北京大学

Peking University

Furong Xu

B.S. Hu, W.G. Jiang, W.J. Chen (Peking University)

James Vary (Iowa State University)

Ab-initio calculations of nuclear structure with MBPT

Nordita Program on “Computational Challenges in Nuclear and Many-Body Physics”

AlbaNova, Stockholm, Sept. 17, 2014

Outline

I. Introduction

What is *ab-initio* ?   Is *ab-initio* enough?

II. Many-Body Perturbation Theory (MBPT) starting from realistic *NN* interactions (e.g., N3LO, JISP16).

preliminary

III. Summary

I. Introduction

What is *ab-initio* calculation?

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

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

1) Realistic nuclear force !

Reproduce experimental two-body *NN* scattering phase shifts .

2) A "good enough" theoretical approach to solve the Hamiltonian and all the symmetries should be preserved!

Realistic nuclear forces:

Chiral EFT (N^3LO), CD Bonn, AV18, JISP16 (bare) …

Renormalization

G-Matrix, UCOM, $V_{low\text{-}k}$, Okubo-Lee-Suzuki (OLS), SRG

ab-initio methods

In coordinate space: **Greens Function Monte Carlo (GFMC)**

In basis space:

No Core Shell Model (NCSM)

No Core Full Configurations (NCFC)

Coupled Cluster (CC)

Many-Body Perturbation Theory (MBPT)

Lattice Nuclear Chiral EFT

. . .

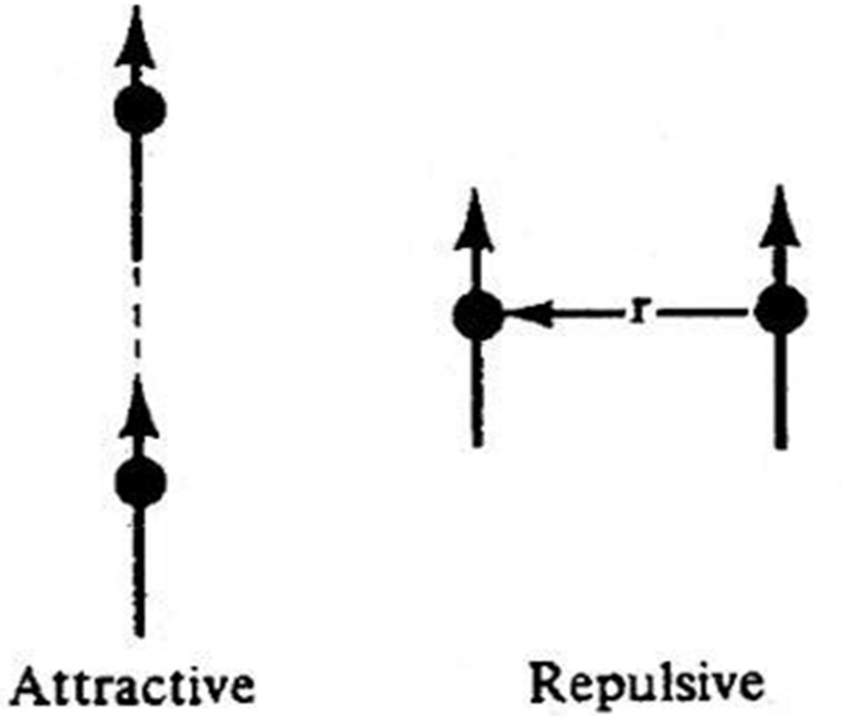
Phenomenological Nuclear Force

In a simple form

$$V = V_c + V_{LS}(\mathbf{L}\cdot\mathbf{S}) + V_T S_{12},$$

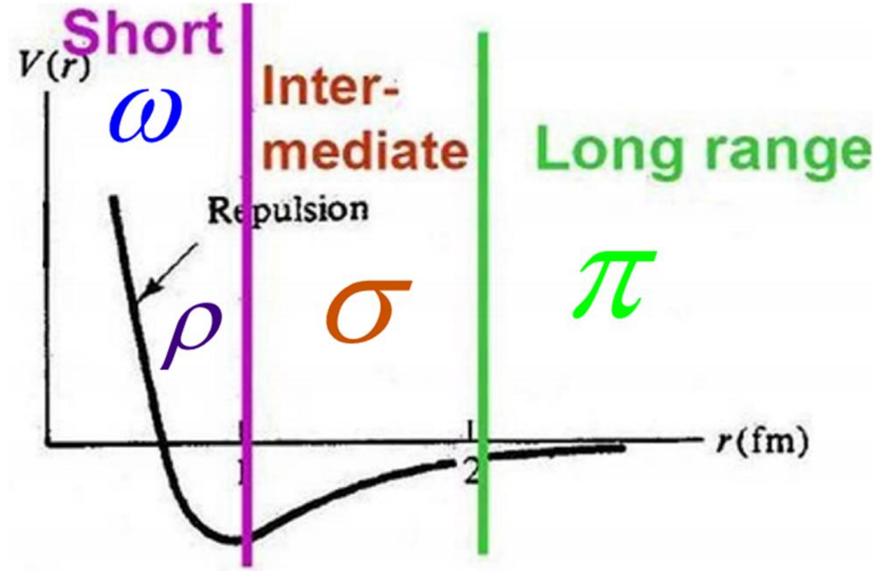
$$S_{12} = \frac{3}{r^2}(\sigma_1\cdot\mathbf{r})(\sigma_2\cdot\mathbf{r}) - \sigma_1\cdot\sigma_2,$$

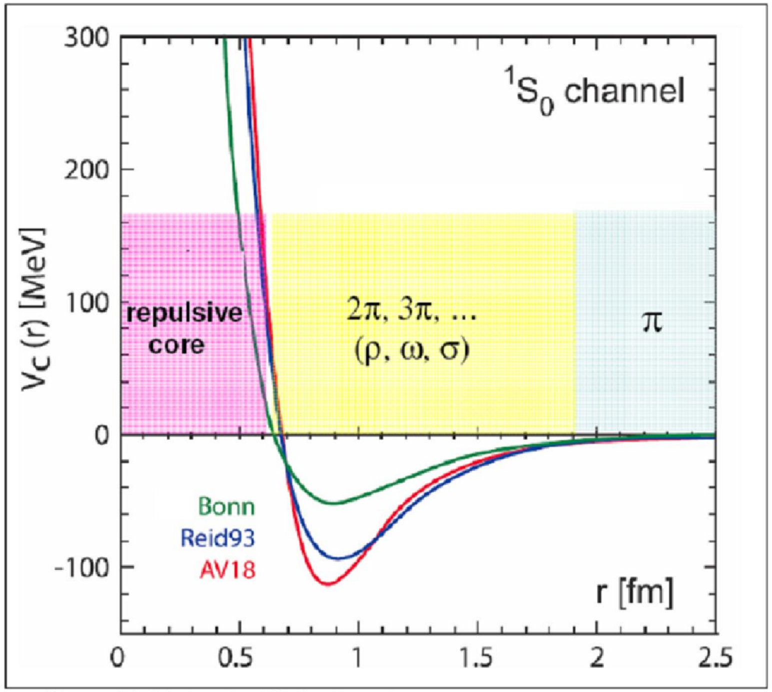
Tensor force



Nuclear force in meson picture

$$V_{\rm OBEP} = \sum_{\alpha=\pi,\sigma,\rho,\omega,\eta,a_0,\ldots} V_\alpha$$

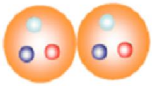




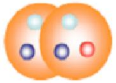
From T. Hatsuda (Oslo 2008)

One-pion exchange
by Yukawa (1935)

Multi-pions
by Taketani (1951)



Repulsive core
by Jastrow (1951)



Bonn *NN* potential

- **70's-80's, University of Bonn.**
- **CD Bonn is a charge-dependent one-boson-exchange *NN* potential.**
- **All mesons with masses below nucleon mass are included (π, ρ, ω, σ)**
- **Fit about 6000 data (proton-proton, neutron-proton scattering phase shifts) and deuteron binding energy.**

NO *3NF*

- **38 parameters**

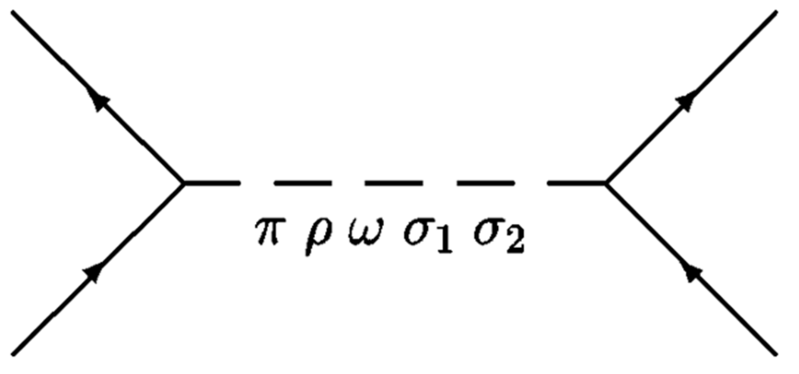


FIG. 1. One-boson exchange Feynman diagrams that define the CD-Bonn *NN* potential.

R. Machleidt, PRC 63, 024001 (2001)

Chiral EFT （N^2LO, N^3LO…)

From QCD to nuclear physics via chiral EFT

- QCD at low energy is strong.

Perturbation is inapplicable !

- Quarks and gluons are confined into colorless hadrons.
- Nuclear forces are residual color forces (similar to van der Waals forces)

From R. Machleidt, “Nuclear Forces - Lecture 4: NF from EFT (CNSSS13)”

QCD=quarks + gluons (symmetries: spin, isosipn, parity, chiral symmetry broken spontaneously)

Weinberg (1990’s)

Chiral EFT=nucleons+pions (symmetries: spin, isosipn, parity, chiral symmetry broken spontaneously)

At low energy, the effective degrees of freedom are nucleon and pion, rather than quark and gluon!

Starting point is an effective chiral πN Lagrangian:

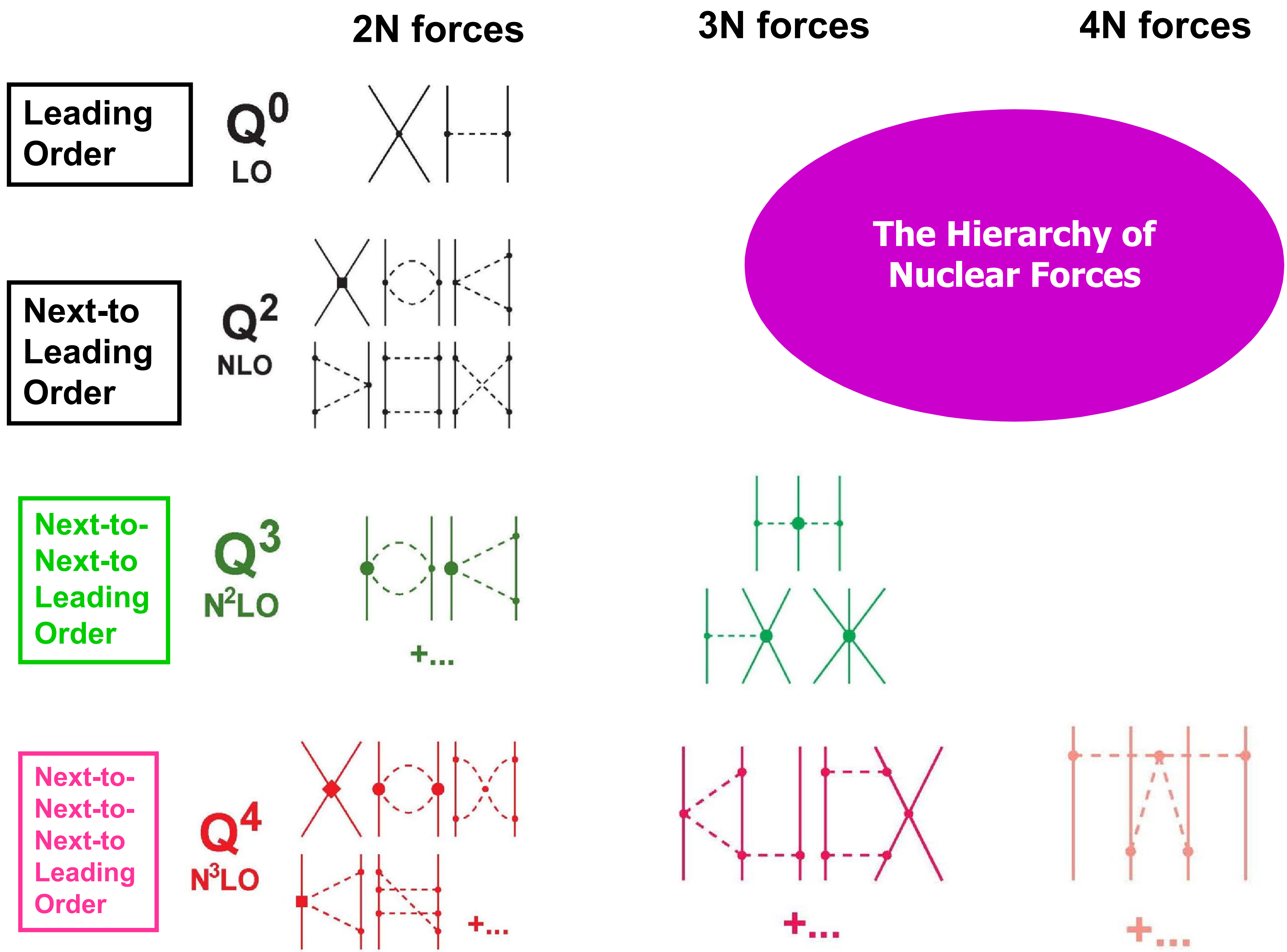
$$L_{\pi N} = L_{\pi N}^{(1)} + L_{\pi N}^{(2)} + L_{\pi N}^{(3)} + \ldots$$

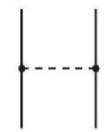
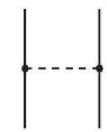
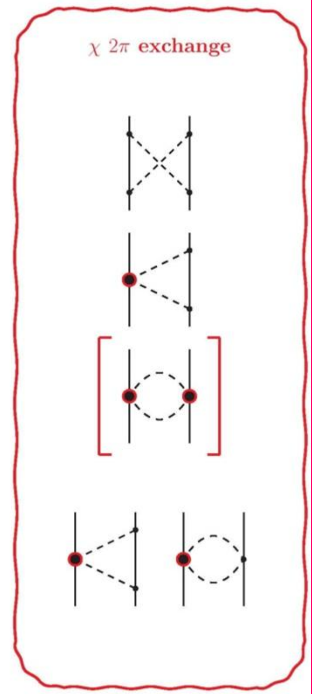
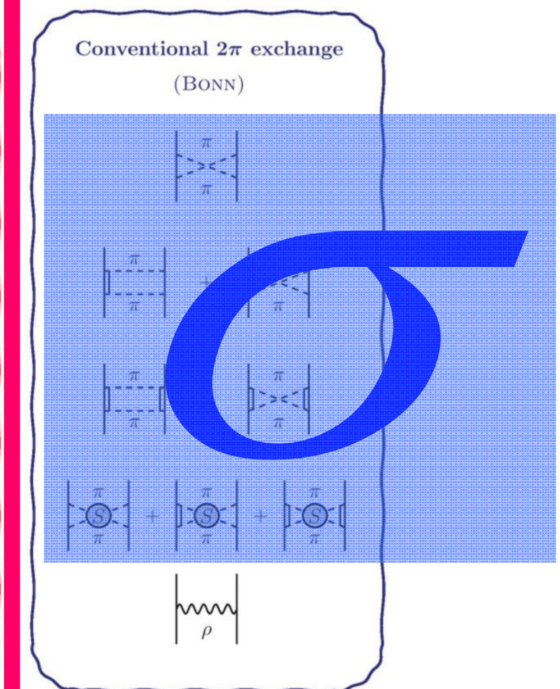
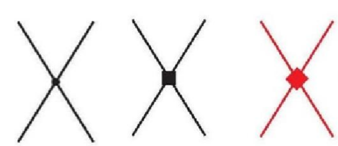
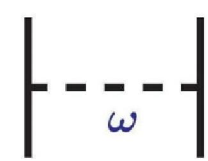
Obeys QCD symmetries (spin, isospin, chiral symmetry breaking)

To develop a low-momentum expansion for chiral EFT (low energy) (Chiral perturbation theory, power counting).

Advantages:

1. **Gives hierarchy of nuclear force**
2. **Naturally generates 3NF, 4NF…**
3. **Provides possibilities to analyze the uncertainties of each hierarchy.**

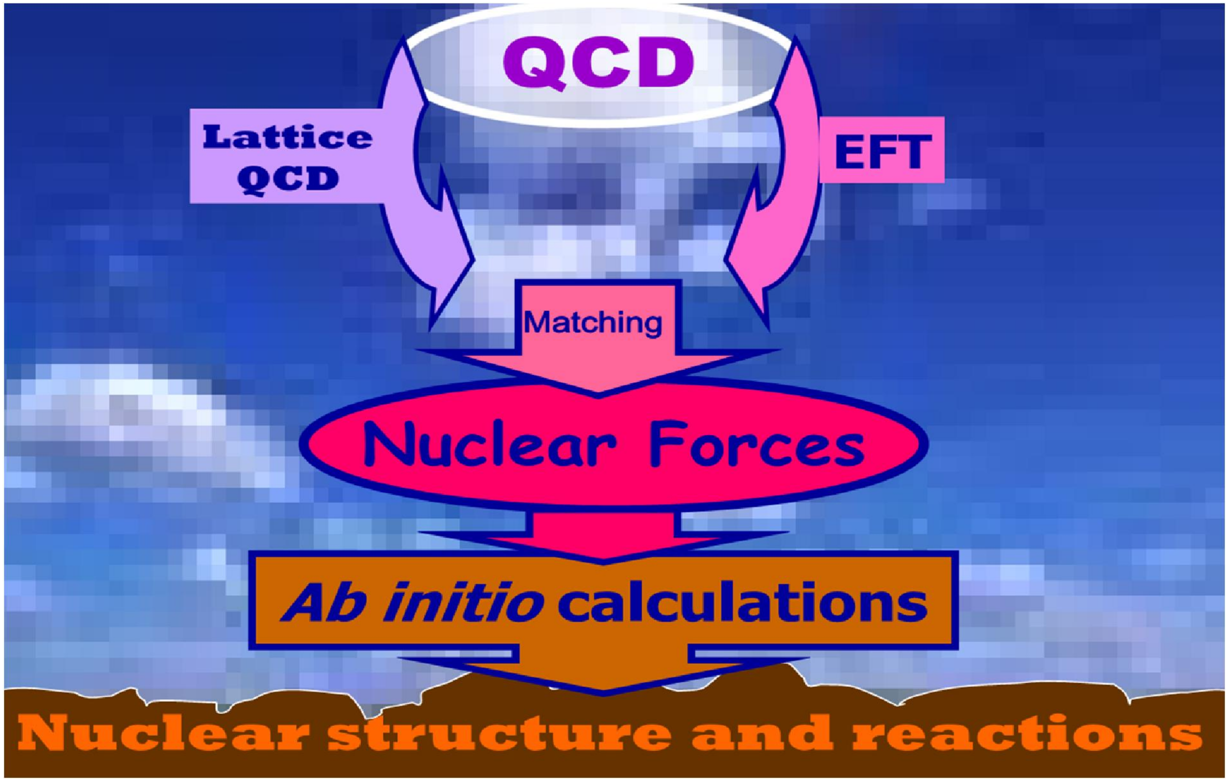

2N forces
3N forces
4N forces
The Hierarchy of Nuclear Forces
Leading Order
Q^0
LO
Next-to Leading Order
Q^2
NLO
Next-to-Next-to Leading Order
Q^3
N^2LO
+...
Next-to-Next-to-Next-to Leading Order
Q^4
N^3LO
+...
+...
+...

	ChPT	Conventional meson theory
OPE		
TPE		
Short range		

Chiral perturbation theory (ChPT) is an expansion in terms of small momenta.

Meson model is an expansion in terms of ranges (masses).

After 80 years of struggle, we have now a proper theory (ChPT) for nuclear force that is based upon the fundamental theory of strong interactions, QCD.



Our *ab-initio* calculations

Many-Body Perturbation Theory (MBPT) with realistic *NN* force.

Hatree-Fock state is chosen as a reference state.

MBPT:

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

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

$$H_0 = \sum_{l_1 l_2} \left(\sum_i \langle l_1 i | T + V | l_2 i \rangle \right) a^\dagger_{l_1} a_{l_2} \quad ; \quad H_0 = \sum_{l_1 l_2} \left(\langle l_1 | T | l_2 \rangle + \sum_i \langle l_1 i | V + Tcor | l_2 i \rangle \right) a^\dagger_{l_1} a_{l_2}$$

The exact solutions of the A-nucleon system are,

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

The zero-order part is,

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

Perturbation (MBPT)

For the ground state:

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

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

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

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

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

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

HF energy

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

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

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

$$\Psi_0 = \Phi_0 + \Psi_0^{(1)} + \Psi_0^{(2)} + \dots$$

HF

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

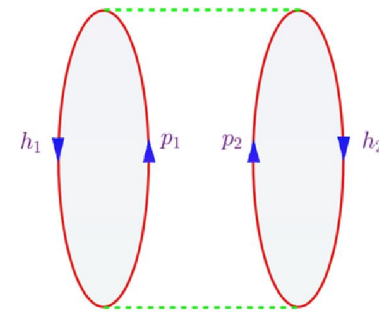
$$\Psi_0^{(2)} = \hat{R}_0 (\hat{V} - E_0^{(1)}) \hat{R}_0 \hat{V} | \Phi_0 \rangle$$

Anti-Symmetrized Goldstone (ASG) diagram expansion

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

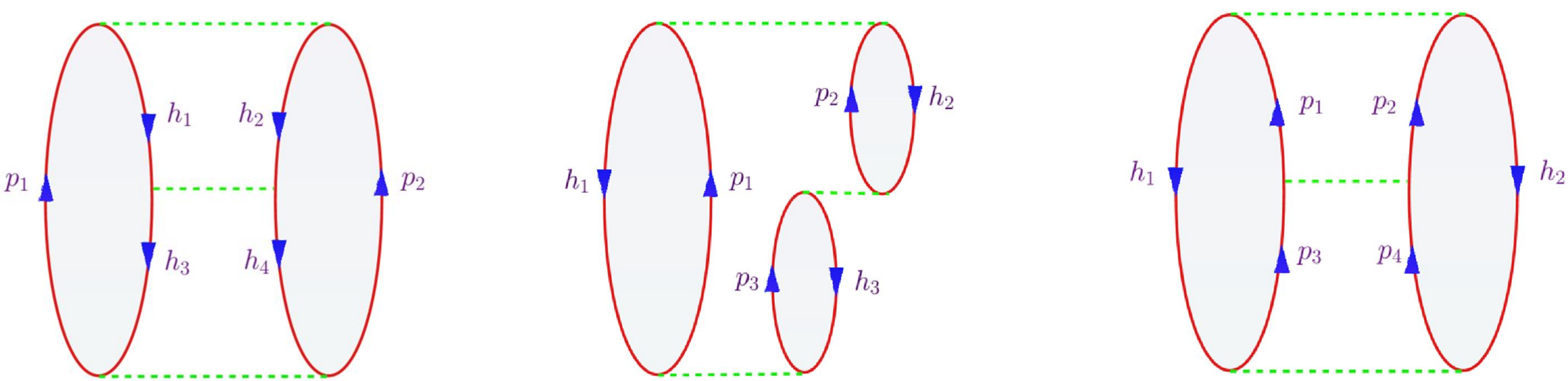
HF energy

$E^{(2)}$



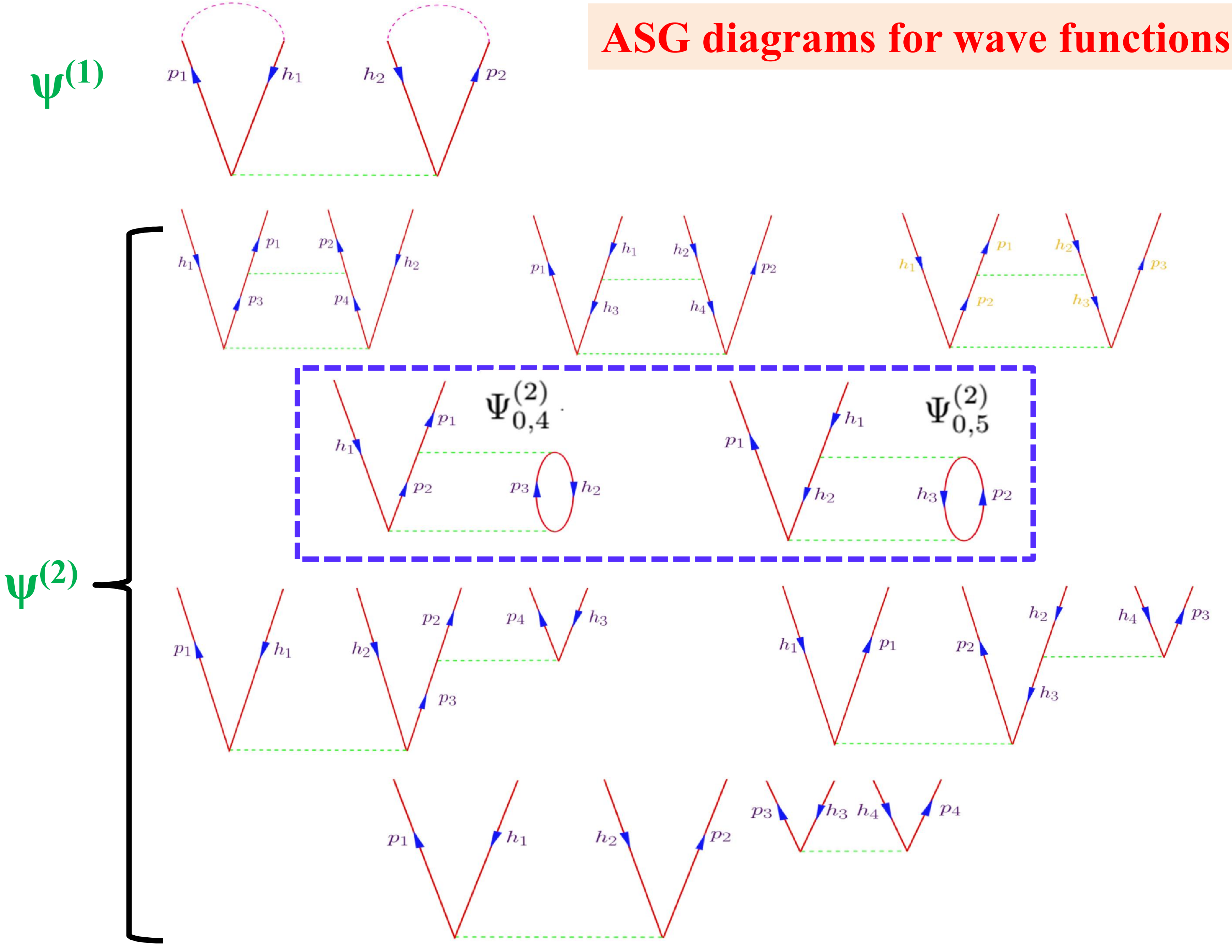
$$\frac{1}{4}\sum_{h_1,h_2<\varepsilon_F}\sum_{p_1,p_2>\varepsilon_F}\frac{|\langle p_1p_2|\hat{\mathrm{H}}_{int}|h_1h_2\rangle|^2}{\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2}}$$

$E^{(3)}$



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



Density

$$\rho(\vec{r}) = \sum_{k=1}^{A} \delta^3\left(\vec{r} - \vec{r}_k\right) = \sum_{k=1}^{A} \frac{\delta\left(r - r_k\right)}{r^2} \sum_{lm} Y^*_{lm}(\hat{\mathrm{r}}_k) Y_{lm}(\hat{\mathrm{r}})$$

In second quantization with HO basis

$$\rho(\vec{r}) = \sum_{K} \sum_{n_1,l_1,j_1} \sum_{n_2,l_2,j_2} \sum_{m_j} R_{n_1,l_1}(r) R_{n_2,l_2}(r) \frac{-Y^*_{K0}(\hat{\mathrm{r}})}{\hat{\mathrm{K}}} \left\langle l_1 \frac{1}{2} j_1 \left|\left| Y_K \right|\right| l_2 \frac{1}{2} j_2 \right\rangle$$
$$(-1)^{j_2+m_j} \left\langle j_1 m_j j_2 - m_j | K0 \right\rangle a^{\dagger}_{n_1,l_1,j_1,m_j} a_{n_2,l_2,j_2,m_j}$$

$$\left\langle l_1 \frac{1}{2} j_1 \left|\left| Y_K \right|\right| l_2 \frac{1}{2} j_2 \right\rangle = \frac{1}{\sqrt{4\pi}} \hat{\mathrm{j}}_1 \hat{\mathrm{j}}_2 \hat{\mathrm{l}}_1 \hat{\mathrm{l}}_2 (-1)^{j_1+\frac{1}{2}} \left\langle l_1 0 l_2 0 | K0 \right\rangle \begin{Bmatrix} j_1 & j_2 & K \\ l_2 & l_1 & \frac{1}{2} \end{Bmatrix}$$

For spherically symmetric system(K=0), we can get a more simple form,

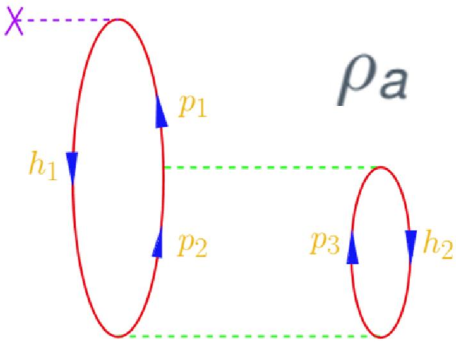
$$\rho(\vec{r}) = \sum_{n_1, n_2} \sum_{l, j, m_j} \left[\frac{R_{n_1, l}(r) R_{n_2, l}(r)}{4\pi} \right] a^{\dagger}_{n_1, l, j, m_j} a_{n_2, l, j, m_j}$$

For the ground state, the 2nd order correction to density is only from the 4th and 5th ASG diagrams of the 2nd-order wave function, others belong to higher-order corrections, i.e.,

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

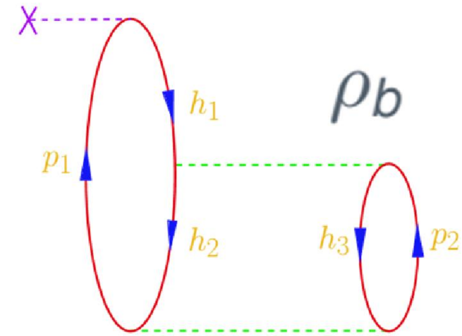
$$\rho(\vec{r}) = \langle\Phi_0|\rho(\vec{r})|\Phi_0\rangle + \underbrace{\langle\Phi_0|\rho(\vec{r})|\Phi_0\rangle\langle\Psi_0^{(1)}|\Psi_0^{(1)}\rangle}_{} + \underbrace{2\rho_a + 2\rho_b + \rho_{c1} + \rho_{c2}}_{} + \ldots$$

HF **1st order** **2nd order**



ρ_a

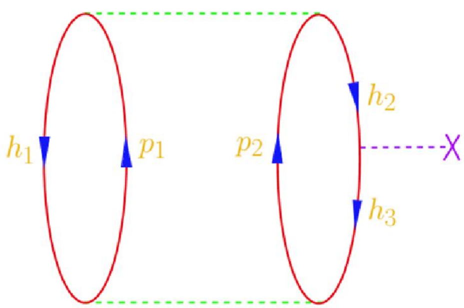
$$\frac{1}{2}\sum_{h_1,h_2<\varepsilon_F}\sum_{p_1,p_2,p_3>\varepsilon_F}\frac{\langle h_1h_2|\hat{H}|p_2p_3\rangle\langle p_2p_3|\hat{H}|p_1h_2\rangle\langle h_1|\rho|p_1\rangle}{(\varepsilon_{h_1}-\varepsilon_{p_1})(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_2}-\varepsilon_{p_3})}$$



ρ_b

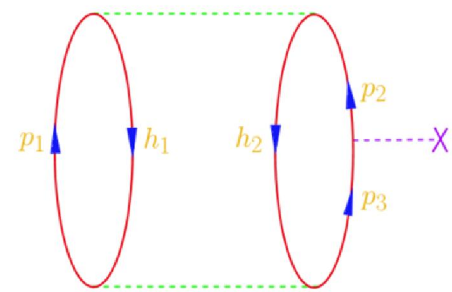
$$-\frac{1}{2}\sum_{h_1,h_2,h_3<\varepsilon_F}\sum_{p_1,p_2>\varepsilon_F}\frac{\langle p_1p_2|\hat{H}|h_2h_3\rangle\langle h_2h_3|\hat{H}|h_1p_2\rangle\langle h_1|\rho|p_1\rangle}{(\varepsilon_{h_1}-\varepsilon_{p_1})(\varepsilon_{h_2}+\varepsilon_{h_3}-\varepsilon_{p_1}-\varepsilon_{p_2})}$$

ρ_{c1}



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

ρ_{c2}



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

Point-particle distribution radii:

$$\langle {r_{pp}}^2 \rangle = \frac{\int r^2 \rho_p(\vec{r}) d^3r}{\int \rho_p(\vec{r}) d^3r} \qquad \langle {r_{nn}}^2 \rangle = \frac{\int r^2 \rho_n(\vec{r}) d^3r}{\int \rho_n(\vec{r}) d^3r}$$

Charge radius:

$$\langle {r_{ch}}^2 \rangle = \langle {r_{pp}}^2 \rangle + {\langle R \rangle_p}^2 \qquad (\langle R \rangle_p = 0.8 fm)$$

NCSM with N^{3}LO+SRG
S.K. Bogner *et al.*, arXiv0708.3754v2 (2007)

Both calculations without 3NF

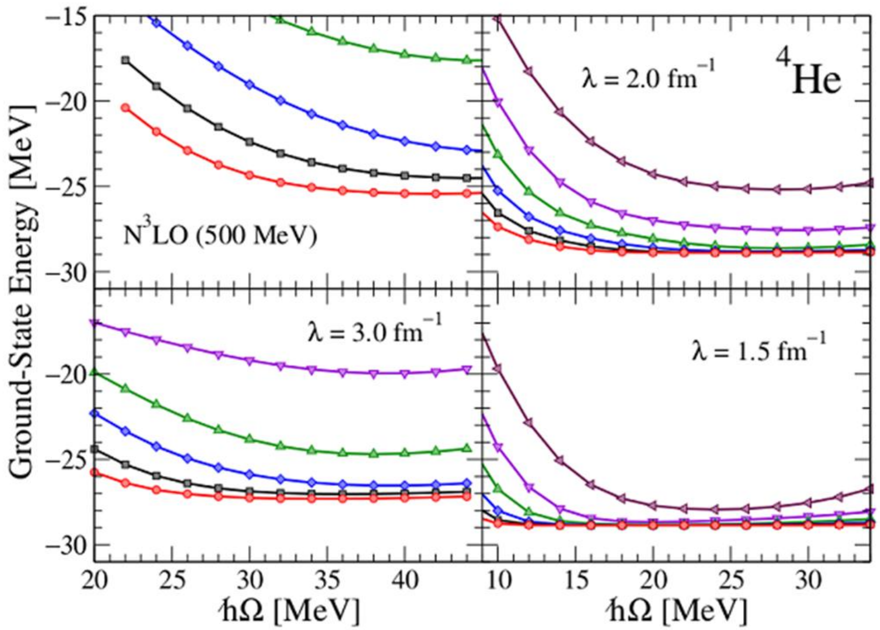
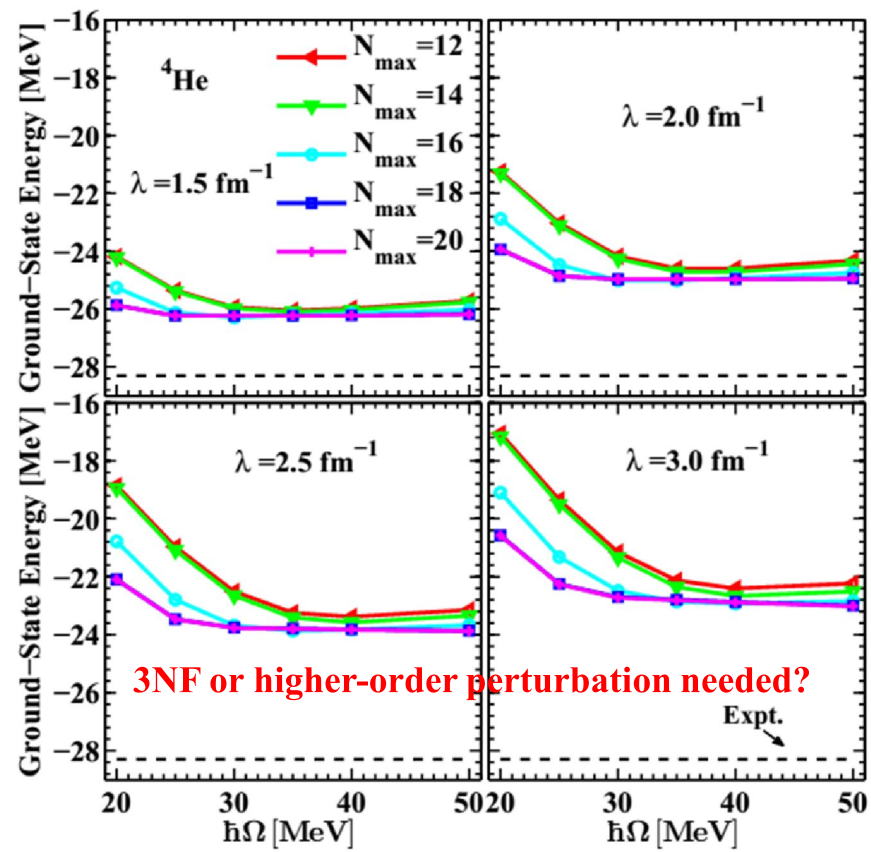


Fig. 3. Ground-state energy of ^{4}He as a function of $\hbar\Omega$ at four different values of λ (∞, 3, 2, 1.5 fm^{-1}). The initial potential is the 500 MeV N^{3}LO NN-only potential from Ref. [13]. The legend from Fig. 1 applies here.

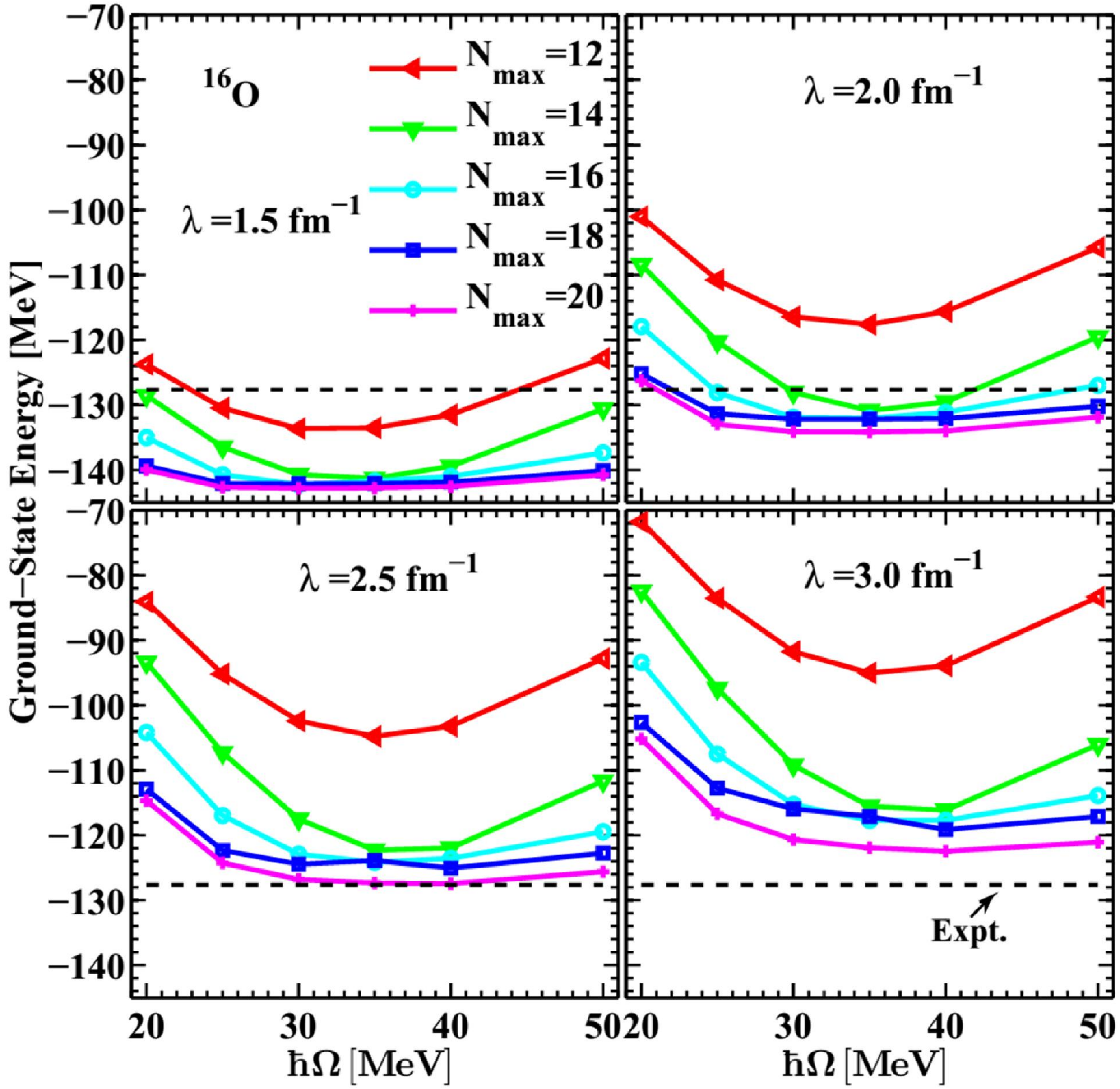
^{4}He

Our MBPT with N^{3}LO+SRG



Our MBPT calculations with N^{3}LO+SRG

^{16}O



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

AV18, UCOM, corrections to 3rd order in energy calculations,
2nd order in radius calculations

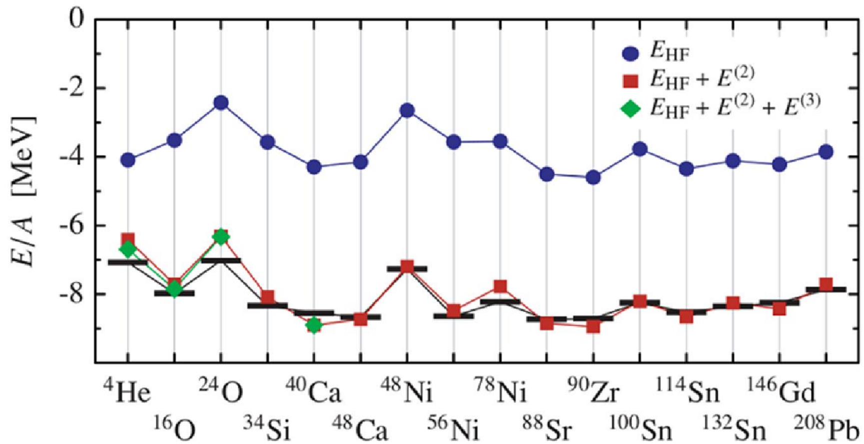


FIG. 5. (Color online) Ground-state energies for selected closed-shell nuclei in HF approximation and with added second- and third-order MBPT corrections. The correlated AV18 potential with $I_\vartheta = 0.09\,\text{fm}^3$ was used. The bars indicate the experimental binding energies [31].

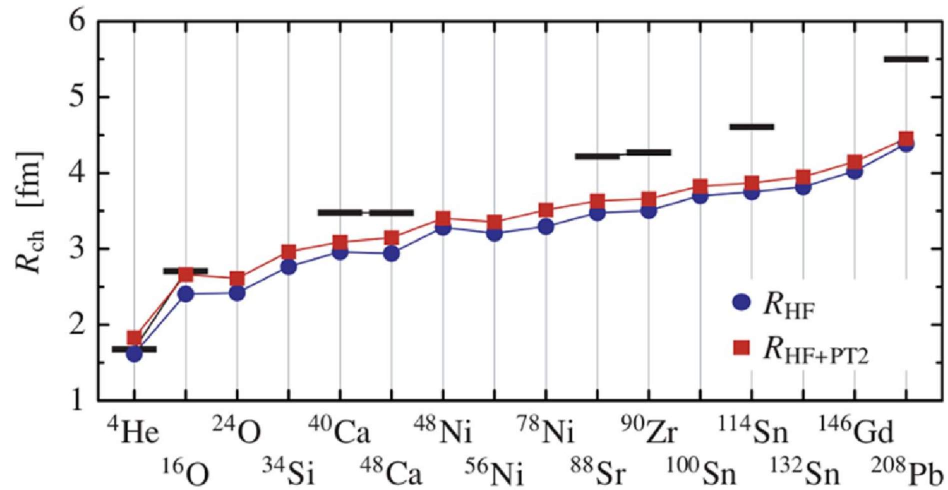


FIG. 8. (Color online) Charge radii for selected closed-shell nuclei in the HF approximation and with added second-order MBPT corrections. The correlated AV18 potential with $I_\vartheta = 0.09\,\text{fm}^3$ was used. The bars indicate experimental charge radii [32].

Our calculations and compared with data

N^3LO[4] with SRG for ^4He ($N_{max} = 20$, $\hbar\Omega = 35MeV$ and $\lambda = 2.0fm^{-1}$)

Observable	p-rms(fm)	$E_{g.s.}$(MeV)
Expreiment	1.450	-28.296
HF	1.8380	-9.1657
Second-order correction	-0.0622	-13.7430
Third-order correction	–	-2.0587
C.M. motion correction	-0.0854	–
MBPT	1.6903	-24.9675

^{4}He

Bare JISP16[10–12] for ^4He ($N_{max} = 14$ and $\hbar\Omega = 10MeV$)

Observable	p-rms(fm)	$E_{g.s.}$(MeV)
Expreiment	1.450	-28.296
NCSH	–	-28.297
HF	1.5714	-22.4143
Second-order correction	0.0160	-4.3126
Third-order correction	–	-0.8031
C.M. motion correction	-0.3695	–
MBPT	1.2179	-27.5301

$N^3LO[4]$ with SRG for ^{16}O ($N_{max} = 20$, $\hbar\Omega = 35MeV$ and $\lambda = 2.0fm^{-1}$)

Observable	p-rms(fm)	$E_{g.s.}$(MeV)
Expreiment	2.58	-127.62
HF	2.3874	-36.6856
Second-order correction	-0.0504	-90.0375
Third-order correction	–	-7.4287
C.M. motion correction	-0.0158	–
MBPT	2.3211	-134.1518

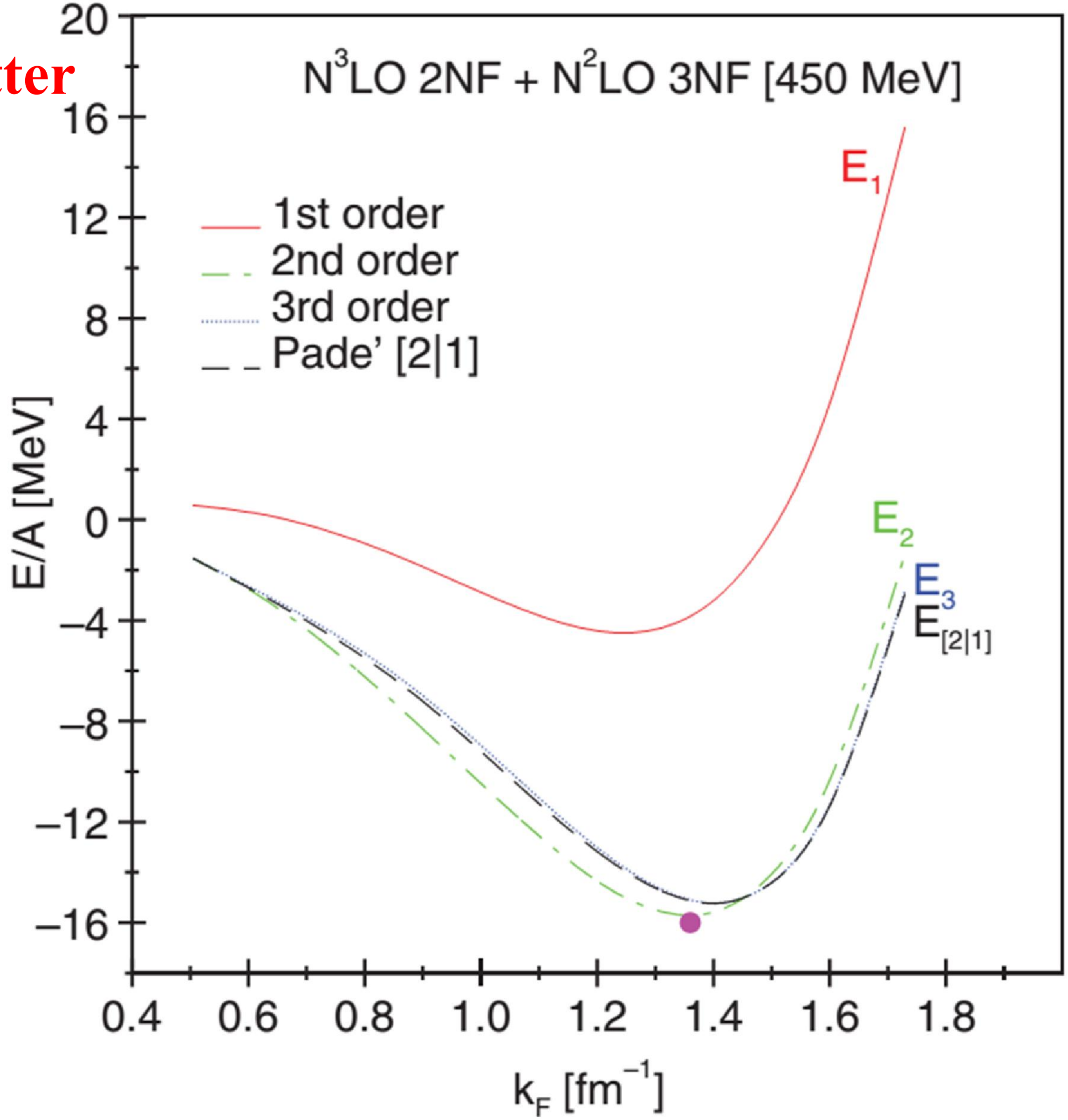
^{16}O

Bare JISP16[10–12] for ^{16}O ($N_{max} = 10$ and $\hbar\Omega = 15MeV$)

Observable	p-rms(fm)	$E_{g.s.}$(MeV)
Expreiment	2.58	-127.62
NCSH($N_{max} = 6$)	–	-126.2
HF	1.8693	-70.8461
Second-order correction	0.0618	-51.7671
Third-order correction	–	-3.2451
C.M. motion correction	-0.0453	–
MBPT	1.8858	-125.8583

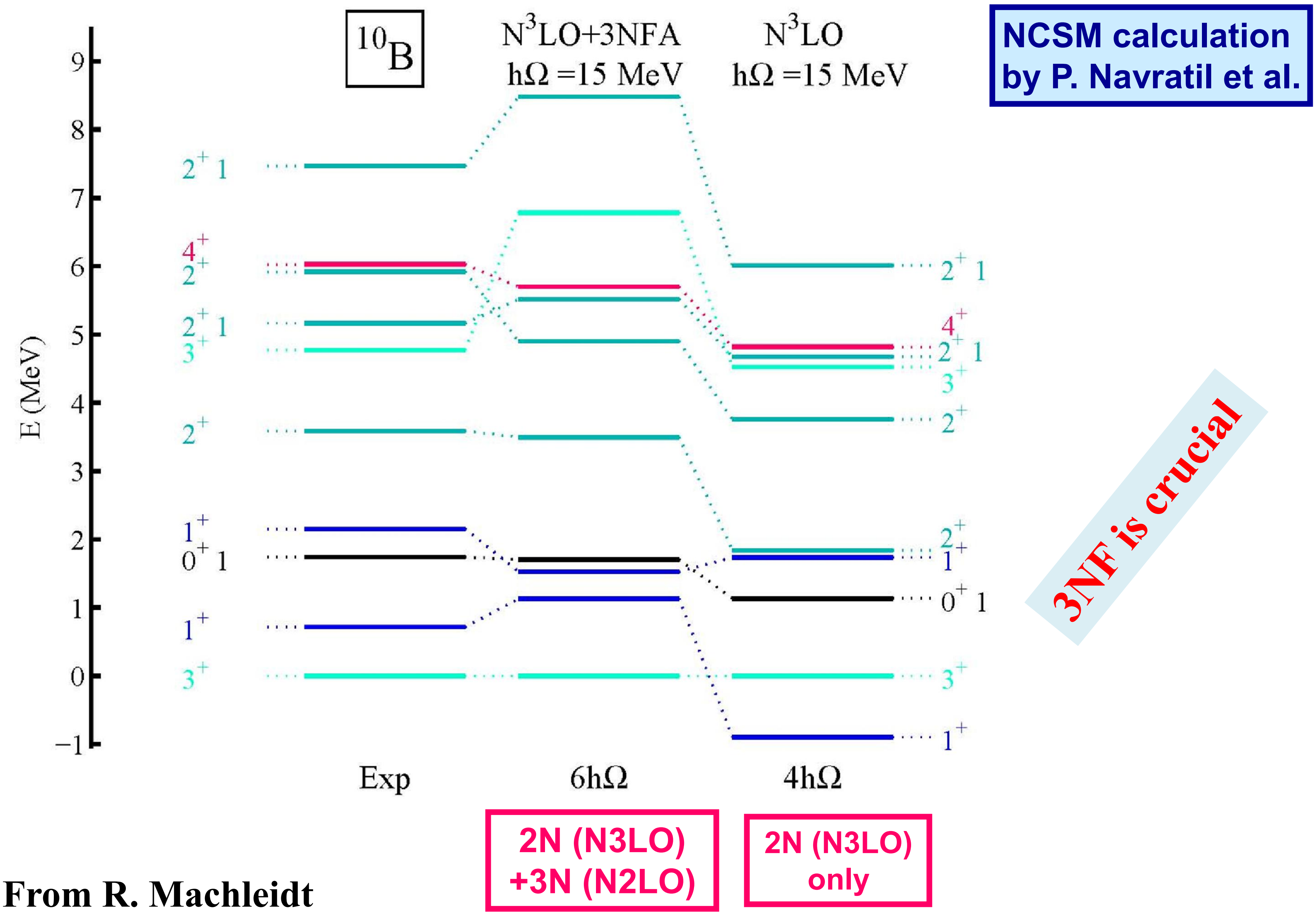
JISP 16 *vs* N3LO: better in energy, worse in radius, in ^{4}He and ^{16}O

MBPT calculations for symmetric nuclear matter



L. Coraggio *et al.*, PRC 89, 044321 (2014)

Calculating the properties of light nuclei using chiral 2N and 3N forces



From R. Machleidt

III. Summary

Ab-initio **MBPT calculations based on realistic interactions**

1. Why *ab-initio*?

i) To understand the nature of nuclear force;

ii) To develop theories or methods with less assumptions or approximations;

2. Why non *ab-initio*?

i) Calculations easier (simpler),

give chance to calculate most nuclei (heavier) in the nuclear chart

ii) May be quantitatively good

……

Thank you for your attention

Peking University Campus

Stockholm, Sept. 17, 2014