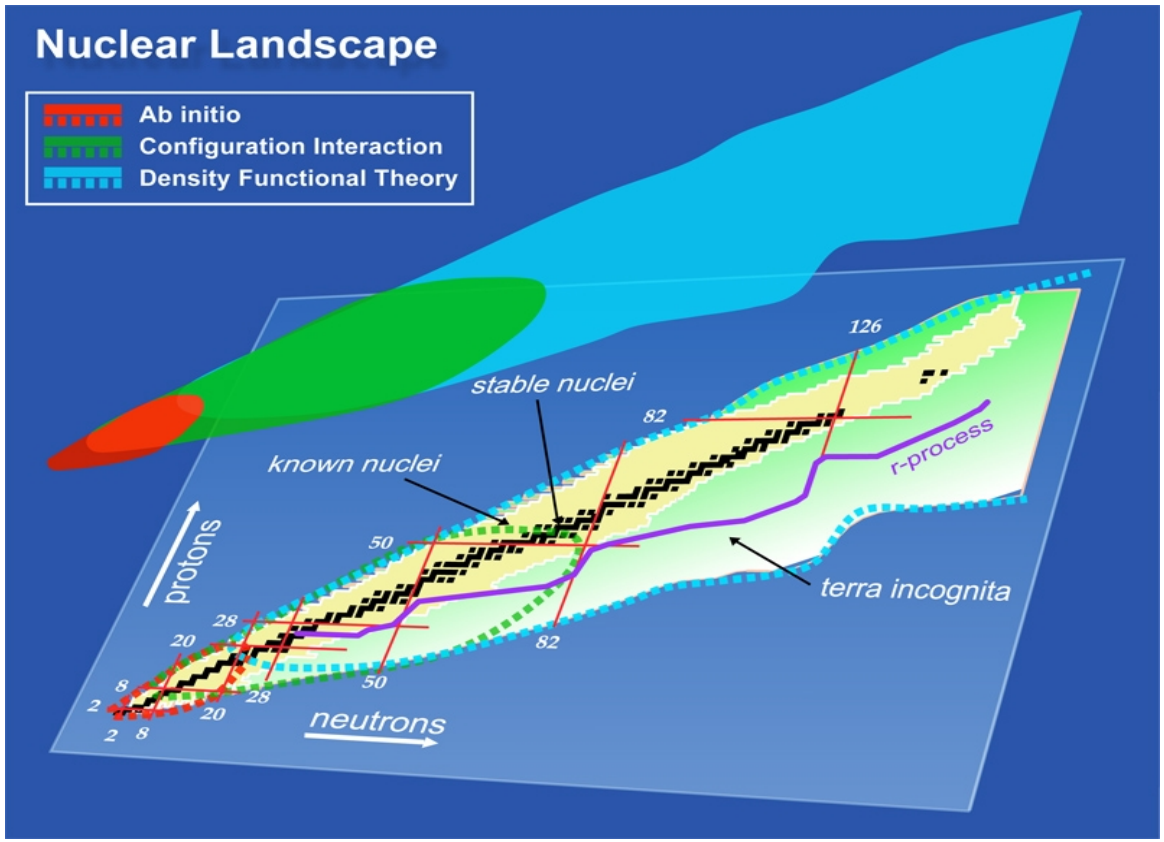
The Nuclear Many-Body Problem
Lecture 4

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.

PHYSICAL REVIEW VOLUME 100, NUMBER 1 OCTOBER 1, 1955

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

K. A. Brueckner
Indiana University, Bloomington, Indiana
(Received April 28, 1955)

505 citations

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)

Derivation of the Brueckner many-body theory

1,062 citations

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.

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

500 citations

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 electrodynamic 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 the modified interaction. The close connexion between this approach and the dielectric theory of plasma oscillations is indicated.

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

Historical Perspective

1.C

Nuclear Physics **7** (1958) 421—424; © *North-Holland Publishing Co., Amsterdam*

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523 citations

BOUND STATES OF A MANY-PARTICLE SYSTEM

F. COESTER

Department of Physics, State University of Iowa, Iowa City, Iowa

Received 10 April 1958

Abstract: Rigorous formal solutions of the bound state Schrödinger equation are constructed in terms of an arbitrary complete set of single particle wave functions. From these solutions one sees without effort that the Rayleigh Schrödinger perturbation expansion of the energy does not contain matrix elements represented by products of unlinked diagrams. The components of the state vector are related in a simple manner to functions represented by linked diagrams only.

The validity of the Brueckner approximation to the bound state energy of a many particle system depends on the absence of "unlinked clusters" in the perturbation expansion of this energy. Brueckner [1]) has shown that such terms are absent from a few orders of the perturbation series. General proofs for all orders of the perturbation series have been given by several authors [2–4]). All these proofs are based on a detailed inspection of perturbation terms of arbitrary order. The purpose of this note is to cast the basic equations into such a form that the absence of unlinked terms from the energy becomes evident without detailed inspection of all n'th order perturbation matrix elements.

1.C:
1.D.1

Nuclear Physics **17** (1960) 477—485; © *North-Holland Publishing Co., Amsterdam*

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578 citations

SHORT-RANGE CORRELATIONS IN NUCLEAR WAVE FUNCTIONS

F. COESTER

Department of Physics and Astronomy, State University of Iowa, Iowa City, Iowa

and

H. KÜMMEL

Max Planck Institut für Chemie, Mainz, Germany †

Received 18 February 1960

Abstract: We assume that the ground state wave functions of a closed shell nucleus is approximated by a Slater determinant in the restricted region of configuration space where all internucleon distances are larger than a certain "healing distance". The remainder of the wave function is given in terms of a series of cluster functions. The overlap integral between the correct wave functions and the Slater determinant is small and depends on the higher cluster functions in a complicated manner. Nevertheless we can show that the one- and two-body density matrices are well approximated by expressions involving only the single-particle wave functions and the two-body cluster functions. The Schrödinger equation yields a coupled set of equations which determine the cluster functions as well as the single-particle wave functions.

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 45, NUMBER 11 1 DECEMBER 1966

On the Correlation Problem in Atomic and Molecular Systems. Calculation of Wavefunction Components in Ursell-Type Expansion Using Quantum-Field Theoretical Methods

1,309 citations

JIŘÍ ČÍŽEK*

Institute of Physical Chemistry, Czechoslovak Academy of Sciences, Prague, Czechoslovakia

(Received 17 May 1966)

A method is suggested for the calculation of the matrix elements of the logarithm of an operator which gives the exact wavefunction when operating on the wavefunction in the one-electron approximation. The method is based on the use of the creation and annihilation operators, hole–particle formalism, Wick's theorem, and the technique of Feynman-like diagrams. The connection of this method with the configuration-interaction method as well as with the perturbation theory in the quantum-field theoretical form is discussed. The method is applied to the simple models of nitrogen and benzene molecules. The results are compared with those obtained with the configuration-interaction method considering all possible configurations within the chosen basis of one-electron functions.

First papers explicitly describing Coupled-Cluster theory

Kummel, Luhrmann, Zabolitsky, Phys. Reps. 36, 1 (1978)
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):

1966: Cizek, J. Chem. Phys. 45, 4256 (1966); Adv. Chem. Phys. 14, 35 (1969)

1971: Cizek and Paldus, Int. J. Quantum Chem. 5, 359

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)

1999: Heisenberg and Mihiala, Phys. Rev. C59, 1440; PRL84, 1403 (2000)

Three nuclei; JJ coupled scheme; bare interactions, approximate V_{3N}

Useful References

Crawford and Schaefer, Reviews in Computational Chemistry, 14, 336 (2000)

Bartlett, Ann. Rev. Phys. Chem. 32, 359 (1981)

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 Ψ

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

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

Coupled Cluster Equations

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

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

$$\bar{H} = \left(H_N exp(T) \right)_C$$

Iterative CCSDT-n approximations to full CCSDT

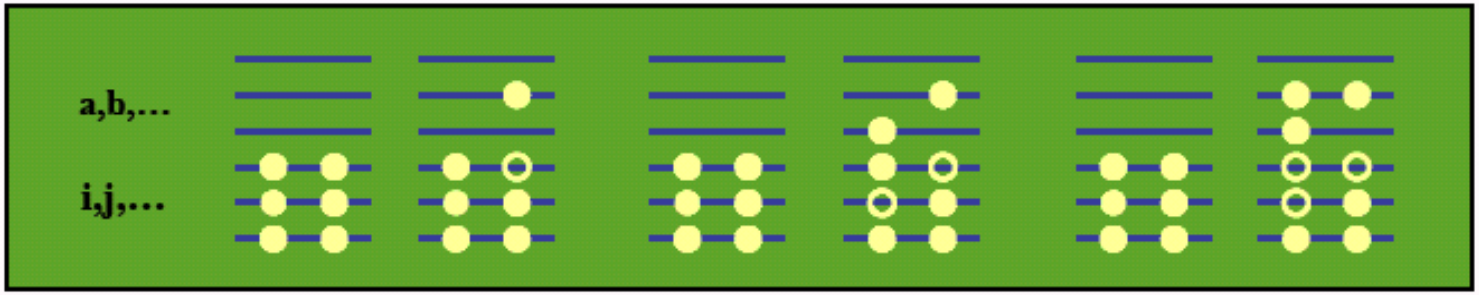
$$\begin{aligned}
\mathrm{CCSDT-1} \quad 0 &= \langle \Phi_{ijk}^{abc} | \left(F_N T_3 + H_N T_2 \right)_C | \Phi_0 \rangle \\
\mathrm{CCSDT-2} \quad 0 &= \langle \Phi_{ijk}^{abc} | \left(F_N T_3 + H_N T_2 + H_N T_2^2/2 \right)_C | \Phi_0 \rangle \\
\mathrm{CCSDT-3} \quad 0 &= \langle \Phi_{ijk}^{abc} | \left(F_N T_3 + H_N \exp(T_1 + T_2) \right)_C | \Phi_0 \rangle \\
\mathrm{CCSDT} \quad 0 &= \langle \Phi_{ijk}^{abc} | \left(H_N \exp(T_1 + T_2 + T_3) \right)_C | \Phi_0 \rangle
\end{aligned}$$

Coupled-Cluster in pictures

(F. Coester, 1958; F. Coester and H. Kümmel, 1960; J. Čížek, 1966, 1969; J. Čížek and J. Paldus, 1971)

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

$$T_1|\Phi\rangle = \sum_{\substack{i \\ a}} t_a^i |\Phi_i^a\rangle, \quad T_2\Phi = \sum_{\substack{i>j \\ a>b}} t_{ab}^{ij}|\Phi_{ij}^{ab}\rangle, \quad T_3\Phi = \sum_{\substack{i>j>k \\ a>b>c}} t_{abc}^{ijk}|\Phi_{ijk}^{abc}\rangle, \quad \text{etc.}$$



$m_A = N$ – exact theory

$m_A < N$ – approximate methods

$m_A = 2$	$T = T_1 + T_2$	CCSD	$n_o^2 n_u^4$ $(n_o^2 n_u^2)$
$m_A = 3$	$T = T_1 + T_2 + T_3$	CCSDT	$n_o^3 n_u^5$ $(n_o^3 n_u^3)$
$m_A = 4$	$T = T_1 + T_2 + T_3 + T_4$	CCSDTQ	$n_o^4 n_u^6$ $(n_o^4 n_u^4)$
$m_A = 5$	$T = T_1 + T_2 + T_3 + T_4 + T_5$	CCSDTQP	$n_o^5 n_u^7$ $(n_o^5 n_u^5)$

The normal ordered Hamiltonian

Wicks theorem:

$$ABC\ldots = \{ABC\ldots\} + \sum_{\substack{\text{all}\\ \text{single}\\ \text{contractions}}} \overline{AB}C\ldots\}$$

$$+ \sum_{\substack{\text{all}\\ \text{double}\\ \text{contractions}}} \{\overline{AB}\overline{C}\ldots\}$$

$$+ \cdots + \sum_{\substack{\text{all}\\ \text{fully}\\ \text{contracted}\\ \text{prdts}}} \{\overline{AB}\overline{C}\ldots\}. \qquad (45)$$

One-body term:

$$p^\dagger q = \{p^\dagger q\} + \{\overline{p^\dagger q}\} = \{p^\dagger q\} + \delta_{pq=i}$$

Two-body term:

$$\begin{aligned} p^\dagger q^\dagger sr &= \{p^\dagger q^\dagger sr\} + \{\overline{p^\dagger q^\dagger sr}\} + \{p^\dagger \overline{q^\dagger sr}\} \\ &+ \{\overline{p^\dagger q^\dagger} sr\} + \{p^\dagger \overline{q^\dagger sr}\} \\ &+ \{\overline{p^\dagger q^\dagger} sr\} + \{\overline{p^\dagger q^\dagger} sr\} \\ &= \{p^\dagger q^\dagger sr\} + \overline{p^\dagger r}\{q^\dagger s\} + \overline{q^\dagger s}\{p^\dagger r\} \\ &- \overline{p^\dagger s}\{q^\dagger r\} - \overline{q^\dagger r}\{p^\dagger s\} \\ &+ \overline{p^\dagger r}\,\overline{q^\dagger s} - \overline{p^\dagger s}\,\overline{q^\dagger r}\,. \end{aligned}$$

The normal ordered Hamiltonian is :

$$H_N = H - \langle 0|H|0\rangle, \quad \text{where} \quad H = \sum_p f_{pp}\{p^\dagger p\} + \sum_{p\neq q} f_{pq}\{p^\dagger q\} + \tfrac{1}{4}\sum \langle pq||rs\rangle\{p^\dagger q^\dagger sr\}$$

$$+ \langle 0|H|0\rangle. \qquad (47)$$

The Coupled-Cluster energy expression

The Baker Hausdorff commutator relation:

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

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

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

The Coupled-Cluster energy expression:

$$E = \langle 0|\bar{H}|0\rangle,$$

$$E = \langle 0|H + (HT_1)_C + (HT_2)_C + (HT_1^2/2)_C|0\rangle$$

Diagramatic representation:

$$T_2 = \sum_{i>j,a>b} t_{ij}^{ab}\{a^\dagger i b^\dagger j\} =$$

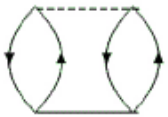
$$T_1 = \sum_{i,a} t_i^a\{a^\dagger i\} =$$

The Coupled Cluster energy expression

$$\langle 0|(WT_2)_C|0\rangle = \frac{1}{4}\sum_{ijab}\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle t_{ij}^{ab}\langle 0|\{p^\dagger q^\dagger sr\}\{a^\dagger ib^\dagger j\}+\{p^\dagger q^\dagger sr\}\{a^\dagger ib^\dagger j\}$$

$$+\{p^\dagger q^\dagger sr\}\{a^\dagger ib^\dagger j\}+\{p^\dagger q^\dagger sr\}\{a^\dagger ib^\dagger j\}|0\rangle$$

$$=\frac{1}{4}\sum_{ai,bj}\langle ij||ab\rangle t_{ij}^{ab} =$$

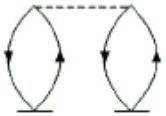


,

$$\langle 0|(WT_1^2/2)_C|0\rangle = \frac{1}{8}\sum_{ijab}\sum_{pqrs}\langle pq||rs\rangle t_i^a t_j^b\langle 0|\{p^\dagger q^\dagger sr\}\{a^\dagger i\}\{b^\dagger j\}+\{p^\dagger q^\dagger sr\}\{a^\dagger i\}\{b^\dagger j\}$$

$$+\{p^\dagger q^\dagger sr\}\{a^\dagger i\}\{b^\dagger j\}+\{p^\dagger q^\dagger sr\}\{a^\dagger i\}\{b^\dagger j\}|0\rangle$$

$$=\frac{1}{2}\sum_{ai,bj}\langle ij||ab\rangle t_i^a t_j^b =$$



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How do we calculate the Coupled-Cluster the particle-hole excitation amplitudes ?

CCSD equations – $n_o^2 n_u^4$ $(\mathcal{N}^6)$

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

$$\begin{aligned} \langle \Phi_{ij}^{ab} | (H_N e^{T_1+T_2})_C | \Phi \rangle \quad \equiv \quad & \langle \Phi_{ij}^{ab} | [H_N (1 + T_1 + T_2 + \tfrac{1}{2} T_1^2 + T_1 T_2 + \tfrac{1}{6} T_1^3 \\ & + \tfrac{1}{2} T_2^2 + \tfrac{1}{2} T_1^2 T_2 + \tfrac{1}{24} T_1^4)]_C | \Phi \rangle = 0 \end{aligned}$$

Two ways to solve the problem:

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

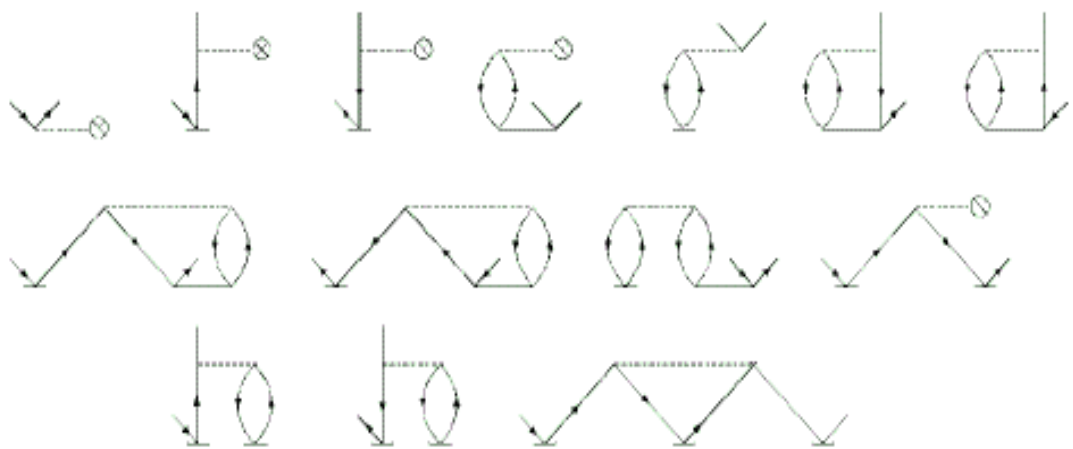
2. Use diagrammatic rules and derive all possible diagrams and convert into algebraic expressions. Intuitive and simple!

Example: the t1 equation

Algebraic expressions for the t1 amplitude equation:

$$\langle \Phi_i^a | (H_N e^{T_1+T_2})_C | \Phi \rangle = f_a^i - f_m^i t_a^m + f_a^e t_e^i - t_e^m v_{ma}^{ie} + f_m^e t_{ea}^{mi} + \frac{1}{2} t_{ea}^{mn} v_{mn}^{ie}$$
$$+ \quad \frac{1}{2} t_{ef}^{mi} v_{ma}^{ef} - t_e^i t_a^m f_m^e + t_a^n t_e^m v_{mn}^{ie} + t_f^i t_e^m v_{ma}^{ef}$$
$$+ \quad \frac{1}{2} t_{ea}^{mn} t_f^i v_{mn}^{fe} + \frac{1}{2} t_{ef}^{ni} t_a^m v_{mn}^{ef} + t_{ea}^{mi} t_f^n v_{nm}^{fe} - t_a^m t_e^i t_f^n v_{nm}^{fe}$$

T_1 equation



Why is Coupled-Cluster so accurate when compared to CI and or shell model calculations ?

$$|\Psi_\alpha\rangle = \left(b^\alpha + b^\alpha_{ai} a^+_a a_i + b^\alpha_{abij} a^+_a a^+_b a_i a_j + \cdots\right)|\Phi_0\rangle$$

1p-1h

2p-2h

"Mean field"

$$B_1 = T_1$$

$$B_2 = T_2 + \frac{1}{2} T_1^2$$

$$B_3 = T_3 + T_2 T_1 + \frac{1}{6} T_1^3$$

$$B_4 = T_4 + T_3 T_1 + \frac{1}{2} T_2^2 + \frac{1}{2} T_2 T_1^2 + \frac{1}{24} T_1^4$$

$$\ldots$$

CCSD

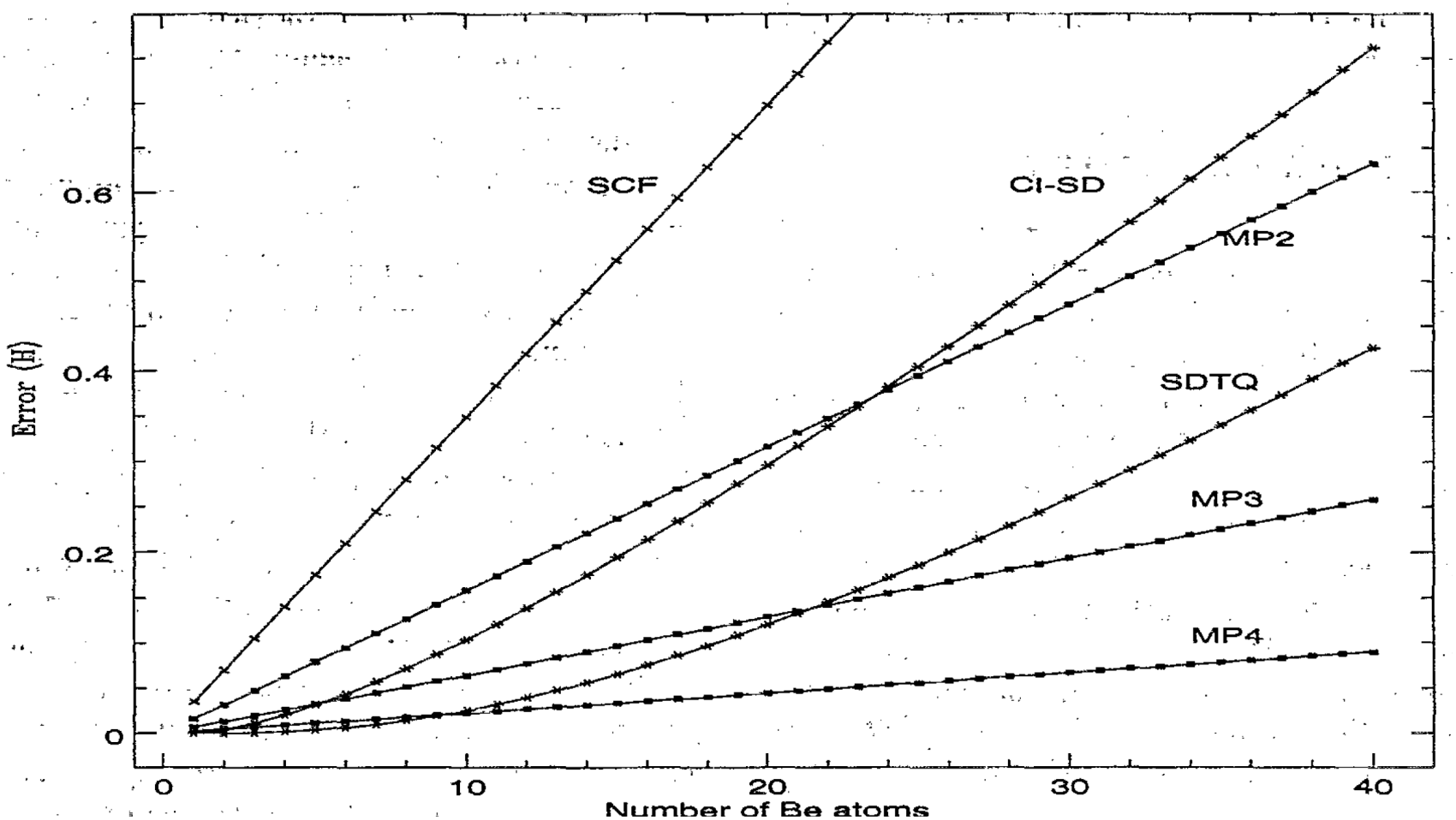
CCSDT

Disconnected quadruples

Connected quadruples

Size (Extensivity) matters !

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



[Duch and Diercksen, J. Chem. Phys. 101 (1994) 3018]

Comparison with other many-body techniques.

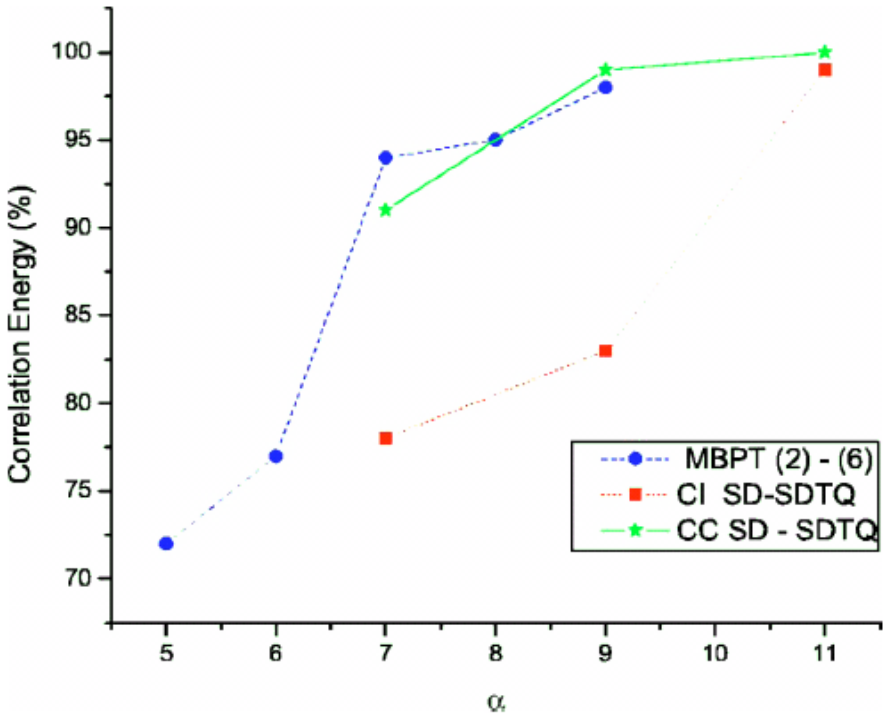


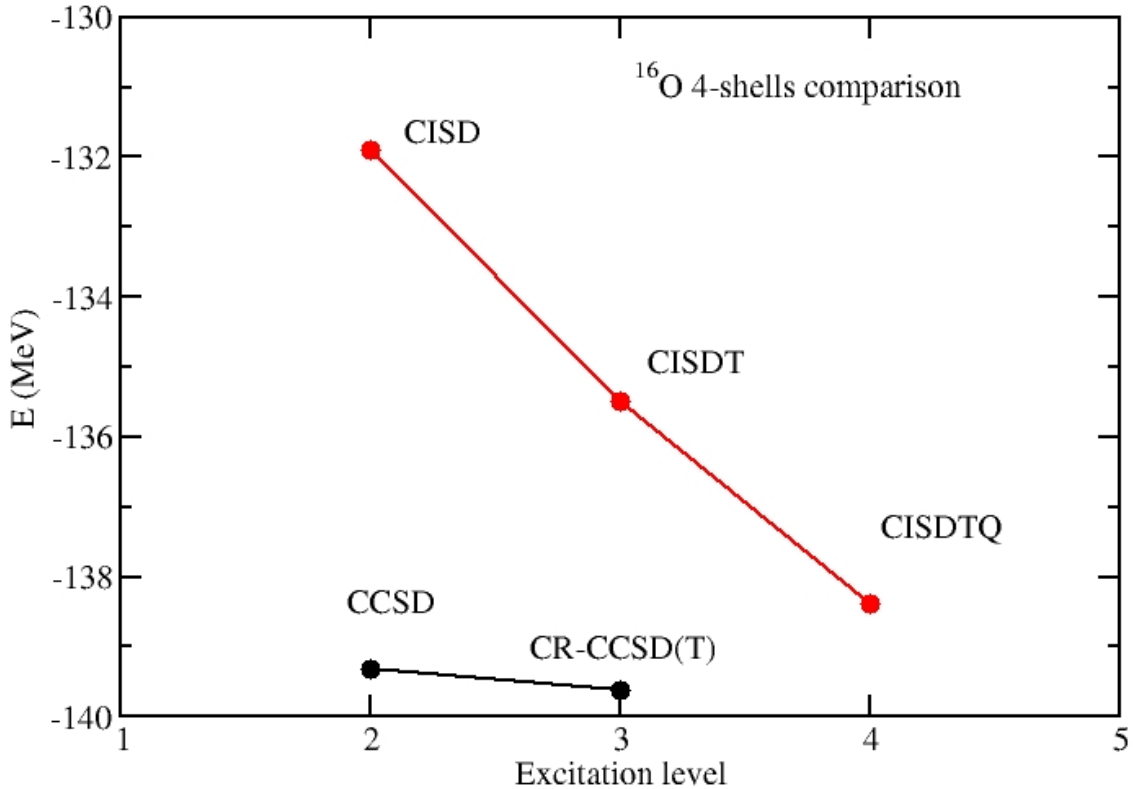
FIG. 3. (Color online) Performance of theories for the correlation energy in small molecules. Graphed is the percentage of the full correlation energy achieved by the CI, CC, and MBPT theories, as a function of the level of approximation. To facilitate comparisons, the ordinate gives the size-scaling 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.

hemistry example (Bartlett et al)

$$\alpha = \alpha_n + \alpha_N + \alpha_{it}$$

$$n^{\alpha_n} N^{\alpha_N} N_{it}^{\alpha_{it}}$$

Comparison with other many-body techniques



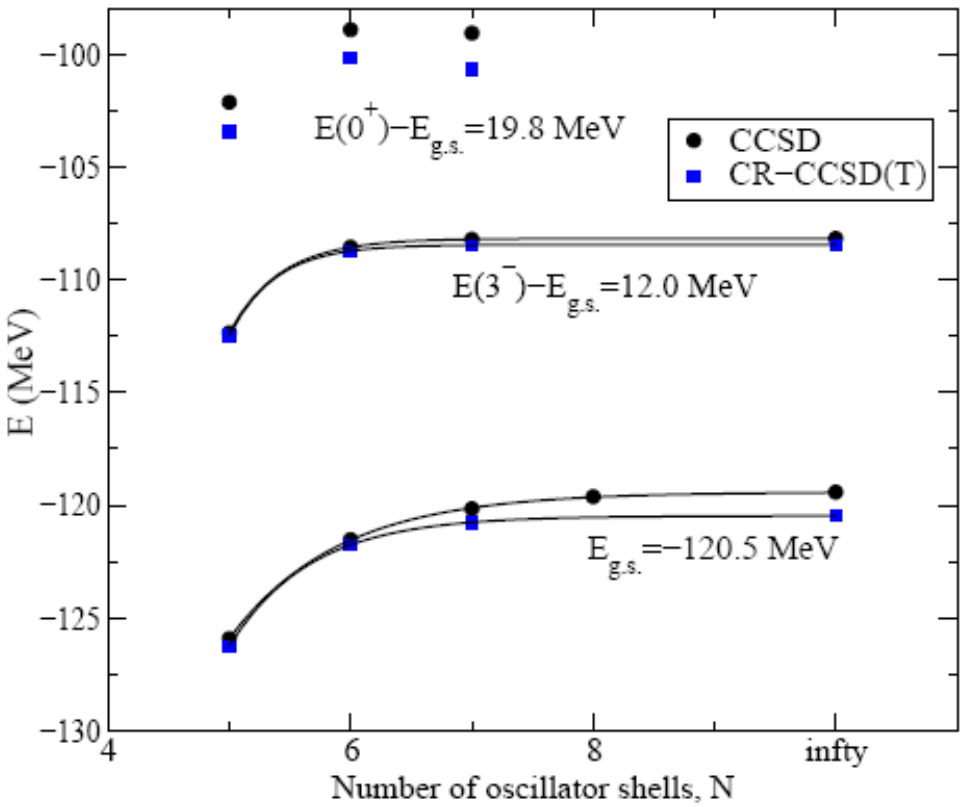
Nuclear Example (Kowalski et al PRL 2004).

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	$O(n^4N^6)N_{it}$

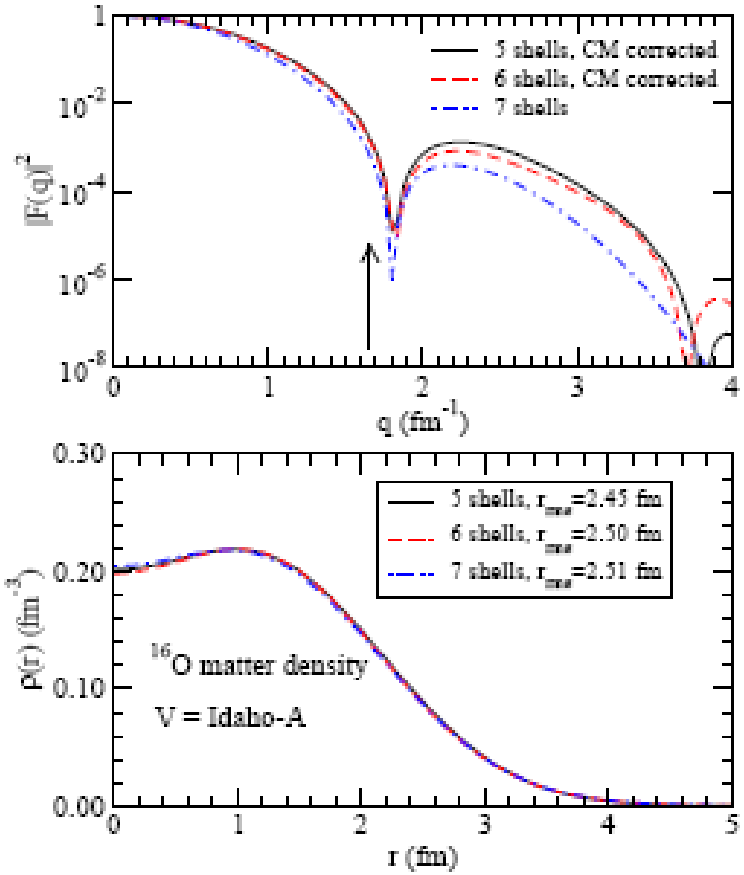
Coupled-cluster calculation for ^{16}O

Interaction: Idaho-A based G-matrix

Model space: Up to 8 oscillator shells



M. Wloch et al, Phys. Rev. Lett. 94, 212501 (2005).



Results converged w.r.t size of model space

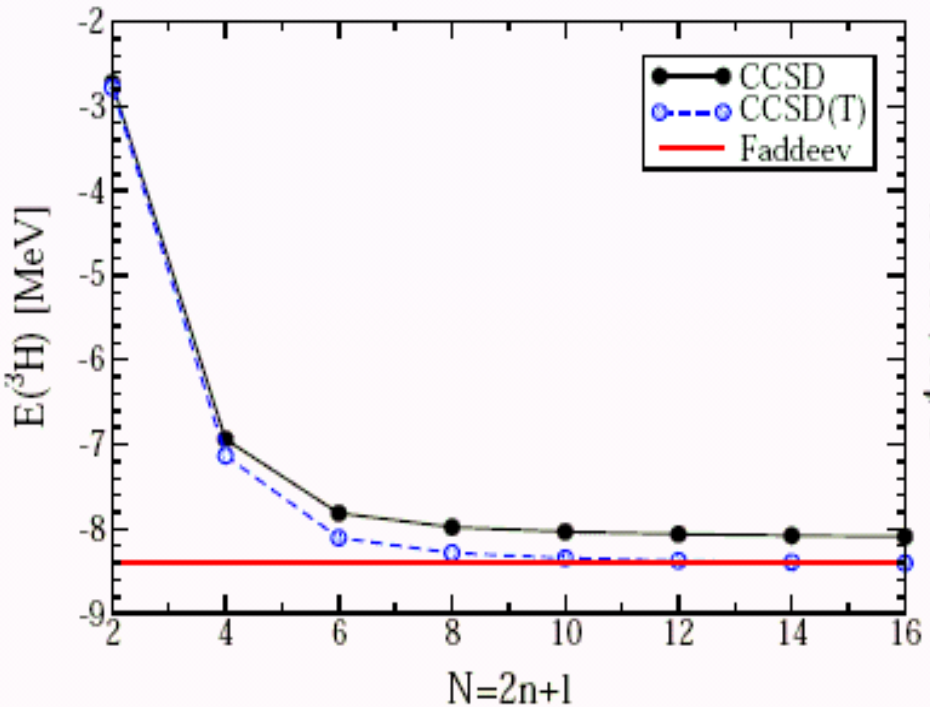
Excited 3^- state: 1p-1h, about 6MeV to high

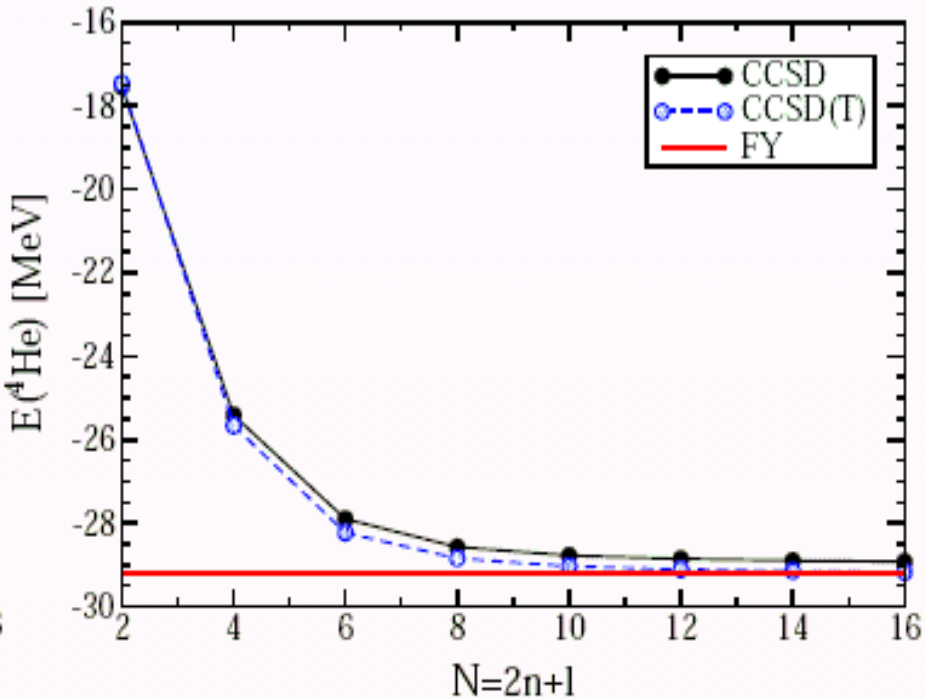
Some deficiencies in form factor.

Three-nucleon force missing.

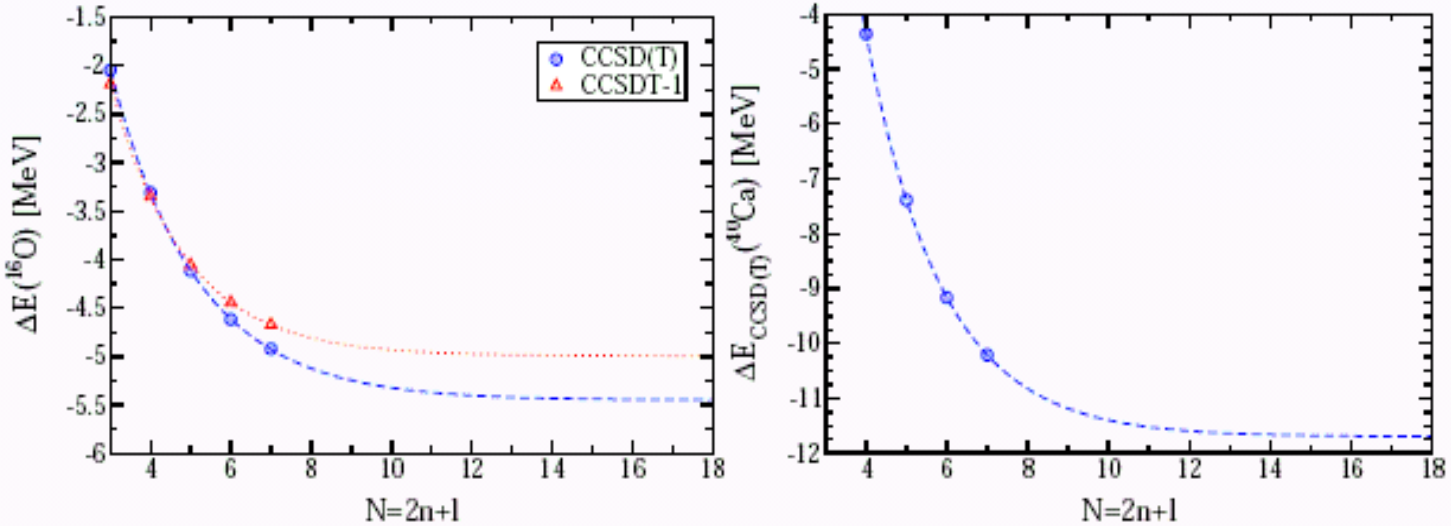
Coupled-Cluster meets benchmarks of 3H and 4He !

CCSD(T) and Faddeev (-Yakubovsky) results for ^{3}H and ^{4}He using $V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 1.9\mathrm{fm}^{-1}$. **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



	^{4}He	^{16}O	^{40}Ca
E_0	-11.815	-60.204	-347.474
ΔE_{CCSD}	-17.107	-82.576	-143.736
$\Delta E_{\mathrm{CCSD(T)}}$	-0.253	-5.450	-11.699
$E_{\mathrm{CCSD(T)}}$	-29.175	-148.232	-502.908
exact (FY)	-29.19(5)		

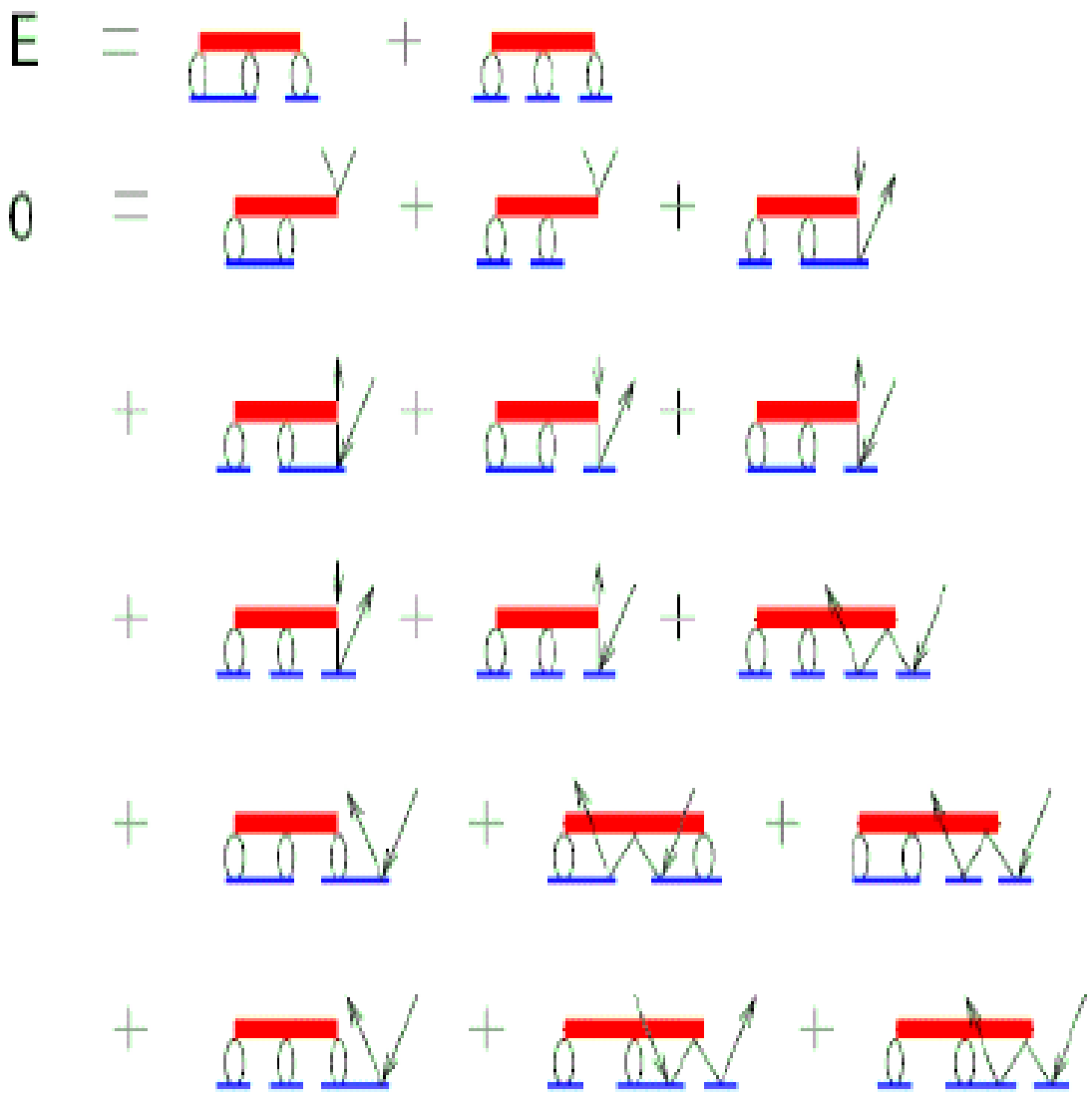
^{40}Ca converged within 1% !

Roth and Navratil PRL 99, 092501 (2007) E_{CISDT} = -462.7MeV. 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



Energy and 1p-1h equation as examples.

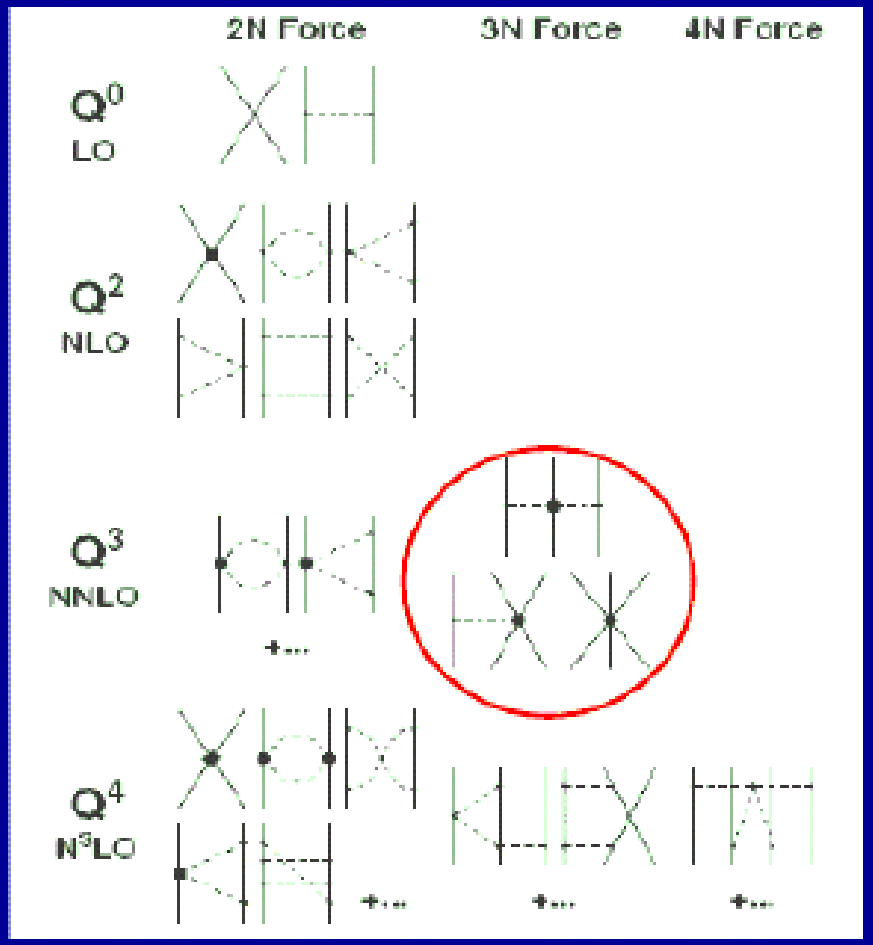
Factorization of diagrams very useful!

1p-1h: 15 diagrams

2p-2h: 51 diagrams

3NF from Chiral Perturbation theory

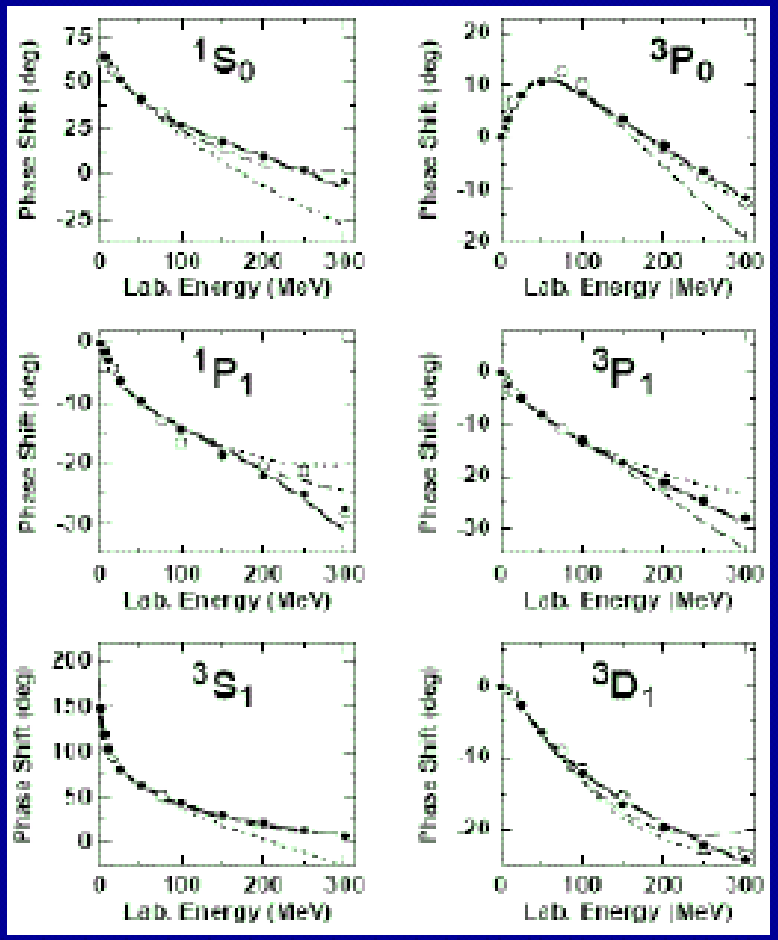
Feynman diagrams



R. Machleidt and D. R. Entem, J. Phys. G 31 (2005) S1235

Phase shifts reproduced to χ^2/datum=1

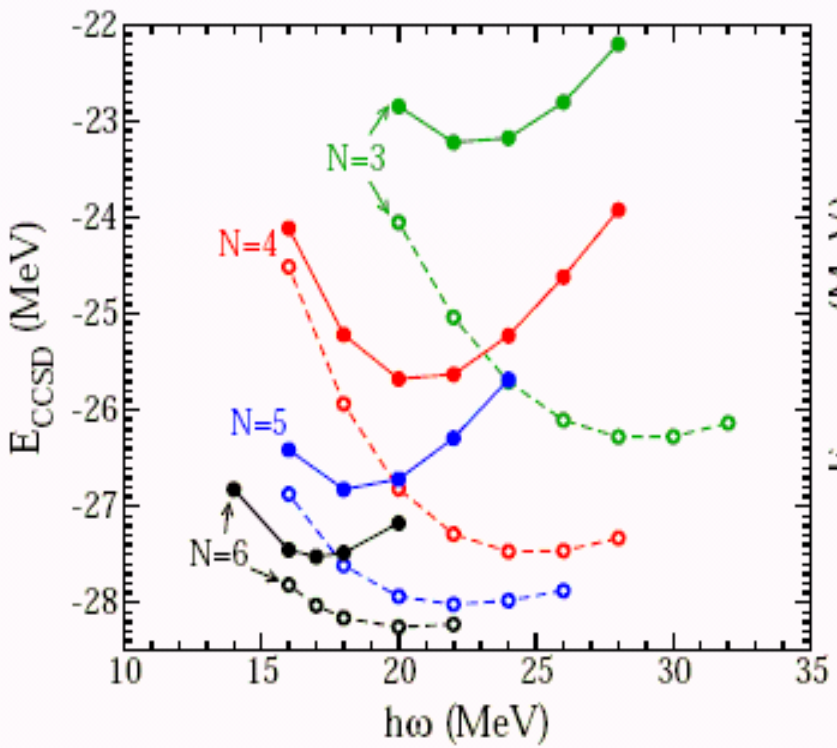
About 24+ parameters

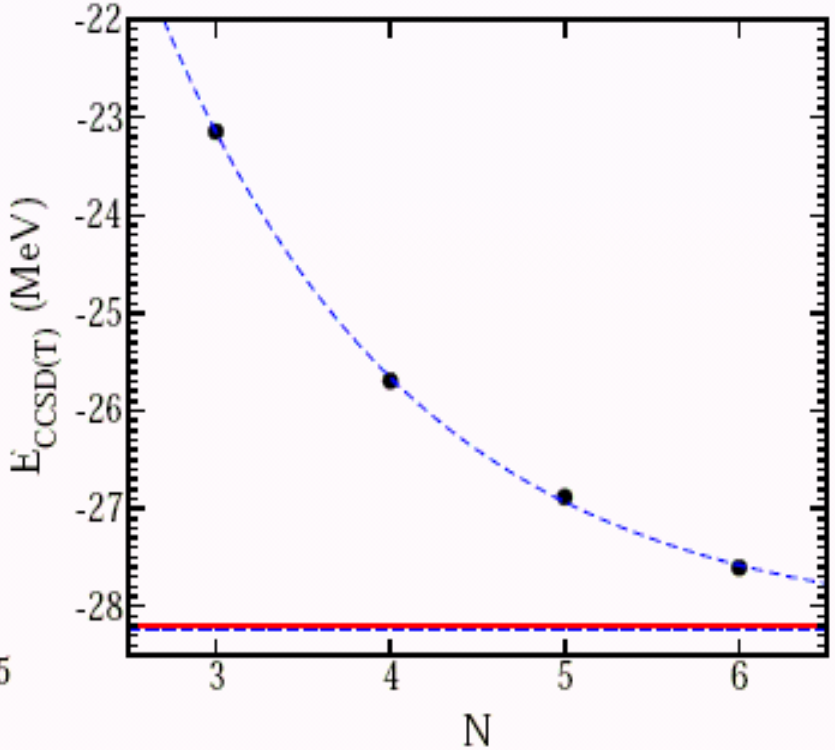


D. R. Entem and R. Machleidt, Phys.Rev. C68 (2003) 041001

Coupled-Cluster results for 4He with 3NF

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

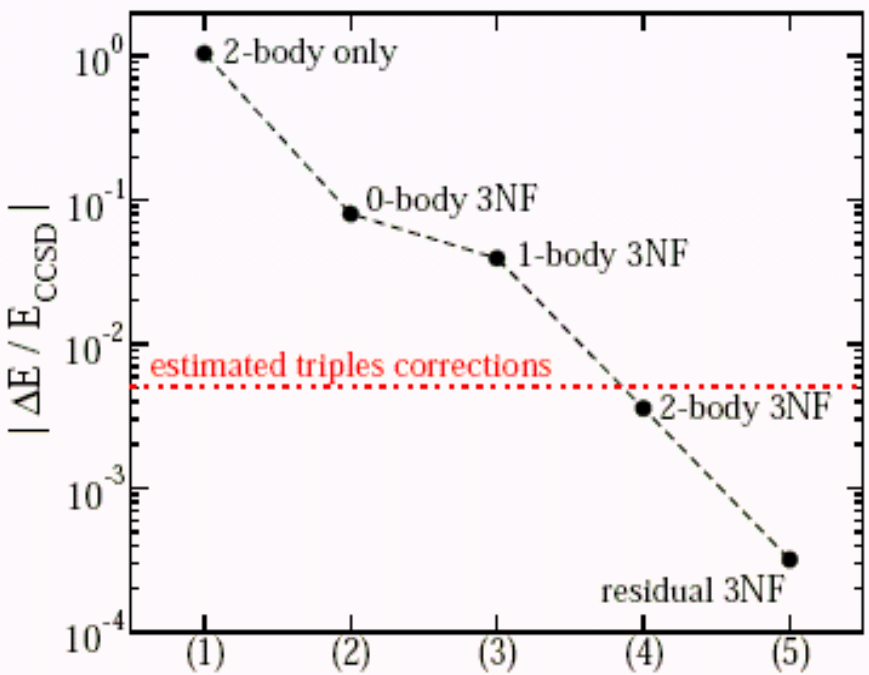




Different contributions to E(CCSD) from 3NF in 4He

Three-body Hamiltonian in normal ordered form:

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



Really good news!

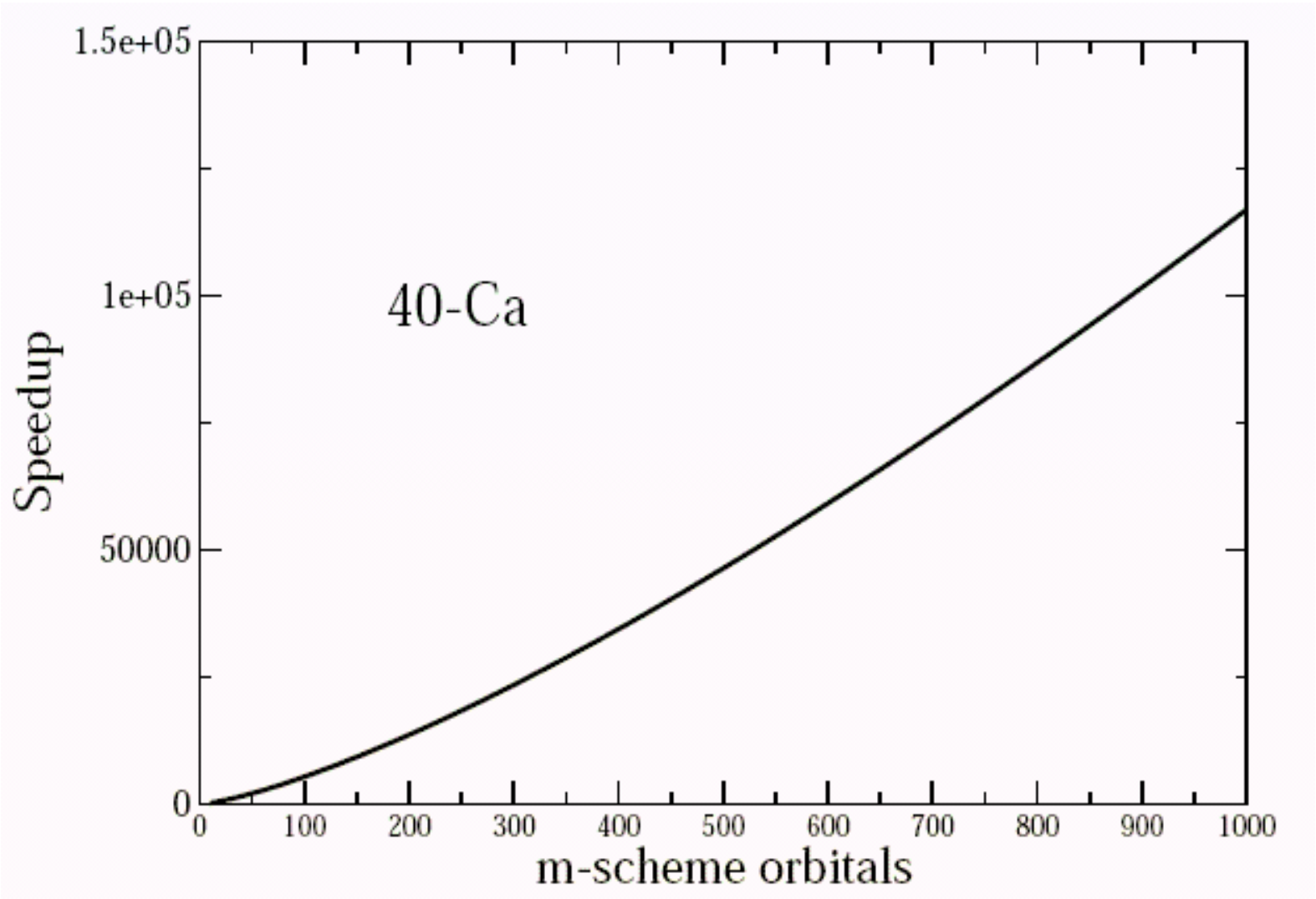
- The "density dependent" terms of 3NF are dominant!
- ϵ from residual 3NF costs $1-\epsilon$ of work !
- "2-body" machinery can be used.
- **Residual three-nucleon force can be neglected!**

Utilize the nuclear total spin symmetry to push further
Potential for 'ab initio' in heavy nuclei

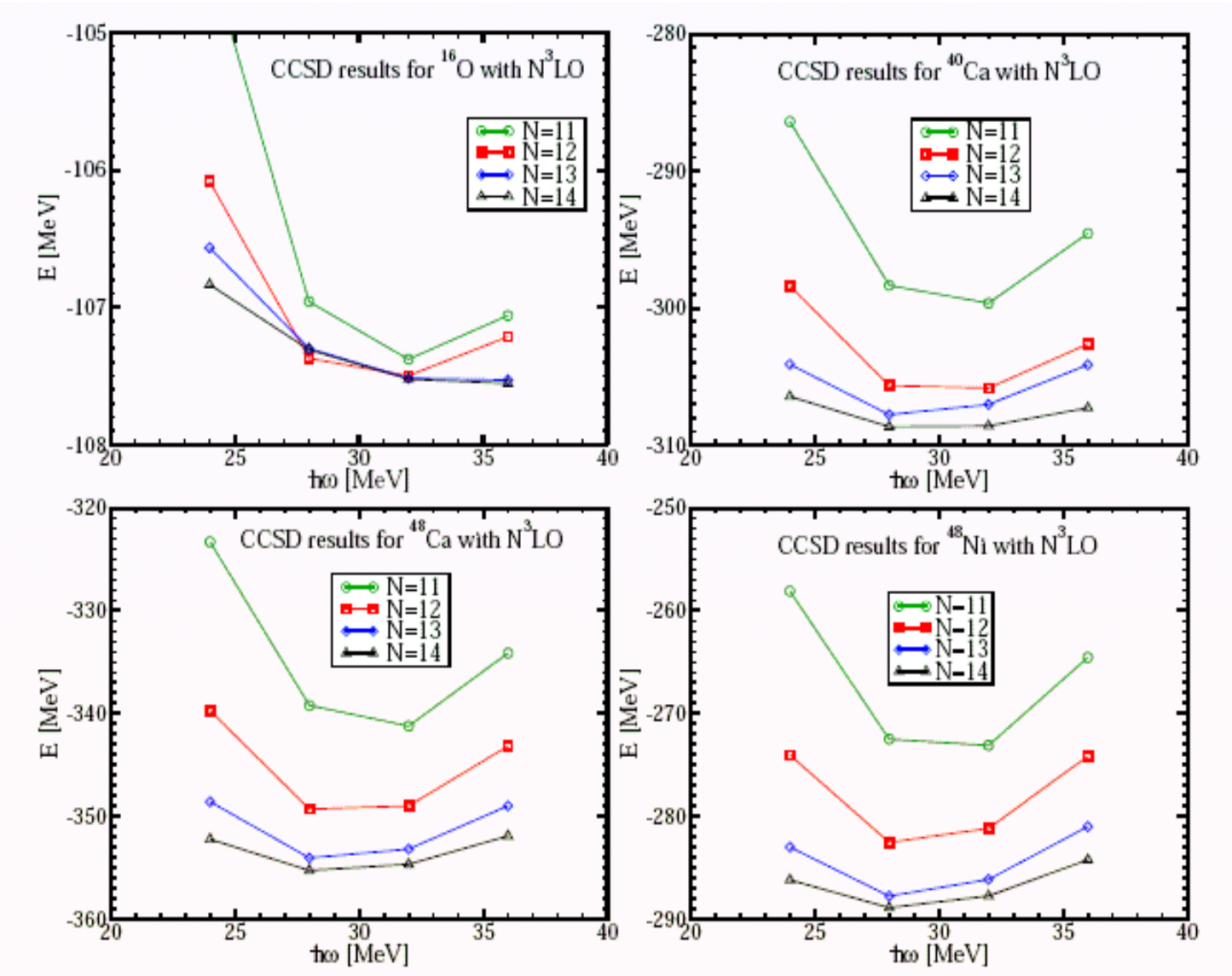
- Implemented a CCSD J-coupled code for heavier nuclei:
- Scaling at CCSD goes from $O(n_o^2 n_u^4)$ to $O(n_o^{4/3} n_u^{8/3})$
- Can do up to 14 complete major shells on a single node.
- CCSDT Gold standard for these heavier nuclei (developing)
- Enables specified calculations for heavy nuclei
- The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

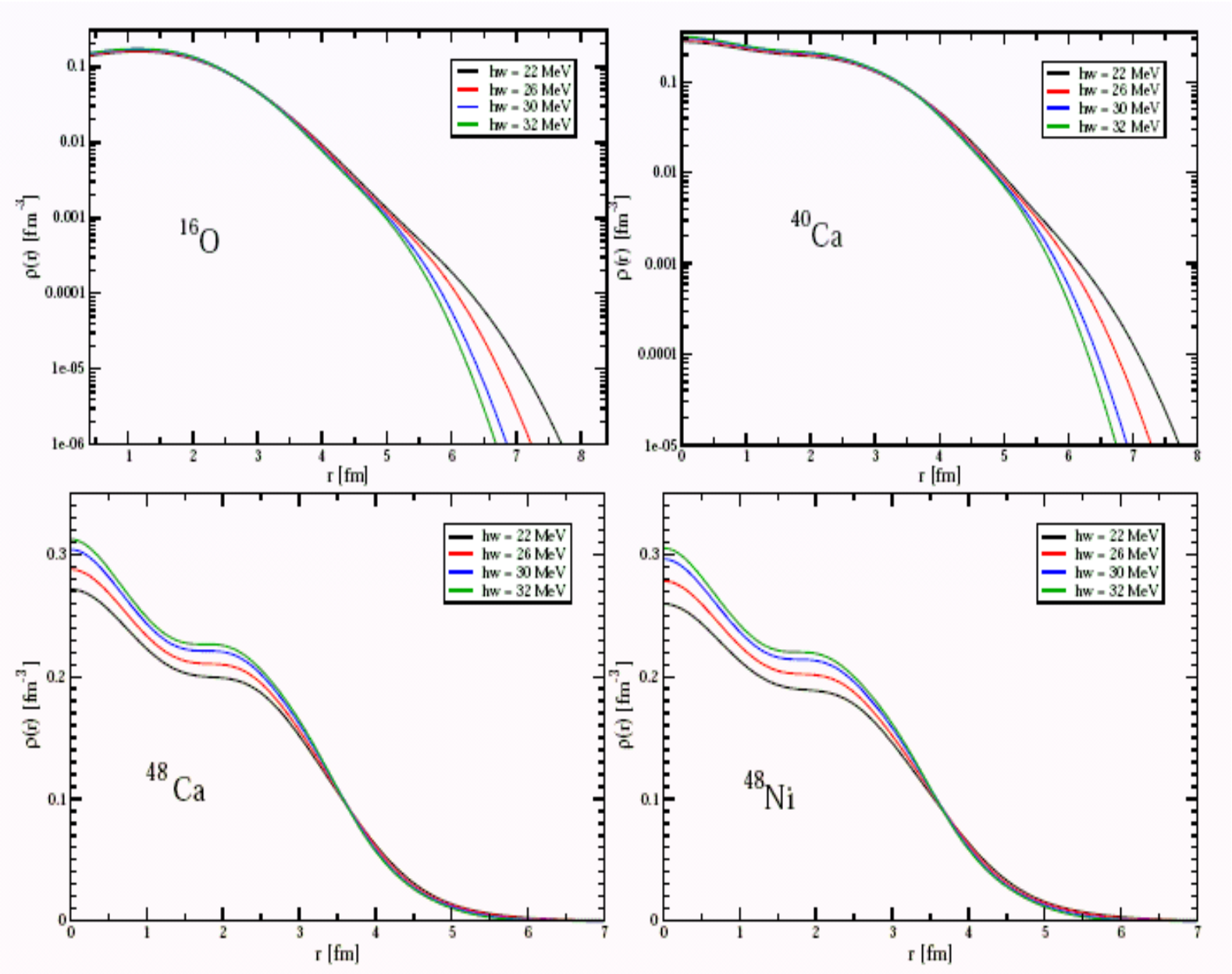
Speedup of J-coupled CCSD code for 40Ca as compared to m-scheme CCSD code



CONVERGED 16O, 40Ca, 48Ca and 48Ni CCSD ground state energies with N3LO !!



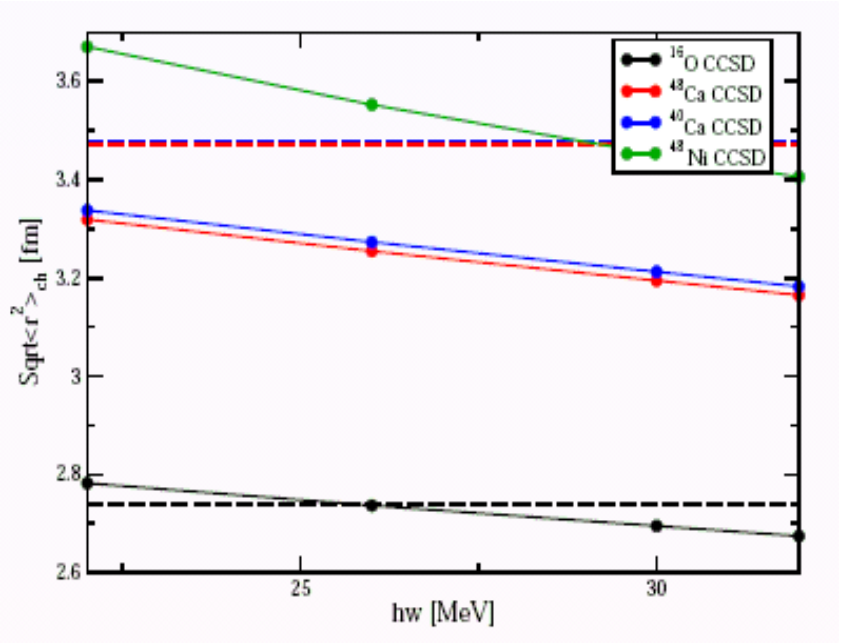
16O, 40Ca, 48Ca and 48Ni CCSD ground state densities



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 !



Nucleus	E/A	V/A	Q	$\Delta E/A$	$< r^2 >_{ch}^{1/2}$	$< r^2 >_{ch}^{1/2}$ (Exp)
^{4}He	-5.99	-22.75	0.90	1.08		1.673(1)
^{16}O	-6.72	-30.69	1.08	1.25	2.72(5)	2.737(8)
^{40}Ca	-7.72	-36.40	1.18	0.84	3.25(9)	3.4764
^{48}Ca	-7.40	-37.97	1.21	1.27	3.24(9)	3.4738
^{48}Ni	-6.02	-36.04	1.20	1.21	3.52(15)	?

Simplicity out of Complexity ! Towards microscopic foundation of the shell-model

Occupation of natural orbitals							
Nucleus	$s_{1/2}$	$p_{3/2}$	$p_{1/2}$	$d_{5/2}$	$s_{1/2}$	$d_{3/2}$	$f_{7/2}$
^{4}He π	0.946						
ν	0.946						
^{16}O π	0.953	0.965	0.962				
ν	0.952	0.964	0.961				
^{40}Ca π	0.986	0.974	0.973	0.983	0.959	0.980	
ν	0.984	0.973	0.972	0.982	0.960	0.979	
^{48} Ca π	0.983	0.971	0.970	0.979	0.959	0.977	
ν	0.987	0.976	0.975	0.983	0.963	0.982	0.987
^{48} Ni π	0.986	0.973	0.972	0.981	0.985	0.979	0.985
ν	0.977	0.966	0.966	0.974	0.956	0.971	
Occupation of Hartree-Fock orbitals							
^{16}O π	0.729	0.638	0.622				
ν	0.737	0.634	0.648				
^{40}Ca π	0.904	0.587	0.584	0.500	0.431	0.489	
ν	0.911	0.604	0.601	0.519	0.448	0.509	

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 easliy 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.