



Exchange correlation effects in nuclear novel phenomena

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Lanzhou University

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OUTLINE

□ Introductions

- Nuclear novel phenomena and the challenges
- Relativistic Hartree-Fock (RHF) theory and the extensions

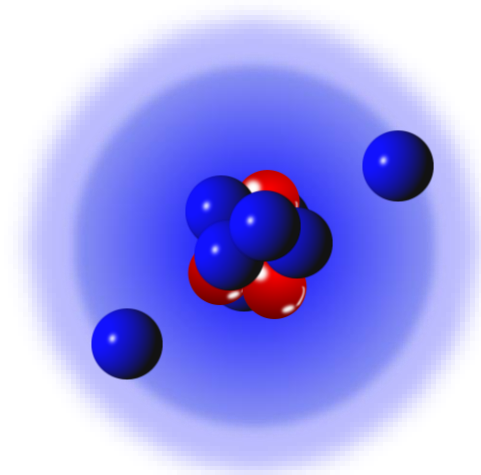
□ Recent developments of the RHF theory

- Deformed relativistic Hartree-Fock-Bogoliubov (D-RHFB) model
- Configuration-Interaction relativistic Hartree-Fock (CI-RHF) model

□ Exchange correlation effects

- Spherical halo phenomena at the drip line of Ce isotopes
- Deformed halo structure in ^{19}C
- Nature of the island of inversion exhibited by ^{32}Mg

□ Conclusions



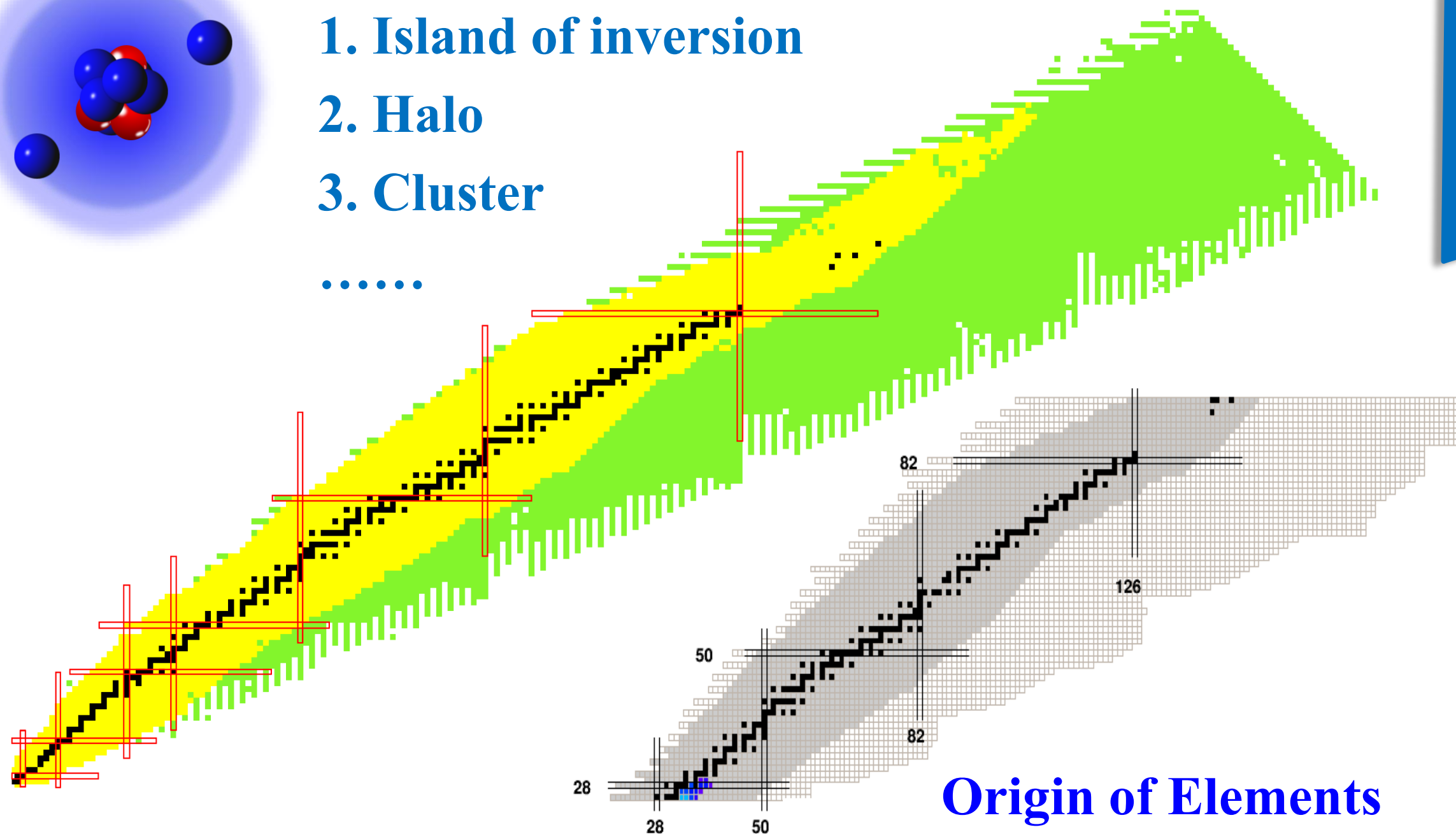
Novel Phenomena

1. Island of inversion

2. Halo

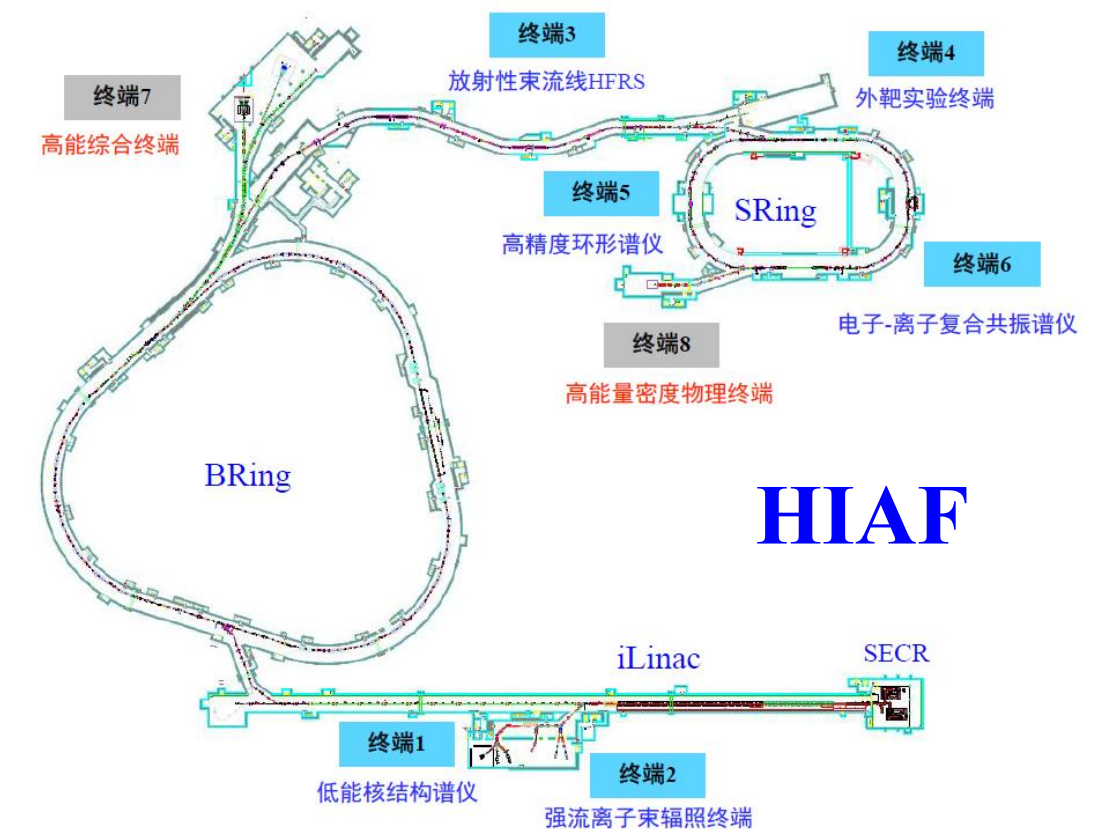
3. Cluster

.....



Origin of Elements

- ☐ Nucleon-Nucleon Interaction
- ☐ Origin of Heavy Elements
- ☐ Island of Superheavy nuclei

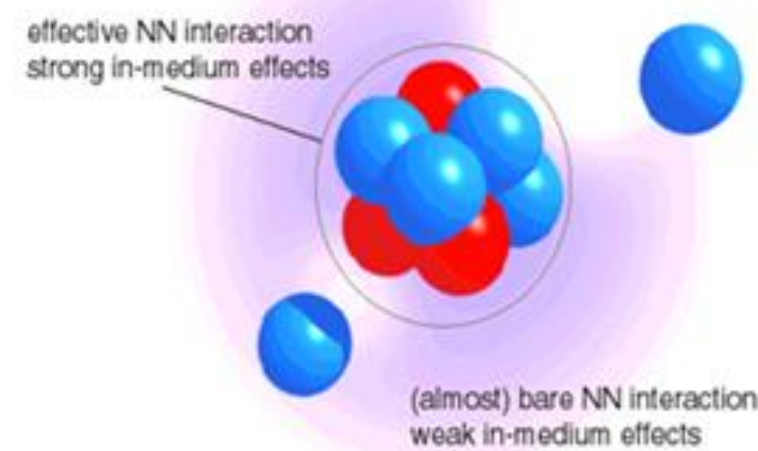
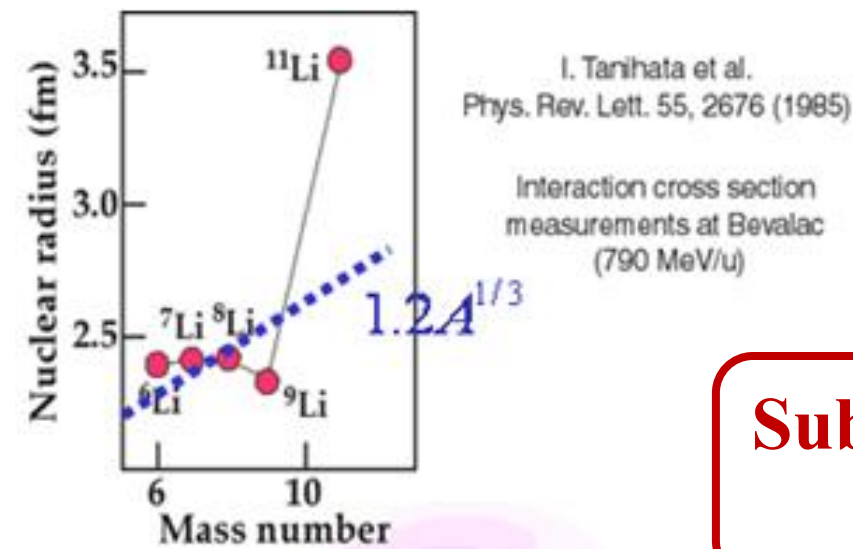


Call for comprehensive understanding on the nature of unstable nuclei



Halo and the challenges

- The first candidate of halo nuclei: ^{11}Li



I. Tanihata et al., PRL **55** (1985) 2676

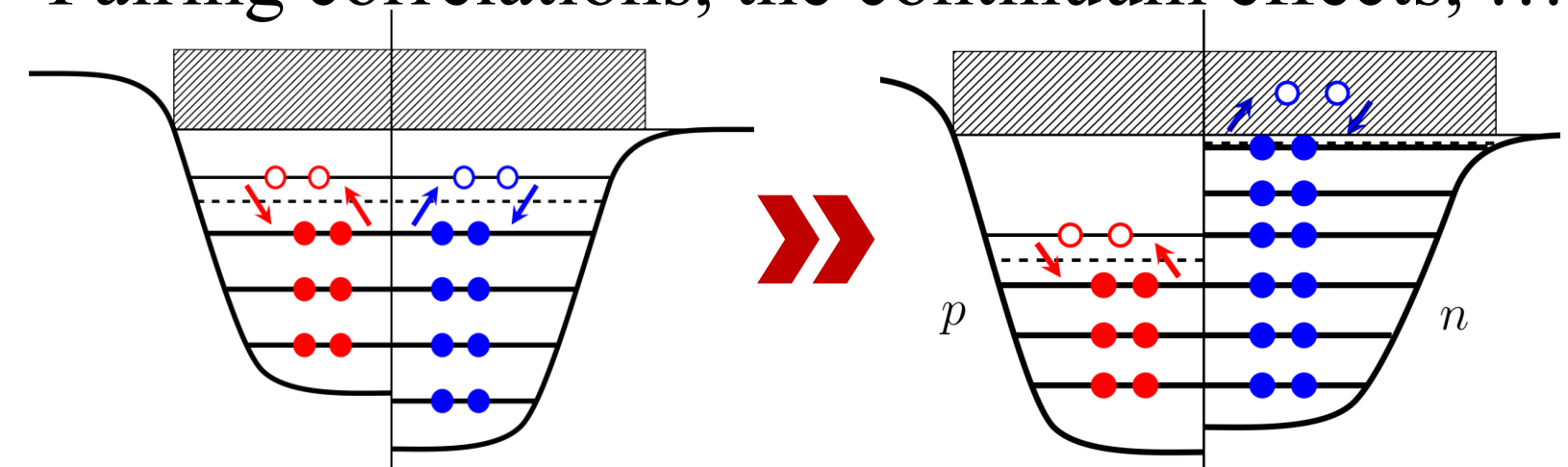
Extraordinary
matter radius

Subvert the conventional
knowledge

Dilute matter
distribution

1. Weak binding mechanism

Pairing correlations, the continuum effects, ...



Meng et al., PPNP **57** (2006) 470

2. Nuclear deformation

Deformed Halo, cluster, island of inversion, ...

3. Nuclear many-body state

Mean field approach, AMP, GCM, SM, ...

How nucleons spontaneously form an atomic nucleus

Nuclear force & Nuclear many-body method



Relativistic Hartree-Fock (RHF) theory

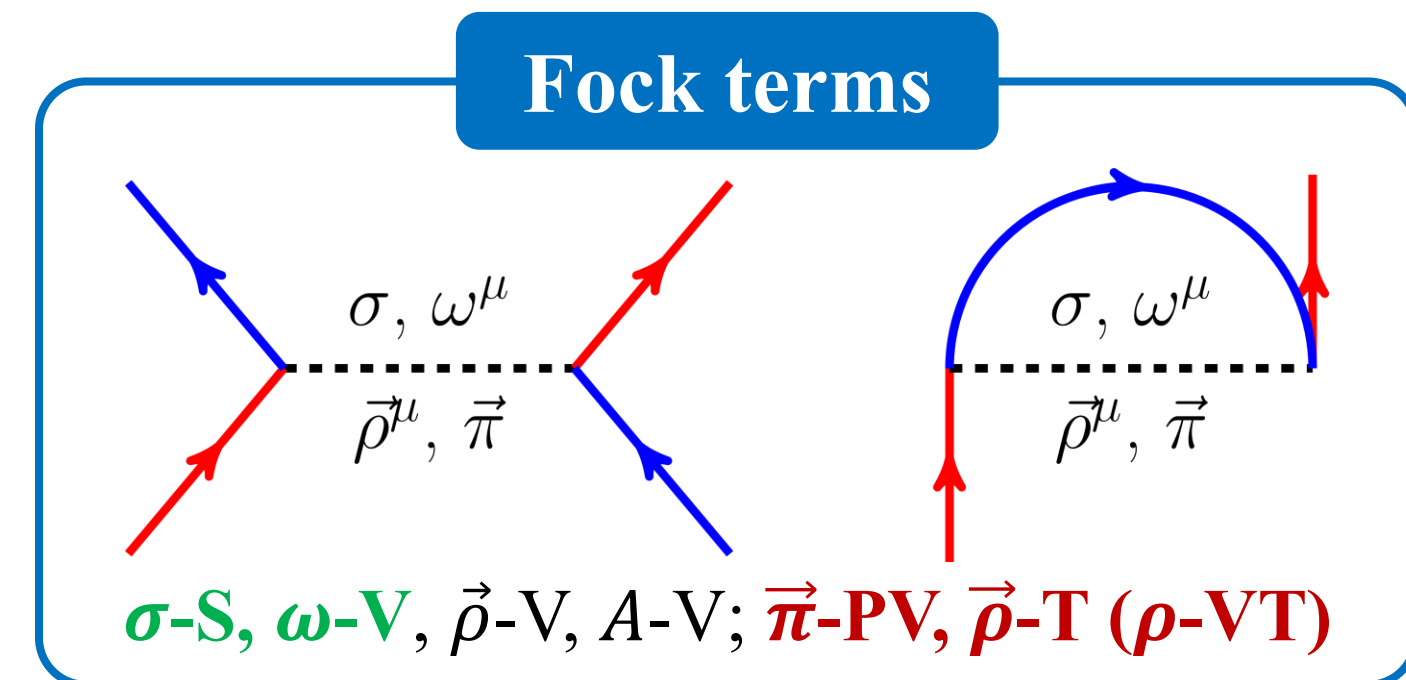
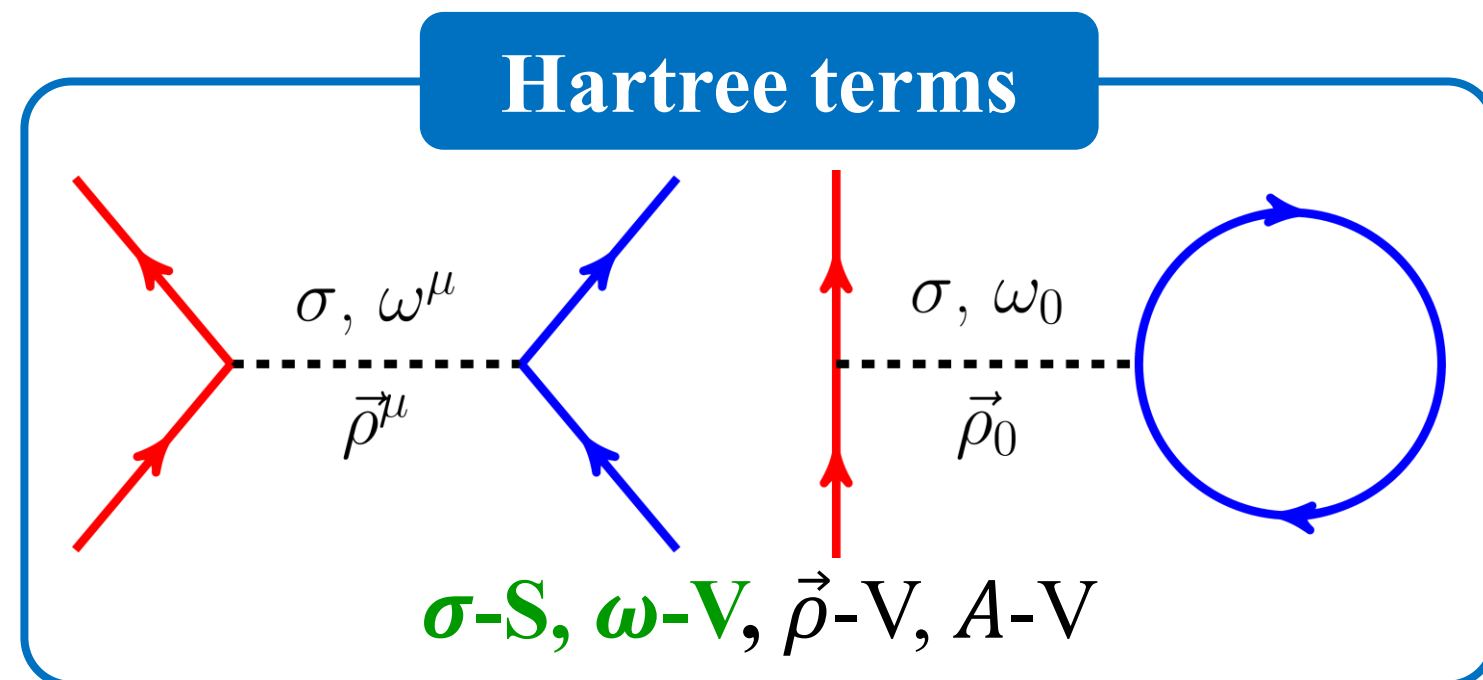


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- **Relativity**: Interplay between **strong scalar attraction** and **vector repulsion**

Natural spin-orbit coupling, the origin of pseudo-spin symmetry and spin symmetry, ...

Meng et al., PPNP **57**, 470 (2006); Ginocchio, PRL **78**, 436 (1997); Meng et al., PRC **58**, R628 (1998); Zhou et al., PRL **91**, 262501 (2003).



- **Fock terms**: pure exchange degrees of freedom (DoF) such as **$\pi\text{-PV}$** and **$\rho\text{-T} (\rho\text{-VT})$**

Impact the modeling of nuclear binding, nuclear tensor force, ...

PRC **100**, 051301(R) (2019)

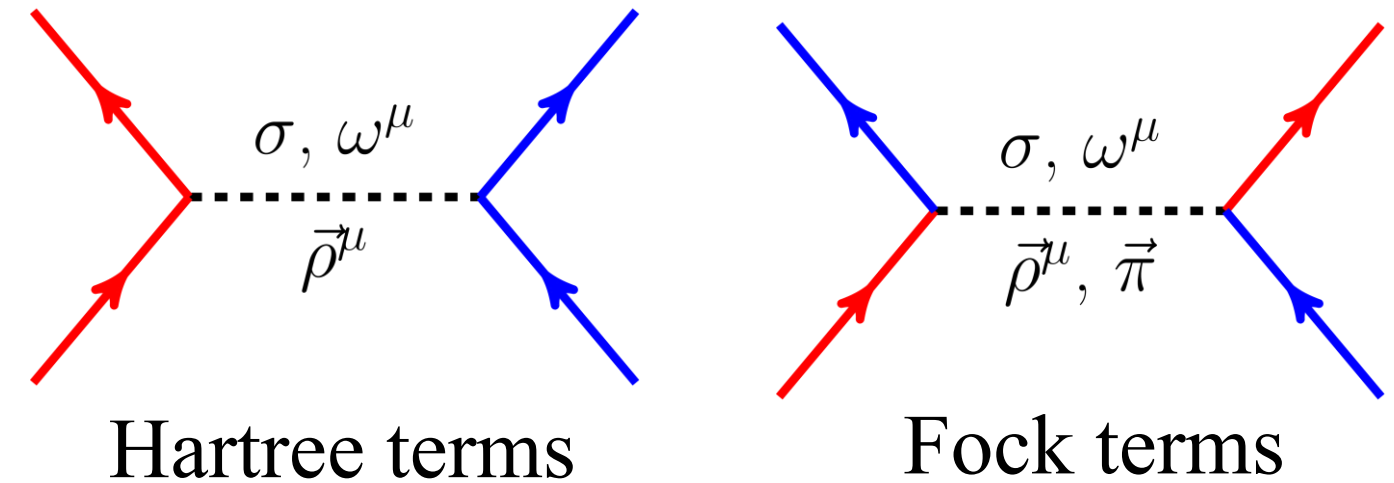
PRC **91**, 034326 (2015); CPC **42**, 024101 (2018); PRC **98**, 034313 (2018); PRC **101**, 064306 (2020)

Exchange correlation effects in nuclear novel phenomena?



- Nuclear in-medium effects
 1. Non-linear self-couplings of meson fields
 2. Density-dependent coupling strengths
- Effects of many-body correlations in nuclei**

- RHF Lagrangians PKO*i* and PKA1
similar quantitative accuracy as popular DFT



WHL, Giai, Meng, PLB **640**, 150 (2006); WHL, Sagawa, Giai, Meng, PRC **76**, 034314 (2007); EPL **82**, 12001 (2008).

PKO2
 σ -S, ω -V
 ρ -V, A-V
Conventional
DoF



PKO1, PKO3
 σ -S, ω -V
 ρ -V, A-V + π -PV
Exchange DoF
 π -PV



PKA1
 σ -S, ω -V
 ρ -V, A-V + π -PV
Exchange DoF
 π -PV & ρ -T

PK: PKU
O: Orsay
A: Aizu

Pave a way to reveal the underlying effects of the exchange correlations



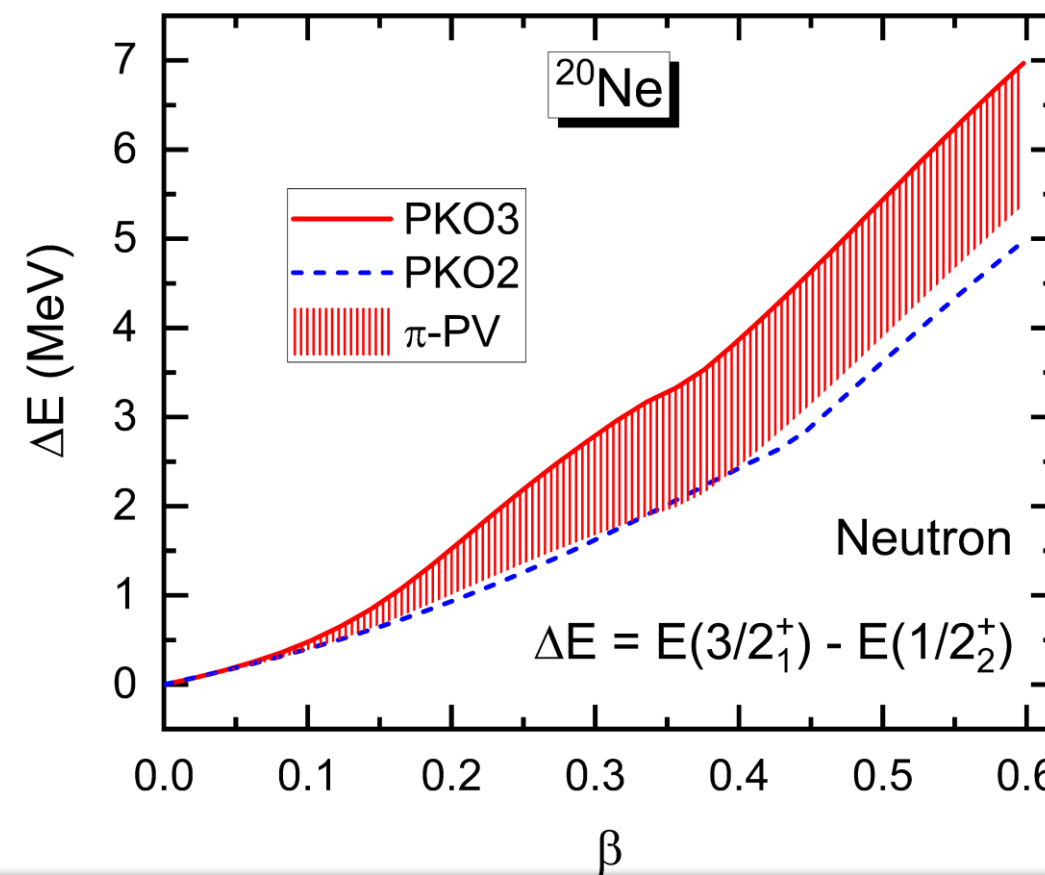
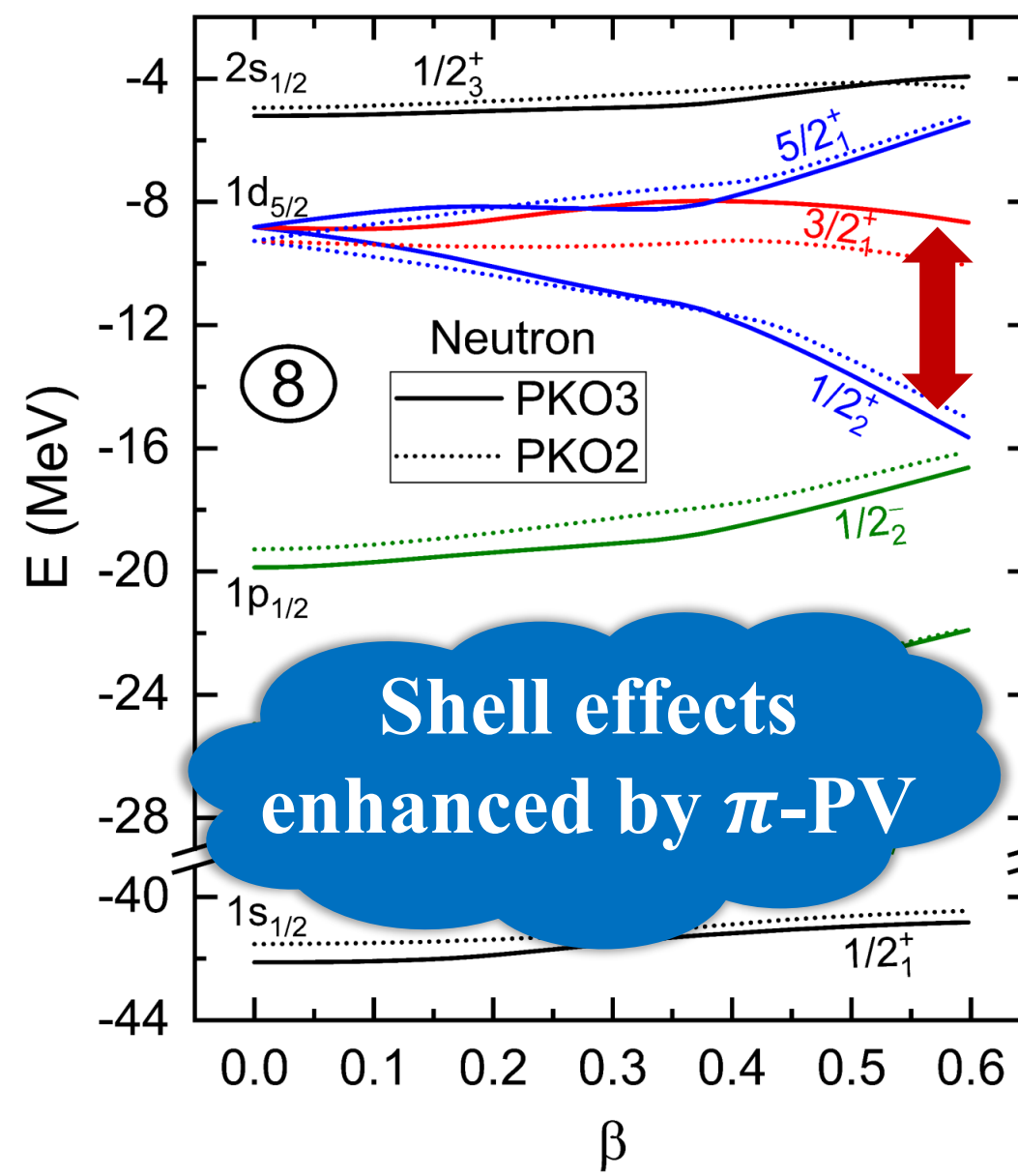
Axially deformed RHF (D-RHF) model: **deformation**

□ Spherical Dirac Woods-Saxon (DWS) basis

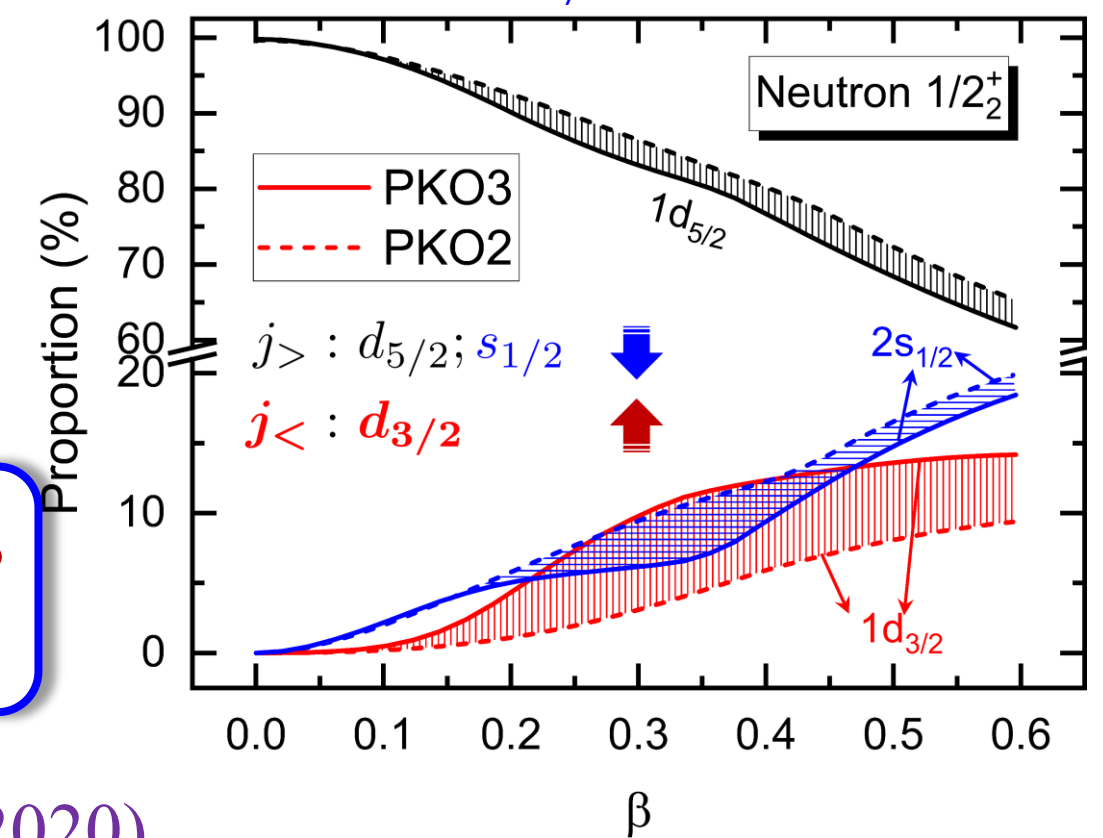
Zhou, Meng, Ring, PRC **68**, 034323 (2003)

- **Appropriate asymptotic behaviors** of wave functions
- **Microscopic insight** into deformed nuclei: tensor force effects

sd 壳 { $1d_{3/2}$
 $2s_{1/2}$
 $1d_{5/2}$ } PKO2
w/o π
VS
(8) PKO3
with π
 $1p_{1/2}$
 $1p_{3/2}$



π -T: more $1d_{3/2}$ but less $1d_{5/2}$ waves mixing in $1/2_2^+$ orbit



Geng, Xiang, Sun, WHL, PRC **101**, 064302 (2020)



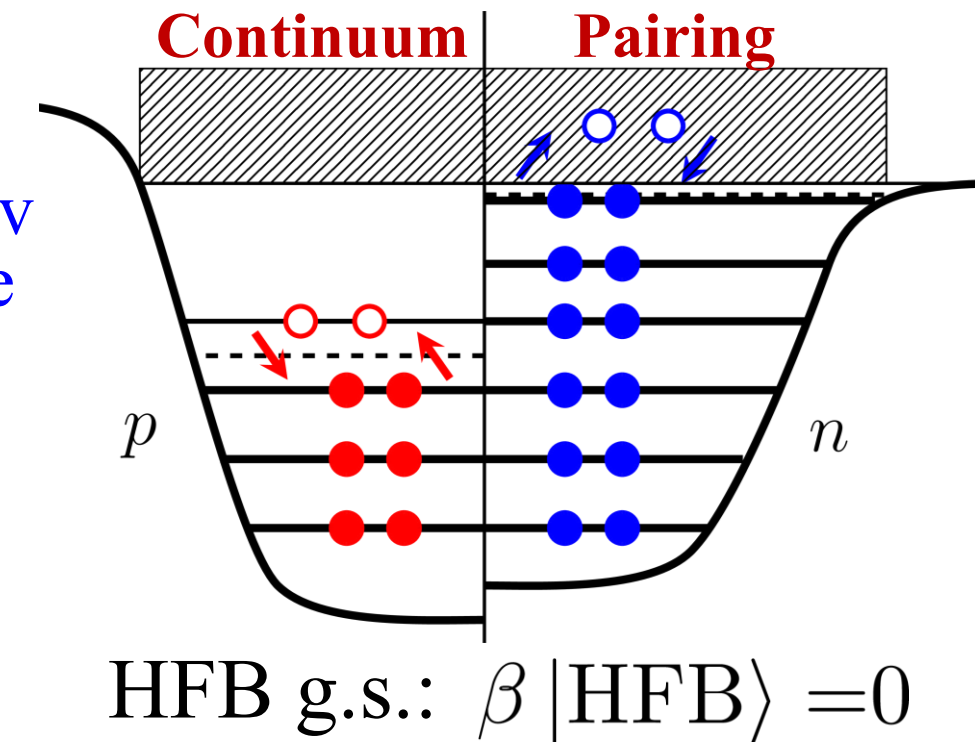
Axially deformed RHFB (D-RHFB) model

□ Bogoliubov transformation: Bloch-Messiah decomposition

$$\text{HF s.p. space } (c, c^\dagger) \xrightarrow{D} (a, a^\dagger) \xrightarrow{\bar{U}, \bar{V}} (\alpha, \alpha^\dagger) \xrightarrow{C} (\beta, \beta^\dagger) \text{ Bogoliubov q.p. space}$$

□ Quantize Dirac spinor in Bogoliubov quasi-particle space

$$\psi(x) = \sum_k \left[\psi_k^U(x) \beta_k + \psi_k^V(x) \beta_k^\dagger \right] \quad H = \hat{T} + \sum_\phi \hat{V}_\phi$$



$$\hat{T} = \int d\mathbf{x} \sum_{kk'} \bar{\psi}_k^V (-i\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} + M) \psi_{k'}^V \beta_k \beta_{k'}^\dagger$$

Geng, WHL, PRC 105, 034329 (2022)

$$\begin{aligned} \hat{V}_\phi = & \frac{1}{2} \iint d\mathbf{x}_1 d\mathbf{x}_2 \sum_{k_1 k'_1} \sum_{k_2 k'_2} \bar{\psi}_{k_1}^V(x_1) \bar{\psi}_{k_2}^V(x_2) \Gamma_\phi D_\phi \psi_{k'_2}^V(x_2) \psi_{k'_1}^V(x_1) \beta_{k_1} \beta_{k_2} \beta_{k'_2}^\dagger \beta_{k'_1}^\dagger \quad \text{Hartree} \\ & \quad \quad \quad \text{Mean field} \\ & \quad \quad \quad \text{Fock} \\ & + \frac{1}{2} \iint d\mathbf{x}_1 d\mathbf{x}_2 \sum_{k_1 k'_1} \sum_{k_2 k'_2} \bar{\psi}_{k_1}^V(x_1) \bar{\psi}_{k_2}^U(x_2) \Gamma_\phi D_\phi \psi_{k'_2}^U(x_2) \psi_{k'_1}^V(x_1) \beta_{k_1} \beta_{k_2}^\dagger \beta_{k'_2} \beta_{k'_1}^\dagger \quad \text{Pairing correlations} \end{aligned}$$

Unified treatment: spin-orbit and tensor forces, deformation, pairing correlations & the continuum



Configuration-Interaction RHF (CI-RHF) model



Effective Hamiltonian based on RHF model

$$H = E_{\text{core}} + \sum_{ii'} \varepsilon_{ii'} :c_i^\dagger c_{i'}: + \frac{1}{4} \sum_{ij i' j'} \bar{V}_{ij i' j'} :c_i^\dagger c_j^\dagger c_{j'} c_{i'}:$$

EKK scheme

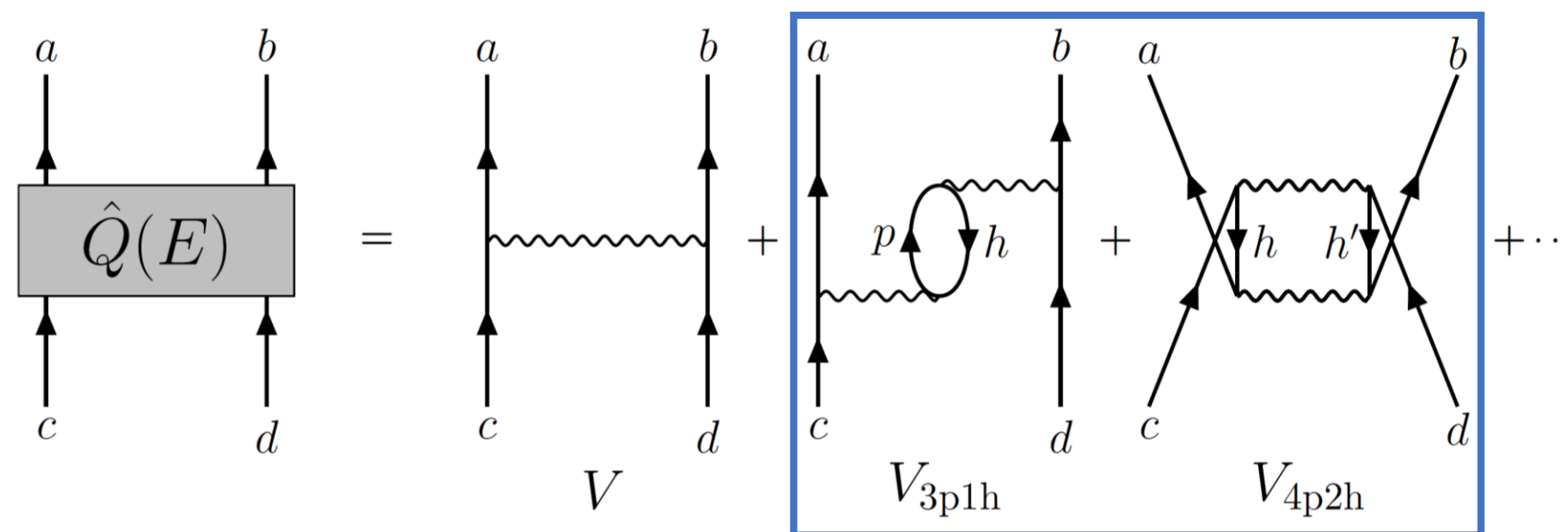
$$H_l^{\text{eff}} = H^{\text{BH}}(E_0) + \sum_{k=1}^{\infty} \frac{1}{k!} \frac{d^k \hat{Q}(E_0)}{dE_0^k} \{H_{l-1}^{\text{eff}} - E_0\}^k$$

Folded terms

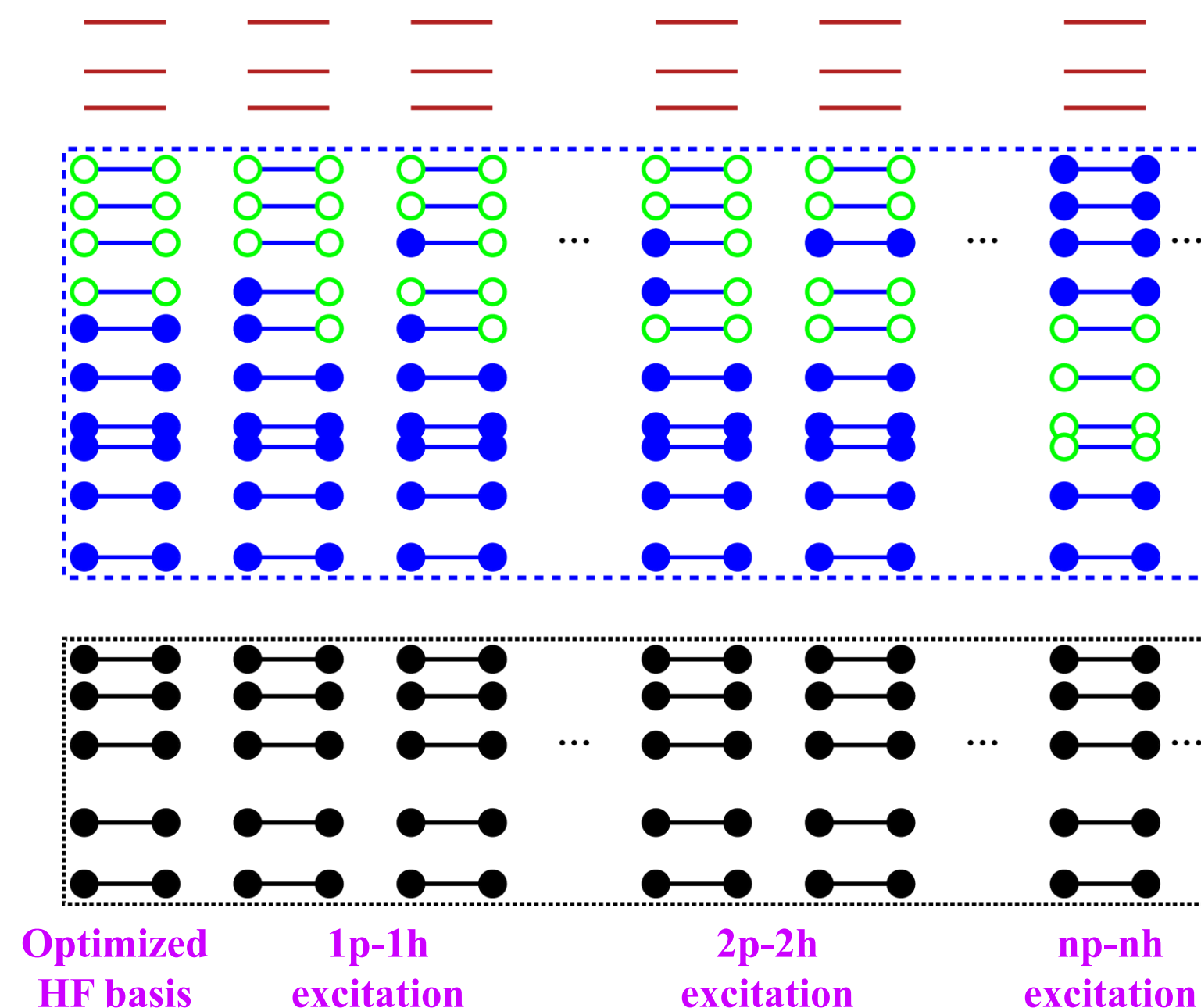
$\hat{Q}$ -box expansion

$$\hat{Q}(E) = \sum_{l=0}^{\infty} P \left[V \frac{Q}{E - H_0} \right]^l V P$$

Core polarization



J. Liu, Y.F. Niu, WHL, CPC **49**, 064104 (2025)



$$|\Psi\rangle = \sum_n C_n |\Phi_n\rangle, \quad |\Phi_n\rangle = \prod_{i=1}^{A-N_{\text{core}}} c_{n_i}^\dagger |\text{core}\rangle$$

Brown et al. PLB **695** (2011) 507...



- Without introducing any new parameters, the effective Hamiltonian constrained by the existing RHF Lagrangians works well for describing the low-lying excitations

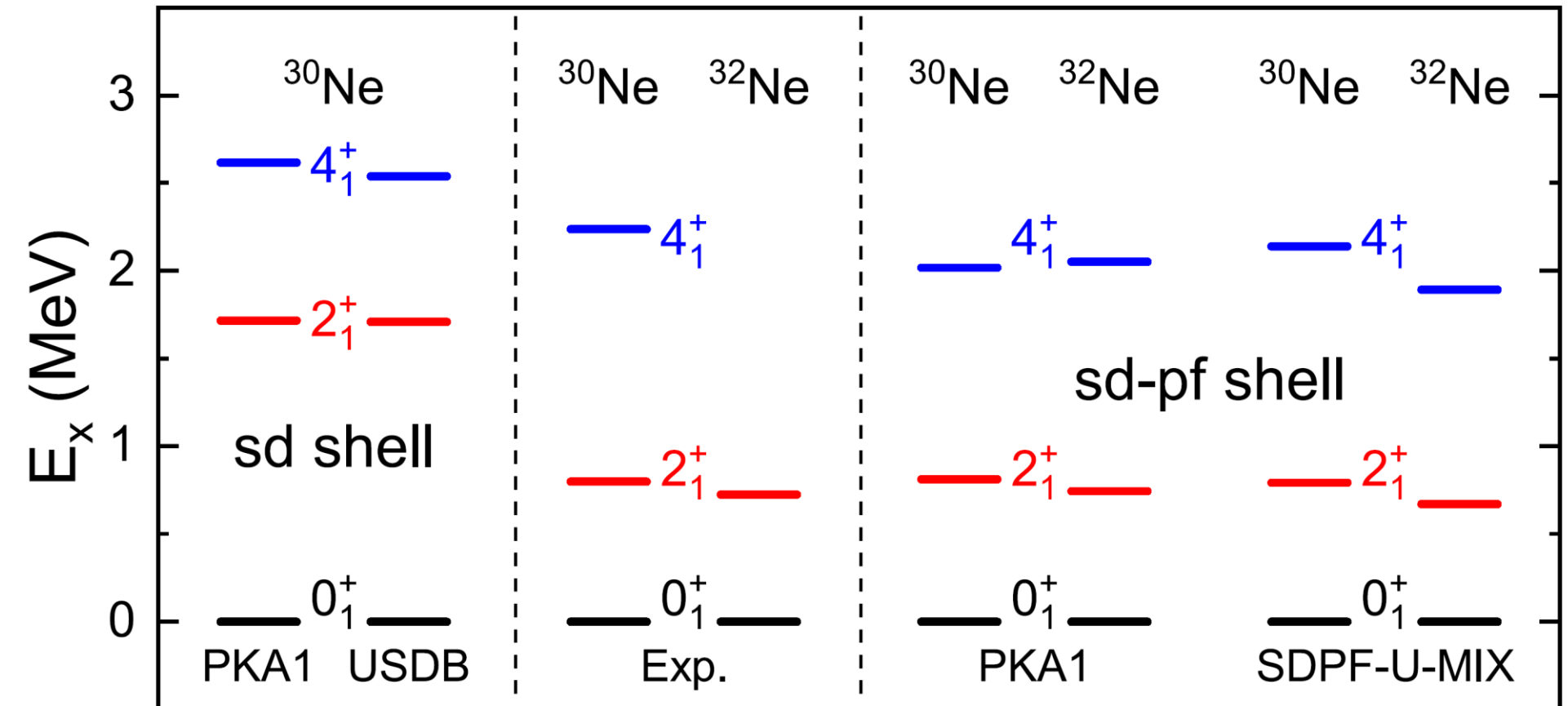
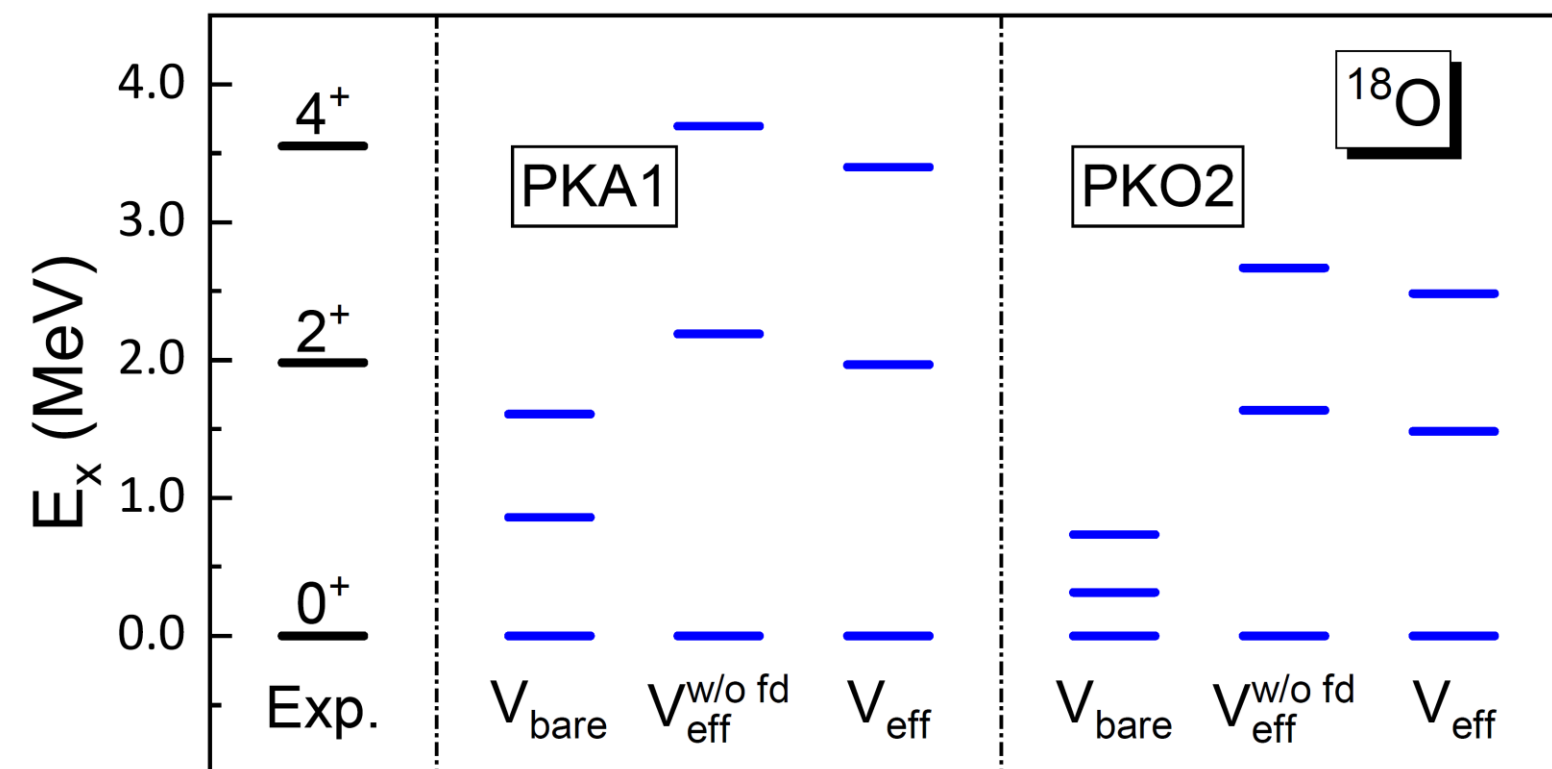
Folded terms & core polarizations

are necessitated for precise description

J. Liu, Y.F. Niu, WHL, CPC 49, 064104 (2025)

Extending from sd shell to sd-pf shell

PKA1 seems better than PKO series



An efficient tool to describe the g.s. and low-lying excitations of unstable nuclei

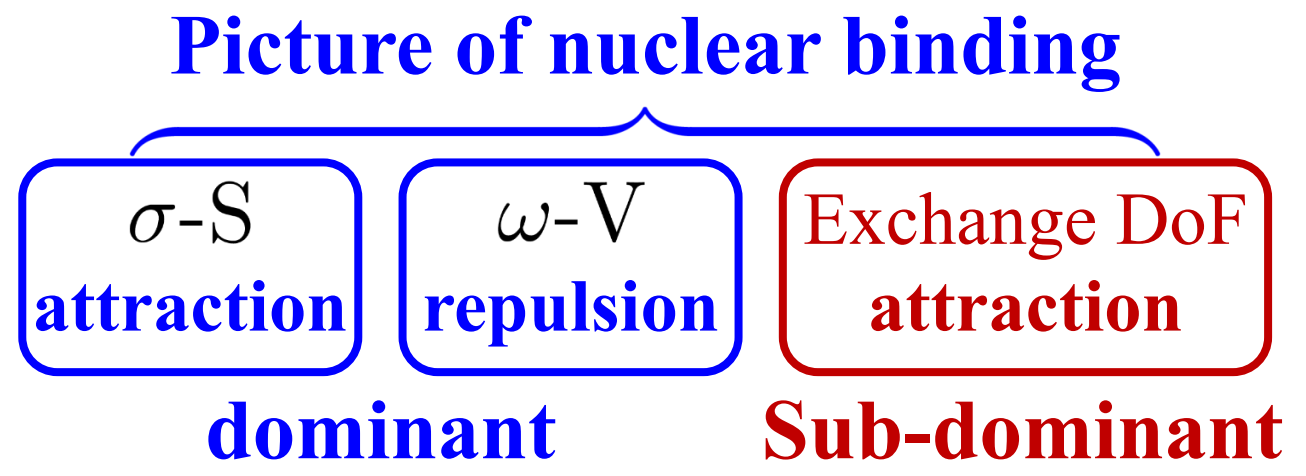


❑ Exchange degrees of freedom (π -PV and ρ -T) change the modeling of nuclear binding

RMF (DD-ME2) $\gg$ RHF (PKO3: plus π -PV) $\gg$ RHF (PKA1: plus π -PV & ρ -T)

Modeling of nuclear binding for ^{208}Pb

Models	$E_{\text{kin.}+\text{c.m.}}$	$E_{\sigma+\omega}$	$E_{\rho+\pi}$	$E_{\text{cou.}}$	Total
DD-ME2	2629.1	-5194.0	+100.3	827.2	-1637.4
PKO3	2823.2	-4609.7	-648.7	798.4	-1636.8
PKA1	2498.9	-3298.9	-1634.8	798.6	-1636.3



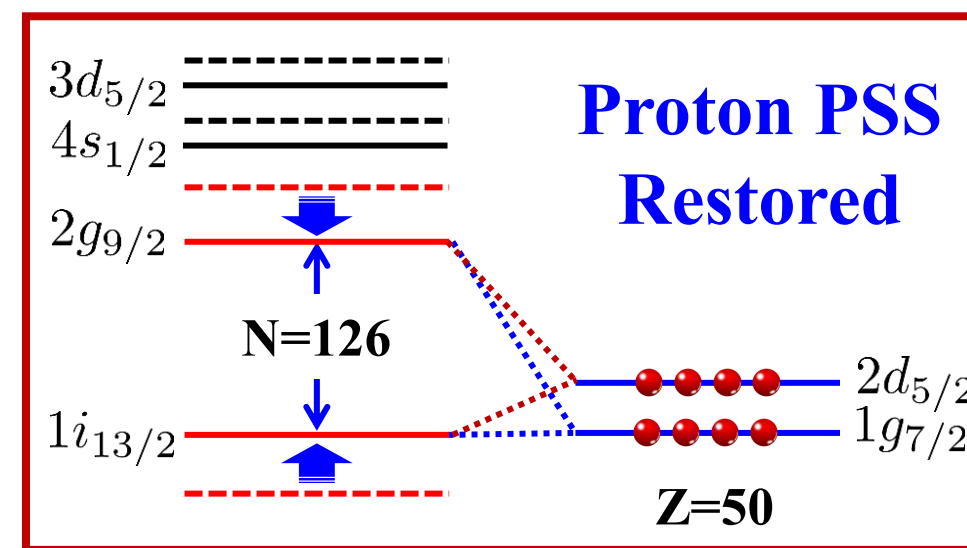
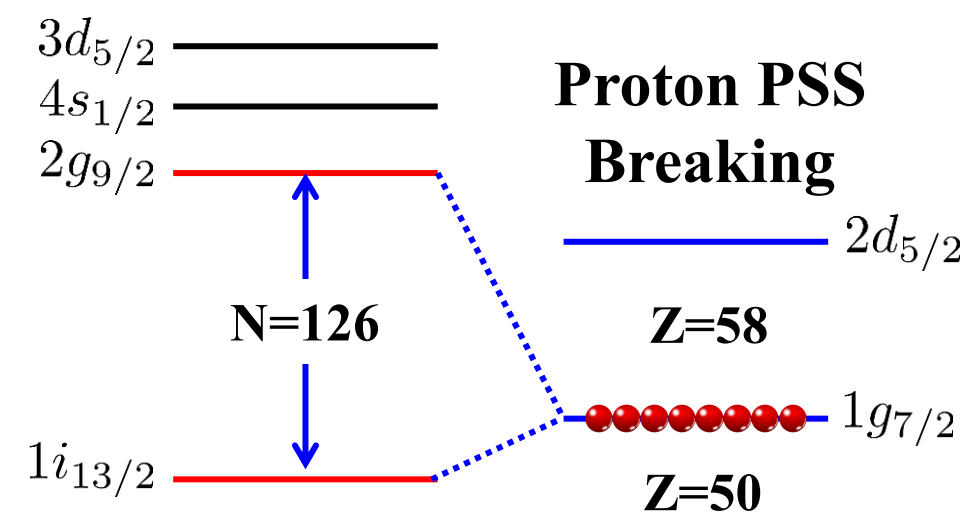
Fock terms, particularly the exchange degrees of freedom (DoF), impact the nuclear binding,

Geng, Li, WHL, Niu, Chang, PRC 100, 051301(R) (2019)



Giant halo in Ce isotopes

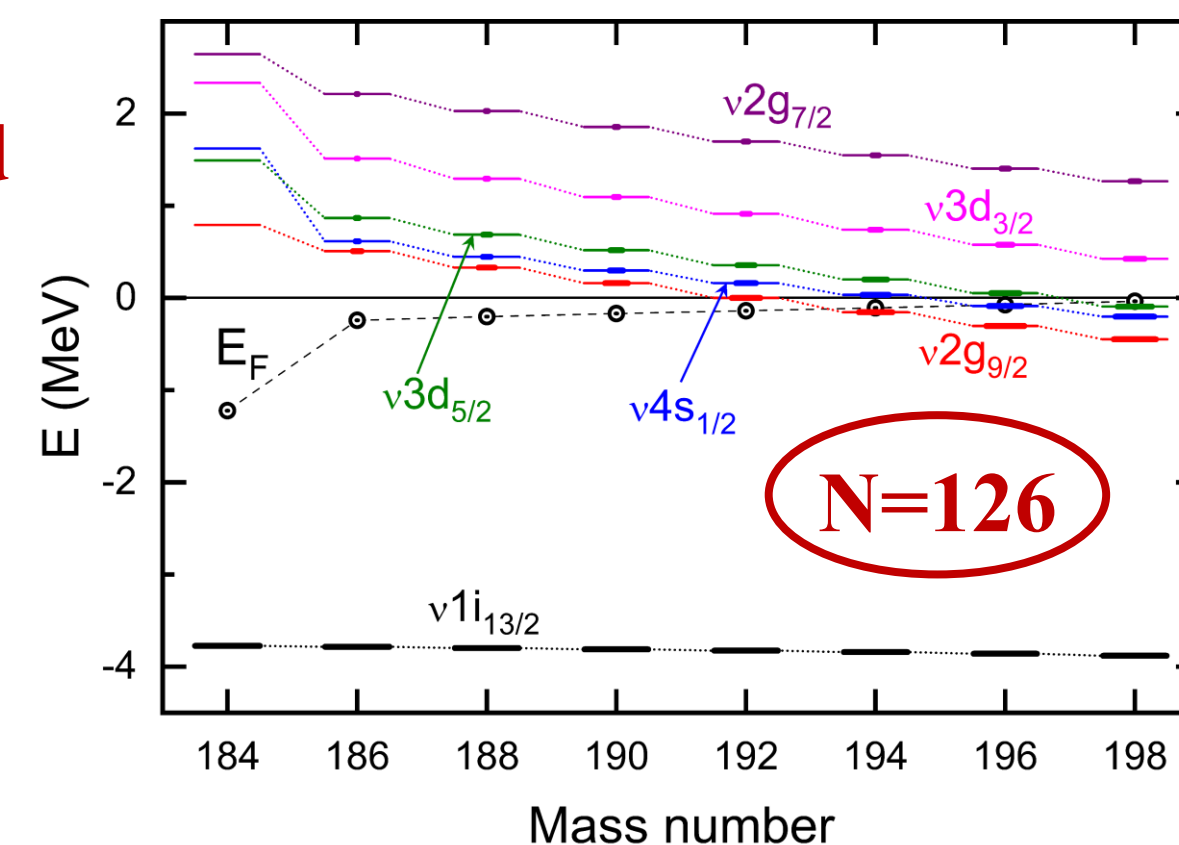
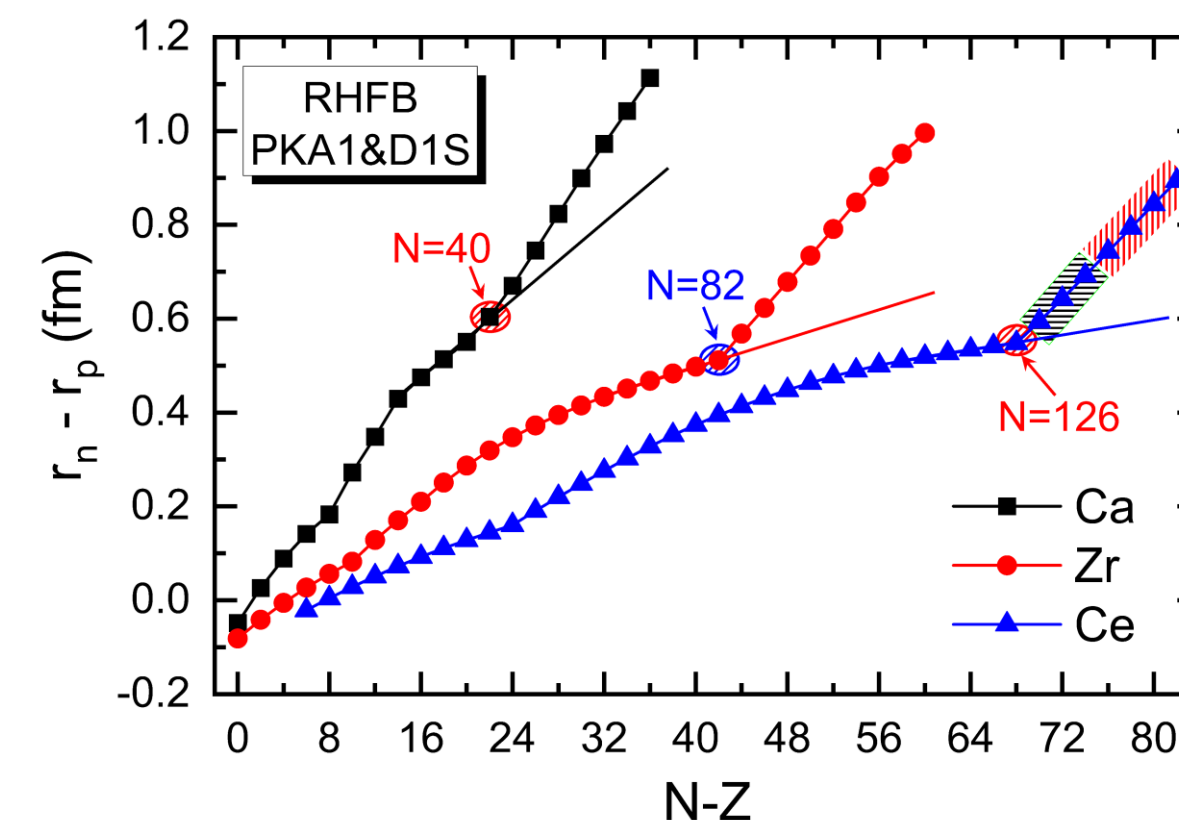
- Exchange DoFs enhance the link between the **restored proton PSS** and the **squeezed N=126 shell**



	$a = \pi 2d_{5/2}$			$a = \pi 1g_{7/2}$		
b	V_{ab}	ρ -T	π -PV	ρ -T	π -PV	V_{ab}
$\nu 1i_{13/2}$	-0.257	25.1%	2.1%	18.5%	9.8%	-0.386
$\nu 4s_{1/2}$	-0.097	17.1%	3.9%	20.2%	3.5%	-0.052
$\nu 2g_{9/2}$	-0.217	24.5%	3.0%	19.0%	8.8%	-0.157

**N=126
squeezed**

**Nodal
effects**



WHL, Ring, Meng, Gai, Bertulani, PRC **81**, 031302(R) (2010)



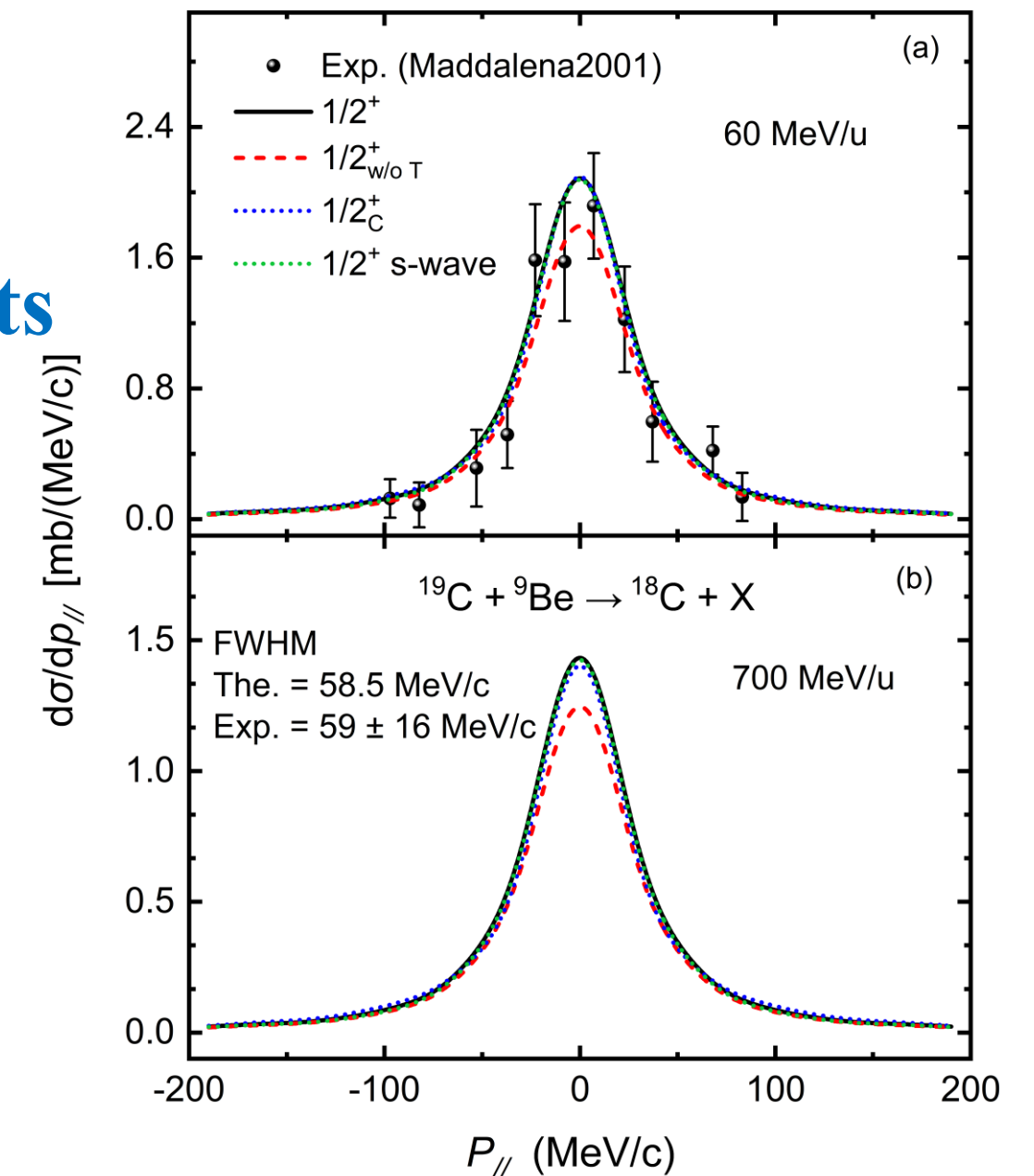
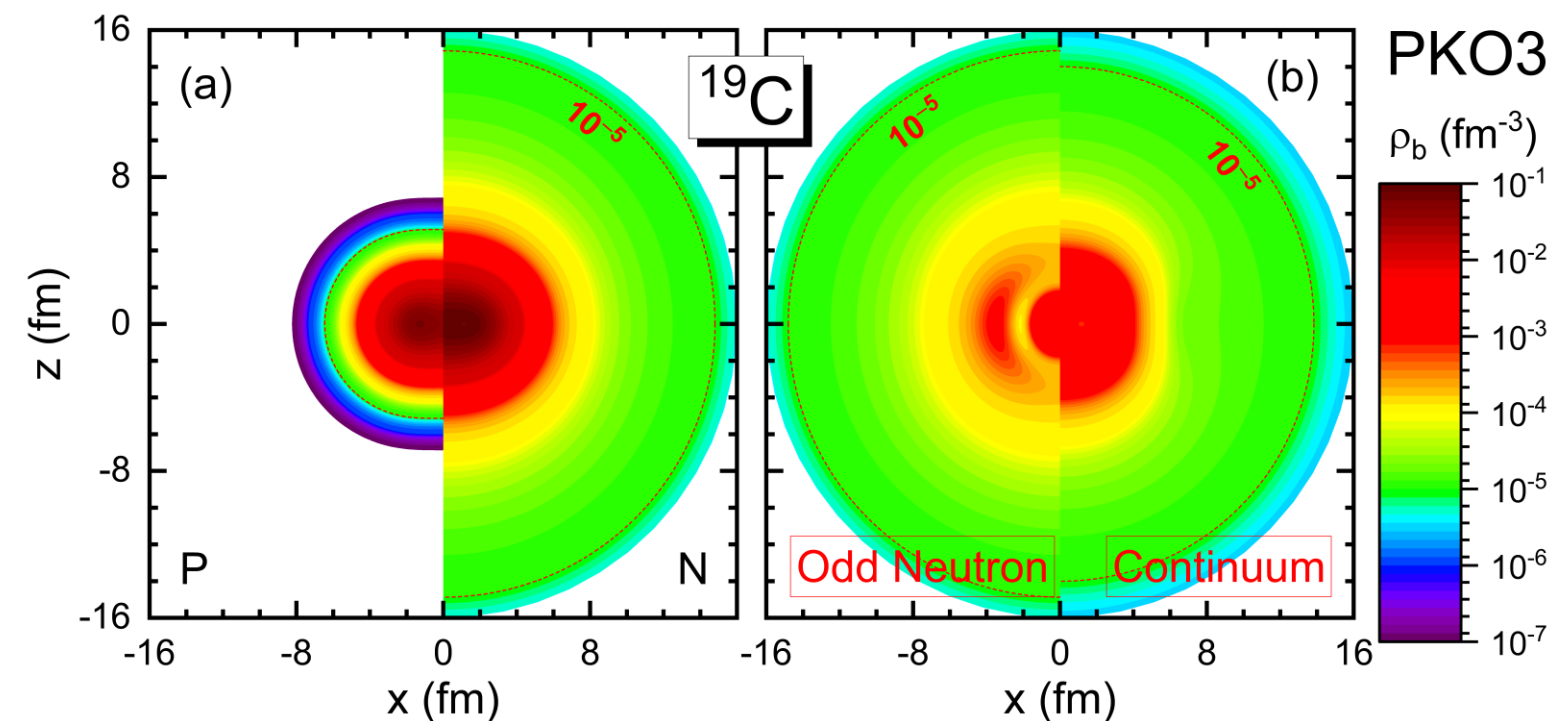
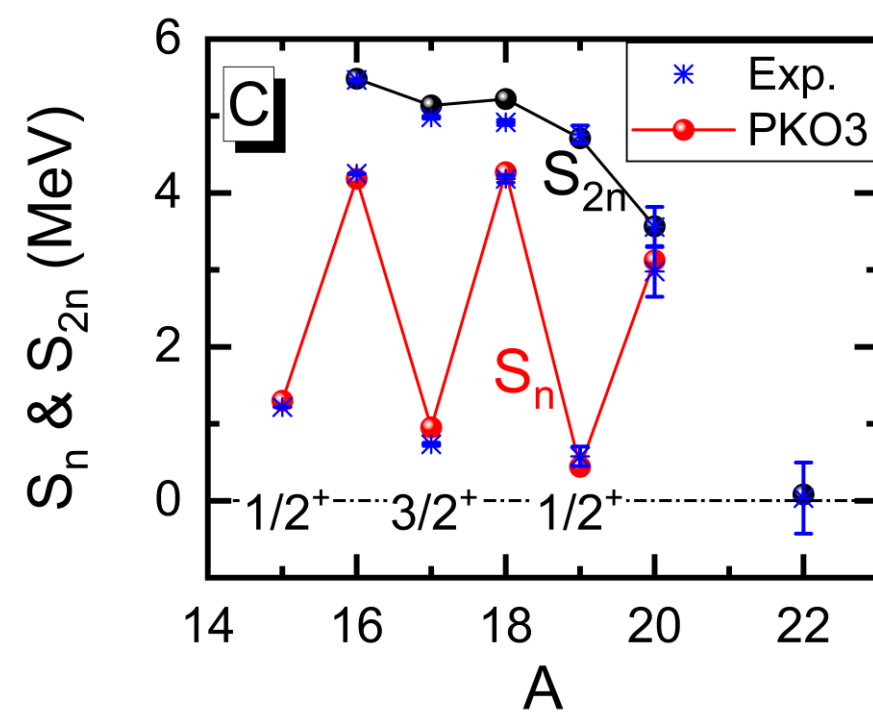
Continuum effects in the halo structure of ^{19}C

□ ^{19}C : single-neutron halo, spin-parity $J^\pi = 1/2^+$

D-RHFB structure & Glauber reaction models

Structure & reaction observables: critical continuum effects

J. L. An, H. C. Li, J. Geng, WHL, S. S. Zhang, JPG 52, 055106 (2025)



Structure: spin-parity, neutron separation energy, density

Reaction: longitude momentum

□ D-RHFB model can provide reliable structure input for the reactions of unstable nuclei



The island of inversion nuclide: ^{32}Mg



□ Nature of the island of inversion exhibited by ^{32}Mg

- **Neutron magic shell $N = 20$ vanishes, accompanying with notable g.s. deformation**
- **Rotational-like g.s. band** and the **co-existence of prolate and spherical shapes**

Motobayashi, Ikedaa *et al.*, PLB **346**, 9 (1995); Pritychenko, Glasmacher *et al.*, PLB **461**, 322 (1999).

Church, Campbell *et al.*, PRC **72**, 054320 (2005); Wimmer, Kroll *et al.*, PRL **105**, 252501 (2010).

□ Shell model with the SDPF-M interaction

A remarkable cross-shell excitation from *sd*- to *pf*-shells is revealed for deformed g.s. 0_1^+

Caurier, Nowacki, Poves, PRC **90**, 014302 (2014); Kitamura, Wimmer, Poves *et al.*, PLB **822**, 136682 (2021).

□ Angular momentum projection based on the mean-field models: **intrusion of *pf*-shell**

Reproduce the deformed g.s. but fail in describing the low-lying excitation energies

Rodríguez-Guzmán, Egido, Robledo, NPA **709**, 201 (2002); Vaquero, Egido, Rodríguez, PRC **88**, 064311 (2013).

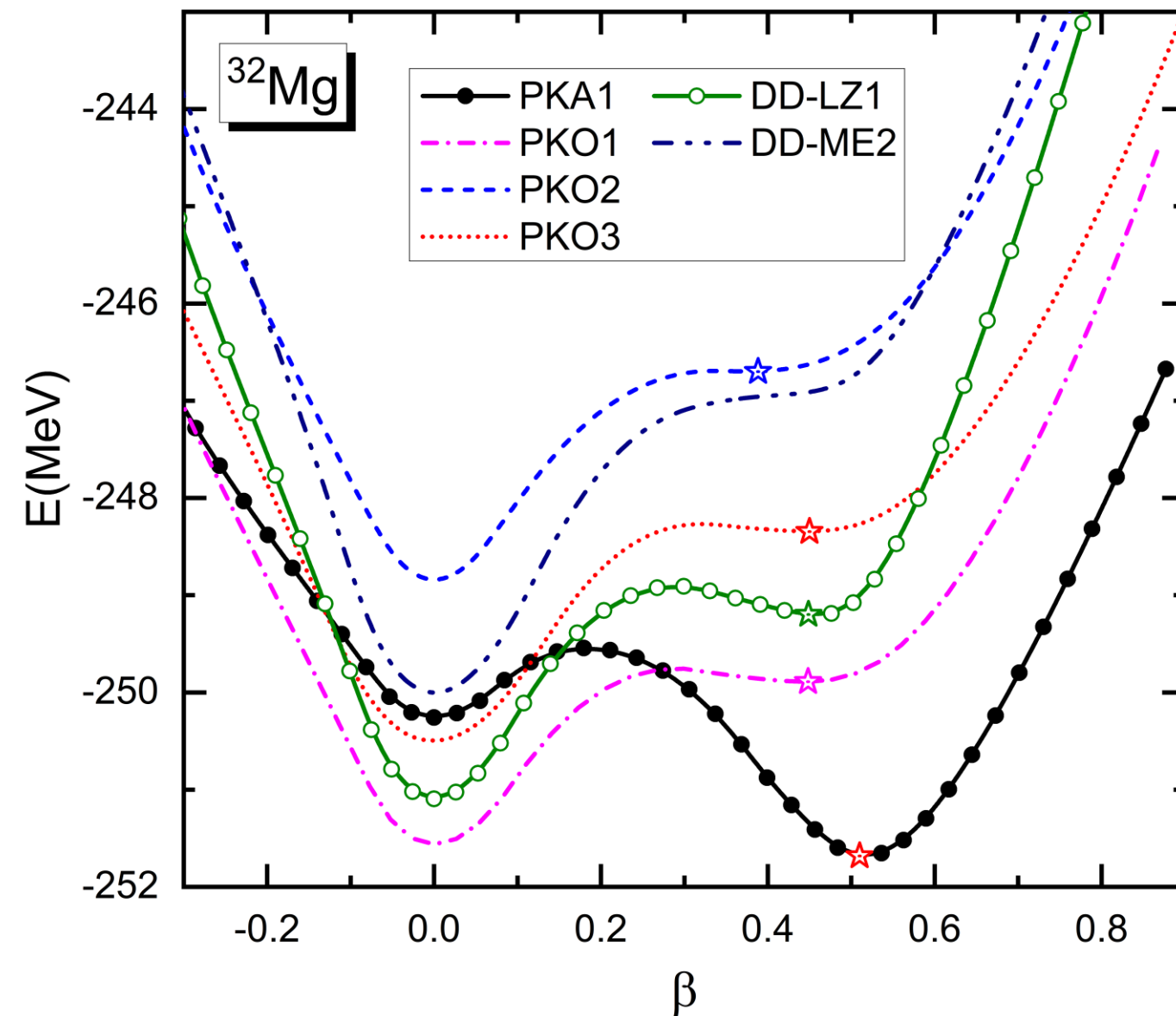
Yao, Meng, Ring *et al.*, PRC **79**, 044312 (2009).

What can we learn from the nature of the island of inversion exhibited by ^{32}Mg

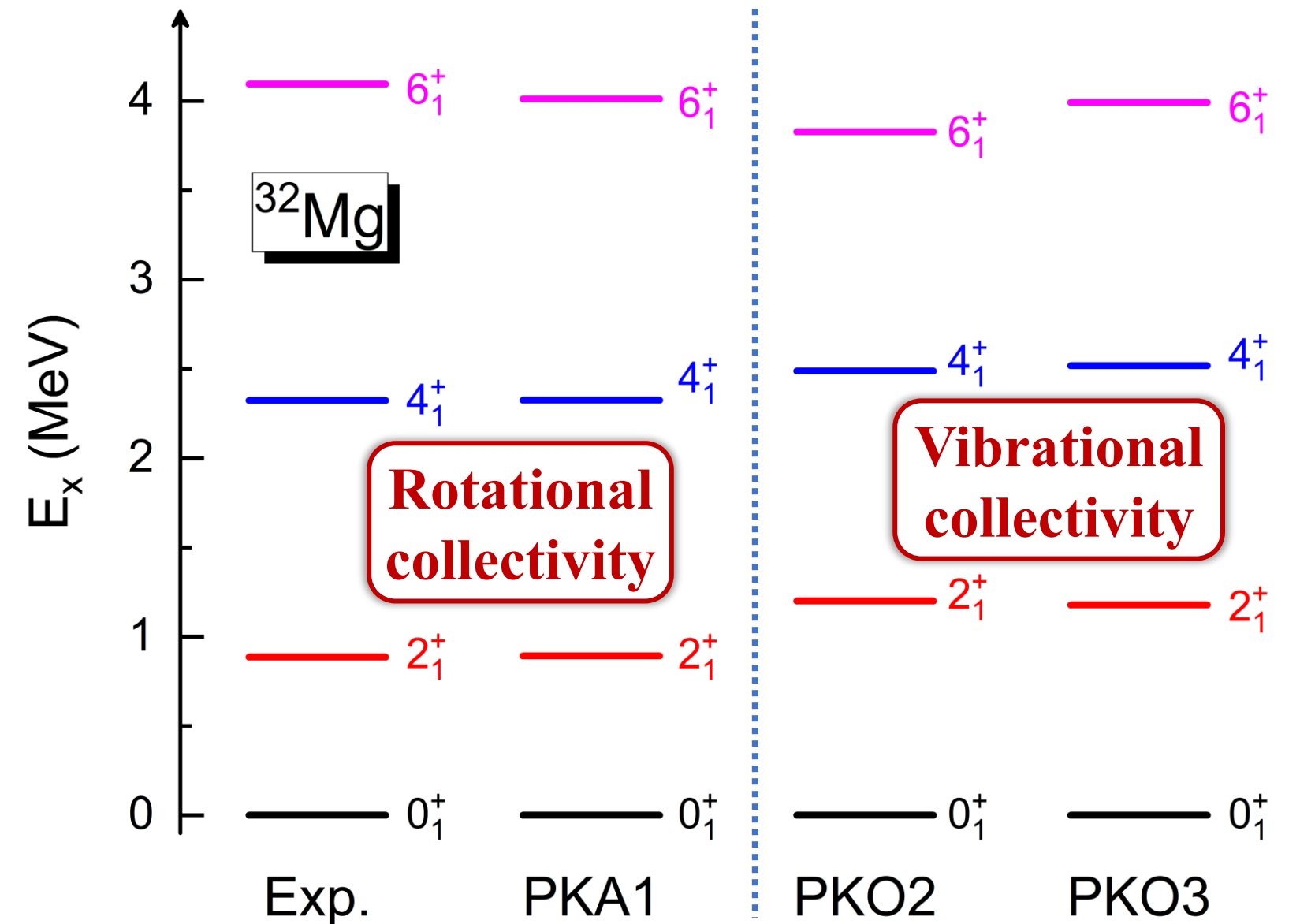


Nature of the island of inversion exhibited by ^{32}Mg

□ D-RHFB calculations: **deformation**



□ CI-RHF calculations: **collectivity**



Link between D-RHFB and CI-RHF

Part of many-body correlations in CI-RHF model are considered by the D-RHFB model

Peng, Liu, Geng, Niu, WHL, CPC 49, 064112 (2025)



Island of inversion: underlying mechanism

□ Cross-shell excitation: deformation picture in ^{32}Mg

$$R = E(4_1^+) / E(2_1^+)$$

	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$	$1f_{7/2}$	$2p_{3/2}$	R
PKA1	5.75	1.91	2.27	1.50	0.56	2.61
PKO2	5.73	1.92	2.38	1.81	0.16	2.07
PKO3	5.73	1.92	2.56	1.57	0.23	2.14

Rotational collectivity
stable deformation

Vibrational collectivity
soft deformation



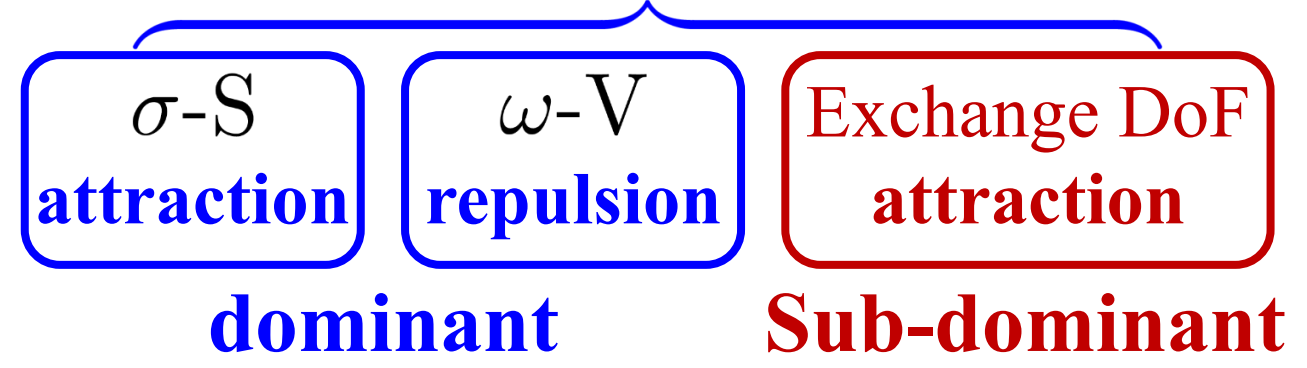
Peng, Liu, Geng, Niu, WHL, CPC 49, 064112 (2025)

□ Impact of exchange DoFs: binding of ^{32}Mg

	$E_{\text{kin.}}$	$E_{\sigma+\omega}$	E_{ρ}	E_{π}	$E_{\text{oth.}}$	E
PKA1	400.8	-417.0	-217.5	-31.5	14.9	-250.2
	409.6	-434.4	-214.4	-29.9	17.4	-251.7
PKO3	438.1	-606.1	-59.7	-37.2	14.4	-250.5
	448.7	-616.3	-59.2	-36.1	14.6	-248.3
DD-LZ1	412.6	-701.3	18.3	—	19.4	-251.1
	414.1	-702.7	17.6	—	21.8	-249.2

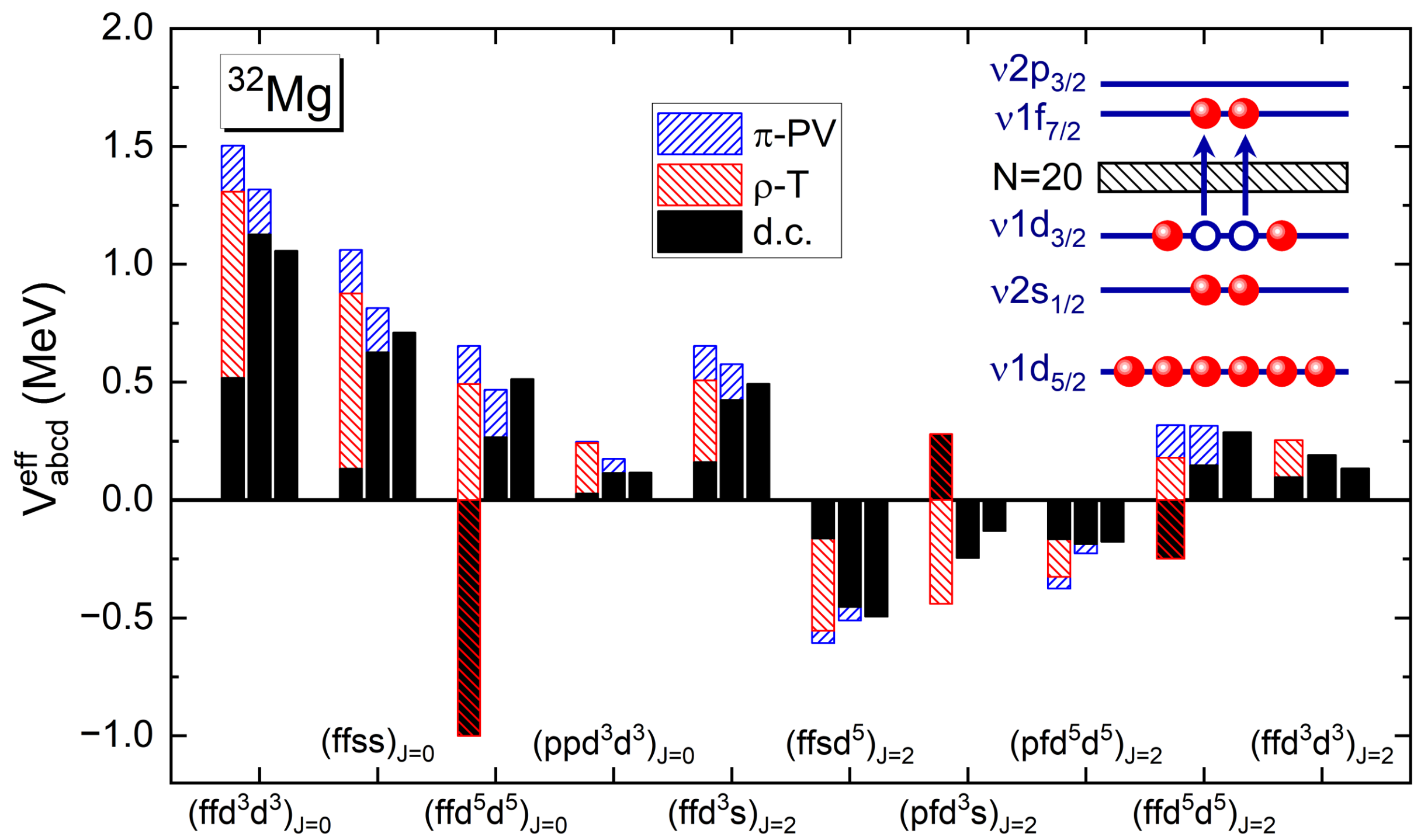
Exchange DoFs exhibit substantial contributions to nuclear binding

Picture of nuclear binding





Configuration Interactions: ρ -T and π -PV



PKA1 (left)
PKO3 (mid.)
PKO2 (right)



Discernible π -PV &
compressive ρ -T



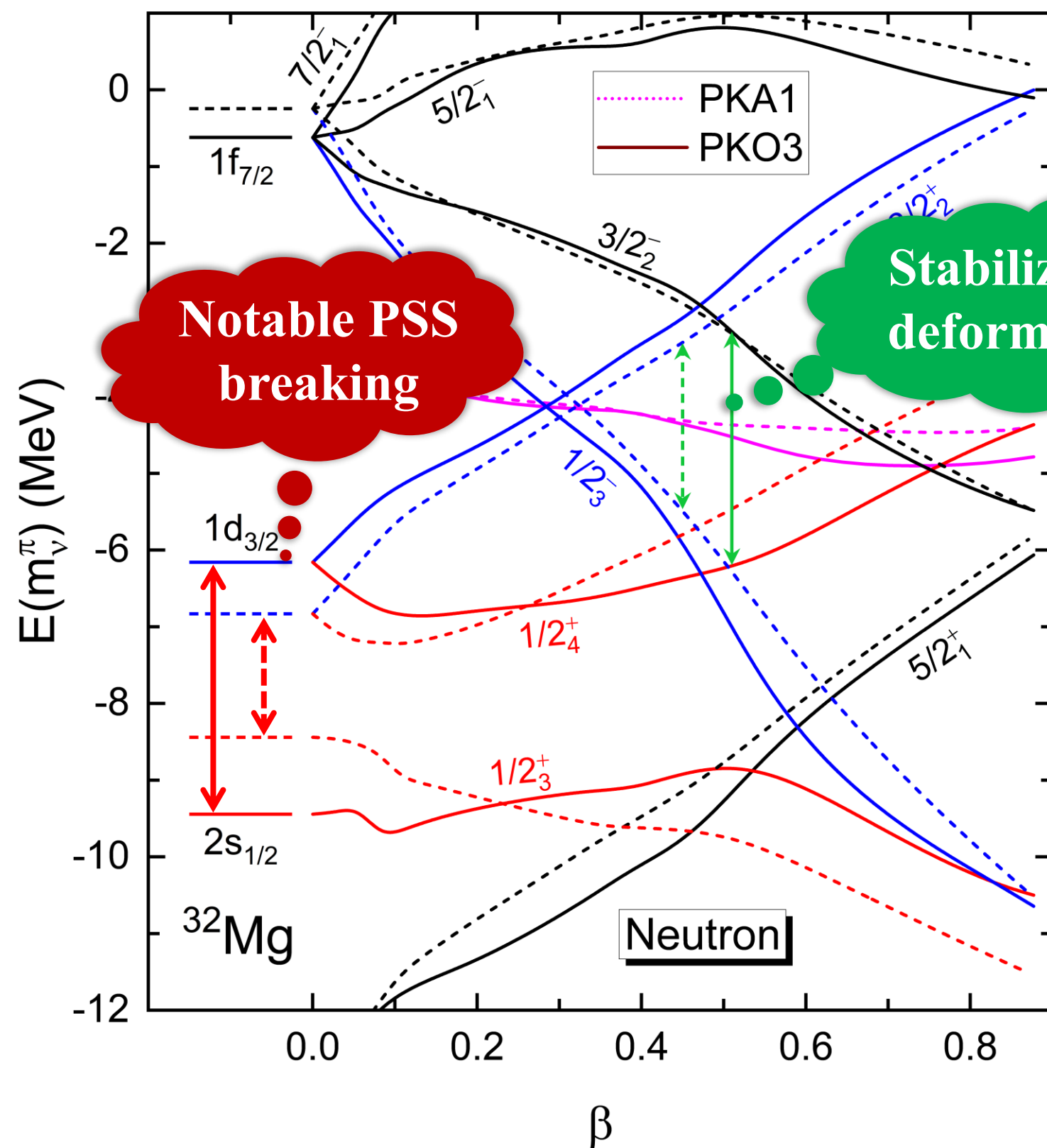
Be determined at the
Hartree-Fock level

Configuration Interactions shaped by the exchange DoFs → deformation stability?

Peng, Liu, Geng, Niu, WHL, CPC 49, 064112 (2025)



PSS breaking: an implemented insight



Notable deformed shell and the breaking of PSS

Underlying effects from exchange DoF

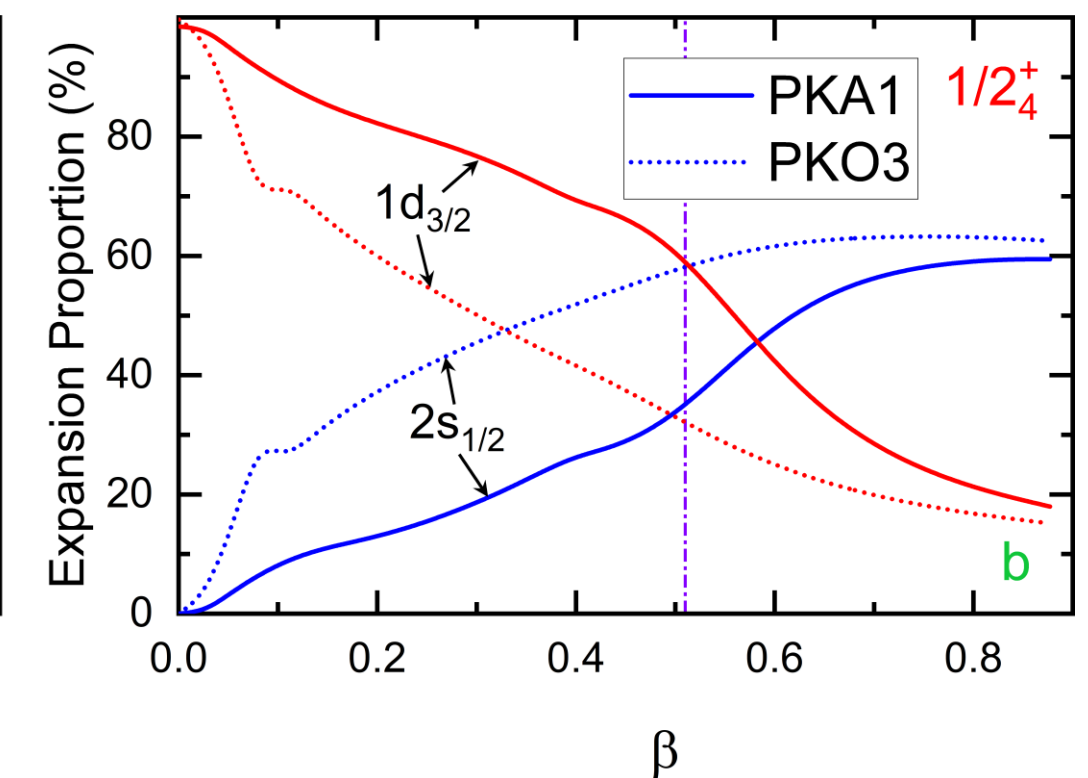
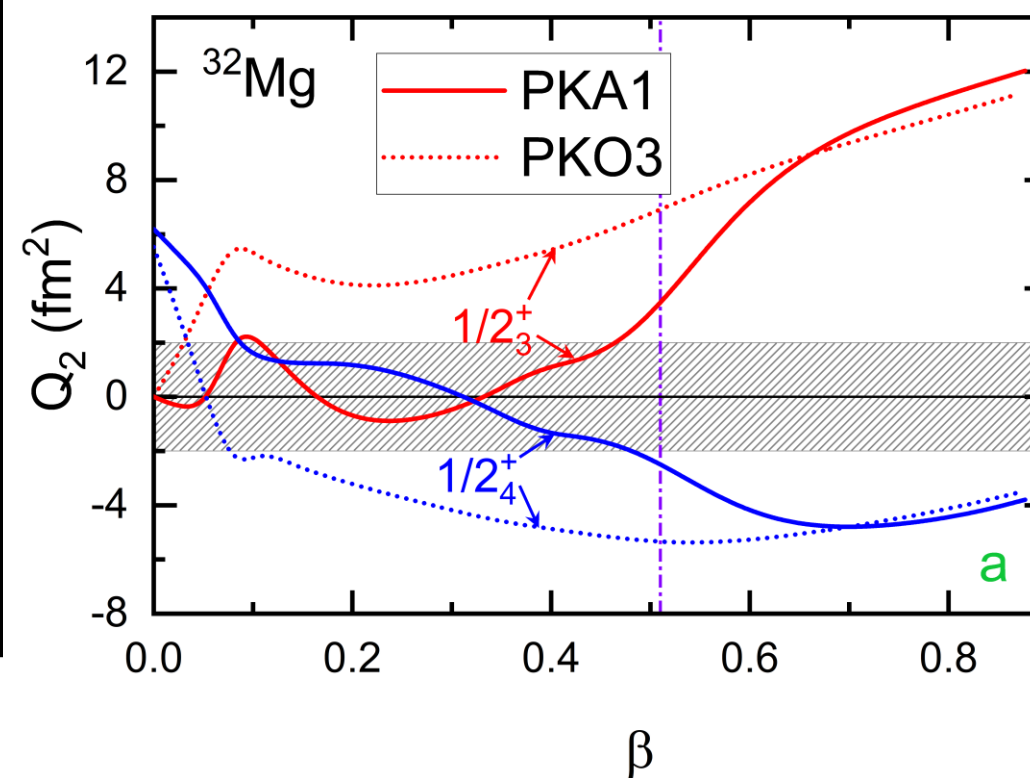
PSS
breaking

Shape
evolution

Deformation

Spherical
Shell

Mixture of
spherical waves

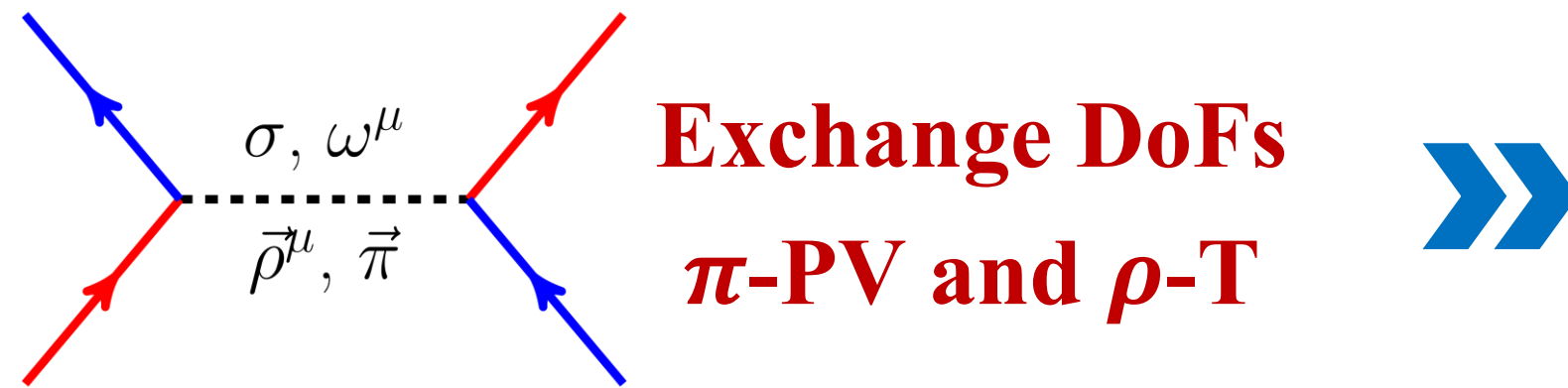


Peng, Liu, Geng, Niu, WHL, CPC 49, 064112 (2025)



Conclusions: exchange correlation effects

- At the mean field level & beyond, exchange DoFs are more important than expected

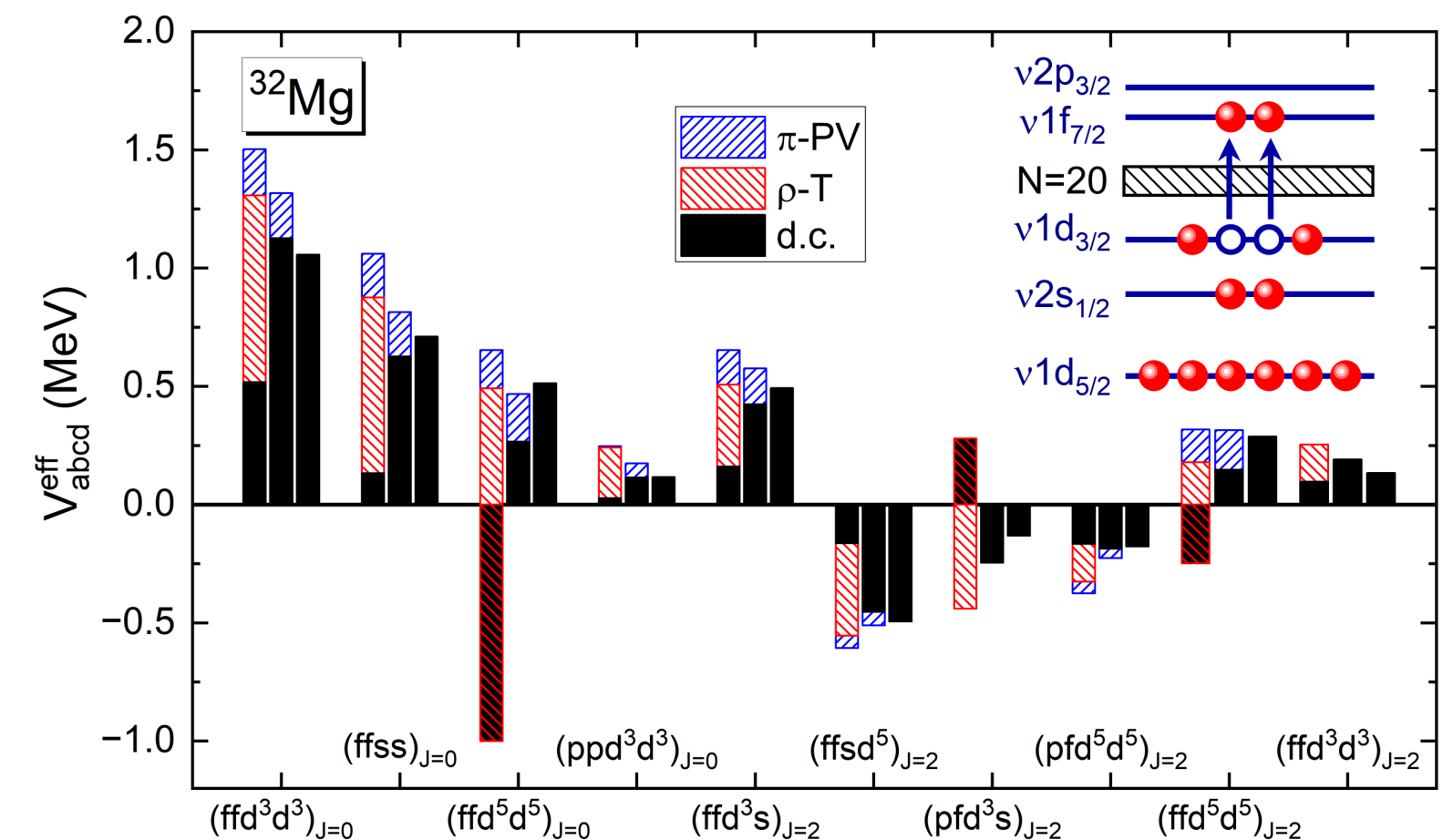
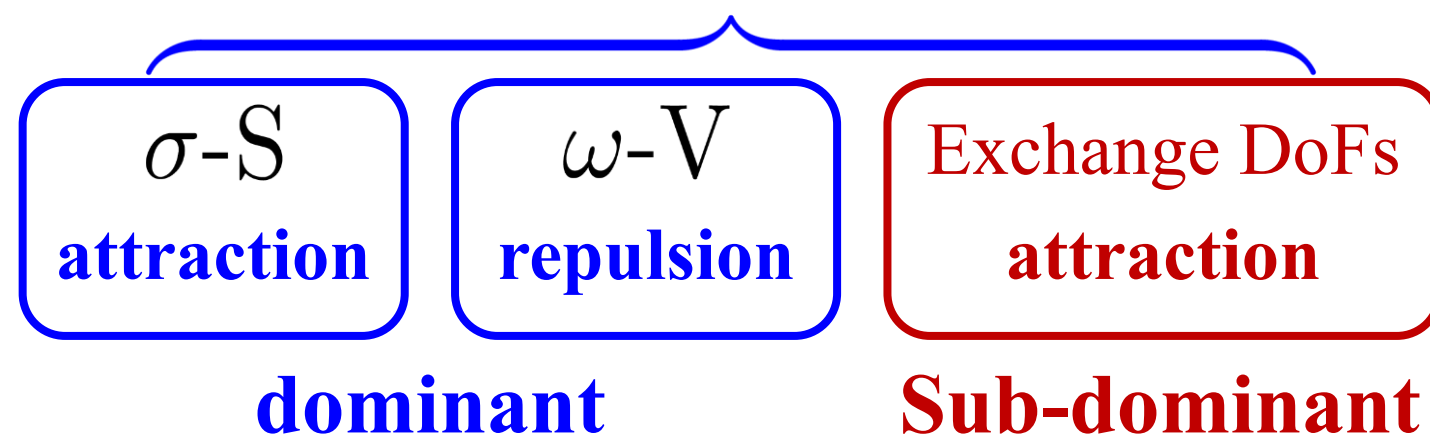


How nucleons form an atomic nucleus

- Impact the modeling of nuclear binding
- Enhance the neutron-proton interactions

- Exchange DoFs shall be predetermined at the mean field level

Picture of nuclear binding



- Explicit Fock terms are complicated, which calls for an economical solution

Acknowledgements

Collaborators:

J. Geng, Y. Peng, Y.F. Niu @LZU

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S.S. Zhang, J.L. An, H.C. Li @BUAA

J. Meng, P.W. Zhao @PKU

J.J. Li, Z.P. Li @SWU

P. Ring @TUM

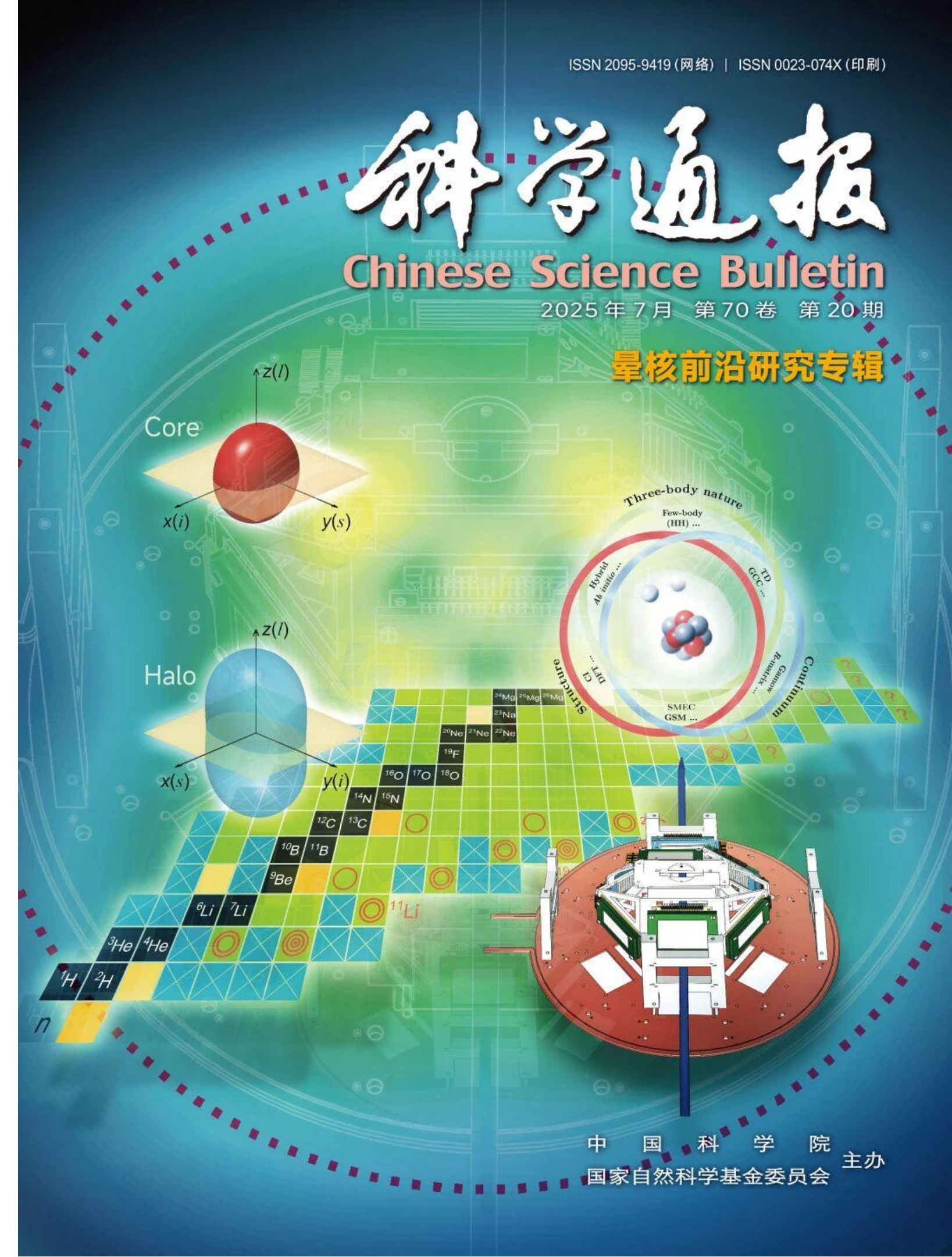
N. Van Gai (@Paris-Saclay University)

C.A. Bertulani @ Texas A&M University-Commerce

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Thank you for your attentions

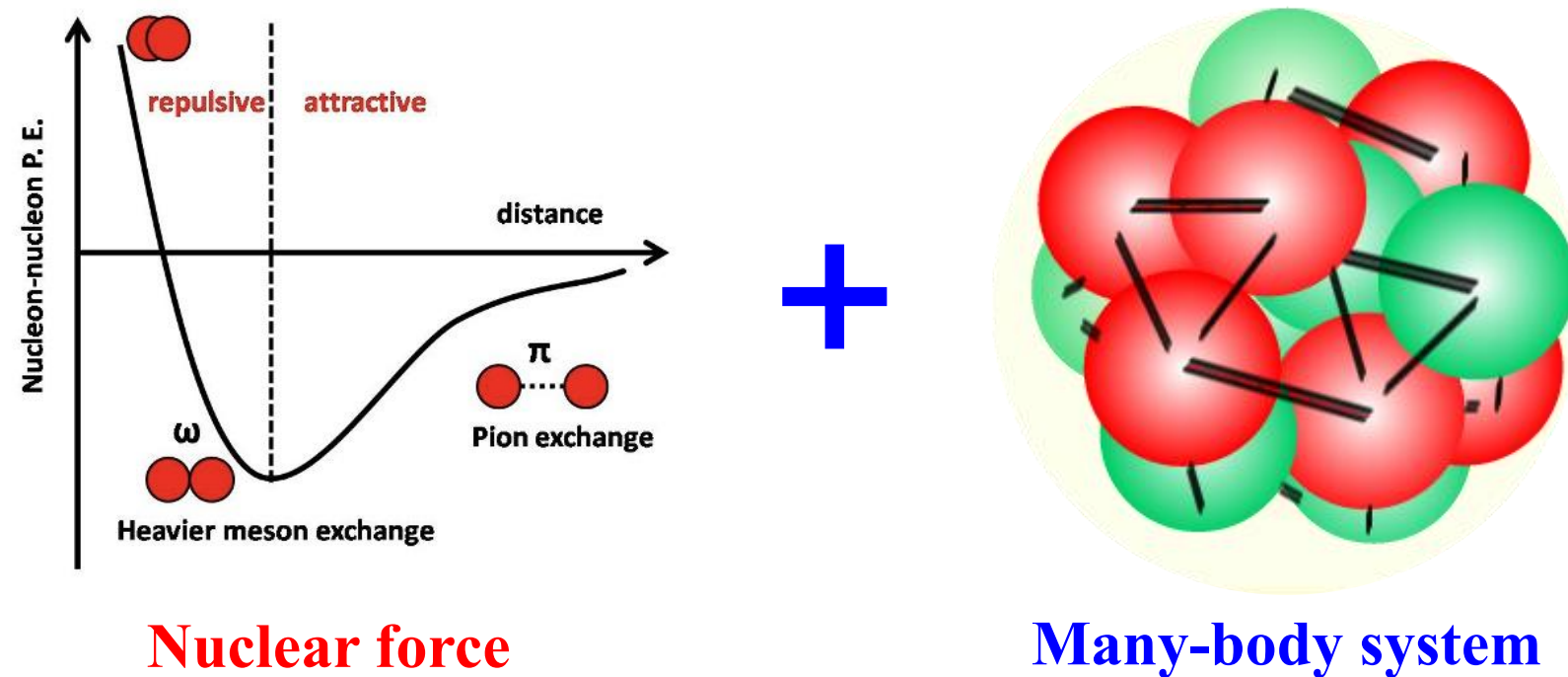
Long, Wen Hui (longwh@lzu.edu.cn)



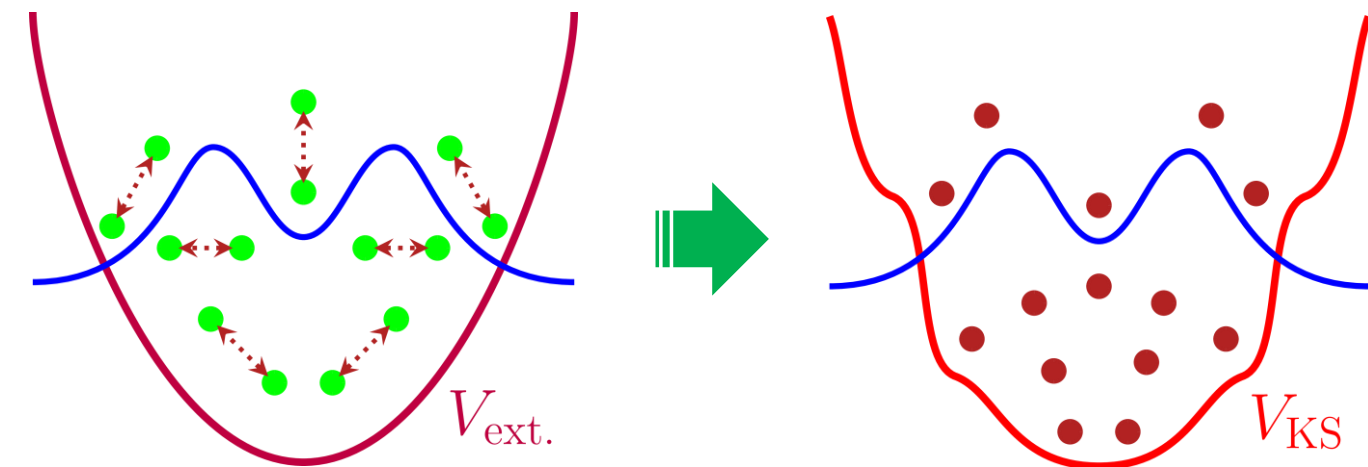


Fundamental issue in nuclear physics

How nucleons spontaneously form atomic nuclei



- **Density functional theory (DFT)**
many-body problem $\rightarrow$ one-body problem



Drut, Furnstahl, Platter, PPNP **64** (2010) 120

- **A relativistic representation** of nuclear binding given by relativistic DFT
Interplay between strong scalar attraction and vector repulsion $\rightarrow$ bound nucleus
Natural spin-orbit coupling, the origin of pseudo-spin symmetry and spin symmetry, ...

Meng et al., PPNP **57**, 470 (2006); Ginocchio, PRL **78**, 436 (1997); Meng et al., PRC **58**, R628 (1998); Zhou et al., PRL **91**, 262501 (2003).

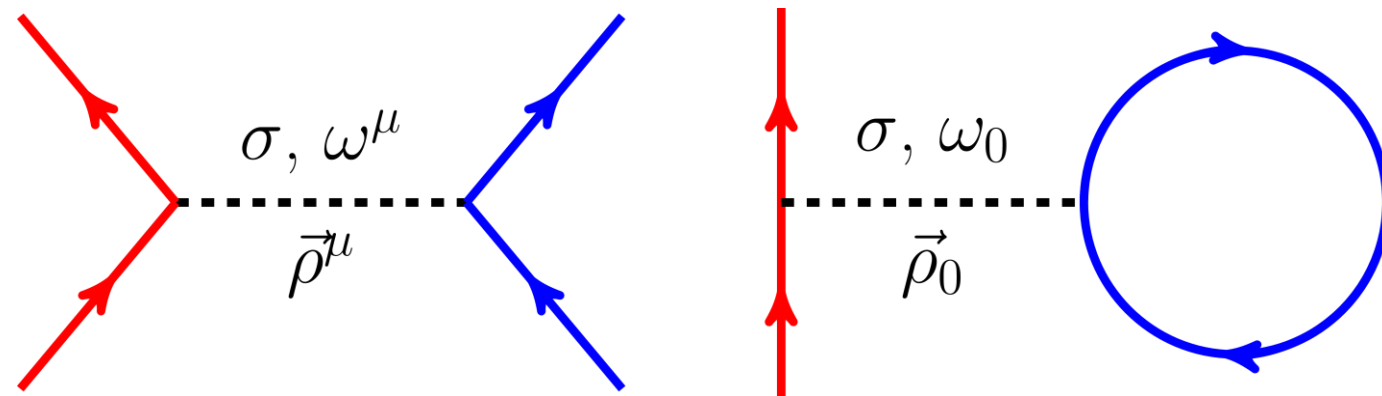
What can we learn from the novel phenomena exhibited by unstable nuclei?



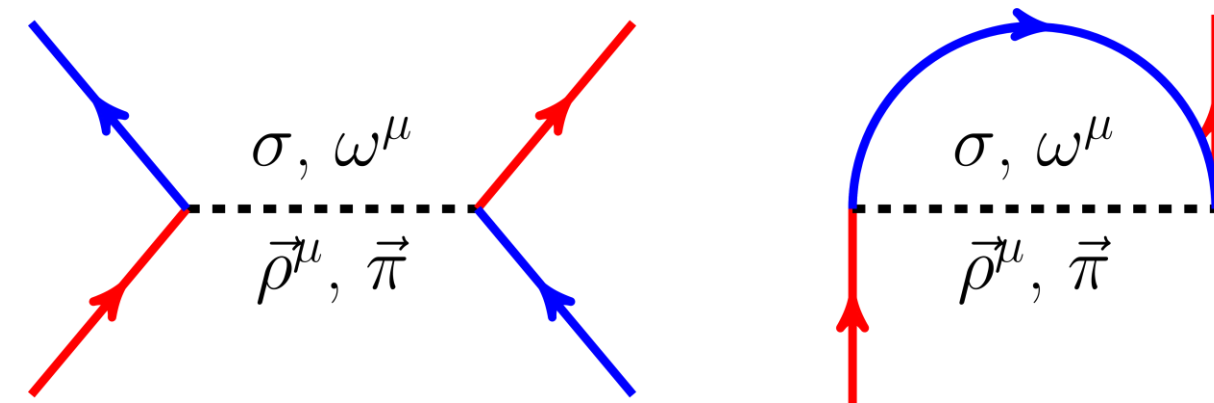
Relativistic Hartree-Fock (RHF) theory



- Fock terms give rise to **pure exchange degrees of freedom**



Hartree terms: σ -S, ω -V, $\vec{\rho}$ -V, A-V



Fock terms: σ -S, ω -V, $\vec{\rho}$ -V, A-V; π -PV, ρ -T (ρ -VT)

Bouyssy (1987), Bernardos (1993), Shi (1995), Marcos (2004), Long (2004-now), Geng (2020-now), ...

- **Exchange degrees of freedom (DoF) impact the modelling of nuclear binding**

π -PV and ρ -T (ρ -VT)

PRC 100, 051301(R) (2019)

- **Nuclear tensor force** can be naturally introduced: e.g., via the π -PV and ρ -T couplings

PRC 91, 034326 (2015); CPC 42, 024101 (2018); PRC 98, 034313 (2018); PRC 101, 064306 (2020)

- **Not exactly a DFT:** **explicit** Fock terms (meson exchange) are **not a functional of local density**

Energy function
of DFT

$$E(\hat{\rho}) = \langle \Psi | \hat{H} | \Psi \rangle \approx \langle \Phi | H_{\text{eff.}} | \Phi \rangle = T + E_H(\rho) + \boxed{E_{\text{xc}}(\rho)} \quad \text{Exchange correlations}$$



Axially deformed RHF (D-RHF) model



□ Spherical Dirac Woods-Saxon (DWS) basis

Zhou, Meng, Ring, PRC 68, 034323 (2003)

- **Appropriate asymptotic behaviors** of wave functions
- **Microscopic insight** into deformed nuclei: effects of tensor force

□ Yukawa propagator: the decomposition in spherical coordinate

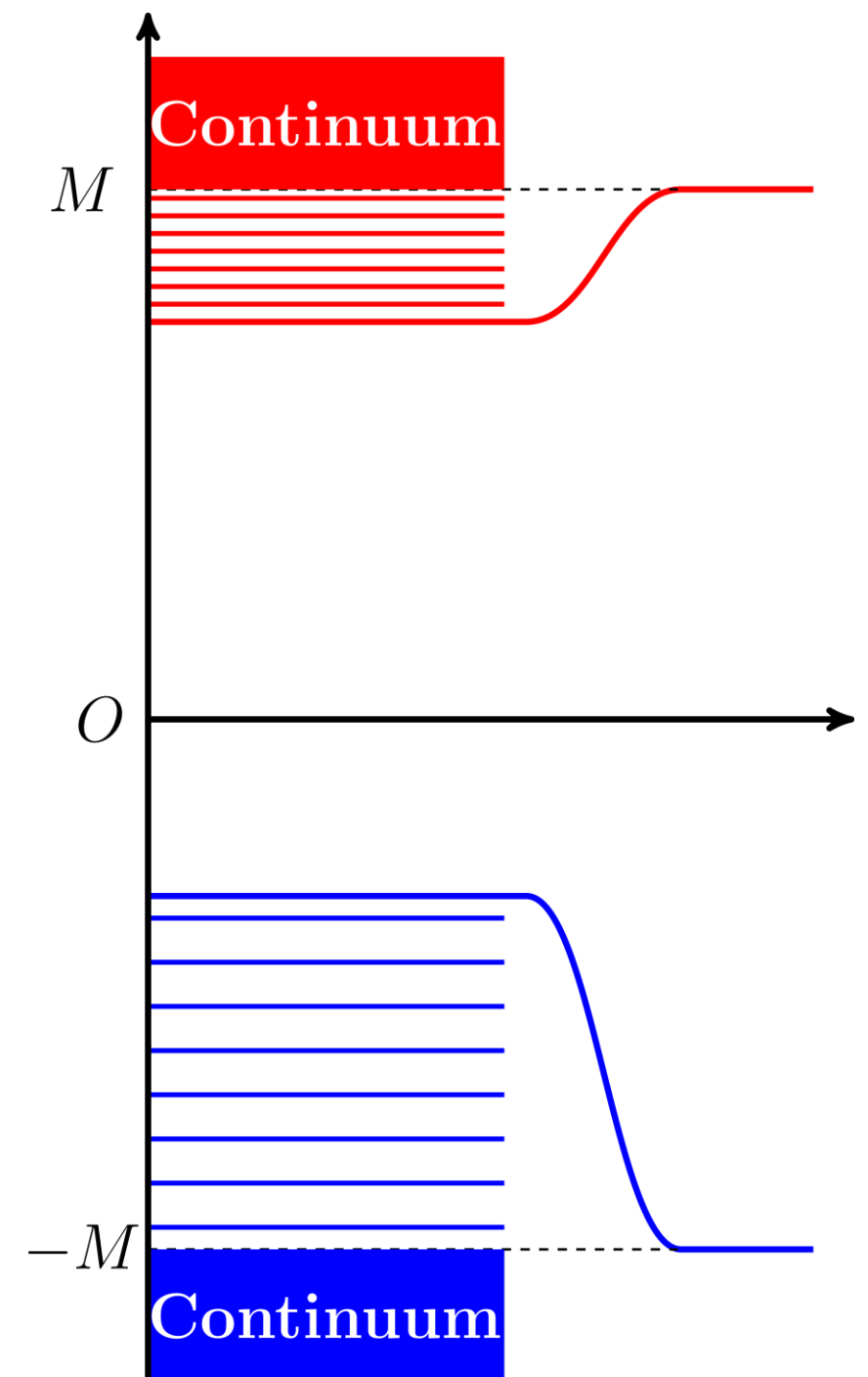
$$\frac{1}{4\pi} \frac{e^{-m|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{rr'} \sum_{\lambda=0}^{\infty} I_{\lambda+\frac{1}{2}}(mr_{<}) K_{\lambda+\frac{1}{2}}(mr_{>}) \sum_{\mu=-\lambda}^{\lambda} Y_{\lambda\mu}(\Omega) Y_{\lambda\mu}^*(\Omega)$$

→ Singularity appears when $\mathbf{x} = \mathbf{x}'$

$$V_{\phi} = \frac{1}{2} \int d\mathbf{x} d\mathbf{x}' \sum_{\alpha\beta;\alpha'\beta'} \left[\bar{\psi}_{\alpha} \Gamma_{\phi} \psi_{\alpha'} \right]_{\mathbf{x}} \frac{1}{4\pi} \frac{e^{-m_{\phi}|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} \left[\bar{\psi}_{\beta} \Gamma^{\phi} \psi_{\beta'} \right]_{\mathbf{x}'} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\beta'} c_{\alpha'}$$

($\lambda\mu$)-terms are truncated by the DWS basis to avoid singularity

Geng, Xiang, Sun, WHL, PRC 101, 064302 (2020)





Tensor force effects in ^{20}Ne

□ Tensor force changes the mixing of spherical waves

sd 壳 { $1d_{3/2}$
 $2s_{1/2}$
 $1d_{5/2}$ } PKO2
w/o π
VS
PKO3
with π
(8)
 $1p_{1/2}$
 $1p_{3/2}$

π -T enhances the
intrude of $1d_{3/2}$ waves

Shell effects
enhanced by π -PV

PRC 101, 064302 (2020)

