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O^{16} in relativistic Brueckner-Hartree-Fock theory

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Outline

- Introduction
- Relativistic Brueckner-Hartree-Fock theory for finite nuclei
- Results and discussion
- Summary & Perspectives

ab initio calculation in nuclear physics

ab initio----- "from the beginning"

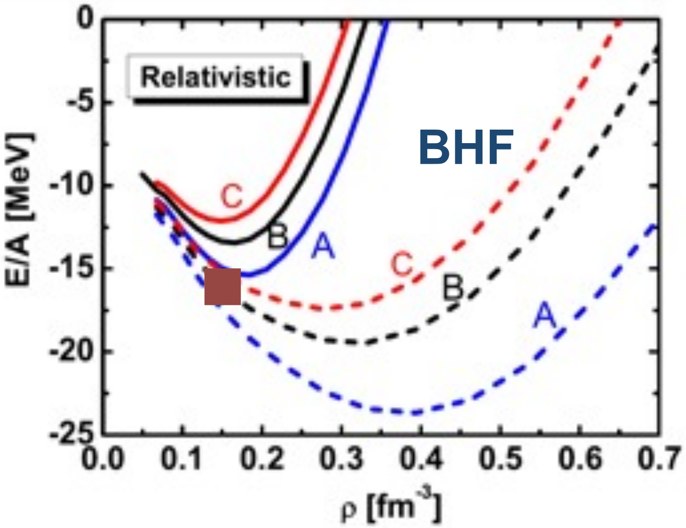
- without additional assumptions
- without additional parameters

ab initio in nuclear physics

- with realistic nucleon-nucleon interaction
- with some few-body methods and many-body methods, such as Monte Carlo method, shell model and energy density functional theory

ab initio in nuclear matter

- Variational method — Akmal PRC1998
- Green's function method — Dickhoff PPNP2004
- Chiral Perturbation theory — Kaiser NPA2002
- Brueckner-Hartree-Fock (BHF) theory — Baldo RPP2012
- Relativistic BHF (RBHF) theory — Brockmann PRC1990
- ………..



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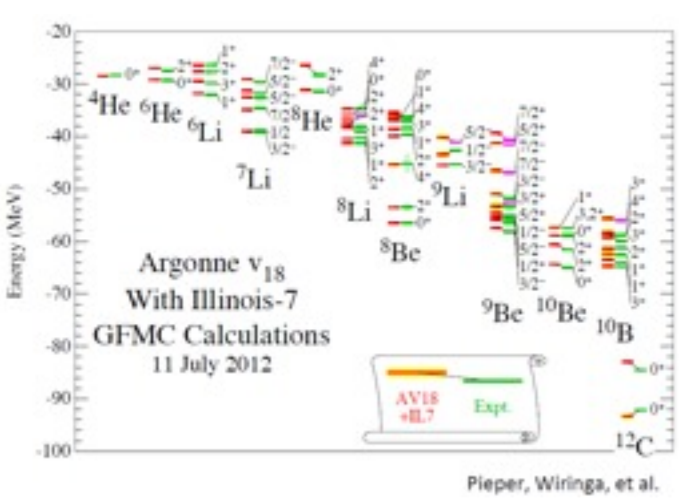
ab initio calculation in nuclear physics

ab initio calculation for light nuclei

- Stochastic Variational Approach — Suzuki LNP1998
- Gaussian Expansion Method — Hiyama PPNP2003
- Green Function Monte Carlo Method — Pieper PRC2004
- Lattice Chiral Effective Field Theory — Lee PPNP2009
- No-Core Shell Model — Barrett PPNP2012
- ……



ab initio calculation for heavier nuclei

- Coupled Channel method — Hagen PRL2009
- BHF theory — Hjorth-Jensen Phys.Rep.1995
  - With HJ potential — Dawson Ann.Phys.1962
  - With Reid potential — Machleidt NPA1975
  - With Bonn potentials — Muether PRC1990

	Bonn C	Bonn B	Bonn A	Exp.
$\varepsilon_{1s_{1/2}}$	−39.73	−44.37	−50.46	-40 ± 8
$\varepsilon_{1p_{3/2}}$	−16.98	−19.49	−22.89	−18.4
$\varepsilon_{1p_{1/2}}$	−11.64	−13.24	−15.44	−12.1
E	−71.84	−85.60	−104.96	−127.68
r_c	2.465	2.380	2.291	2.737

^{16}O in BHF method in Bonn potential

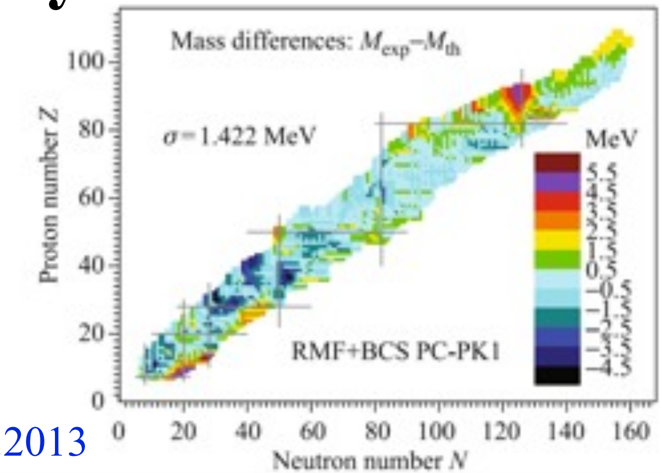
Covariant density functional theory

CDFT is very successful in nuclear physics

Ring PPNP1996, Vretenar Phys.Rep.2005, Meng PPNP2006

- Spin-orbit splitting
- Pseudo-spin symmetry
- Nuclear saturation properties
- Exotic nuclei
- ……

Meng Front. Phys.2013



The attempts to connect ab initio calculation with CDFT

The interaction in CDFT were extracted from the ab initio calculation in nuclear matter

- Density-dependent relativistic mean field theory — Brockmann PRL1992
- Density-dependent relativistic Hartree-Fock theory — Fritz PRL1993

In this work

Calculate the finite nuclei with *ab initio* method in CDFT framework directly, such as relativistic Brueckner-Hartree-Fock theory

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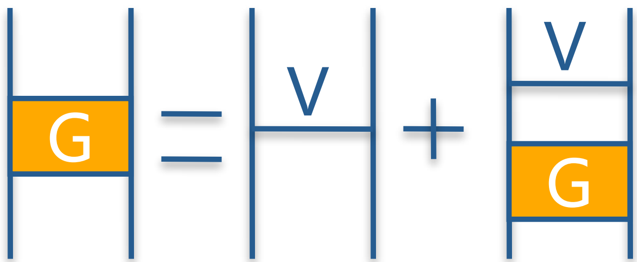
Brueckner-Hartree-Fock theory

Bethe-Goldstone Equation

Brueckner PR1954

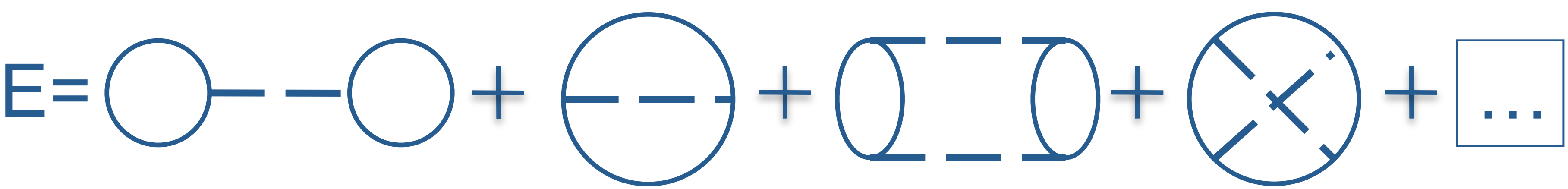
$$G = V + V\frac{Q}{E - H_0}G$$

- E is the starting energy
- Q is the Pauli operator
- V is the realistic NN interaction



Brueckner-Hartree-Fock energy

$$E_{BHF} = \sum_{i<F}\langle i|T|i\rangle + \frac{1}{2}\sum_{i,j<F}\left[\langle ij|G|ij\rangle - \langle ij|G|ji\rangle\right]$$



Bethe-Goldstone equation in basis space

$$\langle nm|G(\omega)|n'm'\rangle = \langle nm|V|n'm'\rangle + \sum_{\varepsilon_i,\varepsilon_j>\varepsilon_F} \frac{\langle nm|V|ij\rangle\langle ij|G(\omega)|n'm'\rangle}{\omega-(\varepsilon_i+\varepsilon_j)}$$

where ε_F is the Fermi energy, $\omega=\varepsilon_m+\varepsilon_n$ is the starting energy and i, j are intermediate states.

Bethe-Goldstone equation in plane wave basis

$$G^{\alpha}_{ll'}(kk'K\omega) = V^{\alpha}_{ll'}(kk') + \sum_{ll'}\int \frac{d^3q}{(2\pi)^3} V^{\alpha}_{ll'}(kq)\frac{Q(q,K)}{\omega-H_0} G^{\alpha}_{ll'}(qk'K\omega)$$

where α is a shorthand notation for J, S, L and T.

Matrix inversion method

$$G = \left(1-\frac{V}{\omega-H_0}\right)^{-1} V$$

Relativistic Hartree-Fock (RHF) equation

$$\sum_{n'}\left(\alpha\cdot p+\beta M+\beta\ \Gamma^{HF}\right)_{nn'}\psi_{n'}=\varepsilon_n\psi_n$$

where $\Gamma^{HF}_{nn'}$ is related with the density matrix $\rho_{nn'}$

$$\Gamma^{HF}_{nn'}=V_{nmn'm'}\rho_{mm'}-V_{nmm'n'}\rho_{mm'}$$

$$\psi_a=\begin{pmatrix}\sum_{n=1}^{n_{\max}}f_n^{(a)}R_{nl_a}(r)\\ \sum_{\tilde{n}=1}^{\tilde{n}_{\max}}g_{\tilde{n}}^{(a)}R_{\tilde{n}\tilde{l}_a}(r)\end{pmatrix}$$

RHF equation in HO basis

$$\begin{pmatrix}A^{RHF}_{nn'} & B^{RHF}_{n\tilde{n}'}\\ B^{RHF}_{\tilde{n}'n} & C^{RHF}_{\tilde{n}\tilde{n}'}\end{pmatrix}\begin{pmatrix}f^{(a)}_{n'}\\ g^{(a)}_{\tilde{n}'}\end{pmatrix}=\varepsilon_a\begin{pmatrix}f^{(a)}_{n}\\ g^{(a)}_{\tilde{n}}\end{pmatrix}$$

where

$$A^{RHF}_{nn'}=(\alpha\cdot p+\beta M)_{nn'}+\sum_b\sum_{m,m'}f_m^{(b)}f_{m'}^{(b)}(v_{nmn'm'}-v_{nmm'n'})$$

$$B^{RHF}_{n\tilde{n}'}=(\alpha\cdot p+\beta M)_{n\tilde{n}'}+\sum_b\sum_{m,\tilde{m}'}f_m^{(b)}g_{\tilde{m}'}^{(b)}(v_{nm\tilde{n}'\tilde{m}'}-v_{nm\tilde{m}'\tilde{n}'})$$

$$C^{RHF}_{\tilde{n}\tilde{n}'}=(\alpha\cdot p+\beta M)_{\tilde{n}\tilde{n}'}+\sum_b\sum_{\tilde{m},\tilde{m}'}g_{\tilde{m}}^{(b)}g_{\tilde{m}'}^{(b)}(v_{\tilde{n}\tilde{m}\tilde{n}'\tilde{m}'}-v_{\tilde{n}\tilde{m}\tilde{m}'\tilde{n}'})$$

RBHF theory for finite nuclei

Relativistic Brueckner Hartree-Fock (RBHF) equation

$$\sum_{n'}\left(\alpha\cdot p+\beta M+\beta\ \Gamma^{BHF}\right)_{nn'}\psi_{n'}=\varepsilon_n\psi_n$$

where $\Gamma^{BHF}_{nn'}$ is related with the density matrix $\rho_{nn'}$

$$\Gamma^{BHF}_{nn'}=G_{nmn'm'}\rho_{mm'}-G_{nmm'n'}\rho_{mm'}$$

RHF equation in HO basis

$$\begin{pmatrix} A^{BHF}_{nn'} & B^{BHF}_{n\tilde{n}'} \\ B^{BHF}_{\tilde{n}'n} & C^{BHF}_{\tilde{n}\tilde{n}'} \end{pmatrix}\begin{pmatrix} f^{(a)}_{n'} \\ g^{(a)}_{\tilde{n}'} \end{pmatrix}=\varepsilon_a\begin{pmatrix} f^{(a)}_{n} \\ g^{(a)}_{\tilde{n}} \end{pmatrix}$$

where

$$A^{BHF}_{nn'}=(\alpha\cdot p+\beta M)_{nn'}+\sum_b\sum_{m,m'}f^{(b)}_m f^{(b)}_{m'}G_{nmn'm'}$$

$$B^{BHF}_{n\tilde{n}'}=(\alpha\cdot p+\beta M)_{n\tilde{n}'}+\sum_b\sum_{m,\widetilde{m}'}f^{(b)}_m g^{(b)}_{\widetilde{m}'}G_{nm\tilde{n}'\widetilde{m}'}$$

$$C^{BHF}_{\tilde{n}\tilde{n}'}=(\alpha\cdot p+\beta M)_{\tilde{n}\tilde{n}'}+\sum_b\sum_{\widetilde{m},\widetilde{m}'}g^{(b)}_{\tilde{m}} g^{(b)}_{\widetilde{m}'}G_{\tilde{n}\tilde{m}\tilde{n}'\widetilde{m}'}$$

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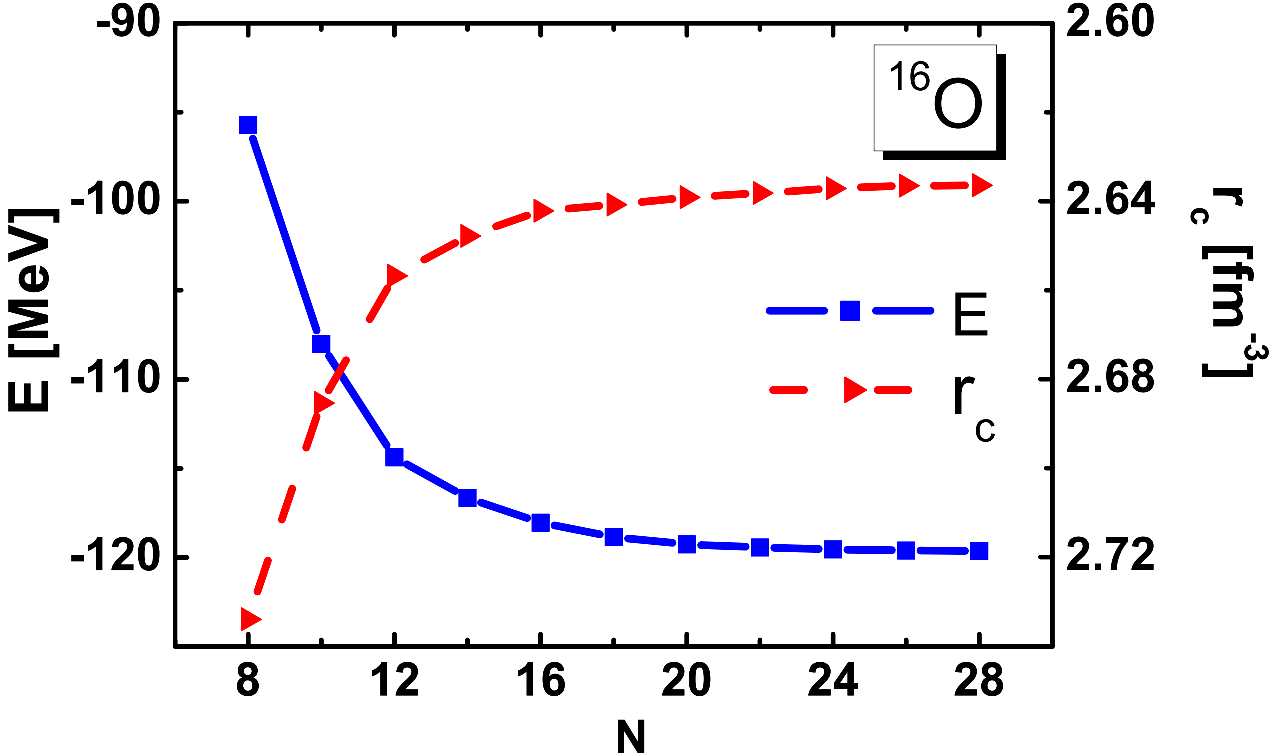
Example

- Object: ^{16}O
- Interaction: Bonn A
- Basis: Harmonics Oscillator (HO)

Machleidt ANP1987

The convergence of RBHF theory for ^{16}O



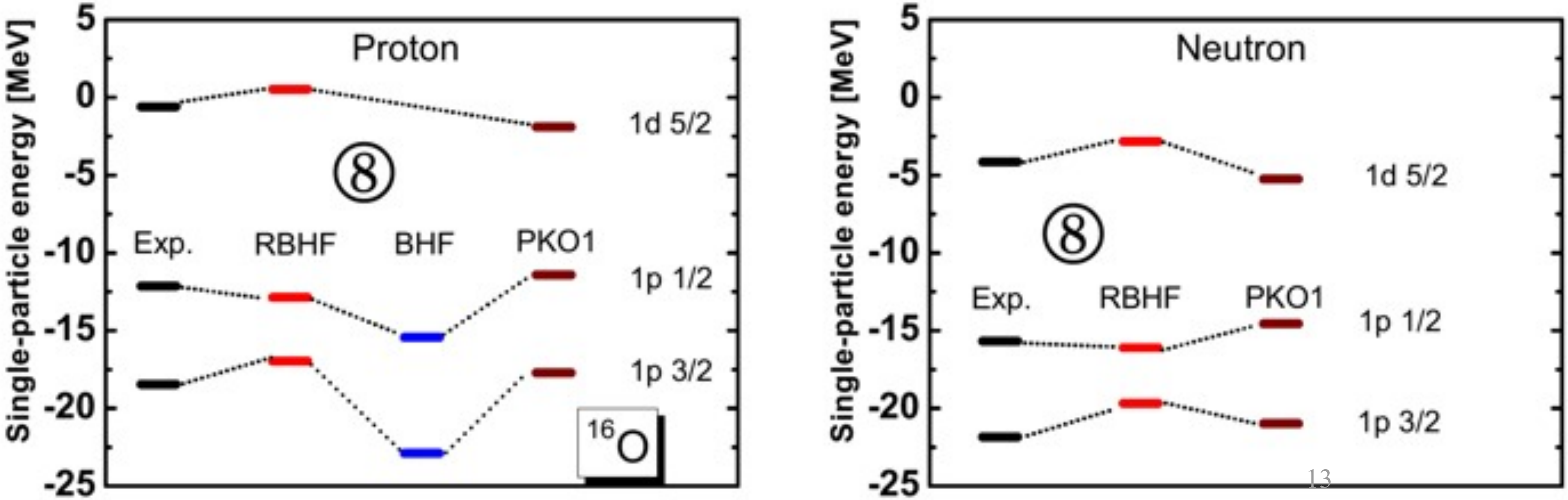
The ground state properties of ^{16}O in RBHF theory

The properties of ^{16}O with different numerical methods

	EXP. [1]	RBHF (N=28)	BHF [2]	PKO1 [3]
E (MeV)	-127.62	-119.552	-104.96	-128.36
r_c (fm)	2.737	2.6357	2.291	2.679
$\varepsilon_{1p_{1/2}} - \varepsilon_{1p_{3/2}}$ (MeV)	6.3	4.1	7.5	6.3

[1] Audi NPA2003, [2] Muether PRC1990, [3]Long PLB2006

The Single particle energies for the orbit level of ^{16}O in RBHF theory



The Lagrangian of Density-dependent RH (DDRH) theory

Brockmann PRL1992

$$L=\bar{\psi}_N(i\gamma_\mu\partial^\mu - M_N - g_{\sigma N}(\rho)\sigma - g_{\omega N}(\rho)\gamma_\mu\omega^\mu - e\gamma_\mu\frac{1-\tau^3}{2}A^\mu)\psi_N + \frac{1}{2}\partial_\mu\sigma\partial^\mu\sigma - \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu$$

$$U_S = g_{\sigma B}(\rho)\sigma$$
$$U_V = g_{\omega B}(\rho)\omega$$

The Lagrangian of Density-dependent RHF (DDRHF) theory

Fritz PRL1993

$$L=\bar{\psi}_N(i\gamma_\mu\partial^\mu - M_N - g_{\sigma N}(\rho)\sigma - g_{\omega N}(\rho)\gamma_\mu\omega^\mu - \frac{f_{\pi N}}{m_\pi}(\rho)\pi^a\gamma_5\gamma_\mu\partial^\mu\pi^a - e\gamma_\mu\frac{1-\tau^3}{2}A^\mu)\psi_N + \frac{1}{2}\partial_\mu\sigma\partial^\mu\sigma - \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu + \frac{1}{2}\partial_\mu\pi^a\partial^\mu\pi^a - \frac{1}{2}m_\pi^2\pi^{a2}$$

$$U_S = g_{\sigma B}(\rho)\sigma$$
$$U_V = g_{\omega B}(\rho)\omega$$

DDRH and DDRHF from RBHF theory

The relativistic Hartree-Fock equation

Bouyssy PRC1987

$$\frac{d}{dr}\begin{pmatrix} G_a(r) \\ F_a(r) \end{pmatrix} = \begin{pmatrix} -\frac{\kappa_a}{r} - \Sigma_{T,a}^D - P_a(r) & M - E_a + \Sigma_{S,a}^D - \Sigma_{0,a}^D + Q_a(r) \\ M - E_a + \Sigma_{S,a}^D + \Sigma_{0,a}^D + R_a(r) & \frac{\kappa_a}{r} + \Sigma_{T,a}^D + S_a(r) \end{pmatrix} \begin{pmatrix} G_a(r) \\ F_a(r) \end{pmatrix}$$

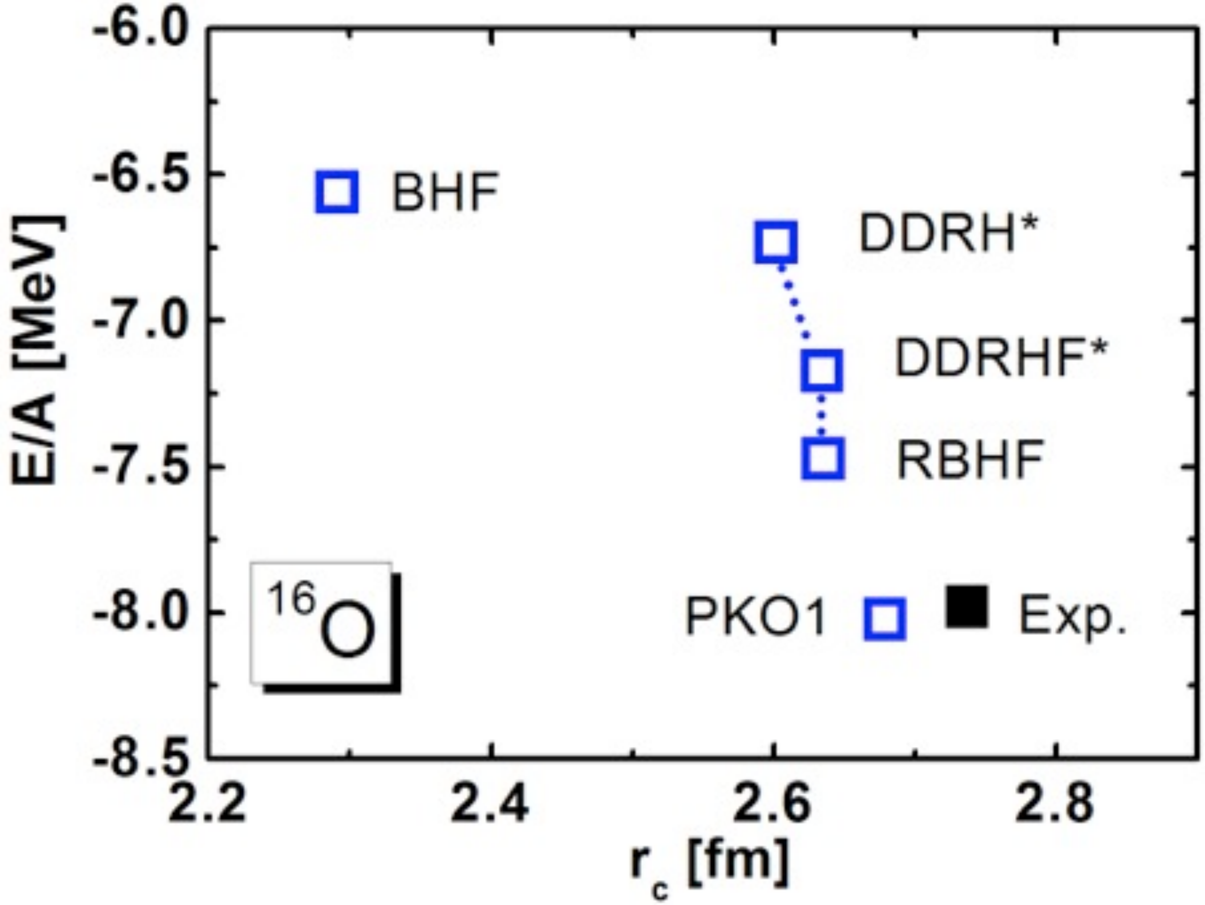
The properties of ^{16}O in different theories

	EXP. [1]	DDRH*	DDRHF*	RBHF (N=28)
E (MeV)	−127.62	−107.72	−114.76	−119.55
r_c (fm)	2.737	2.602	2.634	2.636
$\varepsilon_{1p_{1/2}} - \varepsilon_{1p_{3/2}}$ (MeV)	6.3	5.2	4.8	4.1

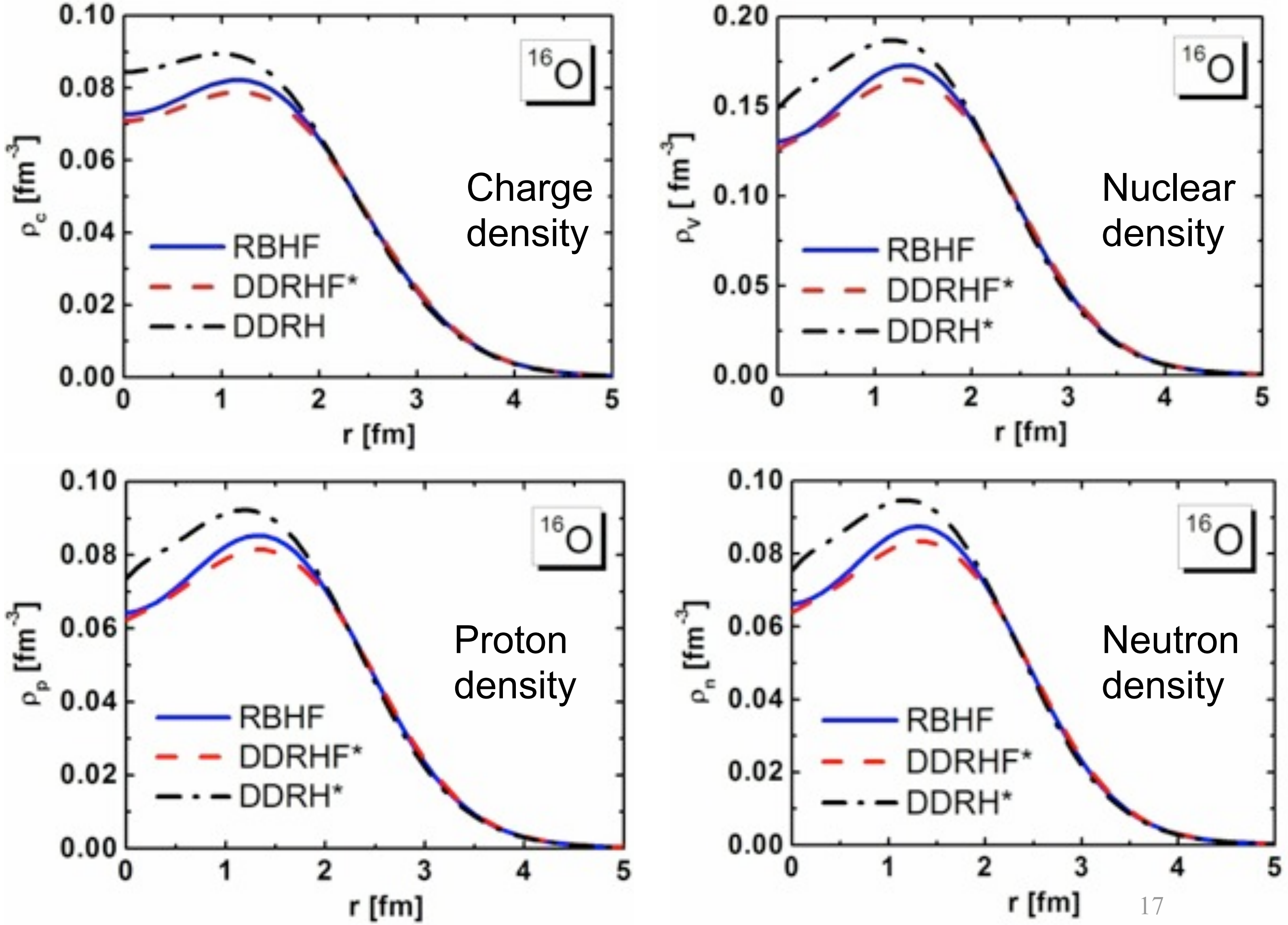
[1] Audi NPA2003

* DD couplings extracted from RBHF theory at nuclear matter

The relation between binding energy and radii of ^{16}O in different theories



The densities of ^{16}O in different theories



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Summary and Perspectives

- The relativistic Brueckner-Hartree-Fock (RBHF) theory is developed for finite nuclei with HO basis.
- The results of RBHF theory with Bonn A potential at N = 28 is reliable, e.g. ^{16}O.
- The binding energy and charge radii from RBHF theory are close to experimental data, and are comparable with the ones from the PKO1.
- In future calculation, the heavier nuclei is feasible.

Thank you very much for your attention!

Appendix

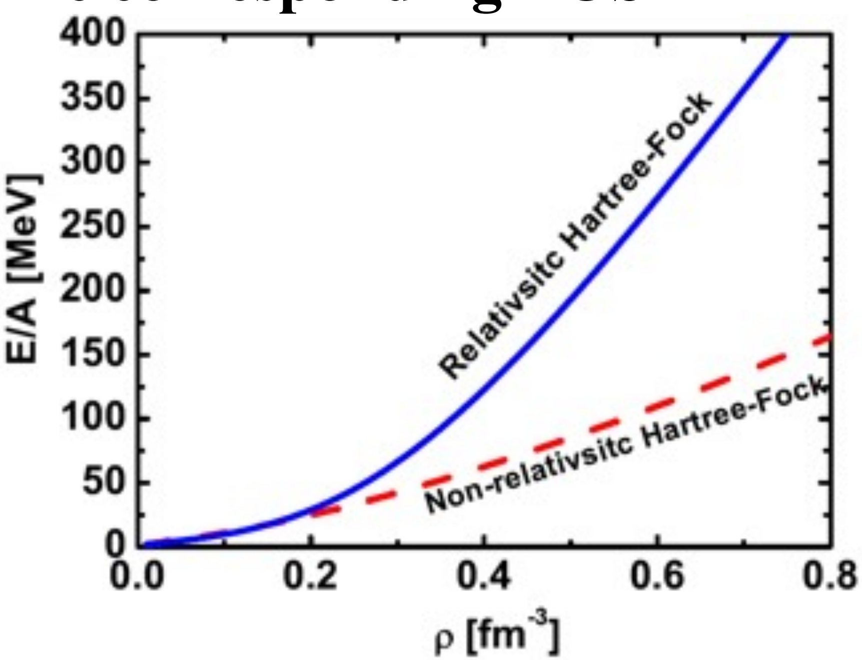
Lippmann-Schwinger Equation

Brown NPA1969

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

- V is the realistic NN interaction
- E is the incident energy
- T-matrix is for two-body scattering

The corresponding EOS in HF



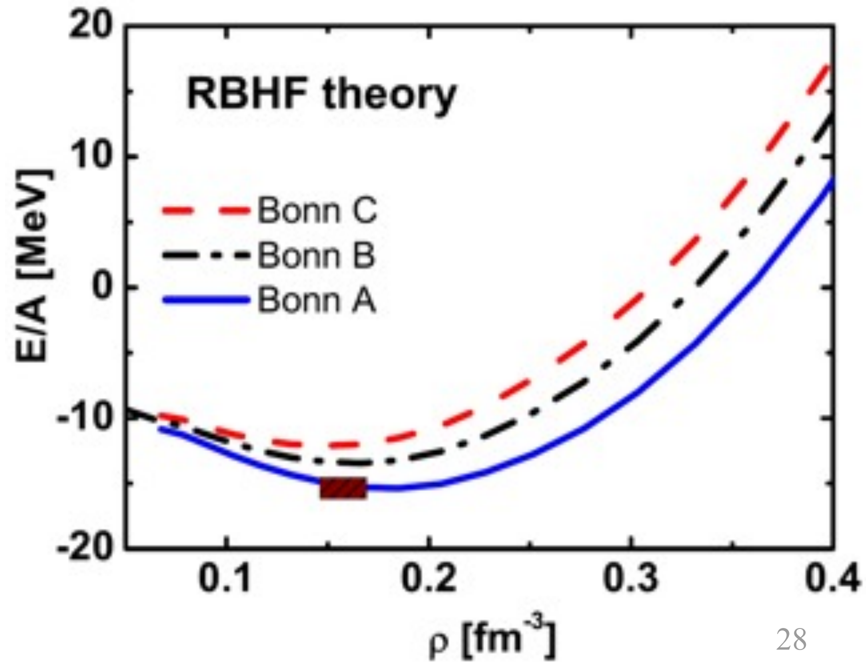
Bethe-Goldstone Equation

Brueckner PRC1969

$$T = V + V\frac{Q}{E - H_0}T$$

- E is the starting energy
- Q is the Pauli operator
- G-matrix is for many-body problem

The corresponding EOS in HF



The ground state properties of other nuclei in RBHF theory

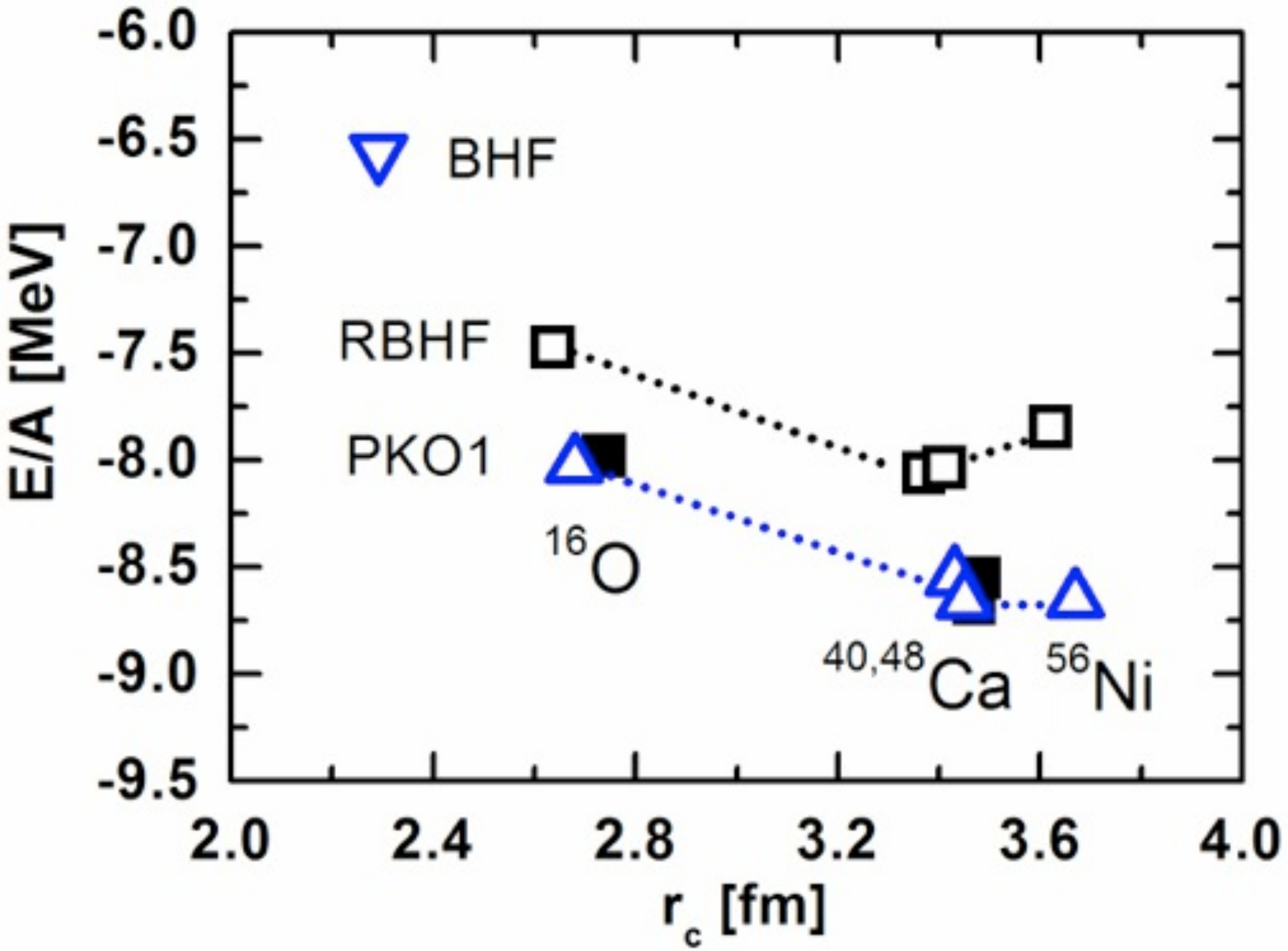
	E (MeV)			r_c (fm)			$\varepsilon_{1p_{1/2}} - \varepsilon_{1p_{3/2}}$ (MeV)		
	Exp.	RBHF	PKO1	Exp.	RBHF	PKO1	Exp.	RBHF	PKO1
^{14}C	−105.73	−98.49	−106.66	2.50	2.42	2.45	–	4.6	6.6
^{14}O	−98.73	−91.51	−100.48	–	2.67	2.68	–	–	–
^{40}Ca	−342.05	−322.41	−341.93	3.48	3.37	3.43	7.2	5.7	6.5
^{48}Ca	−416.16	−385.62	−415.62	3.47	3.41	3.45	4.3	3.1	6.2
^{56}Ni	−483.95	−439.26	−484.61	–	3.62	3.67	–	1.2	1.8

The deviations of binding energy between experiment and RBHF

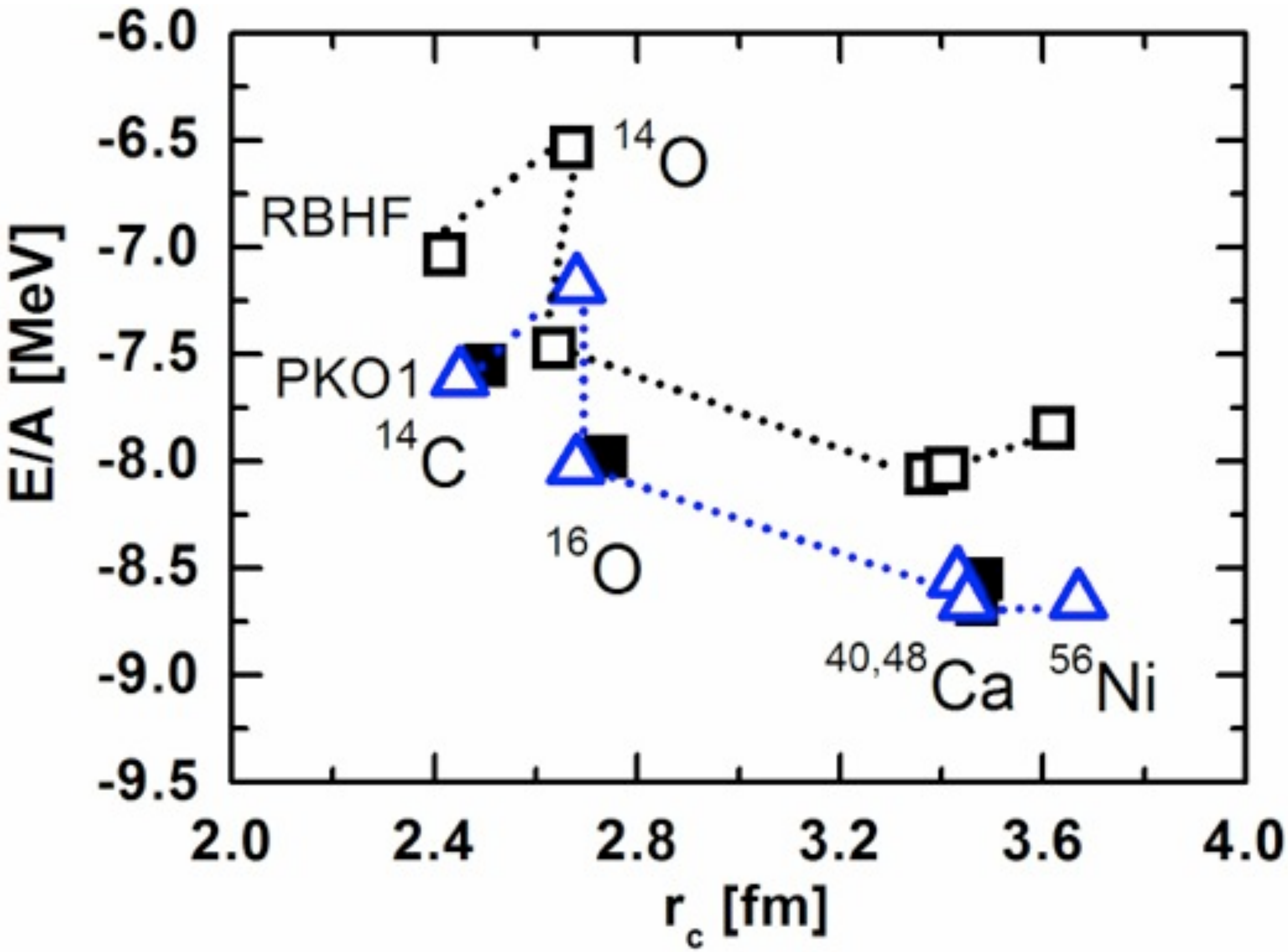
	^{14}C	^{14}O	^{16}O	^{40}Ca	^{48}Ca	^{56}Ni
$(E_{\mathrm{exp.}} - E_{RBHF})/E_{\mathrm{exp.}}(\%)$	6.85	7.31	6.32	5.74	7.34	9.23

- The binding energy is missing less than10% in RBHF comparing with the data
- The spin-orbit splitting is small

The relation between binding energy and radii of doubly magic nuclei in different theories



The relation between binding energy and radii of other nuclei in different theories



The relation between binding energy and radii of other nuclei in different theories