Ab-initio Coupled-Cluster calculations for nuclei

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Outline

1. Status and goals in microscopic nuclear structure approaches
2. From realistic to effective interactions
3. Coupled Cluster approach to nuclear structure
   - Coupled-Cluster theory and application to light and medium mass nuclei
   - Coupled Cluster approach with three-body Hamiltonians
4. Coupled Cluster approach to many-body open quantum systems
   - Non-Hermitian representations - The Berggren ensemble.
   - CCSD calculation of Helium chain
5. Conclusion

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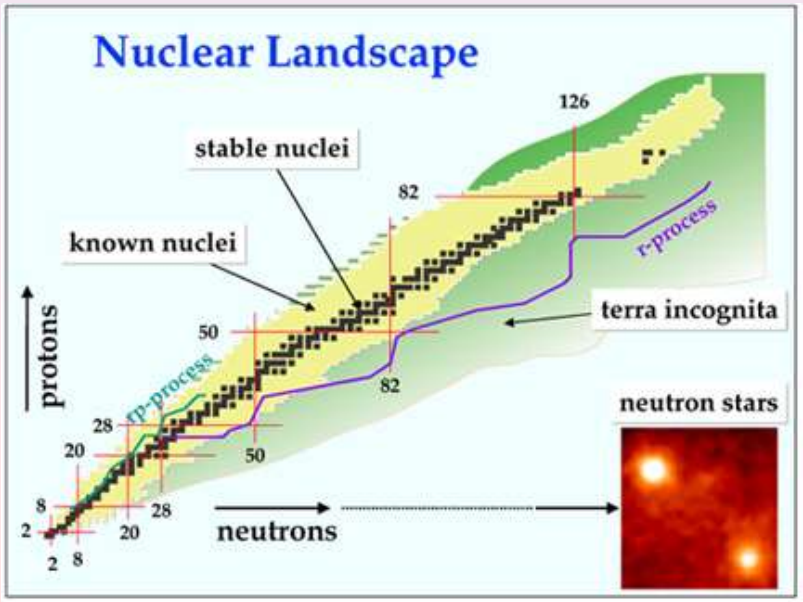
Aims in Nuclear Structure

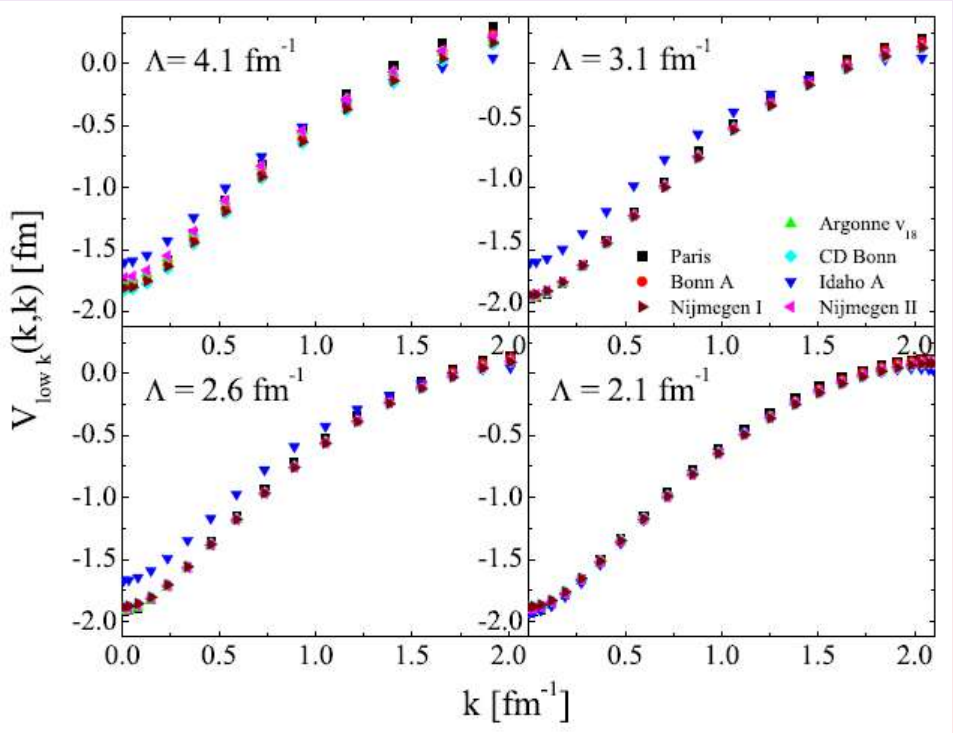
Wish to solve to A-body nuclear Hamiltonian

$$H = T - T_{CoM} + V = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{\mathbf{k}_i^2}{2m} + \sum_{i<j}^{A} \left(V(i,j) - \frac{\mathbf{k}_i \cdot \mathbf{k}_j}{mA} \right) + \sum_{i<j<k}^{A} V(i,j,k).$$



Low-momentum nucleon-nucleon interaction: $V_{\mathrm{low}-k}$

The free N-N interaction generates strongly repulsive and/or diverging matrix elements at short internucleonic distances. Need a **Renormalized Interaction !**



Different high-precision potentials

↓

Universal low-momentum potential

Ref.: S. K. Bogner, T. T. S. Kuo, and A. Schwenk, Phys. Rep. 386 (2003) 1

$V_{\mathrm{low}-k}$; Pros and Cons

1. Energy and nucleus independent interaction.
2. Soft core, suitable for Many-Body perturbation calculations.
3. Means to probe importance of missing Many-Body forces.
4. Generates a cutoff (λ) dependence, which can only be removed by including corresponding Many-Body forces.

Question: Is 3-N force sufficient to remove λ dependence and if so can the 3-N force be treated perturbatively ?

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Coupled Cluster approach to medium mass nuclei

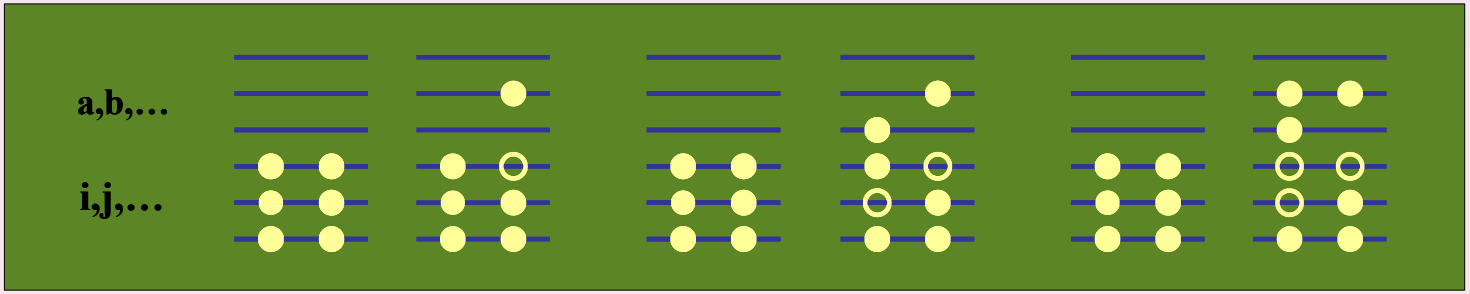
1. Coupled Cluster Theory is fully microscopic .
2. Coupled Cluster is size consistent. The energy of two non-interacting fragments computed separately is the same as that computed for both fragments simultaneously.
3. Low computational cost (CCSD scales as $n_o^2 n_u^4$).
4. Capable of systematic improvements.
5. Amenable to parallel computing.

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

Coupled Cluster in pictures

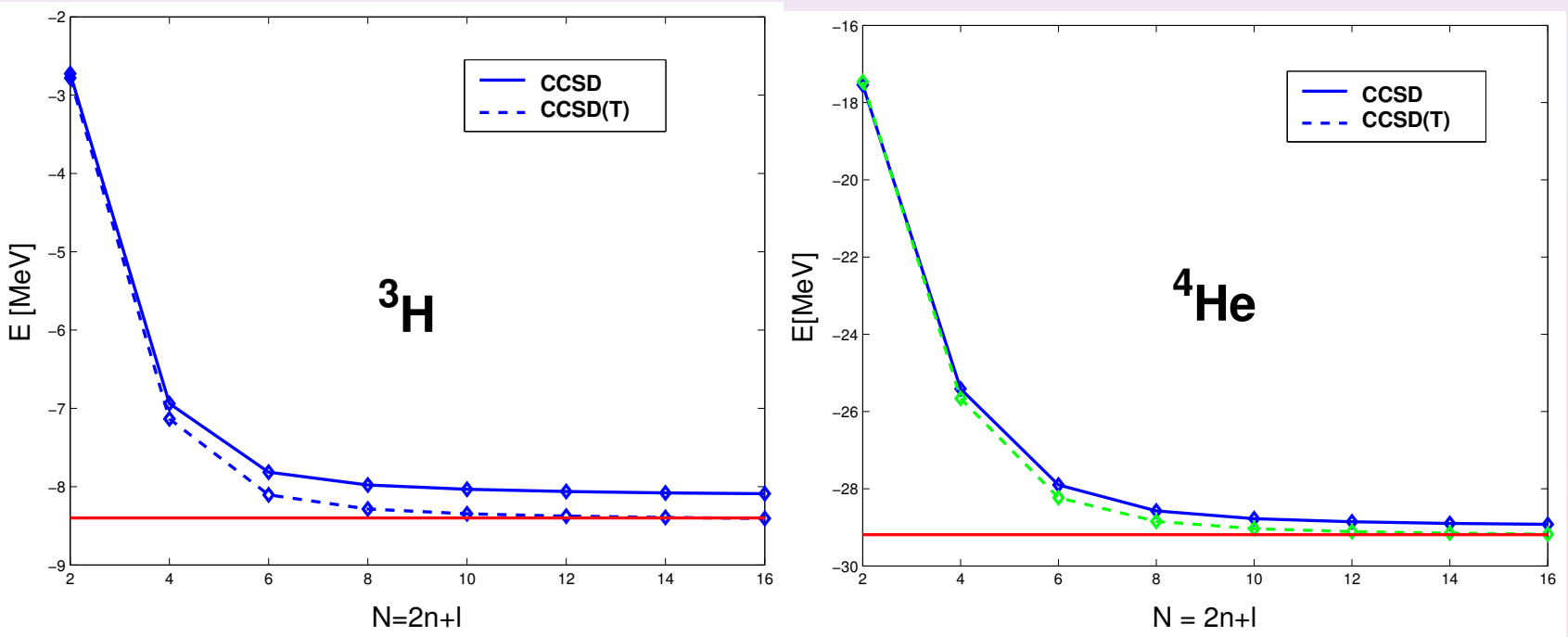
$$\left|\Psi\right\rangle = e^{T^{(A)}}\left|\Phi\right\rangle, \quad T^{(A)} = \sum_{k=1}^{m_A} T_k$$

$$T_1 = \sum_{\substack{i \\ a}} t_i^a \left|\Phi_i^a\right\rangle, \quad T_2 = \sum_{\substack{i>j \\ a>b}} t_{ij}^{ab} \left|\Phi_{ij}^{ab}\right\rangle, \quad T_3 = \sum_{\substack{i>j>k \\ a>b>c}} t_{ijk}^{abc} \left|\Phi_{ijk}^{abc}\right\rangle$$



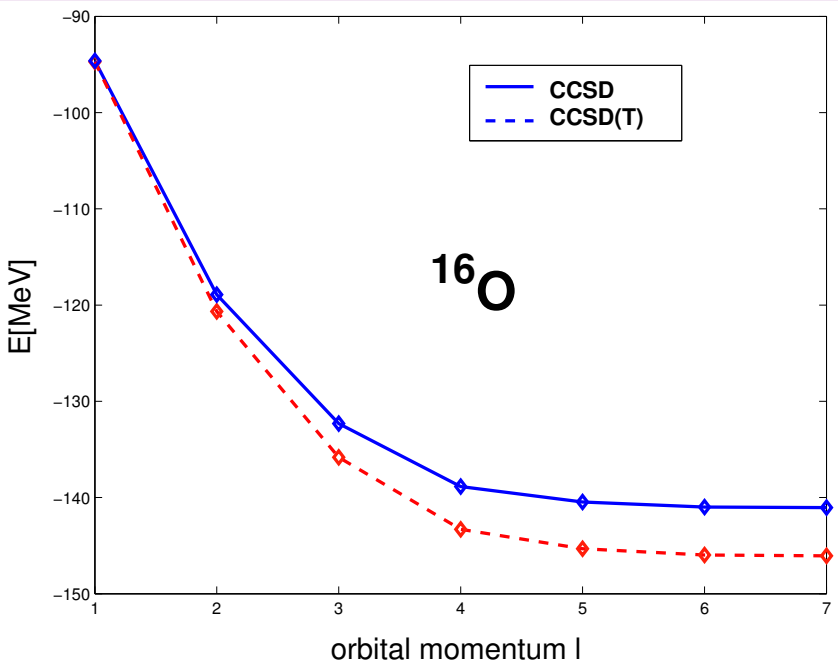
Coupled Cluster meets benchmarks of ^{3}H and ^{4}He!

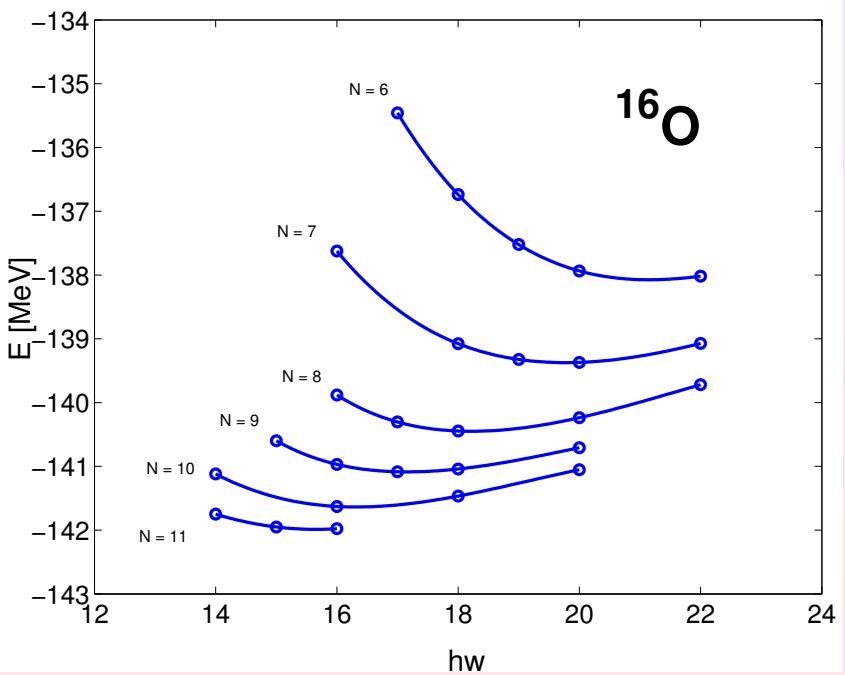
CCSD(T) and Faddeev (-Yakubovsky) results for ^{3}H and ^{4}He using $V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 1.9\mathrm{fm}^{-1}$. **CCSD(T) are within the errors (50 keV) of the Faddeev results!**



Benchmarking ^{16}O with Coupled Cluster Theory

- $V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 2.1\mathrm{fm}^{-1}$.
- $N = 11$ and $l_{max} = 7$ model space gives a shell model dimension of $7E33$!
- An exponential fit to the energy minima yields $E \approx -142.9$MeV.





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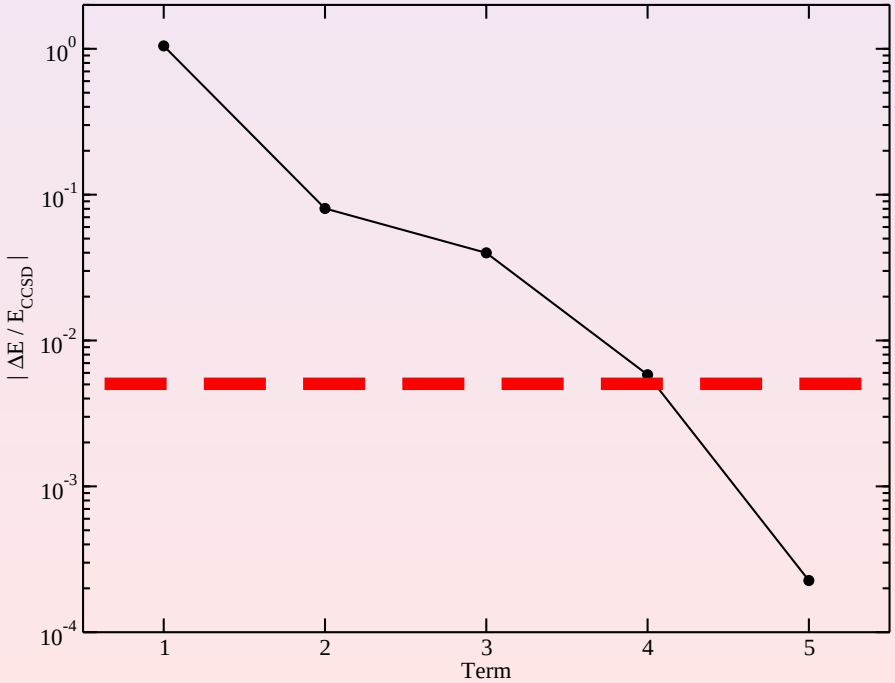
Coupled Cluster Results with TNF

- We have derived and implemented Coupled Cluster equations for three-body Hamiltonians.
- Probe cutoff dependence of $V_{\mathrm{low}-k}$ with three nucleon force in light and medium heavy nuclei.
- Does TNF provide the necessary repulsion/attraction needed to approach experimental mass values ?
- " *Coupled-cluster theory for three-body Hamiltonians* "
  G.Hagen, T.Papenbrock, D. J. Dean, A. Schwenk, A. Nogga, M. Włoch, P. Piecuch.
  To be submitted to PRC.

Different contributions to E_{CCSD} from TNF in ^{4}He

Three-body Hamiltonian in normal ordered form:

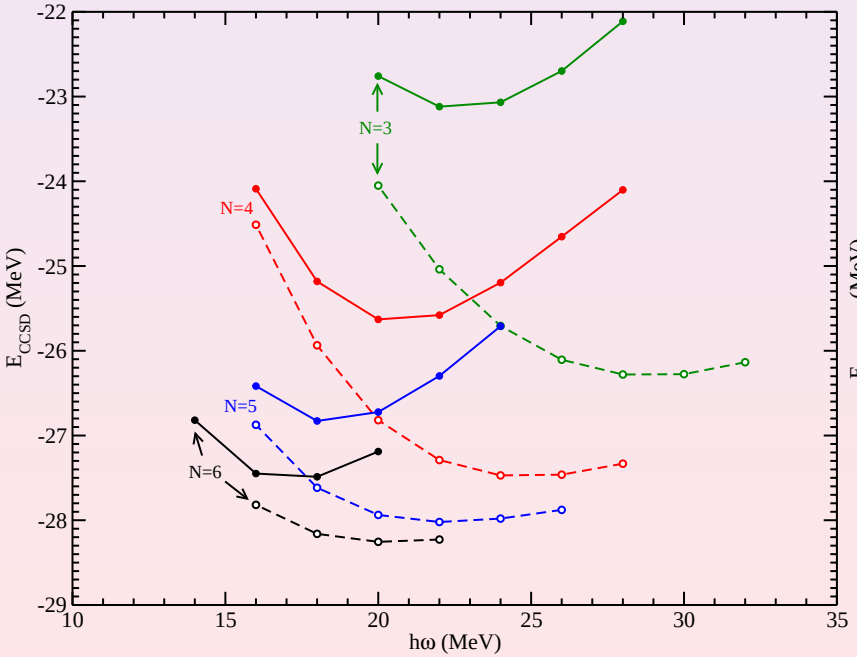
$$\hat{H}_3 = \frac{1}{6}\sum_{ijk}\langle ijk||ijk\rangle + \frac{1}{2}\sum_{ijpq}\langle ijp||ijq\rangle\{\hat{a}_p^\dagger\hat{a}_q\} + \frac{1}{4}\sum_{ipqrs}\langle ipq||irs\rangle\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_s\hat{a}_r\} + \hat{h}_3 \ ,$$

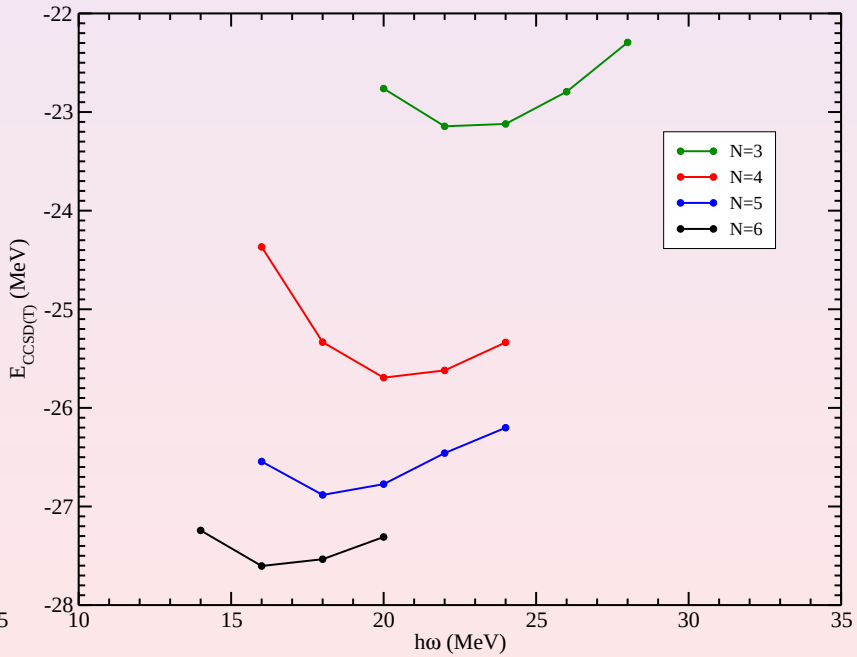


The "density dependent" zero-, one-, and two-body terms of TNF gives the largest contribution to E_{CCSD}.

Coupled Cluster Results for ^{4}He with TNF

- $V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 1.9\mathrm{fm}^{-1}$.
- Exponential fit to the CCSD minima yields $E \approx -28.09$ MeV.
- Exponential fit to the CCSD(T) minima yields $E \approx -28.24$ MeV.
  Fadeev-Yakubovski result: $= -28.29$MeV.





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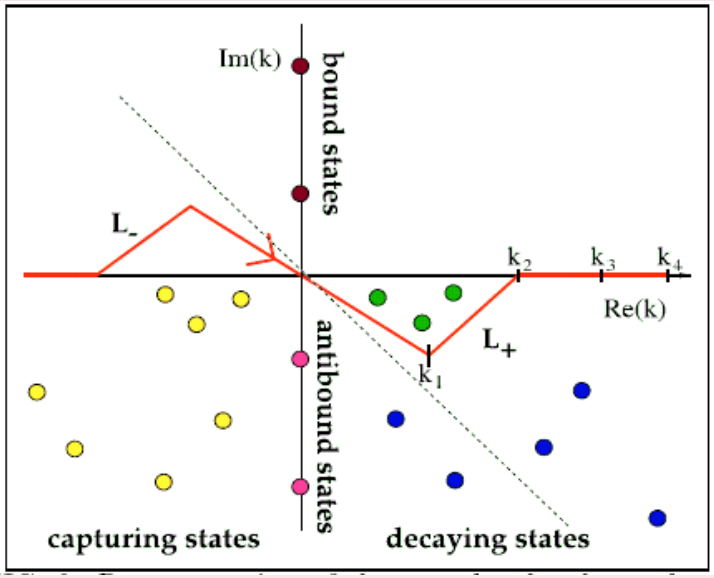
Berggren Single-particle basis

Complex energies requires a generalized completeness relation

$$|\Psi(\mathbf{r},t)|^2 = |\Phi(\mathbf{r})|^2 exp(-\frac{\Gamma}{\hbar}t), \quad E = E_r - i\Gamma/2.$$

$$\mathbf{1} = \sum_{n=a,b,c,d} |\psi_l(k_n)\rangle\langle\tilde{\psi}_l(k_n)| + \int_{L^+} dk\ k^2 |\psi_l(k)\rangle\langle\tilde{\psi}_l(k)|.$$



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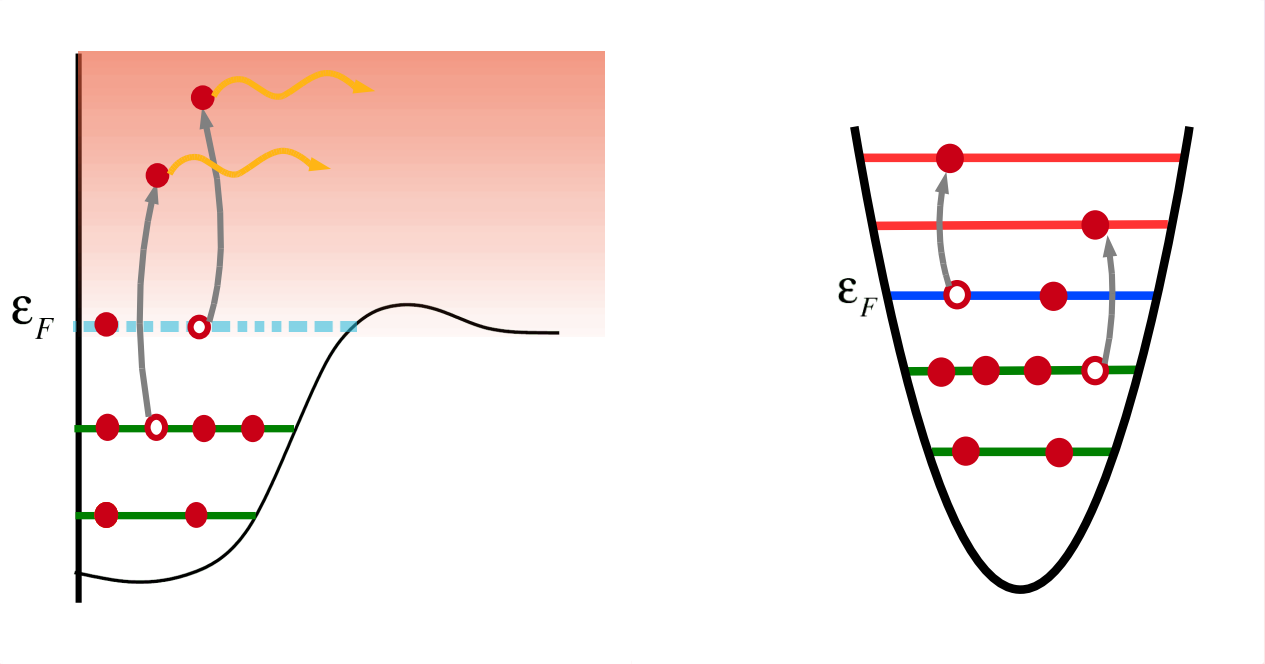
Coupled Cluster for open quantum systems

Open Quantum System.
Coupling with continuum taken into account.

Closed Quantum System.
No coupling with external continuum.

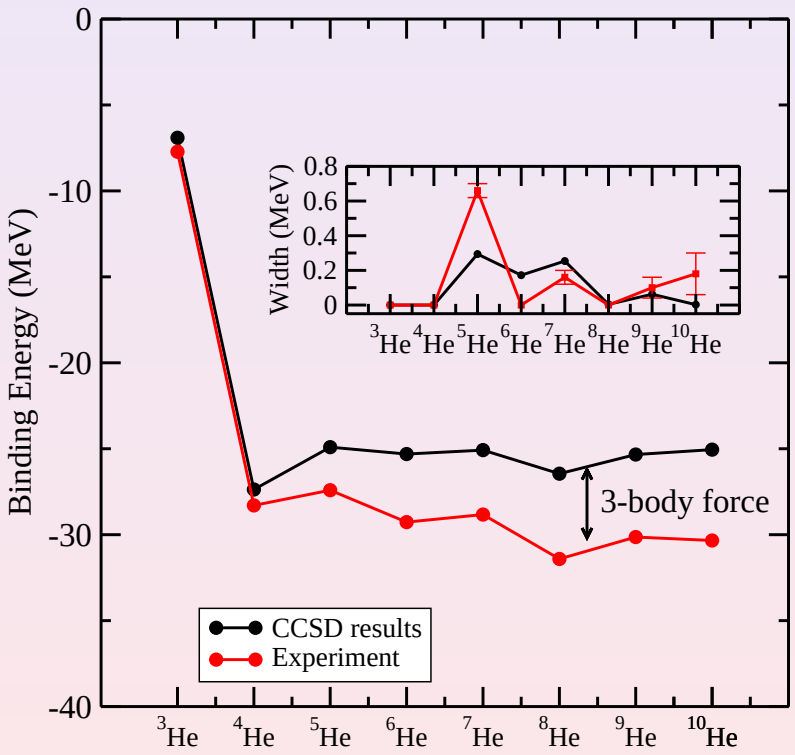


Computational cost in full CI vs. CCSD

- In our largest Coupled Cluster calculations of the He-chain we employed ~ 400 proton and $\sim 500 - 550$ neutron orbitals.
- Large scale shell model codes can reach dimensions: $d \sim 1E10$
- Monte-Carlo based shell model codes can reach dimensions: $d \sim 1E15$

Nucleus	^{4}He	^{6}He	^{8}He	^{9}He	^{10}He
Dim	8E+9	1E+14	1E+18	2E+20	1E+22

CCSD results for Helium chain using $V_{\mathrm{low}-k}$



$V_{\mathrm{low}-k}$ from N3LO with $\Lambda = 1.9\mathrm{fm}^{-1}$.

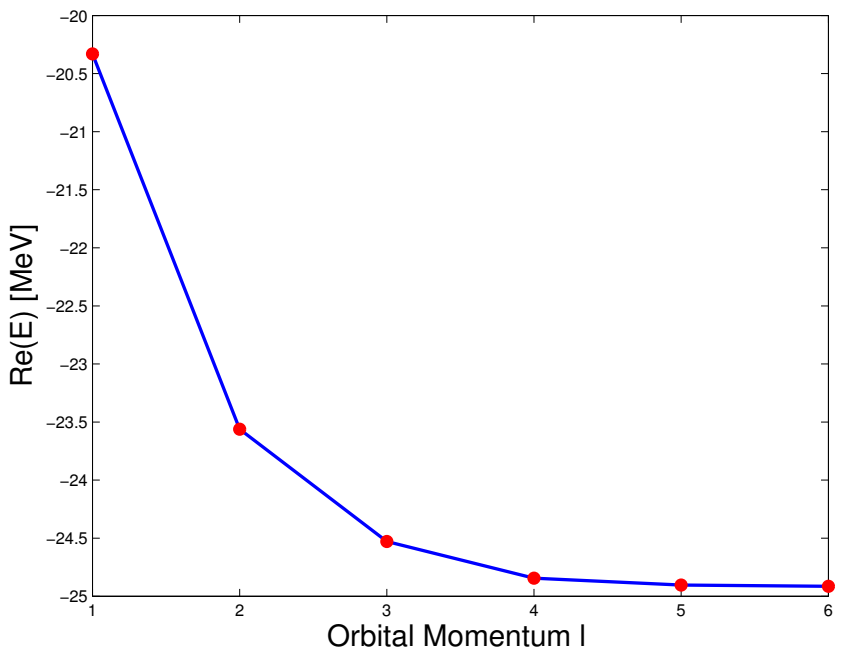
- *spdfghi* partial waves included in basis
- ~ 1000 active orbitals
- Underbinding hints at missing TNF

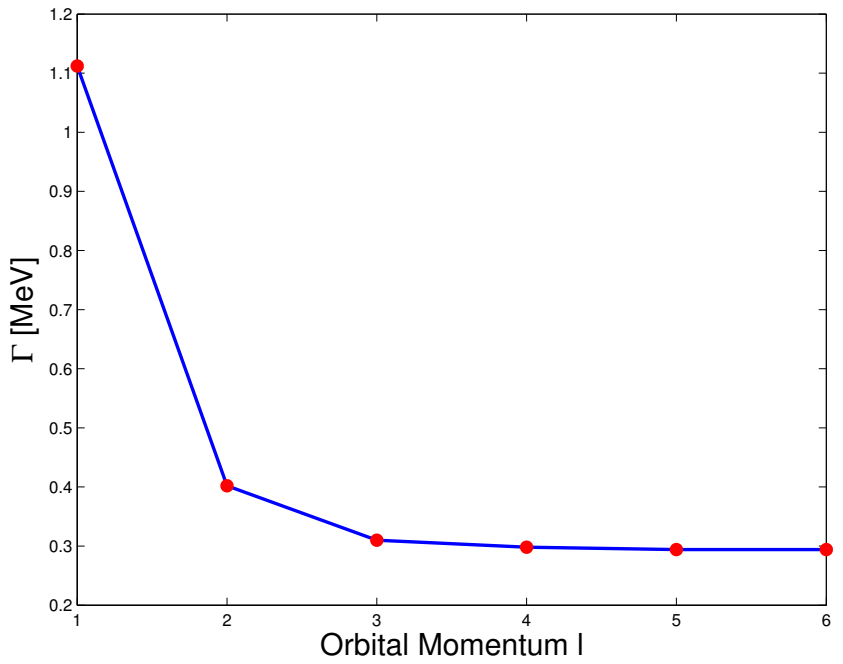
Conclusion and Perspectives

- Coupled Cluster meets few-body benchmark calculations; we have benchmarked ^{16}O with ~ 1000 active single particle orbitals.
- Coupled Cluster theory with TNF has been derived and implemented. Benchmarks of ^{4}He has been met.
- Our study of different contributions from TNF show that the zero-, one- and two-body contributions give the major contributions. Interesting perspective for heavier systems.
- Coupled Cluster theory has been succesfully applied to the description of open-quantum systems. We reproduced basic features of the Helium chain. Location of dripline in the Oxygen chain ?

Convergence of CCSD results

Convergence of ^{5}He ground state energy with increasing number of partial waves in the basis.





CCSD results for Helium chain

CCSD results for the ground state energy of the $^{3-10}$He isotopes using different model spaces. In $s-g$ space we have total of ~ 500 orbitals.

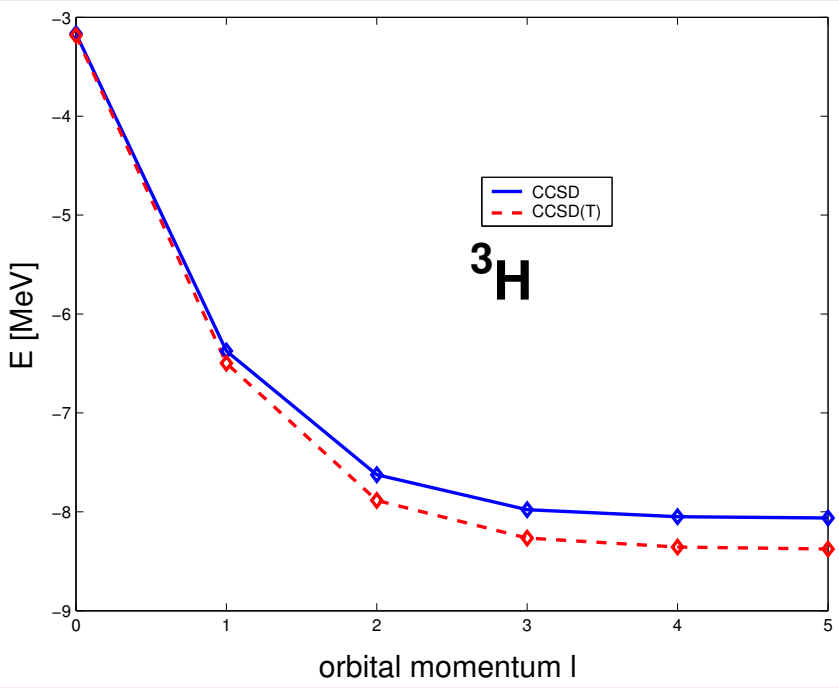
	^{3}He		^{4}He		^{5}He		^{6}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
s-p	-4.94	0.00	-24.97	0.00	-20.08	-0.54	-19.03	-0.18
s-d	-6.42	0.00	-26.58	0.00	-23.56	-0.22	-23.17	-0.08
s-f	-6.81	0.00	-27.27	0.00	-24.56	-0.17	-24.69	-0.07
s-g	-6.91	0.00	-27.35	0.00	-24.87	-0.16	-25.16	-0.06
Expt.	-7.72	0.00	-28.30	0.00	-27.41	-0.33(2)	-29.27	0.00

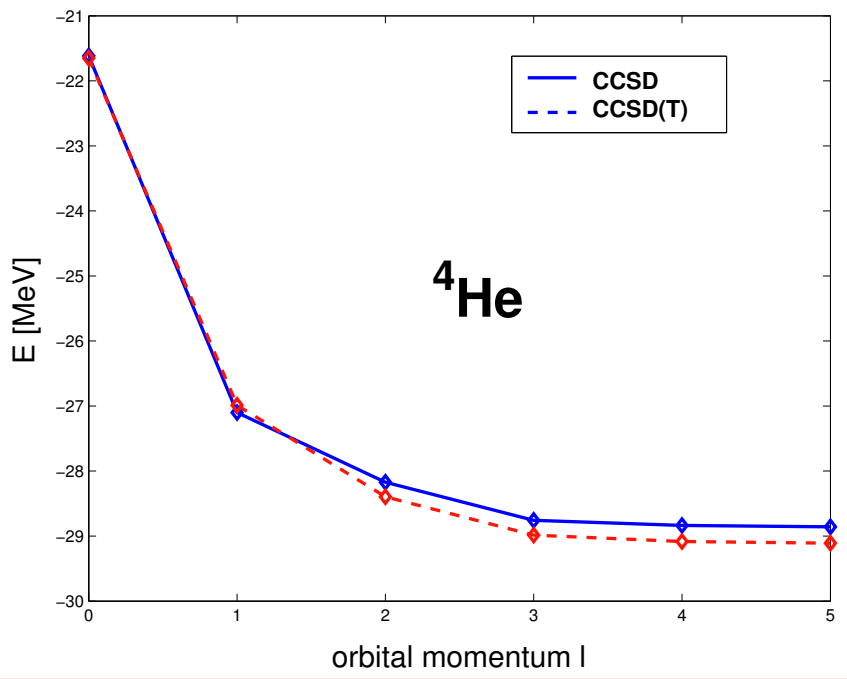
	^{7}He		^{8}He		^{9}He		^{10}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
s-p	-17.02	-0.24	-16.97	-0.00	-15.28	-0.40	-13.82	-0.12
s-d	-22.19	-0.12	-22.91	-0.00	-21.34	-0.15	-20.60	-0.02
s-f	-24.13	-0.11	-25.28	-0.00	-23.96	-0.06	-23.72	-0.00
s-g	-24.83	-0.09	-26.26	-0.00	-25.09	-0.03	-24.77	-0.00
Expt.	-28.83	-0.08(2)	-31.41	0.00	-30.14	-0.05(3)	-30.34	-0.09(6)

Results for ^{3}H and ^{4}He using $V_{\mathrm{low}-k}$

Cusp of $V_{\mathrm{low}-k}$ at cutoff momentum Λ requires a large number of nodes in the basis. Can we truncate orbital momentum l at lower values ?

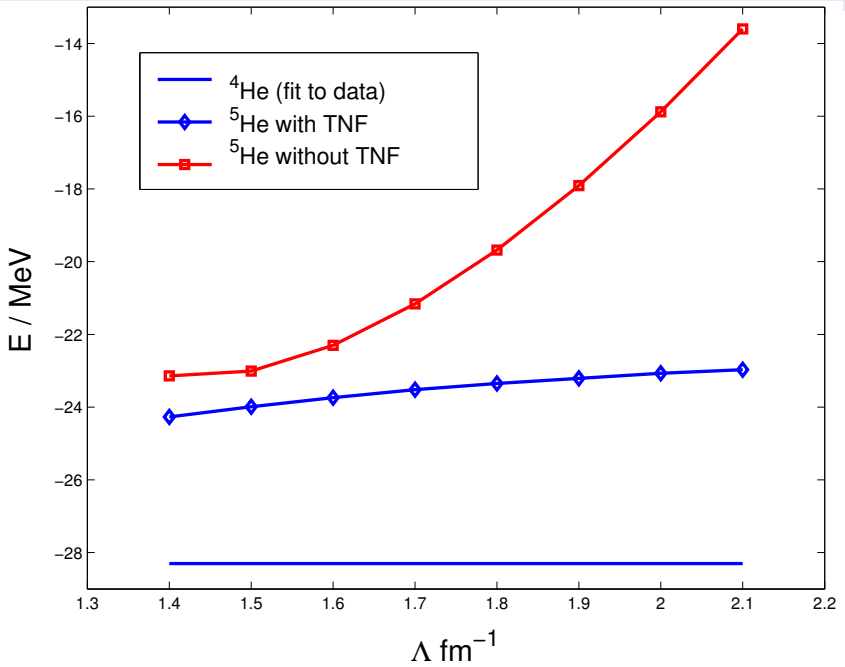
$V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 1.9\mathrm{fm}^{-1}$.

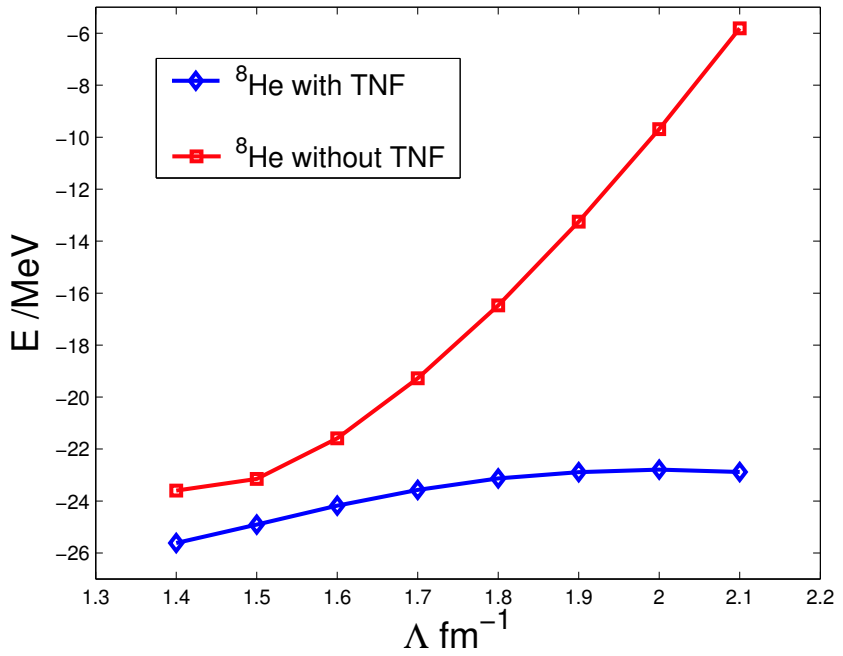




Coupled Cluster Results for Helium isotopes with TNF

CC results with $V_{\mathrm{low}-k}$ from N3LO NN-interaction. Rather limited model-space $N = 3$. Only contact term at NN2LO is retained in the three nucleon force. TNF fitted to reproduce binding energy of ^{4}He.





Coupled Cluster Expansion

Coupled-Cluster : An "Exponential Ansatz" for the wave function

$$\Psi_{CC} = \exp(T)\Phi_0 = \exp(T_1 + T_2 + T_3 + ...)\Phi_0, \quad T_n = \sum_{ab\ldots,ij\ldots} t_{ij\ldots}^{ab\ldots} a_a^\dagger a_b^\dagger \cdots a_j a_i.$$

The CC correlation energy is : $E_{\mathrm{CC}} = \langle\Phi_0|\exp(-T)\hat{H}_N \exp(T)|\Phi_0\rangle$. By the Hausdorff commutator expansion and Wick's theorem the Coupled-Cluster energy is derived,

$$E_{\mathrm{CC}} = \sum_{ia} f_{ia} t_i^a + \frac{1}{4}\sum_{abij}\langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2}\sum_{ijab}\langle ij||ab\rangle t_i^a t_j^b.$$

The algebraic equation for the excitation amplitudes $t_{ij\ldots}^{ab\ldots}$ are given by,

$$\langle\Phi_{ij\ldots}^{ab\ldots}|\exp(-T)H_N \exp(T)|\Phi_0\rangle = 0,$$

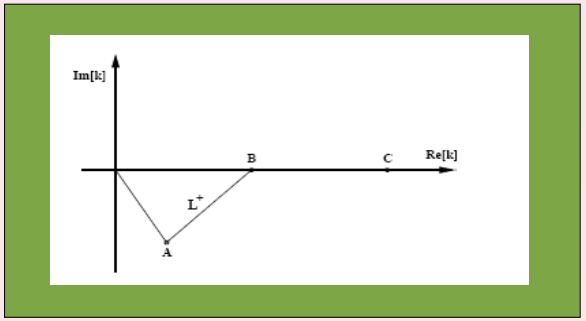
which gives a non-linear set of equations for the excitation amplitudes. Truncation of the Coupled Cluster operator T leads to :

$T = T_1 + T_2 \rightarrow$ CCSD and $T = T_1 + T_2 + T_3 \rightarrow$ CCSDT.

CCSD : How deal with explosion of basis states?

- Very low neutron separation energy. $p-$orbits are the main decay channel and build up the main part of halo-densities.
- Protons have large separation energies (20-30 MeV), mainly occupying deeply bound s-orbits.

Neutron orbitals are Gamow states for s-p partial waves and Oscillators for higher partial waves (d-g)



Neutrons

15s1/2
15p3/2
15p1/2
4d5/2
4d3/2
.
.
.

Proton orbitals are Oscillators restricted by N = 10 major shells and lmax.

Protons

5s1/2
4p3/2
4p1/2
4d5/2
4d3/2
.
.
.

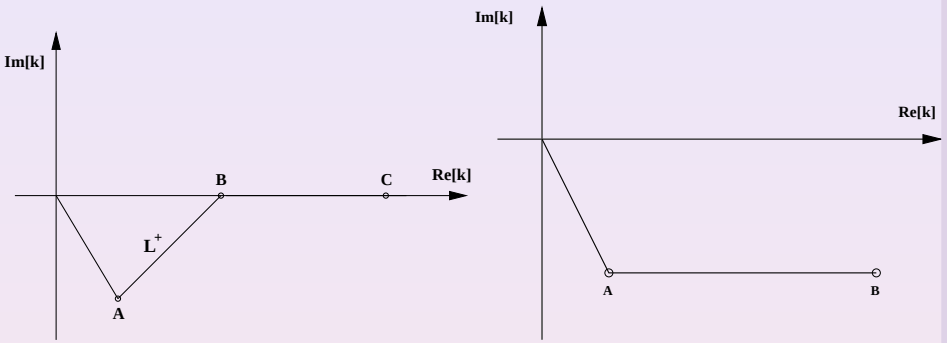
Convergence of CCSD results

- Convergence with respect to the oscillator expansion of the interaction V_{osc},

$$\langle ab|V_{\rm osc}|cd\rangle \approx \sum_{\alpha\leq\beta}^{N}\sum_{\gamma\leq\delta}^{N}\langle ab|\alpha\beta\rangle\langle\alpha\beta|V_{\rm low-k}|\gamma\delta\rangle\langle\gamma\delta|cd\rangle,$$

- Convergence with respect to the finite oscillator basis ($2n + l \leq 10$) used for the proton space and the higher partial waves for the neutron space ?
- How well are the results converged with respect to the discretization of the continuum integral defining the Berggren basis for the $s - p$ partial waves for the neutron space ?

$$\mathbf{1} = \sum_{n=a,b,c,d} |\psi_l(k_n)\rangle\langle\tilde{\psi}_l(k_n)| + \int_{L^+} dk\, k^2 |\psi_l(k)\rangle\langle\tilde{\psi}_l(k)|.$$

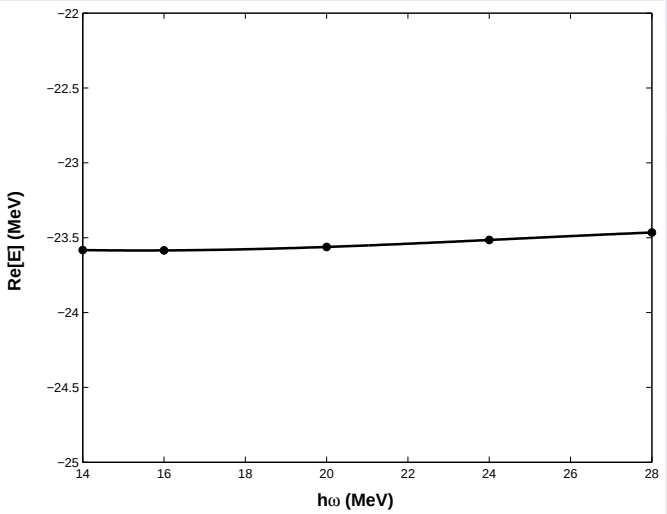


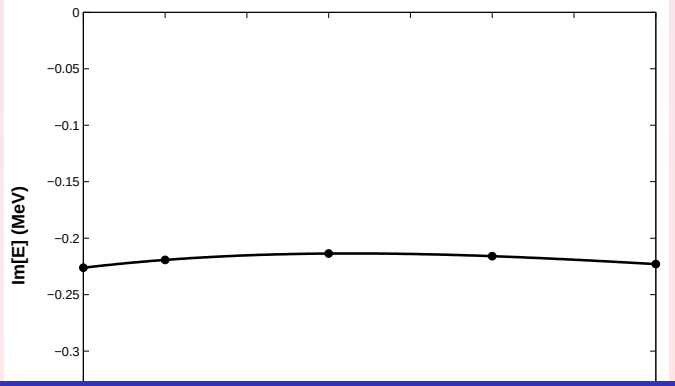
Convergence of the hole and particle neutron states in ^{4}He for two very different contours.
Convergence of the Hartree-Fock energy is typically achieved with $n \sim 20$ points.

	$s_{1/2}$		$p_{3/2}$		$s_{1/2}$		$p_{3/2}$	
n	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
15	-24.323	0.000	1.027	-0.536	-24.324	-0.001	1.003	-0.547
20	-24.323	0.000	1.000	-0.546	-24.323	0.000	1.002	-0.547
25	-24.323	0.000	1.002	-0.548	-24.323	0.000	1.002	-0.548
30	-24.323	0.000	1.002	-0.548	-24.323	0.000	1.002	-0.548

Convergence of CCSD energy with $2n + l \leq 10$ truncation.

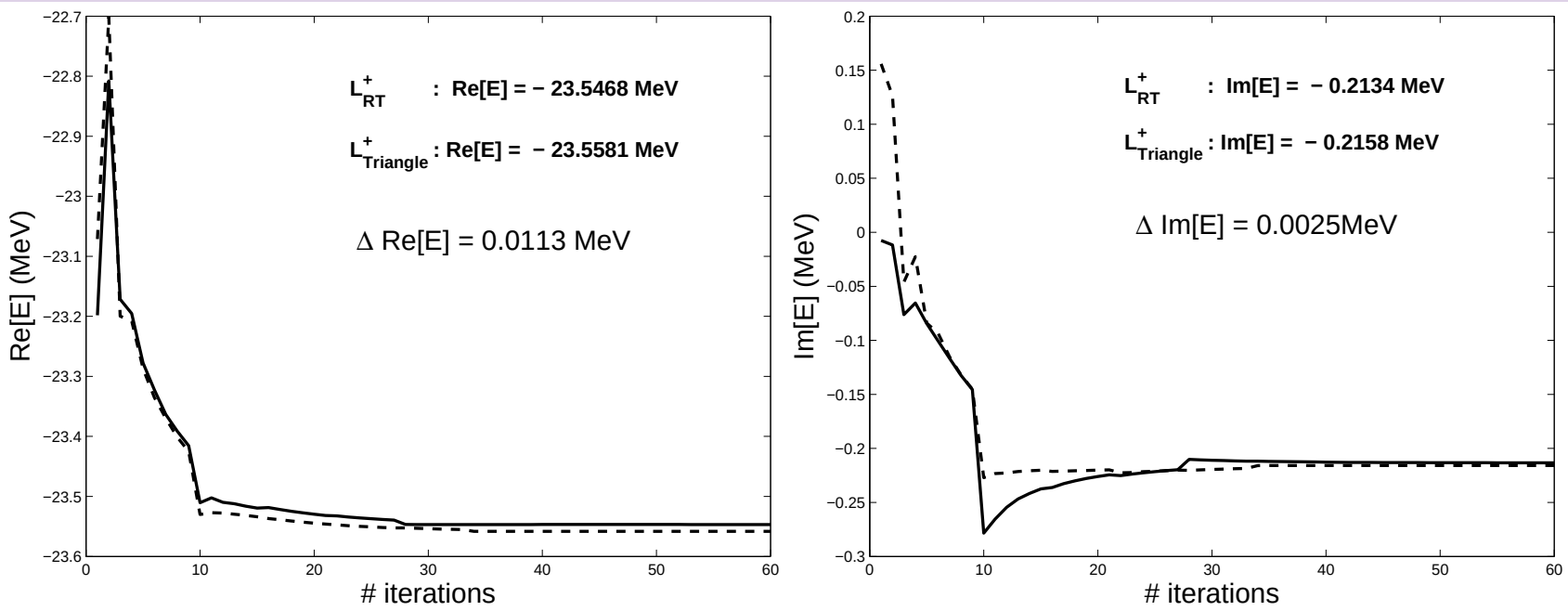
- Calculations of the ^{5}He ground state energy starting with oscillator bases given for different $\hbar\omega$ values.
- Results are well converged with respect to oscillator basis truncation. $\Delta Re[E] \sim 0.1$MeV, $\Delta Im[E] \sim 0.01$MeV





Convergence of CCSD energy.

CCSD convergence of ^{5}He ground state energy for the $s-d$ space (300 orbitals) using $n = 20$ discretization points for L^+. The calculation where performed using two very different L^+ contours



Comparison of CCSD with full CI

Comparison of CCSD and CCSD(T) with exact calculations of the $^{3-6}$He ground states using the low-momentum N^{3}LO nucleon-nucleon interaction. The single particle model space consisted of $4s3p1d$ oscillator states for the proton and neutron side. The energies E are given in MeV.

Method	^{3}He	^{4}He	^{5}He	^{6}He
CCSD (OSC)	-6.21	-26.19	-21.53	-20.96
CCSD (RHF)	-6.10	-26.06	-21.55	-20.99
CCSD (SC-RHF)	-6.11	-26.06	-21.55	-21.04
CCSD(T) (OSC)	-6.40	-26.30	-21.91	-22.83
CCSD(T) (RHF)	-6.35	-26.24	-21.90	-22.56
CCSD(T) (SC-RHF)	-6.34	-26.24	-21.91	-22.62
Exact	-6.45	-26.3	-22.1	-22.7

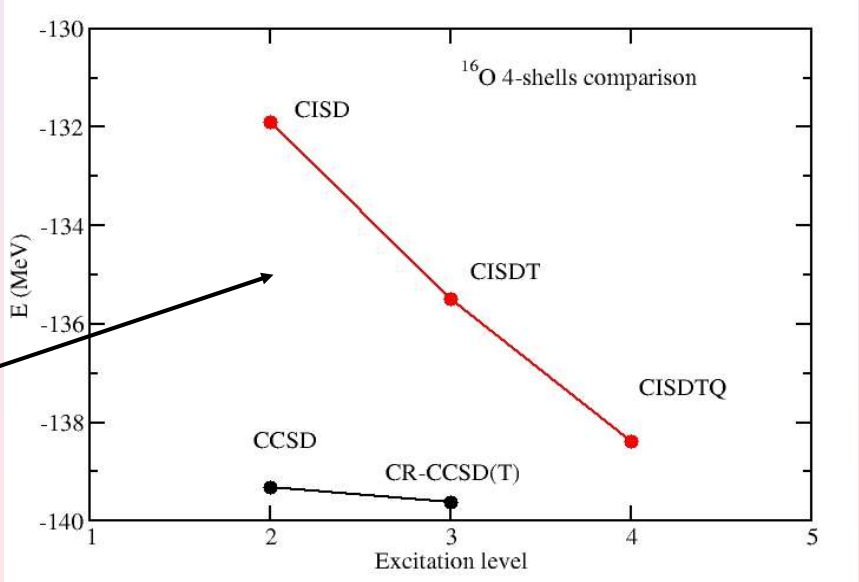
Comparison with Shell Model/Configuration Interaction

In Shell Model appraoch a linear excitation operator is used instead of an exponential. $\Psi = (1 + C)\Phi_0 = (1 + C_1 + C_2 + ...)\Phi_0$

- If truncated disconnected diagrams enter. And it is not size consistent.
- Dimension increases dramatically with number of active particles.

Comparison of CC with CI at given excitation level.

Nuclear Example (Kowalski et al PRL 2004).



Brief outline of the Contour Deformation Method

The Schrödinger equation in Momentum space representation,

$$\int_0^\infty dk'\ k'^2 \langle k|T+V|k'\rangle\langle k'|\psi_\alpha\rangle = E_\alpha \langle k|\psi_\alpha\rangle,$$

Analytic continuation in the complex k-plane may be achieved by deforming the integral giving, (G Hagen et al 2004 J. Phys. A: Math. Gen. 37 8991-9021.)

$$\int_{L^+} dk'\ k'^2 \langle k|T+V|k'\rangle\langle k'|\psi_\alpha\rangle = E_\alpha \langle k|\psi_\alpha\rangle.$$

This is analog with the complex scaling method $r \to r\exp(i\theta), k \to k\exp(-i\theta)$.

Discretizing L^+, a complete basis within the discretization space is obtained:

$$\mathbf{1} = \sum_{p=1}^{\#poles} \psi_p(\vec{k})\psi_p^T(\vec{k}) + \sum_{c=1}^{N-\#poles} \psi_c(\vec{k})\psi_c^T(\vec{k}),\ \ \vec{k} = [k_1, ..., k_N]\,.$$

Here p denotes pole states and c denotes the non-resonant continuum states.

Construction of Berggren many-body basis.

Having constructed a single-particle Berggren basis, a many-body Berggren basis may be constructed in a completely analogous way as when harmonic oscillator states are used. We construct a complete anti-symmetric N-body basis from the Slater determinants consisting of the Berggren orbitals φ_{nljm} i.e.

$$\Phi_{\alpha_1,\ldots,\alpha_N}(1,\ldots,N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_1}(1) & \ldots & \varphi_{\alpha_1}(N) \\ \vdots & & \vdots \\ \varphi_{\alpha_N}(1) & \ldots & \varphi_{\alpha_N}(N) \end{vmatrix}, \tag{1}$$

where α_i labels the single-particle quantum numbers $(n_i l_i j_i m_i)$. We then have at hand a complete set of Slater determinants, i.e.

$$1 = \sum_i^d |\Phi_i\rangle\langle\Phi_i^*|, \tag{2}$$

which the exact many-body wave function may be expanded in. The Shell Model problem then requires the solution of a complex symmetric $N \times N$ matrix eigenvalue equation,

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle, \tag{3}$$

Coupled Cluster Amplitude Equations

In CCSD the single t_i^a and double excitation amplitudes t_{ij}^{ab} may be determined from

$$0 = \langle \Phi_i^a | H | \Phi_0 \rangle, \quad 0 = \langle \Phi_{ij}^{ab} | H | \Phi_0 \rangle;$$

known as the T_1 and the T_2 amplitude equations. Writing the Hamiltonian in normal-ordered form

$$H = \sum_{pq} f_{pq} \left\{ a_p^\dagger a_q \right\} + \frac{1}{4} \sum_{pqrs} \langle pq || rq \rangle \left\{ a_p^\dagger a_q^\dagger a_s a_r \right\} + \langle \Phi_0 | H | \Phi_0 \rangle$$

$$\begin{aligned} 0 \;=\; & f_{ai} + \sum_c f_{ac} t_i^c - \sum_k f_{ki} t_k^a + \sum_{kc} \langle ka || ci \rangle t_k^c + \sum_{kc} f_{kc} t_{ik}^{ac} + \frac{1}{2} \sum_{kcd} \langle ka || cd \rangle t_{ki}^{cd} - \\ & \frac{1}{2} \sum_{klc} \langle kl || ci \rangle t_{kl}^{ca} - \sum_{kc} f_{kc} t_i^c t_k^a - \sum_{klc} \langle kl || ci \rangle t_k^c t_l^a + \sum_{kcd} \langle ka || cd \rangle t_k^c t_i^d - \qquad [152] \\ & \sum_{klcd} \langle kl || cd \rangle t_k^c t_i^d t_l^a + \sum_{klcd} \langle kl || cd \rangle t_k^c t_{li}^{da} - \frac{1}{2} \sum_{klcd} \langle kl || cd \rangle t_{ki}^{cd} t_l^a - \frac{1}{2} \sum_{klcd} \langle kl || cd \rangle t_{kl}^{ca} t_i^d, \end{aligned}$$

Coupled Cluster Amplitude Equations

T_2 amplitudes from:

$$
\begin{aligned}
0 = {} & \langle ab||ij\rangle + \sum_c \left(f_{bc}t_{ij}^{ac} - f_{ac}t_{ij}^{bc}\right) - \sum_k \left(f_{kj}t_{ik}^{ab} - f_{ki}t_{jk}^{ab}\right) + \qquad [153] \\
& \frac{1}{2}\sum_{kl}\langle kl||ij\rangle t_{kl}^{ab} + \frac{1}{2}\sum_{cd}\langle ab||cd\rangle t_{ij}^{cd} + P(ij)P(ab)\sum_{kc}\langle kb||cj\rangle t_{ik}^{ac} + \\
& P(ij)\sum_c \langle ab||cj\rangle t_i^c - P(ab)\sum_k \langle kb||ij\rangle t_k^a + \\
& \frac{1}{2}P(ij)P(ab)\sum_{klcd}\langle kl||cd\rangle t_{ik}^{ac}t_{lj}^{db} + \frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_{ij}^{cd}t_{kl}^{ab} - \\
& P(ab)\frac{1}{2}\sum_{klcd}\langle kl||cd\rangle t_{ij}^{ac}t_{kl}^{bd} - P(ij)\frac{1}{2}\sum_{klcd}\langle kl||cd\rangle t_{ik}^{ab}t_{jl}^{cd} + \\
& P(ab)\frac{1}{2}\sum_{kl}\langle kl||ij\rangle t_k^a t_l^b + P(ij)\frac{1}{2}\sum_{cd}\langle ab||cd\rangle t_i^c t_j^d - P(ij)P(ab)\sum_{kc}\langle kb||ic\rangle t_k^a t_j^c + \\
& P(ab)\sum_{kc} f_{kc}t_k^a t_{ij}^{bc} + P(ij)\sum_{kc} f_{kc}t_i^c t_{jk}^{ab} - \\
& P(ij)\sum_{klc}\langle kl||ci\rangle t_k^c t_{lj}^{ab} + P(ab)\sum_{kcd}\langle ka||cd\rangle t_k^c t_{ij}^{db} + \\
& P(ij)P(ab)\sum_{kcd}\langle ak||dc\rangle t_i^d t_{jk}^{bc} + P(ij)P(ab)\sum_{klc}\langle kl||ic\rangle t_l^a t_{jk}^{bc} + \\
& P(ij)\frac{1}{2}\sum_{klc}\langle kl||cj\rangle t_i^c t_{kl}^{ab} - P(ab)\frac{1}{2}\sum_{kcd}\langle kb||cd\rangle t_k^a t_{ij}^{cd} - P(ij)P(ab)\frac{1}{2}\sum_{kcd}\langle kb||cd\rangle t_i^c t_k^a t_j^d + P(ij)P(ab)\frac{1}{2}\sum_{klc}\langle kl||cj\rangle t_i^c t_k^a t_l^b - \\
& P(ij)\sum_{klcd}\langle kl||cd\rangle t_k^c t_i^d t_{lj}^{ab} - P(ab)\sum_{klcd}\langle kl||cd\rangle t_k^c t_l^a t_{ij}^{db} + \\
& P(ij)\frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_i^c t_j^d t_{kl}^{ab} + P(ab)\frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_k^a t_l^b t_{ij}^{cd} + \\
& P(ij)P(ab)\sum_{klcd}\langle kl||cd\rangle t_i^c t_l^b t_{kj}^{ad} + P(ij)P(ab)\frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_i^c t_k^a t_j^d t_l^b.
\end{aligned}
$$

Nonlinear terms in t2 (4th order)

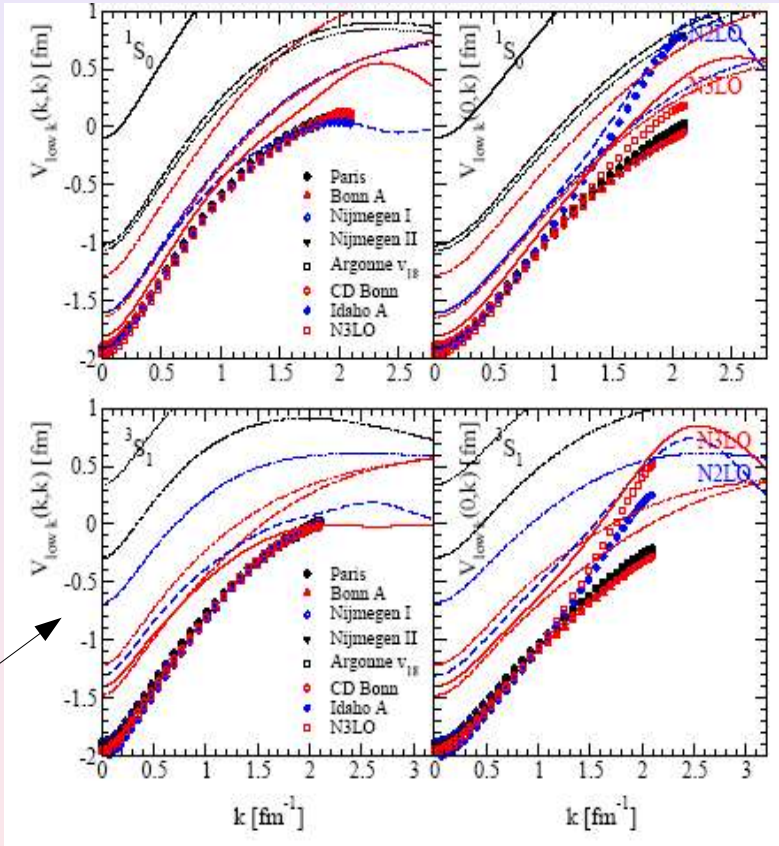
$$P(ij)f(ij) = f(ij) - f(ji)$$

Low-momentum nucleon-nucleon interaction.

1. Modern N-N interactions reproduce two-particle scattering data + deuteron properties.
2. They all differ in strength of tensor force and treatment of the hard-core.
3. V-lowk from different N-N models have the same on-shell and half-offshell behaviour
4. At the two-body level V-lowk is model-independent.

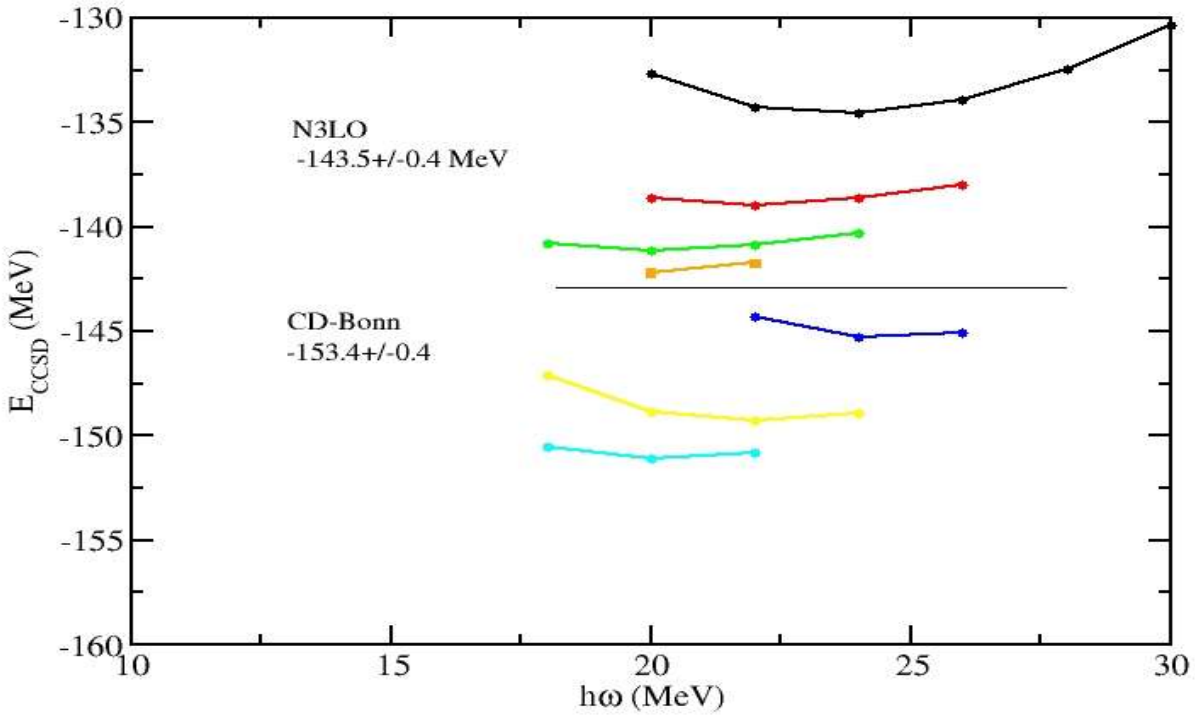
Question: Is this model independence also seen in A > 2 calculations ?

A. Schwenk, J.Phys. G31 (2005) S1273-S1282



Coupled Cluster Results for ^{16}O

V_{lowk} ^{16}O results using N3LO and CD-Bonn



Gamow-Hartree-Fock basis

Two-body matrix elements are calculated numerically in an arbitrary two-particle Gamow basis by truncating the completeness expansion up to N harmonic oscillator two-body states

$$\langle ab|V_{\rm osc}|cd\rangle \approx \sum_{\alpha\leq\beta}^{N}\sum_{\gamma\leq\delta}^{N}\langle ab|\alpha\beta\rangle\langle\alpha\beta|V_{\rm low-k}|\gamma\delta\rangle\langle\gamma\delta|cd\rangle. \tag{4}$$

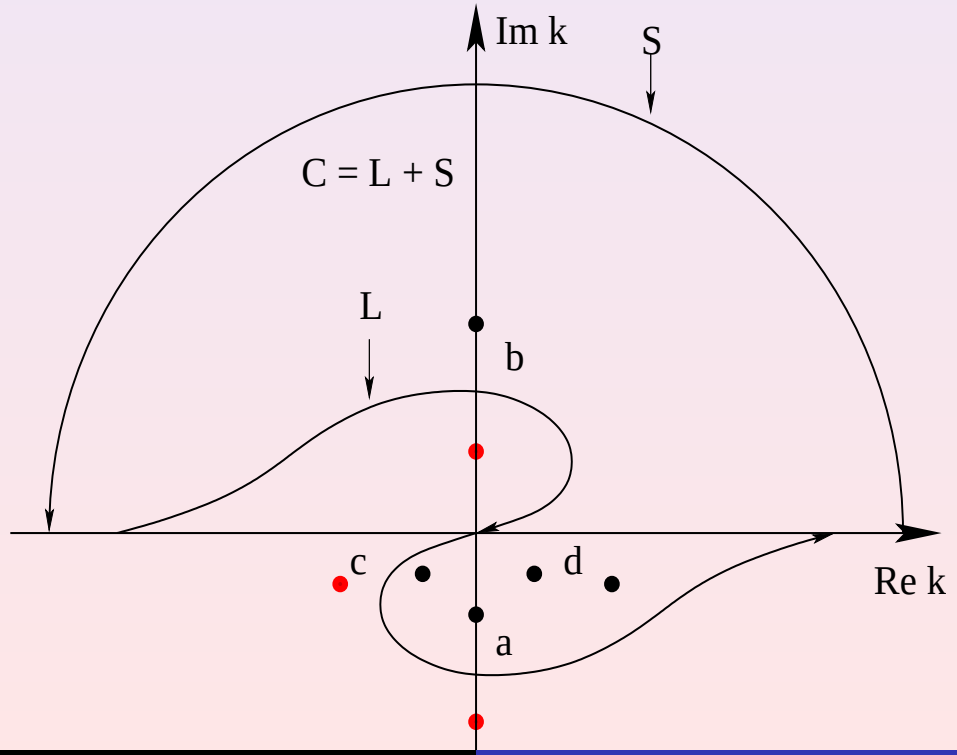
The Gamow-Hartree-Fock basis may then be constructed,

$$\langle p|h_{\rm HF}|q\rangle = \langle p|t|p\rangle\delta_{p,q} + \sum_{i<e_f}\langle pi|V_{\rm osc}|qi\rangle \tag{5}$$

Dripline - Exploring Open Quantum Systems

Berggren Single-Particle Basis

$$\mathbf{1} = \sum_{n=a,b,c,d} |\psi_l(k_n)\rangle\langle\tilde{\psi}_l(k_n)| + \int_{L^+} dk\, k^2 |\psi_l(k)\rangle\langle\tilde{\psi}_l(k)|.$$



Low-momentum nucleon-nucleon interaction.

$V_{\mathrm{low}-k}$ may be constructed by either Renormalization Group Theories (where high momentum modes are integrated out) or Similarity Transformation techniques.

$$P = \left\{ |\bar{k_p}\rangle,\ |k| \leq \Lambda \right\},\ \ Q = \left\{ |\bar{k_q}\rangle,\ \Lambda < |k| < \infty \right\}.$$

$$\tilde{H}\ = X^{-1} H X,\ \ |\Phi_k\rangle = X^{-1} |\Psi_k\rangle.$$

$$\begin{pmatrix} P\tilde{H}P & P\tilde{H}Q \\ Q\tilde{H}P & Q\tilde{H}Q \end{pmatrix} \begin{pmatrix} P\Phi_k \\ Q\Phi_k \end{pmatrix} = E_k \begin{pmatrix} P\Phi_k \\ Q\Phi_k \end{pmatrix},$$

Decoupling equation $Q\tilde{H}P = Q(X^{-1}HX)P = 0$, Lee-Suzuki gives $X = \exp(\omega) = 1 + \omega$ where the wave operator ω satisfies the decoupling condition

$$\omega = Q\omega P.$$

The Lee-Suzuki effective interaction in the P-space is then derived

$$PV_{LS}P = PH(P + \omega) - PH_0P = PVP + PV\omega = PVP + PVQ\omega.$$

Coupled Cluster Amplitude Equations

In CCSD the single t_i^a and double excitation amplitudes t_{ij}^{ab} may be determined from

$$0 = \langle \Phi_i^a | H | \Phi_0 \rangle, \quad 0 = \langle \Phi_{ij}^{ab} | H | \Phi_0 \rangle;$$

known as the T_1 and the T_2 amplitude equations.

$$\begin{aligned} 0 \;=\; & f_{ai} + \sum_c f_{ac} t_i^c - \sum_k f_{ki} t_k^a + \sum_{kc} \langle ka || ci \rangle t_k^c + \sum_{kc} f_{kc} t_{ik}^{ac} + \frac{1}{2} \sum_{kcd} \langle ka || cd \rangle t_{ki}^{cd} - \\ & \frac{1}{2} \sum_{klc} \langle kl || ci \rangle t_{kl}^{ca} - \sum_{kc} f_{kc} t_i^c t_k^a - \sum_{klc} \langle kl || ci \rangle t_k^c t_l^a + \sum_{kcd} \langle ka || cd \rangle t_k^c t_i^d - \qquad [152] \\ & \sum_{klcd} \langle kl || cd \rangle t_k^c t_i^d t_l^a + \sum_{klcd} \langle kl || cd \rangle t_k^c t_{li}^{da} - \frac{1}{2} \sum_{klcd} \langle kl || cd \rangle t_{ki}^{cd} t_l^a - \frac{1}{2} \sum_{klcd} \langle kl || cd \rangle t_{kl}^{ca} t_i^d, \end{aligned}$$

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& P(ab)\sum_{kc} f_{kc}t_k^a t_{ij}^{bc} + P(ij)\sum_{kc} f_{kc}t_i^c t_{jk}^{ab} - \\
& P(ij)\sum_{klc}\langle kl||ci\rangle t_k^c t_{lj}^{ab} + P(ab)\sum_{kcd}\langle ka||cd\rangle t_k^c t_{ij}^{db} + \\
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& P(ij)\sum_{klcd}\langle kl||cd\rangle t_k^c t_i^d t_{lj}^{ab} - P(ab)\sum_{klcd}\langle kl||cd\rangle t_k^c t_l^a t_{ij}^{db} + \\
& P(ij)\frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_i^c t_j^d t_{kl}^{ab} + P(ab)\frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_k^a t_l^b t_{ij}^{cd} + \\
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