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Relativistic *ab initio* calculation in finite nuclear systems and its promotion to nuclear density functional

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Outline

- Relativistic Brueckner-Hartree-Fock (RBHF) Theory
  - Introduction (HF -> BHF -> RBHF)
  - RBHF description for finite nuclei
  - Summary
- Towards an *ab initio* relativistic density functional
  - New functional guided by RBHF calculations
  - Summary

Outline

- Relativistic Brueckner-Hartree-Fock (RBHF) Theory
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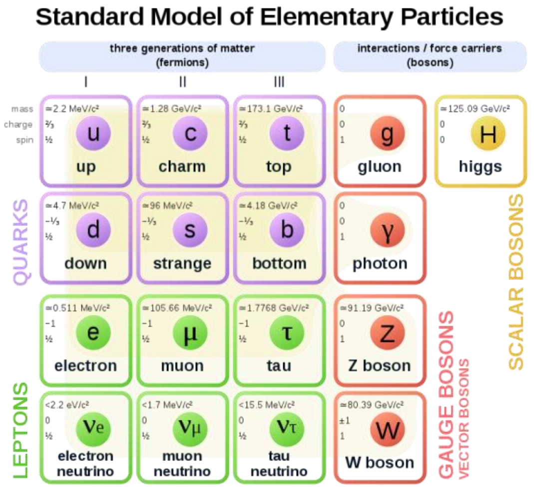
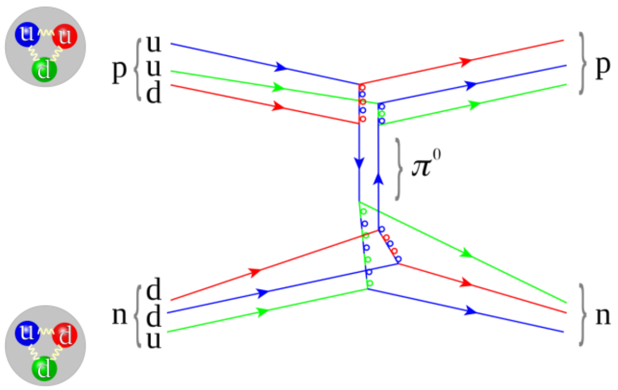
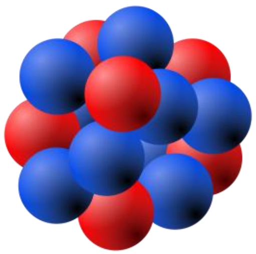
Nuclear *ab initio* Calculations

- Ab initio: from the beginning

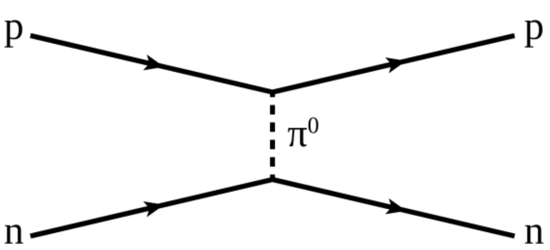


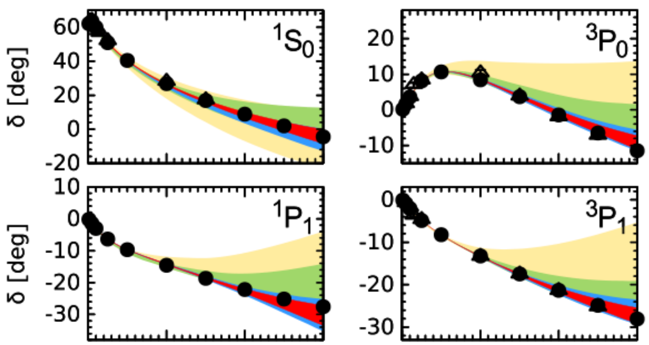




- Chiral effective field theory

At low energy, effective degree of freedom: nucleon and pion





E. Epelbaum, H. Krebs, and U.-G. Meißner, PRL **115**, 122301 (2015)

Nuclear *ab initio* Calculations

- Earlier (realistic) nucleon-nucleon interactions:
  - Reid 93 V. G. J. Stoks, et al., PRC **49**, 2950 (1994)
  - Argonne v18 R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, PRC **51**, 38 (1995)
  - CD Bonn R. Machleidt, PRC **63**, 024001 (2001)
  - …

- Nuclear *ab initio* calculations: realistic NN interaction + many-body framework.

Non-relativistic

- Brueckner-Hartree-Fock (BHF) theory B. Day, RMP **39**, 719 (1967)
- Self-consistent Green's function W. Dickhoff and C. Barbieri, PPNP **52**, 377 (2004)
- Nuclear lattice effective field theory D. Lee, PPNP **63**, 117 (2009)
- No core shell model B. R. Barrett, P. Navrátil, J. P. Vary, PPNP **69**, 131 (2013)
- Coupled-cluster theory G. Hagen, et al., *Rep. Prog. Phys.* **77**, 096302 (2014)
- Quantum Monte Carlo method J. Carlson, et al., RMP **87**, 1067 (2015)
- In medium similarity renormalization group H. Hergert, et al., Phys. Rep. **621**, 165 (2016)
- … …

Relativistic

- Relativistic Brueckner-Hartree-Fock (RBHF) theory M.R. Anastasio, et al., Phys. Rep. **100**, 327 (1983)
- … …

Hartree-Fock Theory

- It is extremely difficult to solve exactly the nuclear many-body Hamiltonian, approximation is unavoidable.

$$H\Psi = E\Psi \qquad H = T + V(\mathbf{r}, \mathbf{r}')$$

$$\Psi_a = \sum_i C_i^{(a)} \Phi_i \qquad \Phi_i(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A) = (A!)^{-1/2} \mathscr{A}(\phi_{i_1}(\mathbf{r}_1)\phi_{i_2}(\mathbf{r}_2) \ldots \phi_{i_A}(\mathbf{r}_A))$$

Dimension explodes easily, N^A

- Hartree-Fock theory

$$\Psi_0 \approx \Phi_0 = (A!)^{-1/2} \mathscr{A}(\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) \ldots \phi_A(\mathbf{r}_A))$$

Dimension, N

$$\frac{\delta \langle \Phi_0 | H | \Phi_0 \rangle}{\delta \phi} = 0 \qquad (T + U)\phi_a = e_a \phi_a$$

$$U(\mathbf{r}) = \int d\mathbf{r}' V(\mathbf{r}, \mathbf{r}') \sum_{a=1}^{A} |\phi_a(\mathbf{r}')|^2 + \text{ exchange term}$$

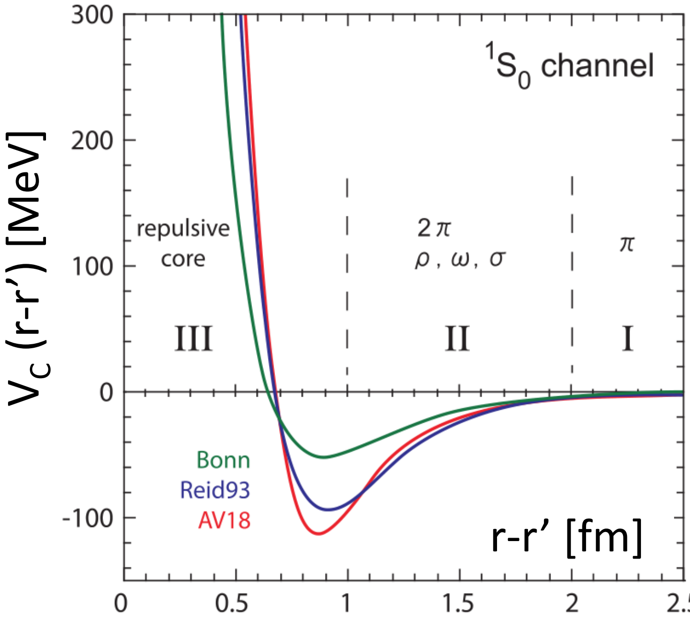
Problem of Hartree-Fock in Nuclear Physics

- Hartree-Fock ground state energy

$$E_0 = \langle \Phi_0 | H | \Phi_0 \rangle = \langle T \rangle + \frac{1}{2} \sum_{a,b=1}^{A} \int d\mathbf{r} d\mathbf{r}' \phi_a^*(\mathbf{r}) \phi_b^*(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \left[\phi_a(\mathbf{r}) \phi_b(\mathbf{r}') - \phi_b(\mathbf{r}) \phi_a(\mathbf{r}') \right]$$

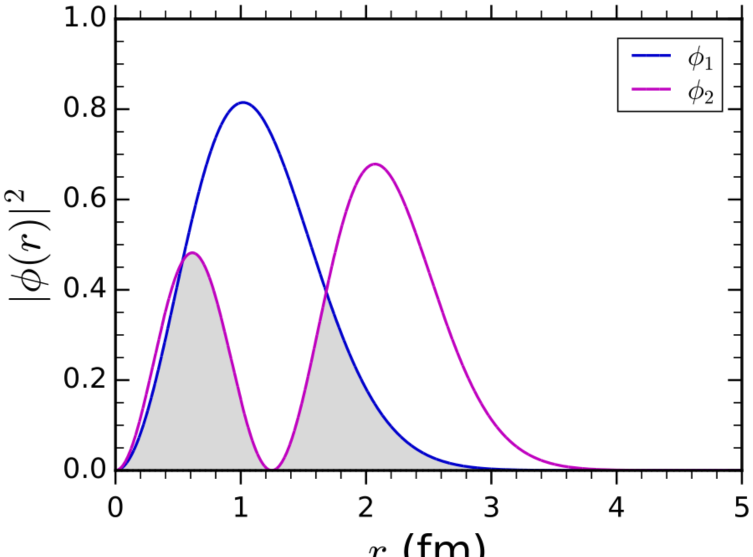
$$\langle ab | \bar{V} | ab \rangle$$

- NN interaction has a very strong repulsive core



N. Ishii, S. Aoki, and T. Hatsuda, *PRL* **99**, 022001 (2007)

For hard core ($V \to \infty$ when $r < r_c$) model, the interacting energy between two nucleons even diverges.



Inspiration from NN Scattering

- Lippmann-Schwinger equation

$$|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\varepsilon} V |\psi^{(\pm)}\rangle \qquad H = H_0 + V \quad H_0 = \frac{\mathbf{p}^2}{2m}$$

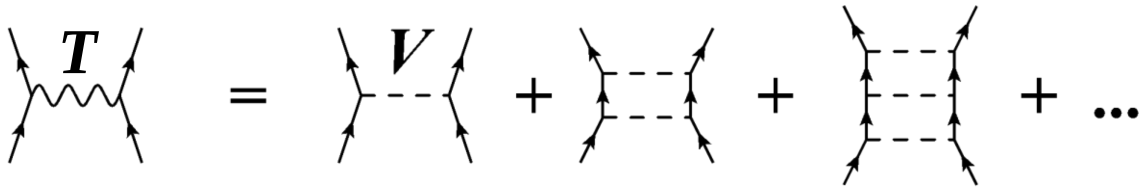
H $\qquad$ H_0

In the form of T-matrix

$$T = V + V \frac{1}{E - H_0 + i\varepsilon} T \qquad V|\psi^{(+)}\rangle = T|\phi\rangle$$

- Born series

$$T = V + V \frac{1}{E - H_0 + i\varepsilon} V + V \frac{1}{E - H_0 + i\varepsilon} V \frac{1}{E - H_0 + i\varepsilon} V + \cdots$$



- If one calculates the T-matrix order by order, the result diverges; if one solve the Lippmann-Schwinger equation exactly, the correct result is obtained.

Re-examine of Hartree-Fock Theory

- Decompose the full many-body Hamiltonian

$$H = H_0 + H_1 \qquad H_0 = T + U, \quad H_1 = V - U$$

Hartree-Fock

Hartree-Fock equation

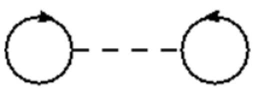
$$(T + U)\phi_a = e_a \phi_a$$

$$\Phi_0 = (A!)^{-1/2} \mathscr{A}(\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\ldots\phi_A(\mathbf{r}_A))$$

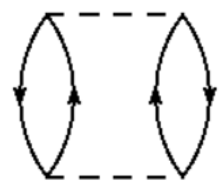
- Many-body perturbation

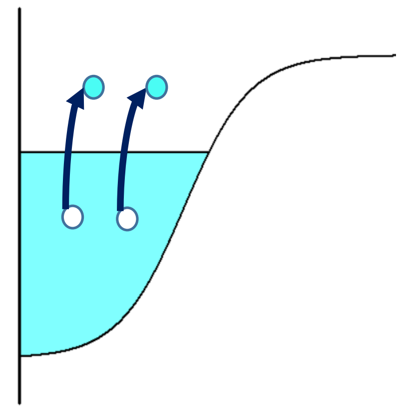
$$E = E_0 + \langle\Phi_0|H_1|\Phi_0\rangle + \langle\Phi_0|H_1(E_0 - H_0)^{-1} P H_1|\Phi_0\rangle + \ldots$$

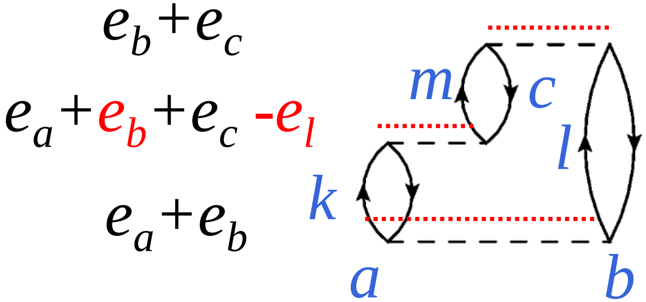
$$= \langle T\rangle + \frac{1}{2}\sum_{a,b\le A}\langle ab|\bar{V}|ab\rangle + \frac{1}{4}\sum_{a,b\le A}\sum_{kl>A}\frac{\langle ab|\bar{V}|kl\rangle\langle kl|\bar{V}|ab\rangle}{e_a + e_b - e_k - e_l} + \ldots$$

direct term: 

Hartree(-Fock)







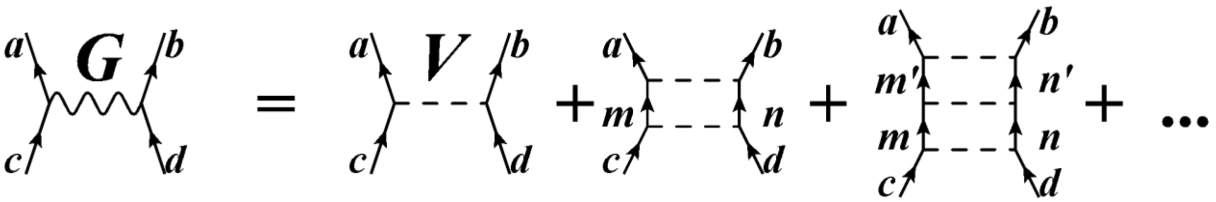
$$\langle cb|V|ml\rangle\langle am|V|kc\rangle\langle kl|V|ab\rangle$$

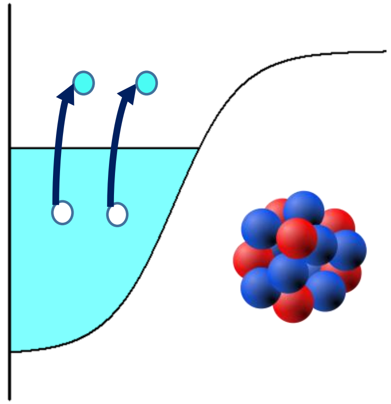
Brueckner theory: sum up ladder diagrams in the many-body perturbation series

K. A. Brueckner, C. A. Levinson, and H. M. Mahmoud, *Phys. Rev.* **95**, 217 (1954)

Brueckner Theory

- Bethe-Goldstone equation





$$\langle ab|G(W)|cd\rangle = \langle ab|V|cd\rangle + \sum_{mn}\langle ab|V|mn\rangle \frac{Q(m,n)}{W - e_m - e_n}\langle mn|G(W)|cd\rangle$$

Dimension: N^2

H. A. Bethe and J. Goldsteon, *Proc. R. Soc. A* **238**, 551 (1957)

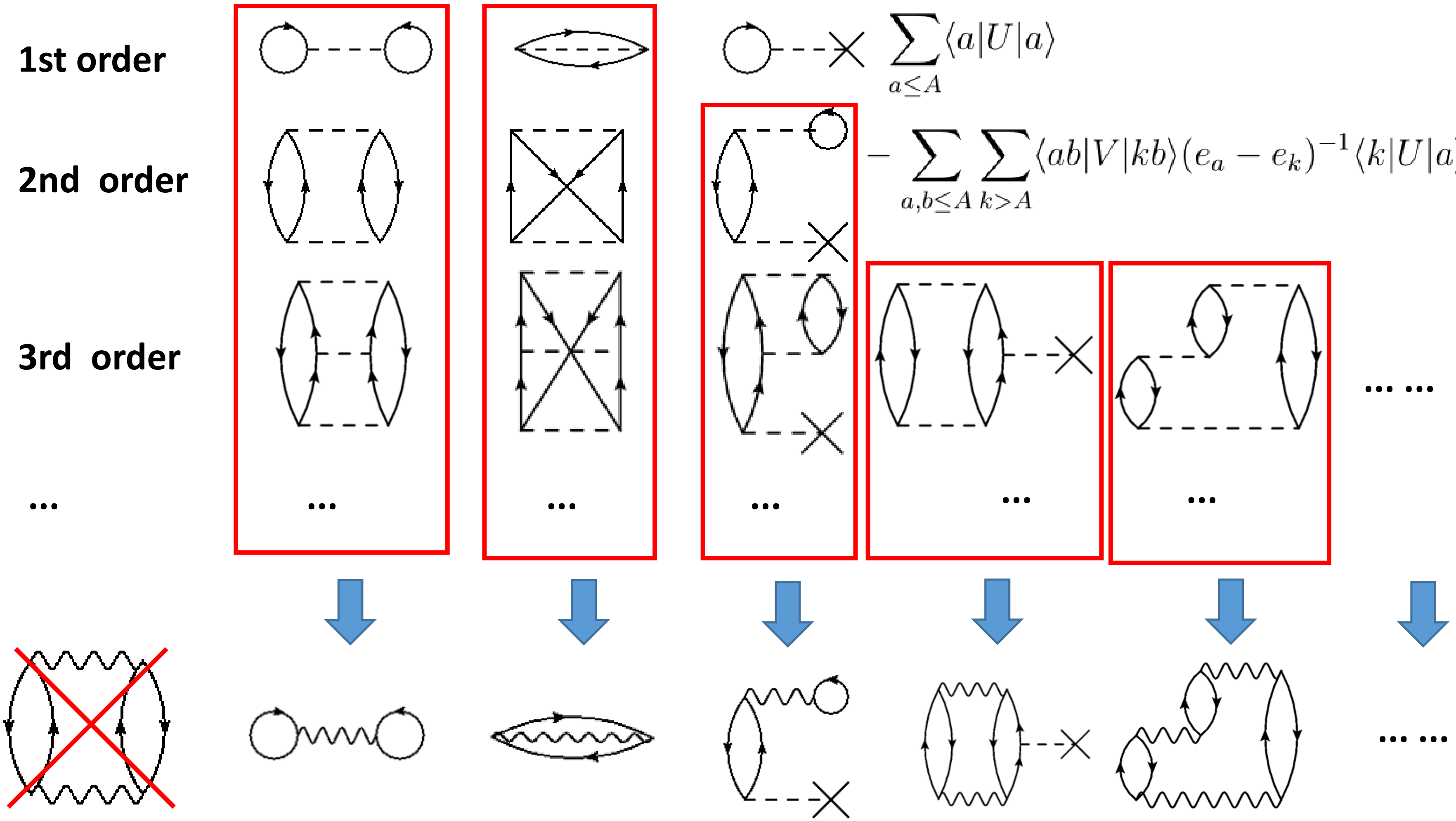
- Q is the Pauli operator which forbids the states being scattered below Fermi surface.

$$Q = \begin{cases} 1, & e_m, e_n > e_F \\ 0, & e_m \le e_F \text{ or } e_n \le e_F \end{cases}$$

- W is the so-called starting energy.

From V-Matrix to G-Matrix

- Transform all the V-matrix diagram to G-matrix diagram:



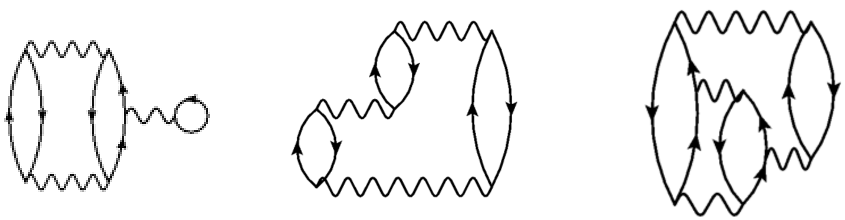
- The G-matrices have small numerical values and are suitable to be used in perturbative expansion.

Hole Line Expansion

- Expansion in powers of G is not converging, but converges in numbers of independent hole lines. R. Rajaraman, *Phys. Rev.* **131**, 1244 (1963)

- Reorganize the diagrams according to the number of independent hole lines:

2 hole line  Brueckner-Hartree-Fock

3 hole line  … …

… … … …

- Convergence properties (hard core as an example): $$\frac{\langle N_{\text{hole}} + 1 \rangle}{\langle N_{\text{hole}} \rangle} \approx 4\pi r_c^3 \rho$$

$$r_c = 0.4 \text{ fm}, \rho = 0.17 \text{ fm}^{-3} \quad \rightarrow 0.14$$

B. D. Day, RMP **39**, 719 (1969)

Moszkowski-Scott hard core interaction: V2 ≈ -38 MeV, V3 ≈ -5 MeV ≈ 13% V2 (T ≈ 23 MeV). M. W. Kirson, NPA **99**, 353 (1967)

Brueckner-Hartree-Fock Theory

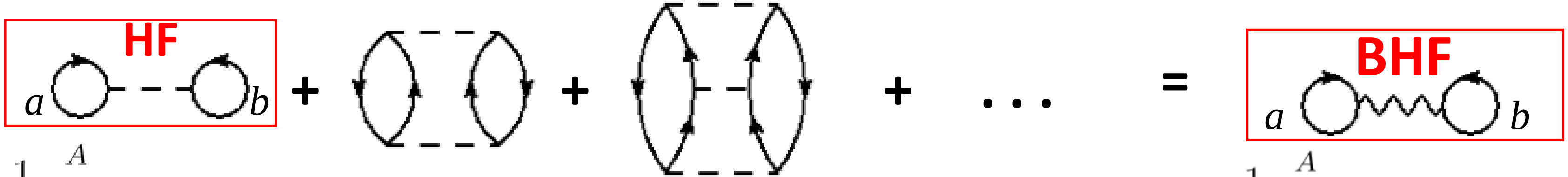
- Hartree-Fock equation in complete basis,

$$\sum_j (T_{ij} + U_{ij}) D_{ja} = e_a D_{ia} \qquad U_{ij} = \sum_{c=1}^{A} \langle ic|\bar{G}(W)|jc\rangle$$

where D are the expansion coefficients: $|a\rangle = \sum_i D_{ia}|i\rangle.$

- G-matrix is obtained by solving Bethe-Goldstone equation.

- BHF total energy



$$\frac{1}{2}\sum_{ab}^{A}\langle ab|V|ab\rangle \qquad \frac{1}{2}\sum_{ab}^{A}\langle ab|G(W)|ab\rangle$$

together with exchange term, $W = e_a + e_b$

$$E = \sum_a^A \langle a|T|a\rangle + \frac{1}{2}\sum_{ab}^{A}\langle ab|\bar{G}(W)|ab\rangle.$$

Brueckner-Hartree-Fock Theory

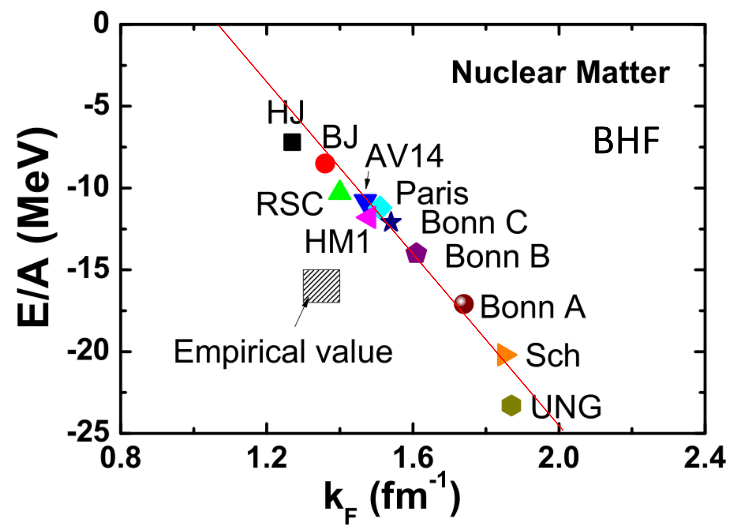
- Systematic investigation of nuclear matter saturation property with BHF:
  Coester line F. Coester, et al., *PRC* **1**, 769 (1970).

- Similar situation in finite nuclei.

BHF for ^{16}O

^{16}O	Bonn C	Bonn B	Bonn A	Exp.
E/A (MeV)	-4.49	-5.35	-6.56	**-7.98**
r_c (fm)	2.465	2.380	2.291	**2.70**

H. Müther, R. Brockmann, and R. Machleidt, *PRC* **42**, 1981 (1990)



R. Brockmann and R. Machleidt, *PRC* **42**, 1965 (1990)

- Variational methods (with correlation function) were developed, but the results were still not in agreement with the data.
  R. Jastrow, PR **98**, 1479 (1955),
  J. W. Clark and E. Feenberg, PR **113**, 388 (1959),
  V. R. Pandhanpande and R. B. Wiringa, NPA **266**, 269 (1976)

Crisis in Nuclear-Matter Theory

Nuclear Physics **A328** (1979) 587–595 © *North-Holland Publishing Co., Amsterdam*

UPDATE ON THE CRISIS IN NUCLEAR-MATTER THEORY: A SUMMARY OF THE TRIESTE CONFERENCE

J. W. CLARK

*McDonnell Center for the Space Sciences and Department of Physics, Washington University, St. Louis, Missouri 63130**

itself. The notion that nuclear saturation can be explained in terms of a non-relativistic system of nucleons alone, interacting by two-body forces fitted to scattering data, would be in doubt (crisis II). The contributions to this meeting

PRL **117,** 052501 (2016) PHYSICAL REVIEW LETTERS week ending 29 JULY 2016

Radii and Binding Energies in Oxygen Isotopes: A Challenge for Nuclear Forces

V. Lapoux,[1,*] V. Somà,[1] C. Barbieri,[2] H. Hergert,[3] J. D. Holt,[4] and S. R. Stroberg[4]

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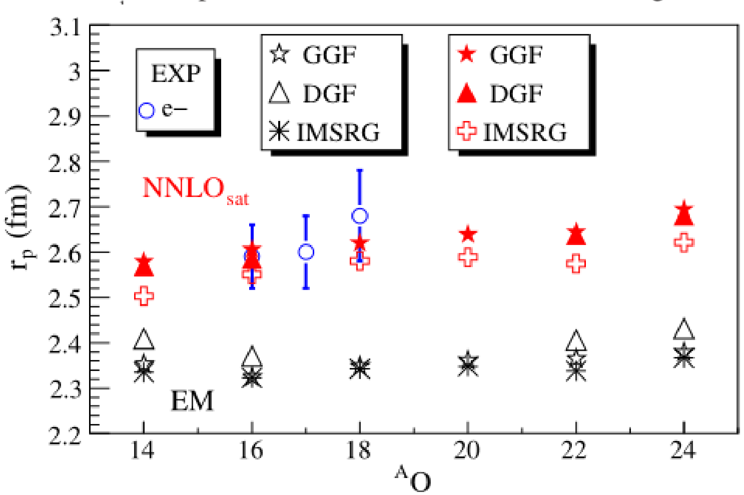
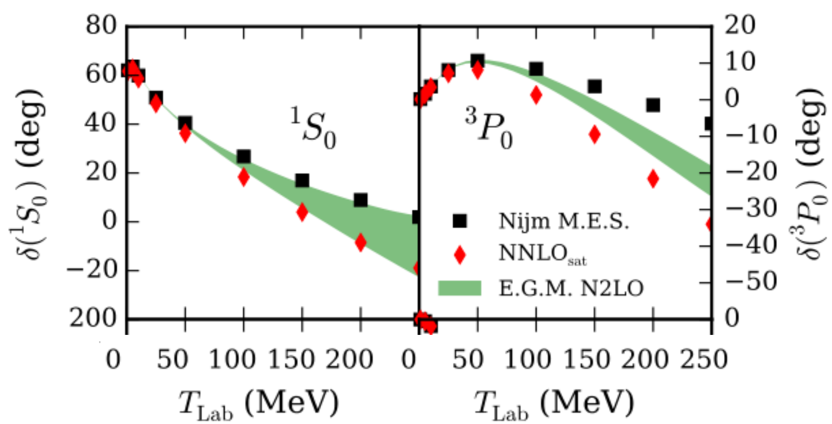


A. Ekström, et al., PRC **91**, 051301(R) (2015)



Relativistic Brueckner-Hartree-Fock Theory

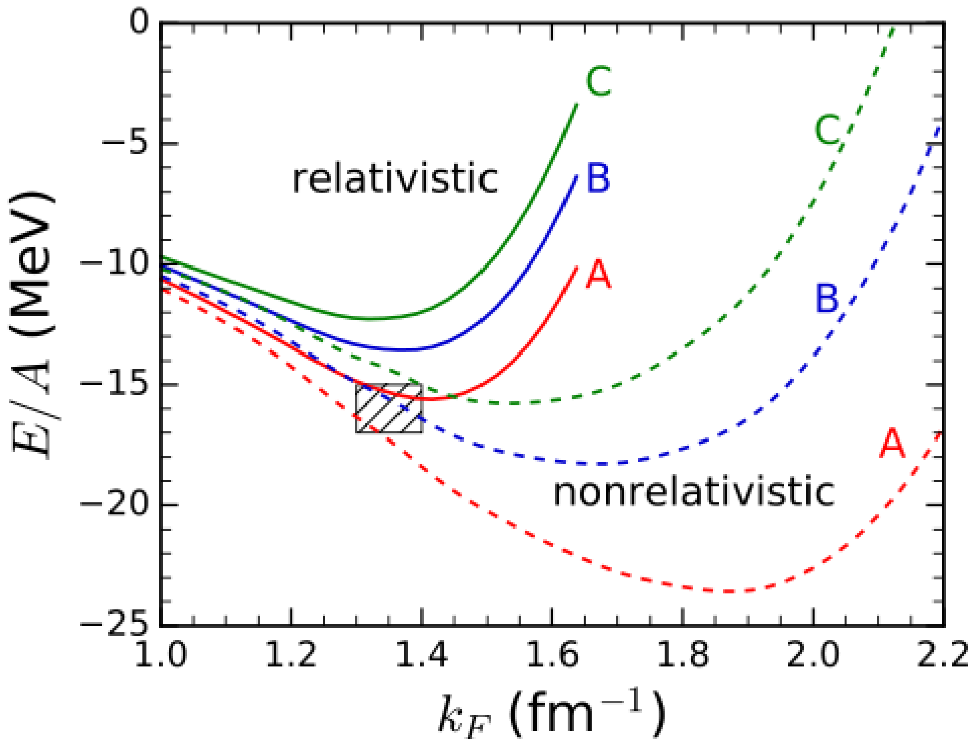
- RBHF for nuclear matter

  M. R. Anastasio, L. S. Celenza, and C. M. Shakin, PRL **45**, 2096 (1980)

  C. J. Horowitz and B. D. Serot, PLB **137**, 287 (1984)

  R. Brockmann and R. Machleidt, PLB **149**, 283 (1984)

  B. ter Haar and R. Malfliet, PRL **56**, 1237 (1986)



Equation of state of symmetric nuclear matter by BHF and RBHF with Bonn A, B, C interactions

R. Brockmann and R. Machleidt, *PRC* **42**, 1965 (1990)

Relativistic Effect

- Relativistic effect in nuclear physics

  G. E. Brown, W. Weise, G. Baym and J. Speth, Comments Nucl. Part. Phys. **17**, 39 (1987)

$$\phi_{\mathbf{k},s}(\mathbf{x}) = u(\mathbf{k},s)e^{i\mathbf{k}\cdot\mathbf{x}} \qquad (\boldsymbol{\gamma}\cdot\mathbf{k} + M + U)u(\mathbf{k},s) = \gamma^0 E_{\mathbf{k}} u(\mathbf{k},s)$$

Free space, U = 0

$$u(\mathbf{k},s) \sim \begin{pmatrix} 1 \\ \frac{\boldsymbol{\sigma}\cdot\mathbf{k}}{E_{\mathbf{k}}+M} \end{pmatrix} \chi_s$$

$$v(\mathbf{k},s) \sim \begin{pmatrix} \frac{\boldsymbol{\sigma}\cdot\mathbf{k}}{E_{\mathbf{k}}+M} \\ 1 \end{pmatrix} \chi_{-s}$$

$$E_{\mathbf{k}}^2 = M^2 + \mathbf{k}^2$$

Nuclear matter, $U(\mathbf{k}) = U_s(\mathbf{k}) + \gamma^\mu U_\mu(\mathbf{k})$

$$u(\mathbf{k},s) \sim \begin{pmatrix} 1 \\ \frac{\boldsymbol{\sigma}\cdot\mathbf{k}}{E^*_{\mathbf{k}}+M^*} \end{pmatrix} \chi_s$$

$$E^*_{\mathbf{k}} = E_{\mathbf{k}} - U_0(\mathbf{k})$$

$$M^* = M + U_s(\mathbf{k})$$

$$E_{\mathbf{k}}^{2*} = M^{*2} + \mathbf{k}^2$$

$$\langle \frac{\mathbf{k}^2}{2M} \rangle \approx 23 \left(\frac{\rho}{\rho_0}\right)^{2/3} \ \mathrm{MeV}$$

$$M \sim 939 \ \mathrm{MeV}$$

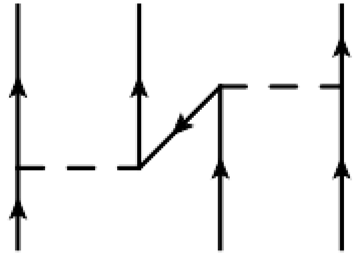
$$\delta E_{\mathbf{k}} \approx \left(\frac{U_s}{M}\right)^2 \frac{\mathbf{k}^2}{2M} \rightarrow \frac{\delta E}{A} \approx 4.2 \left(\frac{\rho}{\rho_0}\right)^{8/3} \ \mathrm{MeV}$$

$$\langle U_s \rangle \approx -400 \frac{\rho}{\rho_0} \ \mathrm{MeV}$$

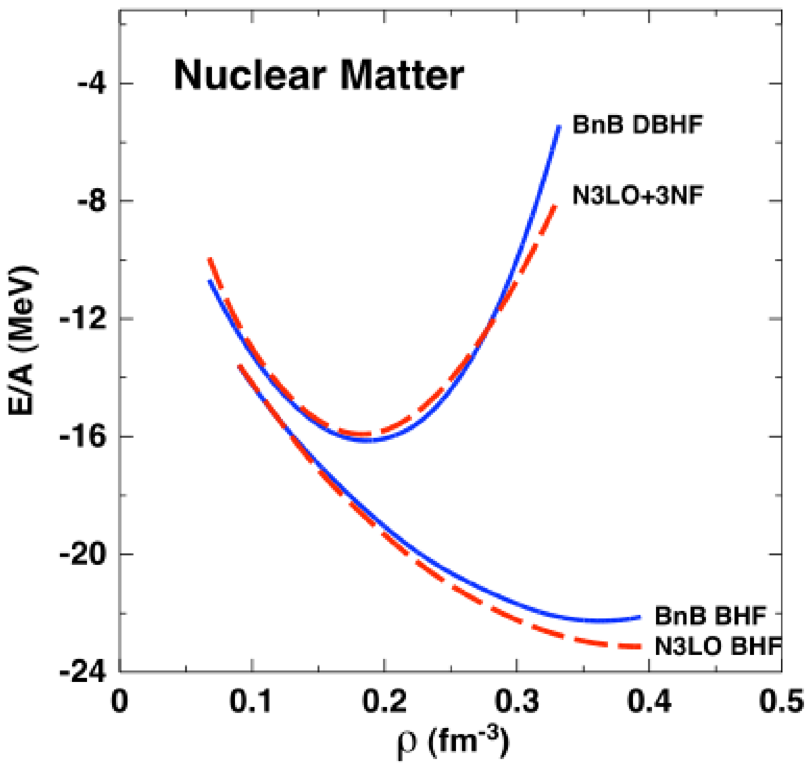
Relativistic Effect

➢ Relativistic origin of 3N interaction

$$\delta E_{\mathbf{k}} \approx \left(\frac{U_s}{M}\right)^2 \frac{\mathbf{k}^2}{2M}$$



G. E. Brown, W. Weise, G. Baym and J. Speth, Comments Nucl. Part. Phys. **17**, 39 (1987)



Equation of state of nuclear matter calculated by

- BHF with Bonn B interaction (BnB BHF)
- RBHF with Bonn B interaction (BnB DBHF)

same interaction, different frameworks

- BHF with 2N interaction N3LO (N3LO BHF)
- BHF with 2N interaction N3LO + 3N interaction N2LO (N3LO+3NF)

same (nonrelativistic) framework, different interactions

F. Sammarruca, et al., PRC **86**, 054317 (2012)

Outline

- Relativistic Brueckner-Hartree-Fock (RBHF) Theory
  - Introduction (HF -> BHF -> RBHF)
  - RBHF description for finite nuclei

    S. Shen, *et al.*, Chin. Phys. Lett. **33**, 102103 (2016)

    S. Shen, *et al.*, PRC **96**, 014316 (2017)
  - Summary

- Towards an ab initio relativistic density functional
  - New functional guided by RBHF calculations
  - Summary

Realistic Nucleon-Nucleon Interaction

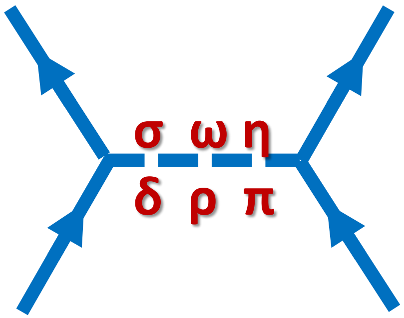
- Starting point: Bonn potential R. Machleidt, *Adv. Nucl. Phys.* **19**, 189 (1989)

  The interaction Lagrangians are defined as

$$\mathscr{L}_{NNpv} = -\frac{f_{ps}}{m_{ps}}\bar{\psi}\gamma^5\gamma^\mu\psi\partial_\mu\varphi^{(ps)},$$

$$\mathscr{L}_{NNs} = g_s\bar{\psi}\psi\varphi^{(s)},$$

$$\mathscr{L}_{NNv} = -g_v\bar{\psi}\gamma^\mu\psi\varphi_\mu^{(v)} - \frac{f_v}{4M}\bar{\psi}\sigma^{\mu\nu}\psi\left(\partial_\mu\varphi_\nu^{(v)} - \partial_\nu\varphi_\mu^{(v)}\right).$$



- Bosons to be exchanged include σ, δ (scalar); ω, ρ (vector); η, π (pseudovector).
- A monopole-type form factor is attached to each vertex. $\frac{\Lambda_\alpha^2 - m_\alpha^2}{\Lambda_\alpha^2 + \mathbf{q}^2}$
- Coupling constants are determined by NN scattering and deuteron properties R. Machleidt, *Adv. Nucl. Phys.* **19**, 189 (1989).

Relativistic Hamiltonian

- Hamiltonian in second quantized form

$$H = \sum_{ab} \langle a|T|b\rangle b_a^\dagger b_b + \frac{1}{2}\sum_i \sum_{abcd} \langle ab|V_i|cd\rangle b_a^\dagger b_b^\dagger b_d b_c,$$

matrix elements are defined as

$$\langle a|T|b\rangle = \int d^3x \bar{\psi}_a(\boldsymbol{x}) \left(-i\boldsymbol{\gamma}\cdot\nabla + M\right) \psi_b(\boldsymbol{x}),$$

$$\langle ab|V_i|cd\rangle = \int d^3x_1 d^3x_2 \bar{\psi}_a(\boldsymbol{x}_1)\bar{\psi}_b(\boldsymbol{x}_2)\Gamma_i(1,2)D_i(\boldsymbol{x}_1,\boldsymbol{x}_2)\psi_c(\boldsymbol{x}_1)\psi_d(\boldsymbol{x}_2).$$

interaction vertex

$$\Gamma_s = g_s,$$

$$\Gamma_{pv} = \frac{f_{ps}}{m_{ps}}\gamma^5\gamma^i\partial_i,$$

$$\Gamma_v^\mu = g_v\gamma^\mu + \frac{f_v}{2M}\sigma^{i\mu}\partial_i.$$

propagator

$$D_\alpha(x_1,x_2) = \pm\int \frac{d^4q}{(2\pi)^4}\frac{1}{m_\alpha^2 - q^2}e^{-iq(x_1-x_2)}$$

Dirac spinor

$$|a\rangle = \frac{1}{r}\begin{pmatrix} F_{n_a\kappa_a}(r)\Omega^{l_a}_{j_a m_a}(\theta,\varphi) \\ iG_{n_a\kappa_a}(r)\Omega^{\tilde{l}_a}_{j_a m_a}(\theta,\varphi) \end{pmatrix},$$

$$\Omega^l_{jm}(\theta,\varphi) = \sum_{m_l m_s} C^{jm}_{l m_l \frac{1}{2} m_s} Y_{l m_l}(\theta,\varphi)\chi_{m_s}.$$

RBHF Equations

- Hartree-Fock equation in complete basis,

$$\sum_j (T_{ij} + U_{ij}) D_{ja} = e_a D_{ia} \qquad U_{ij} = \sum_{c=1}^{A} \langle ic|\bar{G}(W)|jc\rangle$$

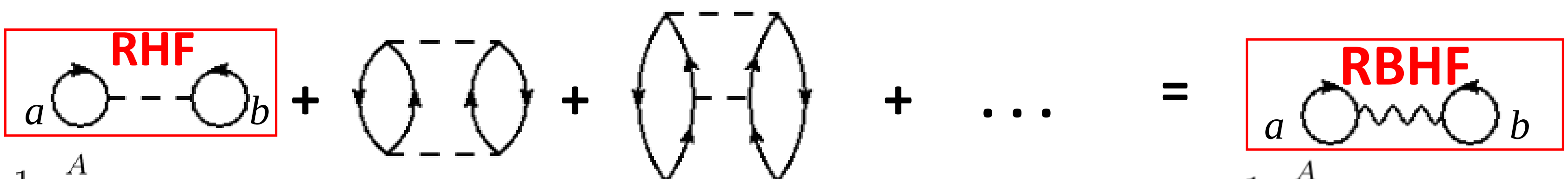
$$U_s, U_v, U_{pv}, U_t$$

where D are the expansion coefficients: $|a\rangle = \sum_i D_{ia}|i\rangle.$

- G-matrix is obtained by solving Bethe-Goldstone equation.

$$\langle ab|G(W)|cd\rangle = \langle ab|V|cd\rangle + \sum_{mn} \langle ab|V|mn\rangle \frac{Q(m,n)}{W - e_m - e_n} \langle mn|G(W)|cd\rangle$$

- RBHF total energy



$$\frac{1}{2}\sum_{ab}^{A} \langle ab|V|ab\rangle \qquad W = e_a + e_b \qquad \frac{1}{2}\sum_{ab}^{A} \langle ab|G(W)|ab\rangle$$

Solution of Bethe-Goldstone Equation

P. Sauer, NPA **150**, 467 (1970)

- One common way to solve the Bethe-Goldstone equation in BHF

$$\langle ab|G(W)|cd\rangle = \langle ab|V|cd\rangle + \sum_{mn} \langle ab|V|mn\rangle \frac{Q(m,n)}{W - e_m - e_n} \langle mn|G(W)|cd\rangle$$

Dimension: N^2

center-of-mass coordinate

$$\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2 \quad \mathbf{k} = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2) \quad \mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

plane wave

$$e^{i\mathbf{k}_1\cdot\mathbf{r}_1} e^{i\mathbf{k}_2\cdot\mathbf{r}_2} = e^{i\mathbf{K}\cdot\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

harmonic oscillator

$$\langle n_1 l_1 n_2 l_2 | N L n l \rangle$$

I. Talmi, Helvetica Physica Acta **25**, 185 (1952)
M. Moshinsky, NP **13**, 104 (1959)

$$\mathbf{K}, \mathbf{R}, NL \quad \mathbf{k}, \mathbf{r}, nl \quad \mathbf{k}_1, \mathbf{r}_1, n_1 l_1 \quad \mathbf{k}_2, \mathbf{r}_2, n_2 l_2$$

Lippmann-Schwinger equation

basis transformation to harmonic oscillator

$$\langle k'|T(W;NL)|k\rangle_{JST} \rightarrow \langle n'l'|T(W;NL)|nl\rangle_{JST}$$

correction for Pauli principle

basis transformation to rest coordinate

$$\rightarrow \langle n'l'|G(W;NL)|nl\rangle_{JST} \rightarrow \langle n_1' l_1', n_2' l_2'|G(W;NL)|n_1 l_1, n_2 l_2\rangle_{JT}$$

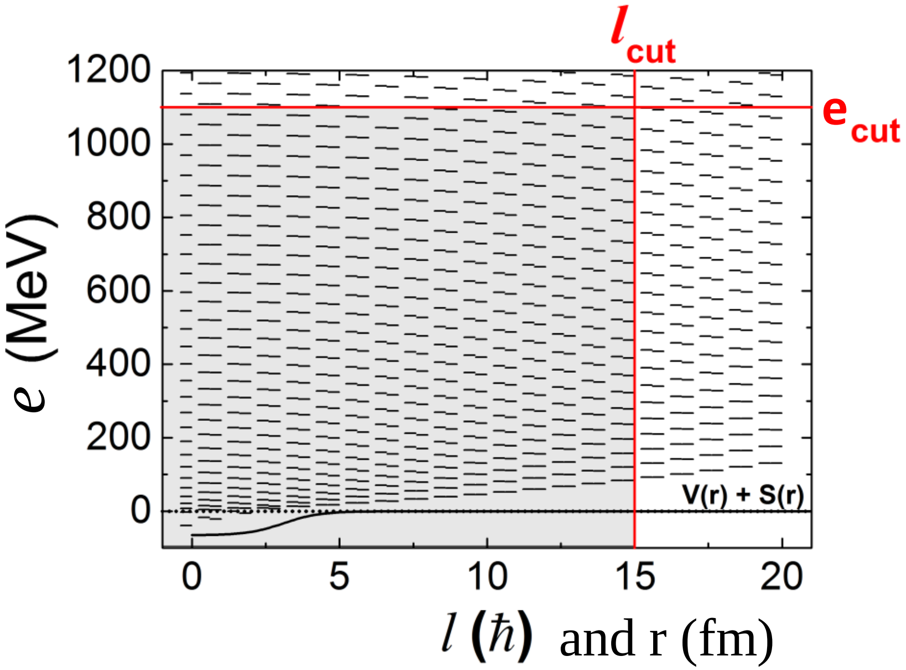
- Not for relativistic.

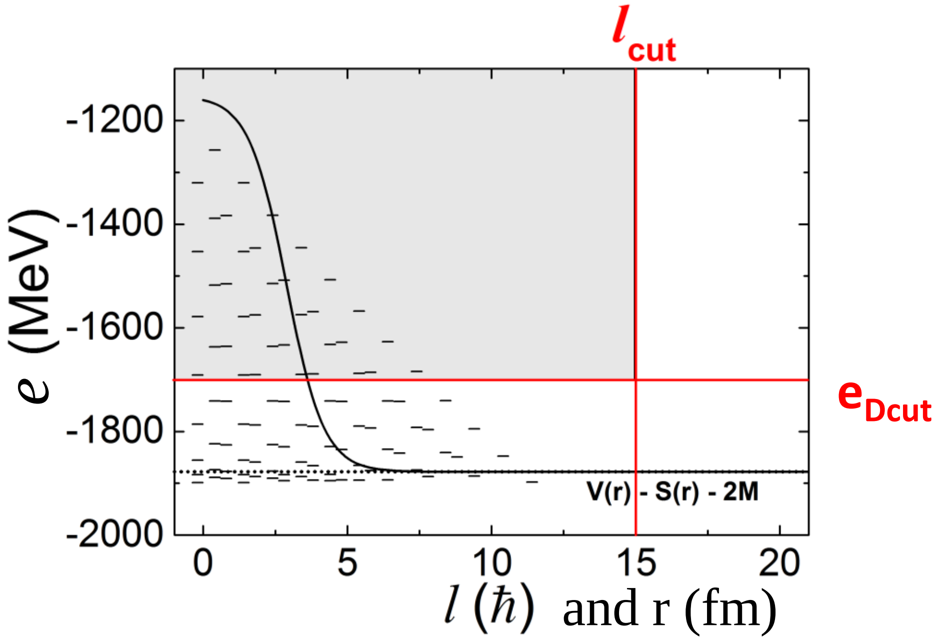
Solution of Bethe-Goldstone Equation

- We solve exactly in the original form of the BG equation in relativistic Brueckner-Hartree-Fock calculations:

$$\langle ab|G(W)|cd\rangle_J = \langle ab|V|cd\rangle_J + \sum_{mn} \langle ab|V|mn\rangle_J \frac{Q(m,n)}{W - e_m - e_n} \langle mn|G(W)|cd\rangle_J$$

- Single-particle basis and example cut-offs with l_{cut} = 15, e_{cut} = 1100 MeV, e_{Dcut} = -1700 MeV.

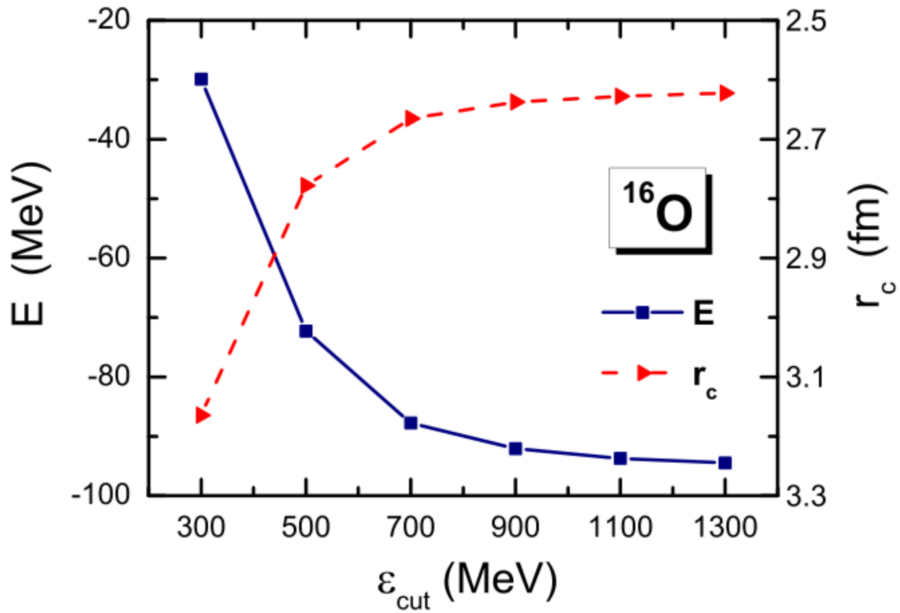




Convergence to Energy Cut-Off

➢ Total energy and charge radius of ^{16}O as a function of energy cut-off. (Center-of-mass motion was not removed)

$$\langle ab|G(W)|cd\rangle = \langle ab|V|cd\rangle + \sum_{mn}\langle ab|V|mn\rangle \frac{Q(m,n)}{W-\varepsilon_m-\varepsilon_n}\langle mn|G(W)|cd\rangle.$$



Rough estimation of the dimension of |ab> :
$(20 \times 2 \times 20)^2$ = 640,000 (symmetry)→ ≈ 60,000
l s n

For one RBHF calculation:
Storage: 256 GB CPU time: 224 h

Intel(R) Xeon(R) CPU E5-4627 v2 @ 3.30GHz

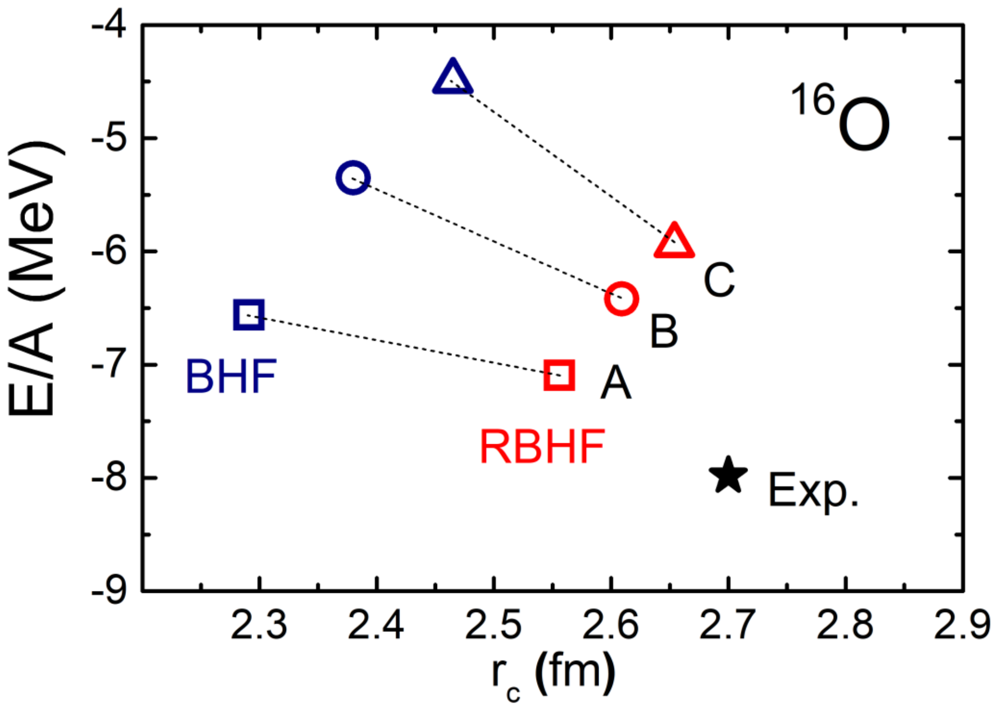
S. Shen, *et al.*, Chin. Phys. Lett. **33**, 102103 (2016)
S. Shen, *et al.*, PRC **96**, 014316 (2017)

- Satisfying convergence is achieved near ε_{cut} = 1100 MeV. From ε_{cut} = 1100 MeV to ε_{cut} = 1300 MeV, E changes 0.79 MeV, r_c changes 0.005 fm.

RBHF for ^{16}O

➢ Total energies and charge radii of ^{16}O calculated by RBHF and BHF with Bonn A, B, and C interactions.

S. Shen, *et al.*, *Chin. Phys. Lett.* **33**, 102103 (2016)
S. Shen, *et al.*, *PRC* **96**, 014316 (2017)
For BHF: H. Müther, R. Brockmann, and R. Machleidt, *PRC* **42**, 1981 (1990).



- Relativistic effect is important to improve the agreement with the data.
- Binding energy and charge radius given by Bonn interactions are smaller than experimental data.

Different ab initio Methods for ^{16}O

- Energy, charge radius, matter radius, and $\pi 1p$ spin-orbit splitting in ^{16}O calculated by RBHF with Bonn A/B/C, in comparison with data, BHF with Bonn A H. Müther, R. Brockmann, and R. Machleidt, *PRC* **42**, 1981 (1990) and with AV18 B. Hu, et al., *PRC* **95**, 034321 (2017), No Core Shell Model (NCSM) R. Roth, et al., *PRL* 107, 072501 (2011), Coupled-Cluster (CC) G. Hagen, et al., *PRC* 80, 021306 (2009), and Nuclear Lattice Effective Field Theory (NLEFT) T. Lähde, et al., PLB 732, 110 (2014).

	E (MeV)	r_c (fm)	r_m (fm)	$\Delta E_{\pi 1p}^{ls}$ (MeV)
Exp.	**-127.6**	**2.70**	**2.54**	**6.3**
RBHF, Bonn A	-120.2	2.53	2.39	5.3
RBHF, Bonn B	-107.1	2.59	2.45	4.5
RBHF, Bonn C	-98.0	2.64	2.50	3.9
BHF, Bonn A	-105.0	2.29	-	7.5
BHF, AV18	-134.2	-	1.92	13.0
NCSM, N^3LO	-119.7(6)	-	-	-
CC, N^3LO	-121.0	-	2.30	-
NLEFT, N^2LO	-121.4(5)	-	-	-

- The results of RBHF are comparable to other state-of-the-art ab initio results.

Different ab initio Methods for ^{40}Ca and ^{48}Ca

- Energies, charge radii, matter radii, and π1d spin-orbit splittings of ^{40}Ca and ^{48}Ca calculated by RBHF with Bonn A, comparing with data, CC with N^3LO G. Hagen, et al., *PRC* **82**, 034330 (2010) and with AV18 G. Hagen, et al., *PRC* **76**, 044305 (2007), BHF B. Hu, et al., *PRC* **95**, 034321 (2017), NCSM R. Roth, et al., *PRL* **99**, 092501 (2007).

	^{40}Ca				^{48}Ca		
	E (MeV)	**r_c (fm)**	**r_m (fm)**	**$\Delta E_{\pi 1d}^{ls}$ (MeV)**	**E (MeV)**	**r_c (fm)**	**$\Delta E_{\pi 1d}^{ls}$ (MeV)**
Exp.	**-342.1**	**3.48**	**-**	**6.6 ± 2.5**	**-416.1**	**3.48**	**4.7**
RBHF, Bonn A	-306.1	3.22	3.10	5.9	-357.3	3.25	2.7
CC, N^3LO	-345.2	-	-	-	-396.5	-	-
CC, AV18	-502.9	-	-	-	-	-	-
BHF, AV18	-552.1	-	2.20	24.9	-	-	-
NCSM, AV18	-461.8	-	2.27	-	-	-	-

For RBHF

Storage: 1100 GB
CPU time: 1720 h

Storage: 1800 GB
CPU time: 4900 h

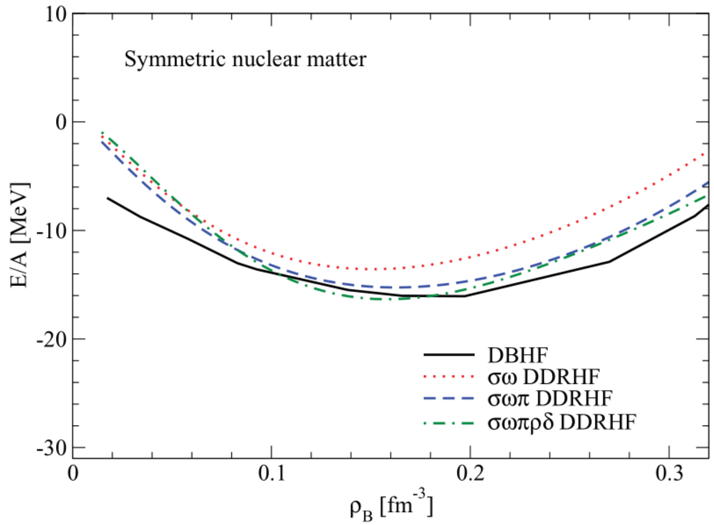
- Results for ^{40}Ca and ^{48}Ca given by RBHF are similar as for ^{16}O.
- CC with N^3LO reproduce the binding energy well, while other non-relativistic calculations give too much binding and too small radii.

Local Density Approximation

- By fitting to RBHF results in nuclear matter at each density, an effective, density-dependent relativistic Hartree(-Fock) interaction can be determined.

RBHF

$$E = \sum_a^A \langle a|T|a\rangle + \frac{1}{2}\sum_{ab}^A \langle ab|\bar{G}(W)|ab\rangle.$$



E. van Dalen and H. Müther, *PRC* **84**, 024320 (2010).

RH/RHF

$$E = \sum_a^A \langle a|T|a\rangle + \frac{1}{2}\sum_{ab}^A \langle ab|\bar{V}_{\text{eff}}(\rho)|ab\rangle$$

$$\mathscr{L}^{(\text{eff})}_{\text{NNs}} = g_s(\rho)\bar{\psi}\psi\varphi^{(s)},$$

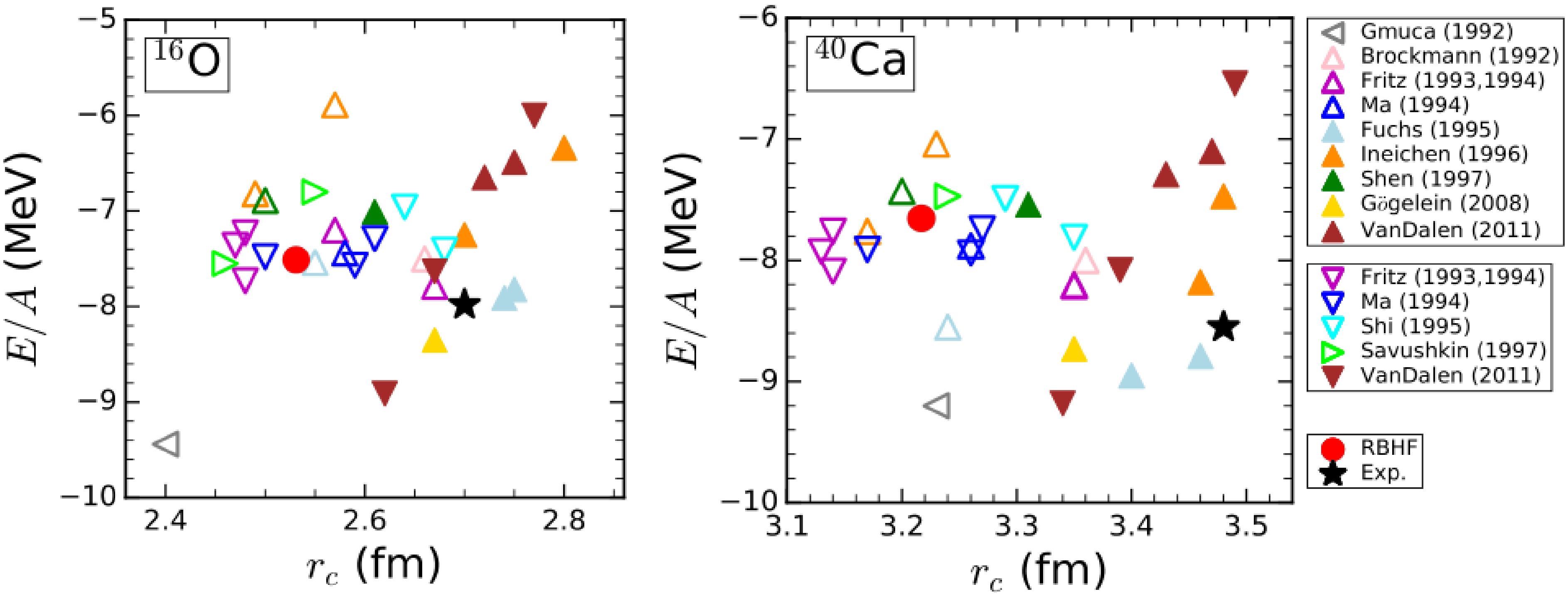
$$\mathscr{L}^{(\text{eff})}_{\text{NNpv}} = -\frac{f_{ps}(\rho)}{m_{ps}}\bar{\psi}\gamma^5\gamma^\mu\psi\partial_\mu\varphi^{(ps)},$$

$$\mathscr{L}^{(\text{eff})}_{\text{NNv}} = -g_v(\rho)\bar{\psi}\gamma^\mu\psi\varphi^{(v)}_\mu - \frac{f_v(\rho)}{4M}\bar{\psi}\sigma^{\mu\nu}\psi\left(\partial_\mu\varphi^{(v)}_\nu - \partial_\nu\varphi^{(v)}_\mu\right),$$

- Such effective interaction can be used to study finite nuclei.

Local Density Approximation

- Energy per nucleon and charge radius of 16O and 40Ca by self-consistent RBHF calculations (red circles), in comparison with results with LDA. All calculations using the same Bonn A interaction.



- Large uncertainty exists in the LDA, and self-consistent RBHF calculation provides a firm benchmark.

Outline

- Relativistic Brueckner-Hartree-Fock (RBHF) Theory
  - Introduction (HF -> BHF -> RBHF)
  - RBHF description for finite nuclei
  - Summary
- Towards an ab initio relativistic density functional
  - New functional guided by RBHF calculations
  - Summary

Summary for RBHF Part

Summary

- Relativistic Brueckner-Hartree-Fock equations have been solved for finite nuclei.
- ^{16}O is taken as an example to show that the convergence is achieved near ε_{cut} = 1.1 GeV.
- ^{16}O, ^{40}Ca and ^{48}Ca have been studied with Bonn A interaction. The resulting binding energies and charge radii have been improved comparing with nonrelativistic case.

Perspectives

- To use state-of-the-art chiral NN interaction.
- To go beyond two hole-line expansion.
- To consider relativistic 3N interaction.
- ... ...

Outline

- Relativistic Brueckner-Hartree-Fock (RBHF) Theory
  - Introduction (HF -> BHF -> RBHF)
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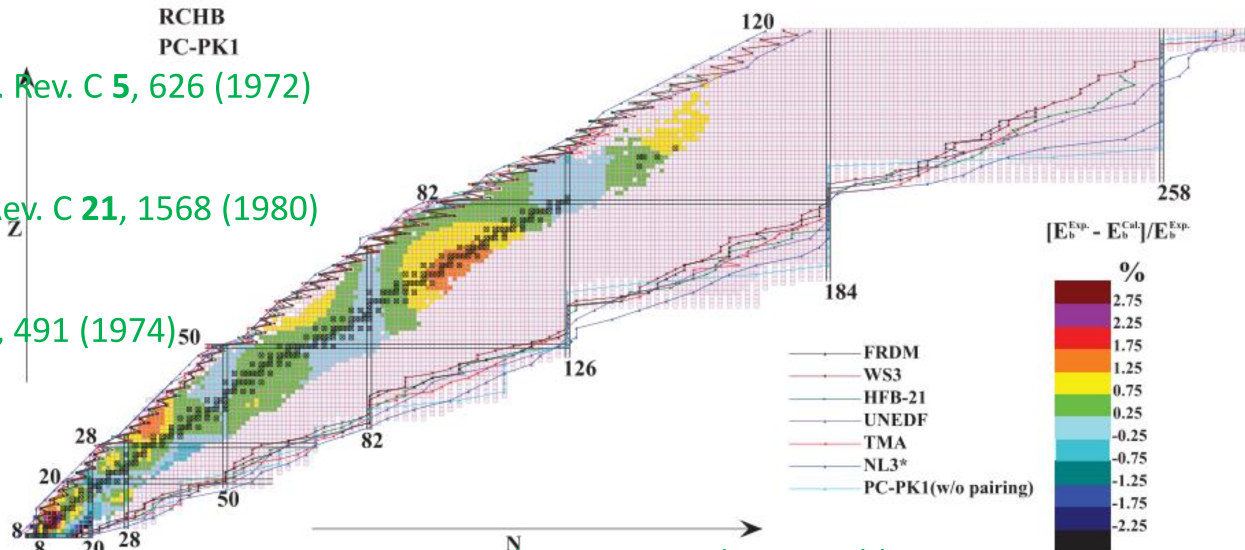
  - Summary
- Towards an ab initio relativistic density functional
  - New functional guided by RBHF calculations
  - Summary

S. Shen, *et al.*, PLB **778**, 344 (2018)
S. Shen, *et al.*, PRC **97**, 054312 (2018)
S. Shen, G. Colo', and X. Roca-Maza, arXiv:1810.09691

Nuclear Energy Density Functional

- Nuclear energy density functional (EDF) is one of the most important tools in nuclear physics M. Bender and P.-h. Heenen, Rev. Mod. Phys. **75**, 121 (2003)
  - Skyrme
    D. Vautherin and D. M. Brink, Phys. Rev. C **5**, 626 (1972)
  - Gogny
    J. Decharg´ e and D. Gogny, Phys. Rev. C **21**, 1568 (1980)
  - Relativistic
    J. D. Walecka, Ann. Phys. (N. Y). **83**, 491 (1974)



X.W. Xia et al. At Data Nucl. Data Tables, 2018, 121–122: 1

- Open questions still exist regarding current functionals:
  - Symmetry energy M. Baldo and G. Burgio, Prog. Part. Nucl. Phys. **91**, 203 (2016)
  - Tensor force H. Sagawa and G. Colò, Prog. Part. Nucl. Phys. **76**, 76 (2014)
  - … …

Tensor Force

- Experimental facts for tensor force in nucleon-nucleon (NN) interaction:
  - Quadrupole moment of deuteron
  - Nonvanishing transition amplitude from L = J – 1 to L = J + 1 in NN scattering

R. Machleidt, *Adv. Nucl. Phys.* **19**, 189 (1989)

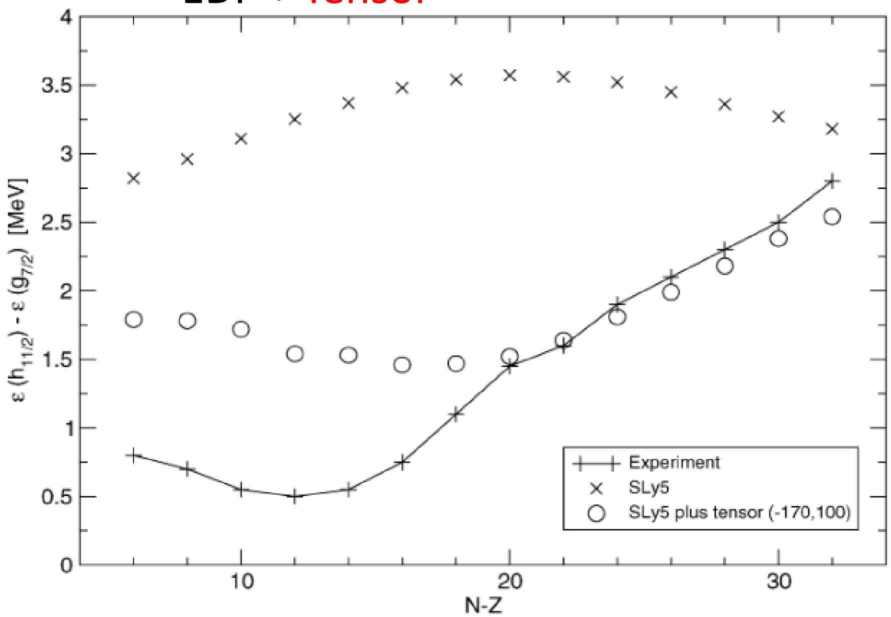
$$V_T = f(r) S_{12},$$

$$S_{12} = 3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

- Tensor force in EDF: still in debate.

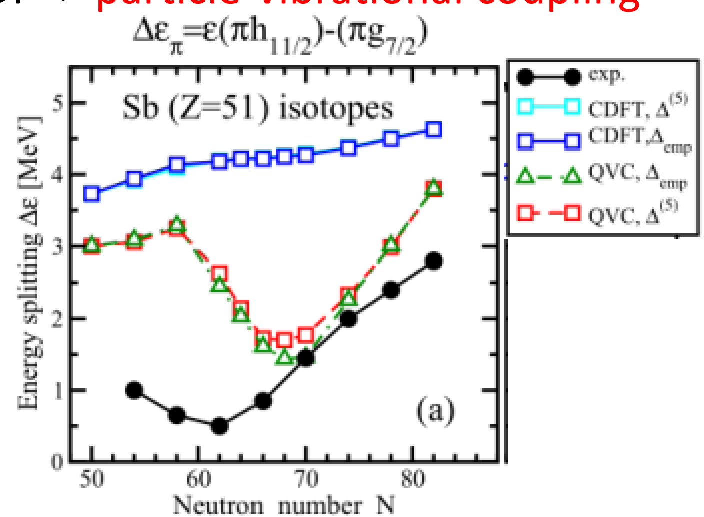
T. Otsuka, *et al.*, *Phys. Rev. Lett.* **95**, 232502 (2005)
H. Sagawa and G. Colò, *Prog. Part. Nucl. Phys.* **76**, 76 (2014)

EDF + Tensor



G. Colò, *et al.*, Phys. Lett. B **646**, 227 (2007)

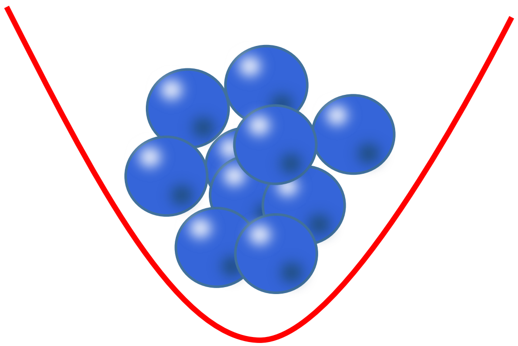
EDF -> particle-vibrational coupling



A. V. Afanasjev, E. Litvinova, *Phys. Rev. C* **92**, 044317 (2015)

ab initio Calculations for Neutron Drops

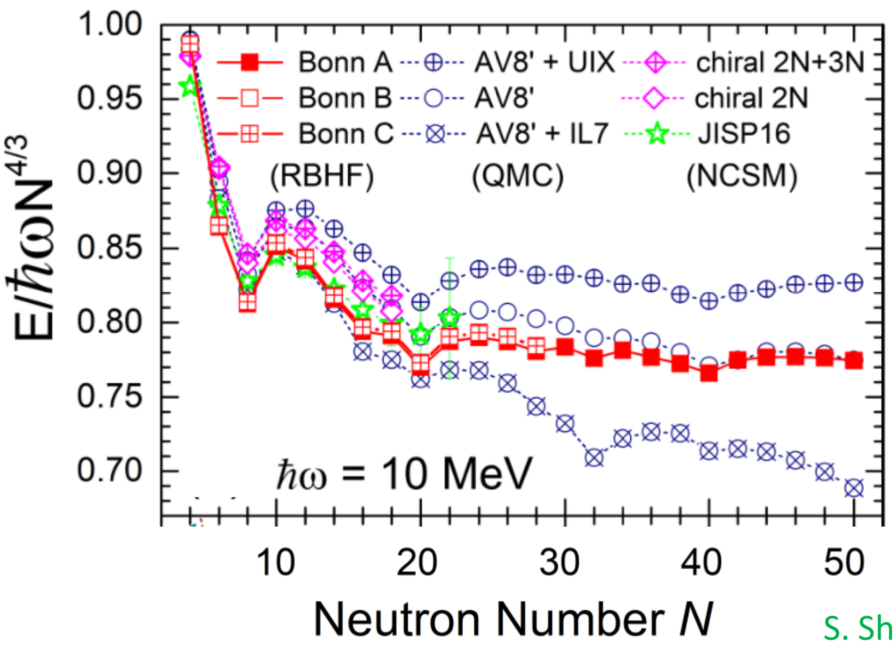
- Neutron drop is an ideal system composed of multi-neutron in an external field.



- Why we study neutron drop?
  - Simple, can be accessed by many ab initio methods S. Gandolfi, J. Carlson, and S. Pieper, *PRL* **106**, 012501 (2011), P. Maris, et al., *PRC* **87**, 054318 (2013).
  - An ideal environment for studying neutron rich system.
  - Provide information for nuclear density functional, such as spin-orbit splitting B. S. Pudliner, *et al.*, *PRL* **76**, 2416 (1996) or tensor force.

Energies of Neutron Drops

➢ Total energies in units of $h\omega N^{4/3}$ for N-neutron drops calculated by RBHF theory using Bonn A, B, C interactions, in comparison with quantum Monte-Carlo (QMC) and no-core shell model (NCSM) calculations S. Gandolfi, J. Carlson, and S. Pieper, *PRL* **106**, 012501 (2011), P. Maris, et al., *PRC* **87**, 054318 (2013), H. D. Potter, et al., *PLB* **739**, 445 (2014).

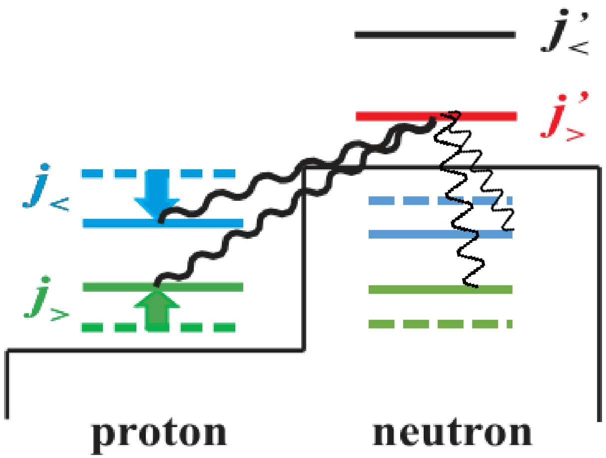


S. Shen, *et al.*, PLB **778**, 344 (2018)
S. Shen, *et al.*, PRC **97**, 054312 (2018)

- Energies given by RBHF with Bonn A are close to JISP16, AV8'+IL7 (for N < 14).

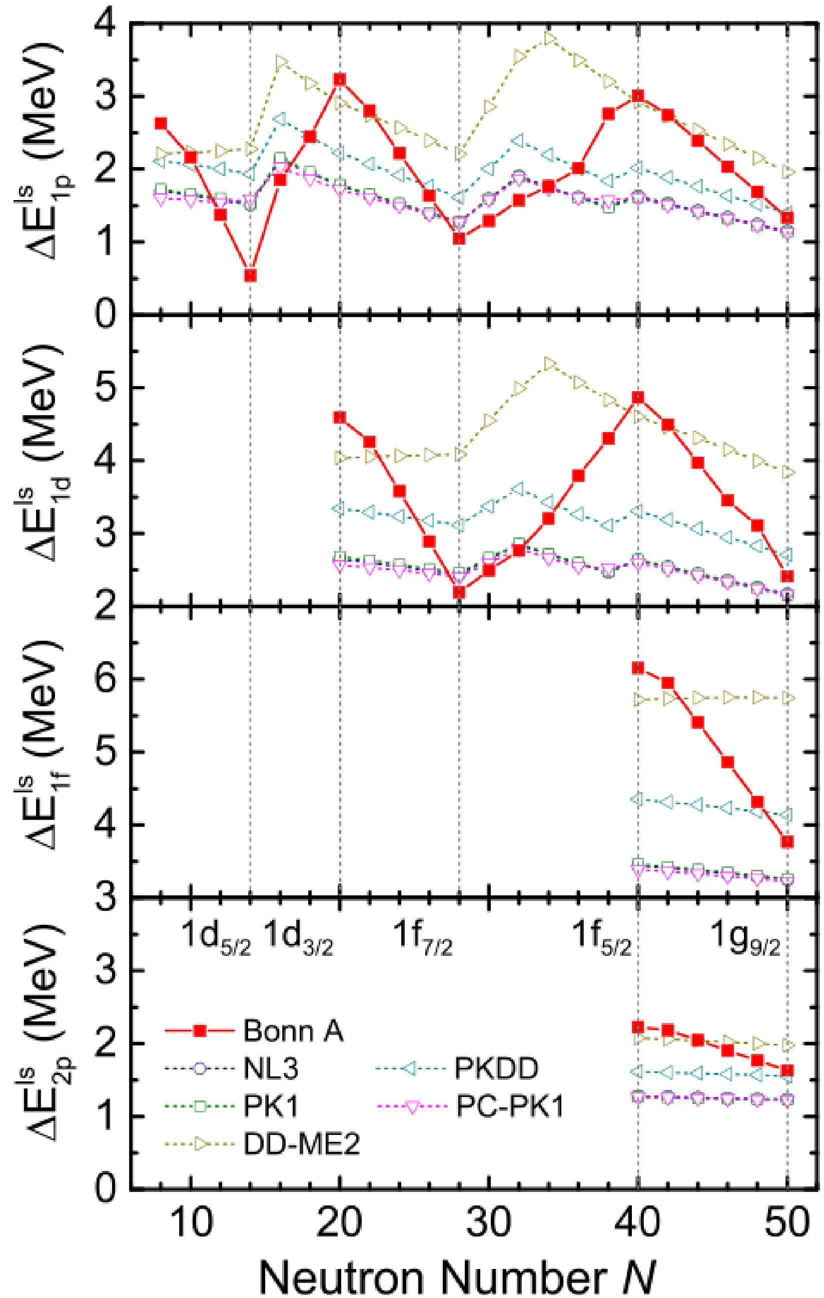
Spin-Orbit Splitting

- Spin-orbit (SO) splittings of 1p, 1d, 1f, and 2p for N-neutron drops calculated by RBHF theory using Bonn A interaction, in comparison with various relativistic functionals without tensor force.



T. Otsuka, *et al.*, *Phys. Rev. Lett.* **95**, 232502 (2005)

- The splitting decreases as the next higher $j_>' = l' + 1/2$ orbit is filled, similar as the effect of tensor force between neutron and proton.
- Such pattern is not obvious in functionals without tensor force.



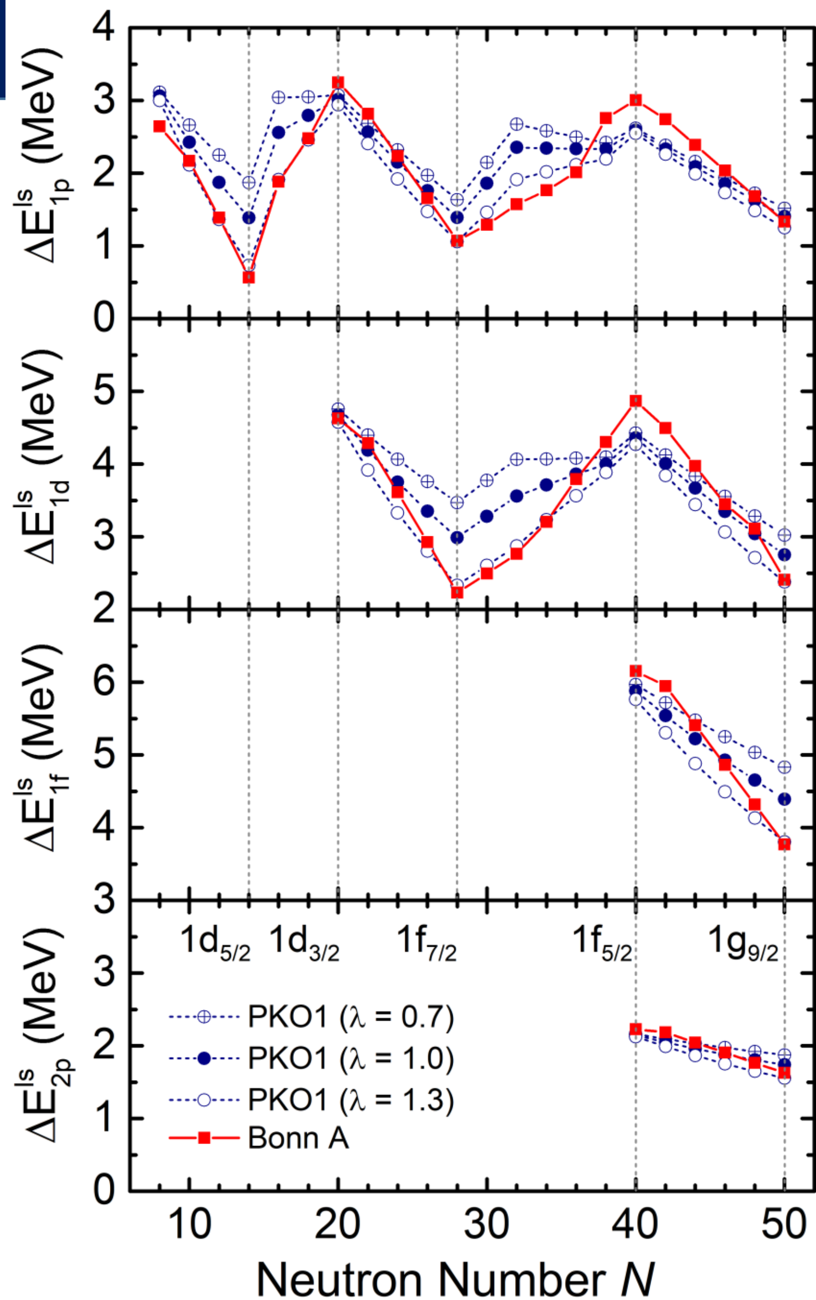
S. Shen, *et al.*, PLB **778**, 344 (2018)
S. Shen, *et al.*, PRC **97**, 054312 (2018)

Spin-Orbit Splitting

- Spin-orbit splitting for N-neutron drops calculated by RBHF theory using Bonn A interaction, in comparison with relativistic functional with tensor force: PKO1 W. Long, N. Van Giai, and J. Meng, *PLB* **640**, 150 (2006).

  different strength of pion coupling characterized by factor λ.

- PKO1 shows similar pattern of SO splitting as RBHF with Bonn A.
- The tensor force induced by pion coupling has large impact on the evolution of SO splitting.
- When the strength of PKO1 pion coupling is enlarged by a factor of 1.3, the results are similar as RBHF.

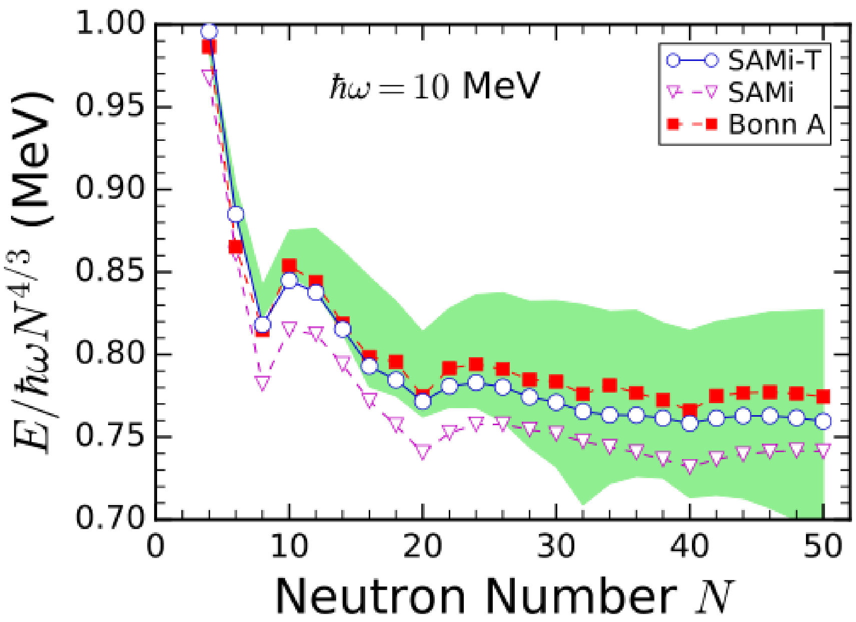


S. Shen, *et al.*, PLB **778**, 344 (2018)
S. Shen, *et al.*, PRC **97**, 054312 (2018)

New Skyrme Functional SAMi-T

- New Skyrme functional SAMi-T was developed, with guidance of RBHF calculations for neutron(-proton) drops.

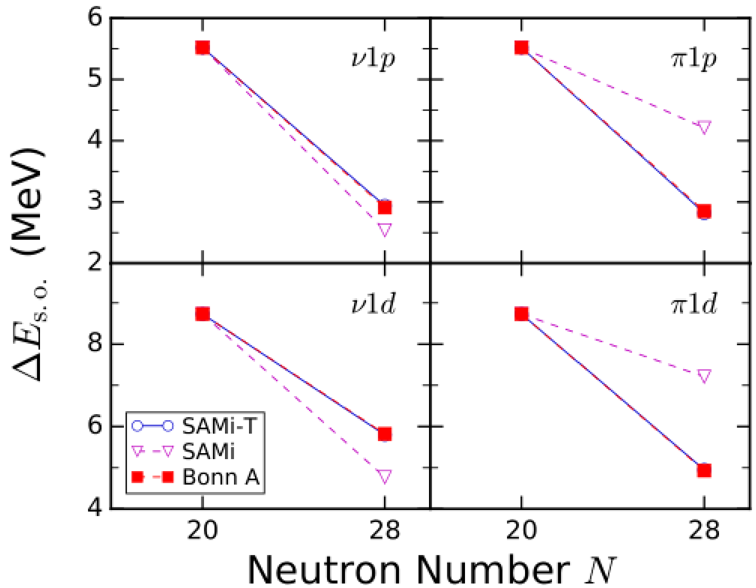
- Data to be fitted:
  - binding energies and charge radii of ^{40}Ca, ^{48}Ca, ^{90}Zr, ^{132}Sn, and ^{208}Pb.
  - Spin-orbit splittings of ^{40}Ca, ^{90}Zr, ^{208}Pb .
  - Relative change of SO splittings of neutron-proton drops (N=20,Z=20) to (Z=20,N=28)
  - Total energy of neutron drops (N=8, 20, 40, 50).

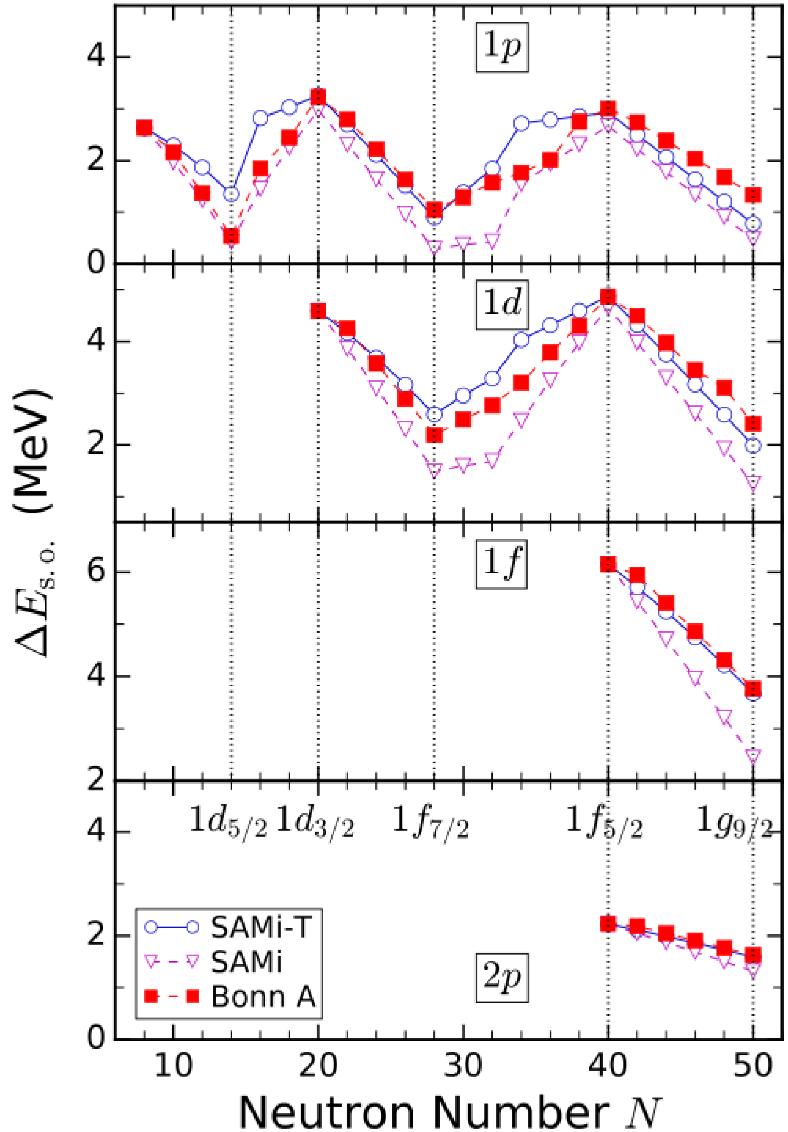


S. Shen, G. Colo', and X. Roca-Maza, arXiv:1810.09691

Pseudodata : Spin-Orbit Splittings

- Neutron and proton 1p and 1d spin-orbit splittings of neutron-proton drops calculated by SAMi-T, in comparison with results of SAMi functional and RBHF theory using the Bonn A interaction.



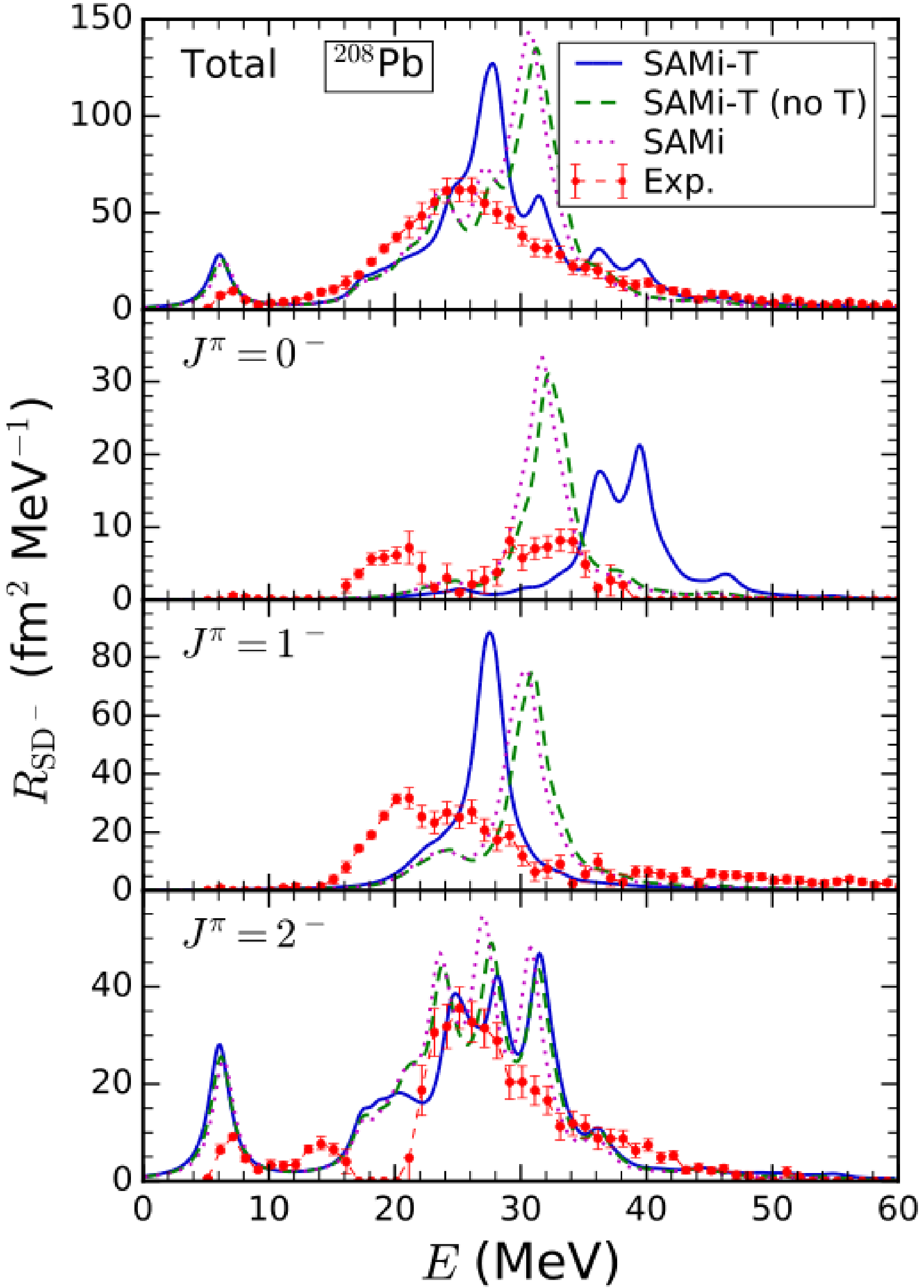


- The relative change of SO splittings in neutron-proton drops by RBHF can be well fitted by SAMi-T.

Spin-Dipole Resonance

- Spin-dipole resonance strength function in the τ− channel for ^{208}Pb calculated by SAMi-T with Skyrme-Hartree-Fock plus random phase approximation.

Exp. T. Wakasa, et al., Phys. Rev. C **85**, 064606 (2012)



- Results of SAMi-T without tensor is similar to those of SAMi.
- Tensor force is important in improving the description of $J^\pi = 1^-$ channel, and improving the total SDR. Consistent with the finding in C. L. Bai, *et al.*, Phys. Rev. Lett. **105**, 072501 (2010)

Summary for Nuclear DFT Part

Summary

- Neutron drops have been studied by RBHF, a systematic and specific pattern due to the effects of the tensor forces is found in the evolution of spin–orbit splittings.
- New Skyrme functional SAMi-T has been developed with tensor force guided by RBHF calculations for neutron-proton drops.
- Besides ground state properties, the excited properties like Gamow-Teller resonance and spin-dipole resonance can be well described by SAMi-T, especially the description for SDR is improved by the tensor force.

Perspectives

- To study more observables with SAMi-T and see the effects of tensor force.
- To consider effect of particle-vibration coupling.
- ... ...

Collaborators

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- Sibo Wang, PKU
- Shuangquan Zhang, PKU

THANK YOU!