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

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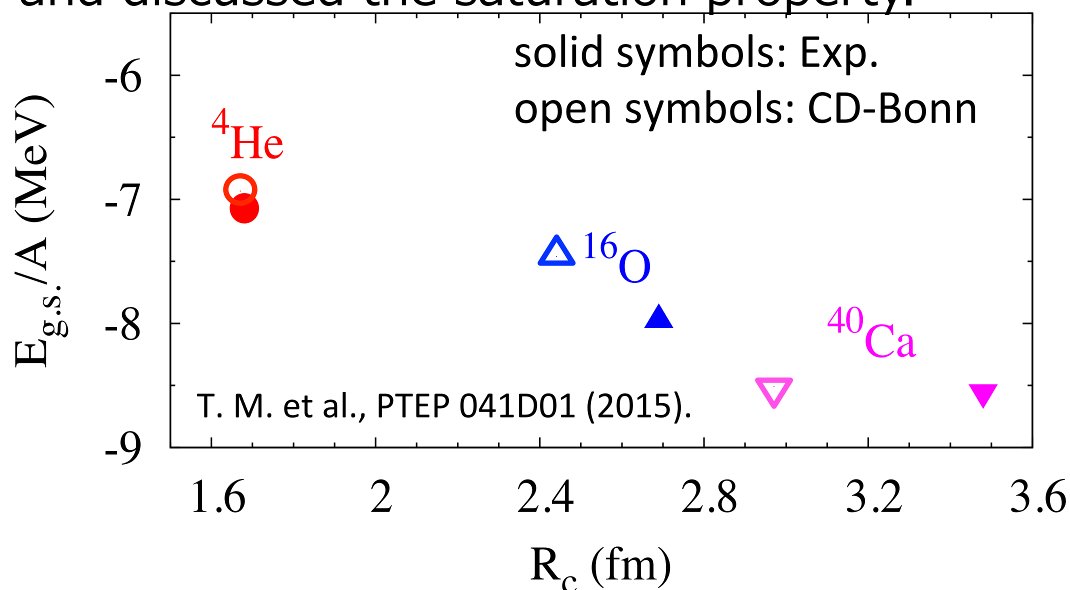
Motivation

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.

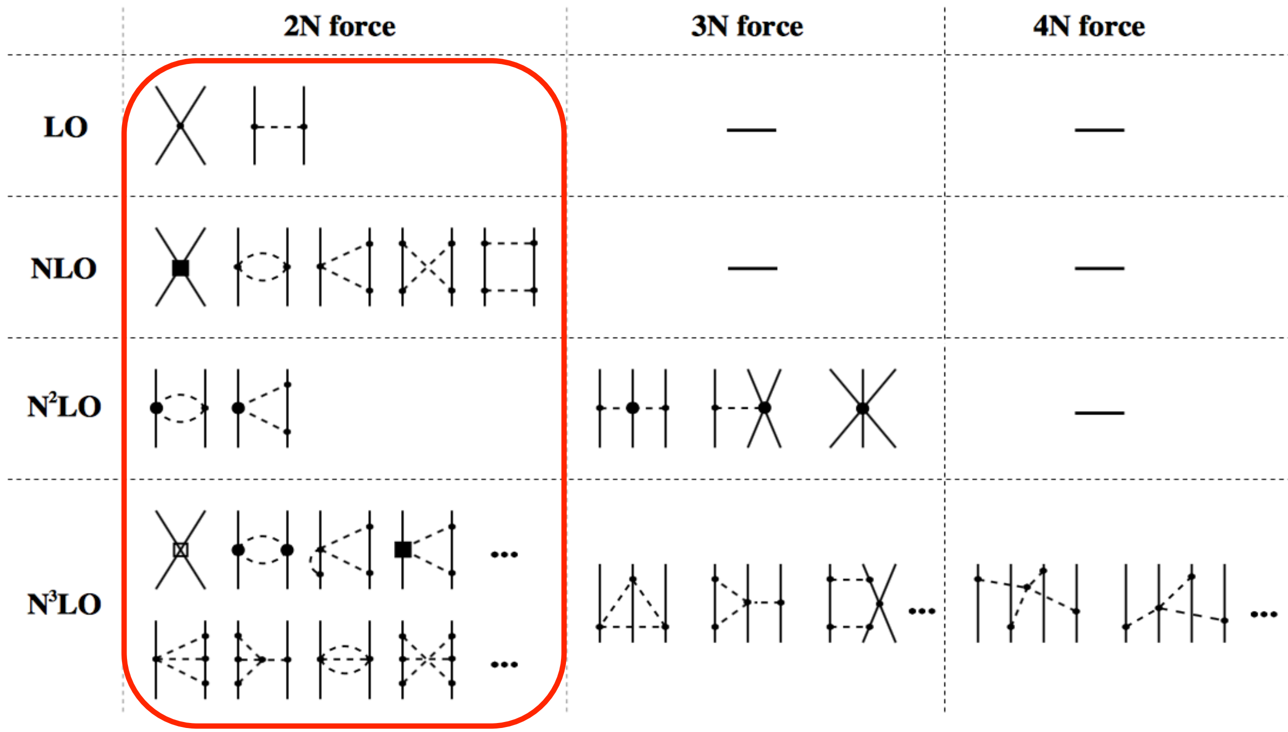
⇒ the chiral effective-field-theory (EFT) interactions

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 systematically 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 ≈ 3-16)

Green's Function Monte Carlo Method

No-Core Shell Model

…

For medium mass nuclei (A ≈ 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}He, ^{16}O, and ^{40}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

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

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

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

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

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

One-body correlation operator two-body correlation operator

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

Cluster expansion of the transformed Hamiltonian

$$\tilde{H} = \tilde{H}^{(1)} + \tilde{H}^{(2)} + \tilde{H}^{(3)} \, + \cdots$$

truncated

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

one-body field determined self-consistently

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

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

$$\tilde{H}^{(3)} = \left(\frac{1}{3!} \right)^2 \sum_{\alpha\beta\gamma\lambda\mu\nu} \langle \alpha\beta\gamma | \tilde{v}_{123} | \lambda\mu\nu \rangle c_\alpha^\dagger c_\beta^\dagger c_\gamma^\dagger c_\nu c_\mu c_\lambda - \left(\frac{1}{2!} \right)^2 \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \tilde{u}_{12} | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

truncated

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

three-body transformed interaction $-(\tilde{h}_1 + \tilde{h}_2 + \tilde{h}_3 + \tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31})$

determination of correlation operator

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

$$H^{(n)}\left|\psi_k^{(n)}\right\rangle = E_k\left|\psi_k^{(n)}\right\rangle$$

n=1, 2 one- and two-body Schrödinger equation

$$\left|\psi_k^{(n)}\right\rangle = \left|\phi_k^{(n)}\right\rangle + \omega^{(n)}\left|\phi_k^{(n)}\right\rangle$$

P-space component

decomposition of the wave function into the P and Q components

mapping operator ω satisfies the decoupling condition.

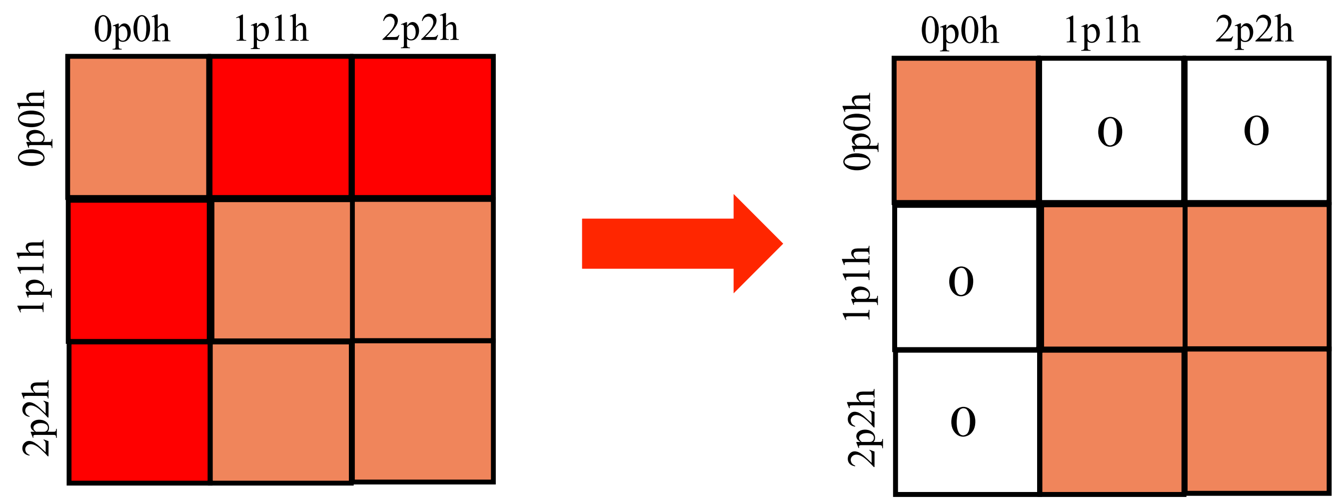
$$Q^{(n)}(1-\omega^{(n)})H^{(n)}(1+\omega^{(n)})P^{(n)} = 0$$

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

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

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

Hamiltonian after the transformation



original Hamiltonian

Ground-state energy

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

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

Charge radius

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

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

R^2_p, R^2_n: mean-square radii of proton and neutron, respectively
R^2_p = 0.832 fm^2 and R^2_n = -0.115 fm^2 are used in this work.

$$r_p^2 \equiv \frac{1}{Z} \sum_{i=1}^{Z} \left(\vec{r}_i - \vec{R}_{c.m.} \right)^2 \Rightarrow \quad r_p^{(1)} + r_p^{(2)}$$

decomposition into one- and two-body parts

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

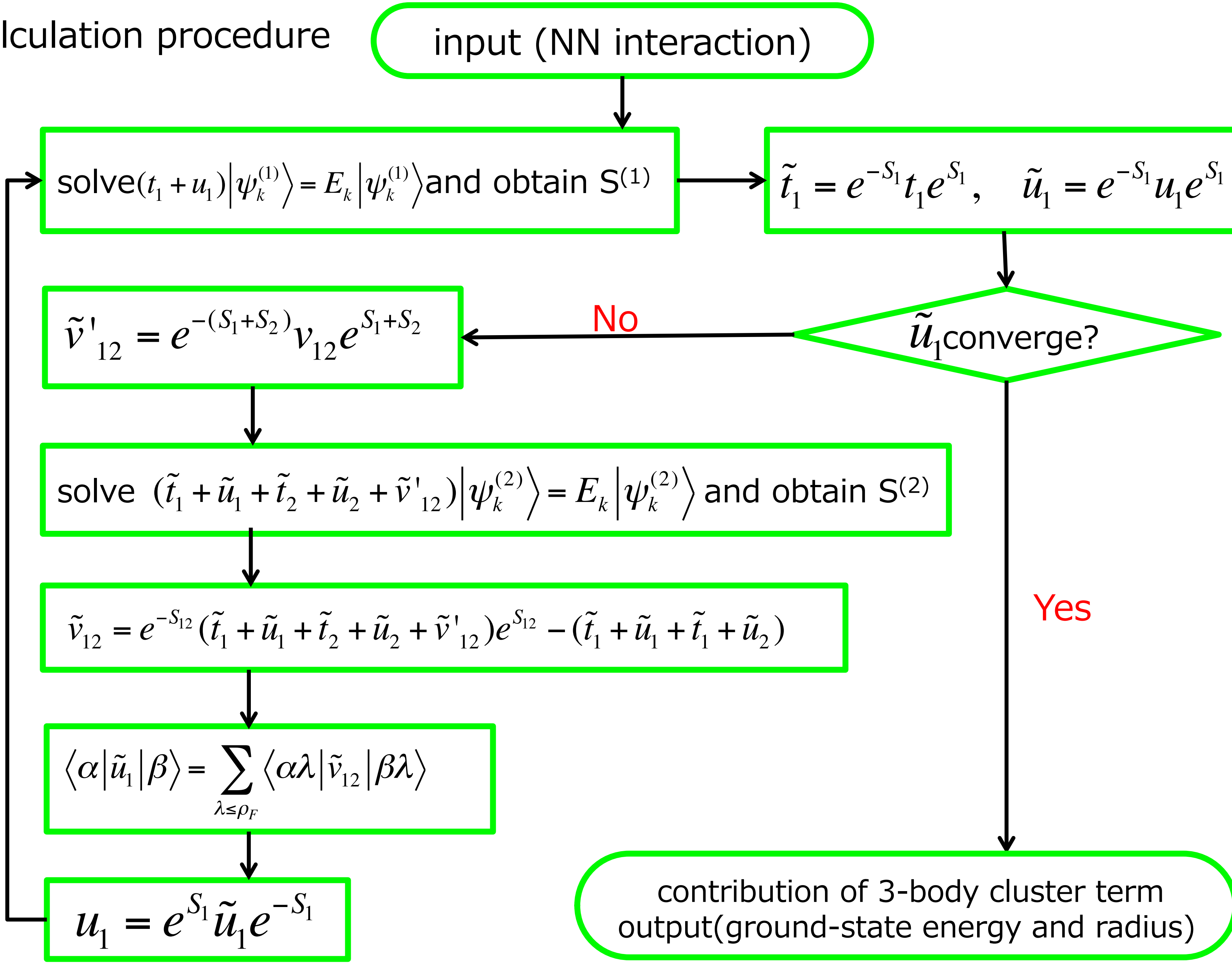
$$\langle \Psi | r_p | \Psi \rangle = \langle \Phi | U^{-1} r_p U | \Phi \rangle = \langle \Phi | \tilde{r}_p | \Phi \rangle \qquad \tilde{r}_p = \tilde{r}_p^{(1)} + \tilde{r}_p^{(2)} + \cdots$$

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

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

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

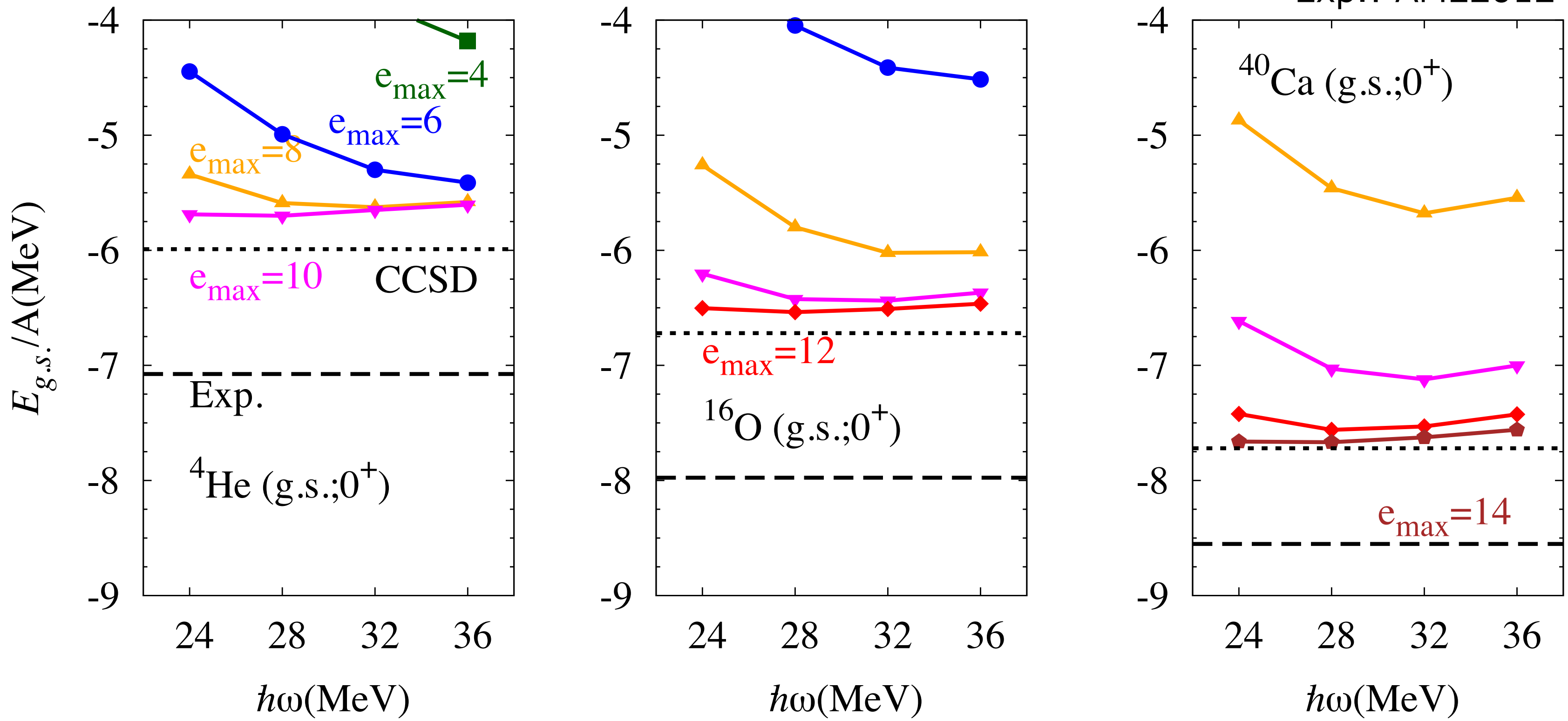
calculation procedure



Ground-state energies

interaction: chiral NN interaction at N^3LO by Entem & Machleidt (Λ=500MeV)
model space: e_{max} = max(2n+l)

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

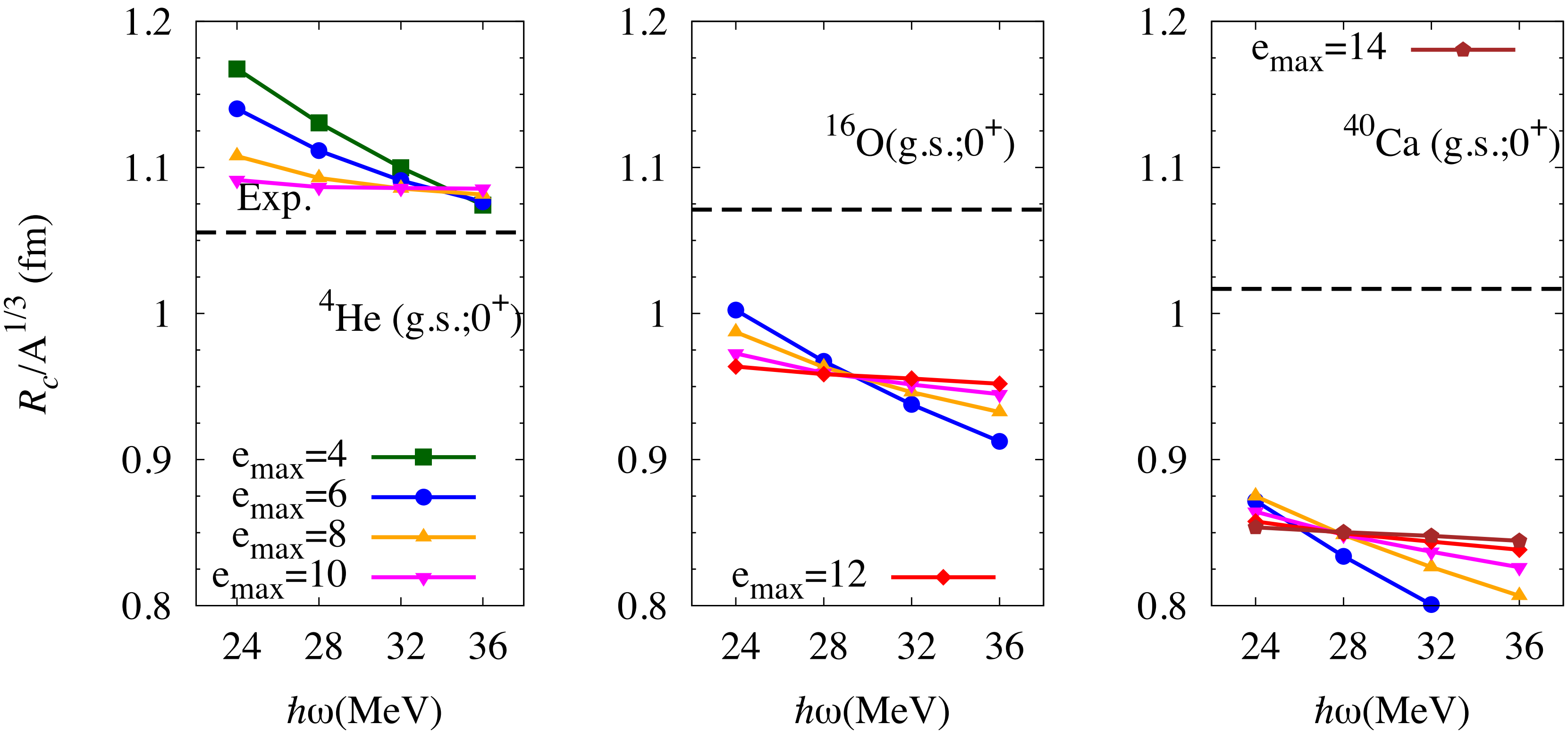


Our results are close to the CCSD results, while underbound to the experimental data.

Charge radii

interaction: chiral NN interaction at N^{3}LO by Entem & Machleidt (Λ=500MeV)
model space: e_{max} = max(2n+l)

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

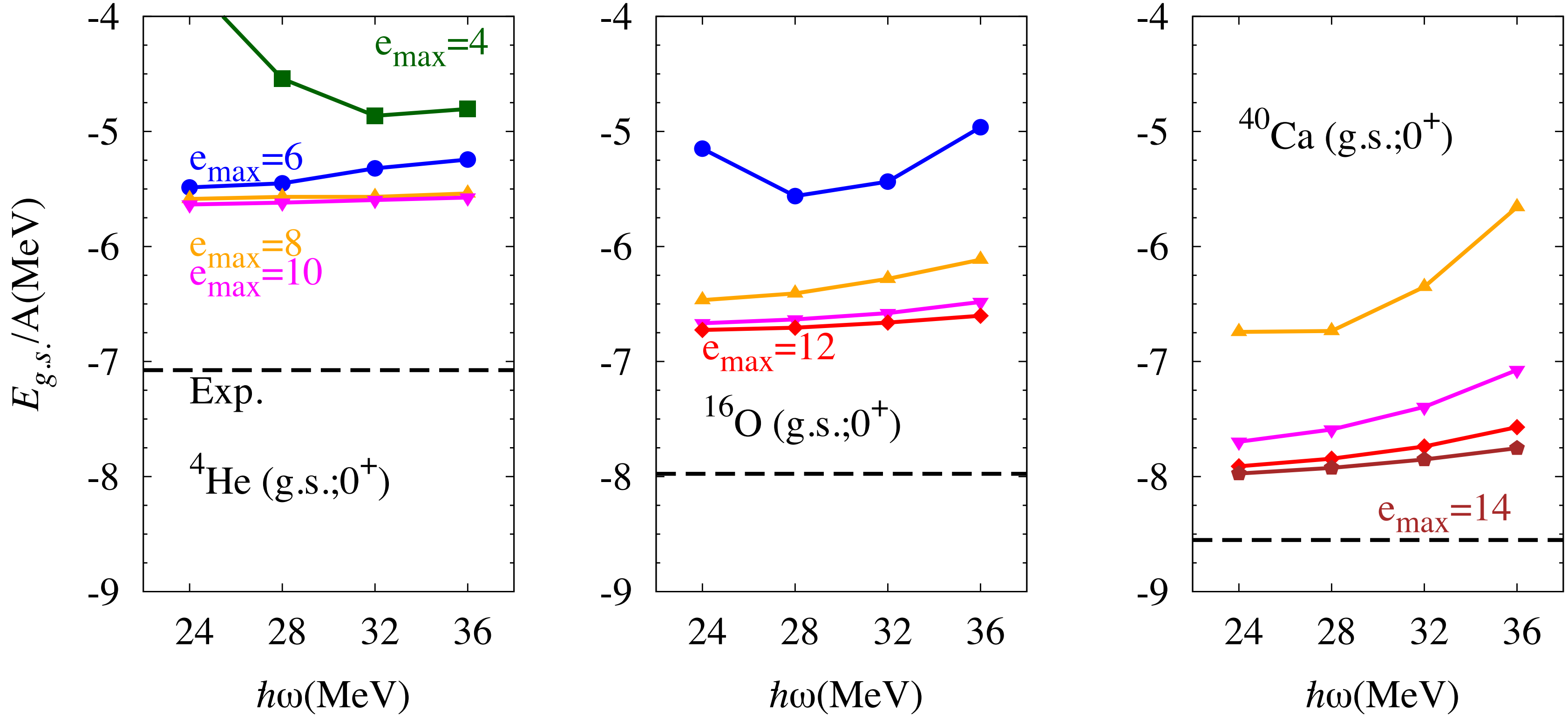


overestimate for ^{4}He, while underestimate for ^{16}O and ^{40}Ca

Ground-state energies

interaction: chiral NN interaction at N^{3}LO by Epelbaum (Λ = 450 MeV)
model space: e_{max} = max(2n+l)

Exp.: AME2012

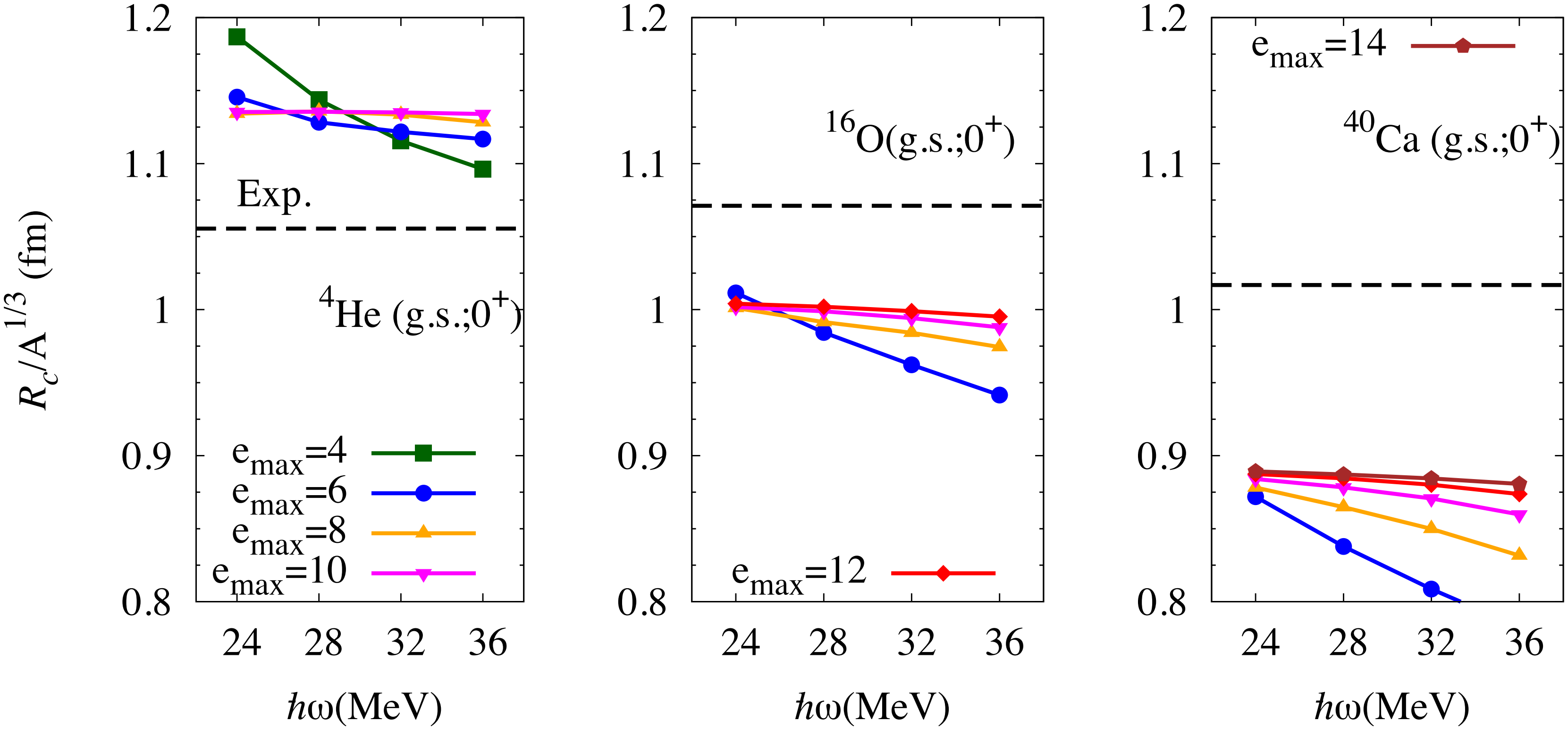


underbound to the experimental data

Charge radii

interaction: chiral NN interaction at N^{3}LO by Epelbaum (Λ = 450 MeV)
model space: e_{max} = max(2n+l)

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

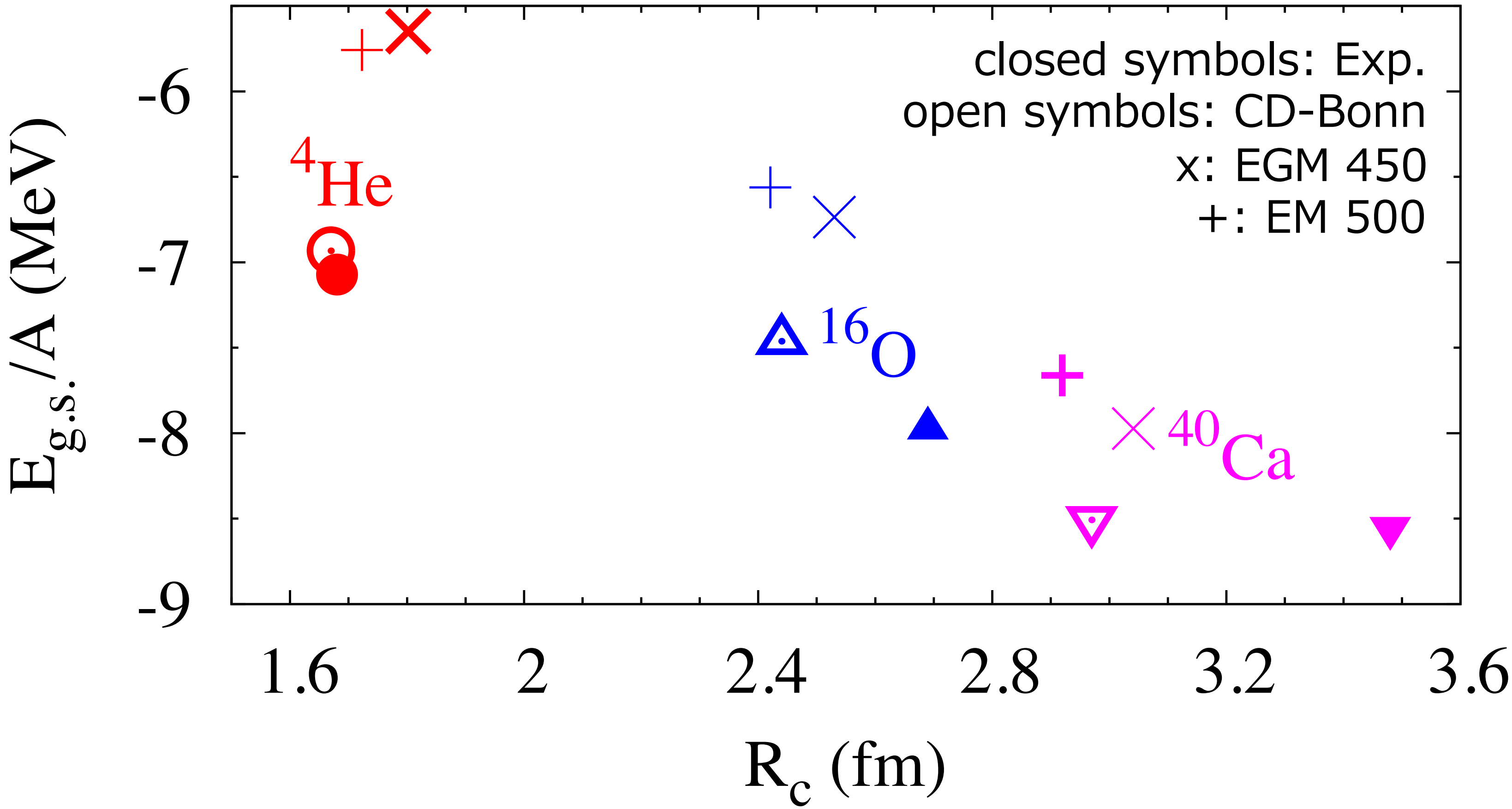


overestimate for ^{4}He, while underestimate for ^{16}O, ^{40}Ca

saturation property

Energy: underbound
radii: small

similar to the results with the CD-Bonn potential



Summary

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

Iterative treatment of the three-body cluster term