Coupled-cluster approach to an *ab-initio* description of nuclei

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Outline

Aims and Motivation

1. Facilities like RIKEN/FAIR/Eurisol/RIA(mini) can offer unprecendeted data on weakly bound systems. Increased experimental intensities.
2. Crucial for Nuclear physics next 10 years : understand how shells evolve
3. Identify and investigate methods that will extend to unstable systems
4. Combine effective interactions for unstable systems and the shell model (CI)
5. Want an 'ab initio' and reductionist approach starting with both NN and NNN interactions
6. Complement the shell model (CI) for heavier systems

Nuclear Many-Body Methods

1. Variational and Diffusion Monte Carlo/GFMC (Benchmark-test $A \leq 12$)
2. Shell-model (CI), Monte Carlo shell model and No-core shell-model
3. Coupled cluster theory
4. Perturbative many-body methods
5. Parquet diagrams, Green's function method, FHNC, ab initio DFT,.....
6. Extention to weakly bound systems : Complex scaling and complex shell model, Gamow shell model.

Progress in our QCD understanding of the NN force

- CEBAF 12 GeV upgrade: Explore the limits of our understanding of the atomic nuclei based on nucleonic and mesonic degrees of freedom
  1. Experimental plans aim at identifying and exploring the transition from the nucleon/meson description of nuclei to the underlying quark and gluon description.
  2. Test the short-range behavior of the NN interaction via deep inelastic scattering
- Effective field theory has made progress in constructing NN and NNN forces from the underlying symmetries of QCD
- Three-body forces emerge naturally and have explicit expressions at every order in the chiral expansion.
- Recent progress in Lattice QCD may hold great promise for the construction/paremetrization of the nucleon-nucleon interaction.

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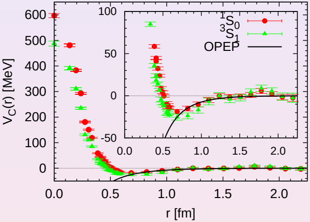
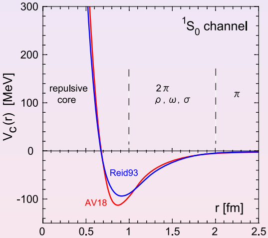
- Recent progress in Lattice QCD may hold great promise for the construction/paremetrization of the nucleon-nucleon interaction.

Lattice QCD, Ishii *et al*, nucl-th/0611096, PRL 2007





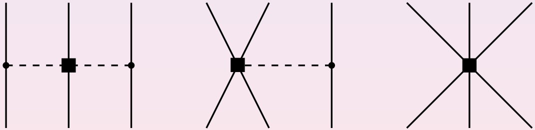
The nucleon-nucleon interaction, Phenomenology vs Lattice calculations.

2N and 3N Interactions from Effective Field Theory

Nucleons and Pions as effective degrees of freedom only. Chiral perturbation theory for different orders (ν) of the expansion in terms of momentum/pion mass.

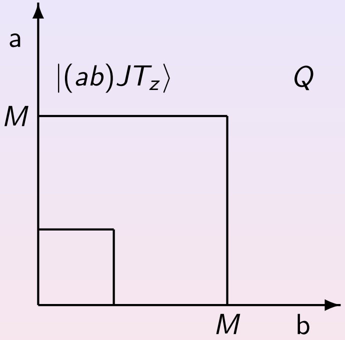
Chiral order	2N force	3N force	4N force
$\nu = 0$	$V_{1\pi} + V_{\mathrm{cont}}$	–	–
$\nu = 1$	–	–	–
$\nu = 2$	$V_{1\pi} + V_{2\pi} + V_{\mathrm{cont}}$	–	–
$\nu = 3$	$V_{1\pi} + V_{2\pi}$	$V_{2\pi} + V_{1\pi,\,\mathrm{cont}} + V_{\mathrm{cont}}$	–
$\nu = 4$	$V_{1\pi} + V_{2\pi} + V_{3\pi} + V_{\mathrm{cont}}$	work in progress	work in progress

Three-Nucleon Force at chiral order $\nu = 3$.



(a) (b) (c)

Effective Hamiltonian and Model Spaces



$$M \leq 2n + l \approx 4 - 20$$

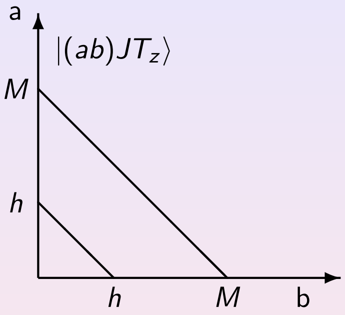
Two-Body Effective Hamiltonian for Large Space

Need to renormalize short-range behavior of V:

$$G_{ijkl} = V_{ijkl} + \sum_{mn \in Q} V_{ijmn} \frac{Q}{\omega - \varepsilon_m - \varepsilon_n} G_{mnkl}$$

- Harmonic oscillator basis.
- Note well energy ω dependence!
- 2N interactions + Coulomb. Compute via matrix inversion.

Effective Hamiltonian for Large Spaces II



$$M \leq 2n + l \approx 200$$
$$h \leq 2n + l \approx 4 - 20$$

Similarity Transformation

- Diagonalize

$$H_2^\Omega = \frac{\vec{p}_1^{\,2} + \vec{p}_2^{\,2}}{2m} + \frac{1}{2} m\Omega^2 (\vec{r}_1^{\,2} + \vec{r}_2^{\,2})$$

$$+ V(\vec{r}_1 - \vec{r}_2) - \frac{m\Omega^2}{2A} (\vec{r}_1 - \vec{r}_2)^2$$

- Use similarity-transformation to obtain V_{eff} for smaller space.
- No energy dependence! HO basis.

Algorithm

Start with the two-body equation

$$H_2^{\Omega} \equiv H_{02}^{\Omega} + V_2^{\Omega} = \frac{\vec{p}_1^{\,2} + \vec{p}_2^{\,2}}{2m} + \frac{1}{2} m\Omega^2 (\vec{r}_1^{\,2} + \vec{r}_2^{\,2}) + V(\vec{r}_1 - \vec{r}_2) - \frac{m\Omega^2}{2A} (\vec{r}_1 - \vec{r}_2)^2 \, .$$

- Define A for the specific nucleus
- Define a large space in terms of the harmonic oscillator shells $2n + l \sim 200 - 300$
- Diagonalize exactly the two-body problem.
- Transform to a smaller space with $2n + l \sim 4 - 20$ via adequate similarity transformations

$V_{\mathrm{low}-k}$ in large spaces

- Diagonalize the two-body Schroedinger equation in momentum space for all momenta
- Choose a cutoff which defines the model space in terms of relative momenta
- Use exact eigenvalues and momenta to perform a similarity transformation
- Obtain effective interaction in relative momenta
- Integrate to get harmonic oscillator matrix elements for relative quantum numbers
- Transform to lab frame

Potential drawback: no connection with harmonic oscillator cutoff. Interaction stays the same irrespective of the number of shells.

All two-body interactions need to be accompanied by at least a three-body interaction.

What do we want?

1. Want a many-body formalism which allows one to include in a systematic way various many-body correlations.
2. These correlations should be summed to infinite order (want a size-extensive theory)
3. Should be able to describe both bound and weakly bound systems.
4. Complement the shell model for heavier systems and extract better effective interactions for the nuclear shell model
5. Strategy: combine coupled cluster with shell-model (CI)

Why Coupled-Cluster theory?

Advantages

- Fully microscopic. Only linked diagrams enter, size extensive
- Can be improved upon systematically, e.g., by inclusion of three-body interactions and more complicated correlations. To be contrasted to many-body perturbation theory.
- Allows for description of both closed-shell systems and valence systems
- Derivation of effective two and three-body interactions for the shell model
- Amenable to parallel computing
- Huge development in Quantum Chemistry. Exploit this for the nuclear many-body problem.

More on Coupled Cluster

More advantages

- Can be used to generate excited spectra for nuclei like ^{16}O or ^{40}Ca with many shells. Hard for the shell model to go beyond one major shell. Huge dimensionalities in shell-model (CI) calcs

System	4 shells	7 shells
^{4}He	4E4	9E6
^{8}B	4E8	5E13
^{12}C	6E11	4E19
^{16}O	3E14	9E24

  Shell-model (CI) codes can today reach dimensionalities of $d \sim 10^{10}$ basis states.
- Can include complex effective interactions

Coupled Cluster with Triple Correlations

Correlated many-body wave function is given by

$$|\,\Psi\rangle = \exp\left(T\right)|\,\Phi_0\rangle\ ,$$

with the reference Slater determinant as $|\,\Phi_0\rangle$ and the correlation operator as $T = T_1 + T_2 + T_3 + \cdots + T_A$

$$T_1 = \sum_{i<\varepsilon_f, a>\varepsilon_f} t_i^a a_a^+ a_i$$

for single excitations (S, 1p-1h)

$$T_2 = \frac{1}{4} \sum_{i,j<\varepsilon_f; ab>\varepsilon_f} t_{ij}^{ab} a_a^+ a_b^+ a_j a_i$$

for double excitations (D, 2p-2h) and

$$T_3 = \frac{1}{36} \sum_{i,jk<\varepsilon_f; abc>\varepsilon_f} t_{ijk}^{abc} a_a^+ a_b^+ a_c^+ a_k a_j a_i$$

for triple excitations (T, 3p-3h)

Coupled Cluster equations

Define:

$$f = \sum_{pq} f_{pq} \{a_p^+ a_q\}$$

with f_{pq} the Fock matrix elements

$$W = \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \{a_p^+ a_q^+ a_r a_s\}$$

where $\langle pq || rs \rangle$ are anti-symmetrized two-body matrix elements. Normal-order creation and annihilation operators.

Coupled Cluster, CCSDT level

The extention to triples gives the following equations for the amplitudes with 1p-1h

$$\langle\Phi_i^a|[fT_1+f(T_2+1/2T_1^2)+WT_1+W(T_2+1/2T_1^2)+W(T_1T_2+1/6T_1^3+T_3)]_C|\Phi\rangle=0,$$

and with 2p-2h

$$\langle\Phi_{ij}^{ab}|[fT_1+f(T_3+T_2T_1)+W+WT_1+W(T_2+1/2T_1^2)+W(T_1T_2+1/6T_1^3+T_3)$$

$$+W(T_1T_3+1/2T_2^2+1/2T_2T_1^2+1/24T_1^4)]_C|\Phi\rangle=0.$$

and with 3p-3h

$$\langle\Phi_{ijk}^{abc}|[fT_3+f(T_3T_1+1/2T_2^2)+WT_2+W(T_3+T_1T_2)+W(1/2T_2+T_3T_11/2T_1^2+T_1)$$

$$+W(T_2T_3+1/2T_2^2T_1+1/2T_3T_1^2+1/6T_2T_1^3)]_C|\Phi\rangle=0.$$

Coupled Cluster

When the equations have been solved we have defined the amplitudes $t_{\cdots}^{\cdots}$

$$T_1 = \sum_{i<\varepsilon_f, a>\varepsilon_f} t_i^a a_a^+ a_i$$

$$T_2 = \frac{1}{4} \sum_{i,j<\varepsilon_f; ab>\varepsilon_f} t_{ij}^{ab} a_a^+ a_b^+ a_j a_i$$

$$T_3 = \frac{1}{36} \sum_{i,jk<\varepsilon_f; abc>\varepsilon_f} t_{ijk}^{abc} a_a^+ a_b^+ a_c^+ a_k a_j a_i$$

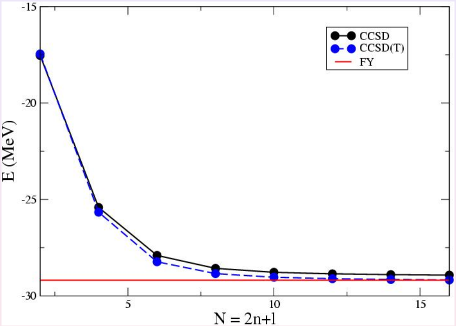
and can then extract effective interactions. Different approximations to the solution of the triples equations yield different CCSDT approximations. CCSD scales as $n_o^2 n_u^4$ while full CCSDT scales as $n_o^3 n_u^5$, with n_o the number of occupied orbits and n_u the number of unoccupied.

Acronyms, summary

1. CCSD: coupled cluster with single and double excitations only
2. CCSD(T) : CCSD energy is augmented by a perturbative treatment of triple excitation effects, normally reliable
3. CCSDT-1: skip WT_1T_3 in 2p-2h part and keep only fT_3 and WT_2 in 3p-3h
4. CCSDT-2: full 2p-2h and 3p-3h as in CCSDT-1
5. CCSDT-3 : All terms in 3p-3h except the fT_3 term.
6. CCSDT: all terms

Excellent review by Bartlett and Musial in Rev. Mod. Phys. 79, 291 (2007).

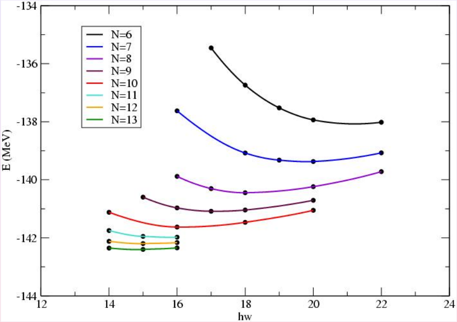
Benchmarks, ^{4}He



$V_{\mathrm{low}-k}$

- $V_{\mathrm{low}-k}$ with $\Lambda = 1.9$ fm^{-1} and $\hbar\omega = 14$ MeV
- Argonne V_{18} interaction
- Comparison with FY calculations, agreement with FY within 10 keV (FY error 50 keV))

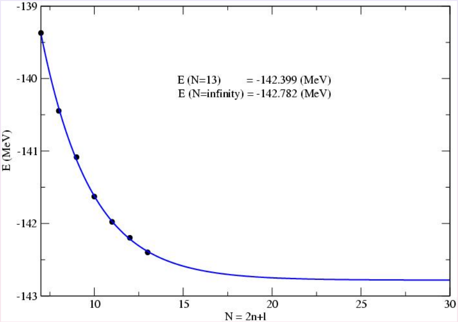
Benchmarks, ^{16}O



$\hbar\omega$ dependence

- $V_{\mathrm{low}-k}$
- Argonne V_{18} interaction
- With increasing number of shells $2n + l$ $\hbar\omega$ dependence disappears.

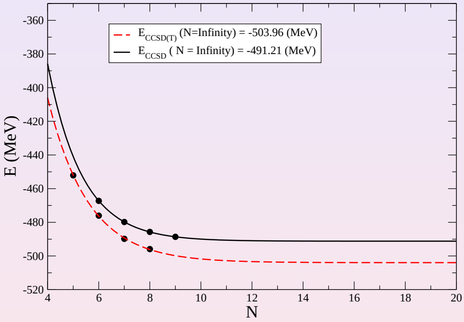
Benchmarks, ^{16}O



Extrapolation

- $V_{\mathrm{low}-k}$ with $\Lambda = 1.9$ fm^{-1} and $\hbar\omega = 14$ MeV
- Argonne V_{18} interaction
- Note overbinding, need to accompany a two-body interaction with three-body interaction

Benchmarks, ^{40}Ca

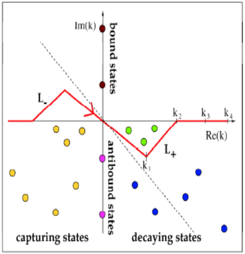


Extrapolation

- $V_{\text{low}-k}$ with $\Lambda = 1.9$ fm^{-1} and $\hbar\omega = 20$ MeV. Argonne V_{18}.
- Note considerable overbinding, need to accompany a two-body interaction with three-body interaction. Different NN forces need different NNN forces. Largest space 10^{66}.

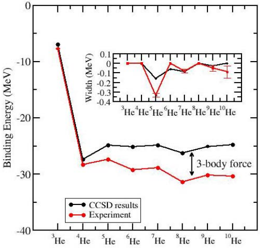
Helium Isotopes

Weakly bound and unbound nuclei – requires continuum states: complex coupled-clusters [Hagen et al, PRL (2006)]



Single-particle basis includes bound, resonant, non-resonant continuum, and scattering states (5s5p5d4f4g protons; 20s20p5d4f4g neutrons)

He Chain Results



N^3LO V_{lowk} (λ=1.9 fm^{-1})

Coupled Cluster, Complex Scaling and He Isotopes

	^{3}He		^{4}He		^{5}He		^{6}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
$s-p$	-4.94	0.00	-24.97	0.00	-20.08	-0.54	-19.03	-0.18
$s-d$	-6.42	0.00	-26.58	0.00	-23.56	-0.22	-23.26	-0.09
$s-f$	-6.81	0.00	-27.27	0.00	-24.56	-0.17	-24.69	-0.07
$s-g$	-6.91	0.00	-27.35	0.00	-24.87	-0.16	-25.16	-0.06
Expt.	-7.72	0.00	-28.30	0.00	-27.41	-0.33(2)	-29.27	0.00

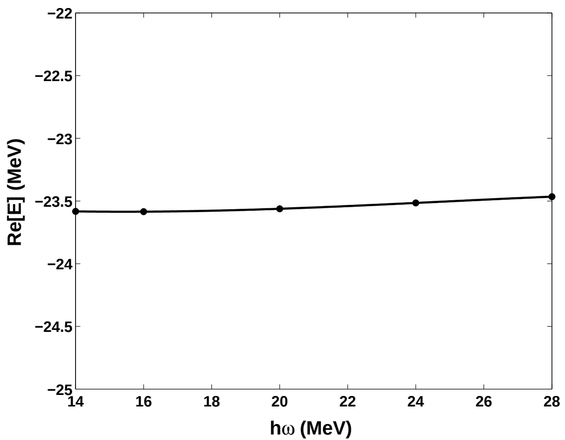
CCSD calculation of the $^{3-6}$He ground states with the low-momentum N^{3}LO nucleon-nucleon interaction for increasing number partial waves. The energies E are given in MeV for both real and imaginary parts. Reference state defined so that total spin projection is maximal. Orbits with largest m_j filled first.

Coupled Cluster, Complex Scaling and He Isotopes

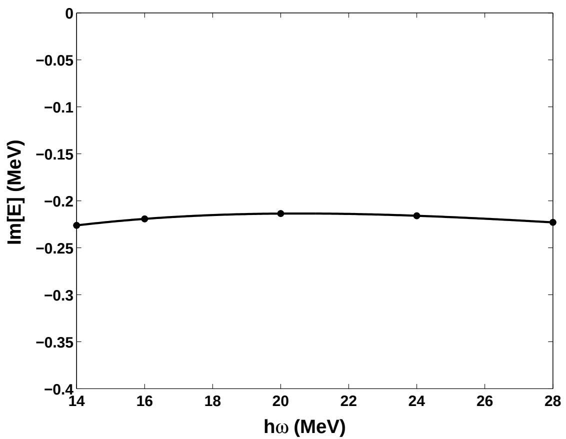
	^{7}He		^{8}He		^{9}He		^{10}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
$s-p$	-17.02	-0.24	-16.97	-0.00	-15.28	-0.40	-13.82	-0.12
$s-d$	-22.19	-0.12	-22.91	-0.00	-21.34	-0.15	-20.60	-0.02
$s-f$	-24.13	-0.11	-25.28	-0.00	-23.96	-0.06	-23.72	-0.00
$s-g$	-24.83	-0.09	-26.26	-0.00	-25.09	-0.03	-24.77	-0.00
Expt.	-28.83	-0.08(2)	-31.41	0.00	-30.26	-0.05(3)	-30.34	0.09(6)

CCSD calculation of the $^{7-10}$He ground states. 850 single-particle orbitals, $5s5p5d4f44h4i$ proton orbitals and $20s20p5d4f44h4i$ neutron orbitals. For ^{10} this is approximately 10^{22} basic states.

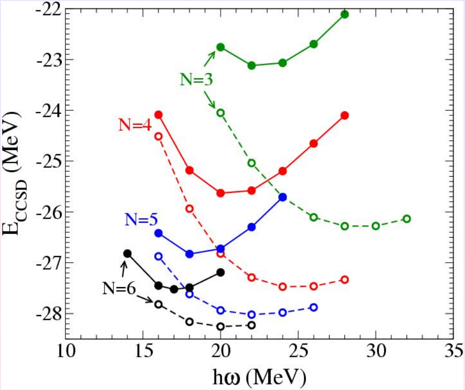
$\hbar\omega$ dependence of the real part of the ^{5}He ground state energy



$\hbar\omega$ dependence of the imaginary part of the ^{5}He ground state energy



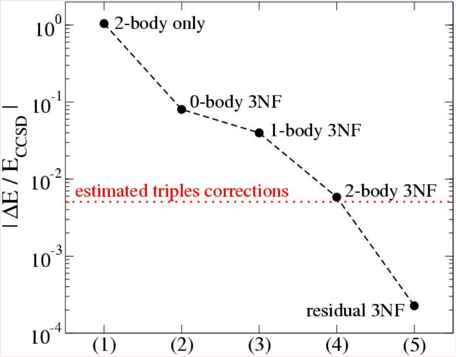
^{4}He and three-body, preliminary



Scheme

- $V_{\mathrm{low}-k}$ Hamiltonian based on V_{18} interaction with (full) three-body interaction added and without (dashed) .
- $V_{\mathrm{low}-k}$ with $\Lambda = 1.9$ fm^{-1}.
- Only $T = 1/2$ and $J = 1/2$ part of three-body interaction.

^{4}He and three-body



Relative contribution $\Delta E / E_{CCSD}$

- Normal-ordered Hamiltonians due to 3NFs
- Dotted line represents the estimated triple corrections

Summary: much Work in Progress

- Three-body forces included in CC calculations, give density dependent two-body forces.
- Can now extract effective interactions for the nuclear shell-model, with and without three-body forces.
- Inclusion of continuum effects, complex coupled-cluster code and complex effective interactions
- Three-body forces included in CC calculations, give density dependent two-body forces.
- Current interest: Helium and Oxygen isotopes, especially from ^{20}O till ^{28}O. several experiments at for example RIKEN and NSCL-MSU, ^{23}O, ^{24}O and ^{25}O.
- Ground state properties of closed-shell nuclei, from ^{4}He to ^{208}Pb: Now ^{56}Ni.
- How much due to three-body forces and how much due to coupling to continuum with only two-body?
- Can we understand how shells evolve? Is it due to three-body effects or continuum effects, or something else?

Selected Articles

- Kowalski *et al*, Phys. Rev. Lett. **92**, 132501 (2004).
- Wloch *et al*, Phys. Rev. Lett. **94**, 132501 (2005).
- Hagen, Hjorth-Jensen, and Michel, Phys. Rev. C **73**, 064307 (2006), complex scaling
- Hagen *et al*, nucl-th/0610072, Phys. Lett. B, in press, complex scaling
- Hagen *et al*, nucl-th/0704.2854, Phys. Rev. C, in press, three-body interaction
- Hagen *et al*, nucl-th/0707.1516, Phys. Rev. C, submitted, benchmark calculations

ORNL-OSLO-Michigan Many-Body project

ORNL

David Dean, Gaute Hagen, Thomas Papenbrock and Achim Schwenk (TRIUMF)

Oslo

Elise Bergli, Morten Hjorth-Jensen, Maxim Kartamychev

Michigan, MSU and CMU

Jeff Grour, Mihai Horoi, Piotr Piecuch, and Marta Wloch