2022 CENS Brown Bag Seminar April 6th

Exchange Terms in Relativistic Density Functional Theory

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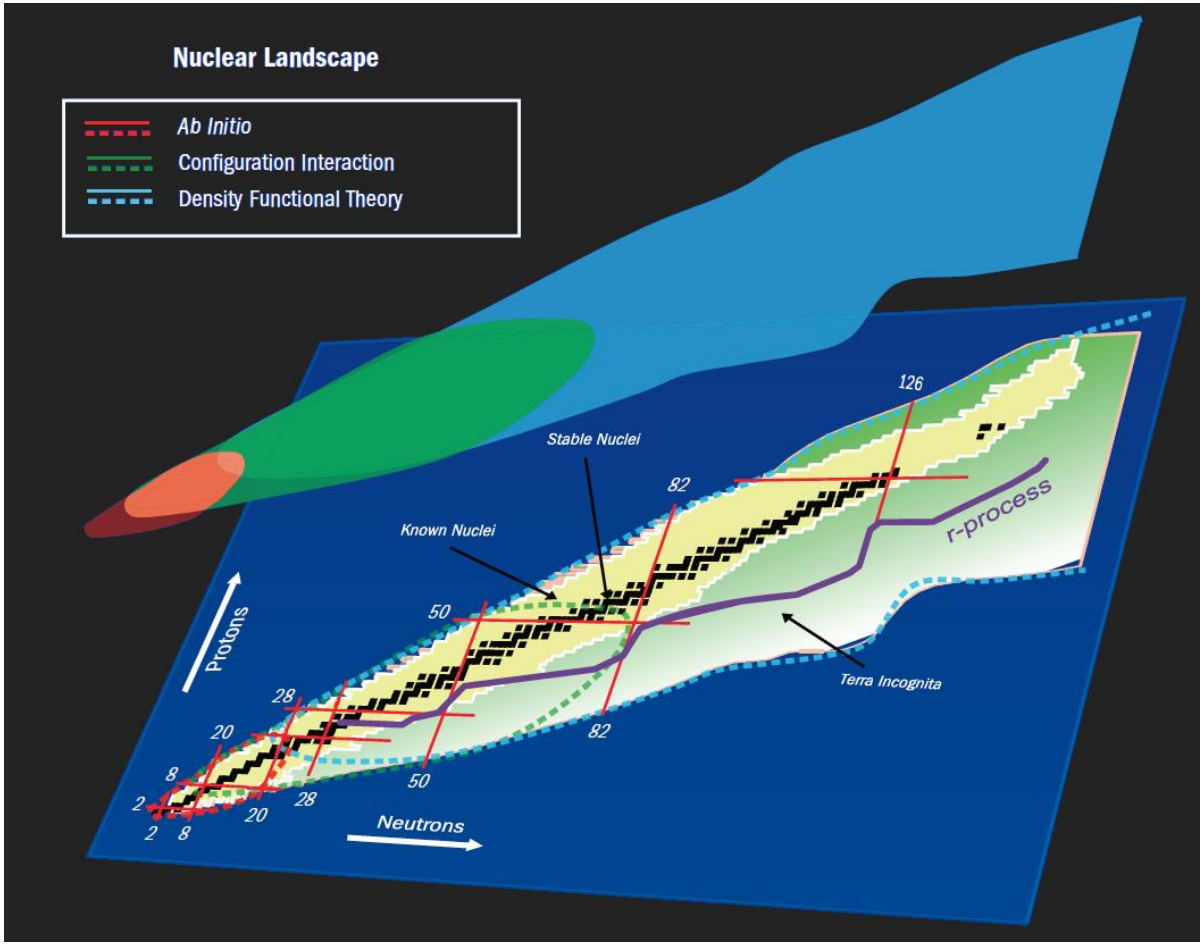
Content

- **Introduction**
- Importance of Exchange Terms
  - Evolution of $N = 40$ Shell Gaps
  - New Magic Numbers $N = 32$ and $N = 34$
  - Self-Consistent Descriptions for Spin-Isospin Excitations
- Solutions to High Computational Cost
  - Localized Exchange Terms
  - Relativistic Optimized Effective Potential Method
  - Relativistic Hartree-Fock on 3D Lattice
- Summary and Prospects

Nuclear Many-Body Theory

- Nuclear system is a complex quantum many-body system



http://unedf.mps.ohio-state.edu/

Nuclear Density Functional Theory (DFT) can provide a self-consistent description across almost the whole nuclear chart.

Relativistic Density Functional Theory

- Wide application of Relativistic Density Functional Theory (RDFT)

  - Ground state
    - ✓ Nuclear Mass

      Zhang et al., ADNDT 144, 101488 (2022)
    - ✓ Exotic Nuclei

      Meng and Ring, PRL 77, 3963 (1996)
  - Nuclear decay
    - ✓ Beta decay

      Niu et al., PLB 723, 172 (2013)
    - ✓ Proton radioactivity

      Zhao et al., PRC 90, 054326 (2014)

      Lim et al., PRC 93, 014314 (2016)
  - Nuclear fission

    Lu, Zhao, and Zhou, PRC 85, 011301(R) (2012)

    Zhou, PS 91, 063008 (2016)

    Agbemava et al., PRC 95, 054324 (2017)
  - Nuclear rotation

    König and Ring PRL 71, 3079 (1993)

    Afanasjev and Abusara PRC 82, 034329 (2010)

    Peng et al., PRC 78, 024313 (2008)

    Zhao et al., PRL 107, 122501 (2011)
  - Nuclear vibration

    Nikšić et al., PRC 66, 064302 (2002)

    Paar et al., PRL 103, 032502 (2009)

    Liang, Giai, and Meng, PRL 101, 122502(2008)

    Niu, Paar, Vretenar, and Meng, PLB 681, (2009)
  - Nuclear reaction

    Ren, Zhao, and Meng, PLB 801, 135194 (2020)

    Ren, Zhao, and Meng, PRC 102, 044603 (2020)

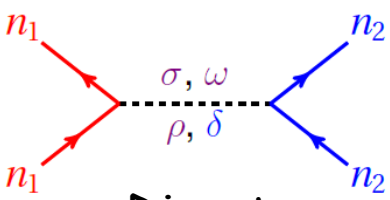
DRHBc Mass Table *Zhang et al., ADNDT 144, 101488 (2022)* (http://drhbctable.jcnp.org/)

Relativistic Density Functional Theory

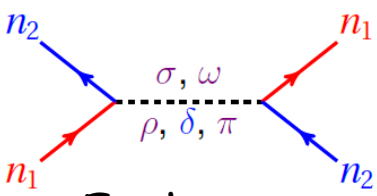
Relativistic Density Functional Theory (RDFT)

Meng, Relativistic Density Functional for Nuclear Structure, World Scientific, 2016

- Meson-exchange: interact via exchange of mesons



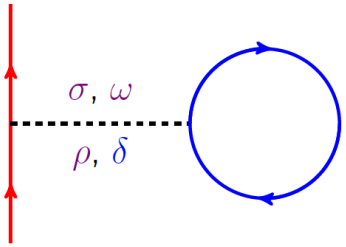
Direct
(Hartree)



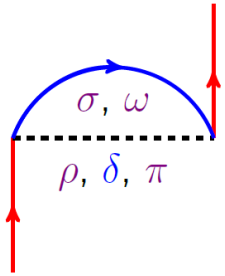
Exchange
(Fock)

- Mean-field (MF) approximation

  move independently in an averaged potential



Local MF



Nonlocal MF

Lagrangian Density for RDFT

- Lagrangian density $\mathcal{L} = \mathcal{L}_I + \mathcal{L}_0$

$$\mathcal{L}_I = -\bar{\psi}[g_\sigma \sigma + g_\delta \vec{\tau}\cdot\vec{\delta} + g_\omega \gamma^\mu \omega_\mu + g_\rho \gamma^\mu \vec{\tau}\cdot\vec{\rho}_\mu + e\gamma^\mu \frac{1-\tau_3}{2} A_\mu]\psi$$

$$-\bar{\psi}[\frac{f_\pi}{m_\pi}\gamma_5\gamma^\mu \partial_\mu \vec{\pi}\cdot\vec{\tau} + \frac{f_\rho}{2M}\sigma_{\mu\nu}\vec{\tau}\cdot\partial^\nu \vec{\rho}^\mu]\psi$$

π pseudo-vector (π-PV) **ρ tensor (ρ-T)**

- Some of the commonly used effective interactions

Method	Interaction	σ(S)	ω(V)	ρ(tV)	π(PV)	ρ(T)
Hartree	PC-PK1	√	√	√		
	DD-ME1	√	√	√		
	DD-ME2	√	√	√		
Hartree-Fock	PKO2	√	√	√		
	PKO1	√	√	√	√	
	PKO3	√	√	√	√	
	PKA1	√	√	√	√	√

Exchange terms in RDFT

- The exchange terms are included within **Relativistic Hartree-Fock model**

  Bouyssy(1987), Long(2006), Geng(2020)

- History of relativistic Hartree-Fock (RHF) model
  - 1987: First systematic applications — *Bouyssy, PRC (1987)*
  - 1993: Employ non-linear terms — *Bernardos, PRC (1993)*
  - 1995: Employ density-dependent coupling constants — *Shi, PRC (1995)*
  - 2006, 2007: Good descriptions for finite nuclei (PKOi and PKA1) — *Long (2006, 2007)*
  - 2010: Relativistic Hartree-Fock-Bogoliubov (RHFB) Model — *Long, PRC (2010)*
  - 2011, 2020, 2022: Axially deformed RHF and RHFB model — *Ebran(2011), Geng (2020, 2022)*

- Importance of the exchange terms — **π-PV, ρ-T**
  - Naturally include tensor force — *Jiang(2015), Wang(2018)*
  - Improvement on the shell evolution — *Long(2007, 2009), Li(2016), Liu(2020)*
  - Self-consistent description of spin-isospin excitation — *Liang(2008,2012)*

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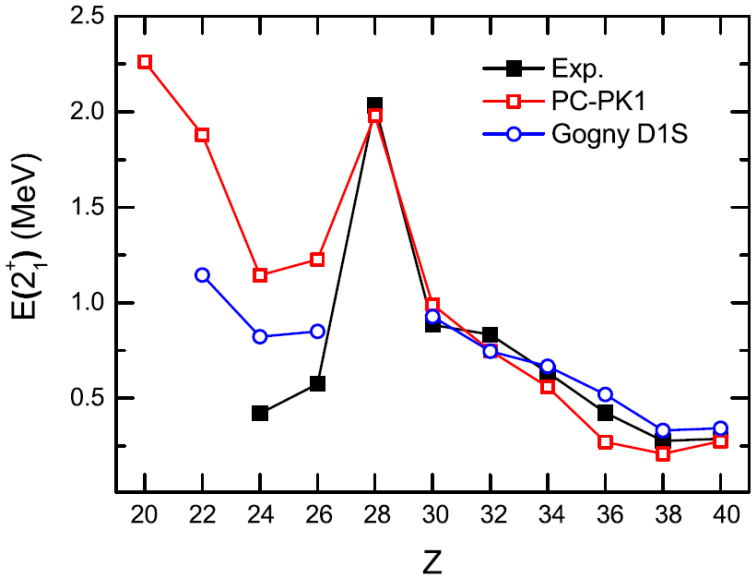
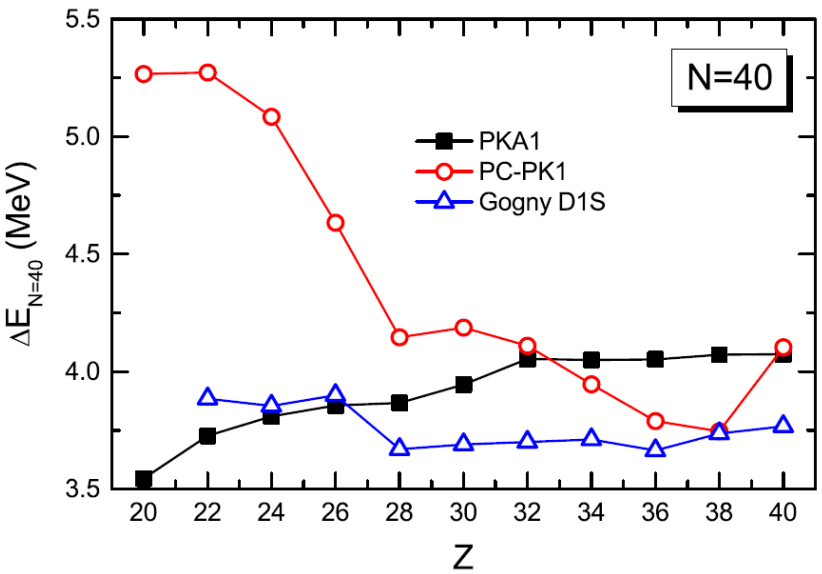
Shell Evolution of $N = 40$ Isotonic Chain

- Energy of first 2^+ excited states



- Spherical shell gaps at $N = 40$



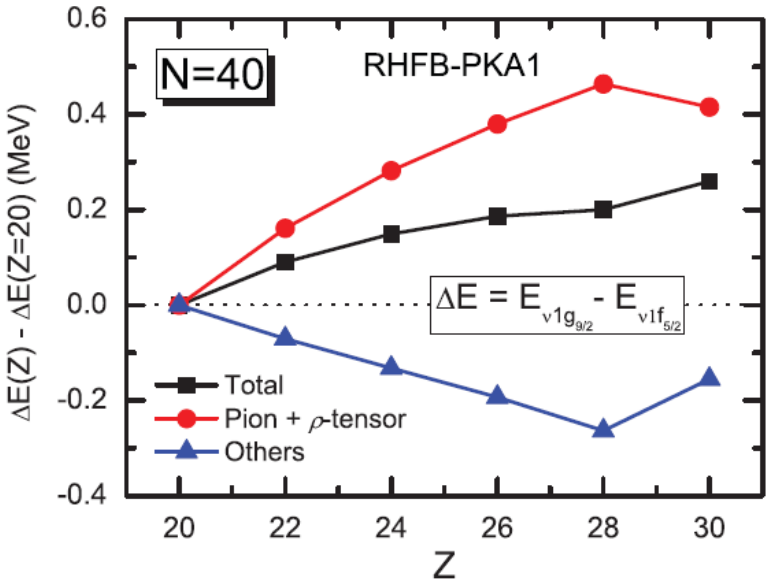
Z.H. Wang et al., JPG 42, 045108 (2015)

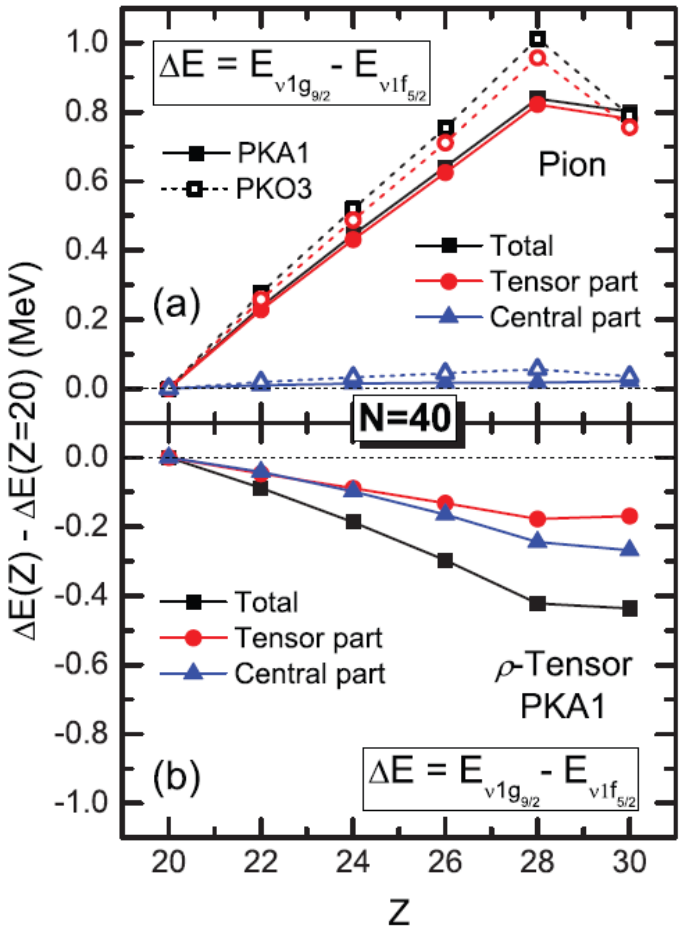
- Enhanced quadrupole collectivity is observed at the neutron-rich side of $N = 40$ isotonic chain

- The effective interaction PKA1 can give a decreasing $N = 40$ gaps for neutron-rich isotones, which agrees with experimental observations.

Shell Evolution of $N = 40$ Isotonic Chain

- Contributions of the π-PV and ρ-T coupling to the $N = 40$ shell gaps





L.J. Wang et al., PRC 87, 047301 (2013)

- The tensor force plays an important role in the shell evolution of $N = 40$.

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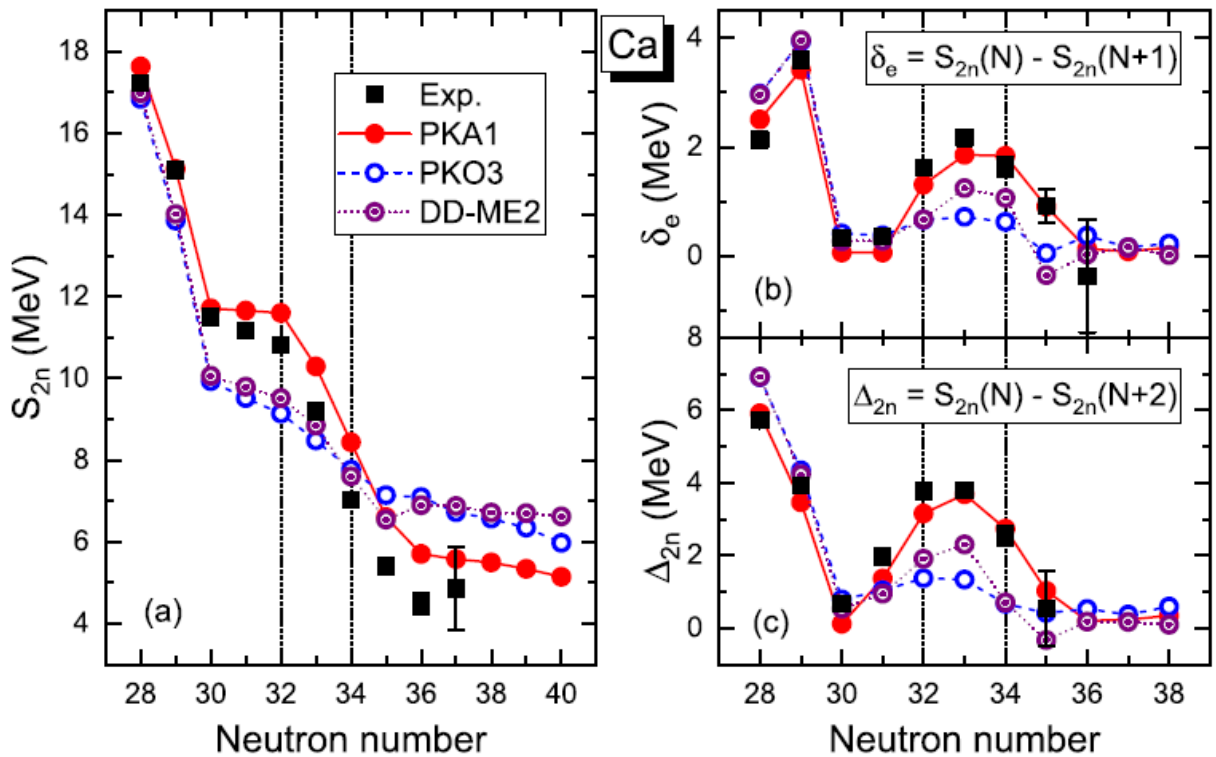
New Magic Numbers N = 32 and 34

- New magic numbers $N = 32$ and 34 have been confirmed in Ca isotopes experimentally according to the 2_1^+ excitation energy and the mass.

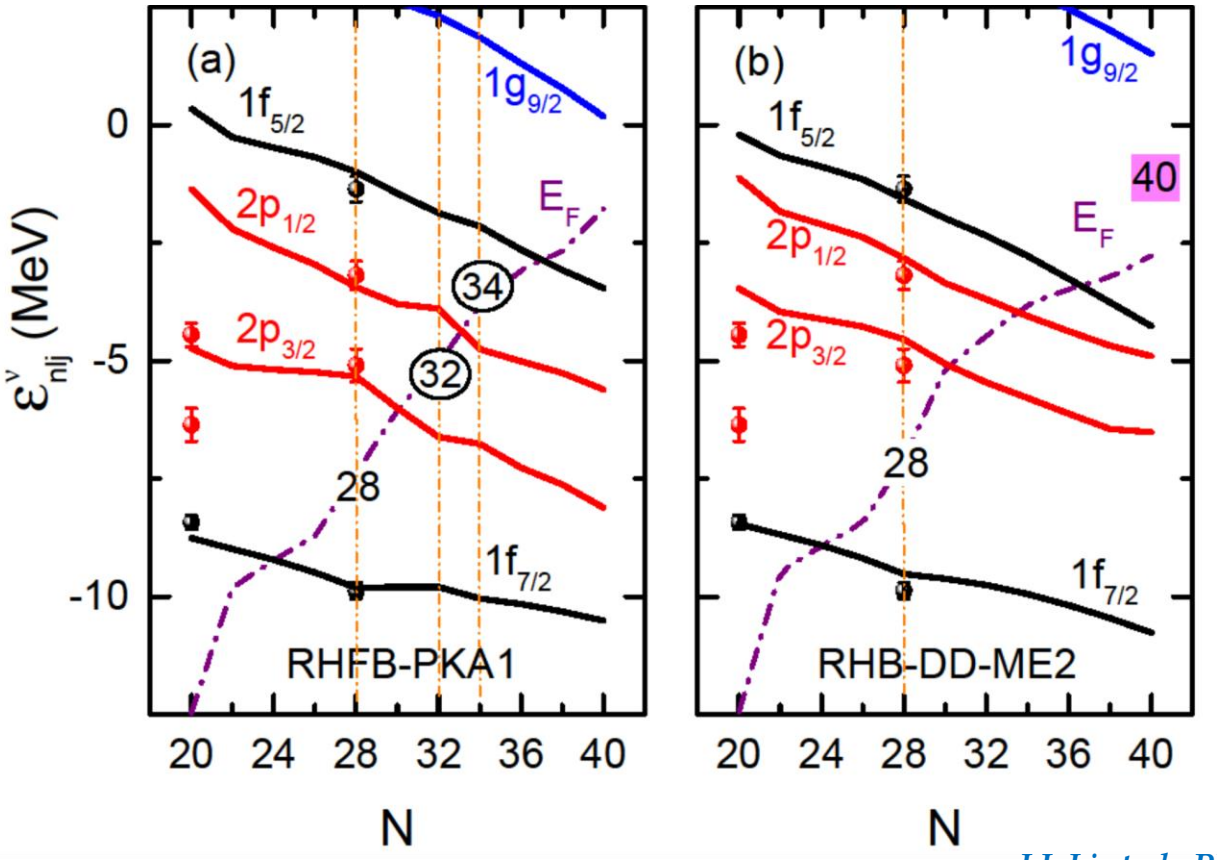


J. Liu et al., PLB 806, 135524 (2020)

PKA1 can reproduce the two-neutron separation energies, that implies new magic numbers at $N = 32$ and 34.

Single-Particle Levels of Ca Isotopes

- Evolution of the neutron single-particle levels for Ca isotopes

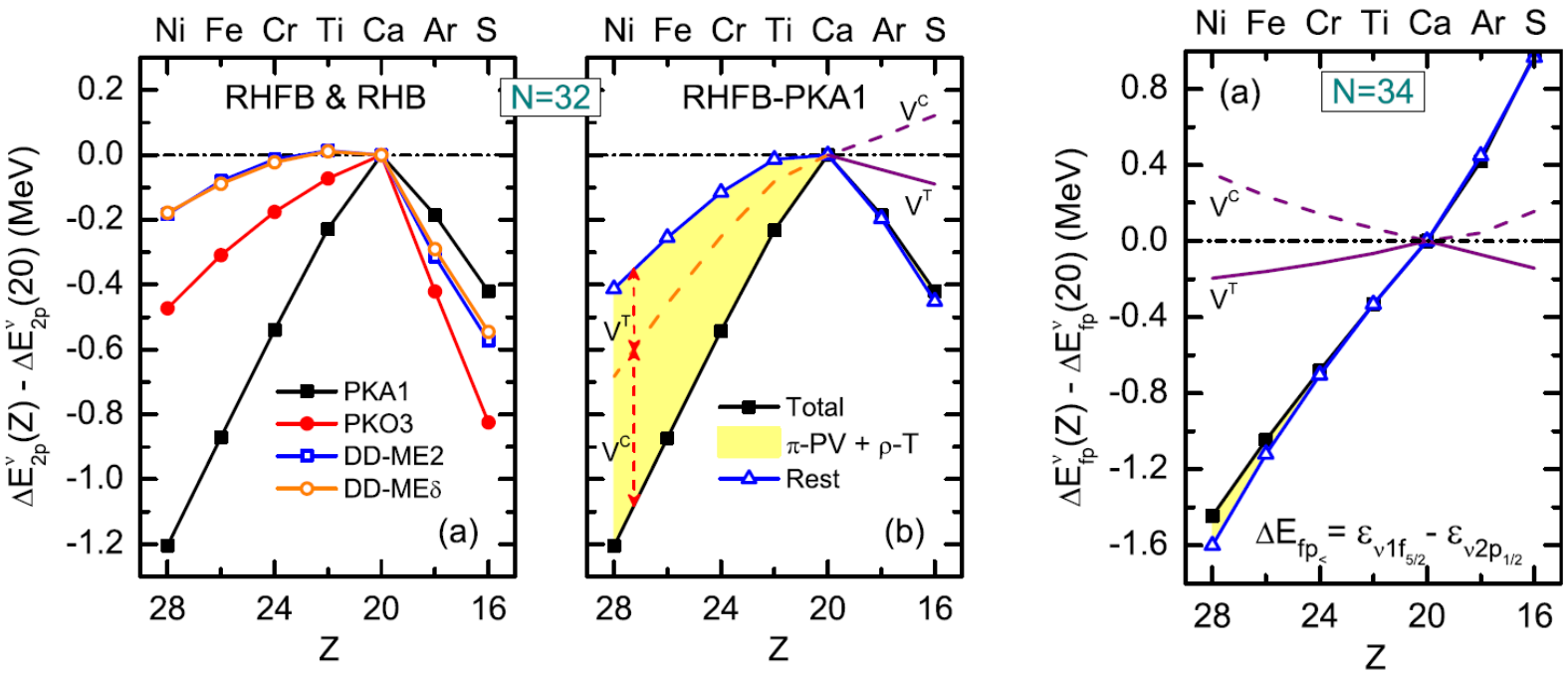


J.J. Li et al., PLB 753, 97 (2016)

The effective interaction PKA1 presents subshells at both $N = 32$ and 34.

Shell Gaps of $N = 32$ and 34 along Isotonic Chains

- Shell gaps at $N = 32$ and 34 along the isotonic chains

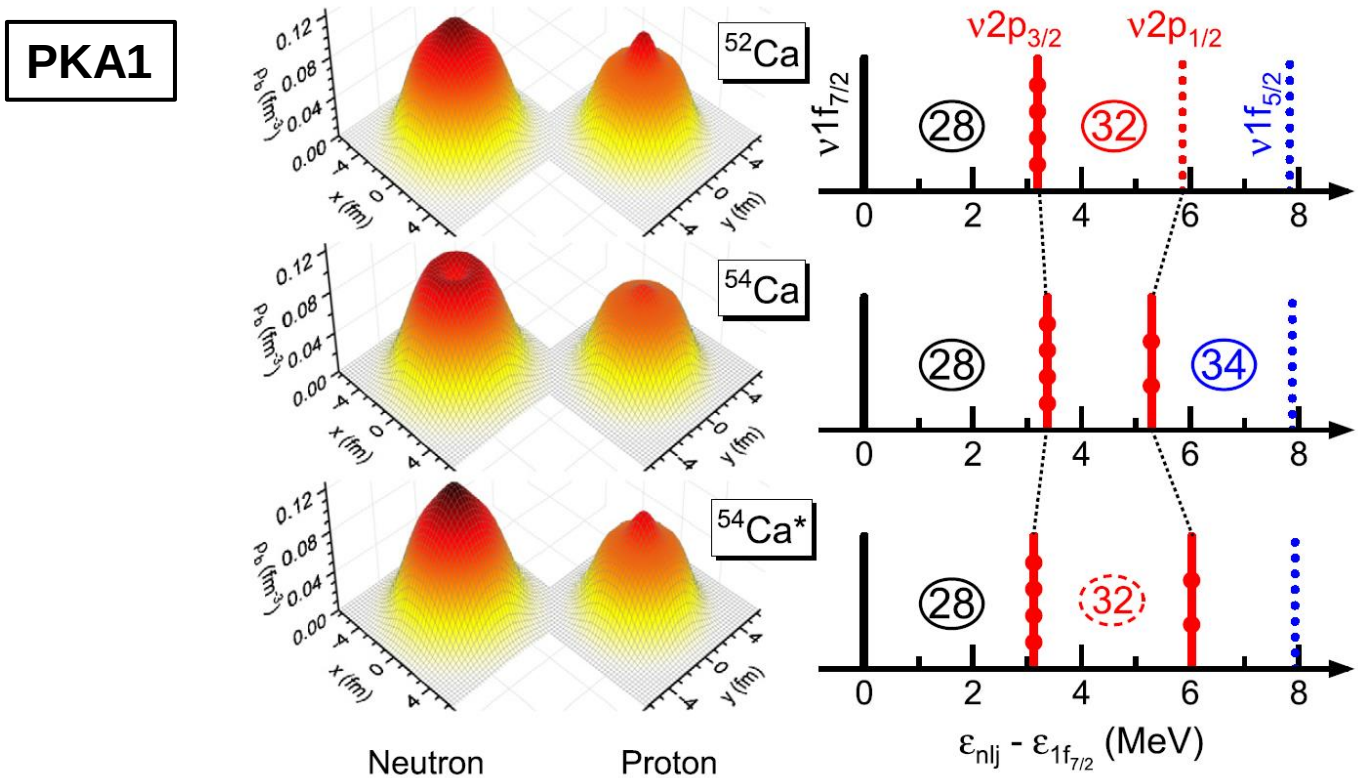


J.J. Li et al., PLB 753, 97 (2016)

The π-PV and ρ-T are **dominant** for the new shell gaps $N = 32$, but tiny contributions to the shell gaps $N = 34$.

Emergence of Subshell at $N = 34$

- The central-depressed density profiles reduce the spin-orbit splitting of $\nu 2p$ states leading to the new magic number $N = 34$



J. Liu et al., PLB 806, 135524 (2020)

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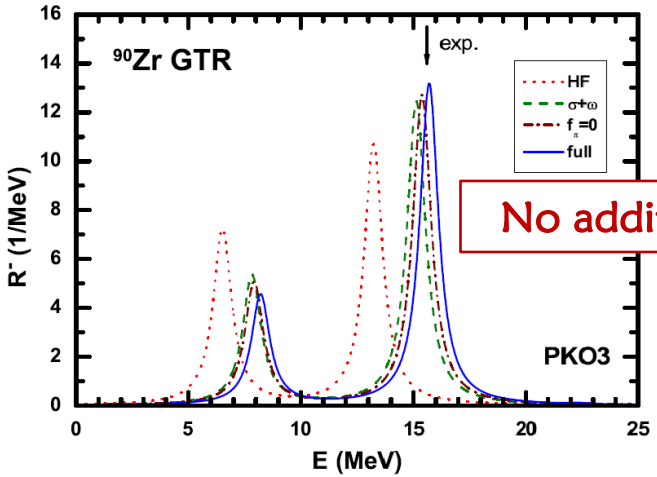
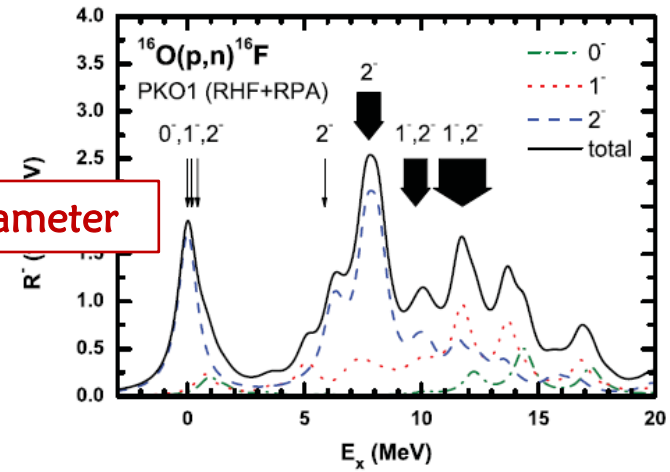
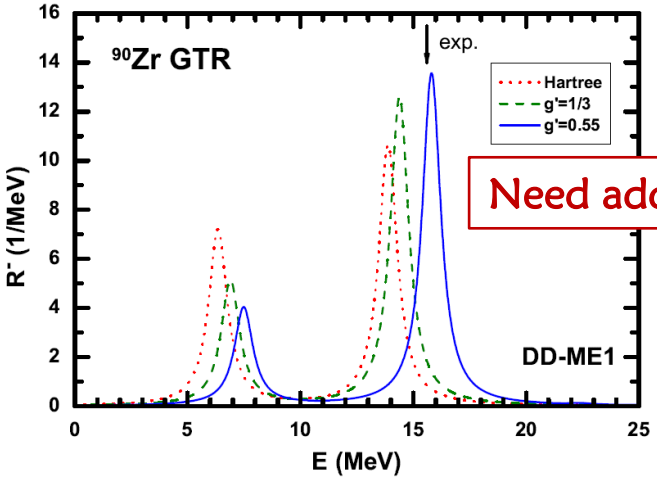
Self-consistent description for Spin-Isospin Excitation

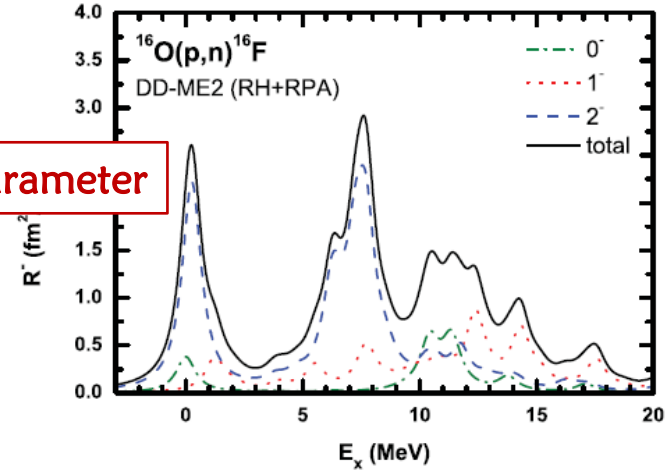
- Gamow-Teller Resonance
- Spin-dipole Resonance





No additional parameter





Need additional parameter

J. Meng et al., AIP CP 1235, 29 (2010)

H.Z. Liang et al., PRC 85, 064302 (2012)

- RHF can self-consistently well describe the spin-isospin excitations without any additional parameters.

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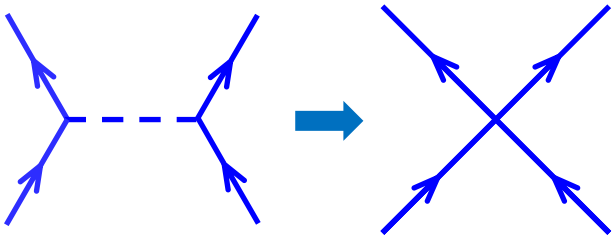
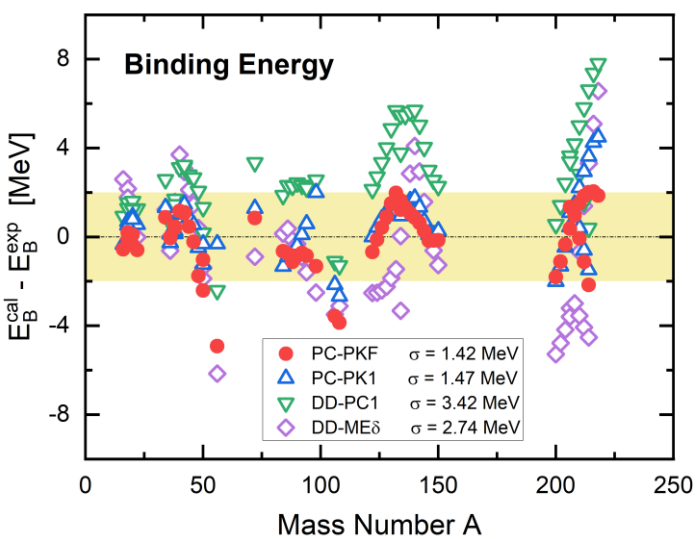
PC-PKF: RDF with Localized Exchange Terms

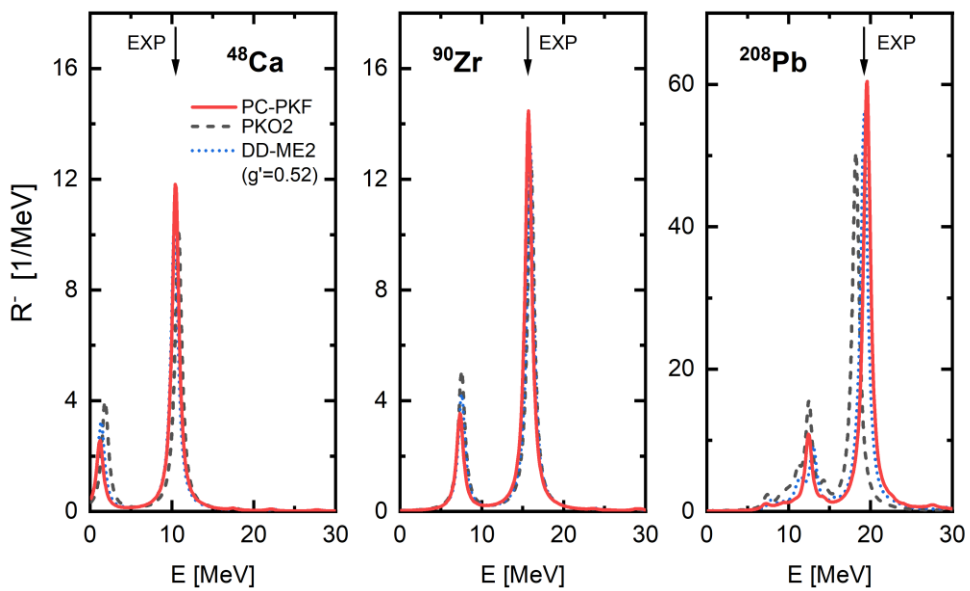
- New relativistic density functional PC-PKF: Localized exchange terms
  - Relativistic point-coupling: zero-range interaction
  - **Fierz transformation**:
    Express the exchange terms as superpositions of Hartree terms

Sulaksono(2003)



- PC-PKF can self-consistently describe the Gamow-Teller resonance excitation energy without adjusting additional parameters





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Relativistic Optimized Effective Potential Method

Kohn-Sham (KS) Density Functional Theory

W. Kohn, L.J. Sham, Phys. Rev. 140 (1965) A1133

Construct the energy density functional with the orbitals from a Kohn-Sham potential which generates the same ground-state density as the interacting system.

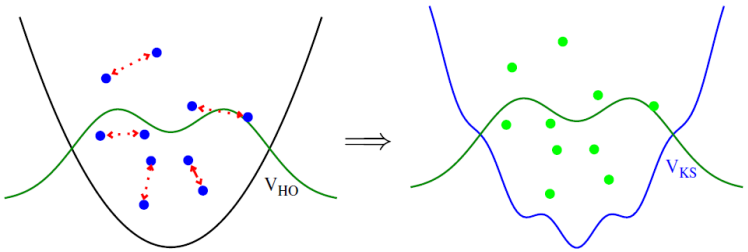


Figure from Drut et al., PPNP 64, 120-168 (2010)

RKS equation $$[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + M + U_{\mathrm{H}}(\boldsymbol{x})]\,\varphi_k^{\mathrm{KS}}(\boldsymbol{x}) + U_{\mathrm{x}}(\boldsymbol{x})\varphi_k^{\mathrm{KS}}(\boldsymbol{x}) = \gamma^0 E_k \varphi_k^{\mathrm{KS}}(\boldsymbol{x})$$

RHF equation $$[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + M + U_{\mathrm{H}}(\boldsymbol{x})]\,\varphi_k^{\mathrm{HF}}(\boldsymbol{x}) + \frac{\delta E_x}{\delta\bar{\varphi}_k^{\mathrm{HF}}(\boldsymbol{x})} = \gamma^0 E_k \varphi_k^{\mathrm{HF}}(\boldsymbol{x})$$

Relativistic Optimized Effective Potential (ROEP) Method

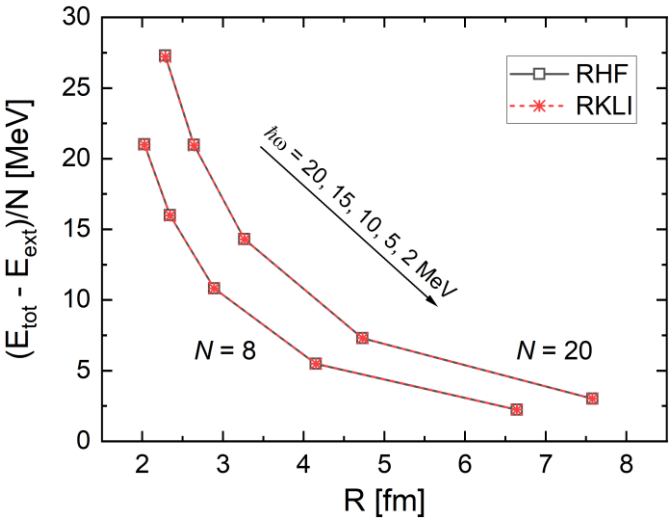
Perturbate Kohn-Sham potential with $$\Delta U_k(\boldsymbol{x}) = \frac{1}{\varphi_k(\boldsymbol{x})}\frac{\delta E_{\mathrm{x}}}{\bar{\varphi}_k(\boldsymbol{x})} - U_{\mathrm{x}}(\boldsymbol{x})$$

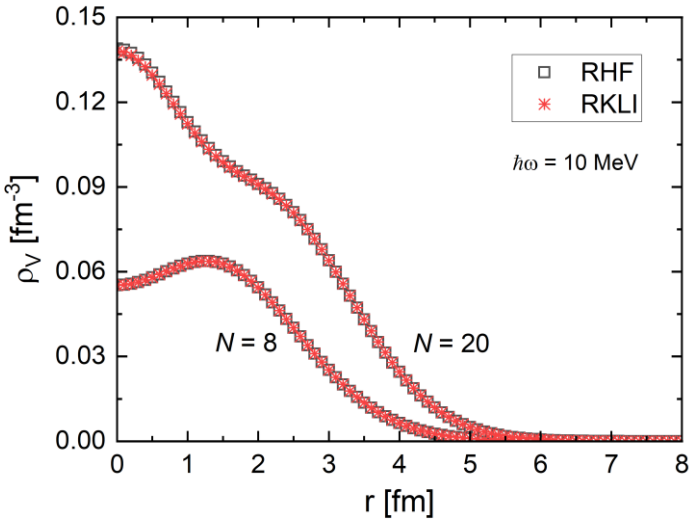
First-order changes on densities and currents
$$\begin{cases} \sum_k^{\mathrm{occ.}} [\Delta\bar{\varphi}_k(\boldsymbol{x})\varphi_k(\boldsymbol{x}) + c.c.] = 0 \\ \sum_k^{\mathrm{occ.}} [\Delta\bar{\varphi}_k(\boldsymbol{x})\gamma_\mu\varphi_k(\boldsymbol{x}) + c.c.] = 0 \end{cases}$$

Relativistic Krieger-Li-Iafrate (RKLI) approximation

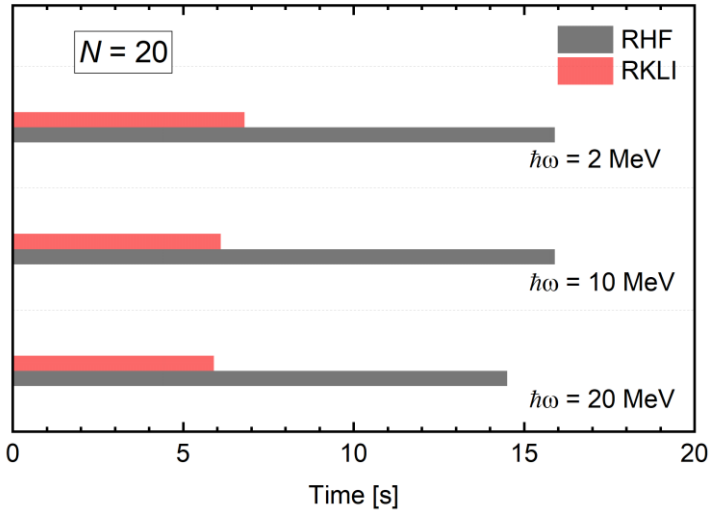
Preliminary Results

- Ground-state properties of neutron drops confined in harmonic potential





- The ground-state energies, radii and density distributions calculated with RKLI approximation are well consistent with the RHF results.
- The time cost is less than half of the RHF calculations. **(~1/3)**



The effective interaction is taken from Bouyssy et al., PRC 36, 380 (1987)

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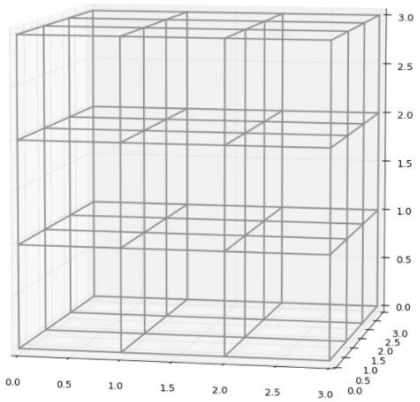
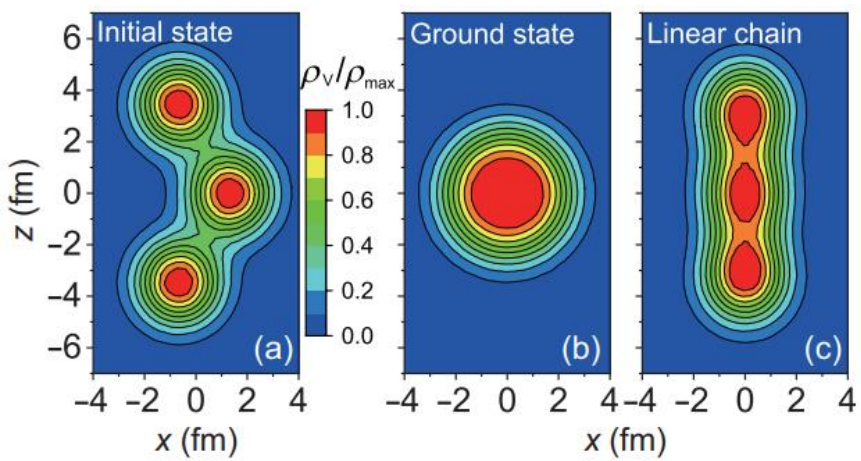
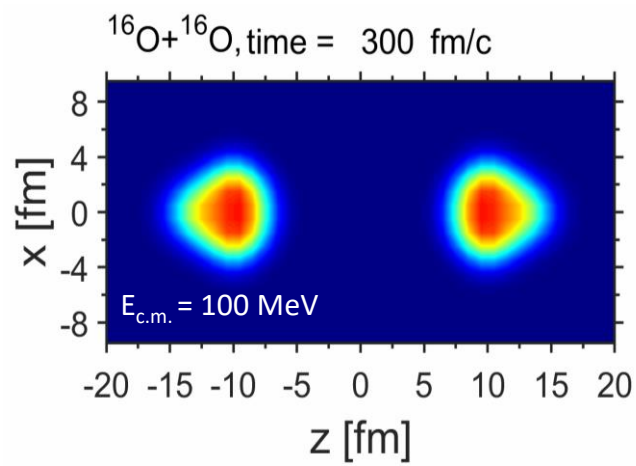
Relativistic Hartree-Fock on 3D Lattice

- Relativistic Hartree-Fock on 3D Lattice
  - No limitation on spatial symmetry
    - ✓ Arbitrary shape: Spherical, axial, triaxial, …
  - Moderate calculation for RHF
    - ✓ Almost only depend on grid number and box size
  - Easy to extend to cranking RHF and time-dependent RHF





Ren et al., SC-PMA 62, 112062 (2019)



Ren et al., PRC 102, 044603 (2020)

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Summary

- Importance of exchange terms:
  - Take into account the **π-PV and ρ-T** couplings (Tensor force)
  - Improve the descriptions of the **shell structures**
  - Self-consistent describe the **spin-isospin excitations**

- Simplify the treatment of exchange terms:
  - Employ **localized exchange terms** (point-coupling interaction)
    - ✓ Good descriptions on properties of finite nuclei
    - ✓ Self-consistent descriptions on Gamow-Teller resonances
  - Apply the **relativistic optimized effective potential method**
    - ✓ Nice agreement with the RHF calculations
    - ✓ Less computational cost (Less time and less memories)

Prospects

- Develop a well optimized **new effective interaction** for RHF/ROEP:
  - Determine the strength of the tensor force
  - Study the correlations between the saturation properties of nuclear matter and properties of finite nuclei
  - Uncertainty analysis for the RHF model

- **Relativistic Hartree-Fock on 3D Lattice**:
  - Combine with the ROEP method
  - Effect of exchange terms on nuclear shapes, low-lying spectrum, …
  - Extend to the time-dependent RHF model

Thank you!