北京大学物理学院
School of Physics, Peking University

Ab initio many-body perturbation theory for atomic nuclei

Furong Xu

Collaborators: James Vary, Baishan Hu, Zhonghao Sun, Tong Li

Outline

I. The concept of MBPT

II. Corrections to the ground-state energy

III. Corrections to ground-state wavefunction, density, root-mean-square radius

IV. The examples of ^{4}He and ^{16}O

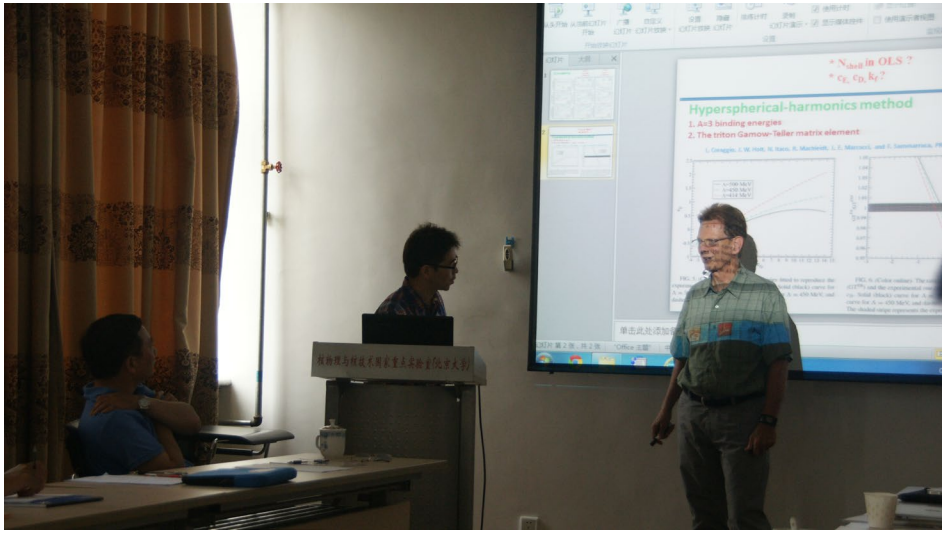
V. Conclusions

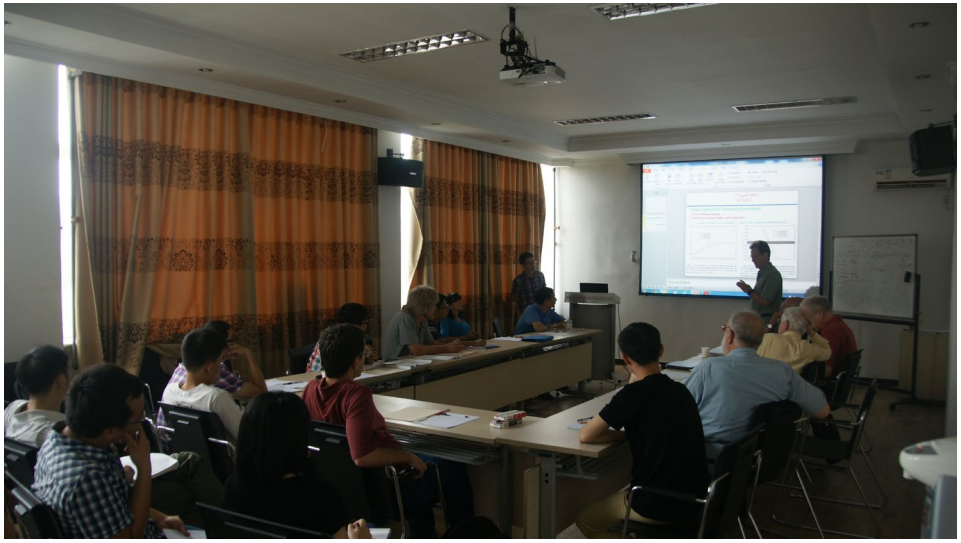
A happy and healthy birthday to our friend, Prof. James Vary

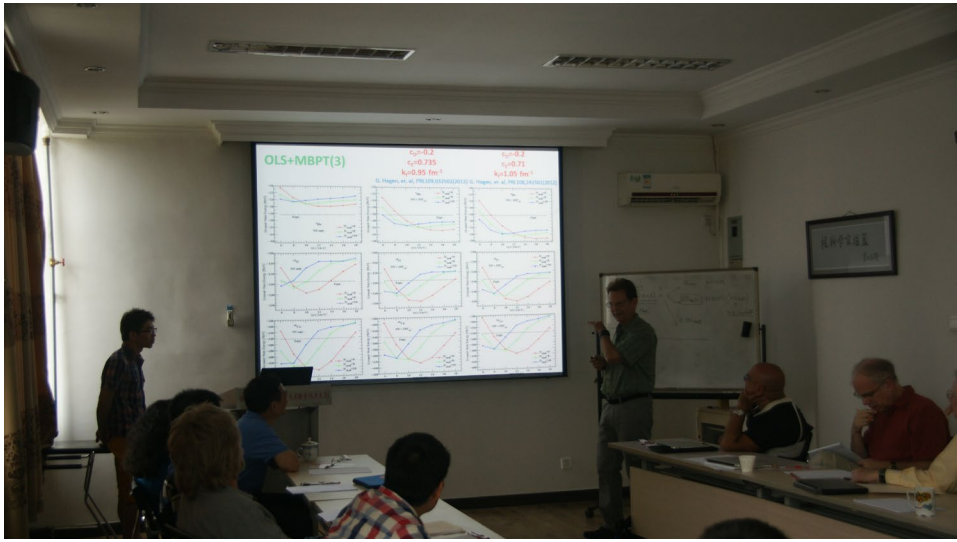
CUSTIPEN workshops, summer 2015

at PKU (organized by Furong Xu's group)

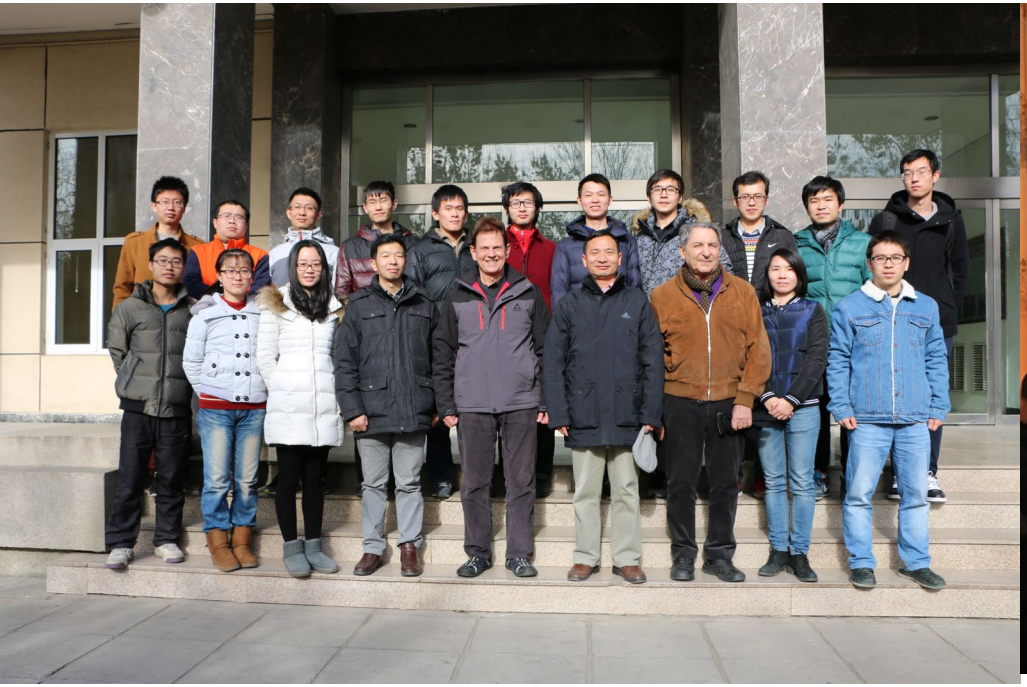
at IMP (organized by Prof. Wei Zuo's group）

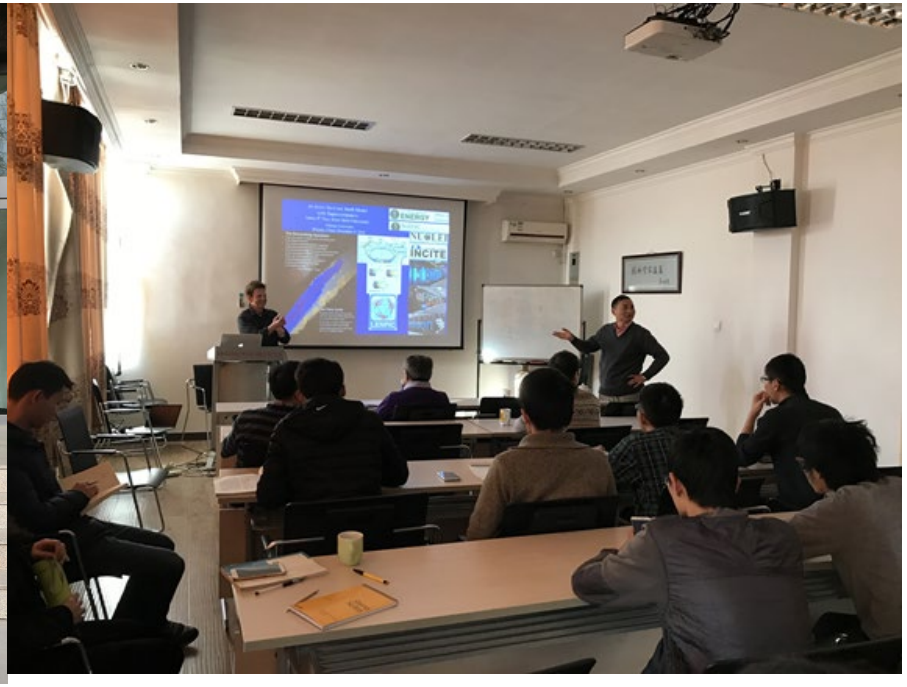






Between workshops at PKU and IMP 2015, one-day discussion session with students at PKU





Mini workshop, 2016 winter, PKU (Beijing)

Workshop for Dr. Nicolas Michel starting his position at IMP,

Organized by Profs. Zuo and Michel

PHYSICAL REVIEW C **94**, 014303 (2016)

Ab initio nuclear many-body perturbation calculations in the Hartree-Fock basis

B. S. Hu (胡柏山),[1] F. R. Xu (许甫荣),[1,*] Z. H. Sun (孙中浩),[1] J. P. Vary,[2] and T. Li (李通)[1]

[1]*State Key Laboratory of Nuclear Physics and Technology, School of Physics, Peking University, Beijing 100871, China*

[2]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*

(Received 25 April 2016; published 6 July 2016)

Starting from realistic nuclear forces, the chiral N^3LO and JISP16, we have applied many-body perturbation theory (MBPT) to the structure of closed-shell nuclei, ^{4}He and ^{16}O. The two-body N^3LO interaction is softened by a similarity renormalization group transformation while JISP16 is adopted without renormalization. The MBPT calculations are performed within the Hartree-Fock (HF) bases. The angular momentum coupled scheme is used, which can reduce the computational task. Corrections up to the third order in energy and up to the second order in radius are evaluated. Higher-order corrections in the HF basis are small relative to the leading-order perturbative result. Using the antisymmetrized Goldstone diagram expansions of the wave function, we directly correct the one-body density for the calculation of the radius, rather than calculate corrections to the occupation probabilities of single-particle orbits as found in other treatments. We compare our results with other methods where available and find good agreement. This supports the conclusion that our methods produce reasonably converged results with these interactions. We also compare our results with experimental data.

DOI: 10.1103/PhysRevC.94.014303

Ab initio many-body perturbation theory - MBPT

Two fundamental problems in nuclear structure calculations:

1) nuclear force; 2) many-body correlation

Ab initio calculations of nuclei

1. Starting from realistic nuclear forces

2. Renormalization (softening) to speed up convergence

3. *Ab-initio* methods to treat many-body problems

$$\hat{H}_{int} = \sum_{i<j}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \sum_{i<j}^{A} V_{NN,ij} + \sum_{i<j<k}^{A} V_{NNN,ijk}$$

$$H_{\rm int} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j} V(|\vec{r}_i - \vec{r}_j|) - \frac{P^2}{2Am} \qquad \vec{P} = \sum_{i=1}^{A} \vec{p}_i$$

MBPT calculations for closed-shell nuclei

$$\hat{H}_{int} = \sum_{i<j}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \sum_{i<j}^{A} V_{NN,ij} \quad ; \qquad H_{\rm int} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j} V(|\vec{r}_i - \vec{r}_j|) - \frac{P^2}{2Am} \quad , \qquad \vec{P} = \sum_{i=1}^{A} \vec{p}_i$$

a) First we performed spherical HF calculation (in HO basis)

b) The HF state is chosen as a reference state, which limits to closed-shell nuclei.

c) In the HF basis, we make MBPT: for energy up to 3rd-order perturbation corrections, and for radius up to 2nd-order corrections, in the *j-j* scheme:

$$H_0 = \sum_{l_1 l_2} h^{HF}_{l_1 l_2} a^{\dagger}_{l_1} a_{l_2}$$

$$\hat{H} = \hat{H}_0 + (\hat{H} - \hat{H}_0) = \hat{H}_0 + \hat{V}$$

The exact solutions of the A-nucleon system are,

$$\hat{H}\Psi_n = E_n \Psi_n, \qquad n = 0, 1, 2, ...$$

The zero-order part is,

$$\hat{H}_0 \Phi_n = E_n^{(0)} \Phi_n, \qquad n = 0, 1, 2, ...$$

For the ground state:

Perturbation (MBPT)

$$\chi_0 = \Psi_0 - \Phi_0$$

$$\Delta E = E_0 - E_0^{(0)}$$

$$\Psi_0 = \sum_{m=0}^{\infty} \left[\hat{R}_0(E_0^{(0)})(\hat{V} - \Delta E)\right]^m \Phi_0$$

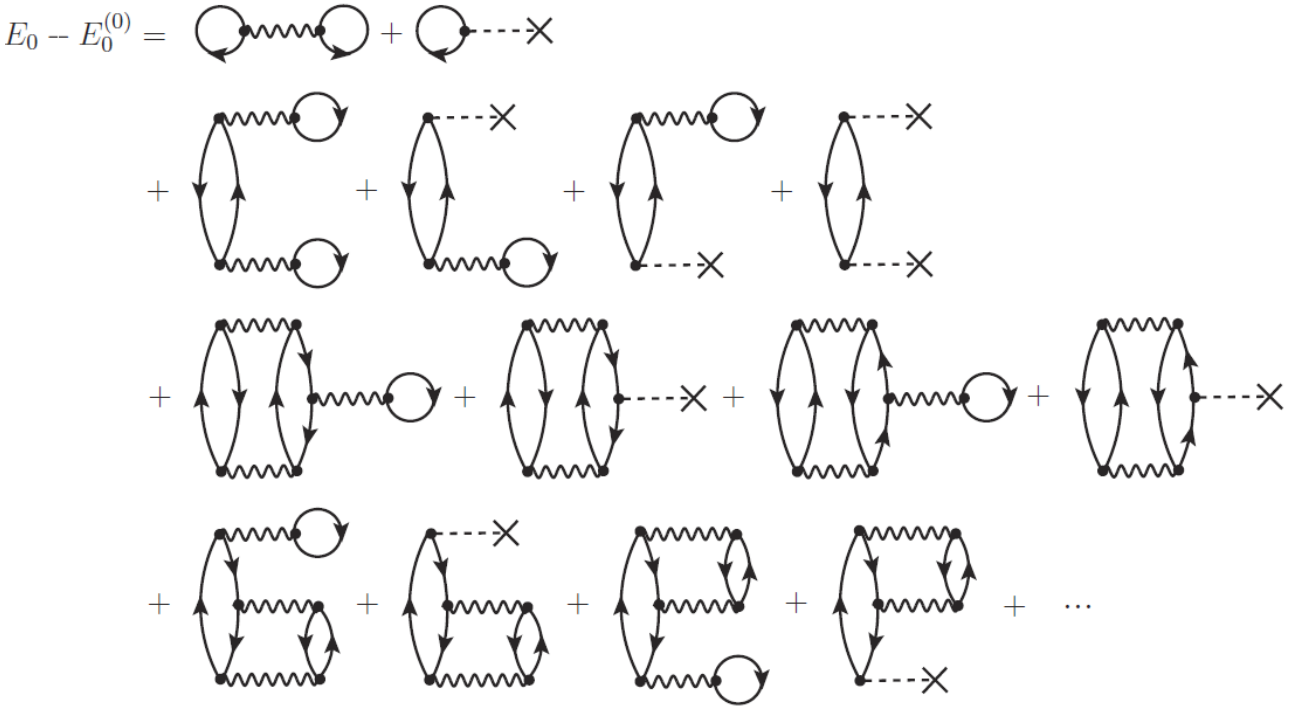
$$\Delta E = \sum_{m=0}^{\infty} \langle \Phi_0 | \hat{V} \left[\hat{R}_0(E_0^{(0)})(\hat{V} - \Delta E)\right]^m | \Phi_0 \rangle$$

where $\hat{R}_0 = \sum_{i \neq 0} \frac{|\Phi_i\rangle\langle\Phi_i|}{E_0^{(0)} - E_i^{(0)}}$ is called the resolvent of $\hat{H}_0$

Rayleigh-Schrodinger method

Advantages in HF basis, compared with HO basis:

1) **faster convergence;**
2) **some-type perturbation diagrams can be cancelled out, but not in HO basis;**
3) **In HO basis, calculations could be $\hbar\omega$ dependent, while less dependent in HF basis.**



$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} + E_0^{(3)} + \dots$$

HF energy $= \langle \phi_0 | H | \phi_0 \rangle$, $\quad \hat{H} = \hat{H}_0 + (\hat{H} - \hat{H}_0) = \hat{H}_0 + \hat{V}$

$$E_0^{(1)} = \langle \Phi_0 | \hat{V} | \Phi_0 \rangle$$

$$E_0^{(2)} = \langle \Phi_0 | \hat{V} \hat{R}_0 \hat{V} | \Phi_0 \rangle$$

$$E_0^{(3)} = \langle \Phi_0 | \hat{V} \hat{R}_0 (\hat{V} - \langle \Phi_0 | \hat{V} | \Phi_0 \rangle) \hat{R}_0 \hat{V} | \Phi_0 \rangle$$

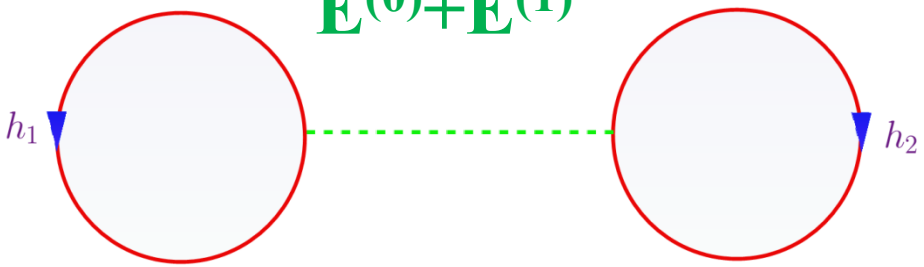
$$\Psi_0 = \underbrace{\Phi_0}_{\text{HF}} + \Psi_0^{(1)} + \Psi_0^{(2)} + \dots$$

$$\Psi_0^{(1)} = \hat{R}_0 \hat{V} | \Phi_0 \rangle$$

$$\Psi_0^{(2)} = \hat{R}_0 (\hat{V} - E_0^{(1)}) \hat{R}_0 \hat{V} | \Phi_0 \rangle$$

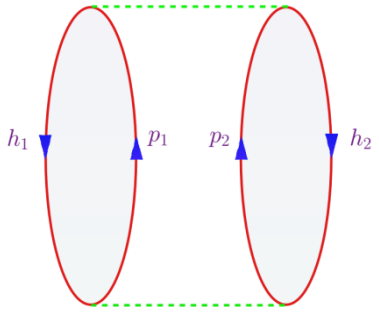
Anti-Symmetrized Goldstone (ASG) diagram expansion

$E^{(0)}+E^{(1)}$



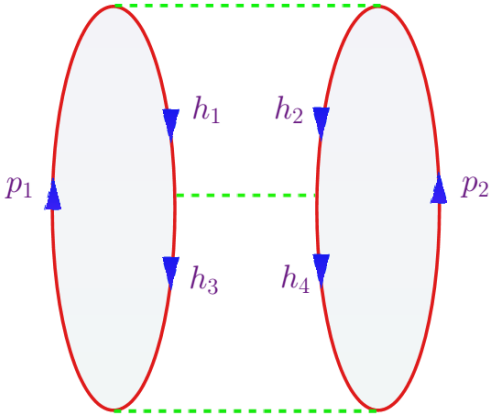
HF energy

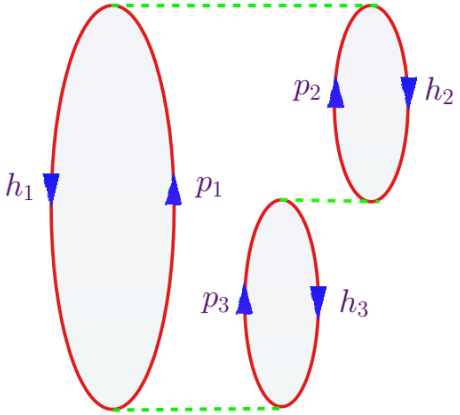
$E^{(2)}$

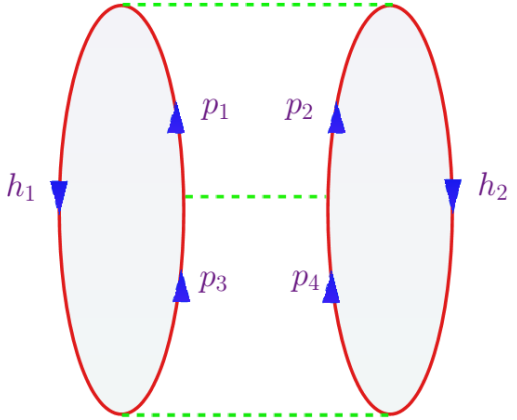


$$\frac{1}{4}\sum_{h_1,h_2<\varepsilon_F}\sum_{p_1,p_2>\varepsilon_F}\frac{|\langle p_1p_2|\hat{\mathrm{H}}_{int}|h_1h_2\rangle|^2}{\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2}}$$

$E^{(3)}$





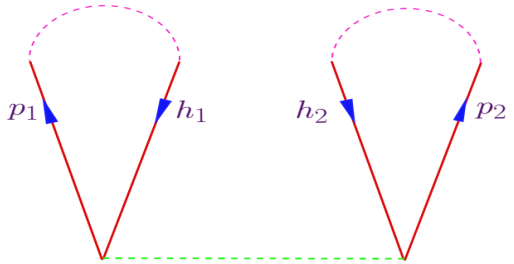


2p4h =

$$\frac{1}{8}\sum_{h_1,h_2,h_3,h_4<\varepsilon_F}\sum_{p_1,p_2>\varepsilon_F}\frac{\langle p_1p_2|\hat{\mathrm{H}}_{int}|h_3h_4\rangle\langle h_3h_4|\hat{\mathrm{H}}_{int}|h_1h_2\rangle\langle h_1h_2|\hat{\mathrm{H}}_{int}|p_1p_2\rangle}{(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2})(\varepsilon_{h_3}+\varepsilon_{h_4}-\varepsilon_{p_1}-\varepsilon_{p_2})}$$

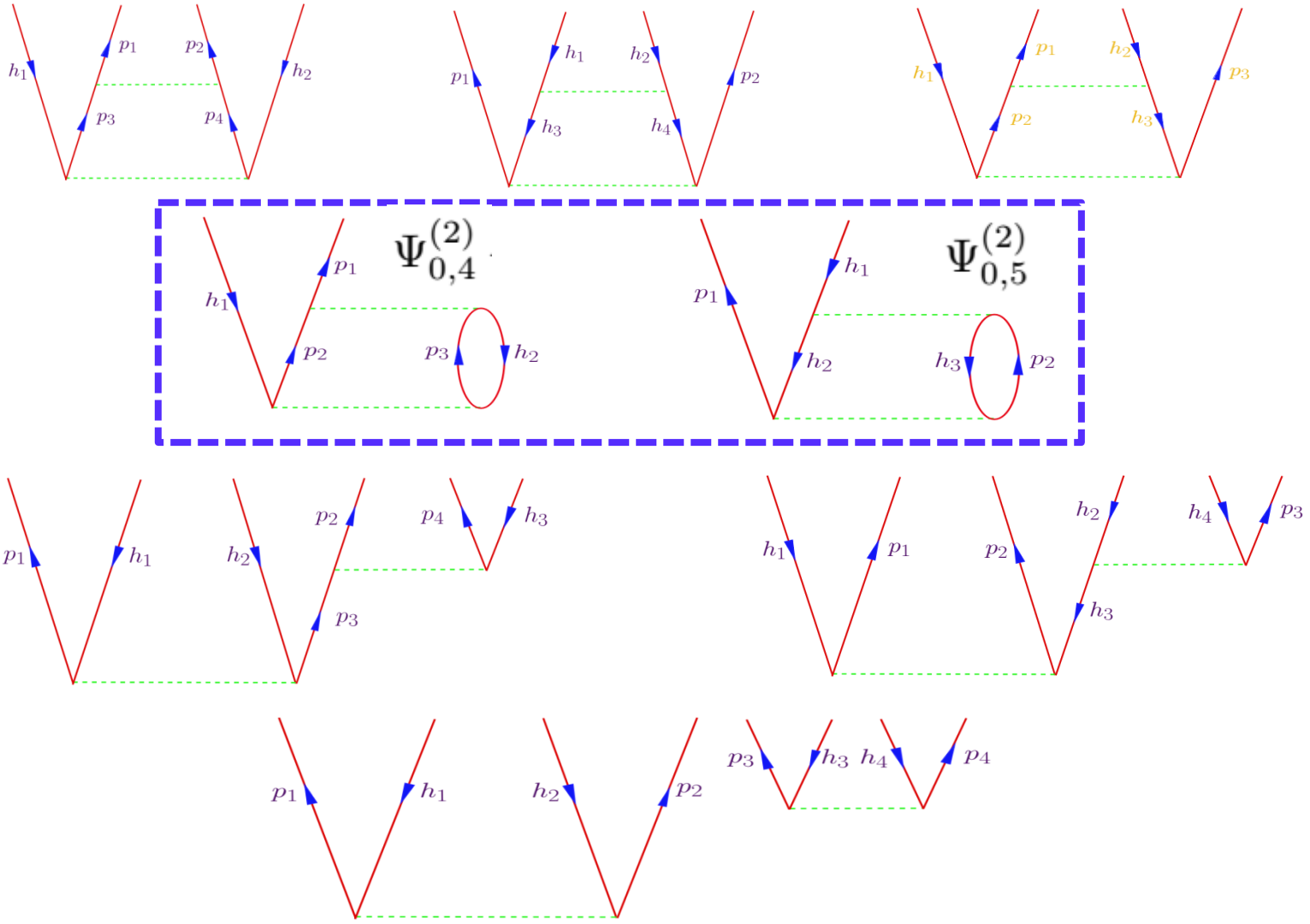
ASG diagrams for wave functions

$\psi^{(1)}$



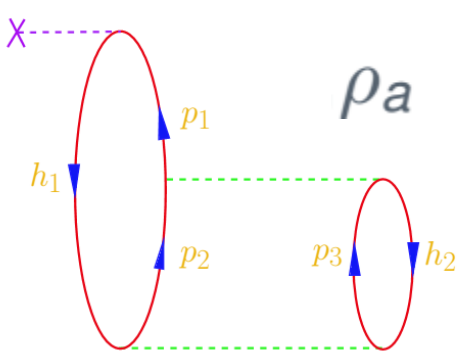
$$\Psi_0' = \Phi_0 + \Psi_0^{(1)} + \Psi_{0,4}^{(2)} + \Psi_{0,5}^{(2)}$$

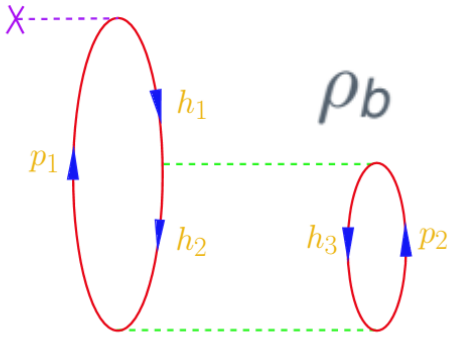
$\psi^{(2)}$



$$\rho(\vec{r}) = \langle\Phi_0|\rho(\vec{r})|\Phi_0\rangle + \underline{\langle\Phi_0|\rho(\vec{r})|\Phi_0\rangle\langle\Psi_0^{(1)}|\Psi_0^{(1)}\rangle} + \underline{2\rho_a + 2\rho_b + \rho_{c1} + \rho_{c2}} + \cdots$$

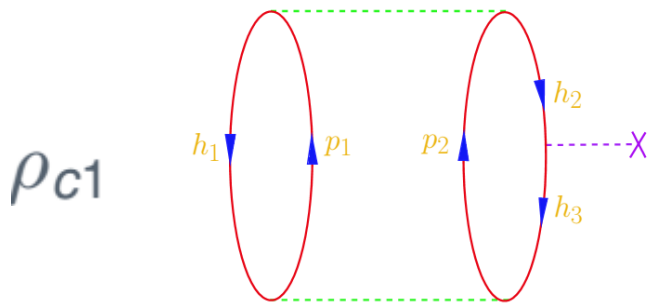
HF — **2nd order** — **2nd order**

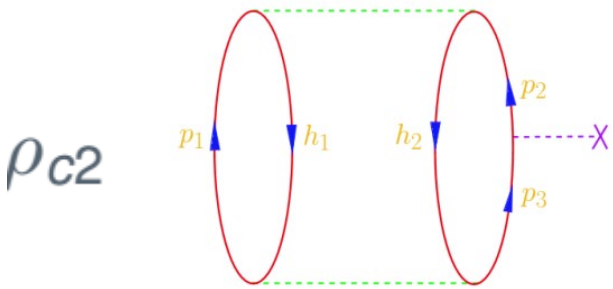




$$\frac{1}{2}\sum_{h_1,h_2<\varepsilon_F}\sum_{p_1,p_2,p_3>\varepsilon_F}\frac{\langle h_1h_2|\hat{H}|p_2p_3\rangle\langle p_2p_3|\hat{H}|p_1h_2\rangle\langle h_1|\rho|p_1\rangle}{(\varepsilon_{h_1}-\varepsilon_{p_1})(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_2}-\varepsilon_{p_3})}$$

$$-\frac{1}{2}\sum_{h_1,h_2,h_3<\varepsilon_F}\sum_{p_1,p_2>\varepsilon_F}\frac{\langle p_1p_2|\hat{H}|h_2h_3\rangle\langle h_2h_3|\hat{H}|h_1p_2\rangle\langle h_1|\rho|p_1\rangle}{(\varepsilon_{h_1}-\varepsilon_{p_1})(\varepsilon_{h_2}+\varepsilon_{h_3}-\varepsilon_{p_1}-\varepsilon_{p_2})}$$





$$-\frac{1}{2}\sum_{h_1,h_2,h_3<\varepsilon_F}\sum_{p_1,p_2>\varepsilon_F}\frac{\langle h_1h_2|\hat{H}|p_1p_2\rangle\langle p_1p_2|\hat{H}|h_1h_3\rangle\langle h_3|\rho|h_2\rangle}{(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2})(\varepsilon_{h_1}+\varepsilon_{h_3}-\varepsilon_{p_1}-\varepsilon_{p_2})}$$

$$\frac{1}{2}\sum_{h_1,h_2<\varepsilon_F}\sum_{p_1,p_2,p_3>\varepsilon_F}\frac{\langle p_1p_3|\hat{H}|h_1h_2\rangle\langle h_1h_2|\hat{H}|p_1p_2\rangle\langle p_2|\rho|p_3\rangle}{(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_3})(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2})}$$

Root-mean-square radius calculation

$$\hat{r}_{\mathrm{m}}^2 = \frac{1}{A}\sum_{i=1}^{A}(\vec{r}_i - \vec{r}_0)^2 = \frac{1}{A^2}\sum_{i<j}^{A}(\vec{r}_i - \vec{r}_j)^2 = \left(1-\frac{1}{A}\right)\left(\sum_{i=1}^{A}\vec{r}_i{}^2/A\right) - \frac{2}{A^2}\left(\sum_{i<j}^{A}\vec{r}_i\cdot\vec{r}_j\right)$$

$$\approx \left(1-\frac{1}{A}\right)\left(\sum_{i=1}^{A}\vec{r}_i{}^2/A\right) \qquad \vec{r}_0 = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i$$

$$\hat{r}_{\mathrm{pp}}^2 = \frac{1}{Z}\sum_{i=1}^{Z}(\vec{r}_i - \vec{r}_0)^2 \approx \left(1-\frac{1}{A}\right)\left(\sum_{i=1}^{Z}\vec{r}_i{}^2/Z\right) \longrightarrow \langle R_{\mathrm{pp}}^2\rangle = \frac{\int r^2\rho_{\mathrm{p}}(\vec{r})d^3r}{\int \rho_{\mathrm{p}}(\vec{r})d^3r}$$

c.m. effect

$$\langle r_{\mathrm{ch}}^2\rangle = \langle r_{\mathrm{pp}}^2\rangle + R_{\mathrm{p}}^2 + \frac{N}{Z}R_{\mathrm{n}}^2 + \frac{3\hbar^2}{4m_{\mathrm{p}}^2c^2}$$

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

$R_{\mathrm{p}} = 0.8775(51)$ fm $\quad \frac{3\hbar^2}{4m_{\mathrm{p}}^2c^2} \approx 0.033$ fm^2, $\quad R_{\mathrm{n}}^2 = -0.1149(27)$ fm^2

$$\Delta r_{\mathrm{c.m.}} = \left[\left(1-\frac{1}{A}\right)\langle R_{\mathrm{pp}}^2\rangle\right]^{1/2} - \langle R_{\mathrm{pp}}^2\rangle^{1/2}$$

Approximate center-of-mass correction for charge radius (point-proton)

NCSM

S.K. Bogner *et al.*, arXiv0708.3754v2 (2007)

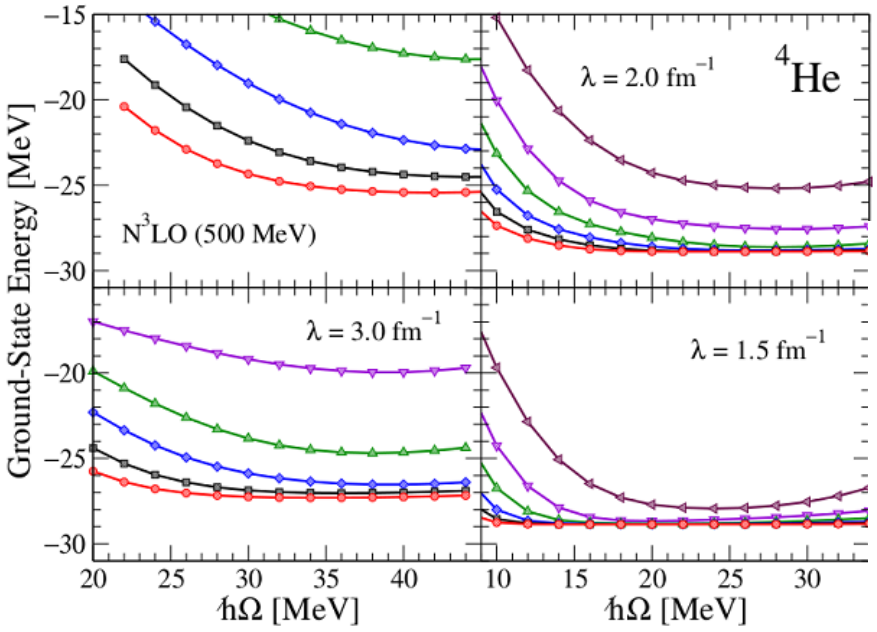


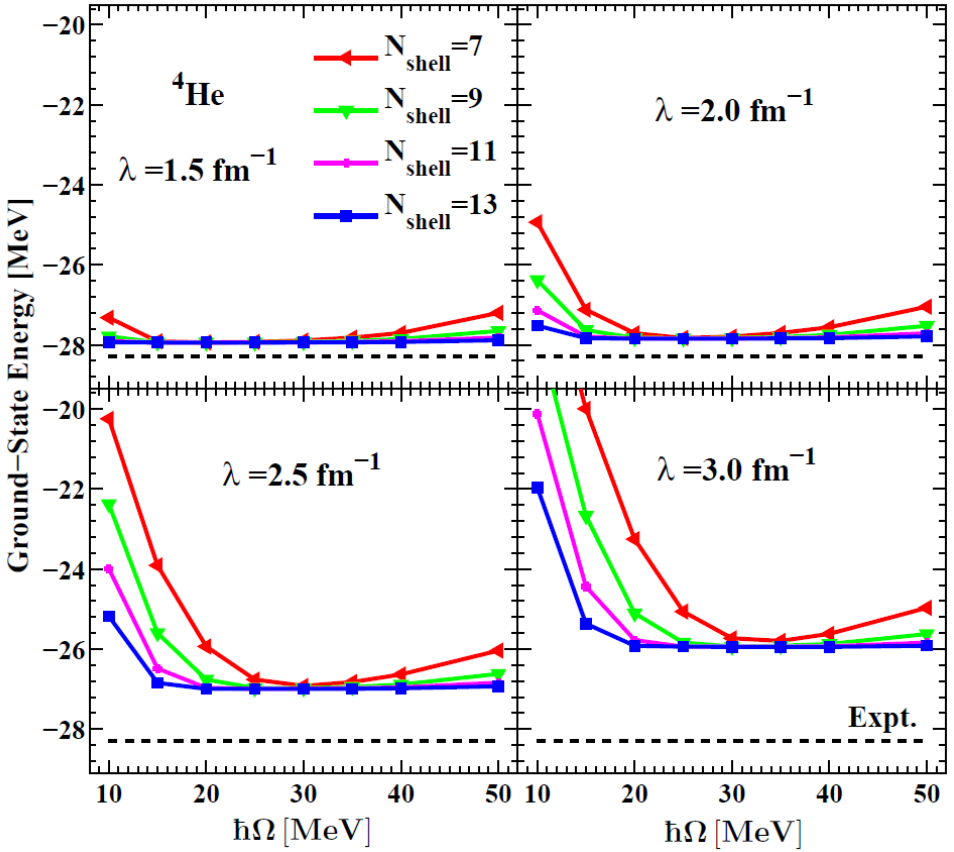
Fig. 3. Ground-state energy of ^{4}He as a function of $\hbar\Omega$ at four different value: (∞, 3, 2, 1.5 fm^{-1}). The initial potential is the 500 MeV N^{3}LO NN-only pot from Ref. [13]. The legend from Fig. 1 applies here.

^{4}He

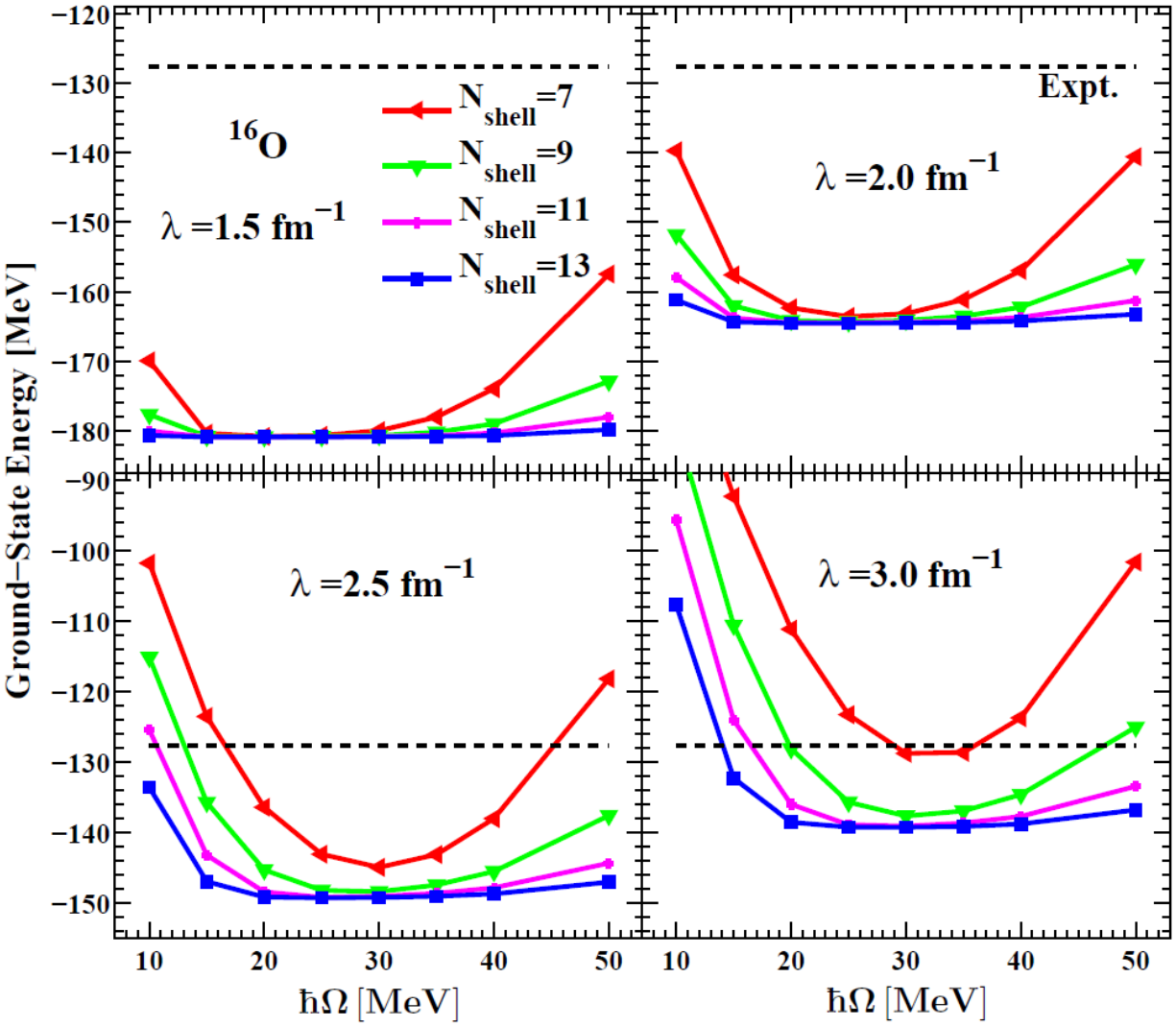
Our MBPT calculations

B.S. Hu, F.R. Xu, Z.H. Sun, J.P. Vary, T. Li, PRC 94, 014303 (2016)

N^{3}LO+SRG without 3NF

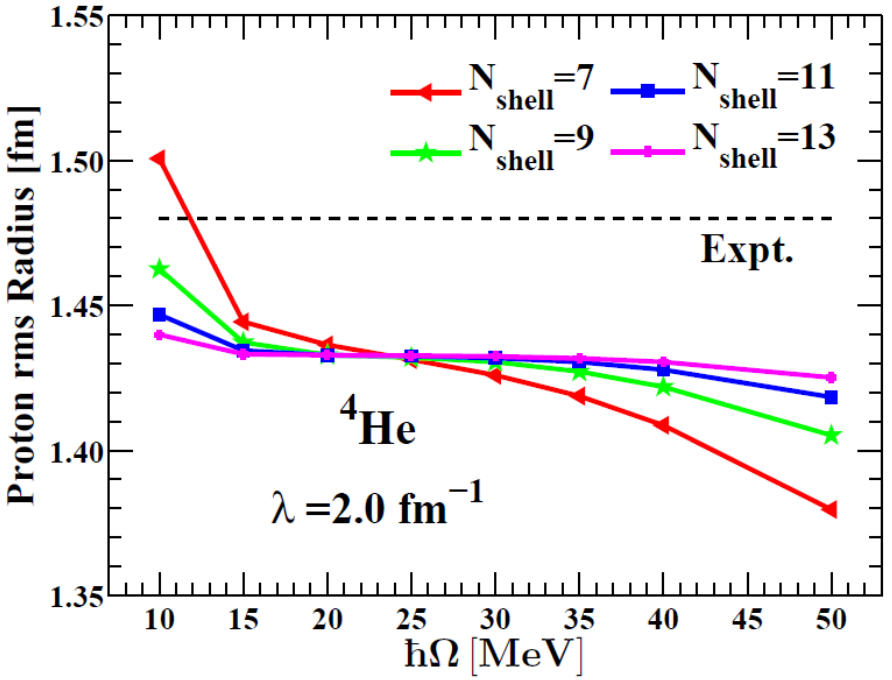


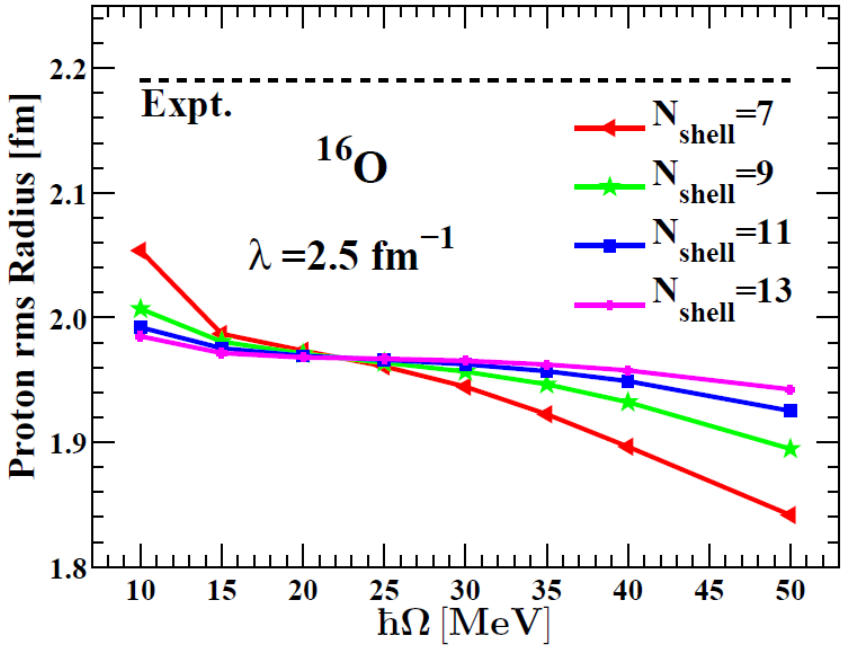
Our MBPT: N^{3}LO+SRG without 3NF



^{16}O

Our MBPT calculations with N^{3}LO+SRG: convergence in radius





HF-MBPT calculations for ^{4}He with N^{3}LO-SRG, N_{shell}=13, hΩ=35 MeV

Binding energy

	SRG flow parameter λ (fm^{-1})			
	1.5	2.0	2.5	3.0
Expt. [60]	-28.296	-28.296	-28.296	-28.296
NCSM [61]	-28.20	-28.41	-27.43	-26.80
SHF	-25.754	-21.864	-15.854	-10.278
PT2	-1.788	-5.088	-9.652	-13.783
PT3	-0.391	-0.899	-1.523	-1.953
SHF+PT2+PT3	-27.933	-27.850	-27.029	-26.013

r_p(NCSM)=1.418 fm with N_{max}=10

Point-proton rms radius

	SRG flow parameter λ (fm^{-1})			
	1.5	2.0	2.5	3.0
Expt.	1.477	1.477	1.477	1.477
SHF	1.677	1.652	1.714	1.816
PT2	0.007	0.001	-0.021	-0.065
$\Delta r_{\text{c.m.}}$	-0.226	-0.222	-0.227	-0.235
SHF+PT2+$\Delta r_{\text{c.m.}}$	1.458	1.431	1.466	1.516

R. Roth *et al*. (2006) PRC 73, 044312

MBPT, but AV18 and UCOM

Corrections to 3rd order in energy, 2nd order in radius

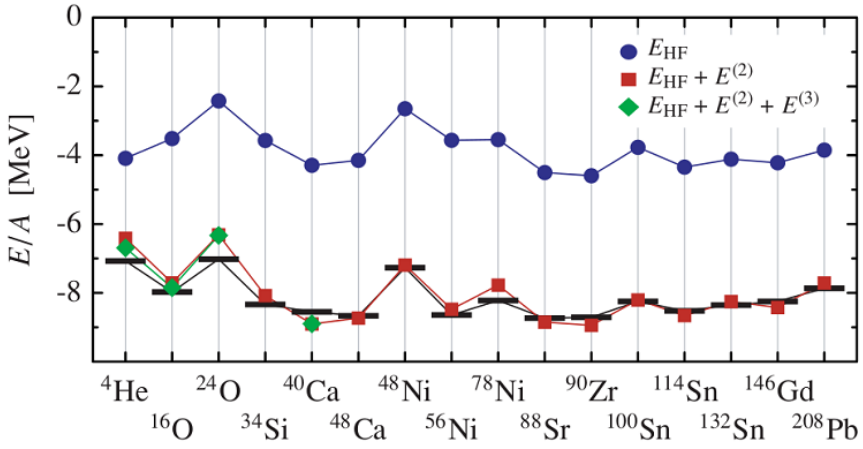


FIG. 5. (Color online) Ground-state energies for selected closed-shell nuclei in HF approximation and with added second- and third-order MBPT corrections. The correlated AV18 potential with $I_\vartheta = 0.09\,\mathrm{fm}^3$ was used. The bars indicate the experimental binding energies [31].

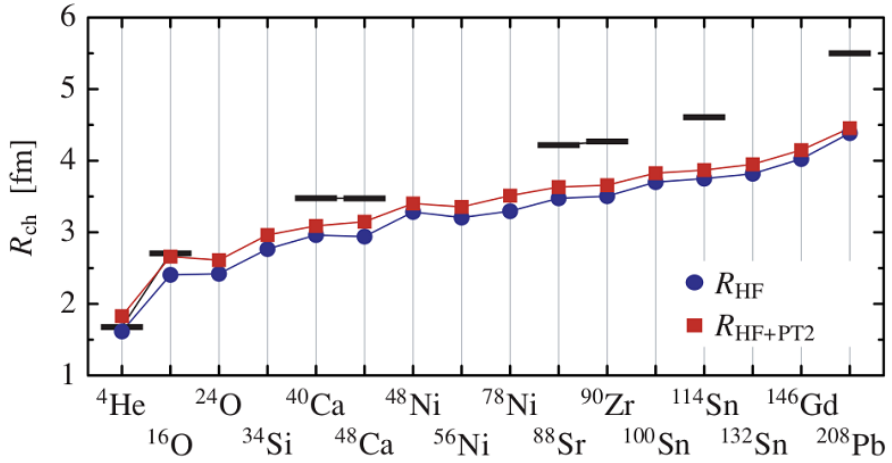


FIG. 8. (Color online) Charge radii for selected closed-shell nuclei in the HF approximation and with added second-order MBPT corrections. The correlated AV18 potential with $I_\vartheta = 0.09\,\mathrm{fm}^3$ was used. The bars indicate experimental charge radii [32].

A. Tichai, J. Langhammer, S. Binder, R. Roth, PLB 756 (2016) 283 (in March)

MBPT, N^{3}LO(NN)+N^{2}LO(NNN), SRG

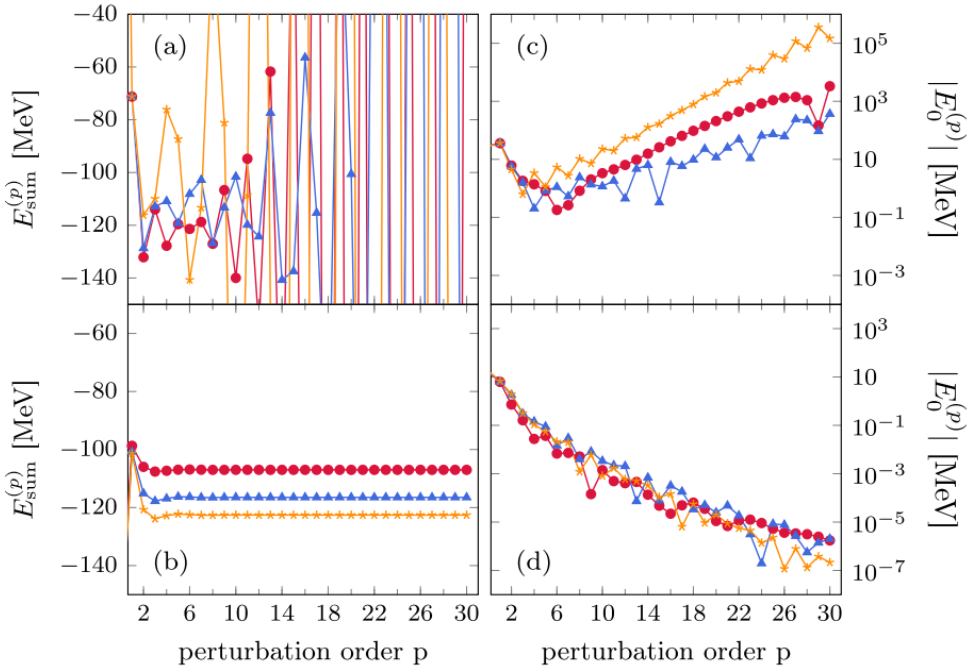


Fig. 1. Partial sums for the ground-state energy of ^{16}O in the HO basis (a) and the HF basis (b) for the NN+3N-full interaction with $\alpha = 0.08\,\mathrm{fm}^4$ and model-space truncation parameters $N_{\max} = 2$ (●), 4 (▲), and 6 (★). The corresponding energy corrections for each order are displayed in panels (c) and (d), respectively. All calculations are performed at frequency $\hbar\Omega = 24\,\mathrm{MeV}$.

MBPT in HO basis

divergent

MBPT in HF basis

well convergent

Conclusions

1) ***Ab initio*** **MBPT calculations of nuclear structures.**
2) **Hartree-Fock provides a good basis to get the MBPT calculation converged.**
3) **It seems that realistic nuclear forces give smaller radii of nuclei compared with data, not only in MBPT but also other ab initio methods.**
4) **3NFs should be required for calculations of heavy nuclei.**

Southern Center for Nuclear-Science Theory (SCNT)

- Located in Huizhou city, Guangdong Province (HIAF is there）
- Hosted by Institute of Modern Physics, Chinese Academy of Sciences

Director: Bingsong Zou (ITP)

Deputy Director: Jujun Xie (IMP)

1. Nuclear structure and reactions (Furong Xu, PKU)
2. Hadron spectroscopy (Fengkun Guo, ITP）
3. Hadron structure (Bowen Xiao, CUHK-Shenzhen)
4. EIC theory （Yuxiang Zhao, IMP)

Best wishes to Prof. James Vary

From Furong and Junchen' groups at PKU (June 5, 2023)