Coupled Cluster theory and its application to medium sized nuclei.
Extending the Ab-Initio program beyond the lightest nuclei.

- Need a theory which scales softly with system size and can be systematically improved.
- Need a theory which scales correctly with system size. *Size Extensivity* ensures that the energy scales linearly with number of particles.
- Coupled Cluster theory a promising candidate.
Quantum many-body theory a historical perspective.

**Many-Body Problem for Strongly Interacting Particles. II. Linked Cluster Expansion**

K. A. Brueckner

Indiana University, Bloomington, Indiana

(Received April 28, 1955)

An approximation method developed previously to deal with many particles in strong interaction is examined in further detail. It is shown that the series giving the interaction energy is a development in a sequence of linked or irreducible cluster terms each of which gives a contribution to the energy proportional to the total number of particles. Consequently the convergence of the expansion is independent of the total number of particles. The origin of this simple feature is illustrated by showing that a similar situation exists in the expansion of standard perturbation theory. The numerical convergence of the expansion is quantitatively discussed for the nuclear problem where it is shown that the correction arising from the first cluster term involving three particles is less than the leading term by a factor of about $10^{-4}$. The smallness of the correction is largely a result of the action of the exclusion principle.

**Size Extensive Theories:** FCI (NCSM), Many-body Perturbation theory, Coupled-Cluster theory

**Size Inextensive Theories:** Particle-hole truncated CI (shell-model)

505 citations

**Derivation of the Brueckner many-body theory**

By J. Goldstone

Trinity College, University of Cambridge

(Communicated by N. F. Mott, F.R.S.—Received 24 August 1956)

An exact formal solution is obtained to the problem of a system of fermions in interaction. This solution is expressed in a form which avoids the problem of unlinked clusters in many-body theory. The technique of Feynman graphs is used to derive the series and to define linked terms. The graphs are those appropriate to a system of many fermions and are used to give a new derivation of the Hartree–Fock and Brueckner methods for this problem.

- BE ~ A
- Series converges for all A
- NO unlinked diagrams in energy evaluation
- Fast convergence in cluster rank
- Precursor to Coupled Cluster theory

1,062 citations

The description of collective motions in terms of many-body perturbation theory

By J. Hubbard

Atomic Energy Research Establishment, Harwell, Didcot, Berkshire

(Communicated by R. E. Peierls, F.R.S.—Received 2 February 1957)

In this and a succeeding paper it is shown how a theory equivalent to the Bohm & Pines collective motion theory of the electron plasma can be derived directly from a perturbation series which gives in principle an exact solution of the many-body problem. This result is attained by making use of a diagrammatic method of analysis of the perturbation series. By a process analogous to the elimination of photon self-energy parts from the electrodynamics S matrix it is found possible to simplify the perturbation series, introducing a modified interaction between the particles. A useful integral equation for this modified interaction can be set up, and it is shown how the energy of the system can be expressed in terms of this modified interaction. The close connexion between this approach and the dielectric theory of plasma oscillations is indicated.

500 citations
Historical Perspective

First papers explicitly describing Coupled-Cluster theory

Bishop, Flynn, Buendia, Guardiola, PRC42, 1341 (1990)
Mihala & Heisenberg, PRL84, 1403 (2000)
A short history of coupled-cluster theory

Formal introduction:
1958: Coester, Nucl. Phys. 7, 421
1960: Coester and Kummel, Nucl. Phys. 17, 477

Introduction into Chemistry (late 60’s):

Numerical implementations
1978: Pople et al., Int. J. Quantum Chem Symp, 14, 545
1978: Bartlett and Purvis, Int. J. Quantum Chem 14, 561

Initial nuclear calculations (1970’s):
1978: Kummel, Luhrmann, Zabolitzky, Phys. Rep. 36, 1 and refs. therein
1980-90s: Bishop’s group. Coordinate space.

Few applications in nuclei, explodes in chemistry and molecular sciences.
  Hard-core interactions; computer power; unclear interactions

Nuclear physics reintroduction: (1/E_{ph} expansion)
  Three nuclei; JJ coupled scheme; bare interactions, approximate V_{3N}

Useful References
Crawford and Schaefer, Reviews in Computational Chemistry, 14, 336 (2000)
Coupled-Cluster theory

- Coupled-Cluster theory is fully microscopic
- Coupled-Cluster theory is size extensive. NO unlinked diagrams enters, and energy scales linearly with number of particles.
- Low computational cost
- Capable of systematic improvements
- Amenable to parallel computing

Computational Chemistry: 100's of publications in any year (Science Citation Index) for applications and developments.
Coupled Cluster theory.

Exponential Ansatz for $\Psi$

$$|\Psi\rangle = e^{\hat{T}} |\Phi_0\rangle, \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$

$$\hat{T}_1 = \sum_{i,a} t_i^a \hat{a}_a^\dagger \hat{a}_i, \quad \hat{T}_2 = \frac{1}{2} \sum_{i<j,a<b} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i.$$

Coupled Cluster Equations

$$\Delta E = \langle \Phi_0 | (H_N \exp(T))_C | \Phi_0 \rangle$$

$$0 = \langle \Phi_p | (H_N \exp(T))_C | \Phi_0 \rangle$$

$$\tilde{H} = (H_N \exp(T))_C$$

Iterative CCSDT-n approximations to full CCSDT

CCSDT - 1

$$0 = \langle \Phi_{ijk}^{abc} | (F_N T_3 + H_N T_2)_C | \Phi_0 \rangle$$

CCSDT - 2

$$0 = \langle \Phi_{ijk}^{abc} | \left( F_N T_3 + H_N T_2 + H_N T_2^2 / 2 \right)_C | \Phi_0 \rangle$$

CCSDT - 3

$$0 = \langle \Phi_{ijk}^{abc} | (F_N T_3 + H_N \exp(T_1 + T_2))_C | \Phi_0 \rangle$$

CCSDT

$$0 = \langle \Phi_{ijk}^{abc} | (H_N \exp(T_1 + T_2 + T_3))_C | \Phi_0 \rangle$$
Coupled-Cluster in pictures


\[ |\Psi\rangle = e^{T^{(A)}} |\Phi\rangle, \quad T^{(A)} = \sum_{k=1}^{m_A} T_k \]

\[ T_1 |\Phi\rangle = \sum_{i} t^i_a |\Phi^a_i\rangle, \quad T_2 |\Phi\rangle = \sum_{i > j} t^{ij}_{ab} |\Phi^{ab}_{ij}\rangle, \quad T_3 |\Phi\rangle = \sum_{i > j > k} t^{ijk}_{abc} |\Phi^{abc}_{ijk}\rangle, \text{ etc.} \]

\[ m_A = N \quad - \quad \text{exact theory} \]
\[ m_A < N \quad - \quad \text{approximate methods} \]

\[ m_A = 2 \quad T = T_1 + T_2 \quad \text{CCSD} \quad n_o^2 n_u^4 (n_o^2 n_u^2) \]
\[ m_A = 3 \quad T = T_1 + T_2 + T_3 \quad \text{CCSDT} \quad n_o^3 n_u^5 (n_o^3 n_u^3) \]
\[ m_A = 4 \quad T = T_1 + T_2 + T_3 + T_4 \quad \text{CCSDTQ} \quad n_o^4 n_u^6 (n_o^4 n_u^4) \]
\[ m_A = 5 \quad T = T_1 + T_2 + T_3 + T_4 + T_5 \quad \text{CCSDTQP} \quad n_o^5 n_u^7 (n_o^5 n_u^5) \]
The normal ordered Hamiltonian

Wicks theorem:

\[ ABC \ldots = \{ ABC \ldots \} + \sum_{\text{all single contractions}} \{ ABC \ldots \} \]

\[ + \sum_{\text{all double contractions}} \{ ABC \ldots \} \]

\[ + \cdots + \sum_{\text{all fully contracted products}} \{ ABC \ldots \} \] (45)

One-body term:

\[ p^\dagger q = \{ p^\dagger q \} + \{ p^\dagger q \} = \{ p^\dagger q \} + \delta_{pq=i} \]

Two-body term:

\[ p^\dagger q^\dagger sr = \{ p^\dagger q^\dagger sr \} + \{ p^\dagger q^\dagger sr \} + \{ p^\dagger q^\dagger sr \} \]

\[ + \{ p^\dagger q^\dagger sr \} + \{ p^\dagger q^\dagger sr \} \]

\[ + \{ p^\dagger q^\dagger sr \} + \{ p^\dagger q^\dagger sr \} \]

\[ = \{ p^\dagger q^\dagger sr \} + p^\dagger r \{ q^\dagger s \} + q^\dagger s \{ p^\dagger r \} \]

\[ - p^\dagger s \{ q^\dagger r \} - q^\dagger r \{ p^\dagger s \} \]

\[ + p^\dagger r q^\dagger s - p^\dagger s q^\dagger r \] .

The normal ordered Hamiltonian is :

\[ H_N = H - \langle 0 \mid H \mid 0 \rangle, \quad \text{where} \quad H = \sum_p f_{pp} \{ p^\dagger p \} + \sum_{p \neq q} f_{pq} \{ p^\dagger q \} + \frac{1}{4} \sum \langle pq \parallel rs \rangle \{ p^\dagger q^\dagger sr \} \]

\[ + \langle 0 \mid H \mid 0 \rangle. \] (47)
The Coupled-Cluster energy expression

The Baker Hausdorff commutator relation:

\[ \tilde{H}_N = H_N + [H, T] + \frac{1}{2}[[H, T]T] + \frac{1}{3!}[[[H, T]T]T] \]

\[ + \frac{1}{4!}[[[[H, T]T]T]T], \]

\[ \tilde{H}_N = \exp(-T)H_N \exp(T) = [H_N \exp(T)]_C \]

The Coupled-Cluster energy expression:

\[ E = \langle 0 | \tilde{H} | 0 \rangle, \]

\[ E = \langle 0 | H + (HT_1)_C + (HT_2)_C + (HT^2_1/2)_C | 0 \rangle \]

Diagramatic representation:

\[ T_2 = \sum_{i>j,a>b} t^a_{ij} \{ a^\dagger b^\dagger j \} = \]

\[ T_1 = \sum_{i,a} t^a_i \{ a^\dagger i \} = \]
The Coupled Cluster energy expression

\[
\langle 0 \vert (WT_2)_c \vert 0 \rangle = \frac{1}{4} \sum_{ijab} \frac{1}{4} \sum_{pqrs} \langle pq \vert rs \rangle t_{ij}^{ab} \langle 0 \vert \{p^\dagger q^\dagger sr\} \{a^\dagger ib^\dagger j\} + \{p^\dagger q^\dagger sr\} \{a^\dagger ib^\dagger j\} \vert 0 \rangle
\\
+ \{p^\dagger q^\dagger sr\} \{a^\dagger ib^\dagger j\} + \{p^\dagger q^\dagger sr\} \{a^\dagger ib^\dagger j\} \vert 0 \rangle
\\
= \frac{1}{4} \sum_{ai,bj} \langle ij \vert ab \rangle t_{ij}^{ab} = \begin{array}{c}
\end{array}
, \quad
\\
\langle 0 \vert (WT_1^2/2)_c \vert 0 \rangle = \frac{1}{8} \sum_{ijab} \sum_{pqrs} \langle pq \vert rs \rangle t_{ij}^{ab} t_{ij}^{ab} \langle 0 \vert \{p^\dagger q^\dagger sr\} \{a^\dagger i\} \{b^\dagger j\} + \{p^\dagger q^\dagger sr\} \{a^\dagger i\} \{b^\dagger j\} \vert 0 \rangle
\\
+ \{p^\dagger q^\dagger sr\} \{a^\dagger i\} \{b^\dagger j\} + \{p^\dagger q^\dagger sr\} \{a^\dagger i\} \{b^\dagger j\} \vert 0 \rangle
\\
= \frac{1}{2} \sum_{ai,bj} \langle ij \vert ab \rangle t_{ij}^{ab} t_{ij}^{ab} = \begin{array}{c}
\end{array}.
\]
How do we calculate the Coupled-Cluster the particle-hole excitation amplitudes?

**CCSD equations –** \( n_o^2 n_u^4 \) \((N^6)\)

\[
\langle \Phi_i^a | (H_N e^{T_1 + T_2})_C | \Phi \rangle \equiv \langle \Phi_i^a | [H_N (1 + T_1 + T_2 + \frac{1}{2} T_1^2 + T_1 T_2 + \frac{1}{6} T_1^3)]_C | \Phi \rangle = 0
\]

\[
\langle \Phi_{ij}^{ab} | (H_N e^{T_1 + T_2})_C | \Phi \rangle \equiv \langle \Phi_{ij}^{ab} | [H_N (1 + T_1 + T_2 + \frac{1}{2} T_1^2 + T_1 T_2 + \frac{1}{6} T_1^3 + \frac{1}{2} T_2^2 + \frac{1}{2} T_1^2 T_2 + \frac{1}{24} T_1^4)]_C | \Phi \rangle = 0
\]

Two ways to solve the problem:

1. Apply wicks theorem and do all possible contractions -> very tedious and prone to error!

2. Use diagrammatic rules and derive all possible diagrams and convert into algebraic expressions. Intuitive and simple!
Algebraic expressions for the t1 amplitude equation:

\[
\langle \Phi_i^q \mid (H_Ne^{T_1+T_2})_C \mid \Phi \rangle = f_{i}^{a} - f_{m}^{i} t_{a}^{m} + f_{a}^{e} t_{e}^{i} - t_{e}^{m} v_{ma}^{i} + f_{m}^{e} t_{ea}^{i} + \frac{1}{2} t_{ea}^{i} v_{mn}^{ie} \\
+ \frac{1}{2} t_{ef}^{i} v_{ma}^{ef} - t_{e}^{i} f_{m}^{e} + t_{a}^{m} v_{mn}^{ie} + t_{f}^{i} t_{m}^{e} v_{ma}^{ef} \\
+ \frac{1}{2} t_{ea}^{i} t_{f}^{i} v_{mn}^{fe} + \frac{1}{2} t_{ef}^{i} t_{a}^{m} v_{mn}^{ef} + t_{ea}^{m} t_{f}^{i} v_{nm}^{fe} - t_{a}^{m} t_{e}^{i} t_{f}^{i} v_{nm}^{fe}
\]
Why is Coupled-Cluster so accurate when compared to CI and or shell model calculations?

\[
|\Psi_\alpha\rangle = (b_\alpha + b_{ai}^\alpha a_i^+ a_i + b_{abij}^\alpha a_i^+ a_j^+ a_i a_j + \ldots) |\Phi_0\rangle
\]

1p-1h  2p-2h  "Mean field"

Connected quadruples  Disconnected quadruples

\[
B_1 = T_1
\]
\[
B_2 = T_2 + \frac{1}{2} T_1^2
\]
\[
B_3 = T_3 + T_2 T_1 + \frac{1}{6} T_1^3
\]
\[
B_4 = T_4 + T_3 T_1 + \frac{1}{2} T_2 T_1^2 + \frac{1}{24} T_1^4
\]

CCSD  CCSDT
Size (Extensivity) matters!

Only size extensive theories produce a result and an error that scale as $A$. 

Comparison with other many-body techniques.

\[ \alpha = \alpha_n^\alpha + \alpha_N^\alpha + \alpha_{it}^\alpha \]

Quantum chemistry example (Bartlett et al)

FIG. 3. (Color online) Performance of theories for the correlation energy in small molecules. Graphed is the percentage of the full correlation energy achieved by the CI, CC, and MBPT theories, as a function of the level of approximation. To facilitate comparisons, the ordinate gives the size-scaling parameter of the approximation \( \alpha = \alpha_n + \alpha_N + \alpha_{it} \) in the computational cost function \( n^{\alpha_n}N^{\alpha_N}N_{it}^{\alpha_{it}} \). Shown are MBPT (solid circles), approximations (2)–(6); CI (solid squares), approximations SD-SDTQ; and CC (stars), approximations SD-SDTQ. The correlation energy is defined with respect to the Hartree-Fock energy for the given basis set, and the full correlation energies are obtained from the FCI calculations quoted in Table I.
Comparison with other many-body techniques

Nuclear Example (Kowalski et al PRL 2004).

- MBPT(4) \(O(n^3N^4)\)
- CCSD \(O(n^2N^4)N_{it}\)
- CCSD(T) \(O(n^2N^4)N_{it}+O(n^3N^4)\)
- CISDTQ \(O(n^4N^6)N_{it}\)
Coupled-cluster calculation for $^{16}$O

Interaction: Idaho-A based G-matrix
Model space: Up to 8 oscillator shells

Results converged w.r.t size of model space
Excited $3^-$ state: 1p-1h, about 6MeV to high
Some deficiencies in form factor.
Three-nucleon force missing.

Coupled-Cluster meets benchmarks of $^3$H and $^4$He!

CCSD(T) and Faddeev (-Yakubovsky) results for $^3$H and $^4$He using $V_{\text{low}-k}$ from AV18 with $\Lambda = 1.9 \text{fm}^{-1}$. CCSD(T) are within the errors (50 keV) of the Faddeev results! (G. Hagen et al., Phys. Rev. C 76, 044305 (2007))
Benchmarking 16O and 40Ca with Coupled-Cluster

\[
\begin{array}{c|c|c|c}
 & ^4\text{He} & ^{16}\text{O} & ^{40}\text{Ca} \\
\hline
E_0 & -11.815 & -60.204 & -347.474 \\
\Delta E_{\text{CCSD}} & -17.107 & -82.576 & -143.736 \\
\Delta E_{\text{CCSD(T)}} & -0.253 & -5.450 & -11.699 \\
E_{\text{CCSD(T)}} & -29.175 & -148.232 & -502.908 \\
\text{exact (FY)} & -29.19(5) & & \end{array}
\]

40Ca converged within 1%!

Roth and Navratil PRL 99, 092501 (2007) \( E_{\text{CISDT}} = -462.7 \text{MeV} \). Our comment: arXiv:0709.0449
Coupled-Cluster Theory with 3NF

- We have derived and implemented Coupled-Cluster equations for three-body Hamiltonians.
- Probe cutoff dependence of interactions with three nucleon force in light and medium mass nuclei.
- Does 3NF provide the necessary repulsion/attraction needed to approach experimental mass values?
- “Coupled-Cluster theory with three-body Hamiltonians”
  G. Hagen et al., PRC 76, 034302 (2007)
3NF contribution to the T1 cluster equation

\[ E = \sum_{j} \sum_{i} \sum_{k} \sum_{l} \text{contributions} \]

Energy and 1p-1h equation as examples.
Factorization of diagrams very useful!
1p-1h: 15 diagrams
2p-2h: 51 diagrams
3NF from Chiral Perturbation theory

Feynman diagrams

2N Force

3N Force

4N Force

\[ Q^0 \]

LO

\[ Q^2 \]

NLO

\[ Q^3 \]

NNLO

\[ Q^4 \]

N^3LO

Phase shifts reproduced to \( \chi^2/\text{datum}=1 \)

About 24+ parameters

\[ ^1S_0 \]

\[ ^3P_0 \]

\[ ^1P_1 \]

\[ ^3P_1 \]

\[ ^3S_1 \]

\[ ^3D_1 \]


Coupled-Cluster results for 4He with 3NF

- $V_{\text{low-k}}$ from AV18 with $\Lambda = 1.9 \text{fm}^{-1}$.
- 3NF brings in repulsion as expected!
- CCSD and CCSD(T) with 3NF meets Faddeev-Yakubovsky benchmark!
  $E_{\text{CCSD(T)}} \approx -28.24 \text{ MeV}$. F-Y $E = -28.20(5) \text{MeV}$. 

![Graphs showing energy levels for different N values and hω](image-url)
Different contributions to $E(\text{CCSD})$ from 3NF in 4He

Three-body Hamiltonian in normal ordered form:

$$\hat{H}_3 = \frac{1}{6} \sum_{ijk} \langle ijk \mid ijk \rangle + \frac{1}{2} \sum_{ijpq} \langle ipq \mid ijq \rangle \{\hat{a}_p^\dagger \hat{a}_q\} + \frac{1}{4} \sum_{ipqrs} \langle ipq \mid irs \rangle \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\} + \hat{h}_3 ,$$

Really good news!

- The “density dependent” terms of 3NF are dominant!
- $\epsilon$ from residual 3NF costs $1 - \epsilon$ of work!
- “2-body” machinery can be used.
- Residual three-nucleon force can be neglected!
Utilize the nuclear total spin symmetry to push further
Potential for ‘ab initio’ in heavy nuclei

- Implemented a CCSD J-coupled code for heavier nuclei:
  - Scaling at CCSD goes from $O(n_o^2 n_u^4)$ to $O(n_o^{4/3} n_u^{8/3})$
  - Can do up to 14 complete major shells on a single node.
- CCSDT  Gold standard for these heavier nuclei (developing)
- Enables specified calculations for heavy nuclei
- The large model spaces mean that we can do BARE interactions!

- Is it technically feasible to go further? (YES)
- Does size extensivity work in the nuclear case? (YES)
- Does power counting hold in medium mass nuclei (YES)
Speedup of J-coupled CCSD code for 40Ca as compared to m-scheme CCSD code
CONVERGED 16O, 40Ca, 48Ca and 48Ni CCSD ground state energies with N3LO!!
16O, 40Ca, 48Ca and 48Ni CCSD ground state densities
Charge and matter radii/Summary of results

Charge radii for various nuclei using N3LO nucleon-nucleon interaction.

~1MeV missing binding energy for all nuclei: Size Extensivity!

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>$E/A$</th>
<th>$V/A$</th>
<th>$Q$</th>
<th>$\Delta E/A$</th>
<th>$\langle r^2 \rangle_{ch}^{1/2}$</th>
<th>$\langle r^2 \rangle_{ch}^{1/2}$ (Exp)</th>
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<tbody>
<tr>
<td>$^4$He</td>
<td>-5.99</td>
<td>-22.75</td>
<td>0.90</td>
<td>1.08</td>
<td></td>
<td>1.673(1)</td>
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<tr>
<td>$^{16}$O</td>
<td>-6.72</td>
<td>-30.69</td>
<td>1.08</td>
<td>1.25</td>
<td>2.72(5)</td>
<td>2.737(8)</td>
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<tr>
<td>$^{40}$Ca</td>
<td>-7.72</td>
<td>-36.40</td>
<td>1.18</td>
<td>0.84</td>
<td>3.25(9)</td>
<td>3.4764</td>
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<tr>
<td>$^{48}$Ca</td>
<td>-7.40</td>
<td>-37.97</td>
<td>1.21</td>
<td>1.27</td>
<td>3.24(9)</td>
<td>3.4738</td>
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<td>$^{48}$Ni</td>
<td>-6.02</td>
<td>-36.04</td>
<td>1.20</td>
<td>1.21</td>
<td>3.52(15)</td>
<td>?</td>
</tr>
</tbody>
</table>
Simplicity out of Complexity! Towards microscopic foundation of the shell-model

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>$s_{1/2}$</th>
<th>$p_{3/2}$</th>
<th>$p_{1/2}$</th>
<th>$d_{5/2}$</th>
<th>$s_{1/2}$</th>
<th>$d_{3/2}$</th>
<th>$f_{7/2}$</th>
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<td></td>
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<tr>
<td>$\nu$</td>
<td>0.946</td>
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<tr>
<td>$^{16}\text{O}$ $\pi$</td>
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<td>0.962</td>
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<td>$\nu$</td>
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<tr>
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<td>0.973</td>
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<td>0.959</td>
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<td>$\nu$</td>
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<td>0.983</td>
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<tr>
<td>$\nu$</td>
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<td>0.966</td>
<td>0.974</td>
<td>0.956</td>
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<table>
<thead>
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<th>Occupation of Hartree-Fock orbitals</th>
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<tbody>
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<td>$^{16}\text{O}$ $\pi$</td>
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<tr>
<td>$\nu$</td>
</tr>
<tr>
<td>$^{40}\text{Ca}$ $\pi$</td>
</tr>
<tr>
<td>$\nu$</td>
</tr>
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Summary

- Coupled-Cluster theory is size-extensive. Energy scales correctly with system size.
- CC scales polynomial with system size allowing to reach medium size and heavier nuclei.
- By using diagrammatic rules systematic improvements can be easily implemented. CCSD -> CCSDT -> CCSDTQ
- CC meets few-body benchmarks.
- We have implemented CC for three-body Hamiltonians, investigate role of 3NF in medium sized nuclei.
- Taking spherical symmetry into account we have been able to reduce dramatically the computational cost. Converged ground states of 40Ca, 48Ca 48Ni using a single workstation.
- Coupled-Cluster theory is an ideal candidate for extending the ab-initio program to beyond the lightest region of the nuclear chart.