Towards the inclusion of three-body forces in the unitary-model-operator approach

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Motivation

- It is well known that effects of three-nucleon forces (3NFs) are indispensable to reproduce and to understand the nuclear structure and reactions.

- Ab initio calculation methods for medium mass nuclei.
  - Coupled-Cluster Method
  - Self-Consistent Green's Function Method
  - In-Medium Similarity Renormalization Group Approach
  - Unitary-Model-Operator Approach (UMOA)

    3NF effects cannot be included in the UMOA so far.

- Purpose of this work is to extend the UMOA framework towards the inclusion of 3NFs.

Unitary-Model-Operator Approach (UMOA)

K. Suzuki and R. Okamoto, Prog. Theor. Phys. 92, 1045 (1994).

- Similarity transformation

$$\widetilde{H} = U^{\dagger} H U$$

$$H = \sum_{i}^{A} t_i + \sum_{i<j}^{A} v_{ij} \qquad H|\Psi\rangle = E|\Psi\rangle \rightarrow \widetilde{H}|\Phi\rangle = E|\Phi\rangle$$

- Unitary operator U

$$U = e^{S^{(1)}} e^{S^{(2)}} e^{S^{(3)}} \qquad S^{(1)} = \sum_{i}^{A} s_i, \quad S^{(2)} = \sum_{i<j}^{A} s_{ij}, \quad S^{(3)} = \sum_{i<j<k}^{A} s_{ijk}$$

- Cluster expansion of the transformed Hamiltonian

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

explicitly treated in this work

Unitary-Model-Operator Approach (UMOA)

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$$\widetilde{H}^{(1)} = \sum_{\alpha\beta} \langle \alpha | \widetilde{h}_1 | \beta \rangle c_\alpha^\dagger c_\beta, \quad \widetilde{h}_1 = \widetilde{t}_1 + \widetilde{w}_1 = e^{-s_1}(t_1 + w_1)e^{s_1}$$

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

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

$$\widetilde{v}_{12} = e^{-s_{12}} e^{-(s_1+s_2)} (h_1 + h_2 + v_{12}) e^{s_1+s_2} e^{s_{12}} - (\widetilde{h}_1 + \widetilde{h}_2)$$

$$\begin{aligned}\widetilde{v}_{123} = {} & e^{-s_{123}} e^{-(s_{12}+s_{23}+s_{31})} e^{-(s_1+s_2+s_3)} \\ & \times (h_1 + h_2 + h_3 + v_{12} + v_{23} + v_{31} + w_{12} + w_{23} + w_{31} + v_{123}) \\ & \times e^{s_1+s_2+s_3} e^{s_{12}+s_{23}+s_{31}} e^{s_{123}} \\ & - (\widetilde{h}_1 + \widetilde{h}_2 + \widetilde{h}_3 + \widetilde{v}_{12} + \widetilde{v}_{23} + \widetilde{v}_{31})\end{aligned}$$

$$\langle \alpha | \widetilde{w}_1 | \beta \rangle = \sum_{\lambda \le \rho_F} \langle \alpha\lambda | \widetilde{v}_{12} | \beta\lambda \rangle - \sum_{\lambda\mu \le \rho_F} \frac{1}{2} \langle \alpha\lambda\mu | \widetilde{v}_{123} | \beta\lambda\mu \rangle \quad w_1 = e^{s_1} \widetilde{w}_1 e^{-s_1}$$

$$w_{12} = e^{-s_{12}} e^{-(s_1+s_2)} (\widetilde{w}_1 + \widetilde{w}_2 + \widetilde{w}_{12}) e^{s_1+s_2} e^{s_{12}}$$

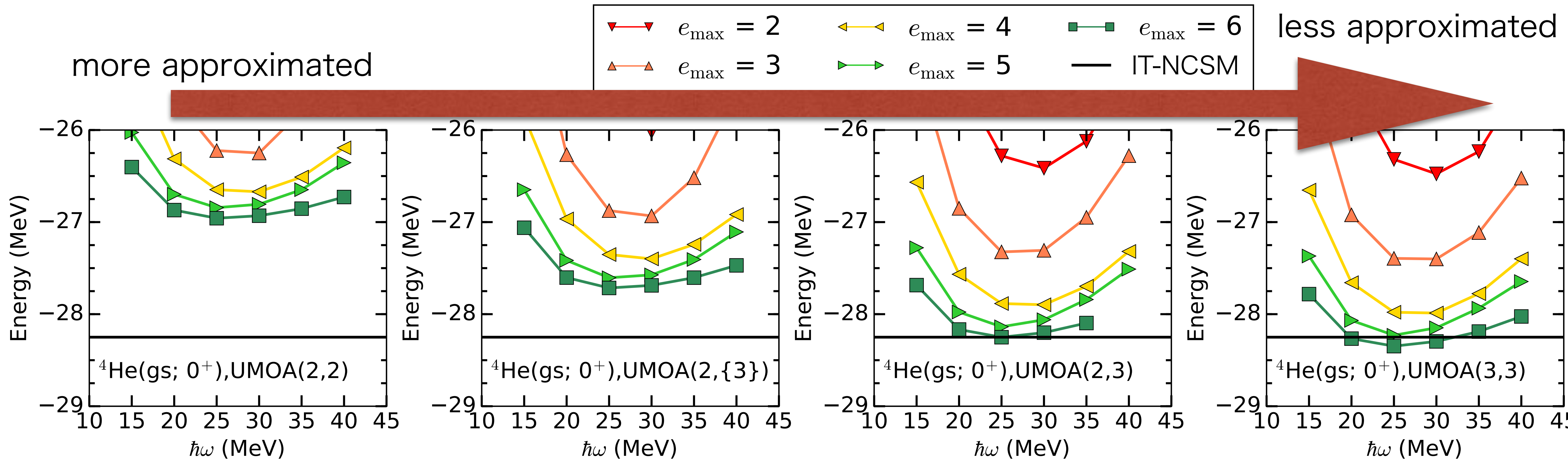
$$\langle \alpha\beta | \widetilde{w}_{12} | \gamma\delta \rangle = \sum_{\lambda \le \rho_F} \langle \alpha\beta\lambda | \widetilde{v}_{123} | \gamma\delta\lambda \rangle$$

Numerical results for ^{4}He

- Calculation setup
  - ★ interaction: SRG transformed NN interaction (NN-only)
  - ★ model space: $e_{max} = \max(2n + l)$
- Calculation rank: UMOA(m, n)

m: $S^{(1)}, \cdots, S^{(m)}$ are included

n: $\tilde{H}^{(1)}, \cdots, \tilde{H}^{(n)}$ are included



2-body level | 3BC, pert. | 3BC, full | 3-body level

effect of the 3-body correlation is small.

IT-NCSM: R. Roth et al., PRL 107, 072501 (2011).

Summary & Future work

- ✦ The extension of the UMOA framework is completed up to the three-body level towards the inclusion of 3NFs.
- ✦ The test calculations are done for ^{4}He with the SRG transformed NN interaction.
- ✦ Our energies are reasonably close to the IT-NCSM energy. The effect of the three-body correlation operator $S^{(3)}$ is small.
- ✦ Inclusion of 3NF is underway.

Techniques for three-body state

- An orthonormal basis set is used.

$$\mathcal{A}|abc:iJ\rangle = |abc:iJ\rangle$$ A is the antisymmetrization operator

i is a label introduced instead of intermediate angular momentum J_{ab}

$$(abc(J_1):J|\mathcal{A}|def(J_2):J') = \sum_{\{m\}} C^{j_a j_b J_1} C^{J_1 j_c J} C^{j_d j_e J_2} C^{J_2 j_f J'} (\alpha\beta\gamma|\mathcal{A}|\delta\epsilon\phi)$$

$$= \frac{1}{6}\Big[\delta_{ad}\delta_{be}\delta_{cf}\delta_{J_1 J_2} - (-1)^{j_a+j_b-J_2}\delta_{ae}\delta_{bd}\delta_{cf}\delta_{J_1 J_2} - (-1)^{j_b+j_c+J_2}\hat{J}_1\hat{J}_2 \begin{Bmatrix} j_a & j_b & J_1 \\ j_c & J & J_2 \end{Bmatrix} \delta_{af}\delta_{bd}\delta_{ce}$$

$$+\hat{J}_1\hat{J}_2 \begin{Bmatrix} j_a & j_b & J_1 \\ j_c & J & J_2 \end{Bmatrix} \delta_{af}\delta_{be}\delta_{cd} - (-1)^{j_a+j_b+J_1}\hat{J}_1\hat{J}_2 \begin{Bmatrix} j_a & j_b & J_1 \\ J & j_c & J_2 \end{Bmatrix} \delta_{ae}\delta_{bf}\delta_{cd}$$

$$+(-1)^{j_a+j_c+J_2}(-1)^{j_a+j_b+J_1}\hat{J}_1\hat{J}_2 \begin{Bmatrix} j_a & j_b & J_1 \\ J & j_c & J_2 \end{Bmatrix} \delta_{ad}\delta_{bf}\delta_{ce}\Big]\delta_{JJ'}$$

$$|abc:iJ\rangle = \sum_{a'b'c'J_1} |a'b'c':J_1 J)(a'b'c':J_1 J|abc:iJ\rangle = \sum_{J_1} P(abc) c^i_{abcJ_1} |abc:J_1 J).$$

non-antisymmetrized three-body state

Techniques for three-body state

- ✦ Matrix elements
  - ★ One-body operator

$$\langle a_1 a_2 a_3 \colon iJ | O^{(1)} | a_4 a_5 a_6 \colon i'J \rangle \\ = 3 \sum_{J_{a_1 a_2} J_{a_4 a_5}} P(a_1 a_2 a_3) P(a_4 a_5 a_6) c^{i*}_{a_1 a_2 a_3 J_{a_1 a_2}} c^{i'}_{a_4 a_5 a_6 J_{a_4 a_5}} o_{a_1 a_4} \delta_{a_2 a_5} \delta_{a_3 a_6},$$

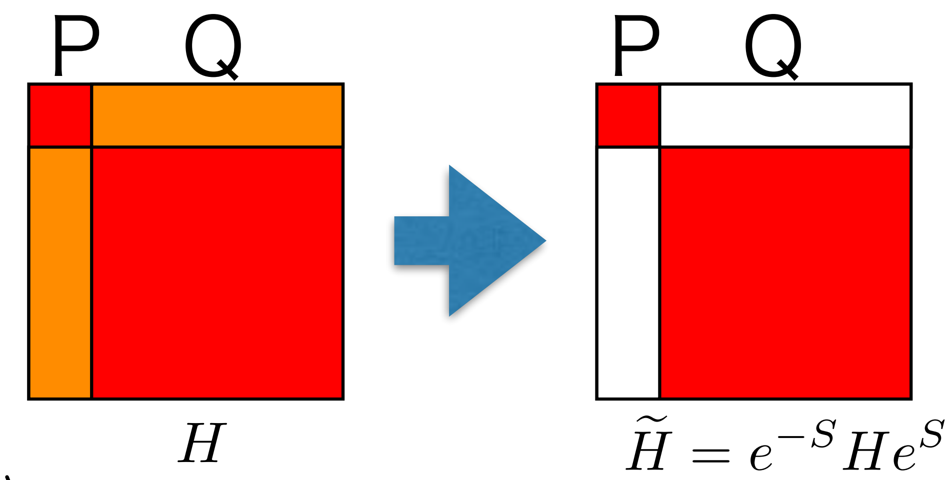
  - ★ Two-body operator

$$\langle a_1 a_2 a_3 \colon iJ | O^{(2)} | a_4 a_5 a_6 \colon i'J \rangle \\ = \frac{3}{2} \sum_{J_{a_1 a_2} J_{a_4 a_5}} P(a_1 a_2 a_3) P(a_4 a_5 a_6) c^{i*}_{a_1 a_2 a_3 J_{a_1 a_2}} c^{i'}_{a_4 a_5 a_6 J_{a_4 a_5}} \delta_{J_{a_1 a_2} J_{a_4 a_5}} \delta_{a_3 a_6} \Delta_{a_1 a_2} \Delta_{a_4 a_5} o^{J_{a_1 a_2}}_{a_1 a_2 a_4 a_5}.$$

$$\begin{aligned} o_{a_1 a_2} &= \langle a_1 | o_1 | a_2 \rangle, \\ o^{J}_{a_1 a_2 a_3 a_4} &= \langle a_1 a_2 \colon J | o_{12} | a_3 a_4 \colon J \rangle, \\ \Delta_{a_1 a_2} &= \sqrt{1 + \delta_{a_1 a_2}}. \end{aligned}$$

UMOA - correlation operator

Okubo-Lee-Suzuki method



- Procedure for correlation operator S
  - solve an eigen value problem

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

  - P and Q are the projection operators
  - The k-th eigen vector can be decomposed into P- and Q-space components

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

  - Formal solution of ω

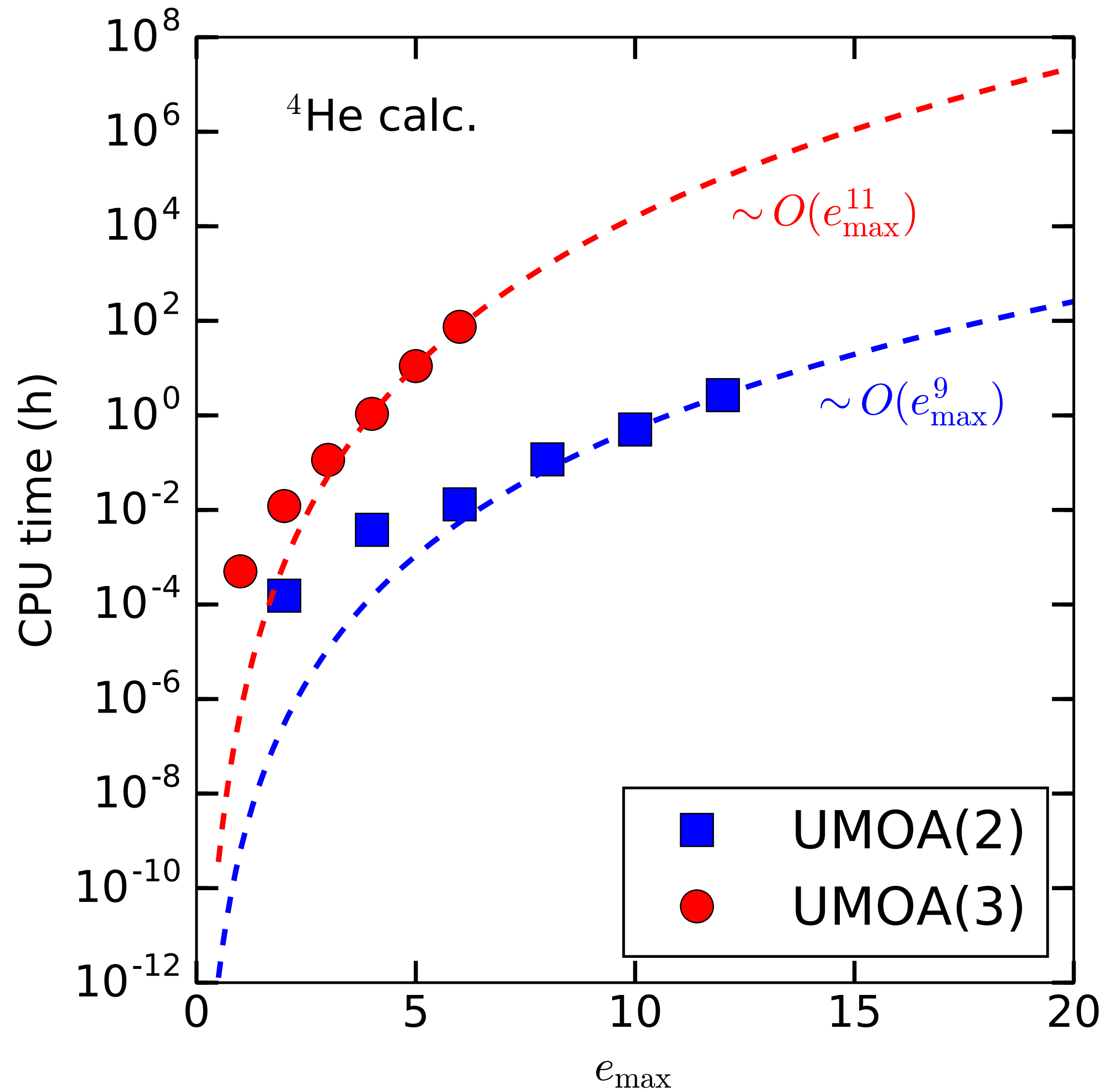
$$\omega = \sum_{k=1}^{d} Q|\psi_k\rangle\langle\widetilde{\phi}_k|P$$

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

- Transformed Hamiltonian satisfies $Q\widetilde{H}P = P\widetilde{H}Q = 0$

Computational aspect

✦ Single node calculation for ^{4}He



Parallel computations are needed.