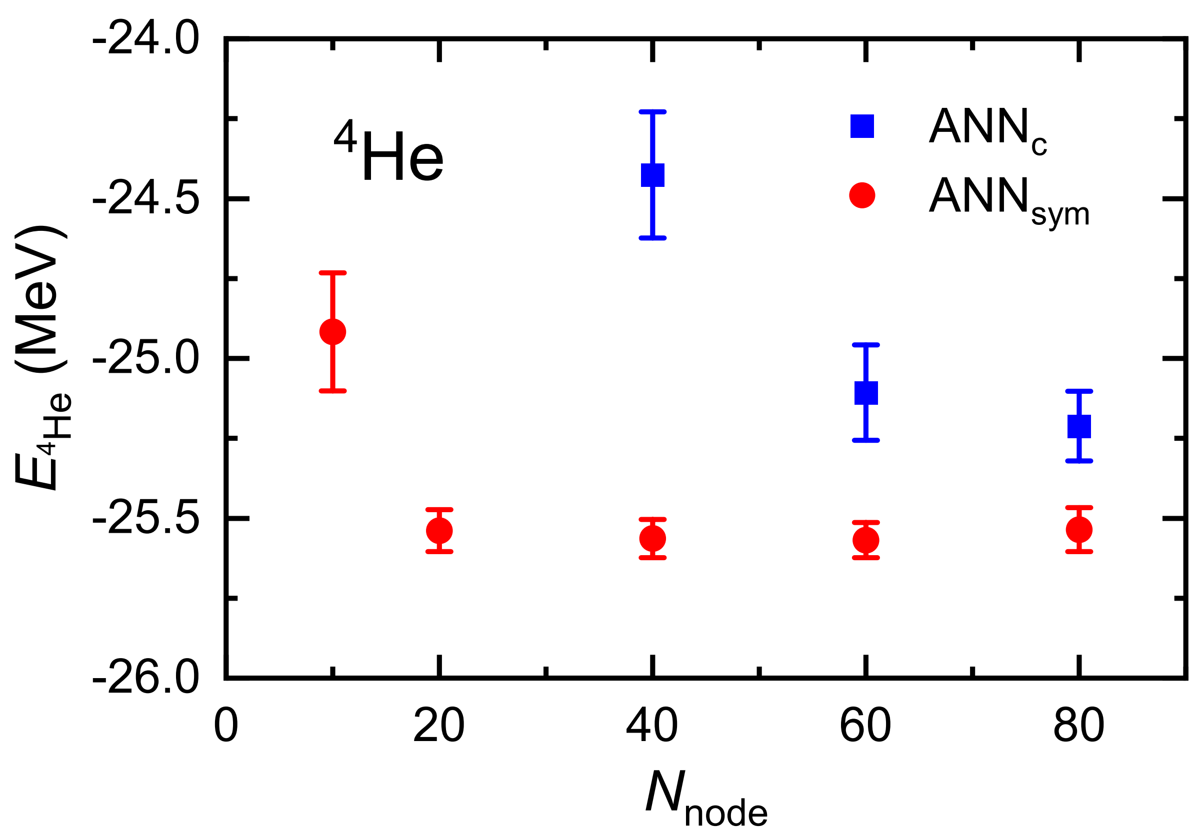
Total energy

$$\frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = E_V$$

Variational wave function

$$| \Psi_V^{\mathrm{ANN}} \rangle = \exp\left[\mathcal{U}(\bar{r}_1, \ldots, \bar{r}_A; r_{12}, \ldots, r_{A-1,A})\right] | \Phi \rangle$$

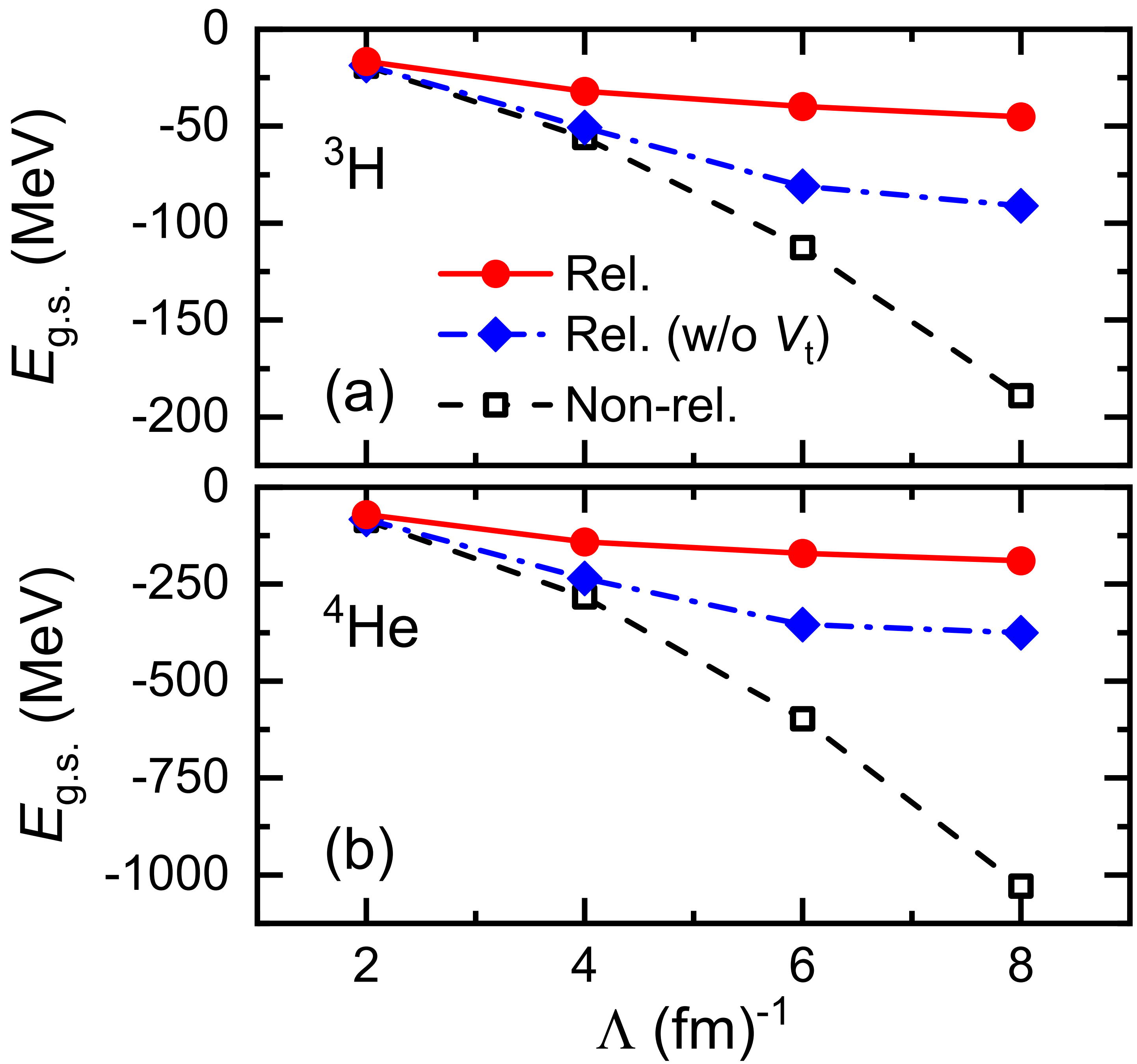




Compatible with the rotational invariance of the Hamiltonian!

Yang, PWZ, arXiv:2206.13208 [nucl-th]

Ground states of three- and four-body nuclei



Thomas collapse avoided

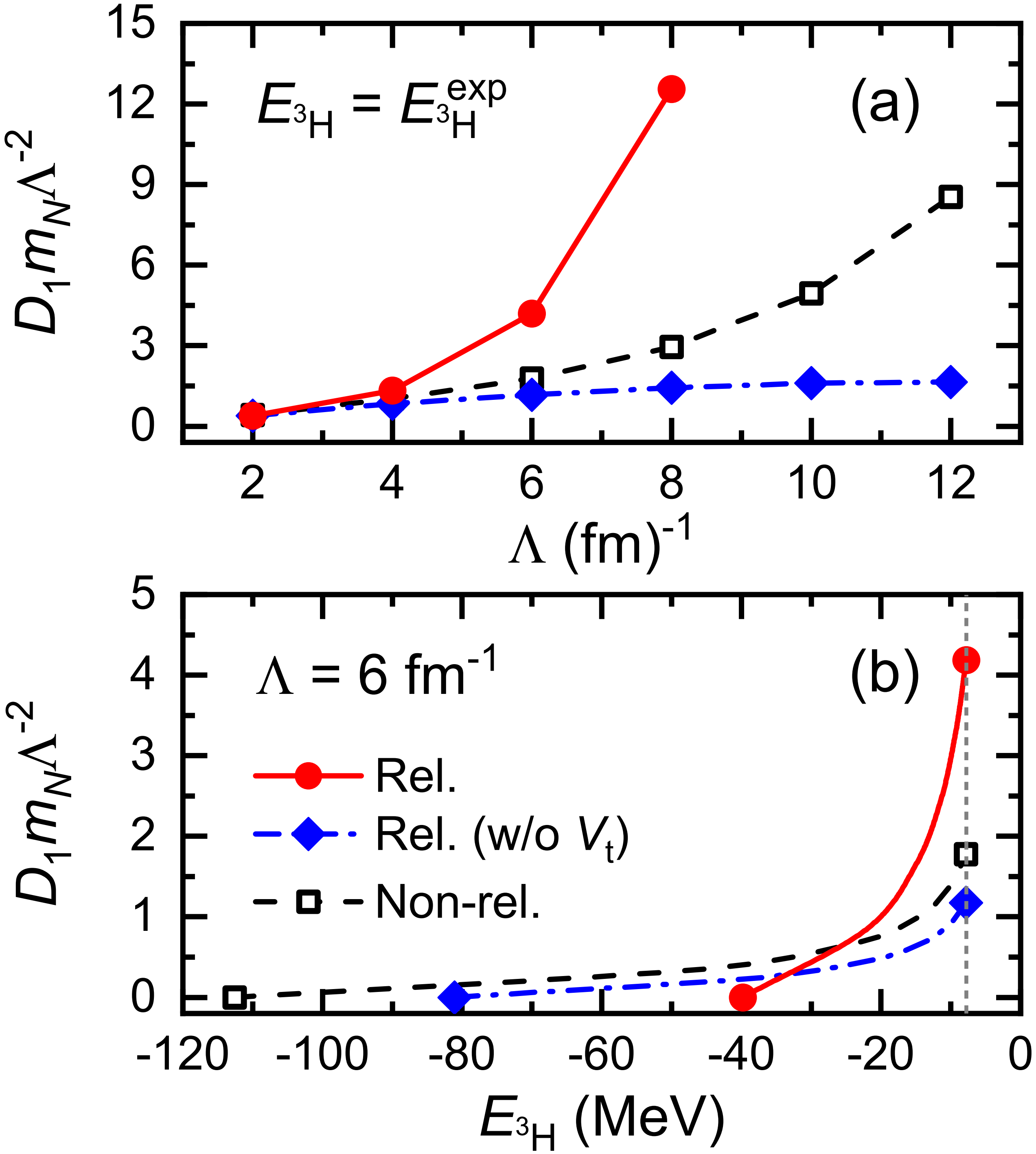
Renormalizability fulfilled

Three-body force needed ?

Four-body force at NLO ?

Yang, PWZ, arXiv:2206.13208 [nucl-th]

The interplay between relativistic effects and three-body force



$$\hat{\boldsymbol{P}}_{12} = \hat{\boldsymbol{p}}_1 + \hat{\boldsymbol{p}}_2 = -\hat{\boldsymbol{p}}_3$$

$$V_{\mathrm{b}}(\boldsymbol{r}_{12}) = -\frac{\hat{\boldsymbol{P}}_{12}^2}{8m_N^2} - \frac{\Lambda^2}{16m_N^2}(\hat{\boldsymbol{P}}_{12}\cdot\boldsymbol{r}_{12})^2,$$

$$V_{\mathrm{b}}(\boldsymbol{r}_{12}) = -\frac{\hat{\boldsymbol{p}}_3^2}{8m_N^2} - \frac{\Lambda^2}{16m_N^2}(\hat{\boldsymbol{p}}_3\cdot\boldsymbol{r}_{12})^2,$$

$$V_{\mathrm{t}}(\boldsymbol{r}_{ij}) = -\frac{\Lambda^2}{4m_N^2}\left[\left(3 - \frac{\Lambda^2}{2}\boldsymbol{r}_{ij}^2\right) + 2\mathrm{i}\boldsymbol{r}_{ij}\cdot\hat{\boldsymbol{p}}_{ij} + 4\frac{\hat{\boldsymbol{p}}_{ij}^2}{\Lambda^2}\right]$$

Repulsive at short-range

Yang, PWZ, arXiv:2206.13208 [nucl-th]

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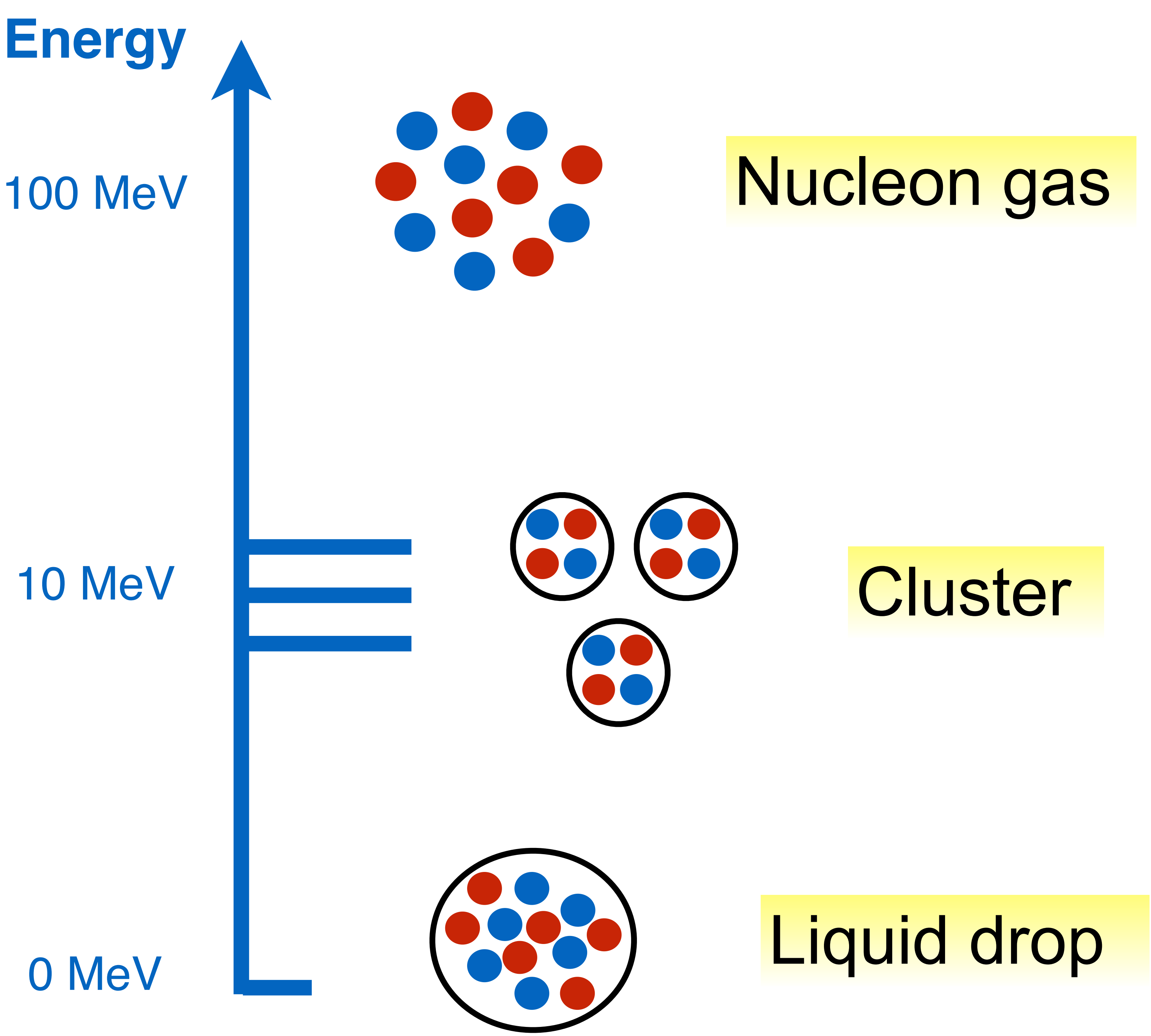
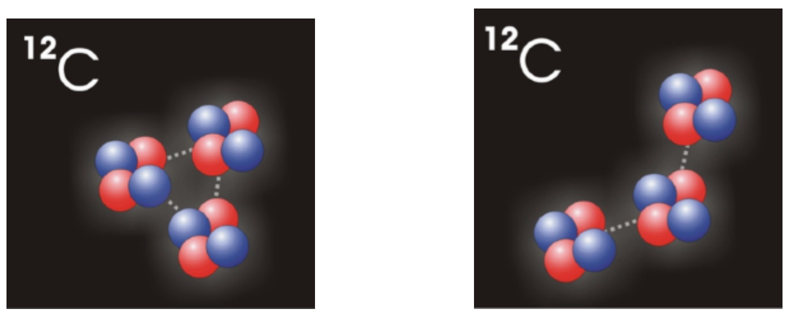
Rod-shaped nuclei

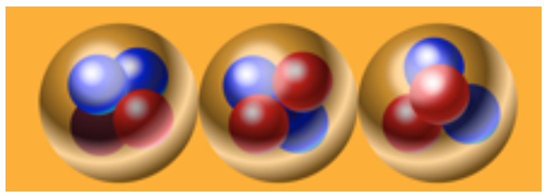
Strongly deformed states towards a hyper-deformation may exist in light N = Z nuclei due to a cluster structure.



^{12}C 6 protons
6 neutrons



No firm evidence



Two difficulties

- ✓ antisymmetrization effects
- ✓ weak-coupling nature

Density functional theory

The many-body problem is mapped onto an 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

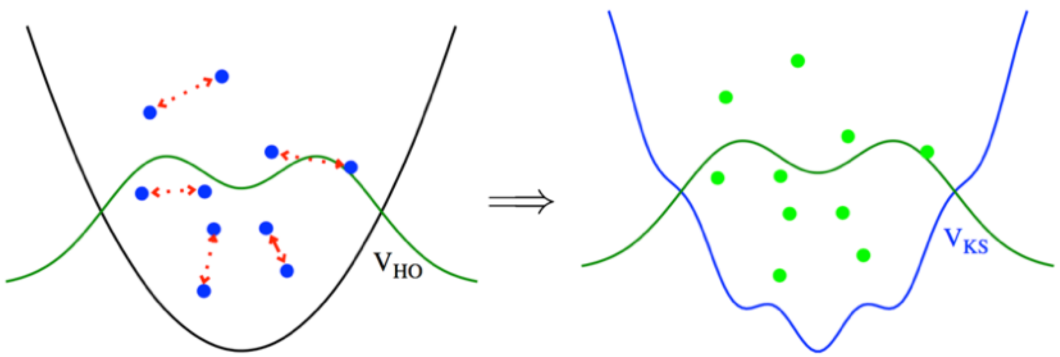


Figure from Drut PPNP 2010

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

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

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

Machine-learning DFT for nuclei

✓ H-K Theorem proves the existence of a universal functional depends solely on density!

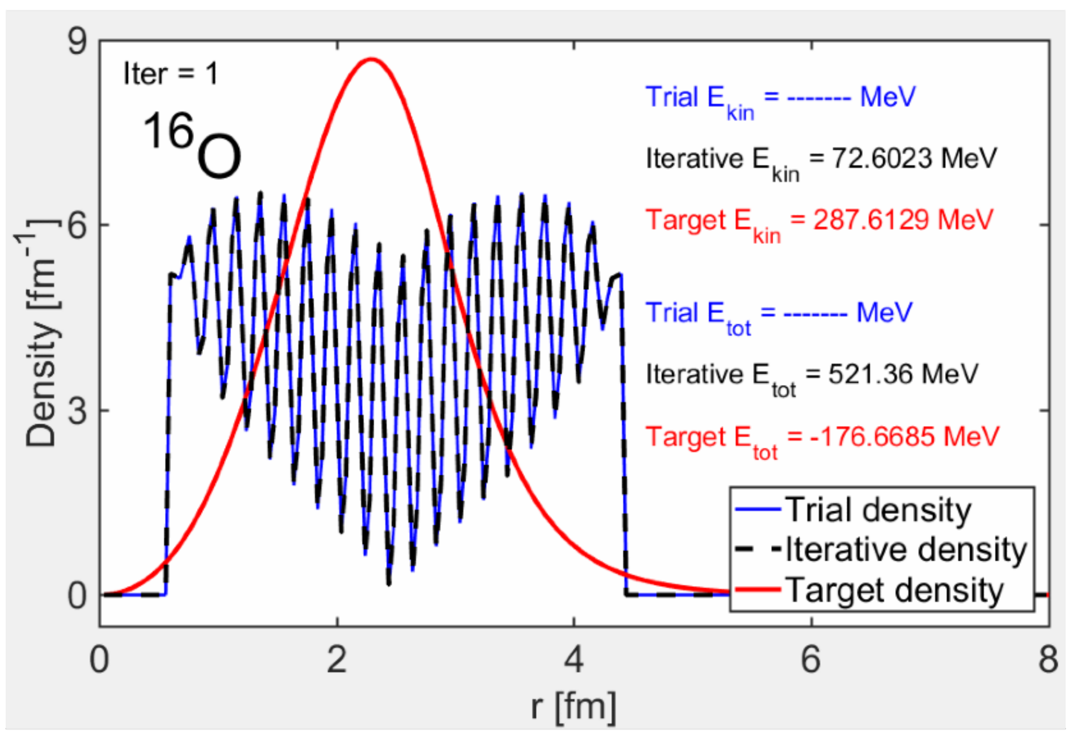
✓ BUT, all previous attempts for a nuclear kinetic energy functional are NOT so accurate.

—〉 One has to introduce Kohn-Sham, i.e., a functional of orbits …

✓ By Machine Learning, a robust and accurate orbital-free density functional is established.

Wu, Ren, PWZ, Phys. Rev. C, *105*, L031303 (2022)

$$E_{\rm tot}[\rho] = E_{\rm kin}^{\rm ML}[\rho] + E_{\rm int}^{\rm SkP}[\rho]$$



Robust self-consistent solution

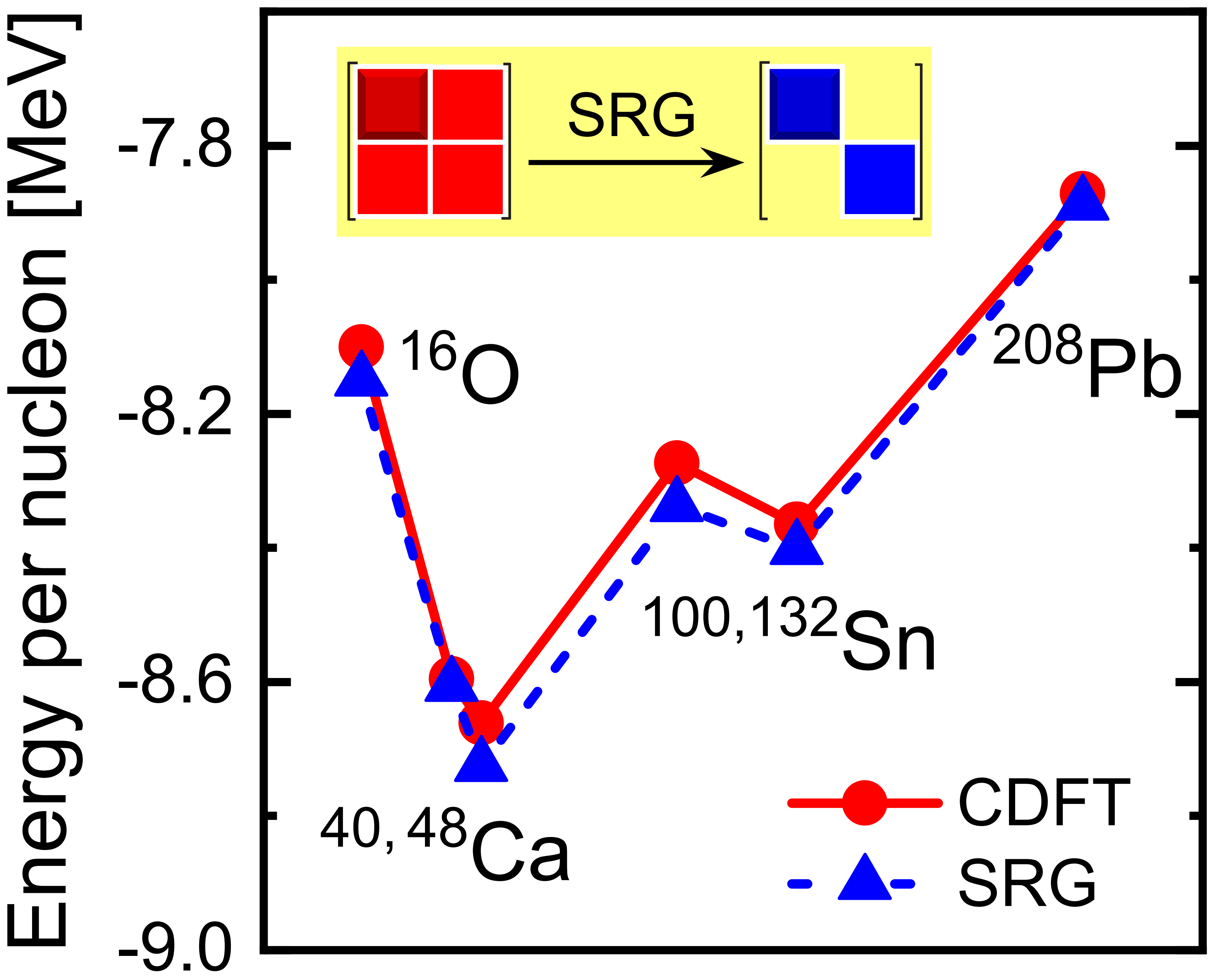
A functional depends solely on density

		Kohn-Sham	Machine-Learning	Experiment
^{4}He	$E_{\rm tot}$	-26.3700	-26.3931 (0.0012)	-28.2957
	$E_{\rm kin}$	35.2138	35.2044 (0.0056)	/
	$\langle r^2 \rangle$	2.1626	2.1628 (0.0002)	1.6755
^{16}O	$E_{\rm tot}$	-127.3781	-127.1622 (0.1584)	-127.6193
	$E_{\rm kin}$	219.2875	218.3458 (0.6882)	/
	$\langle r^2 \rangle$	2.8077	2.8113 (0.0047)	2.6991
^{40}Ca	$E_{\rm tot}$	-342.0645	-341.8027 (0.5724)	-342.0521
	$E_{\rm kin}$	643.1100	642.9145 (1.6875)	/
	$\langle r^2 \rangle$	3.4677	3.4652 (0.0055)	3.4776

Most accurate ever orbit-free DFT for nuclei

Toward a bridge between relativistic and nonrelativistic DFTs

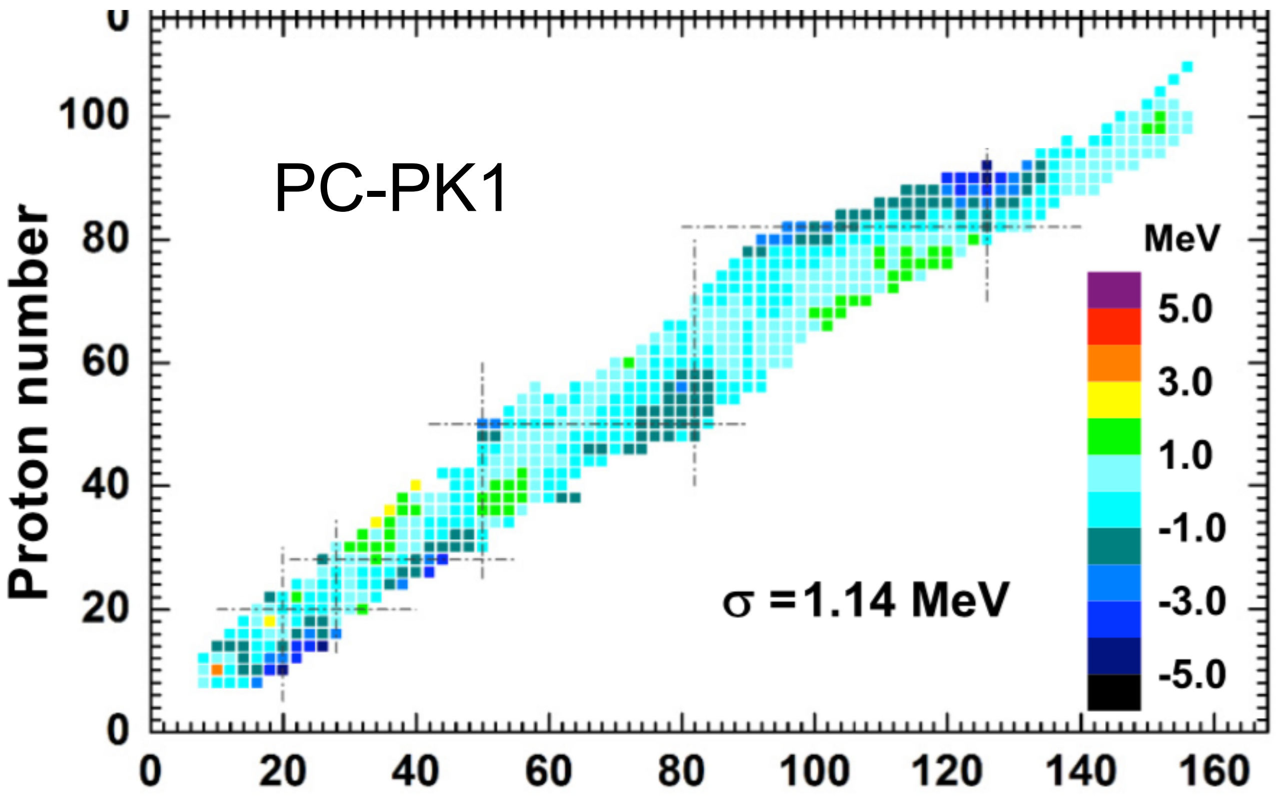
Ren and PWZ, Phys. Rev. C, 102, 021301(R) (2020) **Editors' Suggestion**

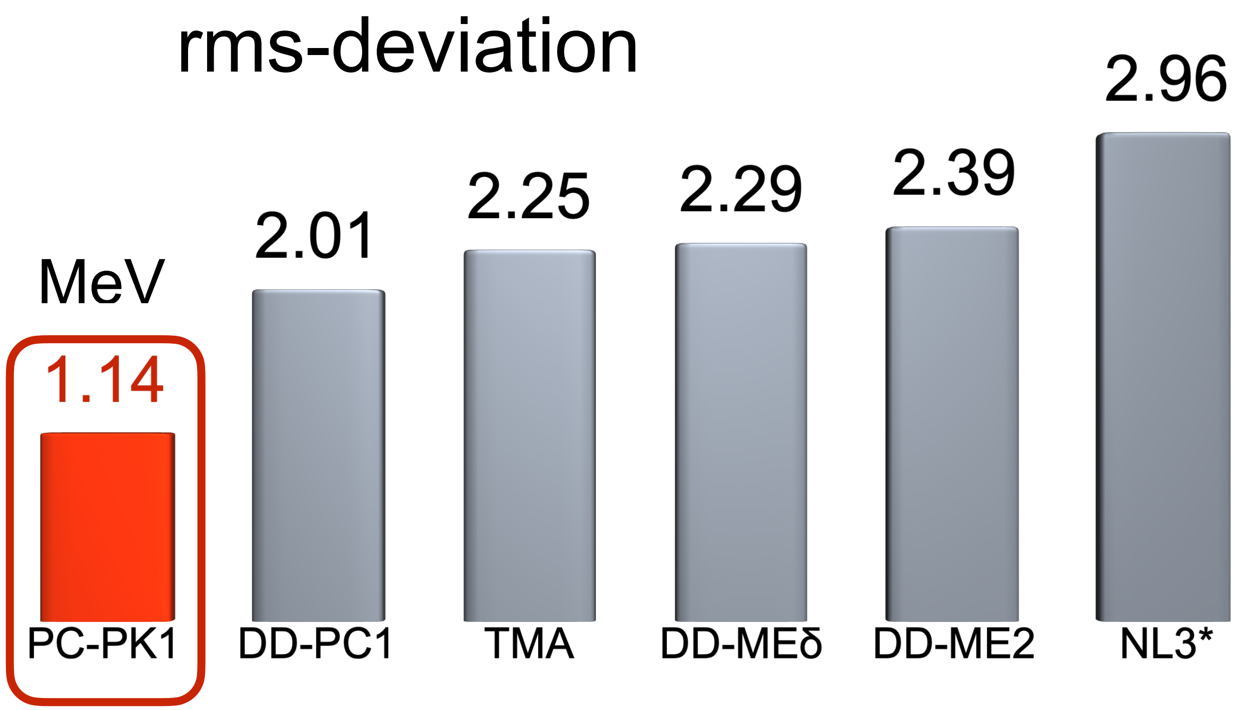


Covariant density functional：PC-PK1

~10 parameters fitted to 60 spherical nuclei …

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





Data from AME2012

Agbemava PRC 2014
Geng PTP 2005

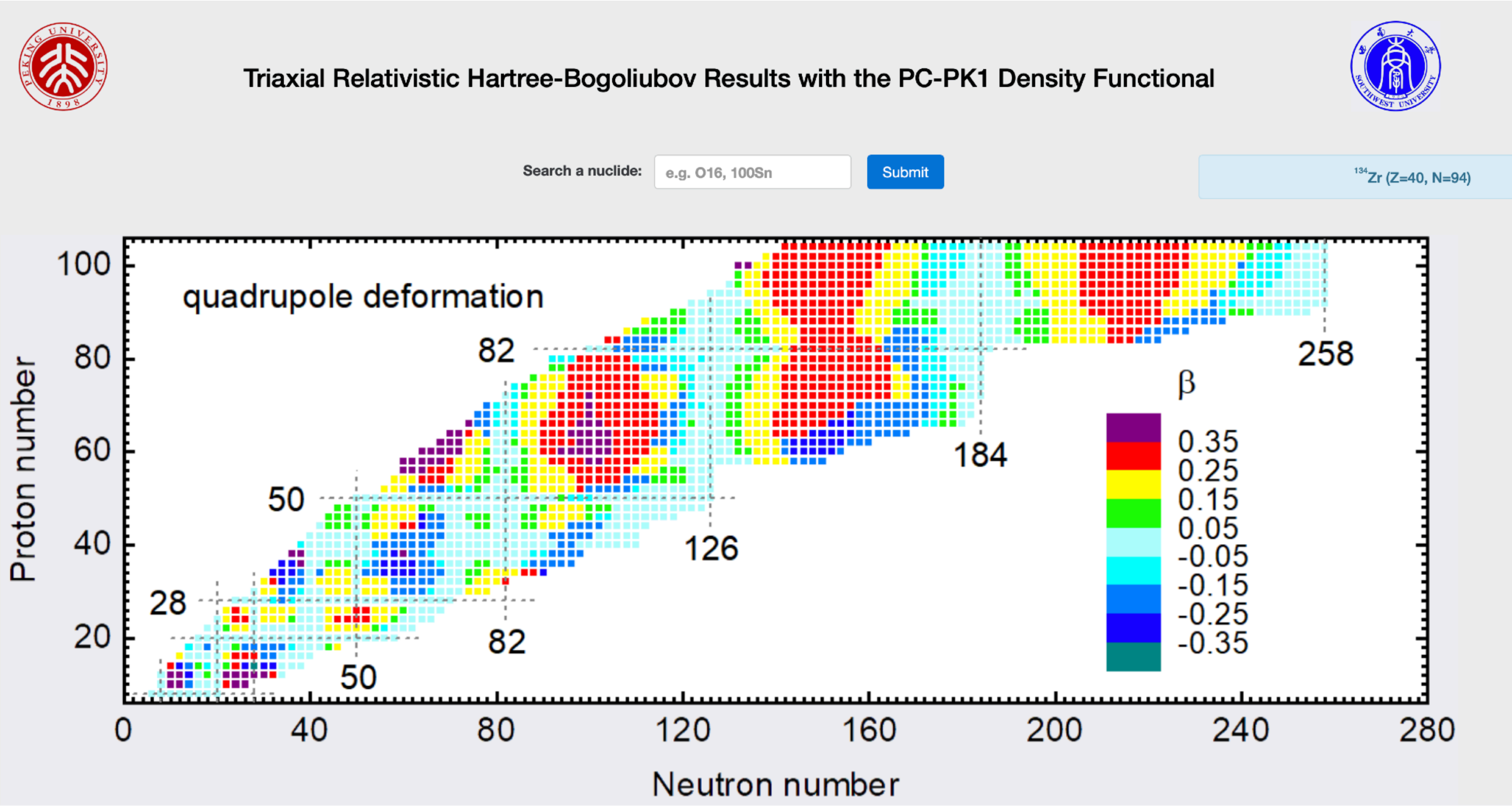
PWZ, Li, Yao, Meng, PRC 82, 054319 (2010)

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

Best density-functional description for nuclear masses so far!

How many nuclei are bound?

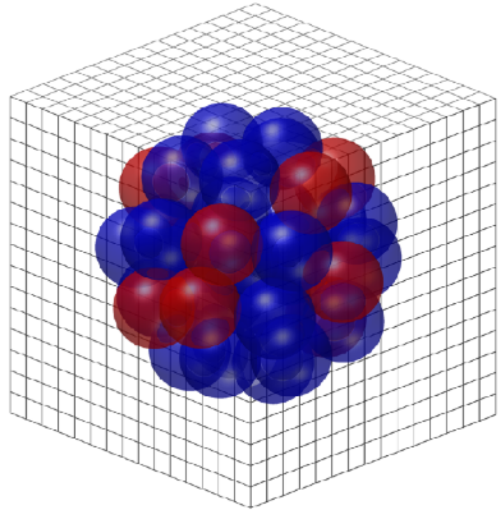
http://nuclearmap.jcnp.org/index.html　三轴+超越平均场关联

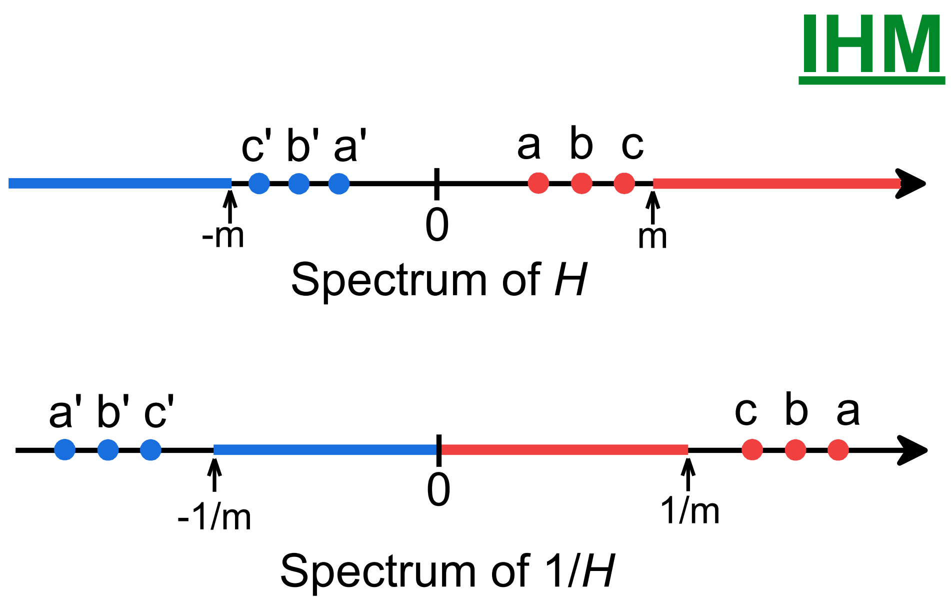


Yang, Wang, PWZ, Li, Phys. Rev. C **104**, 054312 (2021)

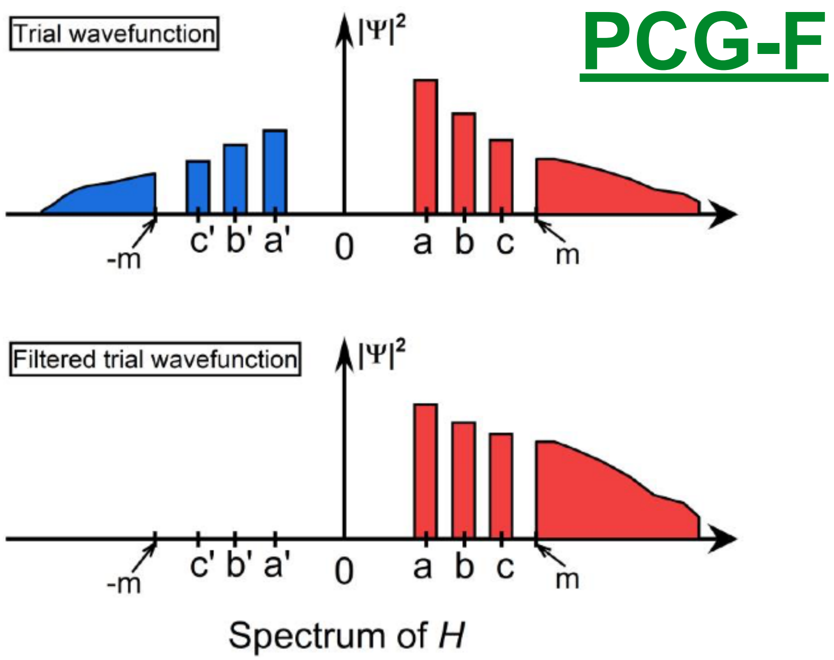
Lattice CDFT

- ✓ No spatial symmetry restriction
- ✓ Appropriate for nuclei with a large space distribution
- ✓ Less computational cost than basis expansion method
- ✓ A long-term challenge due to
  - a) variational collapse problem
  - b) fermion doubling problem





Hagino, Tanimura, PRC 82, 057301 (2010)



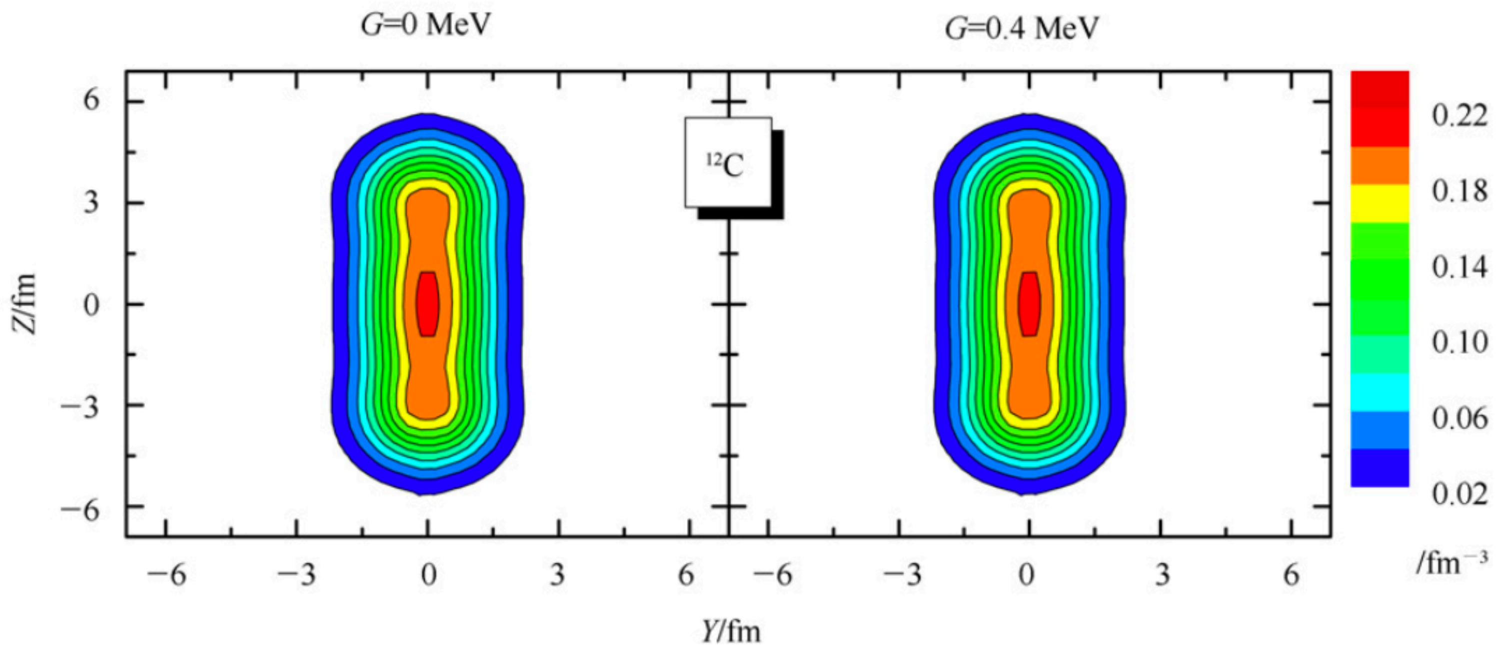
Li, Ren, PWZ, PRC 102, 044307 (2020)

Variational method is used to solve CDFT in 3D lattice efficiently !

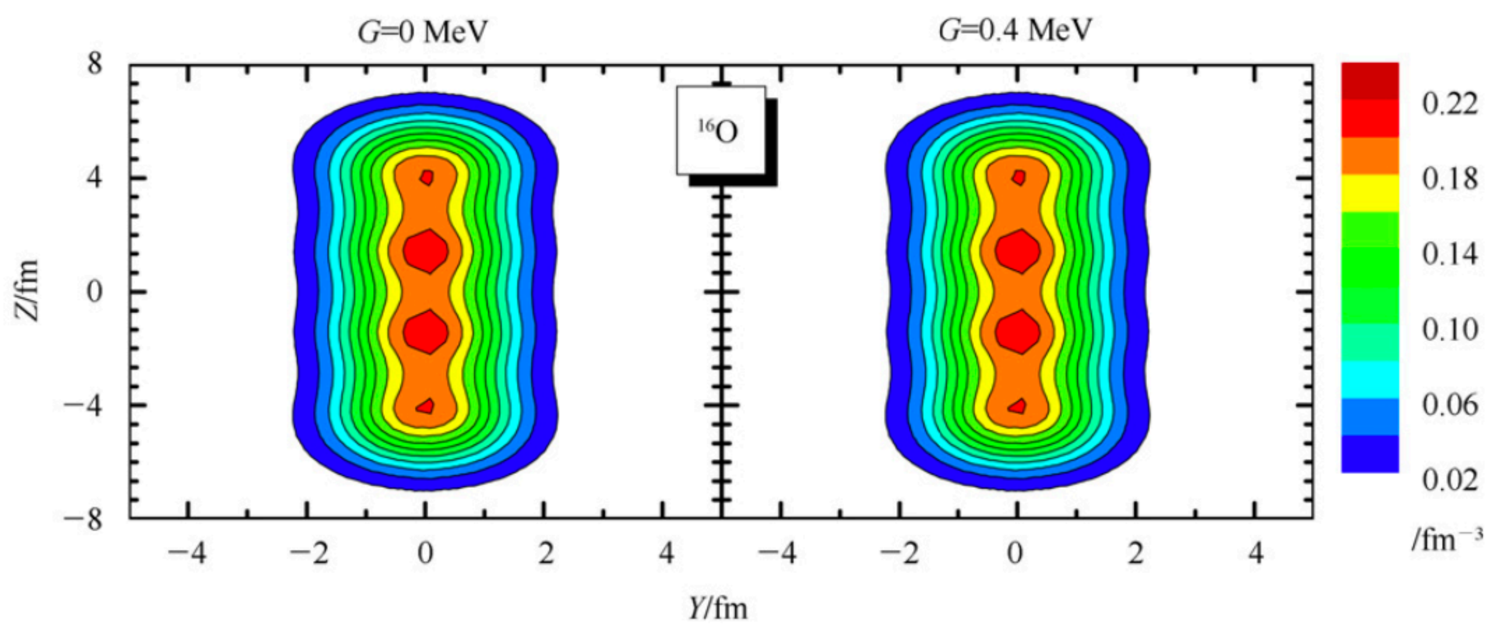
Rod shape against bending and fission

Static calculations with axial symmetry

^{12}C



^{16}O

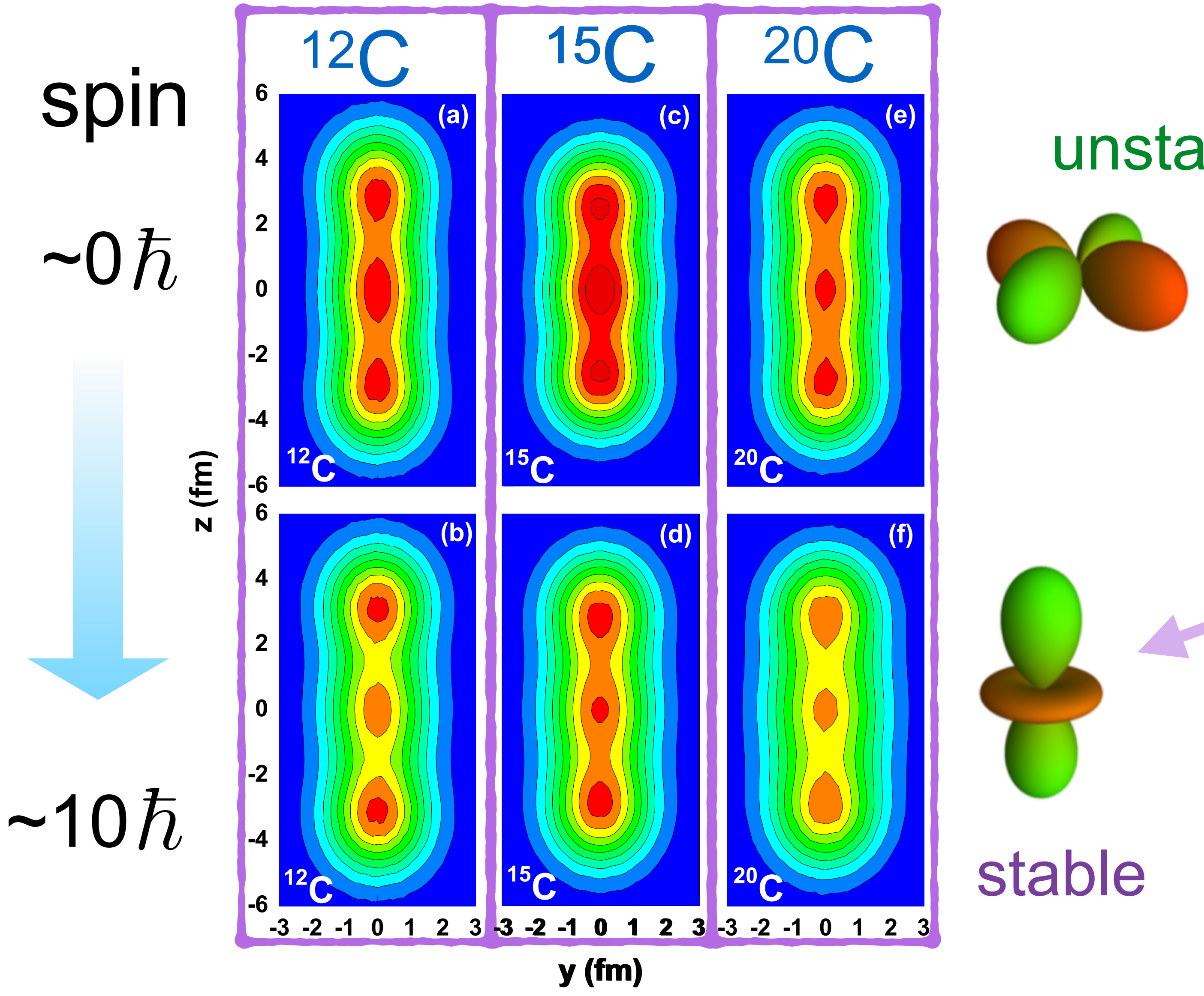


Liu and PWZ, Chin. Phys. C **36**, 818 (2012)

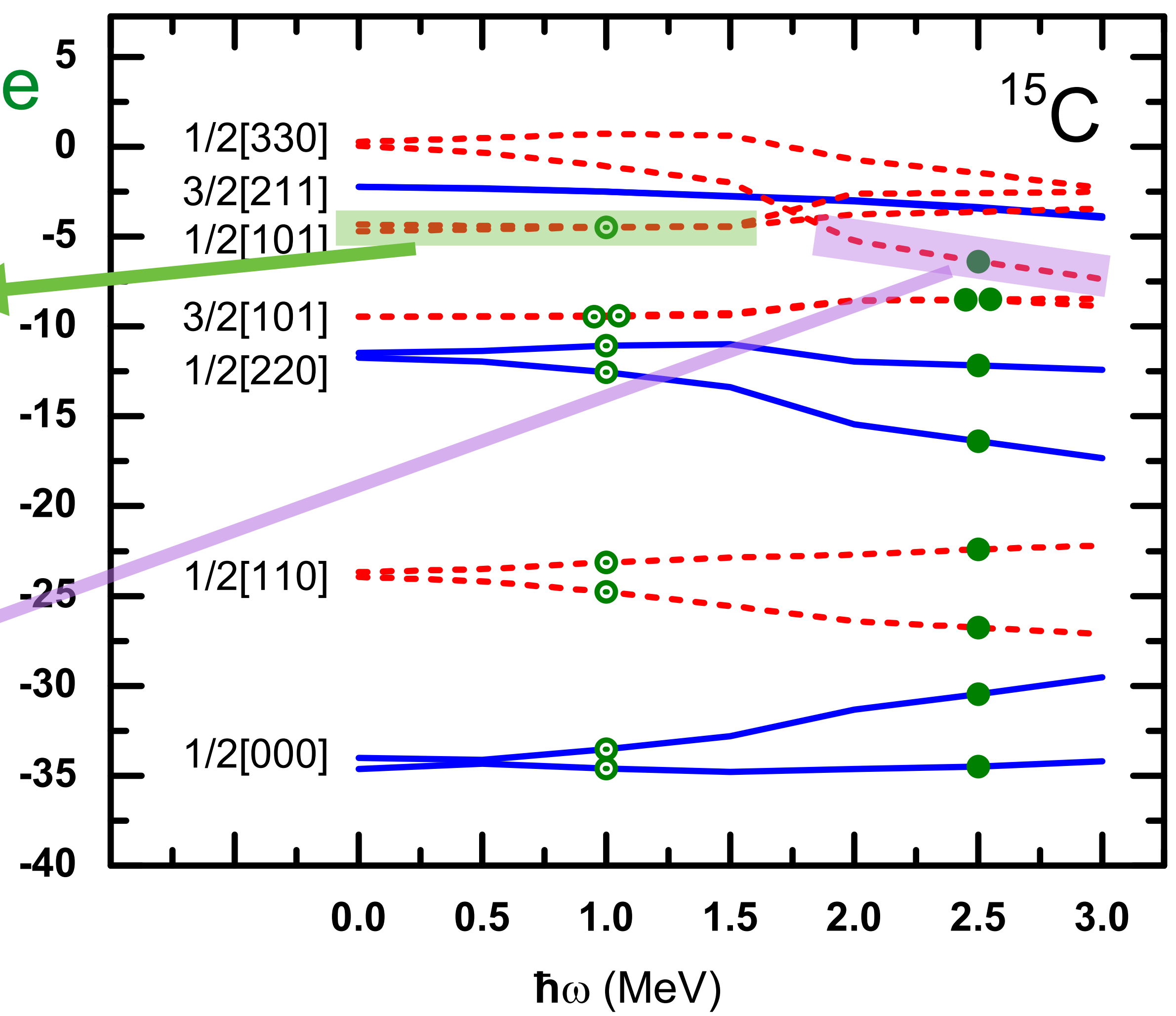
Spin and Isospin Coherent Effects

Static calculations with reflection-symmetry

Proton density distribution



neutron orbitals



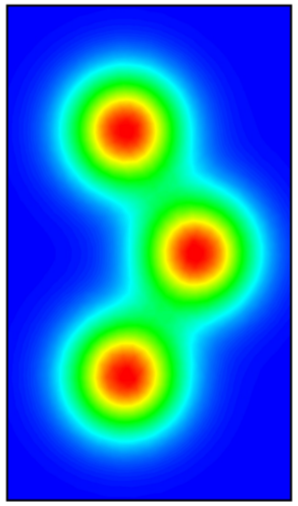
PWZ, Itagaki, Meng, PRL 115, 022501 (2015)

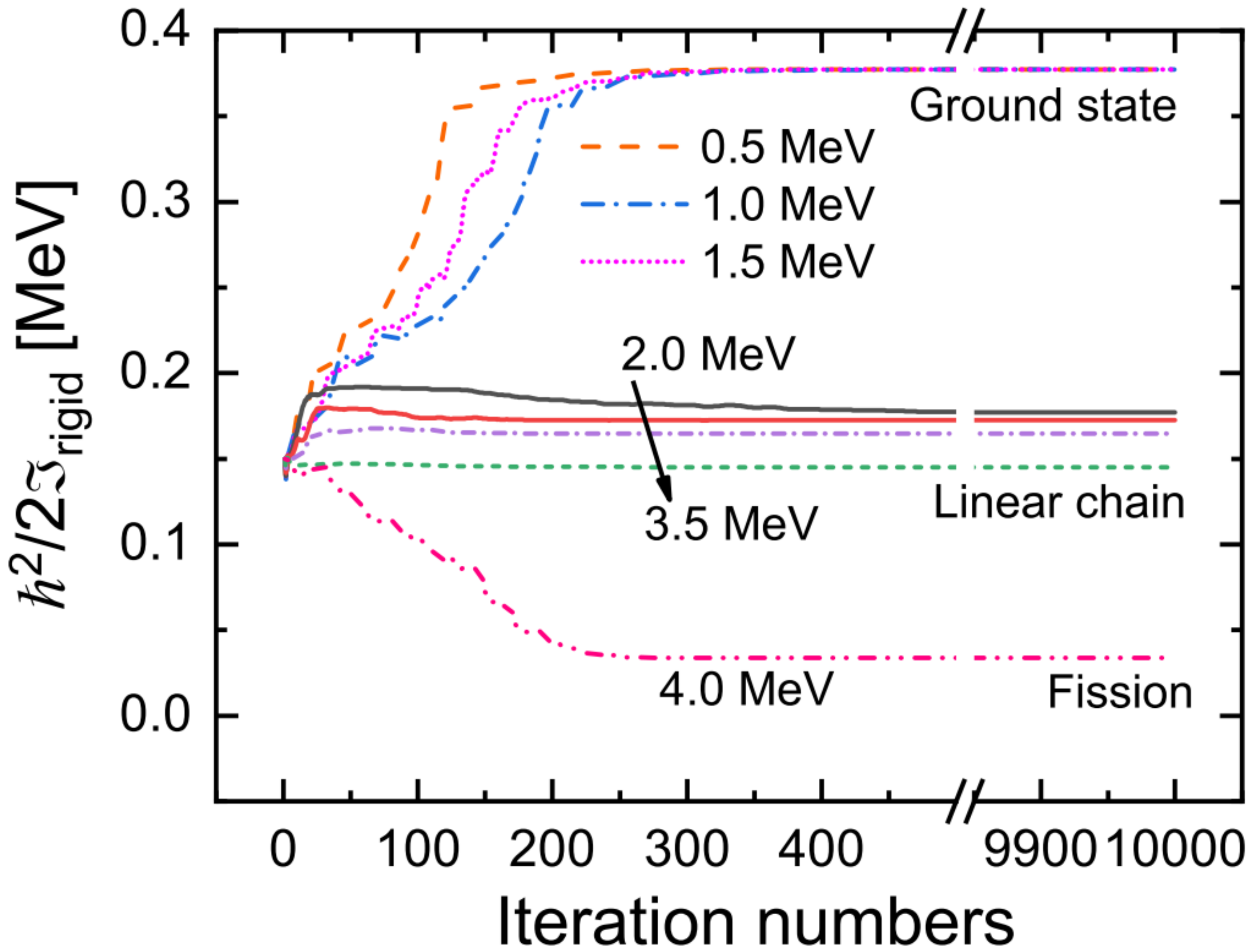
Rod shapes could be realized towards extreme spin and isospin!

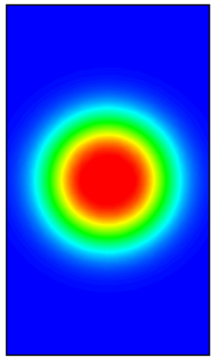
Rod shape against bending and fission

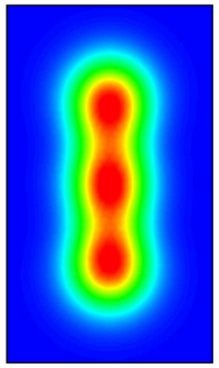
Static calculations in 3D lattice

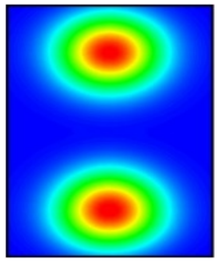
^{12}C











Rod shapes are generated as energy minima at a certain range of rotational frequencies.

Ren, Zhang, PWZ, Itagaki, Maruhn, Meng, Sci. China-Phys. Mech. Astron., 62, 112062 (2019)

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Time-dependent CDFT in 3D lattice

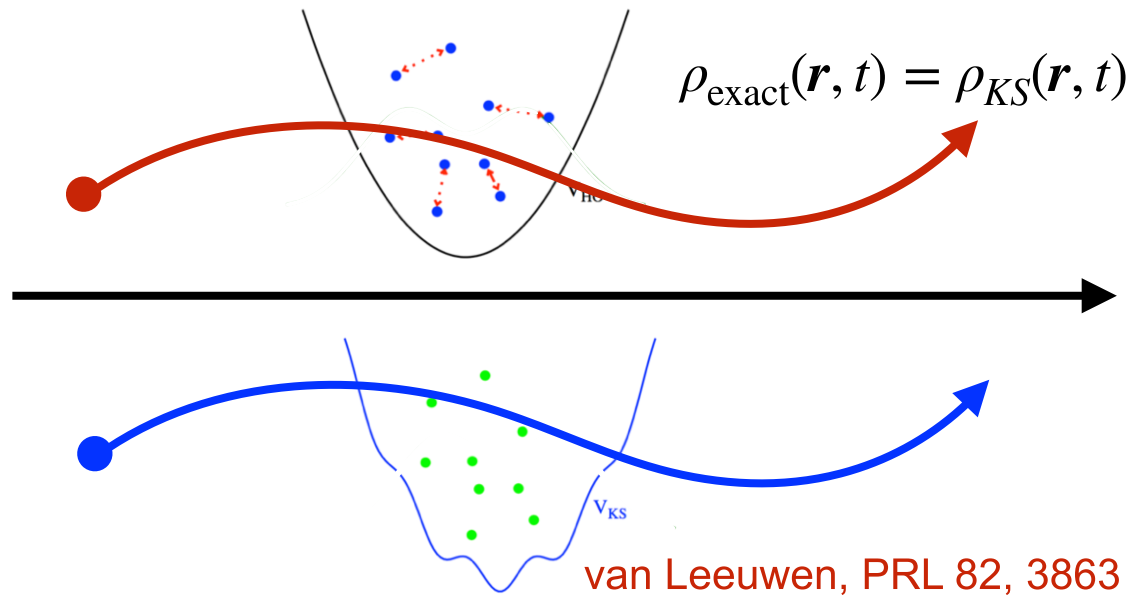
The many-body problem is mapped onto a one-body problem

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)

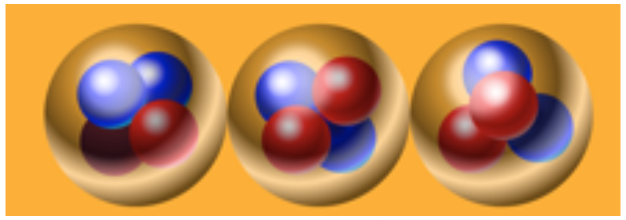
Ren, PWZ, Meng, PLB 801,135194 (2020)

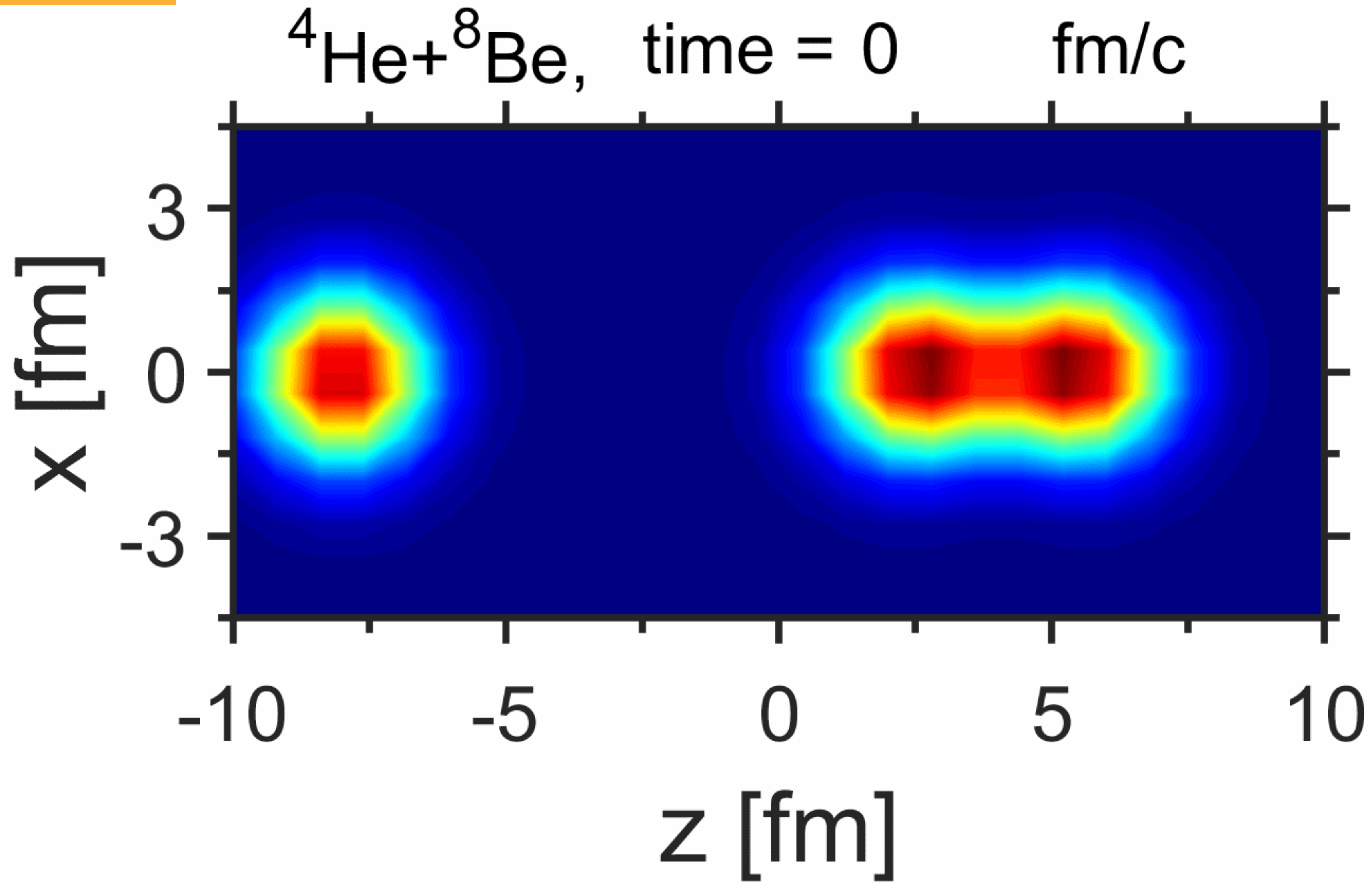
$$i\partial_t \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} m + V + S & \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} & -m + V - S \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}$$

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

Resonant scattering of ^{4}He + ^{8}Be

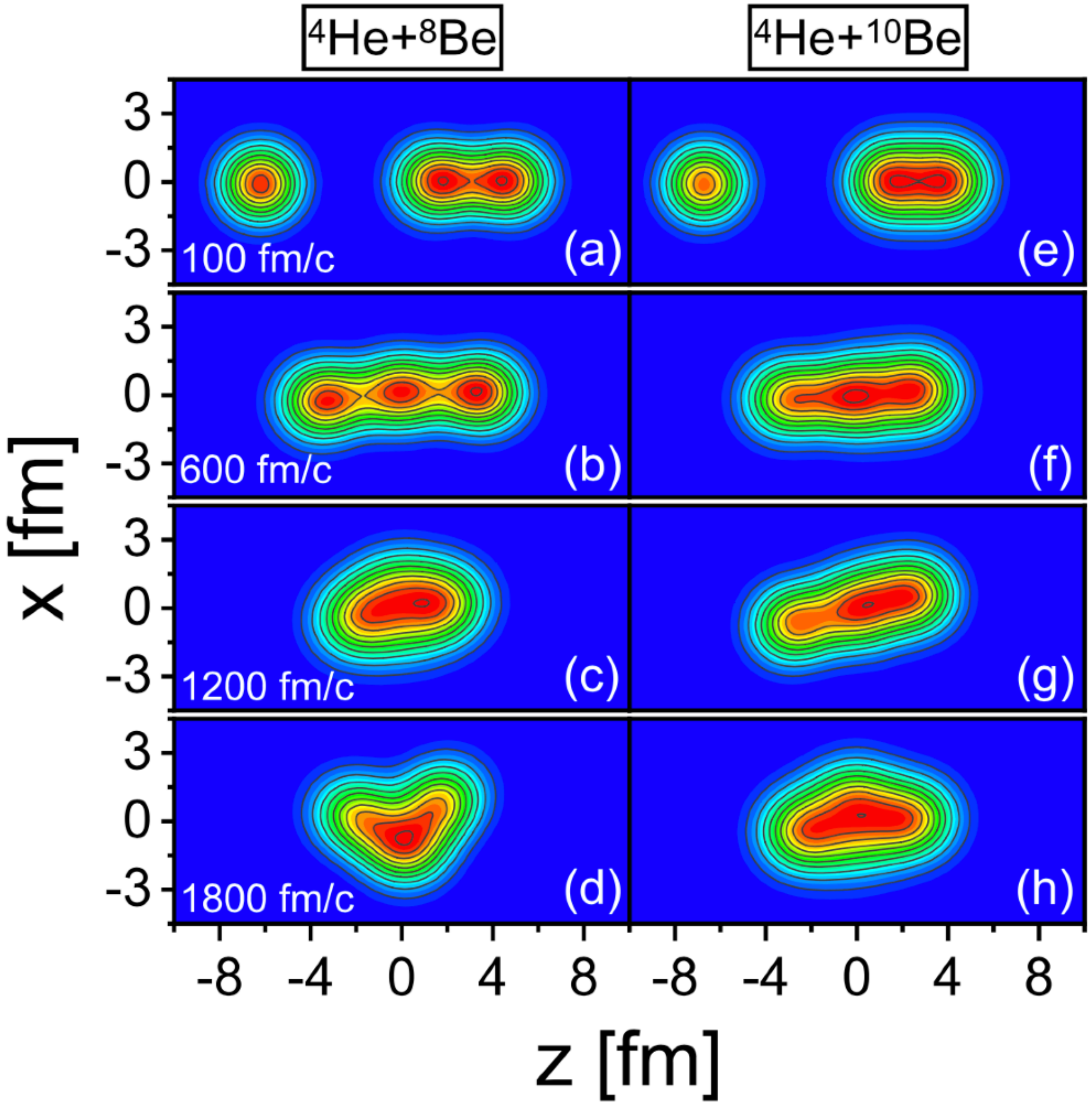
Ren, PWZ, Meng, PLB 801, 135194 (2020)

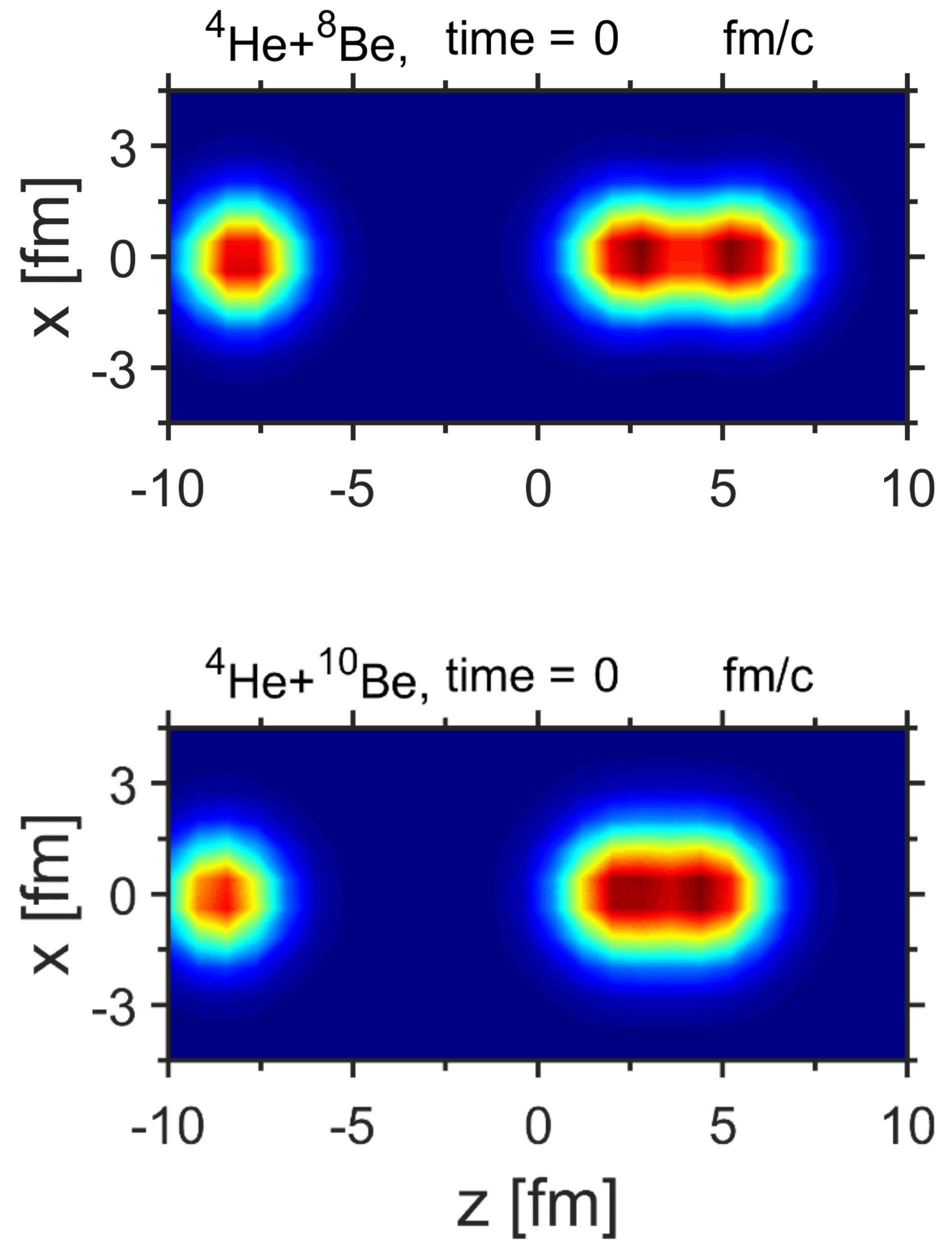




The linear-chain states are generated, and then evolve to a triangular configuration, and finally to a more compact shape.

$^4He + ^{10}Be$



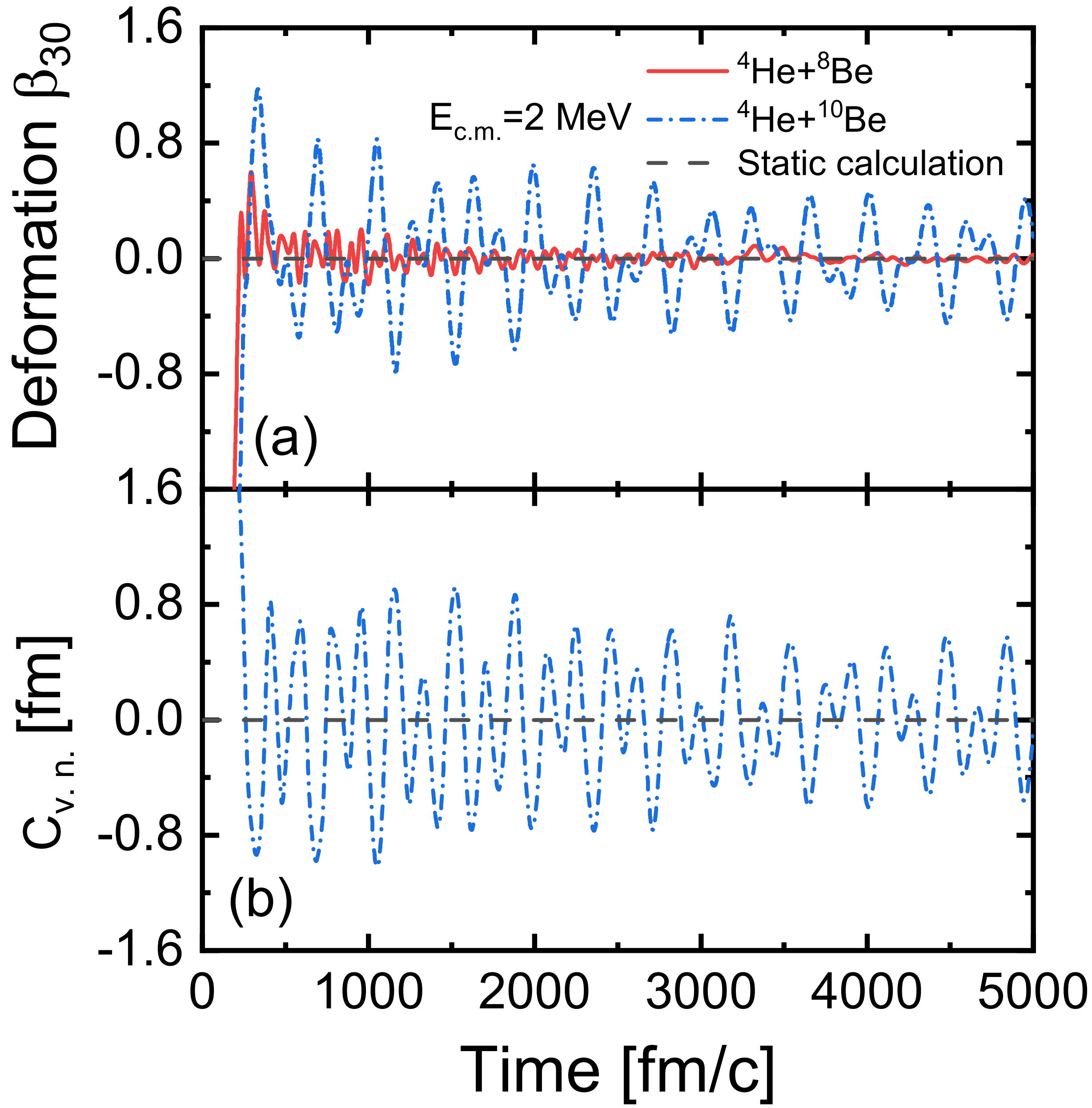


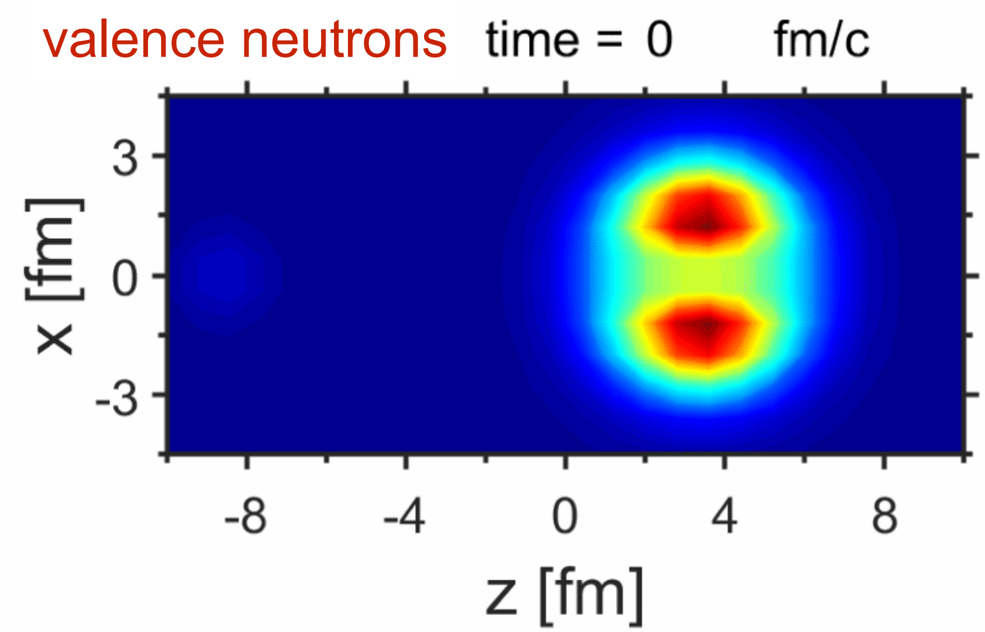
Ren, PWZ, Meng, PLB 801, 135194 (2020)

✓ The metastable linear chains can be formed in $^4He+^8Be$ and $^4He+^{10}Be$ collisions.

✓ During the time evolution of the linear-chain configuration, moving clusters can be found.

Octupole deformation



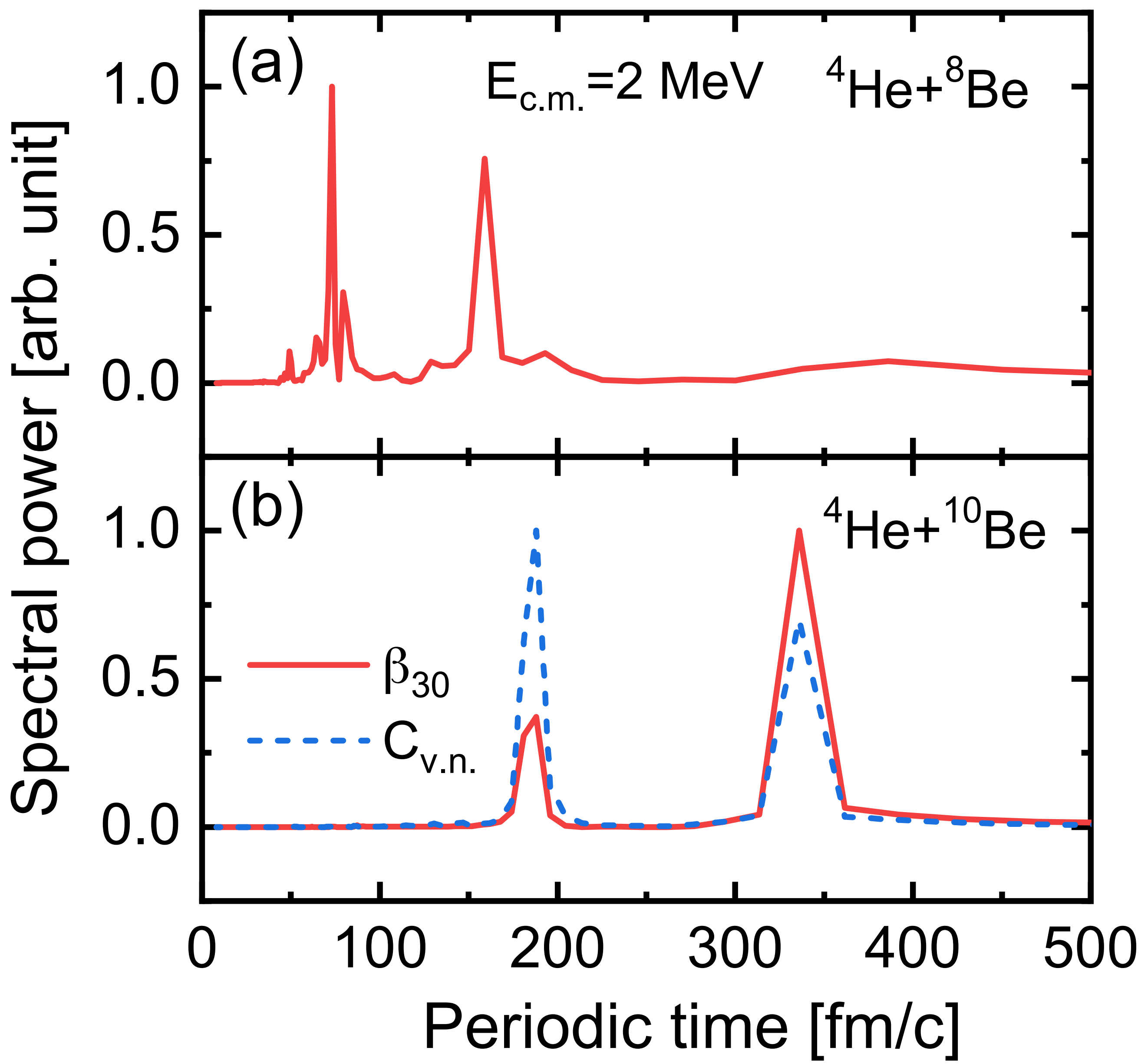


center of valence neutrons

$$C_{\mathrm{v.n.}} = \frac{\int d^3\boldsymbol{r}\, z(\rho_n - \rho_p)}{\int d^3\boldsymbol{r}\, (\rho_n - \rho_p)}$$

The oscillation of the two valence neutrons in the longitudinal direction induces the strong oscillation of the octupole deformation.

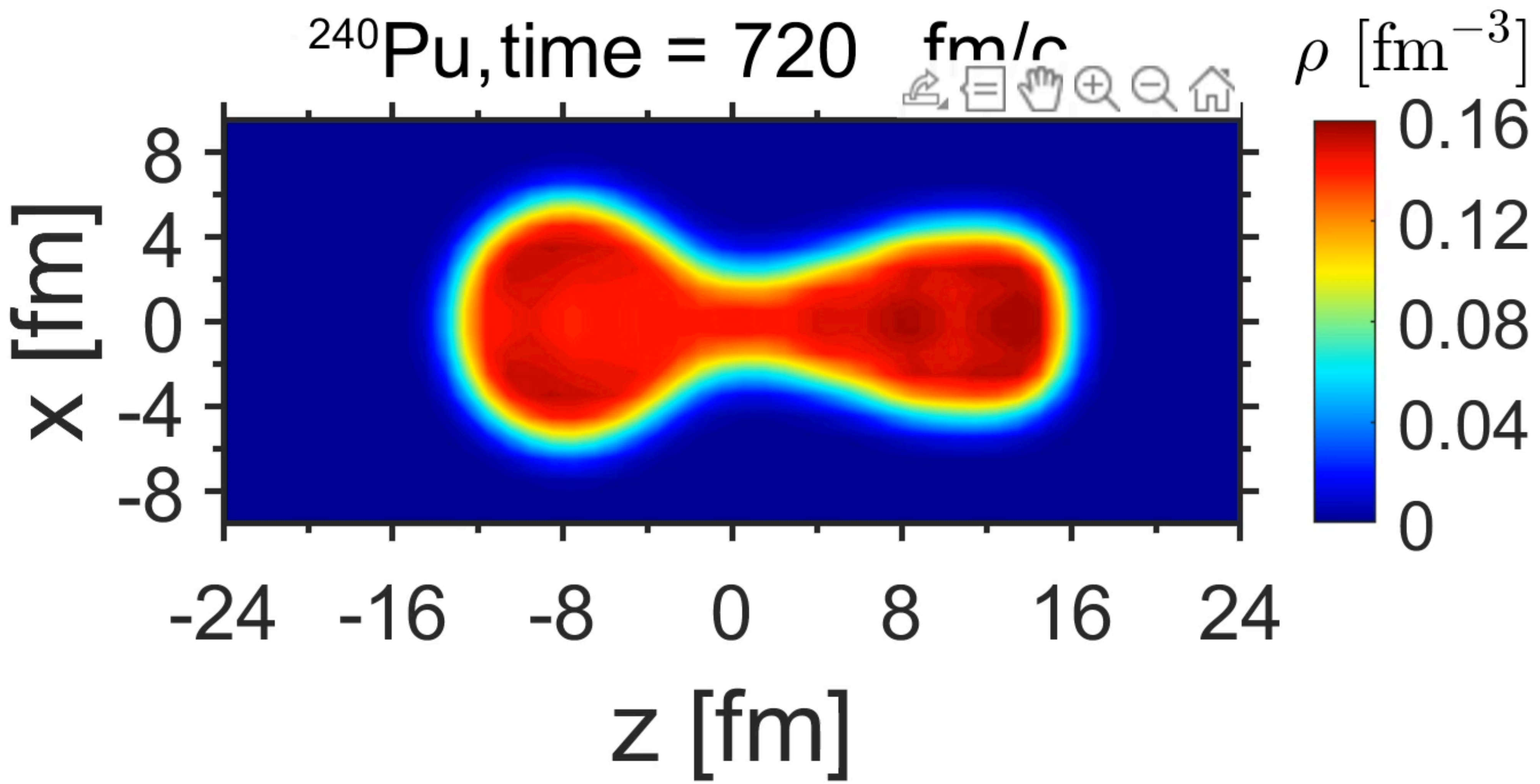
Dynamical isospin effects



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

Dynamical isospin effects: slowing down the longitudinal oscillations by the two valence neutrons.

^{240}Pu的裂变：核子密度分布



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

费米子局域化函数

$$D_{q\sigma}(\boldsymbol{r}) = \left[\sum_{\alpha\in q} |\boldsymbol{\nabla}\phi_\alpha(\boldsymbol{r},\sigma)|^2 - \frac{\left|\sum_{\alpha\in q}\phi_\alpha^*(\boldsymbol{r},\sigma)\boldsymbol{\nabla}\phi_\alpha(\boldsymbol{r},\sigma)\right|^2}{\rho_{q\sigma}(\boldsymbol{r})}\right]$$

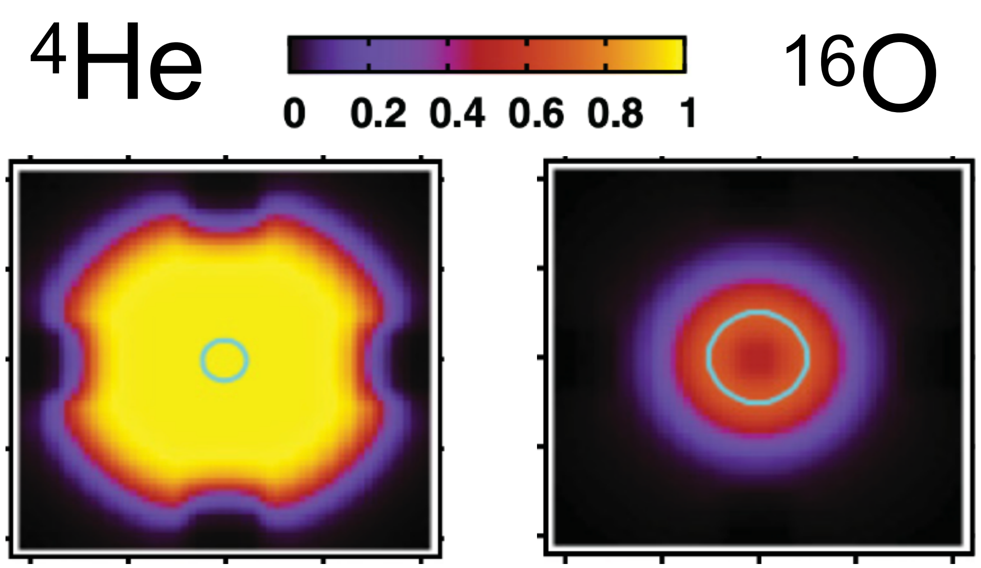
the probability of finding two like-particles in the vicinity of each other —〉 Localization!

Becke and Edgecombe, J. Chem. Phys., **92**, 5397 (1990)

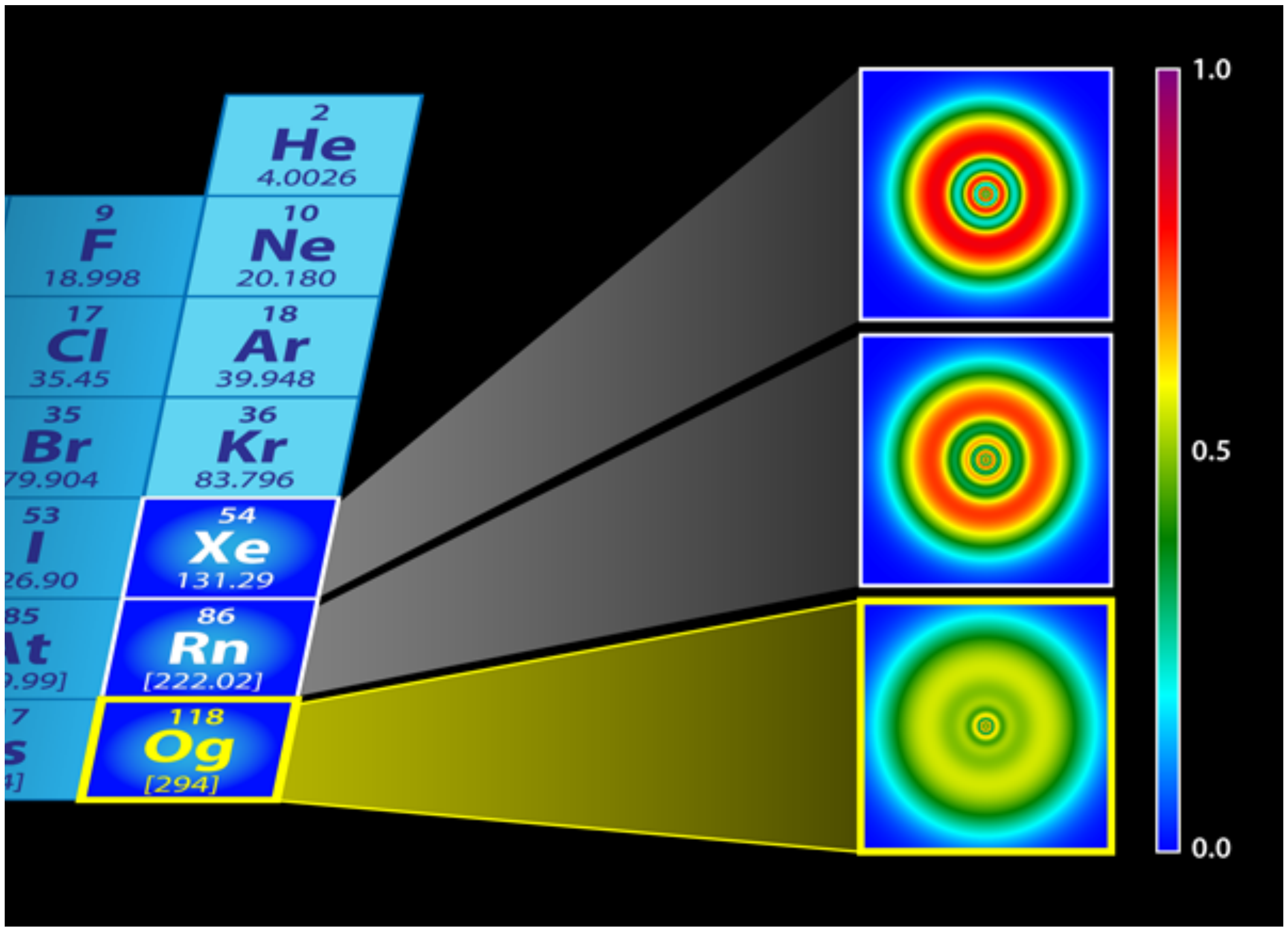
$$\mathcal{C}_{q\sigma}(\boldsymbol{r}) = \left[1 + \left(\frac{D_{q\sigma}(\boldsymbol{r})}{\tau_{q\sigma}^{\mathrm{TF}}(\boldsymbol{r})}\right)^2\right]^{-1}$$

C = 1/2; Thomas-Fermi Gas

C = 1; Highly Localized



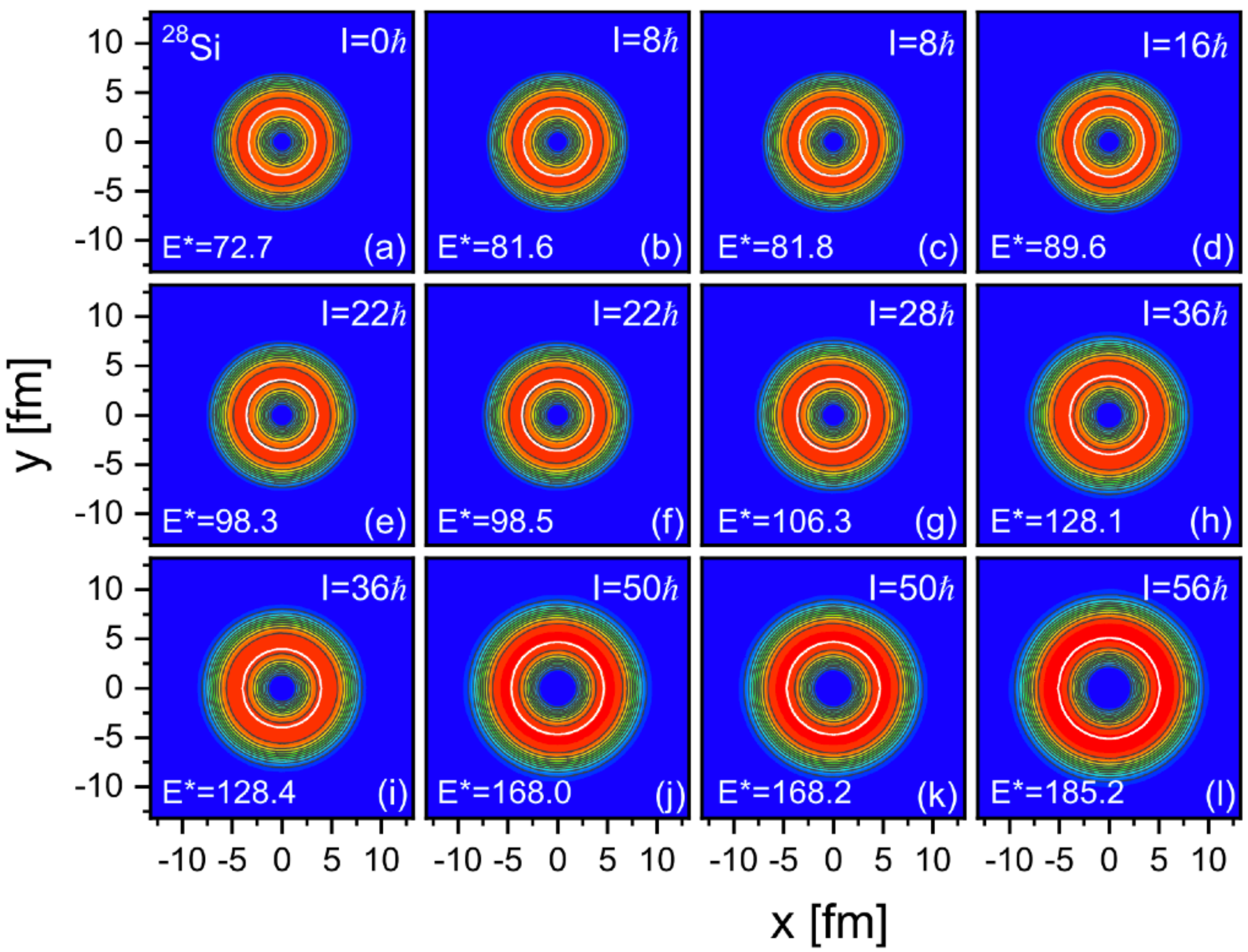
Reinhard, et al., Phys. Rev. C **83**, 034312 (2011)



Jerabek et al., Phys. Rev. Lett. 120, 053001 (2018)

核子局域化函数

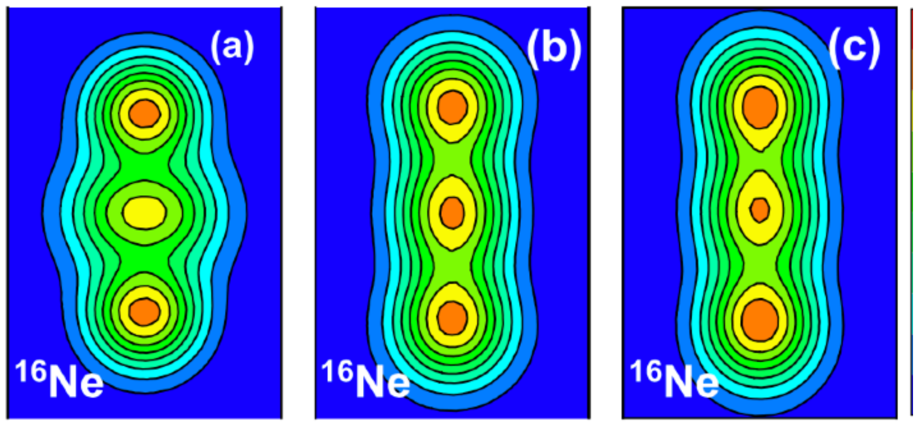
Toroidal states in ^{28}Si



Cao et al., Phys. Rev. C, **99**, 014606 (2019)

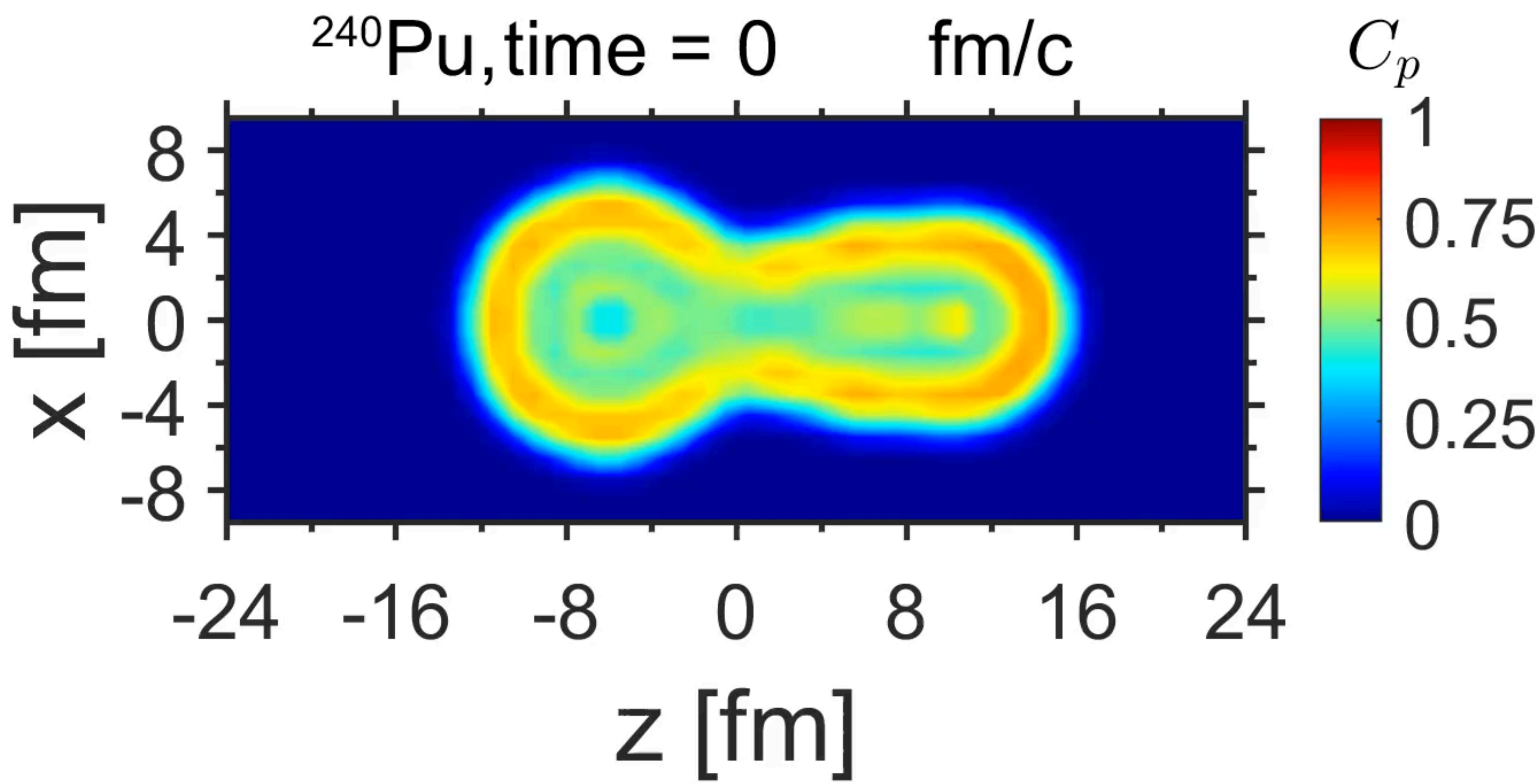
Ren, PWZ, Zhang, Meng, Nucl. Phys. A, **996**, 121696, (2020)

molecular α-chain nuclei



Zhang, Ren, PWZ, Vretenar, Nikšić, Meng, PRC, 105, 024322 (2022)

240Pu的裂变：核子局域化函数



三分裂、四分裂?

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

Take away message

Alpha and alpha cluster in nuclei have been investigated by developing the relativistic variational Monte Carlo method and the relativistic density functional theory.

- **A single alpha**
  - ✓ Relativistic VMC with artificial neural network

    relativistic effects avoid the energy collapse

    a strong interplay between the relativistic effects and three-body force

- **Anomalously rod-shaped nuclei**
  - ✓ Static calculations with reflection symmetry imposed

    coherent effects between spin and isospin could stabilize the rod shape
  - ✓ Static calculations without any symmetry imposed

    rod shapes as energy minima at a certain range of rotational frequencies
  - ✓ Dynamic calculations with the time dependent CDFT

    dynamical isospin effects slowing down the longitudinal oscillations

- **Fission dynamics**
  - ✓ Timescale of neck formation coincides with the assembly of two α-like clusters
  - ✓ The neck ruptures at a point exactly between the two α-like clusters
  - ✓ Opens exciting possibilities for a microscopic study of ternary fission

Collaborations

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Thank you for your attention!