Recent progress in the unitary-model-operator approach

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Introduction

- ✦ One of the fundamental problems is to understand the nuclear structure and reactions based on underlying nuclear interaction.

Nuclear interaction

many-body problem

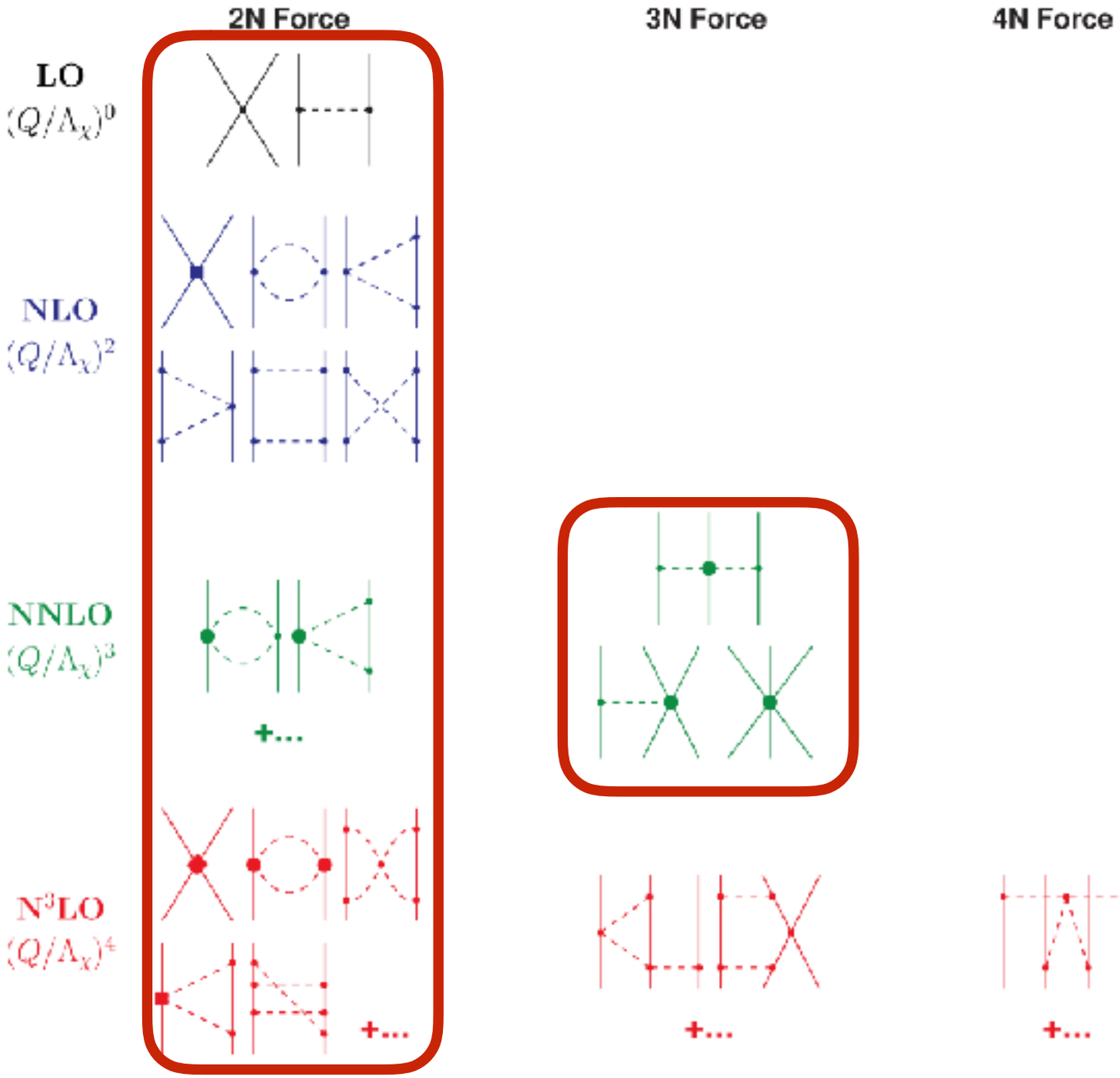
major issues

- ✦ Nuclear interaction : progress in chiral EFT
  - ★ High-precision NN force
  - ★ 3N force consistent with NN force
- ✦ Many-body problem : Ab initio calculation methods

Nuclear force from chiral EFT

✦ Chiral effective field theory

Weinberg, van Kolck, Kaiser, Epelbaum, Glöckle, Meißner, Entem, Machleidt, ⋯



SRG evolution - 1

- Bare nuclear interactions are too “hard” to be applied for usual many-body methods.

- We usually need the “soft” interactions that provides the rapid convergence with respect to the model-space size.

S. K. Bogner, R. J. Furnstahl, and R. J. Perry, PRC **75**, 061001 (2007).

$$\frac{dH(s)}{ds} = [\eta(s), H(s)] \qquad H(s) = U^{\dagger}(s) H U(s)$$

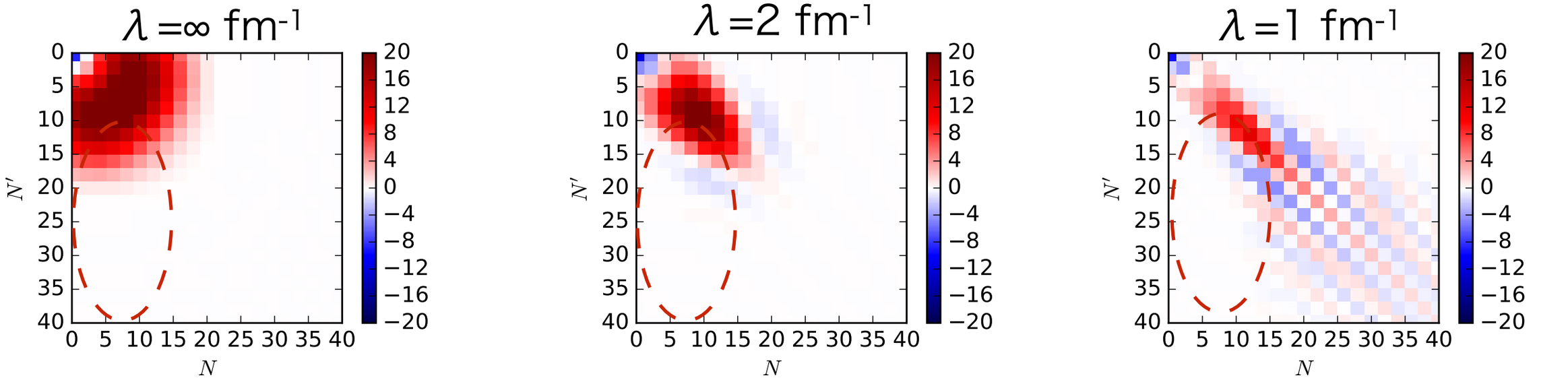
$$\frac{dU(s)}{ds} = -\eta(s) U(s)$$

s: resolution scale in unit of fm^4

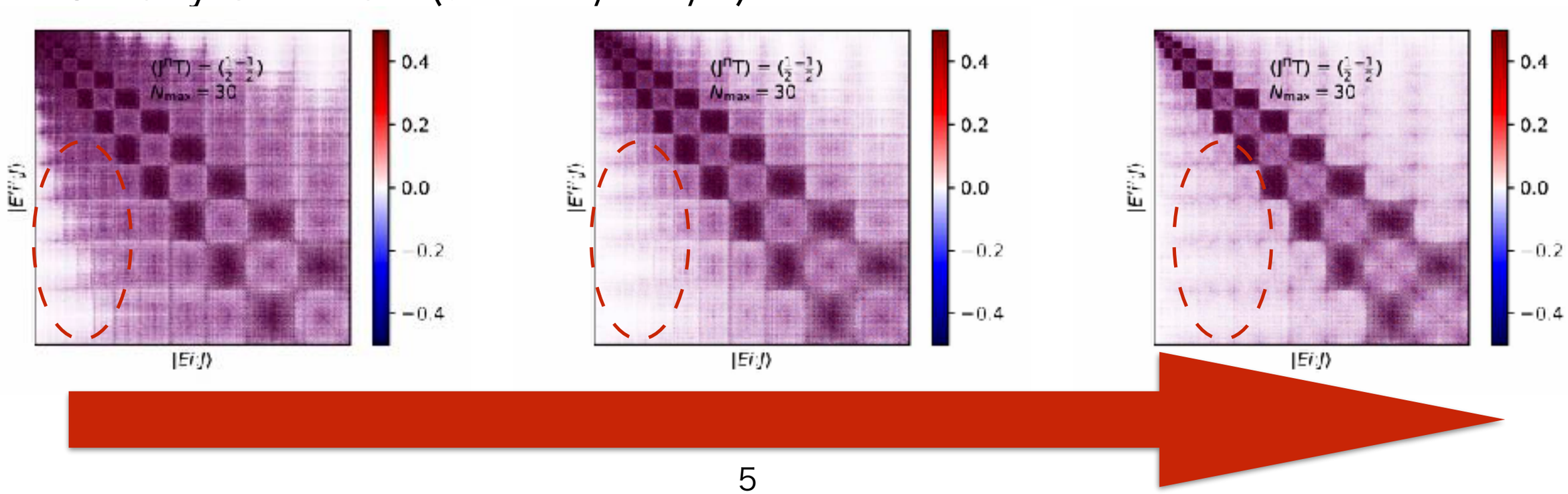
λ : momentum scale $s^{-1/4}$

SRG evolution - 2

- 2-body SRG flow ($^1S_0$ channel)



- 3-body SRG flow ($J^{\pi}T$ = 1/2+1/2)



Normal Ordering Approximation

R. Roth et al., PRL 109 (2012).
S. Binder et al., PRC 87 (2013).
…

- Explicit treatment of 3BF is difficult

$$V_{3N} = \frac{1}{36} \sum_{a_1 a_2 a_3 b_1 b_2 b_3} V^{a_1 a_2 a_3}_{b_1 b_2 b_3} A^{a_1 a_2 a_3}_{b_1 b_2 b_3}, \quad V^{a_1 a_2 a_3}_{b_1 b_2 b_3} = \langle a_1 a_2 a_3 | V_{3N} | b_1 b_2 b_3 \rangle, \quad A^{a_1 a_2 \cdots}_{b_1 b_2 \cdots} = c^\dagger_{a_1} c^\dagger_{a_2} \cdots c_{b_2} c_{b_1}$$

$A^{a_1 a_2 \cdots}_{b_1 b_2 \cdots} |0\rangle = 0$ |0> : nucleon vacuum

- Rearrangement of 3BF w.r.t the ref. state

$$V_{3N} = W + \sum_{a_1 b_1} W^{a_1}_{b_1} \widetilde{A}^{a_1}_{b_1} + \frac{1}{4} \sum_{a_1 a_2 b_1 b_2} W^{a_1 a_2}_{b_1 b_2} \widetilde{A}^{a_1 a_2}_{b_1 b_2} + \frac{1}{36} \sum_{a_1 a_2 a_3 b_1 b_2 b_3} W^{a_1 a_2 a_3}_{b_1 b_2 b_3} \widetilde{A}^{a_1 a_2 a_3}_{b_1 b_2 b_3}$$

Important ← less important

$\widetilde{A}^{a_1 a_2 \cdots}_{b_1 b_2 \cdots} |\Phi\rangle = 0$ |Φ>: reference state $\quad \widetilde{A}^{a_1 a_2 \cdots}_{b_1 b_2 \cdots} = A^{a_1 a_2 \cdots}_{b_1 b_2 \cdots} - (\text{all contracted terms})$

If the reference state is sufficiently close to the true ground state, the effect of the residual 3BF should be small. HF reference state is employed in practical applications.

Discard the residual 3BF term => NO2B approximation

Many-body methods

- ✦ Ab initio calculation methods related with this work
  - ✳ Few-body system (Faddeev equation, Faddeev-Yakubovsky equation, etc.)
  - ✳ Green's Function Monte Carlo
  - ✳ No-Core Shell Model
  - ✳ Nuclear Lattice Effective Field Theory
  - ✳ Coupled-Cluster Method
  - ✳ Self-Consistent Green's Function Method
  - ✳ In-Medium Similarity Renormalization Group Approach
  - ✳ Unitary-Model-Operator Approach (UMOA)
  - ✳ ⋯

Unitary-Model-Operator Approach (UMOA)

K. Suzuki and R. Okamoto, PTP **92**, 1045 (1994).
TM et al., PRC **96**, 054312 (2017).

- Many-body Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle$$

$$(U^\dagger H U)(U^\dagger|\Psi\rangle) = E(U^\dagger|\Psi\rangle)$$

$$\widetilde{H}|\Phi\rangle = E|\Phi\rangle$$

$$H = E_0 + \sum_i^A t_i + \sum_{i<j}^A v_{ij}$$

Uncorrelated single-Slater determinant

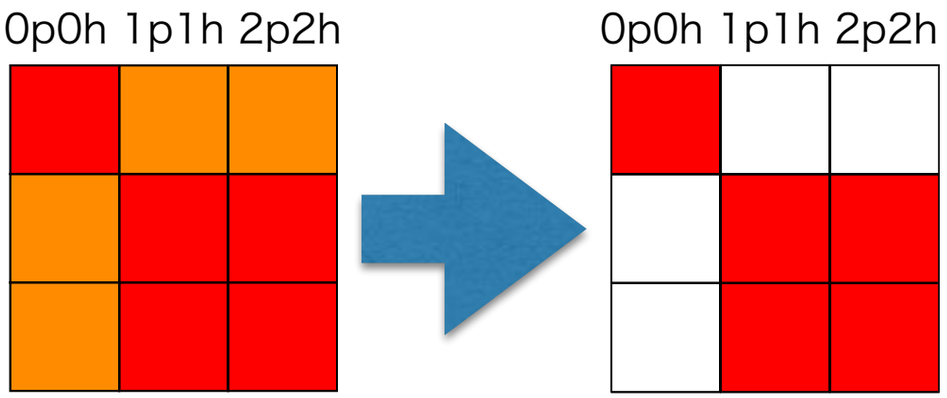
- Unitary operator U

$$U = e^{S^{(1)}} e^{S^{(2)}} \qquad S^{(1)} = \sum_i^A s_i, \quad S^{(2)} = \sum_{i<j}^A s_{ij}$$

- Cluster expansion

$$\widetilde{H} \approx E_0 + \widetilde{H}^{(1)} + \widetilde{H}^{(2)} + \left(\widetilde{H}^{(3)}\right)$$

perturbative treatment



Unitary-Model-Operator Approach (UMOA)

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- Cluster expansion

$$\widetilde{H} \approx E_0 + \widetilde{H}^{(1)} + \widetilde{H}^{(2)} + \widetilde{H}^{(3)}$$

$$\widetilde{H}^{(1)} = \sum_i \widetilde{h}_i;\ \widetilde{h}_i = e^{-s_i}(t_i + w_i)e^{s_i}$$

$$\widetilde{H}^{(2)} = \sum_{i<j} \widetilde{v}_{ij} - \sum_i \widetilde{w}_i$$

$$\widetilde{v}_{ij} = e^{-s_{ij}} e^{-(s_i+s_j)}(t_i + w_i + t_j + w_j + v_{ij})e^{s_i+s_j} e^{s_{ij}} - (\widetilde{h}_i + \widetilde{h}_j)$$

$$\widetilde{w}_i = e^{-s_i} w_i e^{s_i}$$

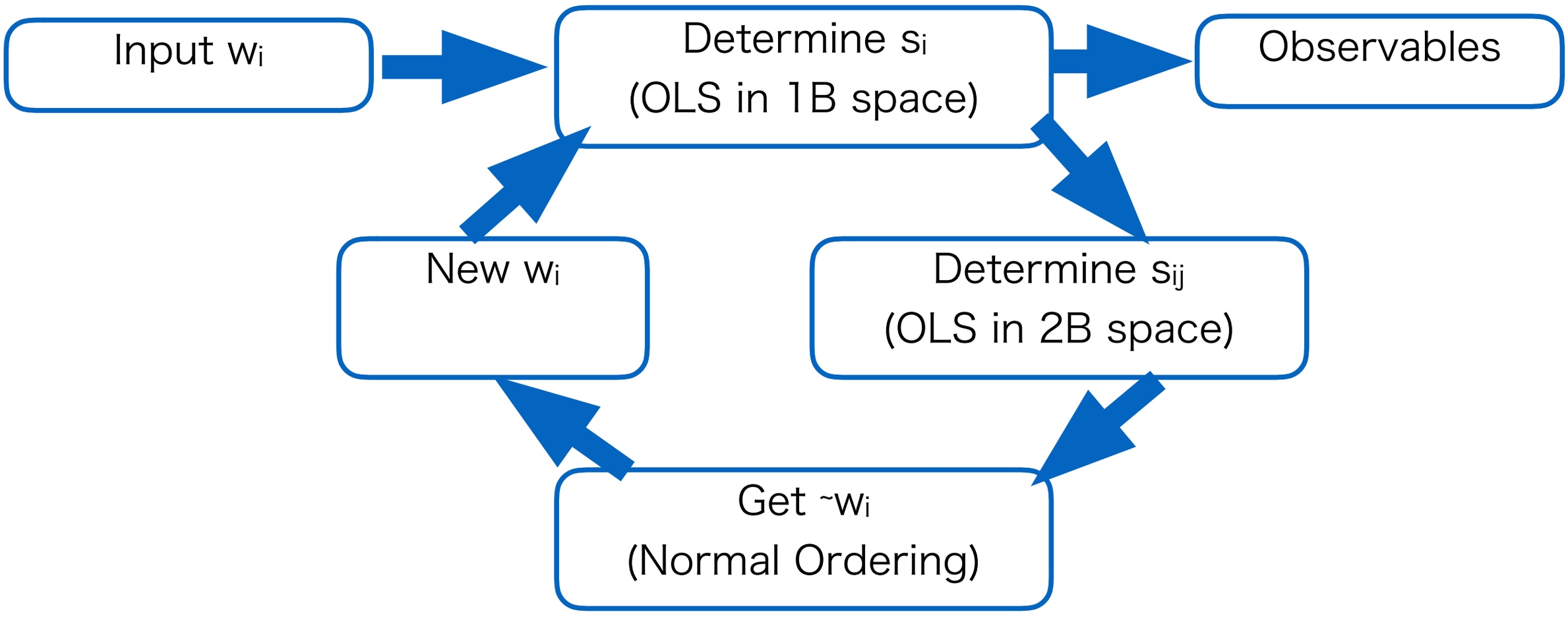
$$\langle a|\widetilde{w}|b\rangle = \sum_{c\le\rho_F} \langle ac|\widetilde{v}|bc\rangle$$

$$\widetilde{H}^{(3)} = \sum_{i<j<k} \widetilde{v}_{ijk} - \sum_{i<j} \widetilde{w}_{ij}$$

Unitary-Model-Operator Approach (UMOA)

K. Suzuki and R. Okamoto, PTP **92**, 1045 (1994).
TM et al., PRC **96**, 054312 (2017).

- Actual calculation procedure



Calculation setup

★ Interaction:

✤ NN: chiral N^3LO (Λ = 500 MeV/c)

D. R. Entem and R. Machleidt, Phys. Rev. C C68, 041001 (2003).

✤ 3N: chiral N^2LO local form (Λ = 400 MeV/c)

R. Roth, et al., Phys. Rev. Lett. 109, 052501 (2012).

★ NO2B approximation through the Hartree-Fock calculations

✤ 3-body matrix elements e_{3max} = 14.

$e_{3max} = \max(2n_1+l_1+2n_2+l_2+2n_3+l_3)$

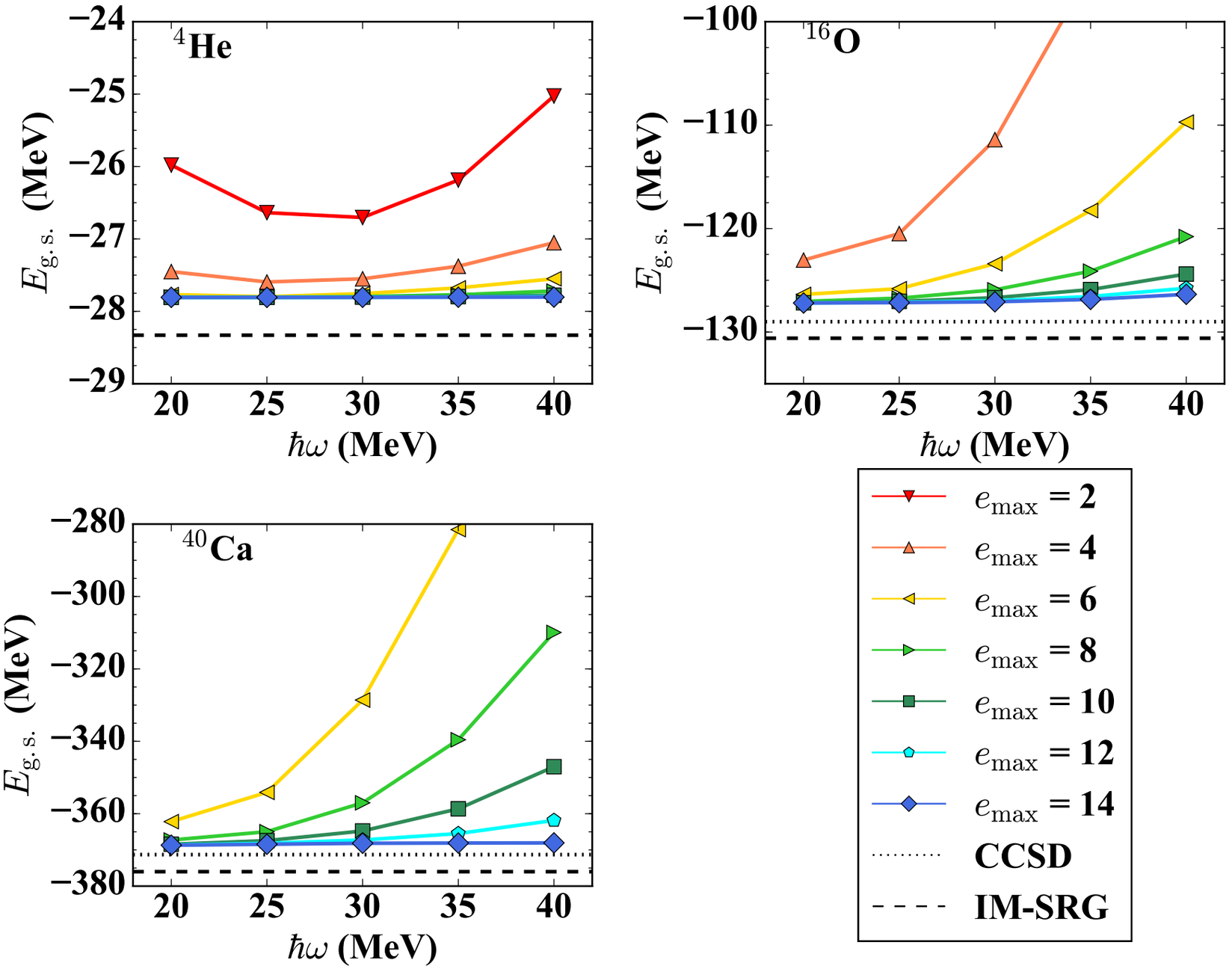
★ UMOA calculations are done with the e_{max} truncation.

$e_{max} = \max(2n+l)$

Convergence (NN+3N-full $\lambda = 1.88$ fm^{-1})

Converged results are found.

UMOA results are close to the CCSD and IM-SRG results.



CCSD: S. Binder, J. Langhammer, A. Calci, P. Navrátil, and R. Roth, Phys. Rev. C **87**, 021303 (2013).

IM-SRG: H. Hergert, S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C **87**, 034307 (2013).

Accuracy of UMOA calc.

perturbative estimation

$$\widetilde{H} \approx E_0 + \widetilde{H}^{(1)} + \widetilde{H}^{(2)} + \widetilde{H}^{(3)}.$$

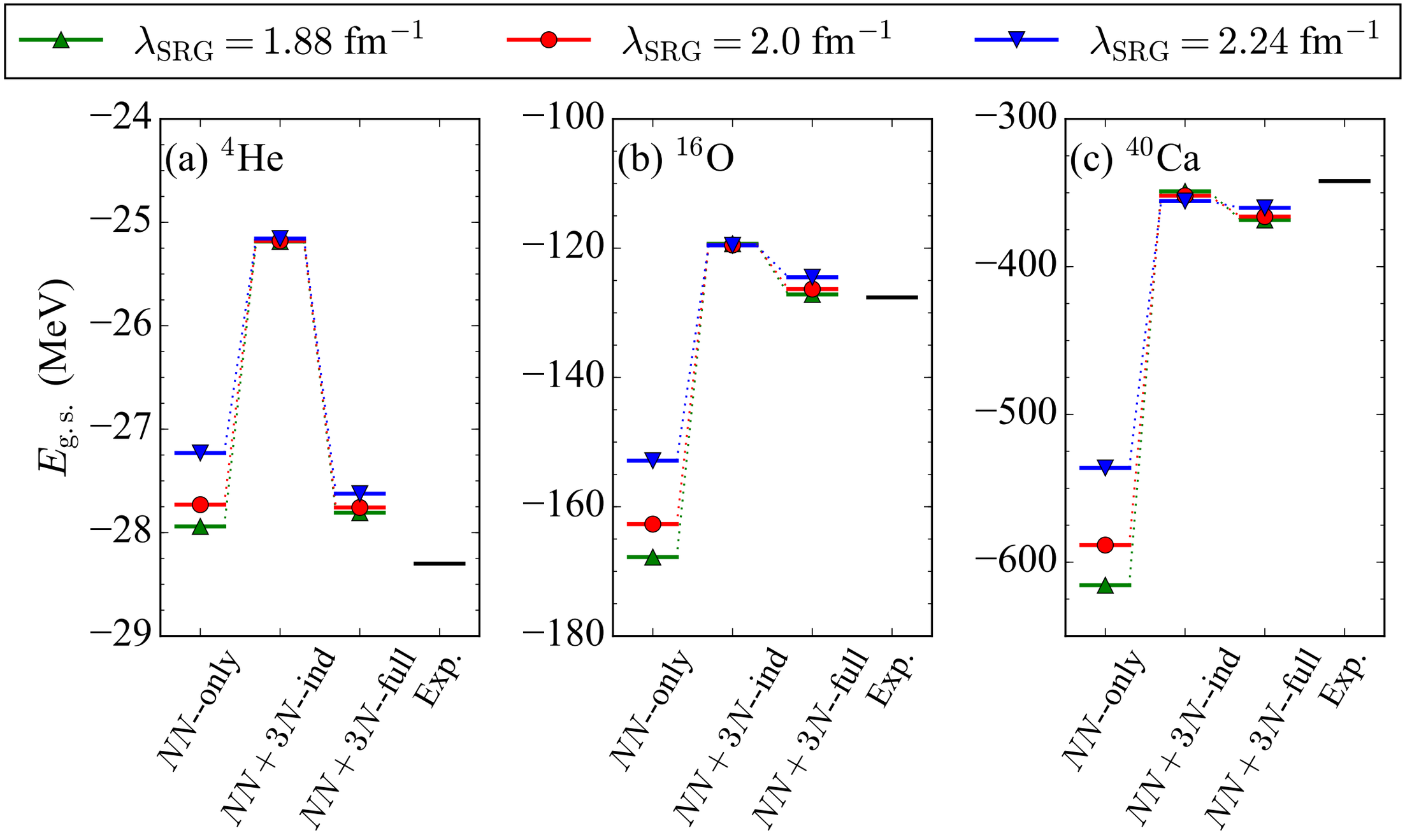
@ e_{max} = 14, hw = 25 MeV, NN+3N-full (λ =1.88 fm^{-1})

	E_0	$\langle H^{(1)} \rangle$	$\langle H^{(2)} \rangle$	$\langle H^{(3)} \rangle$	E_{tot}	$\lvert \langle H^{(3)} \rangle / E_{tot} \rvert$
^{4}He	-0.40	-107.15	80.46	-0.71	-27.81	0.03
^{16}O	32.42	-514.12	357.59	-3.04	-127.16	0.02
^{40}Ca	173.85	-1440.6	905.42	-7.08	-368.44	0.02

Cluster expansion works well

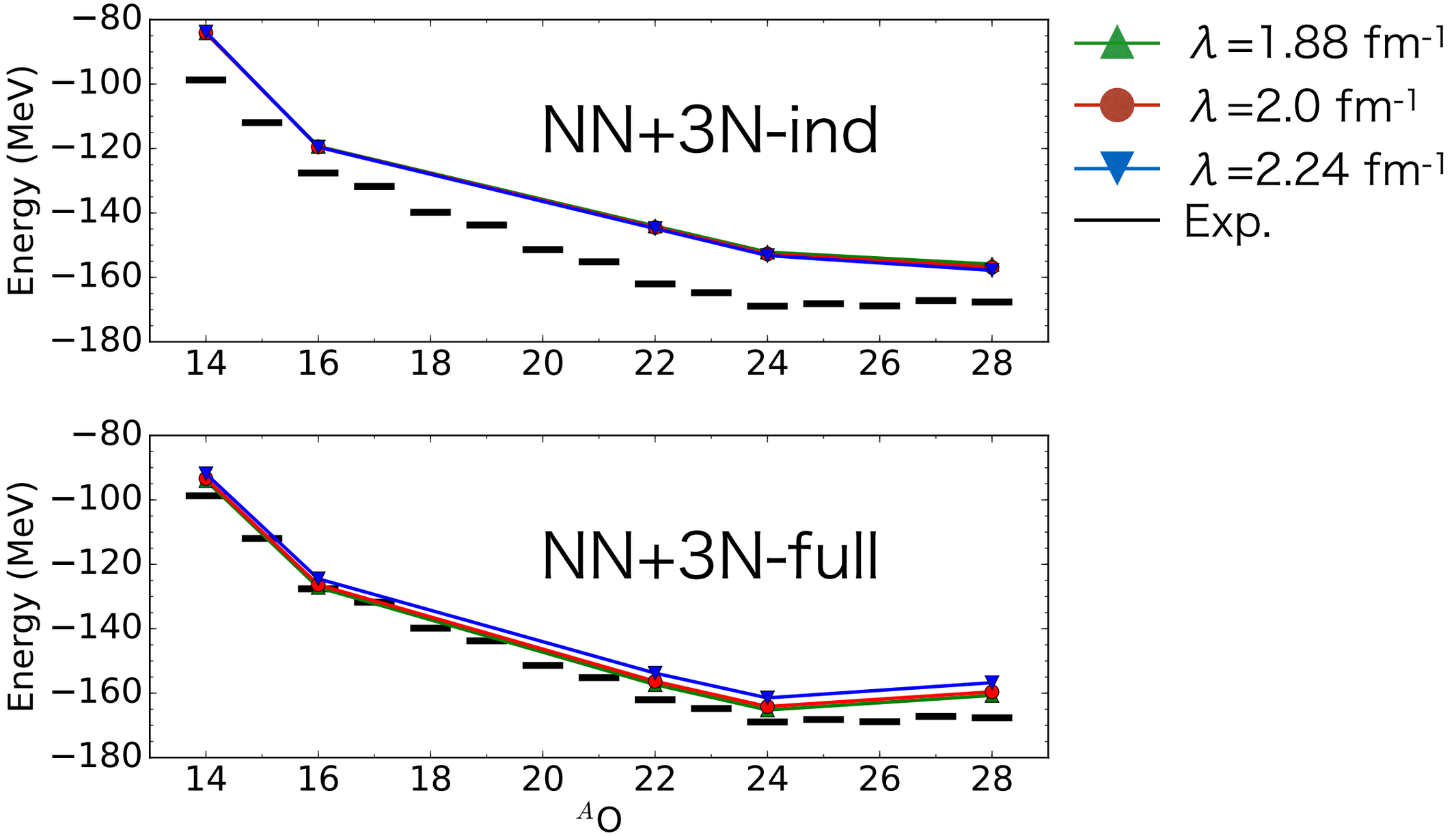
$\langle H^{(3)} \rangle / E_{tot}$ can be thought as the error of UMOA calc.

λ-dependence



Ground-state energies for oxygen isotopes

@e_{max}=14 hw = 25 MeV



Consistent with recent ab initio results

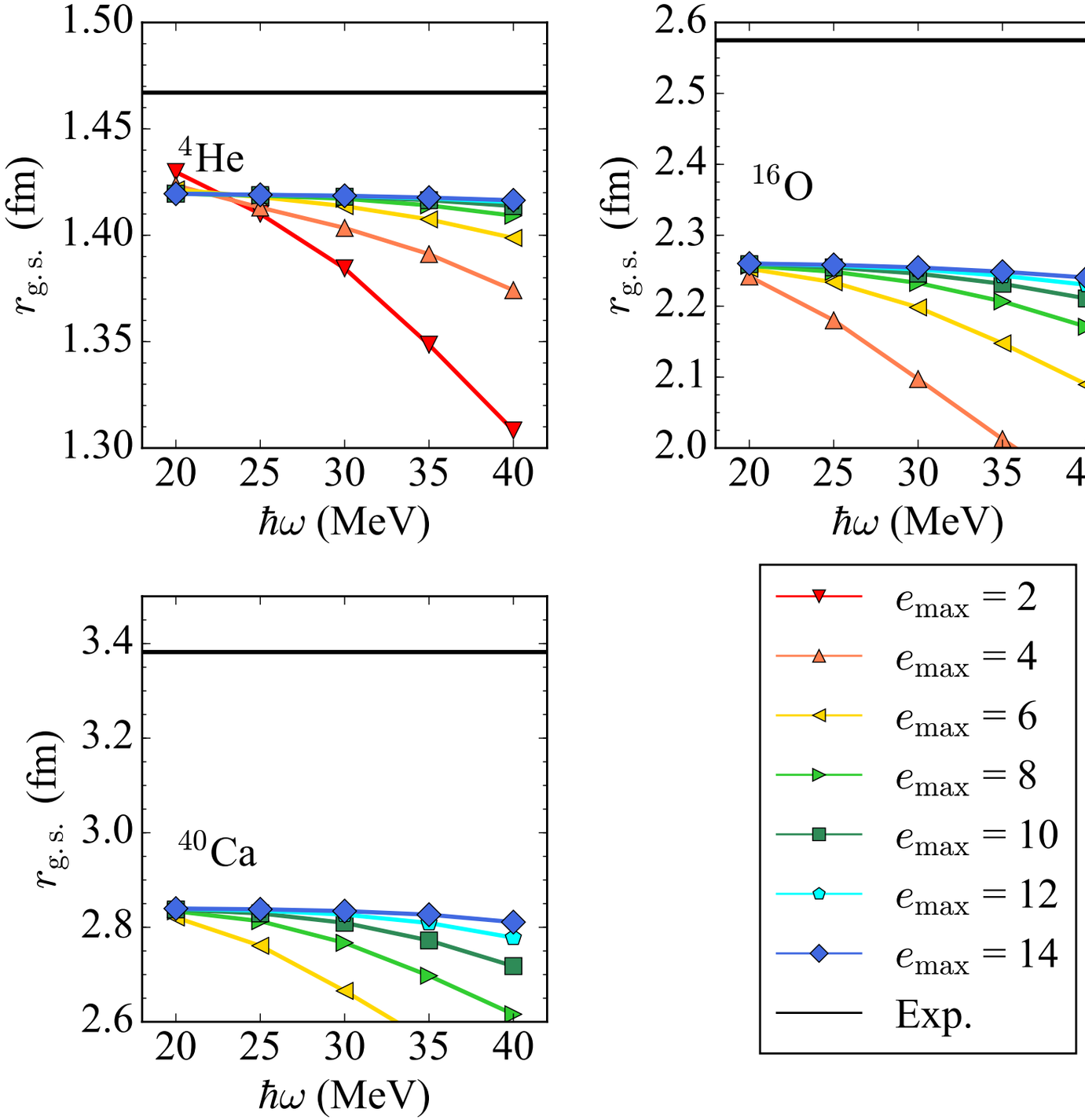
Exp.: AME2012

Root-mean-squared radii

Converged results are found.

Results are significantly smaller than experimental data.

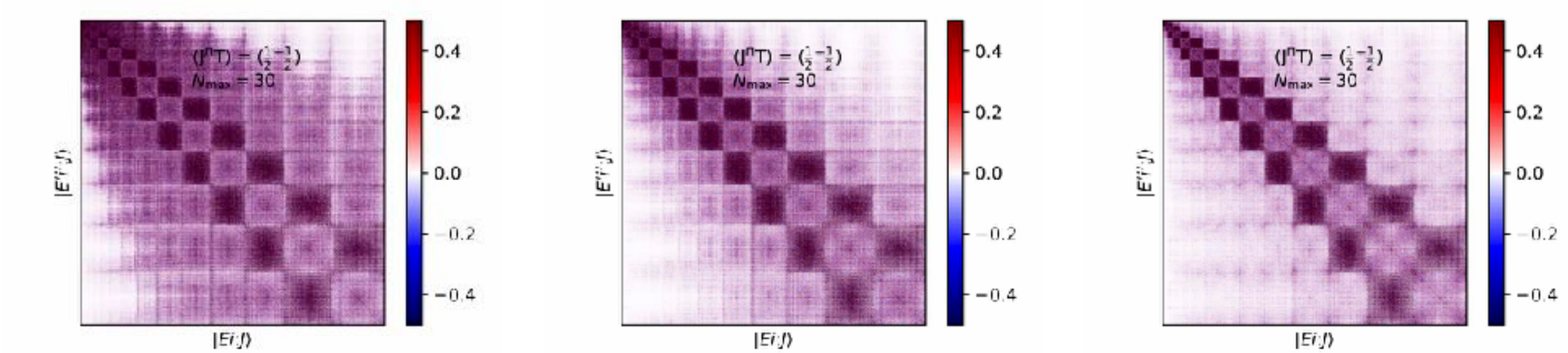
Experimental data are estimated from charge radii.



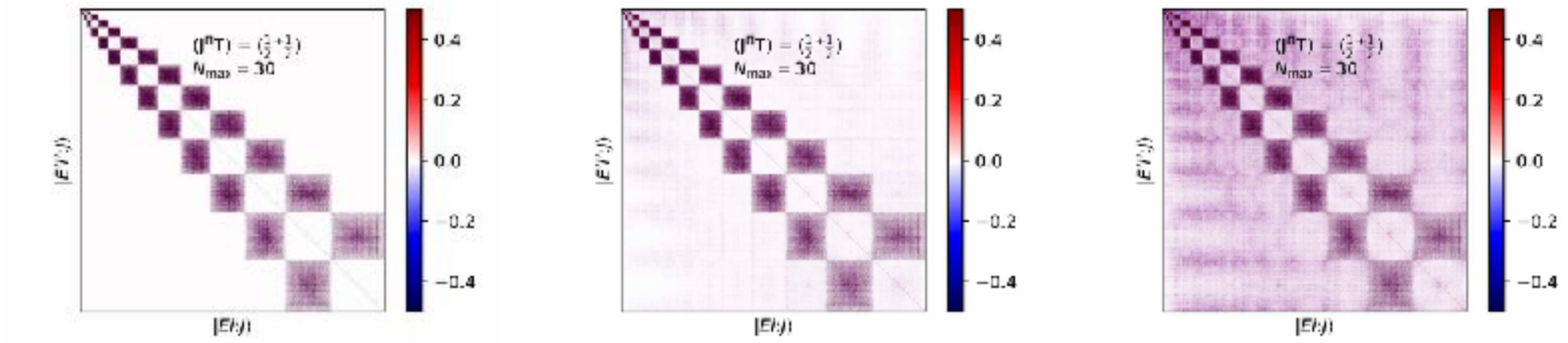
SRG evolution of radius operator

3-body SRG flow

Hamiltonian



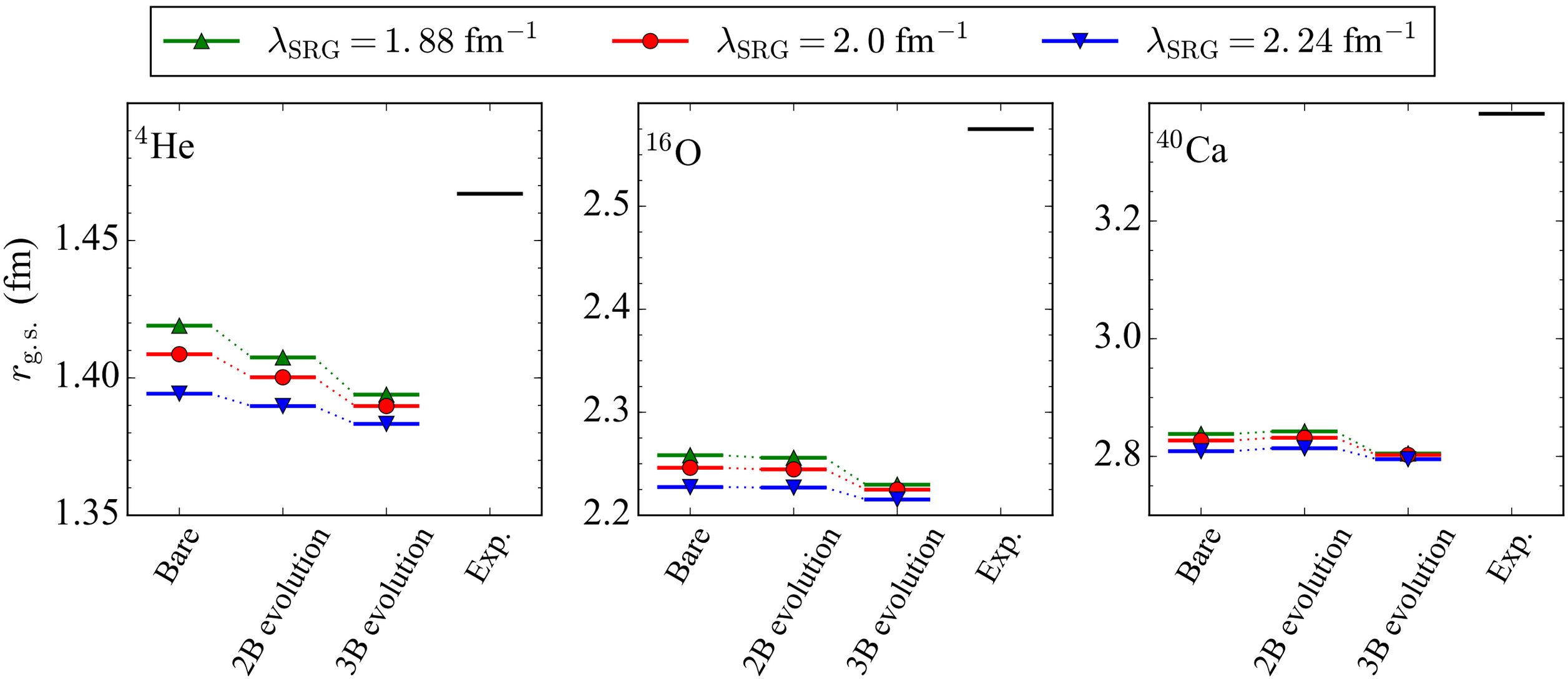
Radius



SRG flow

SRG evolution of radius operator

NN+3N-full, e_{max}=14, hw=25 MeV



Reduction of λ dependence M. D. Schuster, et al., Phys. Rev. C **90**, 011301 (2014).

Radii are still small

Summary

- UMOA works well similar to the other ab initio calculation methods.

- Radii are still small even if the 3NF effect is taken into account.

- SRG evolution gives minor modification for the radius operator.

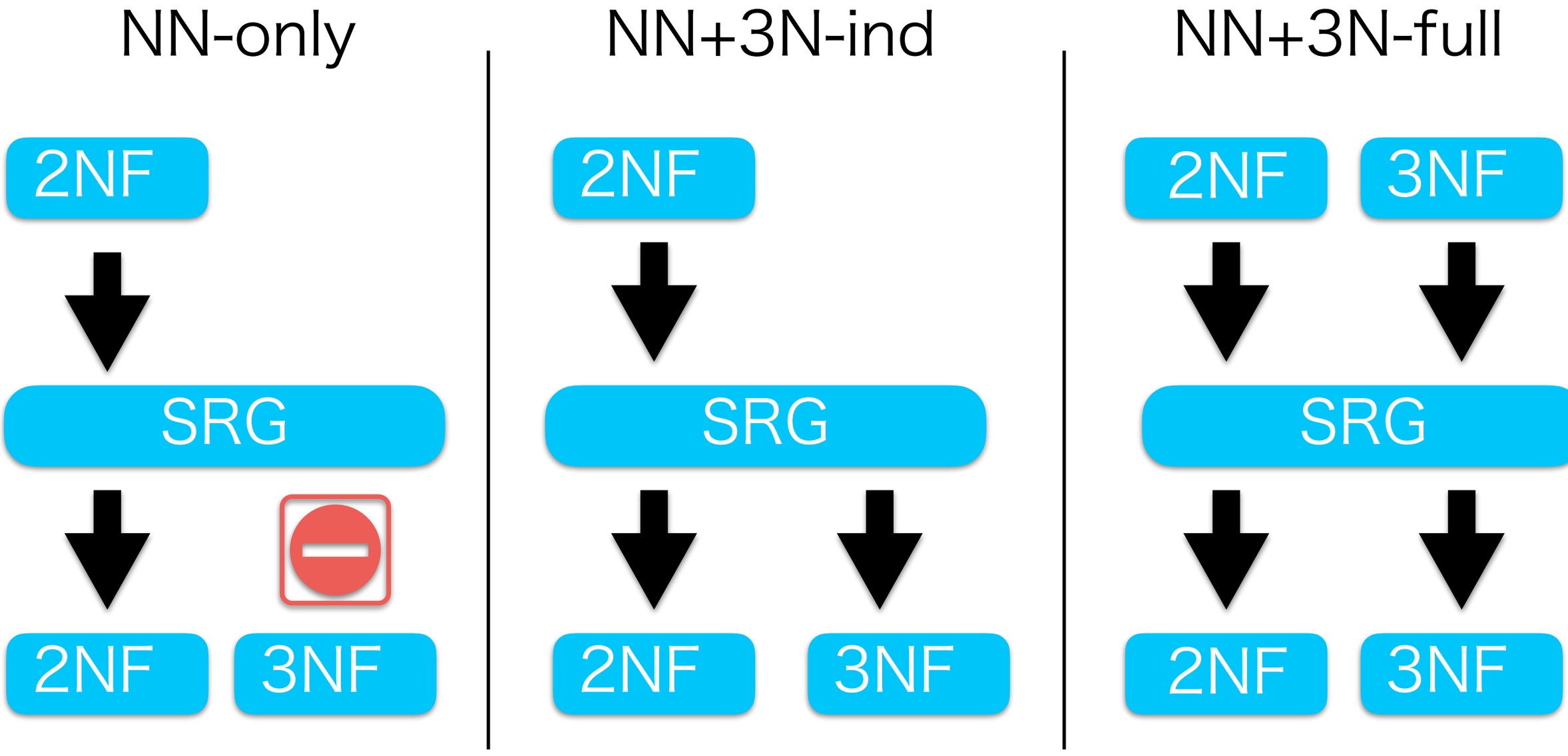
Future works

- Extension of the UMOA framework for direct treatment of 3NF.

Backup

SRG evolution - 3

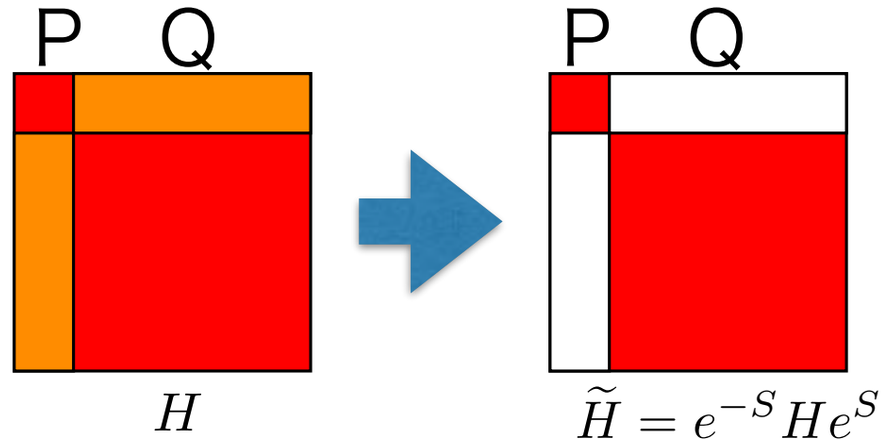
✦ SRG transformation induces many-body forces



E. D. Jurgenson, P. Navratil, and R. J. Furnstahl, PRL **103**, 082501 (2009).
E. D. Jurgenson, P. Navratil, and R. J. Furnstahl, PRC **83**, 034301 (2011).
...

UMOA - determination of S

Okubo, PTP 1954.
Lee and Suzuki, PLB 1980.



- Procedure for S
  - Solve eigenvalue problem

$$(P+Q)H(P+Q)|\psi_k\rangle = \epsilon_k |\psi_k\rangle$$

  - P and Q are the projection operator
  - Decomposition of eigenvector into P and Q component

$$|\phi_k\rangle = P|\psi_k\rangle, \quad \omega|\phi_k\rangle = Q|\psi_k\rangle$$

  - Formal solution of ω

$$\omega = \sum_{k=1}^{d} Q|\psi_k\rangle\langle\widetilde{\phi}_k|P$$

$$S = \mathrm{arctanh}(\omega - \omega^\dagger) \Rightarrow \widetilde{H} = e^{-S} H e^{S}$$

- Decoupling condition is satisfied

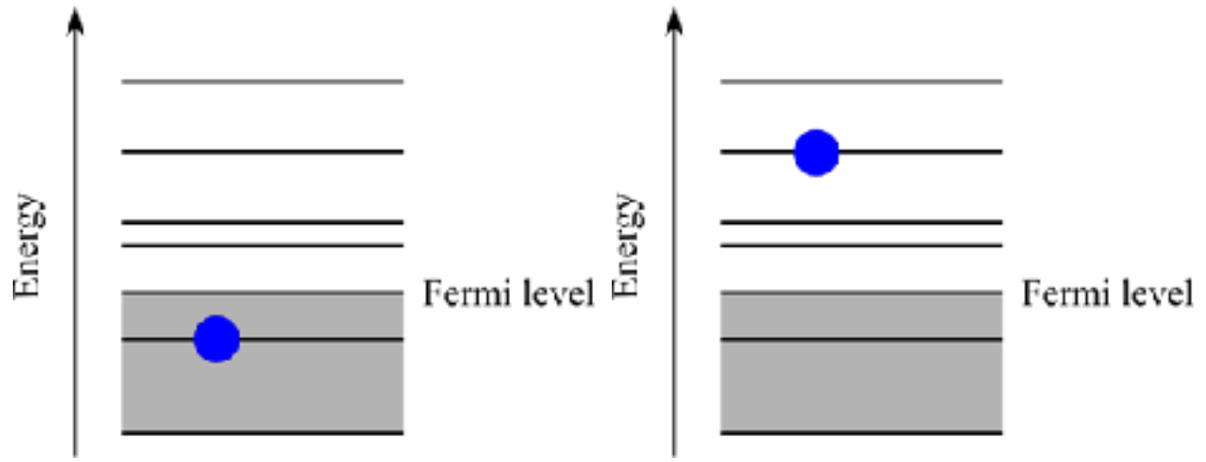
$$Q\widetilde{H}P = P\widetilde{H}Q = 0$$

UMOA - definition of P and Q

- ✦ Choice of P and Q is crucial in actual calculations.
  - ★ P and Q for $S^{(1)}$

$$P^{(1)} = \sum_{a \leq \text{Fermi level}} |a\rangle\langle a|$$

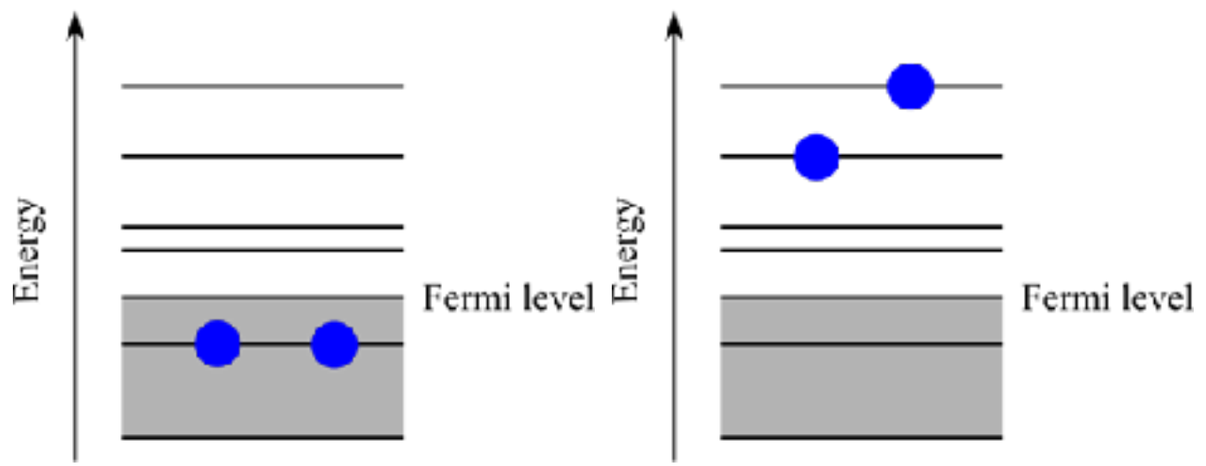
$$Q^{(1)} = \sum_{a > \text{Fermi level}} |a\rangle\langle a|$$



★ P and Q for $S^{(2)}$

$$P^{(2)} = \frac{1}{2} \sum_{ab \leq \text{Fermi level}} |ab\rangle\langle ab|$$

$$Q^{(2)} = \frac{1}{2} \sum_{ab > \text{Fermi level}} |ab\rangle\langle ab|$$



- ✦ For any $S^{(n)}$, P and Q can be determined systematically.

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K. Suzuki and R. Okamoto, PTP **92**, 1045 (1994).
TM et al., PRC **96**, 054312 (2017).

✦ Cluster expansion

$$\widetilde{H} \approx E_0 + \widetilde{H}^{(1)} + \widetilde{H}^{(2)} + \widetilde{H}^{(3)}$$

$$\widetilde{H}^{(1)} = \sum_i \widetilde{h}_i;\ \widetilde{h}_i = e^{-s_i}(t_i + w_i)e^{s_i}$$

$$\widetilde{H}^{(2)} = \sum_{i<j} \widetilde{v}_{ij} - \sum_i \widetilde{w}_i$$

$$\widetilde{v}_{ij} = e^{-s_{ij}} e^{-(s_i+s_j)}(t_i + w_i + t_j + w_j + v_{ij})e^{s_i+s_j} e^{s_{ij}} - (\widetilde{h}_i + \widetilde{h}_j)$$

$$\widetilde{w}_i = e^{-s_i} w_i e^{s_i}$$

$$\widetilde{H}^{(3)} = \sum_{i<j<k} \widetilde{v}_{ijk} - \sum_{i<j} \widetilde{w}_{ij}$$

$$\widetilde{v}_{ijk} = e^{-(s_{ij}+s_{jk}+s_{ki})} e^{-(s_i+s_j+s_k)}(t_i + w_i + t_j + w_j + t_k + w_k + v_{ij} + v_{jk} + v_{ki})e^{s_i+s_j+s_k} e^{s_{ij}+s_{jk}+s_{ki}} - (\widetilde{h}_i + \widetilde{h}_j + \widetilde{h}_k + \widetilde{v}_{ij} + \widetilde{v}_{jk} + \widetilde{v}_{ki})$$

$$\widetilde{w}_{ij} = e^{-s_{ij}} e^{-(s_i+s_j)}(w_i + w_j)e^{s_i+s_j} e^{s_{ij}}$$

Unitary-Model-Operator Approach (UMOA)

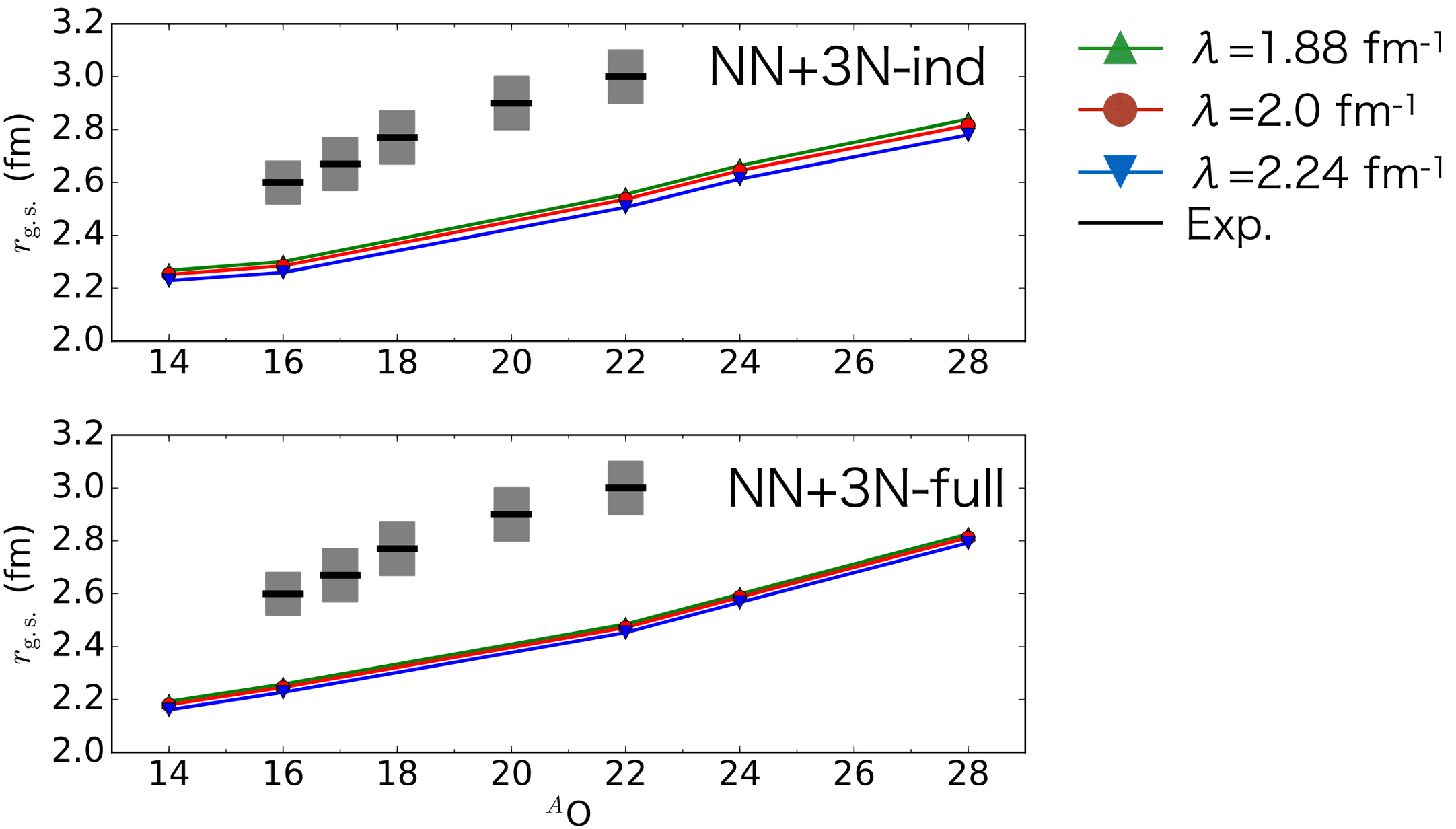
K. Suzuki and R. Okamoto, PTP **92**, 1045 (1994).
TM et al., PRC **96**, 054312 (2017).

- Perturbative evaluation for three-body term

$$\langle \widetilde{H}^{(3)} \rangle \approx \frac{1}{4} \sum_{ab>\rho_F} \sum_{ijkl\leq\rho_F} \langle ij|\widetilde{v}|kl\rangle\langle kl|s|ab\rangle\langle ij|s|ab\rangle$$
$$+ \sum_{abc>\rho_F} \sum_{ijk\leq\rho_F} \langle ia|\widetilde{v}|jb\rangle\langle kj|s|ca\rangle\langle ik|s|cb\rangle$$

Radii for oxygen isotopes

@e_{max}=14 hw = 25 MeV

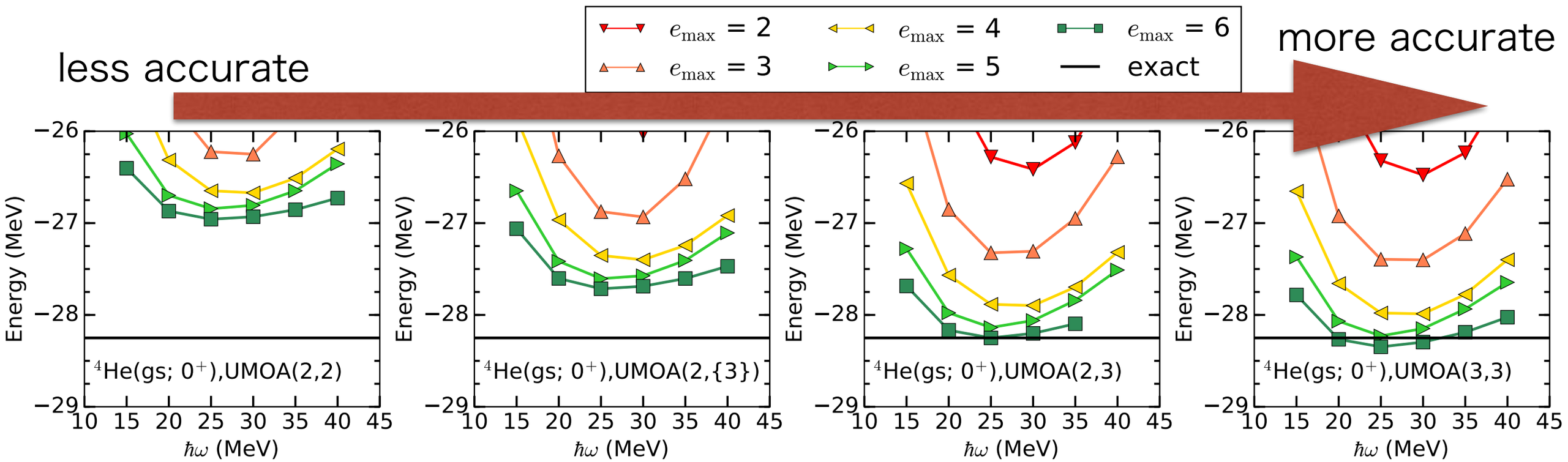


Radii are significantly small

Exp.: V. Lapoux, et al, Phys. Rev. Lett. **117**, 052501 (2016).

Extension of UMOA Framework

- Ground-state energy for ^{4}He (NN-only @ λ =2 fm^{-1})



$U \approx e^{S^{(1)}} e^{S^{(2)}}$

$\widetilde{H} \approx \widetilde{H}^{(1)} + \widetilde{H}^{(2)}$

$U \approx e^{S^{(1)}} e^{S^{(2)}}$

$\widetilde{H} \approx \widetilde{H}^{(1)} + \widetilde{H}^{(2)} + (\widetilde{H}^{(3)})$

$U \approx e^{S^{(1)}} e^{S^{(2)}}$

$\widetilde{H} \approx \widetilde{H}^{(1)} + \widetilde{H}^{(2)} + \widetilde{H}^{(3)}$

$U \approx e^{S^{(1)}} e^{S^{(2)}} e^{S^{(3)}}$

$\widetilde{H} \approx \widetilde{H}^{(1)} + \widetilde{H}^{(2)} + \widetilde{H}^{(3)}$