Applications of the unitary-model-operator approach to the closed sub-shell nuclei

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Motivation
ab-initio calculations related to this work

To understand microscopically structure of 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

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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)

…

So far, we calculated the ground-state energies and charge radii of ^{4}He, ^{16}O, ^{40}Ca, and ^{56}Ni in the UMOA. (TM et al., PTEP (2015).)

To examine the applicability of the UMOA to the sub-shell closed nuclei, we calculate the oxygen isotopes in this work.

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

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

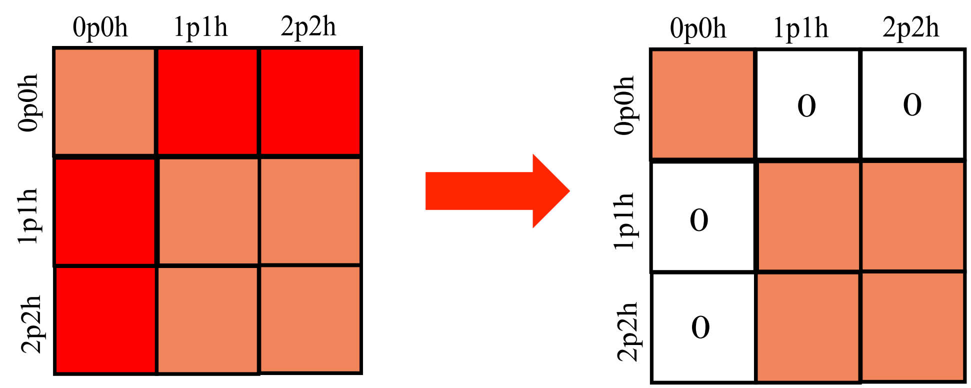
$$U = e^{S^{(1)}} e^{S^{(2)}}$$

$$S^{(1)} = \sum_{\alpha\beta} \langle \alpha | S_1 | \beta \rangle c_\alpha^\dagger c_\beta$$

one-body correlation operator

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

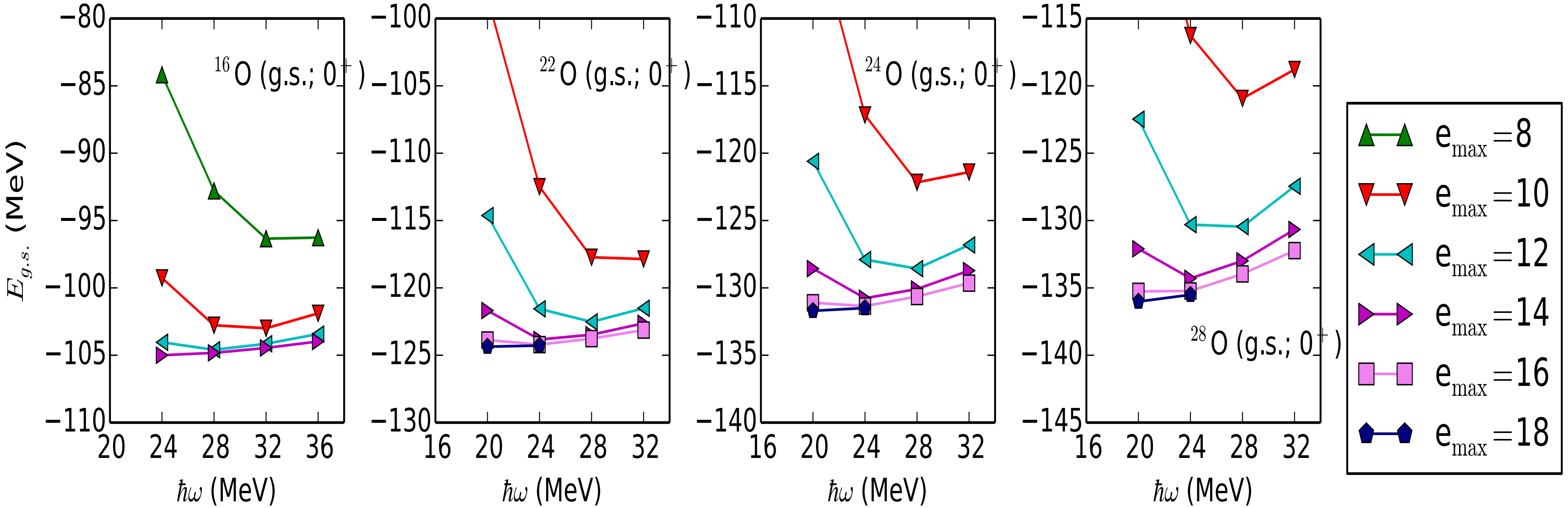
two-body correlation operator



S$^{(1)}$ and S$^{(2)}$ are determined self-consistently.

Ground-state energies of oxygen isotopes

interaction: chiral NN interaction at N^{3}LO (EM Λ=500 MeV)
model space: $e_{\max} = \max(2n+l)$

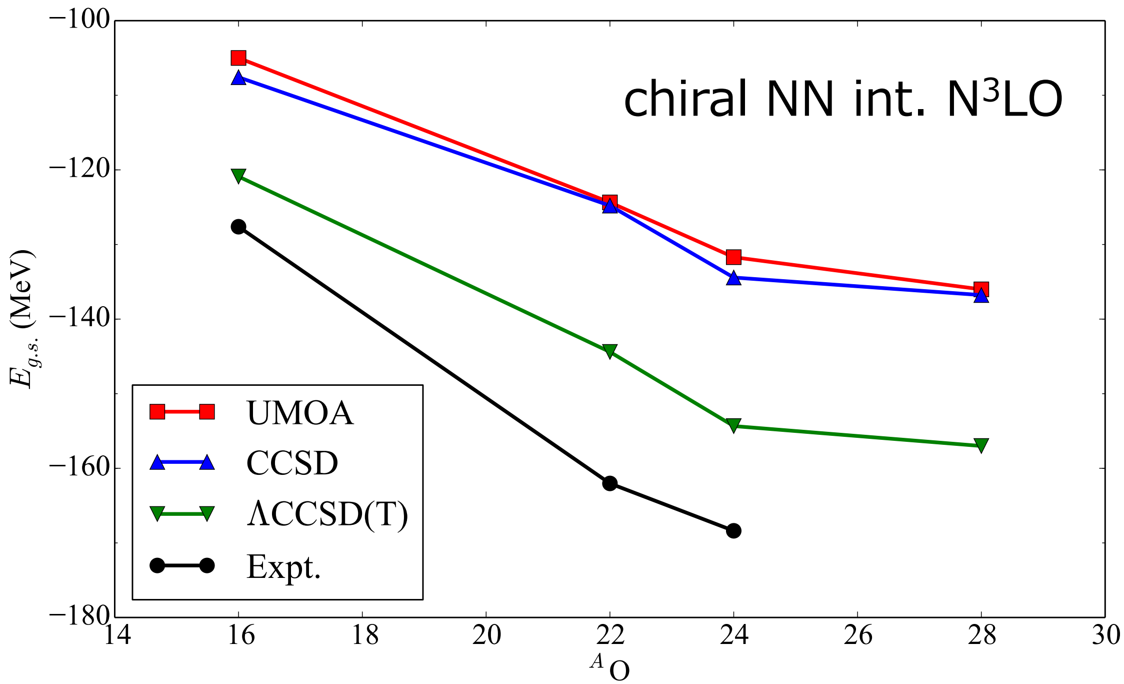


Our energies obtained with largest model space are almost converged.

Summary

We calculated the ground-state energies of the sub-shell closed oxygen isotopes.

Our energies are close to the CCSD results with the same interaction.



CCM results : G. Hagen et al., PRC (2009).

Future work

According to the CCSD and ΛCCSD(T) results, the contribution of triple excitations is not so small. The introduction of the three-body correlation operator ($S^{(3)}$) would be needed, if we use the bare interactions.

Backup

Unitary-Model-Operator Approach (UMOA)

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

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

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

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

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

One-body correlation operator two-body correlation operator

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

Cluster expansion of the transformed Hamiltonian

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

truncated

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

one-body field determined self-consistently

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

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

two-body transformed interaction

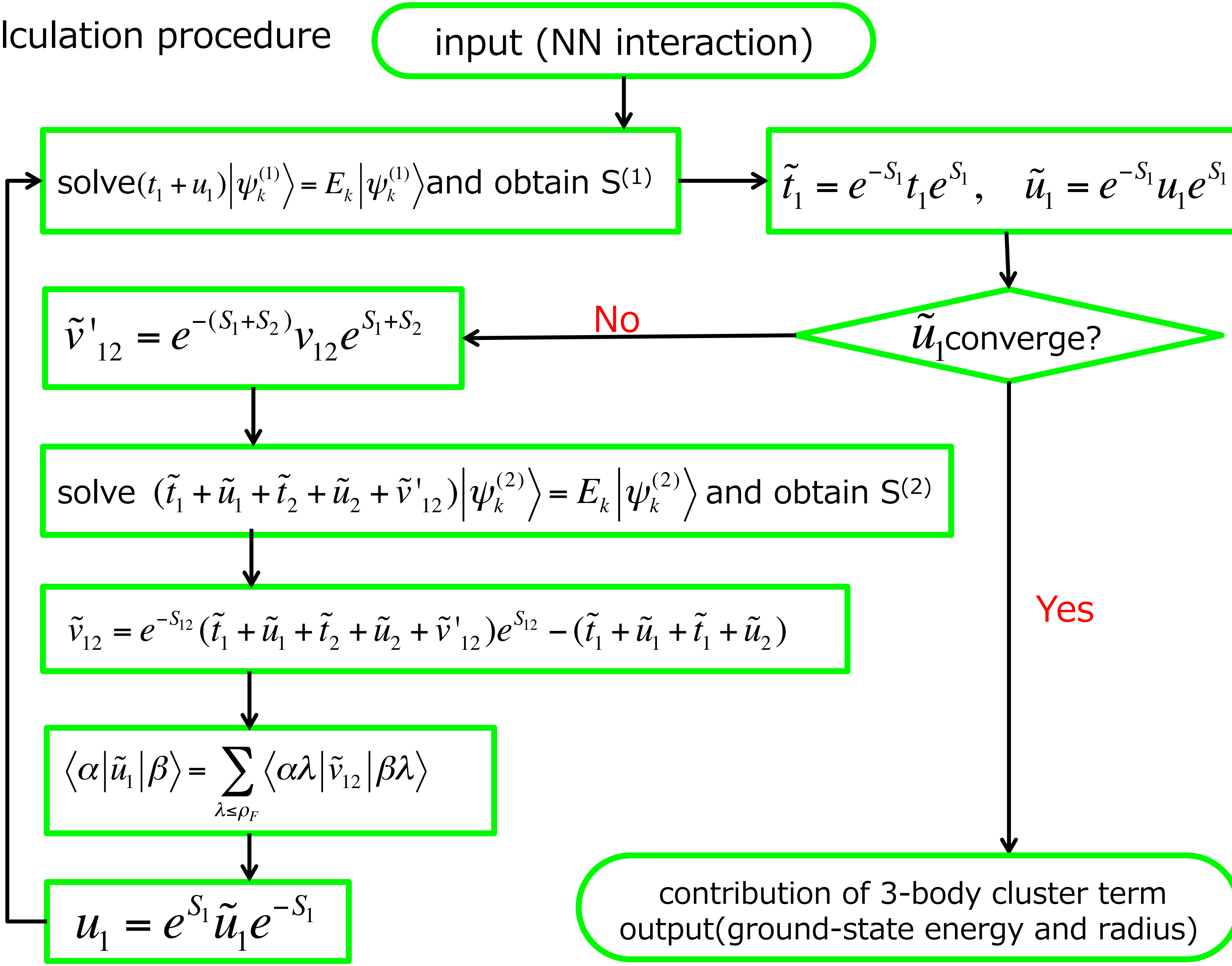
$$\tilde{H}^{(3)} = \left(\frac{1}{3!} \right)^2 \sum_{\alpha\beta\gamma\lambda\mu\nu} \langle \alpha\beta\gamma | \tilde{v}_{123} | \lambda\mu\nu \rangle c_\alpha^\dagger c_\beta^\dagger c_\gamma^\dagger c_\nu c_\mu c_\lambda - \left(\frac{1}{2!} \right)^2 \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta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

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

calculation procedure



$S^{(1)}$ and $S^{(2)}$ are determined self-consistently.

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

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

decomposition of the wave function into the P and Q components

P-space component

mapping operator ω satisfies the decoupling condition.

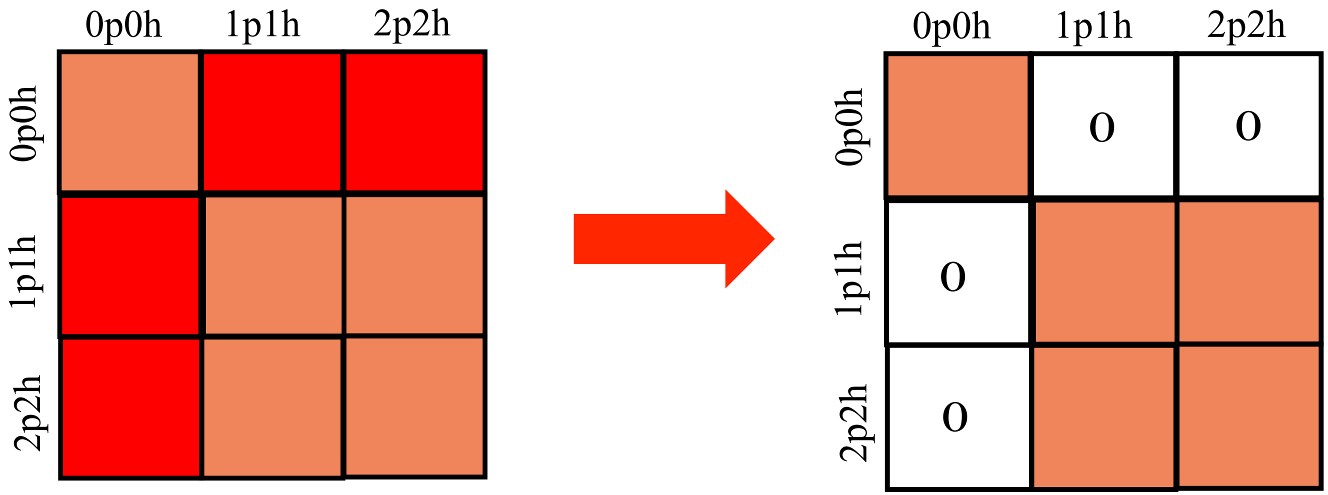
$$Q^{(n)}(1-\omega^{(n)})H^{(n)}(1+\omega^{(n)})P^{(n)} = 0$$

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

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

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

Hamiltonian after the transformation



original Hamiltonian

Ground-state energy

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

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