*First Tsukuba-CCS-RIKEN joint workshop*
*on microscopic theories of nuclear structure and dynamics*
*December 12-16, 2016*

# Relativistic Brueckner-Hartree-Fock Theory for Finite Nuclei

December 14, 2016

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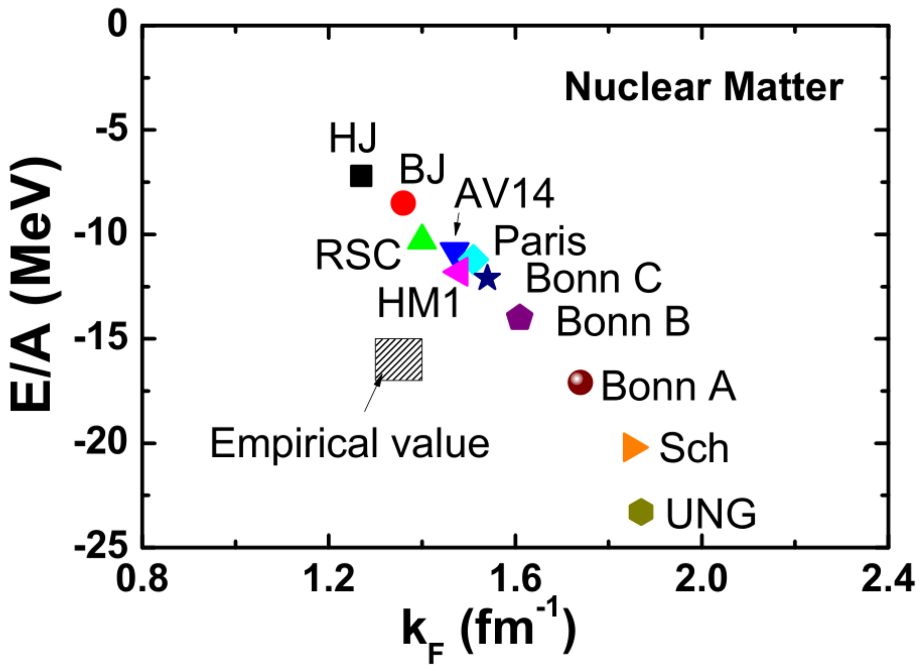
# Introduction

- Describe nuclei from first principle (ab initio)
  1. Realistic nucleon-nucleon (NN) interaction: Chiral force Epelbaum2009RMP, Machleidt2011PR, LQCD Aoki2012PTEP, Beane2011PPNP, OBEP Machleidt2001PRC, …
  2. Many-body framework: no core shell model Barrett2013PPNP, quantum Monte Carlo theory Carlson2015RMP, Coupled Cluster theory Hagen2014RPP, nuclear lattice effective field theory Lee2009PPNP, Brueckner-Hartree-Fock (BHF) theory Bethe1971ARNS, …
- Brueckner-Hartree-Fock theory with two-body interaction only



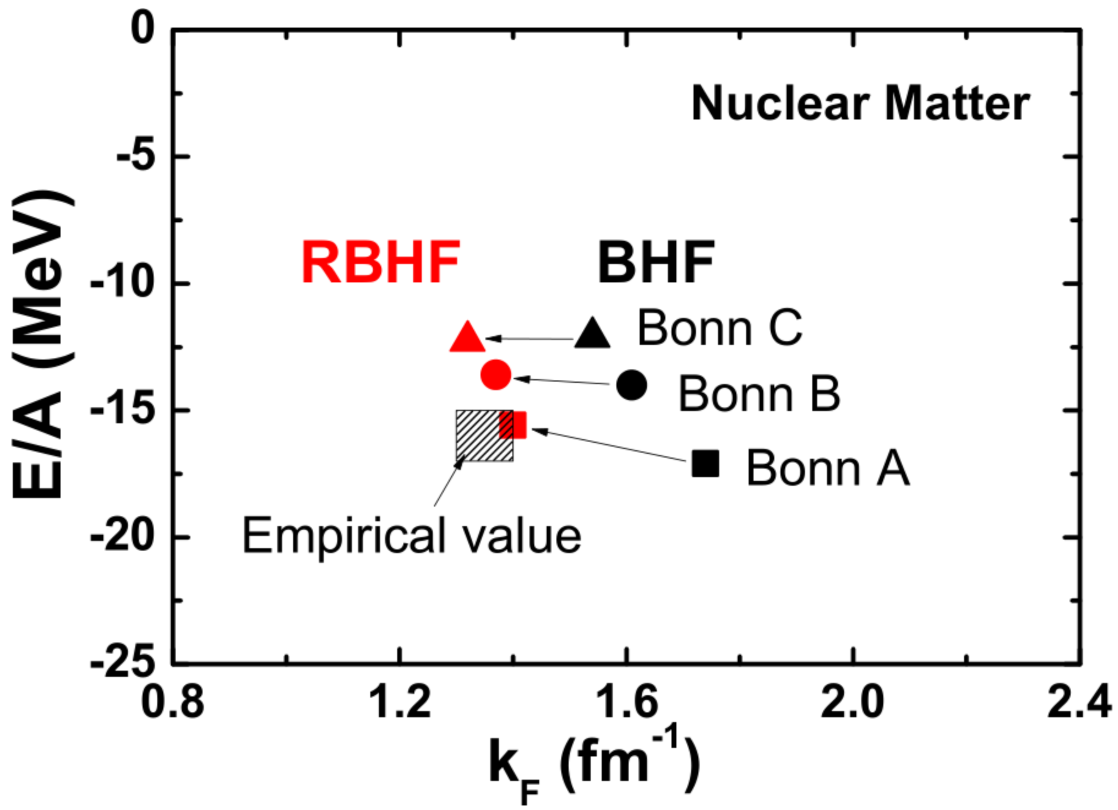

| $^{16}O$ | Bonn C | Bonn B | Bonn A | Exp. |
|---|---|---|---|---|
| E/A (MeV) | -4.49 | -5.35 | -6.56 | **-7.98** |
| $r_c$ (fm) | 2.465 | 2.380 | 2.291 | **2.70** |

BHF for nuclear matter (left) Brockmann1990PRC and $^{16}O$ (up) Müther1990PRC.

# Introduction

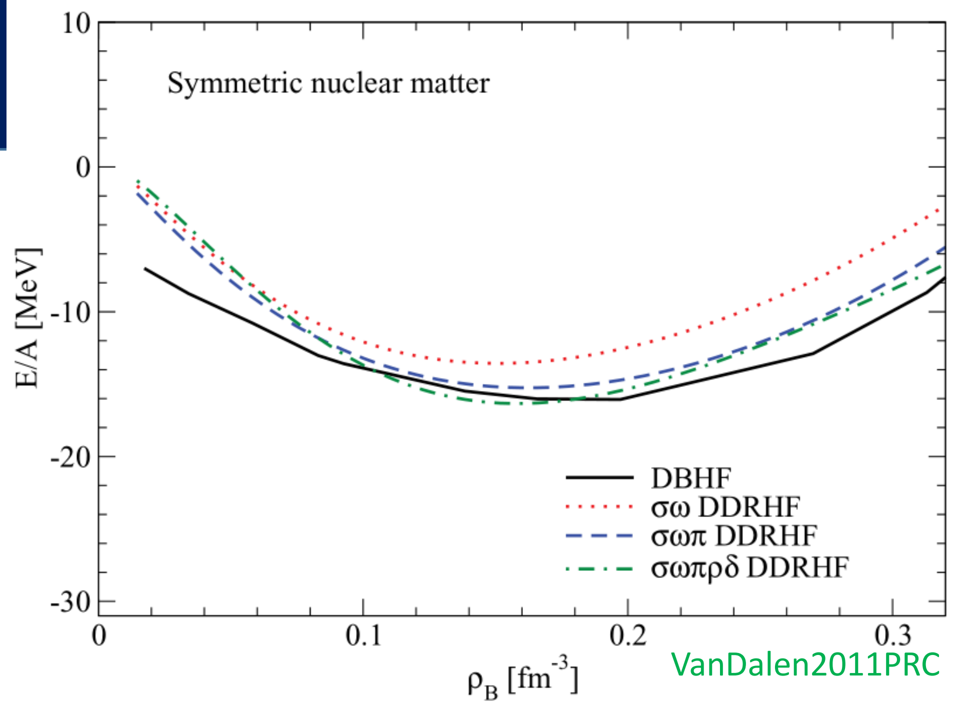
➢ Relativistic Brueckner-Hartree-Fock (RBHF) theory for nuclear matter

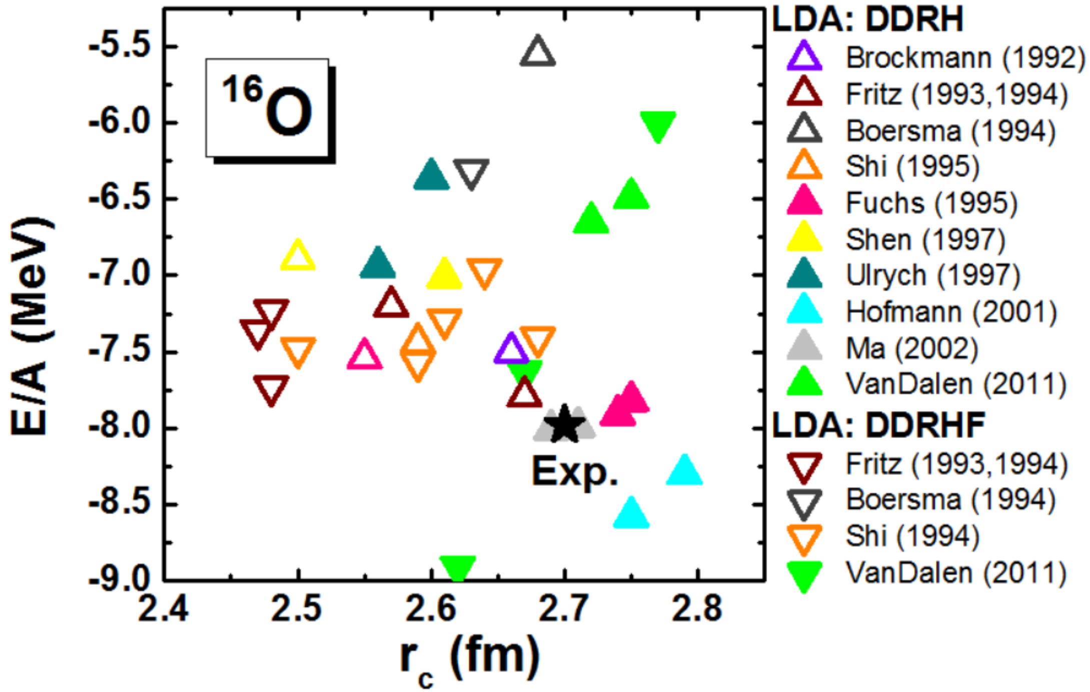
Brockmann1990PRC.



# Introduction

- RBHF theory for finite nuclei
  - BHF theory with effective density approximation Müther1990PRC.
  - RBHF theory with Local density approximation: density dependent relativistic Hartree (DDRH) theory Brockmann1992PRL and DDRHF theory Fritz1993PRL.
  - Self consistent RBHF is still not done yet.



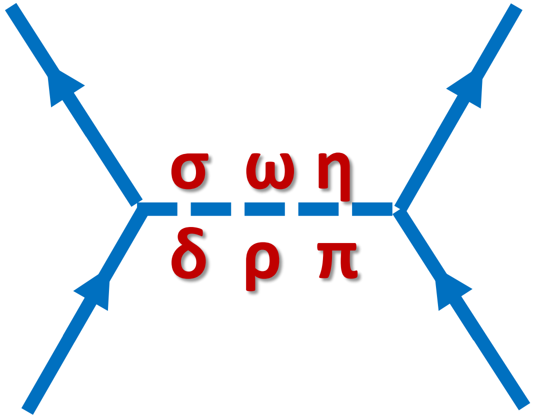




❑ Present work: **self-consistent RBHF theory** for finite nuclei.

# Theoretical Framework

# Nucleon-Nucleon Interaction

- Realistic NN Bonn potential Machleidt1989ANP :




- Bosons: scalar σ, δ; vector ω, ρ; pseudoscalar η, π.
- Coupling constants were determined by fitting to the NN scattering and deuteron properties.

# Relativistic Hamiltonian

➢ Hamiltonian in second quantized form Brockmann1978PRC, where |a> is complete basis of Dirac spinors with both positive energy and negative energy states.

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

where *i* are for mesons and photon. The matrix elements are defined as

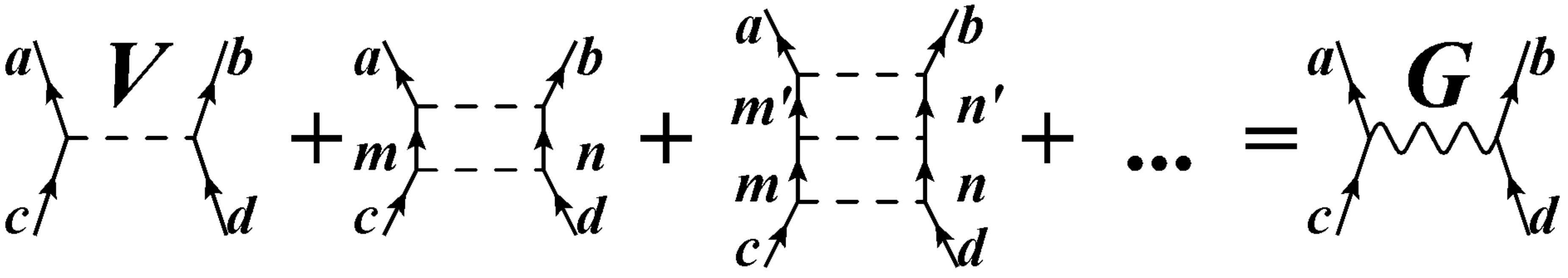
$$\langle a|T|b\rangle=\int d^3x\bar{\psi}_a(\boldsymbol{x})\left(-i\boldsymbol{\gamma}\cdot\nabla+M\right)\psi_b(\boldsymbol{x}),$$

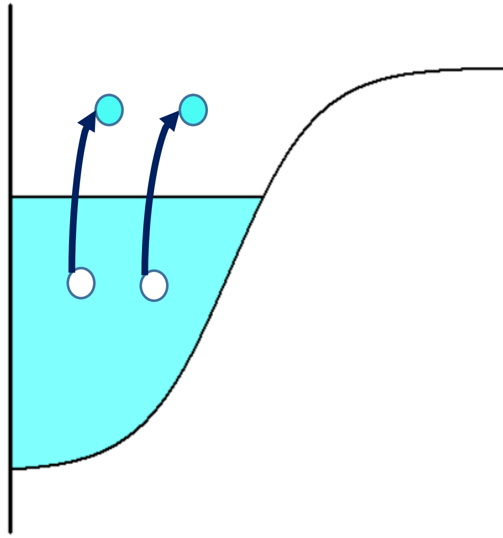
$$\langle ab|V_i|cd\rangle=\int d^3x_1 d^3x_2\bar{\psi}_a(\boldsymbol{x}_1)\bar{\psi}_b(\boldsymbol{x}_2)\Gamma_i(1,2)D_i(\boldsymbol{x}_1,\boldsymbol{x}_2)\psi_c(\boldsymbol{x}_1)\psi_d(\boldsymbol{x}_2).$$

$\Gamma_i$ is the interaction vertex, and $D_i$ is the propagator.

# Bruckner G-matrix

➢ Sum up ladder diagrams to infinite order Brueckner1954PR



Bethe-Goldstone equation Bethe1971ARNS

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

where $W = \varepsilon_c + \varepsilon_d$ is the starting energy, and $\varepsilon_m$ ,$\varepsilon_n$ are the RHF single particle energies. $Q$ is the Pauli operator which forbids the states being scattered below Fermi surface.

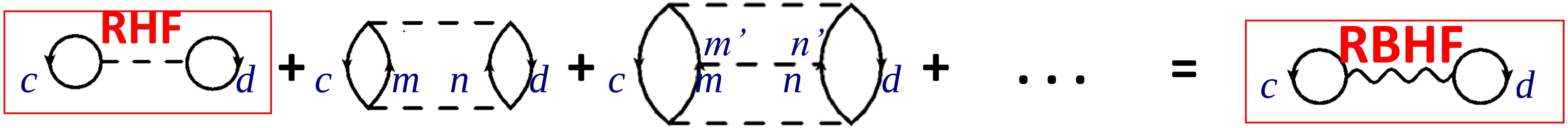
# Relativistic Brueckner-Hartree-Fock Theory

- Relativistic Hartree-Fock equation in complete basis Long2005

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

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

- RBHF total energy




$\sum_{cd} \langle cd|V|cd\rangle$

$\sum_{cd} \langle cd|G(W = \varepsilon_c + \varepsilon_d)|cd\rangle$

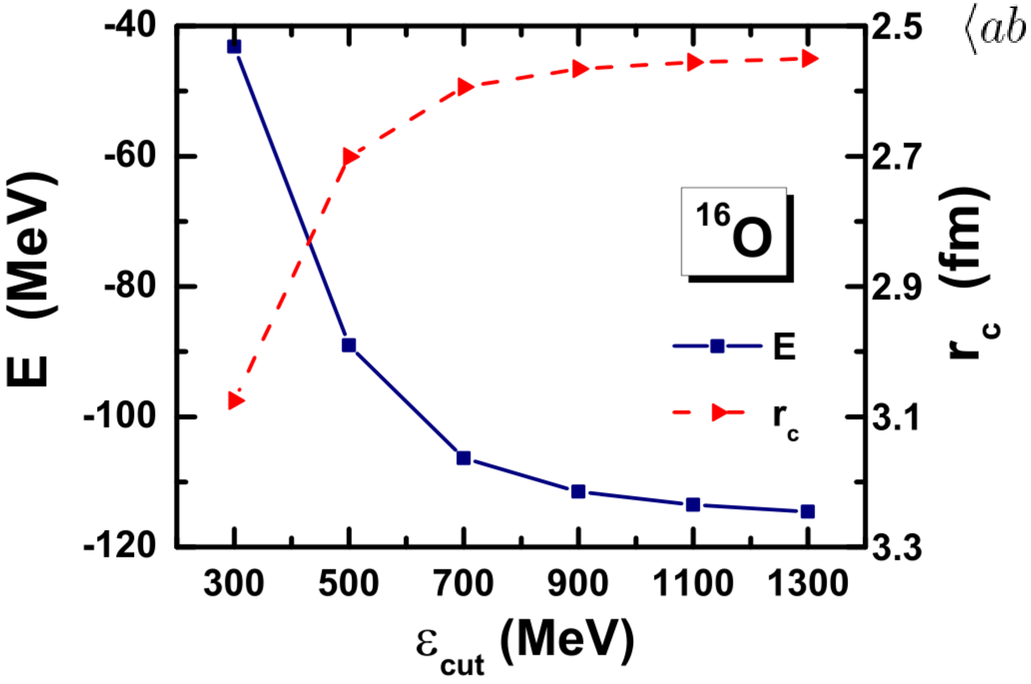
# Results and Discussion

# Numerical Details

- Object: $^{16}O$, $^{40}Ca$
- Interaction: Bonn A potential Machleidt1989ANP
- Cut-offs for basis space: $l_{cut}$ = 20, $\varepsilon_{cut}$ = 1100 MeV, $\varepsilon_{Dcut}$ = -1700 MeV
- Basis: self-consistent RHF basis (for fixed Dirac Woods-Saxon basis, see S. Shen, J. Hu, H. Liang, J. Meng, P. Ring, and S. Zhang, *Chin. Phys. Lett*. **10**, 102103 (2016) )
- Coulomb exchange term: relativistic local density approximation Gu2013PRC
- Center-of-mass correction: included in RHF variation Chabanat1998NPA
- Box size: R = 7 fm

# Convergence to Energy Cut-Off

- Total energy and charge radius of $^{16}O$ as a function of energy cut-off.




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

$$Q(m,n) = \begin{cases} 1, & |m\rangle \text{ and } |n\rangle \text{ are particles,} \\ 0, & |m\rangle \text{ or } |n\rangle \text{ is hole.} \end{cases}$$

Rough estimation of the dimension of |ab> :

$(20 \times 2 \times 20)^2$ = 640,000 (symmetry)→ ≈ 60,000

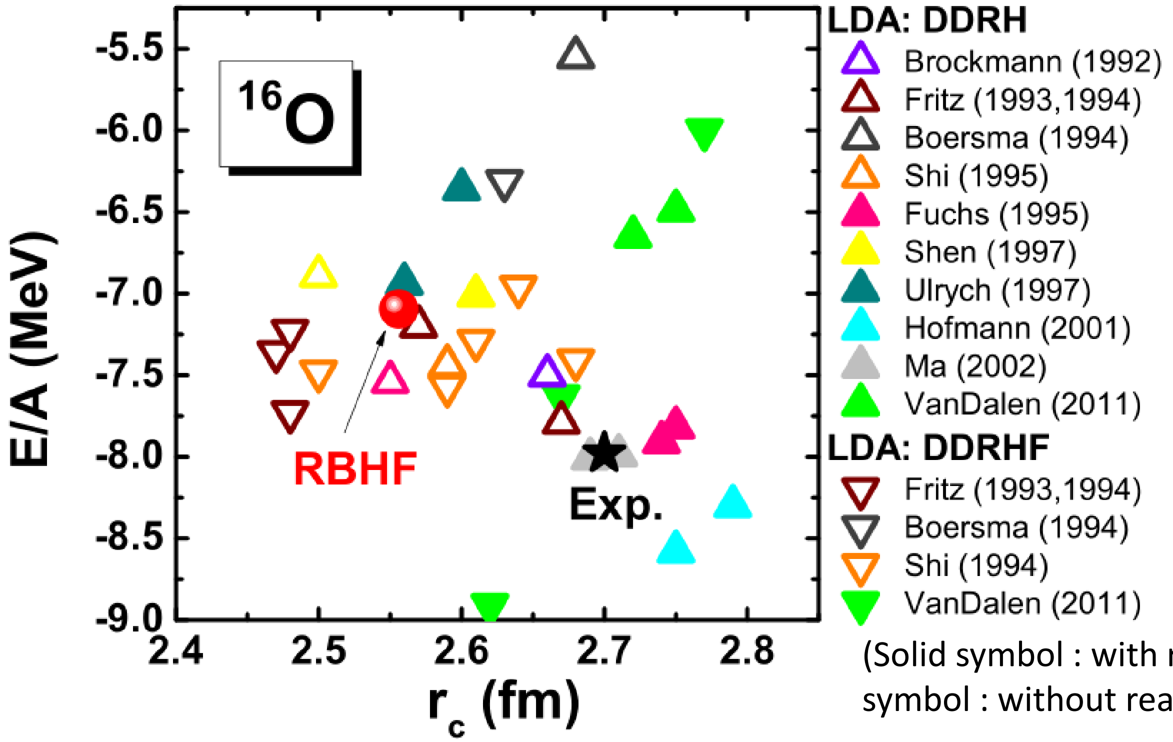
$l \quad s \quad n$

Storage: 256 Gb CPU time: 230 H

- Satisfying convergence is achieved for $\varepsilon_{cut}$ = 1.1 GeV.

# RBHF and RBHF with Local Density Approximation

➢ Total energy and charge radius of $^{16}O$ calculated by RBHF and DDRH or DDRHF (RBHF with LDA ). All calculations using Bonn A potential.




(Solid symbol : with rearrangement term Open symbol : without rearrangement term)

- There is big uncertainty in LDA calculation, where the present self-consistent RBHF calculation can provide a solid benchmark.

# Different ab initio Methods for $^{16}O$

- Energy, charge radius, point matter radius, and π1p spin-orbit splitting in $^{16}O$ with Bonn A in RBHF; with Bonn A in nonrelativistic renormalized BHF Muether1990PRC; with $V_{low-k}$ derived from Argonne v18 in BHF Hu2016PRC; with $N^3LO$ in NCSM Roth2011PRL and Couple-Cluster method (CC) Hagen2009PRC.

| | 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 | -113.5 | 2.56 | 2.42 | 5.4 |
| 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 | - |

- Relativistic effect is important to improve description.
- The results of RBHF are similar to other state-of-the-art ab initio results.

# RBHF for $^{40}$Ca

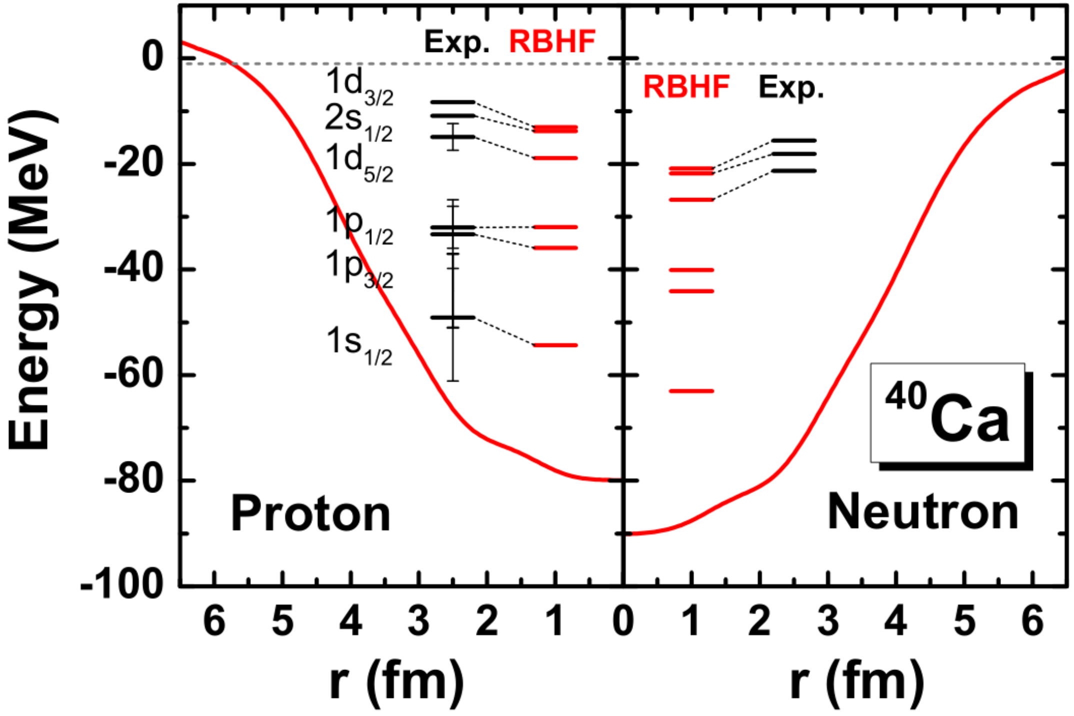
- Energy, charge radius, point matter radius, and π1d spin-orbit splitting of $^{40}$Ca. Results of Bonn A in RBHF, comparing with $V_{low-k}$ derived from Argonne v18 in non-relativistic BHF Hu2016, importance-truncated no-core shell model (IT-NCSM) Roth2007PRL; and coupled cluster (CC) Hagen2007PRC;

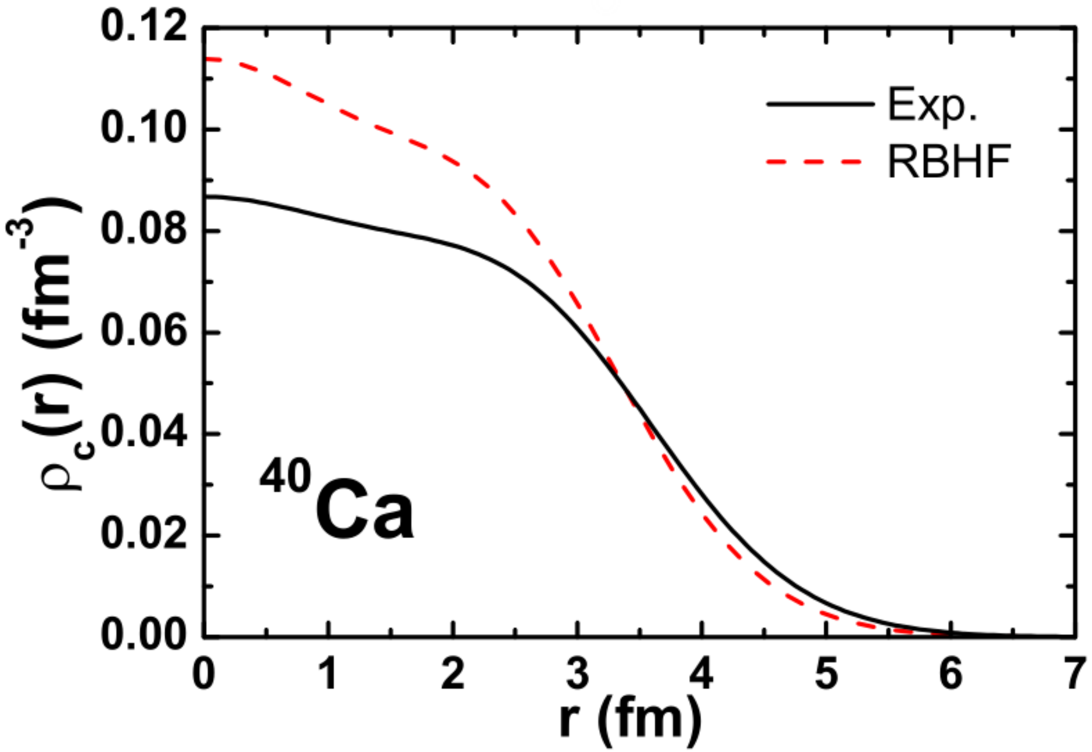
| | E (MeV) | $r_c$ (fm) | $r_m$ (fm) | $\Delta E_{\pi 1p}^{ls}$ (MeV) |
|---|---|---|---|---|
| **Exp.** | **-342.1** | **3.48** | **-** | **6.6 ± 2.5** |
| RBHF, Bonn A | -290.8 | 3.23 | 3.11 | 5.9 |
| BHF, AV18 | -552.1 | - | 2.20 | 24.9 |
| IT-NCSM, AV18 | -461.8 | - | 2.27 | - |
| CC, AV18 | -502.9 | - | - | - |

Storage: 1100 Gb
CPU time: 1720 H

# RBHF for $^{40}$Ca

- Single-particle spectrum (left) and charge density distribution (right) of $^{40}$Ca in RBHF with Bonn A interaction.




- RBHF theory is very promising to describe the heavy nuclei.

# Summary and Perspective

- Full relativistic Brueckner-Hartree-Fock equations have been solved self-consistently for the first time for finite nuclei.
- $^{16}$O is taken as an example, and convergence is achieved near $\varepsilon_{cut}$ = 1.1 GeV.
- $^{16}$O, and $^{40}$Ca have been studied with Bonn A interaction. The resulting binding energies and charge radii are reasonably good. Also the spin-orbit splitting are well reproduced.

**Future Work**

- To improve the convergence, e.g. by using V-low k or SRG technique.
- To investigate with relativistic LQCD force or relativistic chiral force (Ren *et al*. arXiv:1611.08475).
- To learn from the G-matrix and provide information to nuclear energy density functional and other studies.
- …

# THANK YOU!