

# Calculations for medium-mass nuclei with chiral EFT interactions in the unitary-model-operator approach

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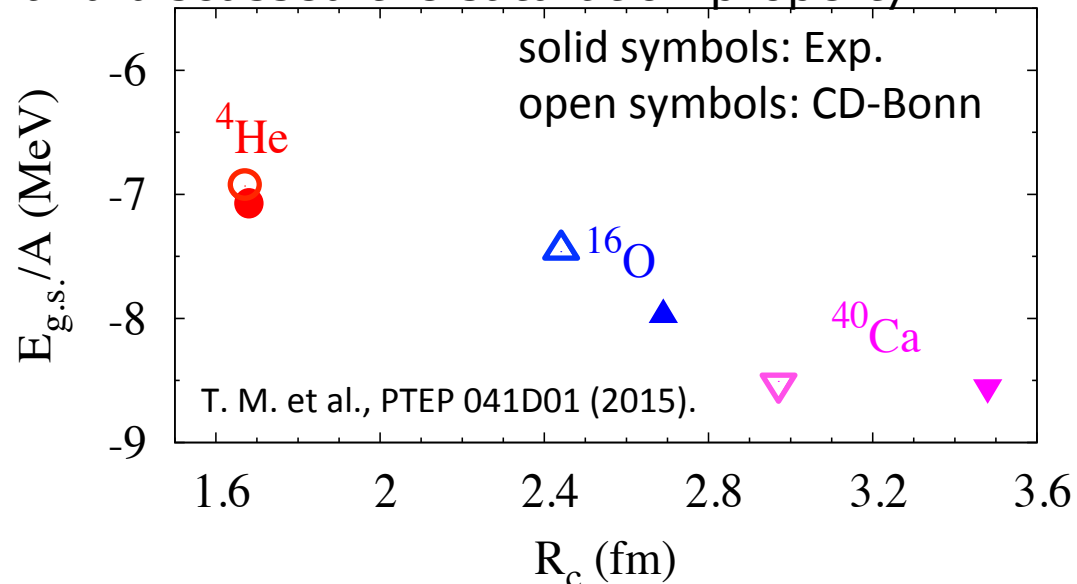
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# Motivation

So far, we calculated the ground-state energies and charge radii for double closed-shell nuclei with the only nucleon-nucleon (NN) interaction and discussed the saturation property.



Then, the binding energies and charge radii were **underbound** to and **smaller** than the experimental data, respectively.

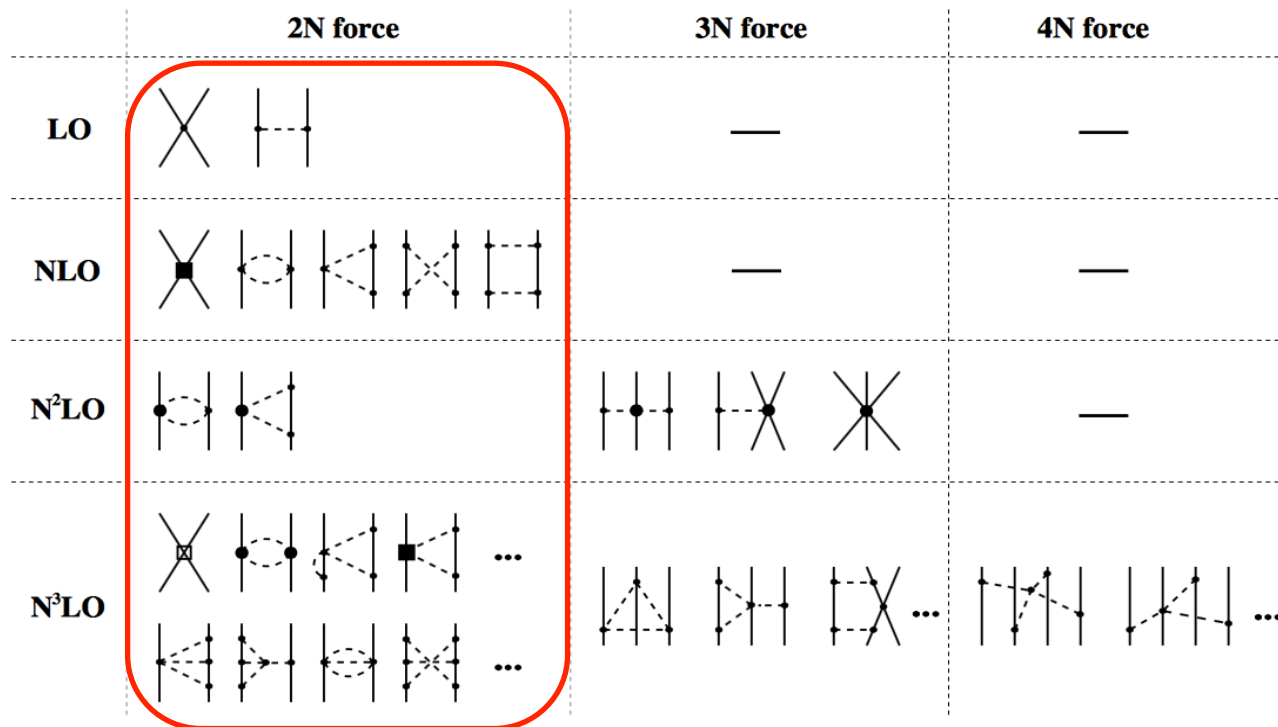
The three-nucleon force effect is one of the important issues.  
⇒ the chiral effective-field-theory (EFT) interactions

# Chiral EFT interactions

E. Epelbaum, Prog. Part. Nucl. Phys. **57**, 654 (2006).  
 R. Machleidt and D. R. Entem, Phys. Rep. **503**, 1 (2011).

Many-body interactions can be automatically derived.  
 Further improvements can be expected by going to higher orders.

E. Epelbaum, arXiv: 1001.3229 [nucl-th] (2010).



As the first application, the NN interaction is used in this work.

# ab-initio calculations related to this work

To understand microscopically the saturation property of finite nuclei, it is desirable to use ab initio calculation methods.

For light nuclei ( $A \approx 3-16$ )

Green's Function Monte Carlo Method

No-Core Shell Model

For medium mass nuclei ( $A \approx 16-56$ )

Coupled-Cluster Method

Self-Consistent Green's Function Method

In-Medium Similarity Renormalization Group

Unitary-Model-Operator Approach(UMOA)

We calculate the ground-state energies and charge radii of  ${}^4\text{He}$ ,  ${}^{16}\text{O}$ , and  ${}^{40}\text{Ca}$  in the UMOA with the chiral nucleon-nucleon interaction.

# Unitary-Model-Operator Approach (UMOA)

K. Suzuki and R. Okamoto, PTP **92**, 1045 (1992).

The original non-relativistic nuclear Hamiltonian

$$H = \sum_{\alpha\beta} \langle \alpha | t_1 | \beta \rangle c_{\alpha}^{\dagger} c_{\beta} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v_{12} | \gamma\delta \rangle c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma} + \dots$$

$$H |\Psi_k\rangle = E_k |\Psi_k\rangle \quad \rightarrow \quad \tilde{H} |\Phi_k\rangle = E_k |\Phi_k\rangle \quad \text{Reference state}$$

$\tilde{H} = U^{-1} H U$  unitary transformation of the original Hamiltonian

$$U = e^{S^{(1)}} e^{S^{(2)}}$$

$$S^{(1)} = \sum_{\alpha\beta} \langle \alpha | S_1 | \beta \rangle c_{\alpha}^{\dagger} c_{\beta} \quad S^{(2)} = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | S_{12} | \gamma\delta \rangle c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}$$

One-body correlation operator      two-body correlation operator

$$U \text{ is unitary} \quad \leftrightarrow \quad S^{(n)\dagger} = -S^{(n)} \quad n = 1, 2$$

# Cluster expansion of the transformed Hamiltonian

$$\tilde{H} = \tilde{H}^{(1)} + \tilde{H}^{(2)} + \tilde{H}^{(3)} + \dots \quad \text{truncated}$$

$$\tilde{H}^{(1)} = \sum_{\alpha\beta} \langle \alpha | \tilde{h}_1 | \beta \rangle c_\alpha^\dagger c_\beta, \quad \tilde{h}_1 = e^{-S_1} (t_1 + u_1) e^{S_1}, \quad \langle \alpha | \tilde{u}_1 | \beta \rangle = \sum_{\lambda \leq \rho_F} \langle \alpha \lambda | \tilde{v}_{12} | \beta \lambda \rangle$$

one-body field determined self-consistently

$$\tilde{H}^{(2)} = \left( \frac{1}{2!} \right)^2 \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \tilde{v}_{12} | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma - \sum_{\alpha\beta} \langle \alpha | \tilde{u}_1 | \beta \rangle c_\alpha^\dagger c_\beta$$

$$\tilde{v}_{12} = e^{-S_{12}} e^{-(S_1+S_2)} (h_1 + h_2 + v_{12}) e^{S_1+S_2} e^{S_{12}} - (\tilde{h}_1 + \tilde{h}_2) \quad \text{two-body transformed interaction}$$

truncated

$$\tilde{H}^{(3)} = \left( \frac{1}{3!} \right)^2 \sum_{\alpha\beta\gamma\lambda\mu\nu} \langle \alpha\beta\gamma | \tilde{v}_{123} | \lambda\mu\nu \rangle c_\alpha^\dagger c_\beta^\dagger c_\gamma^\dagger c_\nu c_\mu c_\lambda - \left( \frac{1}{2!} \right)^2 \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \tilde{u}_1 | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

$$\tilde{v}_{123} = e^{-(S_{12}+S_{23}+S_{31})} e^{-(S_1+S_2+S_3)} (h_1 + h_2 + h_3 + v_{12} + v_{23} + v_{31}) e^{S_1+S_2+S_3} e^{S_{12}+S_{23}+S_{31}} - (\tilde{h}_1 + \tilde{h}_2 + \tilde{h}_3 + \tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31})$$

three-body transformed interaction

# determination of correlation operator

$P^{(n)}$ ,  $Q^{(n)}$ : projection operators onto the n-particle state below and above the Fermi level, respectively

$$H^{(n)} |\psi_k^{(n)}\rangle = E_k |\psi_k^{(n)}\rangle \quad n=1, 2 \text{ one- and two-body Schrödinger equation}$$

$$|\psi_k^{(n)}\rangle = \underbrace{|\phi_k^{(n)}\rangle}_{\text{P-space component}} + \omega^{(n)} |\phi_k^{(n)}\rangle \quad \text{decomposition of the wave function into the P and Q components}$$

mapping operator  $\omega$  satisfies the decoupling condition.

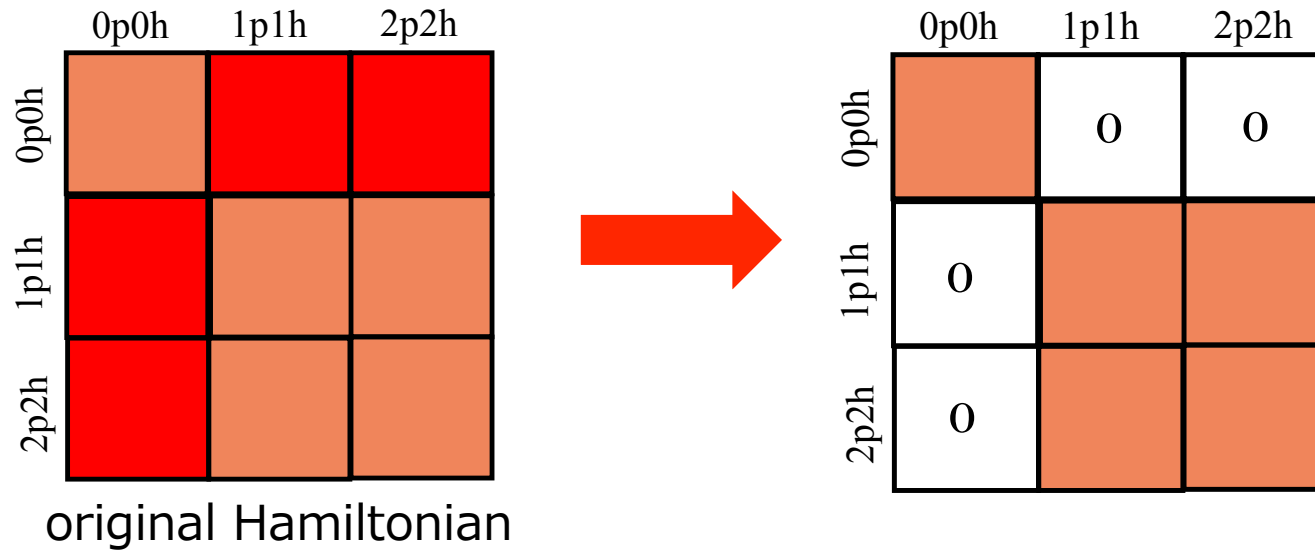
$$Q^{(n)} (1 - \omega^{(n)}) H^{(n)} (1 + \omega^{(n)}) P^{(n)} = 0$$

$$\omega^{(n)} = \sum_{k=1}^d Q^{(n)} |\psi_k^{(n)}\rangle \langle \tilde{\phi}_k^{(n)}| P^{(n)}$$

$$S^{(n)} = \text{arctanh}(\omega^{(n)} - \omega^{(n)\dagger})$$

$$Q^{(n)} \tilde{H}^{(n)} P^{(n)} = P^{(n)} \tilde{H}^{(n)} Q^{(n)} = 0$$

# Hamiltonian after the transformation



Ground-state energy

Normal ordered zero-body term with respect to the reference state

$$E_{g.s.} \approx \sum_{\lambda \leq \rho_F} \langle \lambda | \tilde{t}_1 | \lambda \rangle + \frac{1}{2!} \sum_{\lambda \mu \leq \rho_F} \langle \lambda \mu | \tilde{v}_{12} | \lambda \mu \rangle + \frac{1}{3!} \sum_{\lambda \mu \nu \leq \rho_F} \langle \lambda \mu \nu | \tilde{v}_{123} | \lambda \mu \nu \rangle$$



# Charge radius

$$R_c^2 \equiv \langle \Psi | r_p^2 | \Psi \rangle + R_p^2 + \frac{N}{Z} R_n^2 + \dots$$

J. Carlson, V. R. Pandharipande, NPA **401**, 59-85 (1983).  
J. L. Friar, J. W. Negele, Advances in Nuclear Physics **3**, 219 (1967).

$R_p^2, R_n^2$ : mean-square radii of proton and neutron, respectively

$R_p^2 = 0.832 \text{ fm}^2$  and  $R_n^2 = -0.115 \text{ fm}^2$  are used in this work.

$$r_p^2 \equiv \frac{1}{Z} \sum_{i=1}^Z (\vec{r}_i - \vec{R}_{c.m.})^2 \Rightarrow r_p^{(1)} + r_p^{(2)} \quad \text{decomposition into one- and two-body parts}$$

The cluster expansion can be applied to the evaluation of the point-proton radius

$$\langle \Psi | r_p | \Psi \rangle = \langle \Phi | U^{-1} r_p U | \Phi \rangle = \langle \Phi | \tilde{r}_p | \Phi \rangle \quad \tilde{r}_p = \tilde{r}_p^{(1)} + \tilde{r}_p^{(2)} + \dots$$

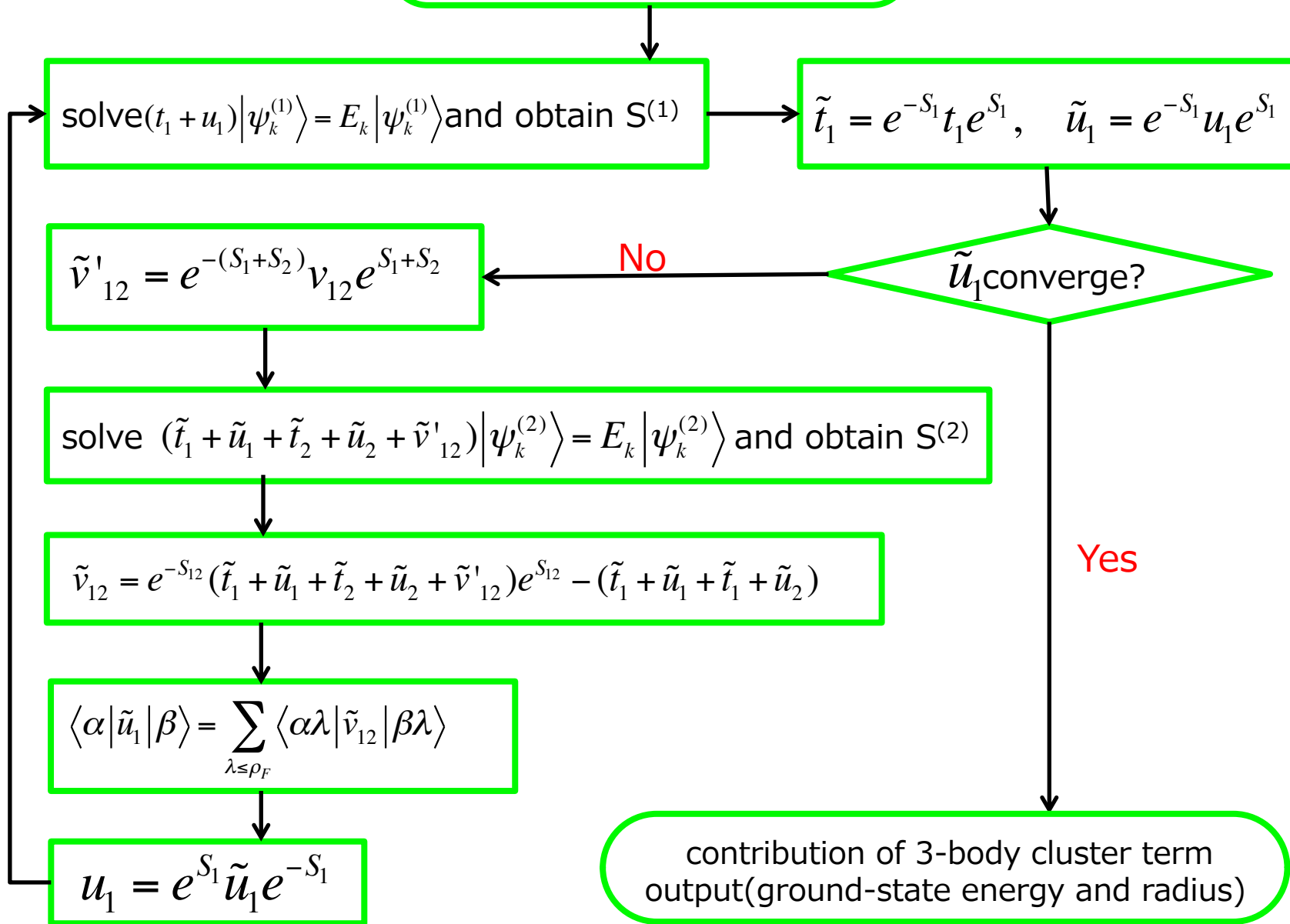
$$\tilde{r}_p^{(1)} = \sum_{\alpha\beta} \langle \alpha | \tilde{r}_{p1} | \beta \rangle c_\alpha^\dagger c_\beta \quad \tilde{r}_{p1} = e^{-S_1} r_{p1} e^{S_1}$$

$$\tilde{r}_p^{(2)} = \left( \frac{1}{2!} \right)^2 \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \tilde{r}_{p12} | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \quad \tilde{r}_{p12} = e^{-S_{12}} e^{-(S_1+S_2)} (r_{p1} + r_{p2} + r_{p12}) e^{S_1+S_2} e^{S_{12}} - (\tilde{r}_{p1} + \tilde{r}_{p2})$$

$$\langle r_p \rangle \approx \sum_{\lambda \leq \rho_F} \langle \lambda | \tilde{r}_{p1} | \lambda \rangle + \frac{1}{2!} \sum_{\lambda\mu \leq \rho_F} \langle \lambda\mu | \tilde{r}_{p12} | \lambda\mu \rangle$$

calculation procedure

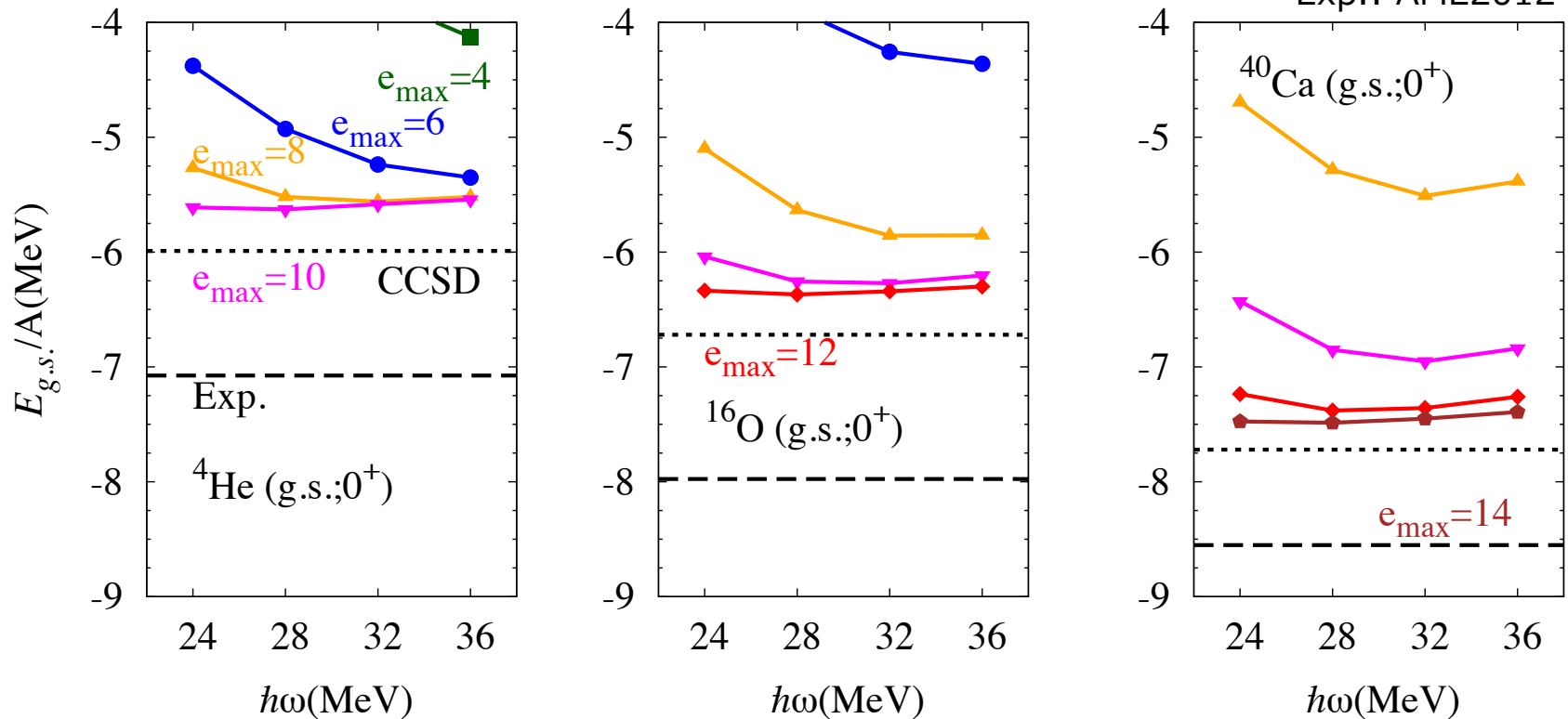
input (NN interaction)



# Ground-state energies

interaction: chiral NN interaction at N<sup>3</sup>LO by Entem & Machleidt ( $\Lambda=500\text{MeV}$ )  
 model space:  $e_{\text{max}} = \max(2n+1)$

CCSD: G. Hagen et al., PRL **101**, 092502 (2008).  
 Exp.: AME2012

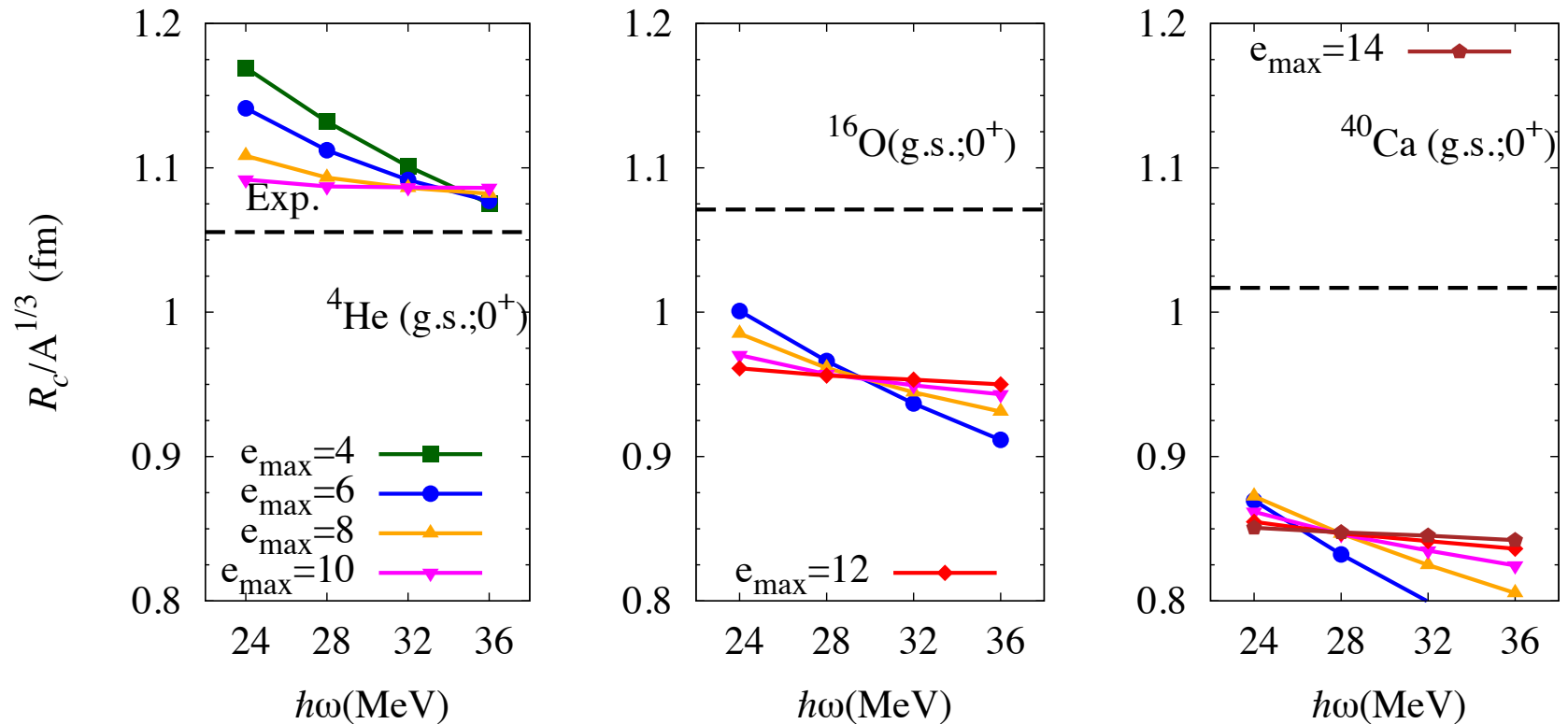


Our results are close to the CCSD results, while underbound to the experimental data.

# Charge radii

interaction: chiral NN interaction at N<sup>3</sup>LO by Entem & Machleidt ( $\Lambda=500\text{MeV}$ )  
 model space:  $e_{\text{max}} = \max(2n+1)$

Exp.: I. Angeli and K.P. Marinova, *atom. data nucl. data* **99**, 69 (2013).

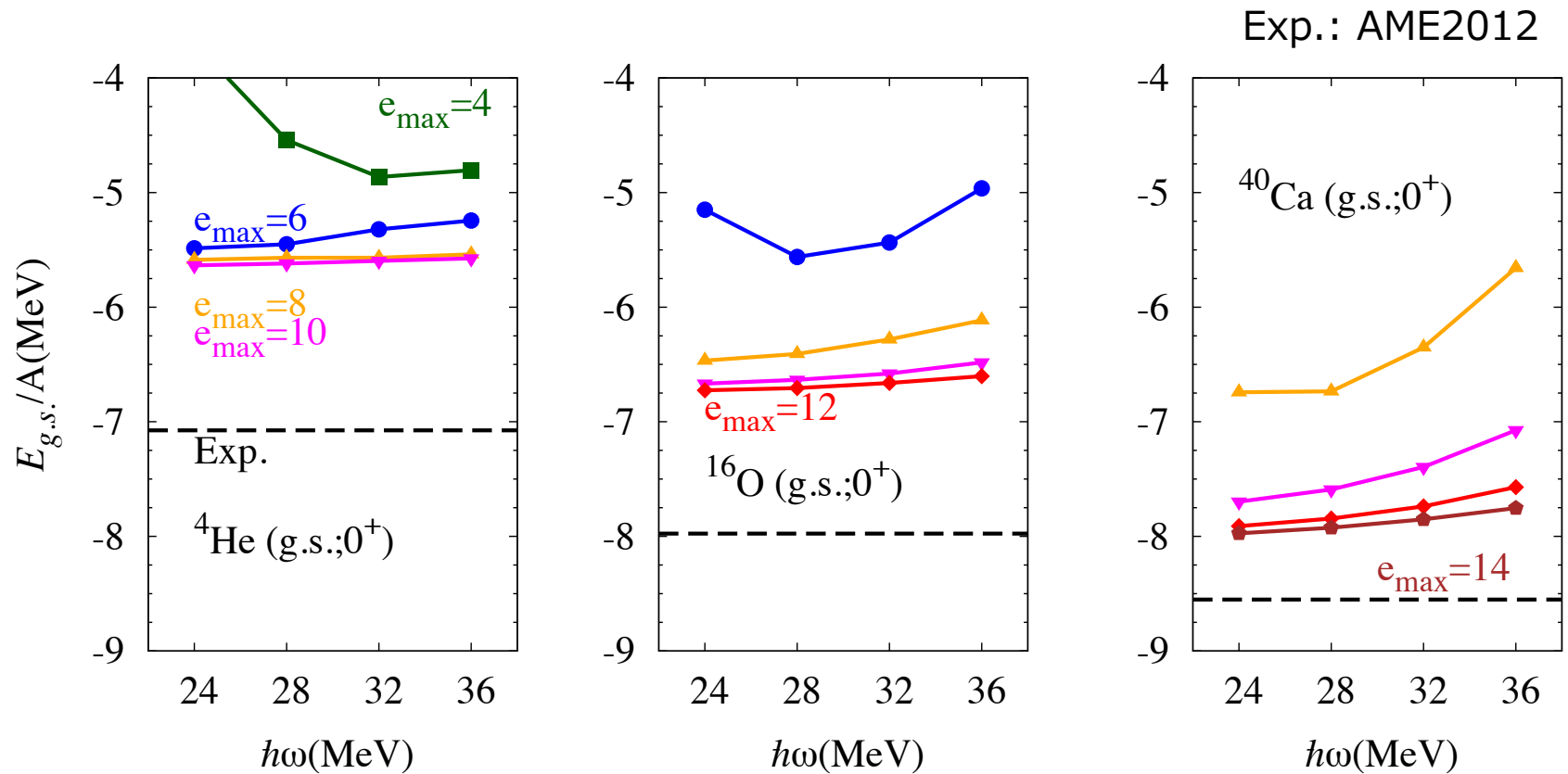


overestimate for  ${}^4\text{He}$ , while overestimate for  ${}^{16}\text{O}$  and  ${}^{40}\text{Ca}$

# Ground-state energies

interaction: chiral NN interaction at N<sup>3</sup>LO by Epelbaum ( $\Lambda = 450$  MeV)

model space:  $e_{\max} = \max(2n+1)$

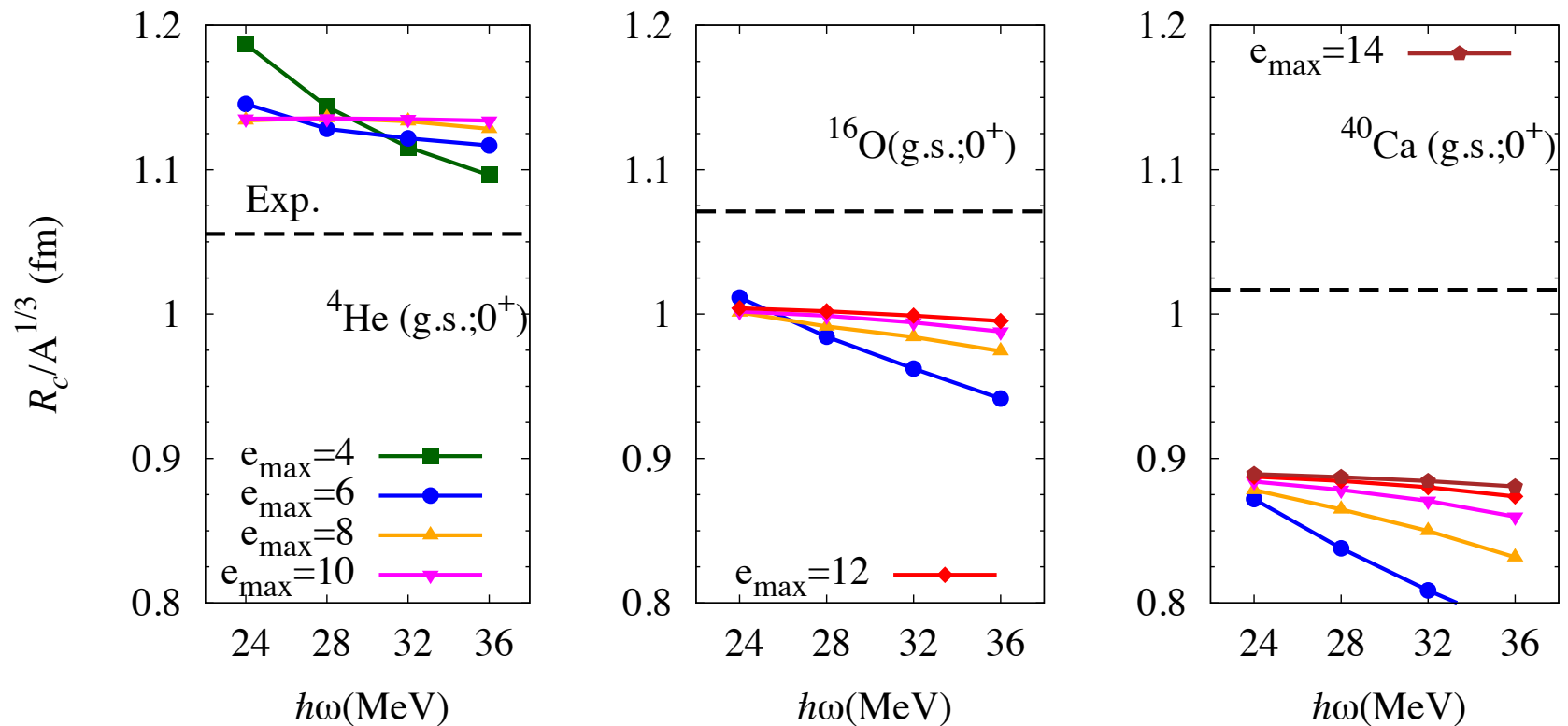


underbound to the experimental data

# Charge radii

interaction: chiral NN interaction at N<sup>3</sup>LO by Epelbaum ( $\Lambda = 450$  MeV)  
 model space:  $e_{\max} = \max(2n+1)$

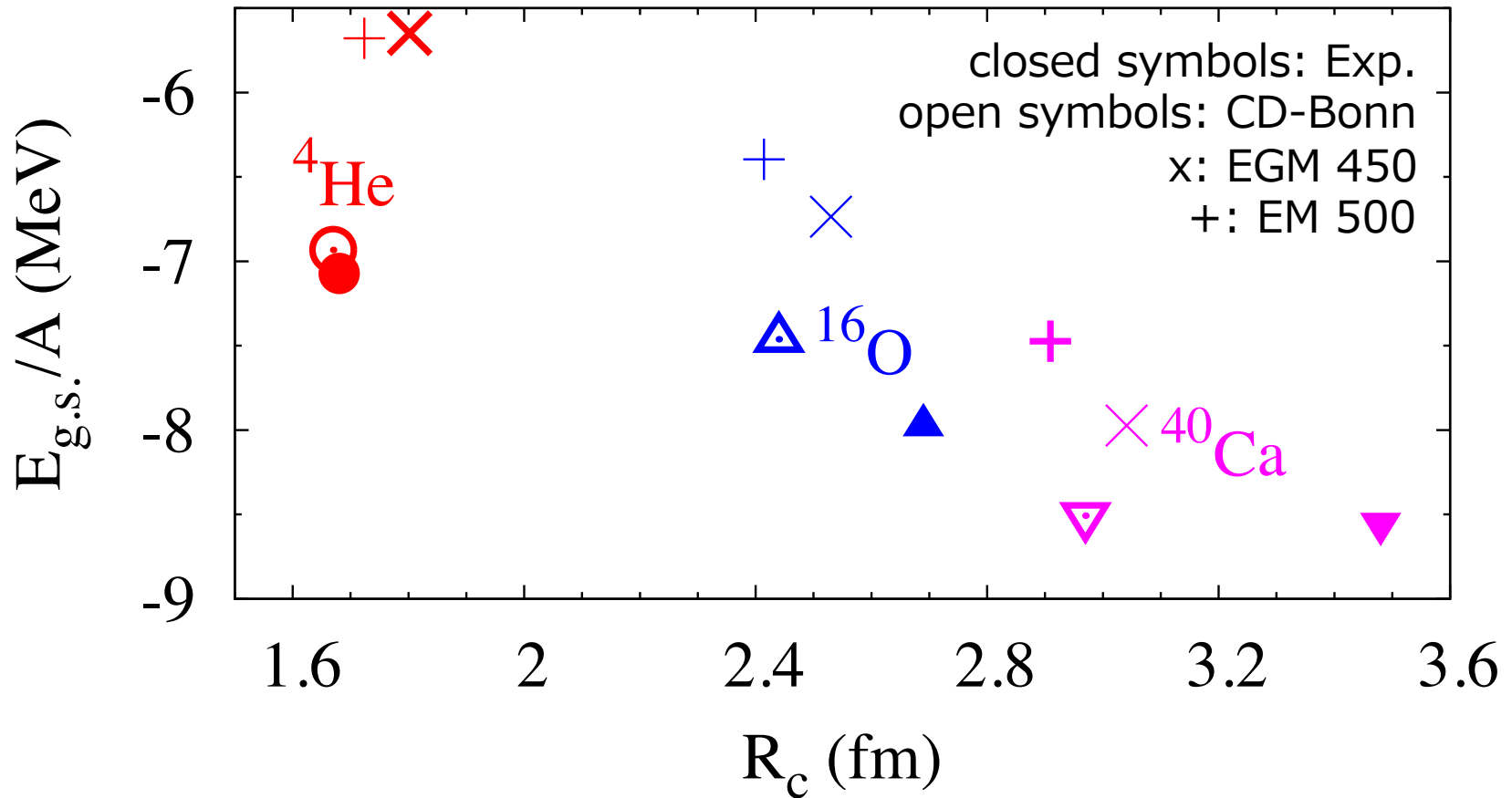
Exp.: I. Angeli and K.P. Marinova, atom. data nucl. data **99**, 69 (2013).



overestimate for  ${}^4\text{He}$ , while underestimate for  ${}^{16}\text{O}$ ,  ${}^{40}\text{Ca}$

# saturation property

Energy: underbound } similar to the results with  
radii: small } the CD-Bonn potential



# Summary

We calculated the ground-state energies and charge radii of  ${}^4\text{He}$ ,  ${}^{16}\text{O}$ , and  ${}^{40}\text{Ca}$  with the chiral NN interaction at  $\text{N}^3\text{LO}$ .

ground-state energies : underbound

charge radii : tend to be smaller than the experimental data

The situation is similar to our previous work with the CD-Bonn potential.

# Future work

Application of chiral three-nucleon interaction to the UMOA