Calculating ab initio nuclear structure with coupled-cluster theroy

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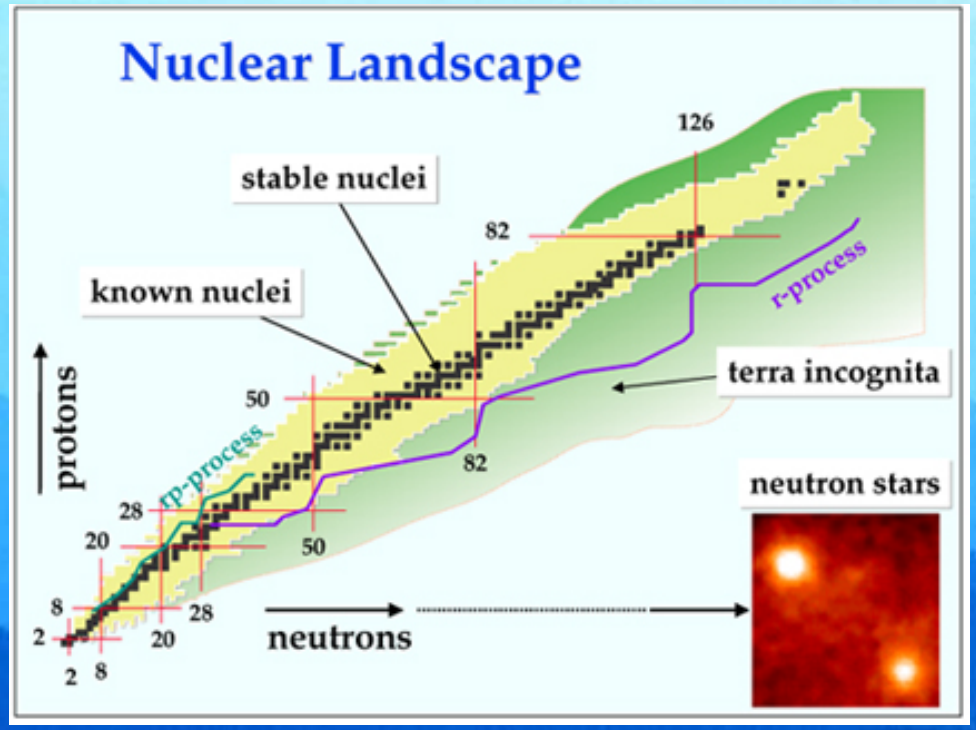
Outline

I. Motivations
II. Ab initio coupled-cluster theory
    A. The CC method
    B. The space and the Hamiltonian
    C. Results in ^{16}O and neighbors
III. Future directions

The physics of nuclei



The big questions:

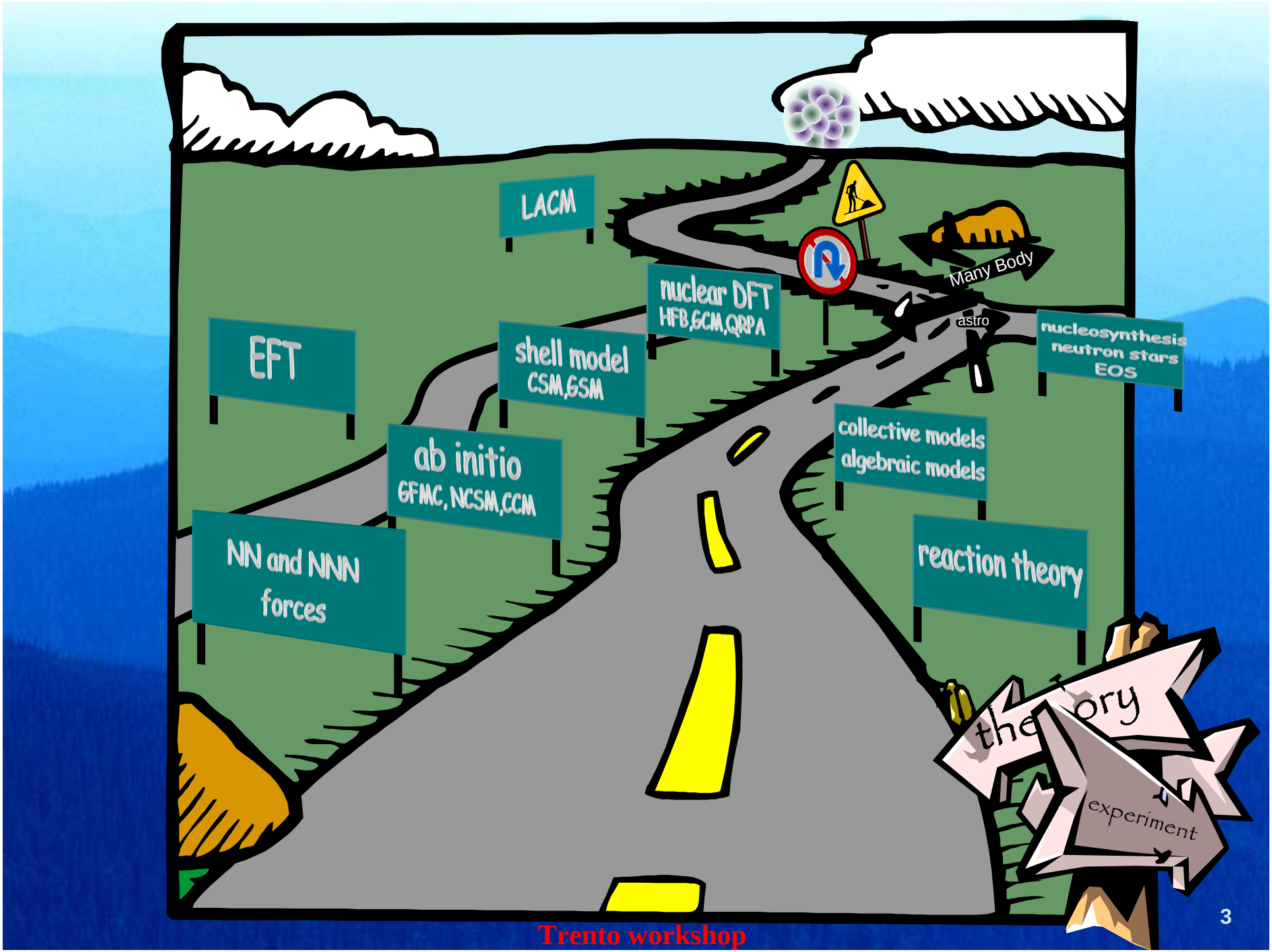
- How do nuclei bind?
- What are their limits of existence?
- What are their symmetries?
- How/where are they produced?
- How can they be used for societal benefit?

Scientific Thrusts:

- How do complex systems emerge from simple ingredients (interaction question)?
- What are the simplicities and regularities in complex systems (shell/symmetries question)?
- How are elements produced in the Universe (astrophysics question)?

Broad impact of neutron-rich nuclei:

- Nuclei as laboratories for tests of 'standard model physics'.
- Nuclear reactions relevant to astrophysics.
- Nuclear reactions relevant to Science Based Stockpile Stewardship.
- Nuclear transportation, safety, and criticality issues.


LACM
nuclear DFT
HFB,GCM,QRPA
Many Body
astro
nucleosynthesis
neutron stars
EOS
EFT
shell model
CSM,GSM
collective models
algebraic models
ab initio
GFMC, NCSM,CCM
NN and NNN
forces
reaction theory
experiment

The ORNL-Oslo-MSU collaboration on nuclear many-body problems

OAK RIDGE NATIONAL LABORATORY

David Dean (CC methods for nuclei and extensions to V_{3N})
Thomas Papenbrock
David Bernholdt (Computer Science and Mathematics)
Trey White, Kenneth Roche (Computational Science)

MICHIGAN STATE UNIVERSITY
Department of Chemistry

Piotr Piecuch (CC methods in chemistry and extensions)
Karol Kowalski (to PNNL)
Marta Wloch
Jeff Gour

UNIVERSITY OF OSLO

Morten Hjorth-Jensen (Effective interactions)
Maxim Kartamychev (3-body forces in nuclei)
Gaute Hagen (effective interactions for weakly bound systems, to ORNL)

Research Plan
-- Excited states (!)
-- Observables (!)
-- Triples corrections (!)
-- Open shells (start)
-- V_{3N} (start)
-- 50<A<100
-- Reactions
-- TD-CCSD??

Steps toward solutions

Begin with a bare NN (+3N) Hamiltonian

$$H = -\frac{\hbar}{2}\sum_{i=1}^{A}\frac{\nabla_i^2}{m_i} + \frac{1}{2}\sum_{i<j} V_{2N}\left(\vec{r}_i, \vec{r}_j\right) + \frac{1}{6}\sum_{i<j<k} V_{3N}\left(\vec{r}_i, \vec{r}_j, \vec{r}_k\right)$$

Bare (GFMC)

Basis expansion

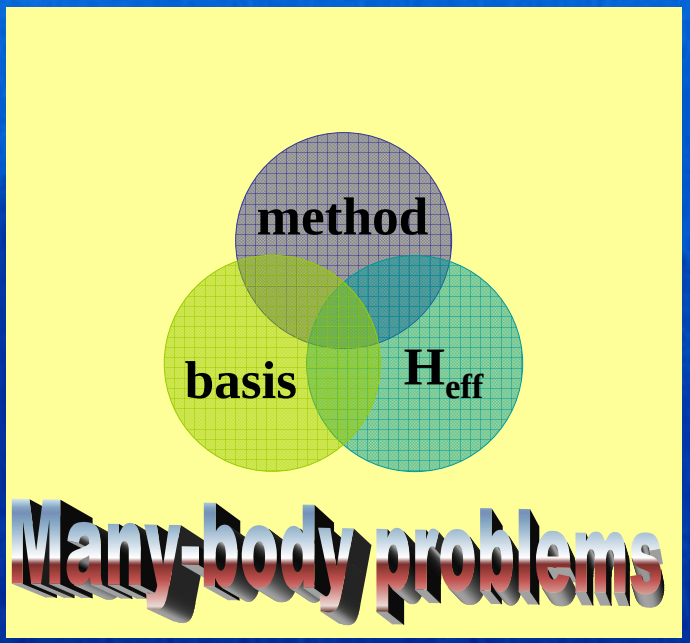
Basis expansions:

- **Choose the method of solution**
- **Determine the appropriate basis**
- **Generate H_{eff}**

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

Oscillator single-particle basis states

Many-body basis states



The Method:
Coupled Cluster Theory

Fascinating Many-body approach: Coupled Cluster Theory

Some interesting features of CCM:

- **Fully microscopic**
- **Size extensive:**
  only linked diagrams enter
- **Size consistent:**
  the energy of two non-interacting fragments computed separately is the same as that computed for both fragments simultaneously
- **Capable of systematic improvement**
- **Amenable to parallel computing**

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

A short history

Formal introduction:

1958: Coester, Nucl. Phys. 7, 421

1960: Coester and Kummel, Nucl. Phys. 17, 477

Introduction into Chemistry (late 60's):

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

$$|\Psi\rangle = \exp(T)|\Phi\rangle$$

Correlated Ground-State wave function

Correlation operator

Reference Slater determinant

$$T = T_1 + T_2 + T_3 + \cdots$$

$$T_1 = \sum_{\substack{i<\varepsilon_f \\ a>\varepsilon_f}} t_{ai} a_a^+ a_i$$

$$T_2 = \sum_{\substack{ij<\varepsilon_f \\ ab>\varepsilon_f}} t_{abij} a_a^+ a_b^+ a_j a_i$$

Energy

$$E = \langle \Phi | \exp(-T) H \exp(T) | \Phi \rangle$$

Amplitude equations

$$\langle \Phi_{ij\cdots}^{ab\cdots} | \exp(-T) H \exp(T) | \Phi \rangle = \langle \Phi_{ij\cdots}^{ab\cdots} | \overline{H} | \Phi \rangle = 0$$

- **Nomenclature**
  - **Coupled-clusters in singles and doubles (CCSD)**
  - **…with triples corrections CCSD(T);**

Dean & Hjorth-Jensen, PRC69, 054320 (2004); Kowalski, Dean, Hjorth-Jensen,Papenbrock, Piecuch, PRL92, 132501 (2004); Wloch, Dean, Gour, Hjorth-Jensen, Papenbrock, Piecuch, PRL 94, 212501 (2005).

Derivation of CC equations

Use Baker-Hausdorff

$$\exp(-T)H\exp(T) = H + [H,T_1] + [H,T_2] + \frac{1}{2}[[H,T_1],T_1] + \frac{1}{2}[[H,T_2],T_2] + [[H,T_1],T_2] + \dots$$

Terminates at quadruply nested commutators (for $H=H_1+H_2$) for all T.

Normal order the Hamiltonian

$$H = \sum_{pq} f_{pq}\{a_p^+ a_q\} + \frac{1}{4}\sum_{pqrs}\langle pq \| rs\rangle\{a_p^+ a_q^+ a_s a_r\} + \sum_i \langle i|t_{osc}|i\rangle + \frac{1}{2}\sum_{ij}\langle ij \| ij\rangle$$

$$f_{pq} = \langle p|t_{osc}|q\rangle + \sum_i \langle pi \| qi\rangle$$

Fock operator

$$\langle \Phi_0 | H | \Phi_0 \rangle$$

Derivation of CC equations

T_1 amplitudes from: $\left\langle \Phi_i^a \middle| \exp(-T) H \exp(T) \middle| \Phi \right\rangle = 0$

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

Note T_2 amplitudes also come into the equation.

T_2 amplitudes from: $\left\langle \Phi_{ij}^{ab} \middle| \exp(-T) H \exp(T) \middle| \Phi \right\rangle = 0$

$$
\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} - \quad 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}
$$

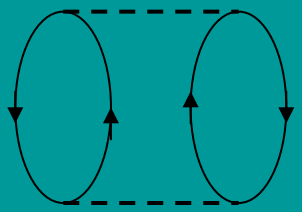
Nonlinear terms in t2 (4th order)

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

An interesting mess. But solvable….

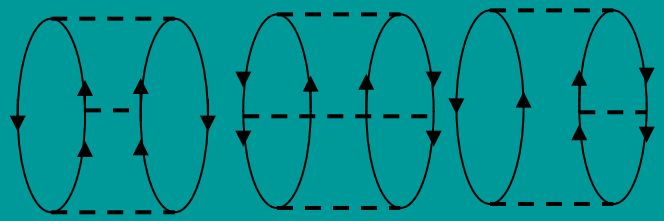
Correspondence with MBPT

2nd order



$$t_{ij}^{ab}(1) = \langle ab \| ij \rangle / D_{ijab}$$

$$E_2 = \sum_{\substack{a>b \\ i>j}} \langle ab \| ij \rangle t_{ij}^{ab}(1)$$



3rd order

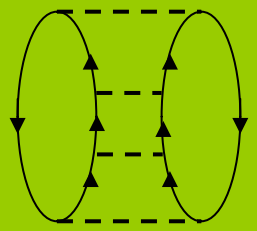
$$t_{ij}^{ab}(2) = \frac{1}{2} \sum_{kl} \langle kl \| ij \rangle t_{kl}^{ab}(1) +$$

$$\frac{1}{2} \sum_{cd} \langle ab \| cd \rangle t_{ij}^{cd}(1) + P(ij)P(ab) \sum_{kc} \langle kb \| cj \rangle t_{ik}^{ac}(1)$$

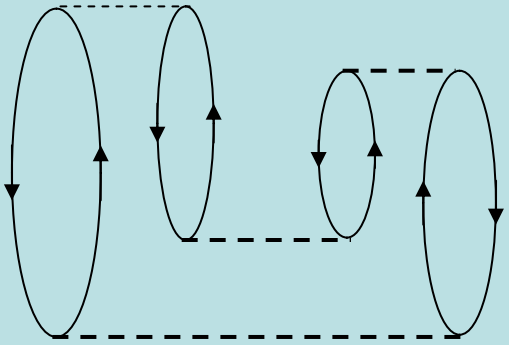
$$E_3 = \sum_{\substack{a>b \\ i>j}} \langle ab \| ij \rangle t_{ij}^{ab}(2)$$

$$D_{ijab} = f_{ii} + f_{jj} - f_{aa} - f_{bb}$$

A few more diagrams



+ all diagrams of this kind (11 more) 4th order
[replace t(2) and repeat above 3rd order calculation]



+ all diagrams of this kind (6 more) 4th order

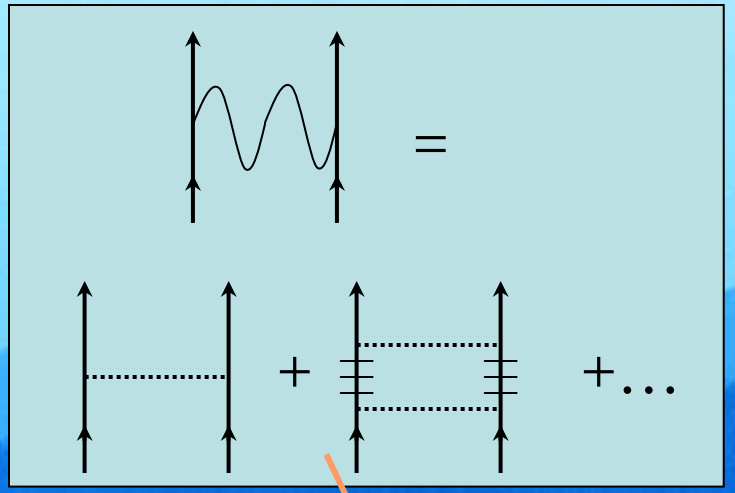
$$t_{ij}^{ab}(3;N)=\frac{1}{2}P(ij)P(ab)\sum_{klcd}\left\langle kl\middle\|cd\right\rangle t_{ik}^{ac}(1)t_{lj}^{db}(1)+\frac{1}{4}\sum_{klcd}\left\langle kl\middle\|cd\right\rangle t_{ij}^{cd}(1)t_{kl}^{ab}(1)$$

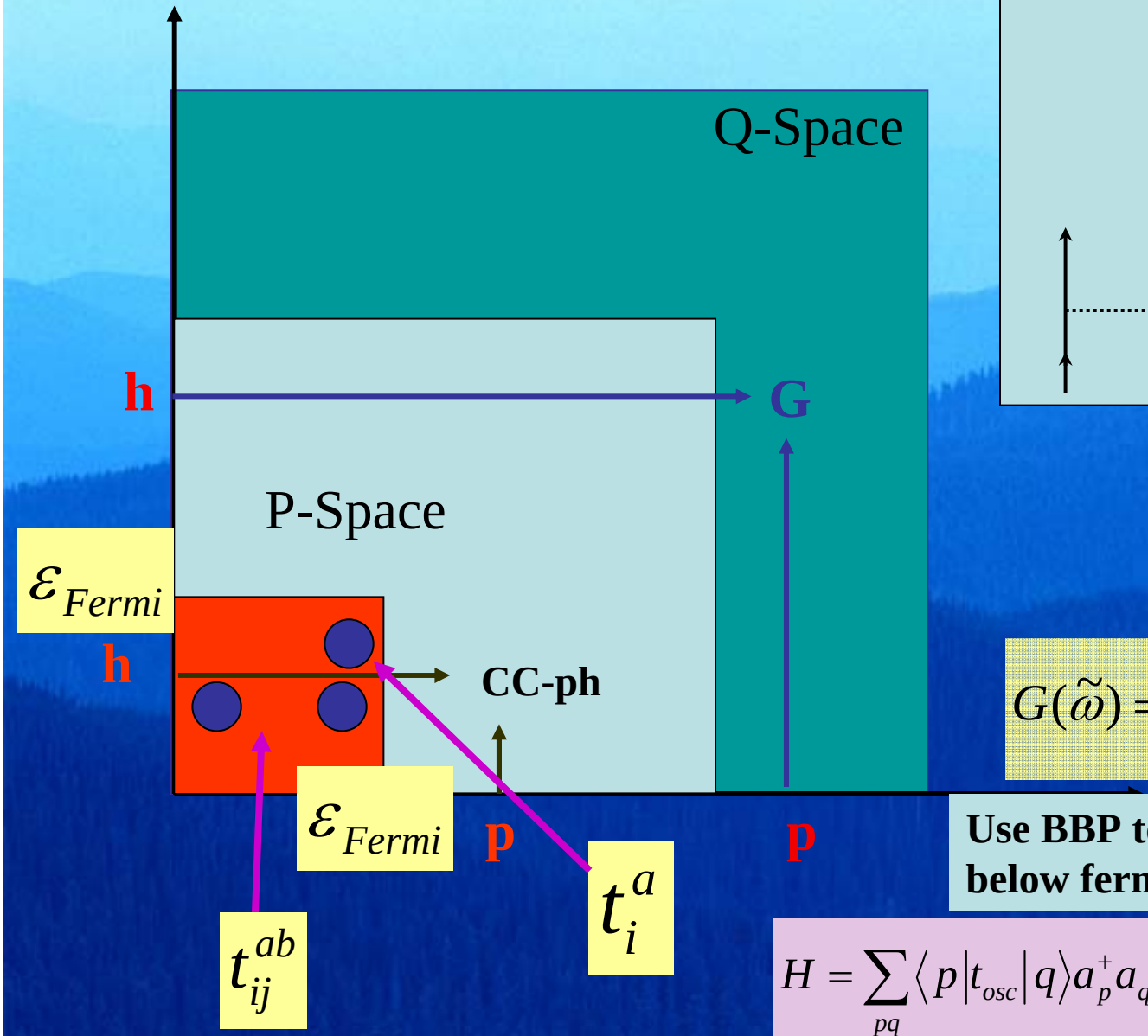
$$-\frac{1}{2}P(ab)\sum_{klcd}\left\langle kl\middle\|cd\right\rangle t_{ij}^{ac}(1)t_{kl}^{bd}(1)-\frac{1}{2}P(ij)\sum_{klcd}\left\langle kl\middle\|cd\right\rangle t_{ik}^{ab}(1)t_{jl}^{cd}(1)$$

$$E_4^Q=\sum_{\substack{a>b\\ i>j}}\left\langle ab\middle\|ij\right\rangle t_{ij}^{ab}(3;N)$$

The model space and the effective Hamiltonian

Choice of model space and the G-matrix





ph intermediate states

$$G(\tilde{\omega}) = V + V\frac{Q}{\tilde{\omega} - QtQ}G(\tilde{\omega})$$

Use BBP to eliminate w-dependence below fermi surface.

$$H = \sum_{pq}\langle p|t_{osc}|q\rangle a_p^+ a_q + \frac{1}{4}\sum_{pqrs}\langle pq|G|rs\rangle a_p^+ a_q^+ a_s a_r$$

In the near future (now?): similarity transformed H

$$H\left|k\right\rangle = E_k\left|k\right\rangle;\ P+Q=1$$

$$Qe^{-\omega}He^{\omega}P=0 \quad \Rightarrow \quad \left\langle \alpha_Q\left|k\right.\right\rangle = \sum_{\alpha_P}\left\langle \alpha_Q\left|\omega\right|\alpha_P\right\rangle\left\langle \alpha_P\left|k\right.\right\rangle$$

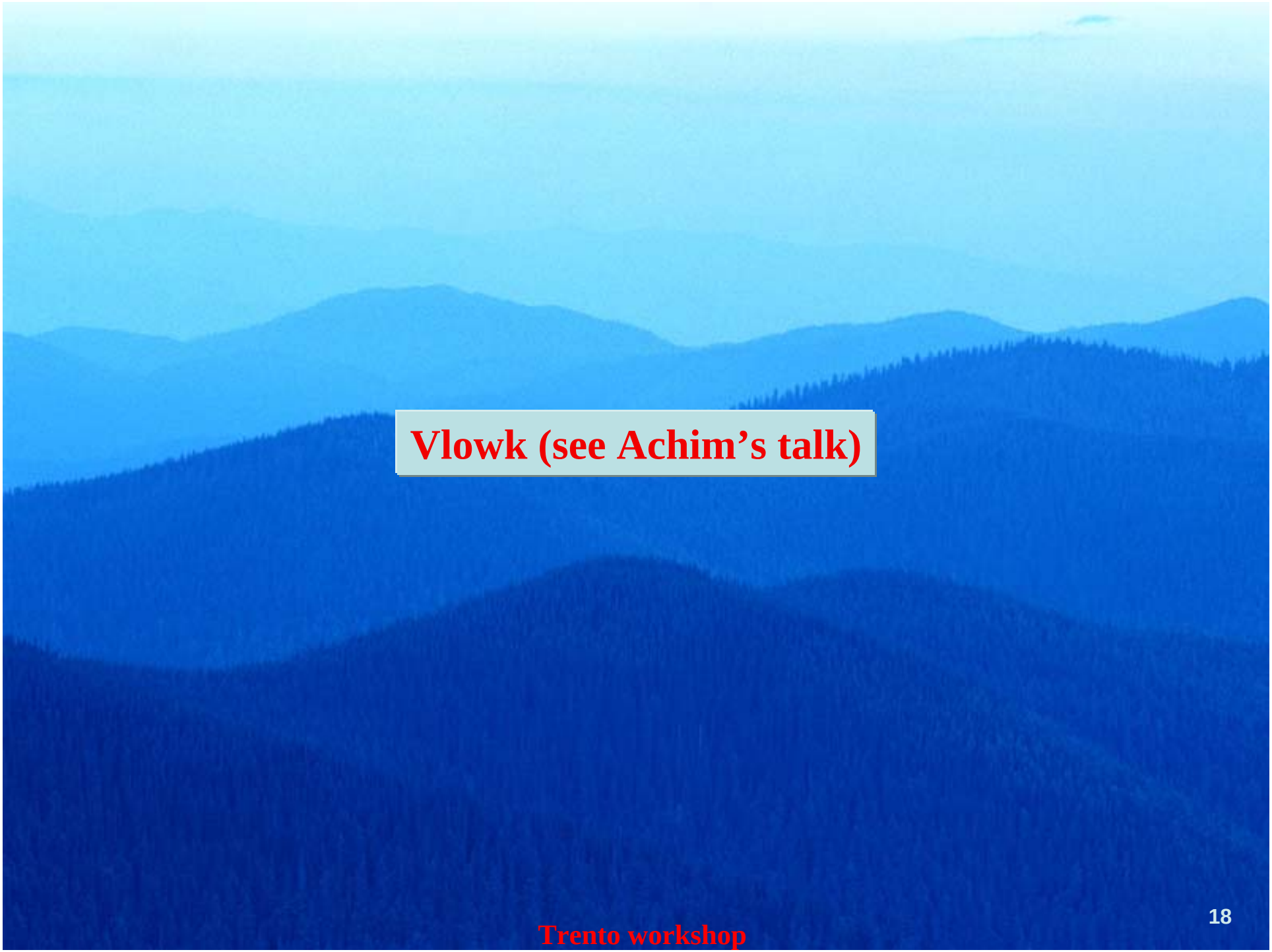
$$\overline{H}_{eff} = \left[P\left(1+\omega^{+}\omega\right)P\right]^{1/2} PH\left(P+Q\omega P\right)\left[P\left(1+\omega^{+}\omega\right)P\right]^{-1/2}$$

K. Suzuki and S.Y. Lee, Prog. Theor. Phys. 64, 2091 (1980)
P. Navratil, G.P. Kamuntavicius, and B.R. Barrett, Phys. Rev. C61, 044001 (2000)
Zuker, Phys. Repts. (1981).

Advantage: no parameter dependence in the interaction

Current status

- **Exact deuteron energy obtained in P space**
- **Working on full implementation in CC theory.**
- **G-matrix + all folded-diagrams+…**
- **Implemented, new results cooking….stay tuned.**

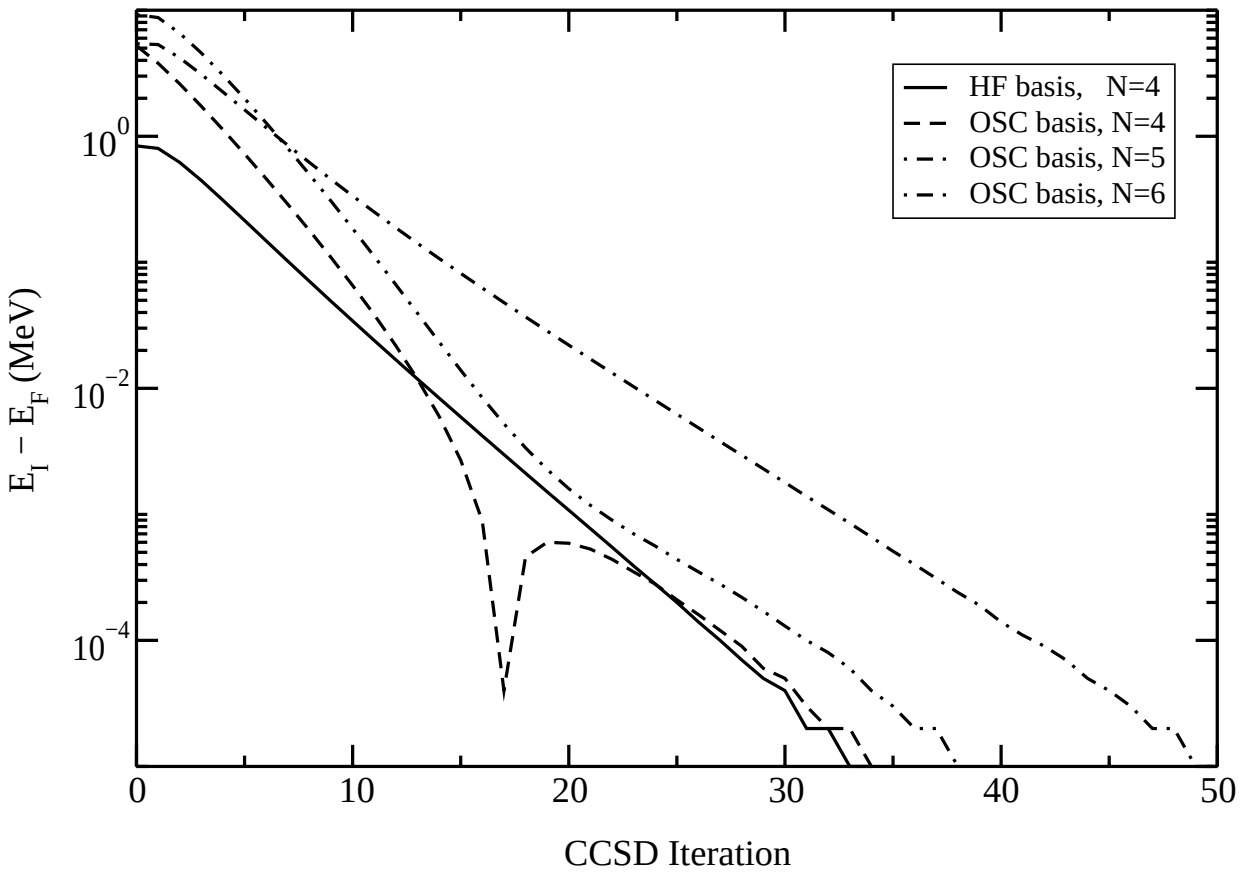

Vlowk (see Achim's talk)

Iterative solution

On the first iteration: use first and second-order many-body perturbation theory as a guide. This gives:

$$= f_{ai} \Big/ D_i^a$$

$$= \langle ab \| ij \rangle \Big/ D_{ij}^{ab}$$



rt into the RHS and
in new amplitudes

tinue until
vergence

: HF vs OSC:
39.31 MeV (OSC)
38.47 MeV (HF)
1% difference

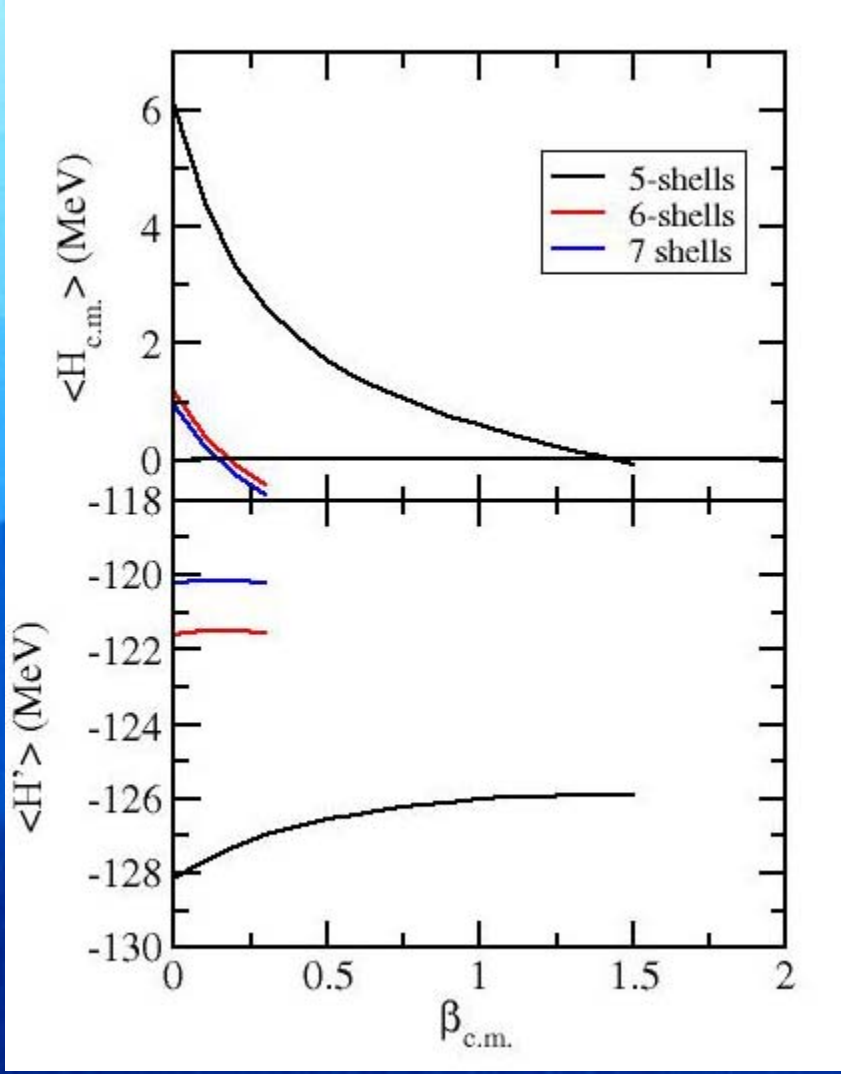
Comparison of HF and OSC basis (Idaho-A)

	E_{corr}	Term 1	Term 2	Term 3	E_0	<H>
OSC	-29.865	-9.669	-1.757	-18.439	-109.45	-139.31
HF	-16.498	7.0e-6	-0.3e-3	-16.498	-121.98	-138.47

$$E_{corr} = E_{ccsd} - E_0 = \sum_{ia} f_{ia} t_i^a + \frac{1}{2} \sum_{aibj} \langle ij \| ab \rangle t_i^a t_j^b + \frac{1}{4} \sum_{aibj} \langle ij \| ab \rangle t_{ij}^{ab}$$

Changing the basis hardly affects the solutions.

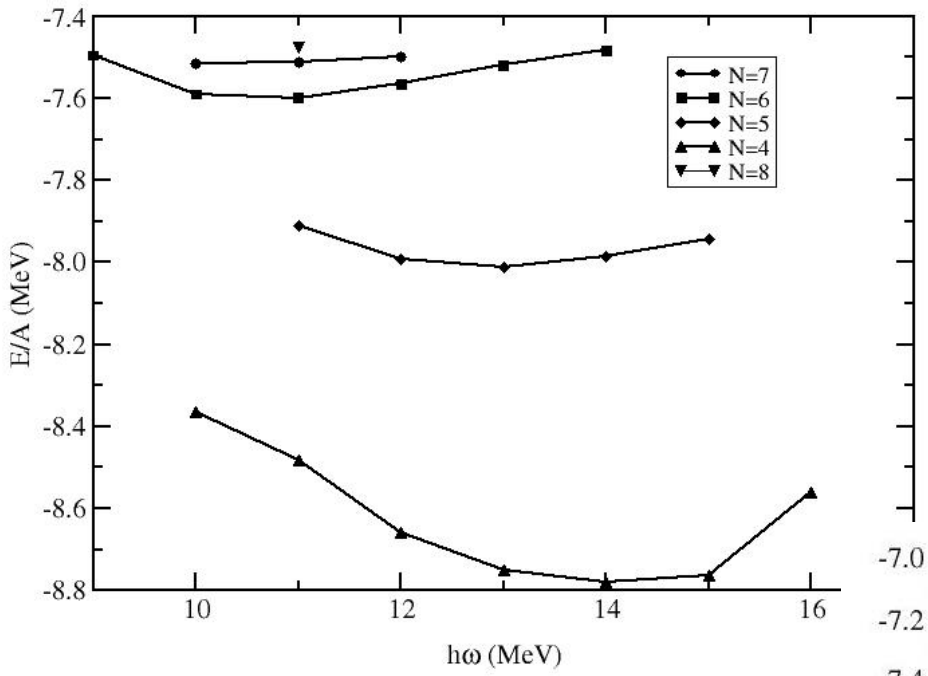
Another center of mass correction on ^{16}O



$$H' = H + \beta_{c.m.} H_{c.m.}$$

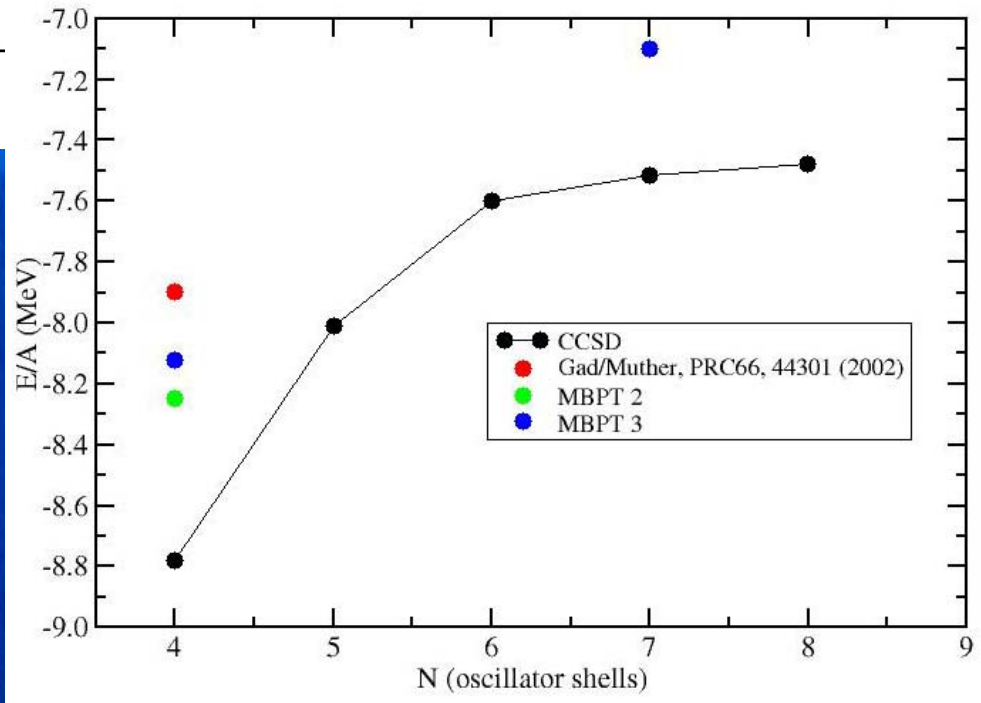
Controls COM contamination of both ground and excited states. Used to isolate "REAL" states.

Calculations for ^{16}O



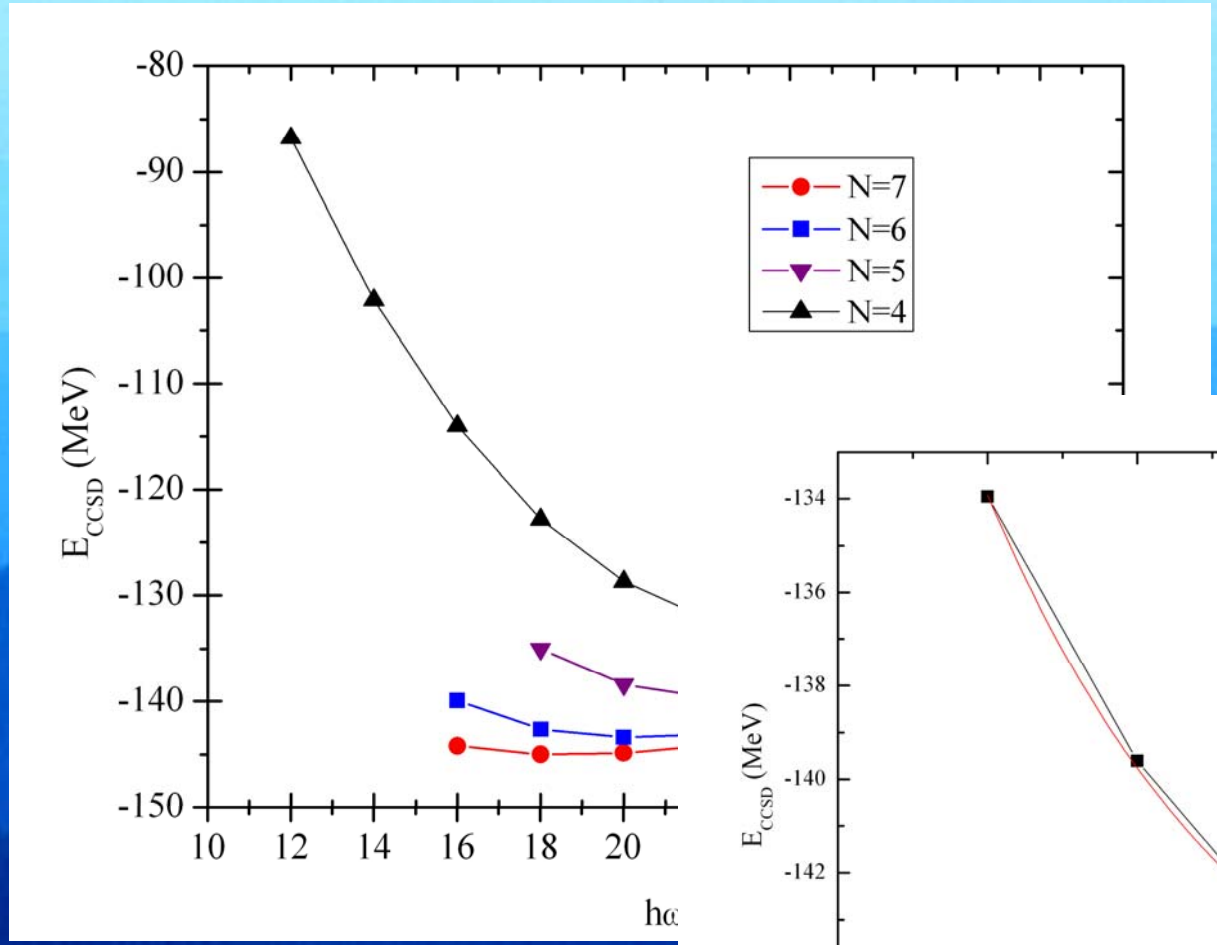
Reasonably converged

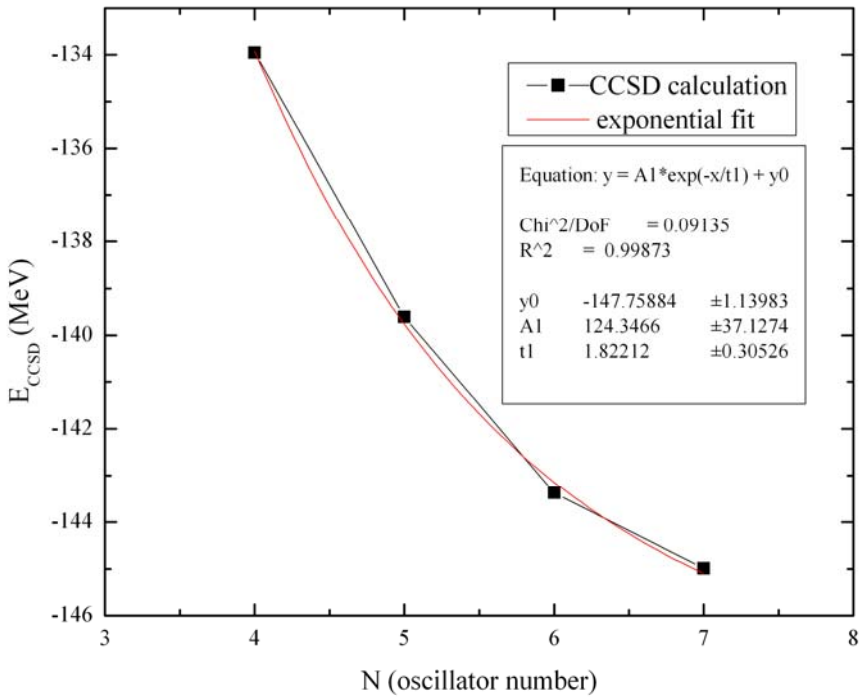
(N3LO gives -6.95 MeV/A)



- **Idaho-A: No Coulomb**
- **Coulomb: +0.7 MeV**
- **Expt result is -8.0 MeV/A**

Initial V_{lowk} results (w/A. Schwenk)





Correcting the CCSD results by non-iterative methods

Goal: Find a method that will yield the complete diagonalization result in a given model space

How do we obtain the triples correction?

How do our results compare with 'exact' results in a given model space, for a given Hamiltonian?

"Completely Renormalized Coupled Cluster Theory"
P. Piecuch, K. Kowalski, P.-D. Fan, I.S.O. Pimienta, and M.J. McGuire, Int. Rev. Phys. Chem. 21, 527 (2002)

Completely renormalized CC in one slide

CC generating functional

$$\Lambda_{CC}[\Psi] = \frac{\sum_{n=1}^{N} \left\langle \Psi \left| \left(H - E_0^{(A)}\right) e^{T(A)} \right| \Phi \right\rangle}{\left\langle \Psi \left| e^{T(A)} \right| \Phi \right\rangle}$$

T(A) = model correlation

if $\Psi \to \Psi_0$

then $\Lambda_{CC} = \delta = E_0 - E_0^{(A)}$

$$\delta = \frac{1}{36} \sum_{ijk,abc} \left\langle \tilde{\Psi} \left| \Phi_{abc}^{ijk} \right\rangle M_{ijk}^{abc} \right/ \Delta$$

$$\Delta = \left\langle \tilde{\Psi} \left| e^{T(CCSD)} \right| \Phi \right\rangle$$

$$M_{abc}^{ijk} = \left\langle \Phi_{ijk}^{abc} \left| \overline{H}^{CCSD} \right| \Phi \right\rangle$$

$$\left| \tilde{\Psi} \right\rangle = P e^{\left(T^{(CCSD)} + \tilde{T}_3\right)}$$

Different choices of Ψ will yield slightly different triples corrections

Leading order terms in the triples equation

Triples correction to the ground state energy
He-4 (4 major oscillator shells)

Method	Energy (MeV)
CCSD	-21.978
CR-CCSD[T],a	-22.665
CR-CCSD[T],a/D=1	-23.214
CR-CCSD[T],c	-22.841
CR-CCSD[T],c/D=1	-23.524
SM-SD	-20.175
SM-SDT	-22.235
FULL SM	-23.484

Different many-body approaches to the energy denominator

$$H' = H + \beta_{c.m.} H_{c.m.}$$

Able to reproduce the 'exact' (full diag) result to within 0.08 MeV.

^{16}O in four major oscillator shells

Method	Energy (MeV)
CCSD	-139.310
CR-CCSD(T),a	-139.465
CR-CCSD(T),a/D=1	-139.621
CR-CCSD(T),b	-139.375
CR-CCSD(T),b/D=1	-139.440
CR-CCSD(T),c	-139.391
CR-CCSD(T),c/D=1	-139.467
Shell model SD	-131.887
Shell model SDT	-135.489
Shell model SDTQ	-138.387

1) Relative size of terms:
   a) T_1 and T_2 of similar order
   b) T_1T_2 disconnected
      >> T_3 connected triples
   c) diff between SM-SD and CCSDT
      comes mainly from T_1T_2
   d) If T_3 were large CCSD(T)
      would be far below CCSD
2) Size extensive nature of CC
3) CCSD + CR-CCSD(T) bring
   $T_1^3T_2$, $T_1T_2^2$, T_2^3 not in SM-SDTQ
4) Scaling

$$\text{CCSD} : n_o^2 n_u^4$$

$$\text{CCSD(T)} : n_o^3 n_u^4$$

$$\text{SM-SDTQ} : n_o^4 n_u^6$$

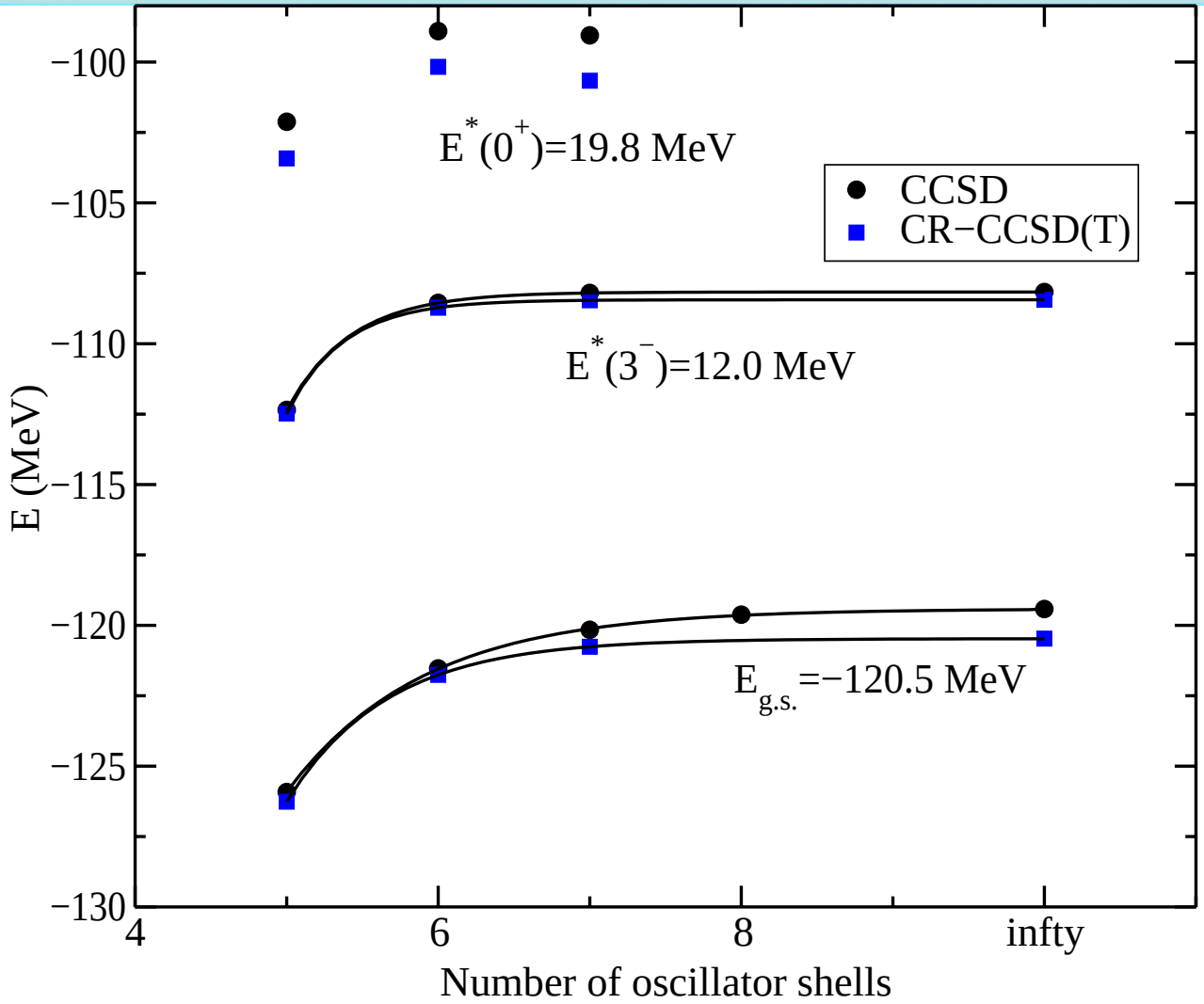
M. Horoi

SM within 0.1 MeV of our CR-CCSD(T) results

Extrapolations: EOMCCSD level

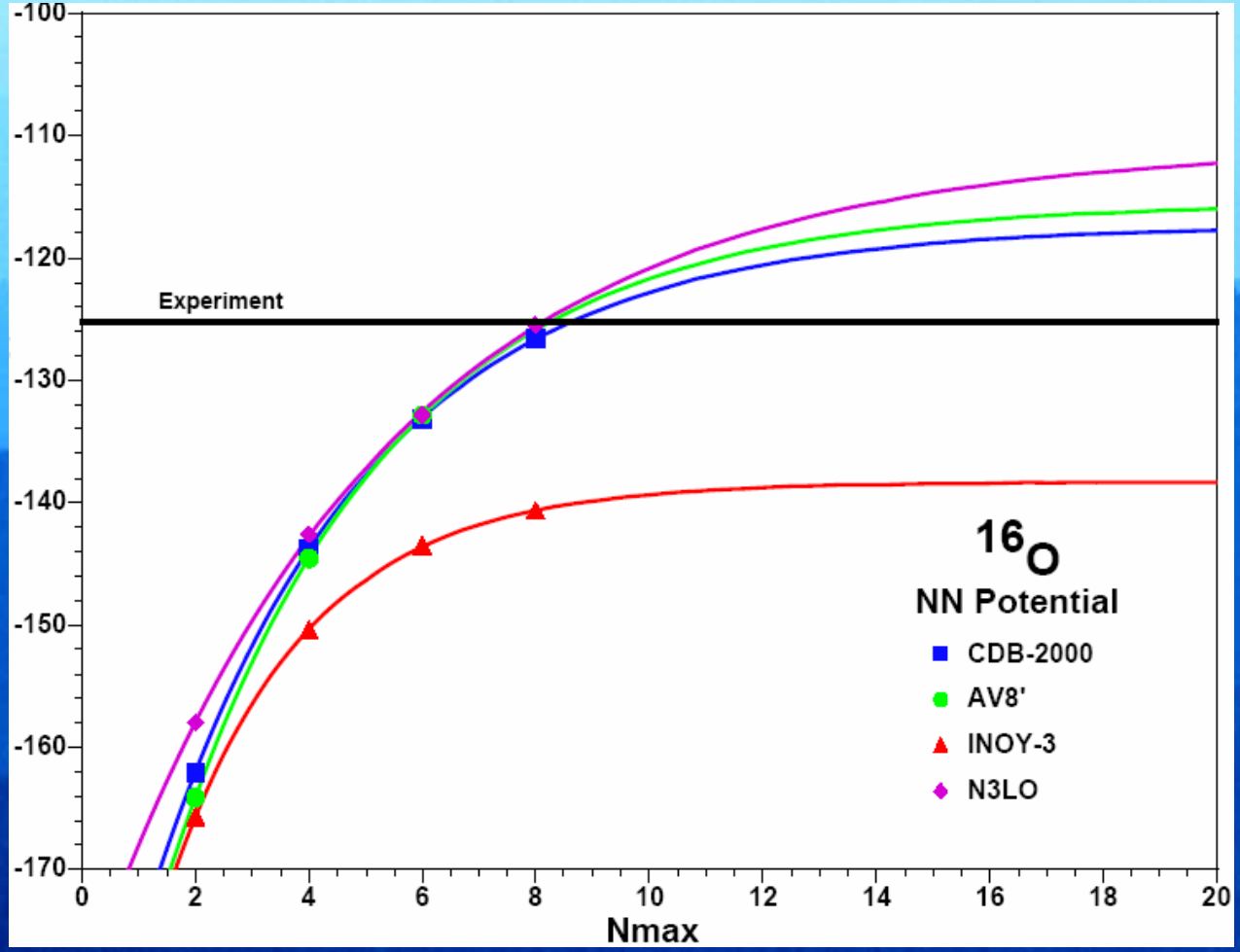
Diagonalize $\overline{H}^{(CCSD)}$ in the space of 1p-1h and 2p-2h excitations

$$R_K^{(CCSD)} = 1 + R_1 + R_2; \left|\Psi_K\right\rangle = R_K^{(CCSD)} e^T \left|\Phi\right\rangle$$



Wloch, Dean, Gour, Hjorth-Jensen, Papenbrock, Piecuch, PRL 94, 212501 (2005)

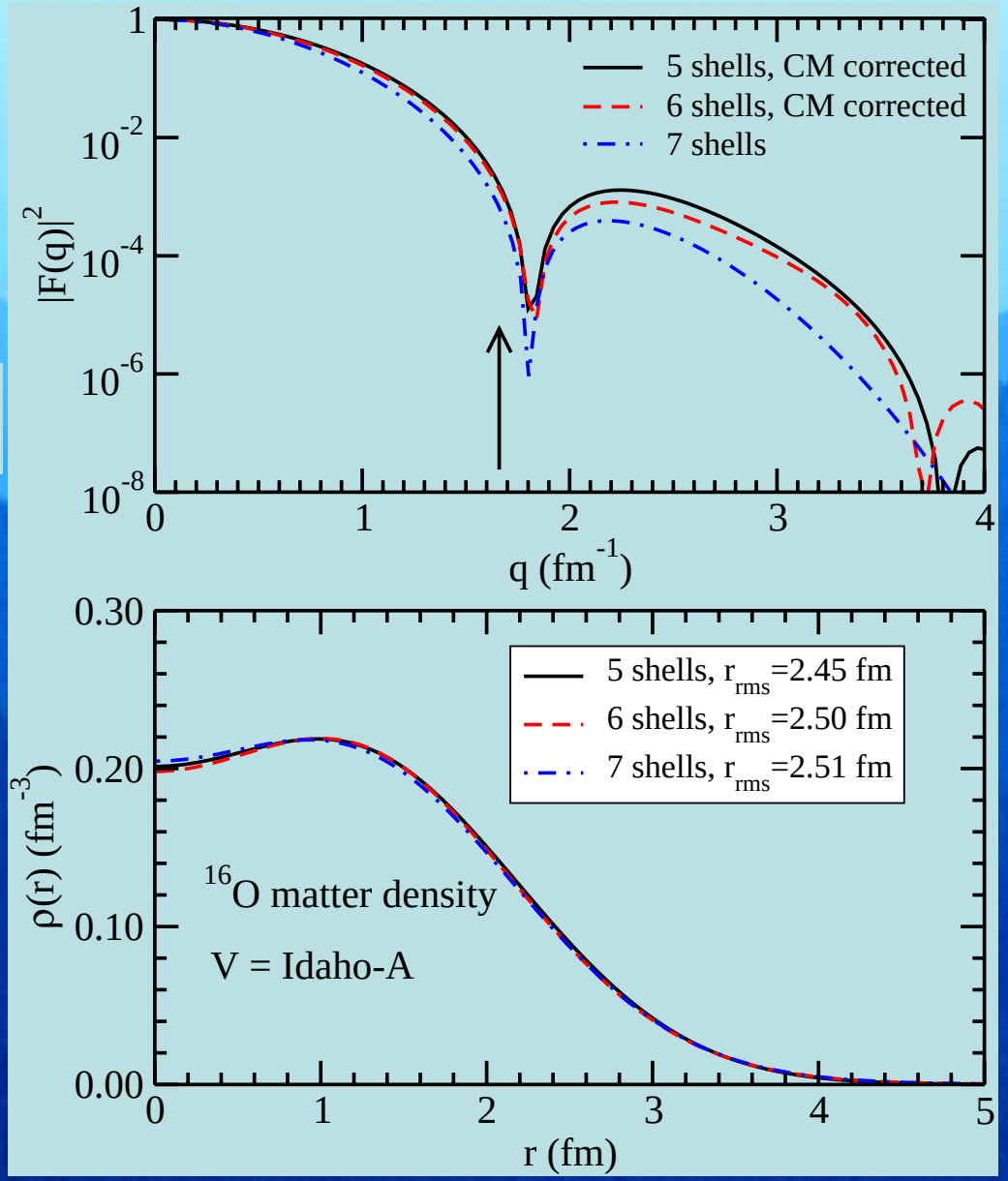
NCSM results for ^{16}O (Vary and Navratil, private communication)



Nuclear Properties

$$\rho_{\alpha\beta} = \left\langle \Phi \middle| L^{(\mu)} \left[e^{-T} a_\alpha^+ a_\beta e^T \right] R^{(\mu)} \middle| \Phi \right\rangle$$

Also includes second-order corrections from the two-body density.



N=8 results for ^{15}O, ^{17}O

Diagonalize $\overline{H}$ (T's solved for n nucleons) in the $n \pm 1$ Fock space.

BE/A	Expt.	N^{3}LO	CD-Bonn
^{15}N	7.7	6.34	
^{15}O	7.46	6.16	6.64
^{16}O	7.98	6.95	7.44
^{17}0	7.75	6.72	7.20
^{17}F	7.54	6.56	

All N=8
O.1 MeV changes from
N=7 to N=8 for excited states (relative).

On going calculations for
CD-Bonn and AV18…

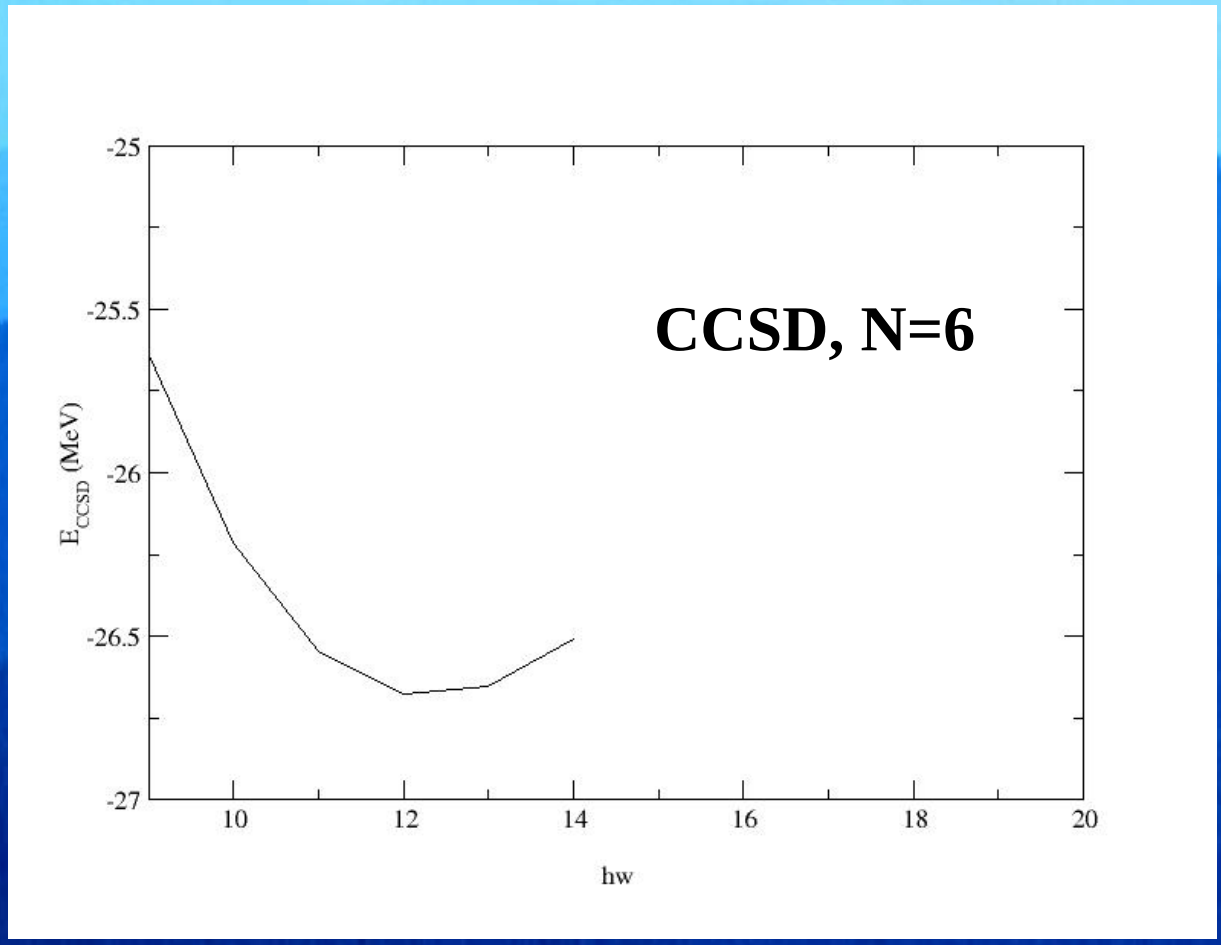
^{15}O	Expt.	N^{3}LO	CD-Bonn
3/2$^-$	6.176	6.26	7.35
1/2$^-$	0.0	0.0	0.0

^{15}N	Expt.	N^{3}LO
3/2$^-$	6.323	6.318
1/2$^-$	0.0	0.0

^{17}O	Expt.	N^{3}LO	CD-Bonn
3/2$^+$	5.085	5.68	6.41
1/2$^+$	0.870	-0.025*	0.31
5/2$^+$	0.0	0.0	0.0

^{17}F	Expt.	N^{3}LO	CD-Bonn
3/2$^+$	5.000	5.891	
1/2$^+$	0.495	0.428*	
5/2$^+$	0.0	0.0	0.0

First similarity-transform calculation
^{4}He Idaho-A (-27.4 MeV exact result)



Moving to larger model spaces always requires innovation

- CCSD code written for IBM using MPI.
- Performs at 0.18 Tflops on 100 processors on shared memory Ithaniam cluster.
- Requires further optimization for new science.

- Problem size increases by about a factor of 5 for each major oscillator shell
- Number of unknowns by a factor of 2 (for each step in N)
- Number of unknowns by a factor of 20 (for 4 times the particles)

N	Single particle basis states	^{4}He (unknowns)	^{16}O (unknowns)	Matrix element memory (Gbyte)
4	80	1792	24,960	0.165
5	140	4000	77,880	1.5
6	224	7,976	176k	10.1
7	336	14,112	345k	51
8	480	---	604k	212

Diagonalization: configuration-interaction, interacting shell model

Yields eigenfunctions which are linear combinations of particle-hole amplitudes

$$\left|\Psi_\alpha\right\rangle = \left(1 + b_i^a a_a^+ a_i + b_{ij}^{ab} a_a^+ a_b^+ a_i a_j + \cdots\right)\left|\Phi_0\right\rangle$$

1p-1h **2p-2h**

How does this compare to CC theory?

Relationship between shell model and CC amplitudes

$$B_1 = T_1$$

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

$$B_3 = T_3 + T_2T_1 + \frac{1}{6}T_1^3$$

$$B_4 = T_4 + T_3T_1 + \frac{1}{2}T_2^2 + \frac{1}{2}T_2T_1^2 + \frac{1}{24}T_1^4$$

$\ldots$

CCSD

CR-CCSD(T)

“Disconnected quadruples”

“Connected quadruples”

Factorization of the equations: intermediates

$$t_2(ab,ij) = \sum_{\substack{kl<\varepsilon_f \\ cd>\varepsilon_f}} \langle kl \| cd \rangle t_{ij}^{cd} t_{kl}^{ab}$$

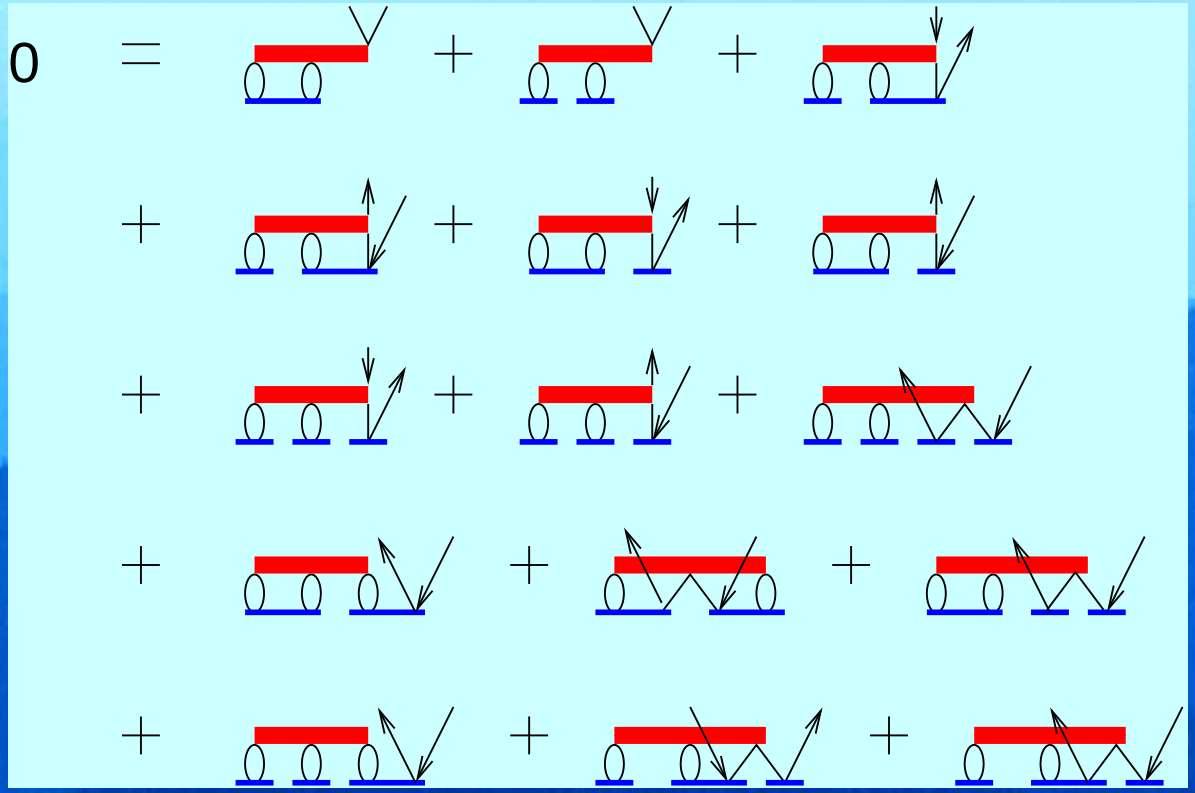
Break summation

$$= \sum_{kl<\varepsilon_f} \left\{ \sum_{cd>\varepsilon_f} \langle kl \| cd \rangle t_{ij}^{cd} \right\}_{kl,ij} t_{kl}^{ab}$$

Intermediate vectors

This leads to a very nice diagrammatic approach to the equations (a la Papenbrock), and to extensions to V3N inclusion in CC theory.

Inclusion of three-body forces: Amplitude equation for t_1:



Results including three-body forces coming soon…..

Conclusions and perspectives

- **Recall objective: development of robust many-body techniques for NN and NNN nuclear potentials….what is the nuclear Hamiltonian?**

- **Solution of the nuclear many-body problems requires extensive use of computational and mathematical tools. Numerical analysis becomes extremely important; methods from other fields (chemistry, CS) invaluable.**

- **Detailed investigation of triples corrections via CR-CCSD(T) indicates convergence at the triples level for ^{16}O calculation. ^{16}O (nearly) converged at 8 shells (not Nhω) using G-matrix and Vlowk.**

- **Excited states calculated for the first time (in huge space) using EOMCCSD and CR-EOMCCSD(T) in ^{16}O (3- high)**

- **Continuing work on the effective interaction; efforts to move to similarity transformed G are almost complete.**

- **Ca-40 underway; V_{3N} beginning; Multi-reference CC theory beginning.**