Coupled-Cluster Theory for Nuclei Past, Present, Future

David J. Dean
Oak Ridge National Laboratory

INT, Seattle, October 2007

"The shell must break before the bird can fly." – Tennyson
"

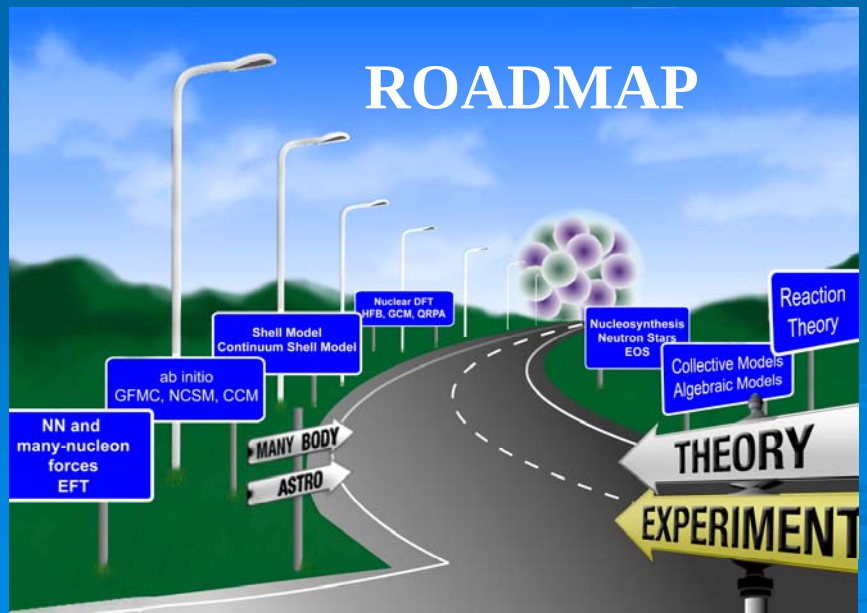
"Plans are useless, but planning is indispensable." – Eisenhower

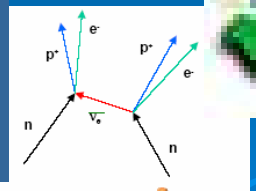
OAK RIDGE National Laboratory
Office of Science U.S. DEPARTMENT OF ENERGY
Office of Nuclear Physics Exploring Nuclear Matter - Quarks to Stars
NERSC

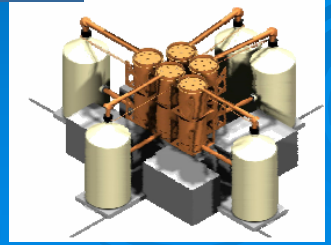
Key science drivers of rare isotopes

- Test the predictive power of models by extending experiments to new regions of mass and proton-to-neutron ratio
- Identify new phenomena that will challenge existing many-body theory

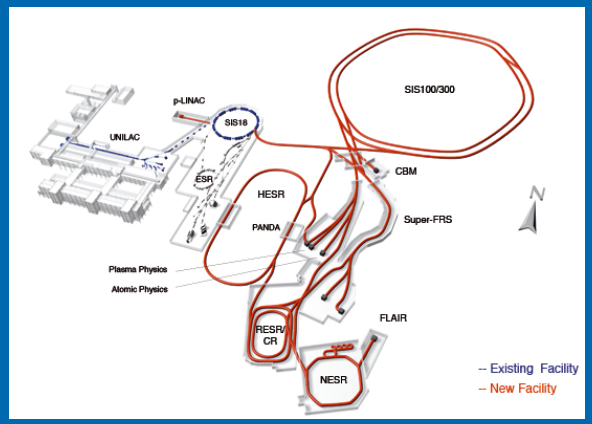
- Create and study super heavy nuclei
- Characterize neutron skins and excitation modes
- Constrain r-process site and explosive nucleosynthesis
- Constrain nuclear equation of state (neutron star crusts)
- Societal Applications: Energy, Security
- Beyond 'Standard Model': $\beta\beta0\nu$ decay; Dark Matter, EDM…

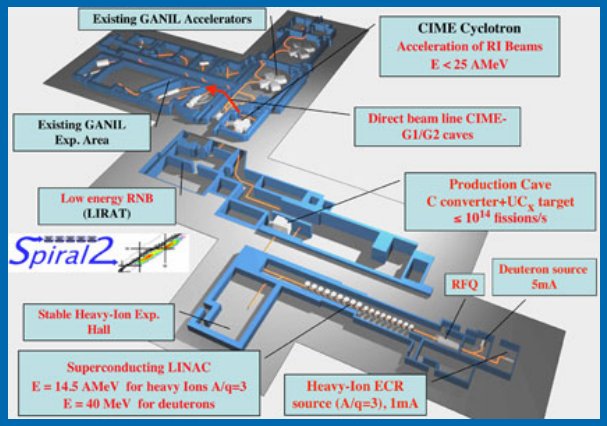




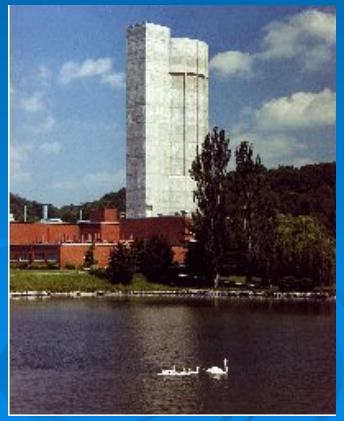


Present and next Generation Radioactive Ion Beam facilities (multi $100M investments world wide)



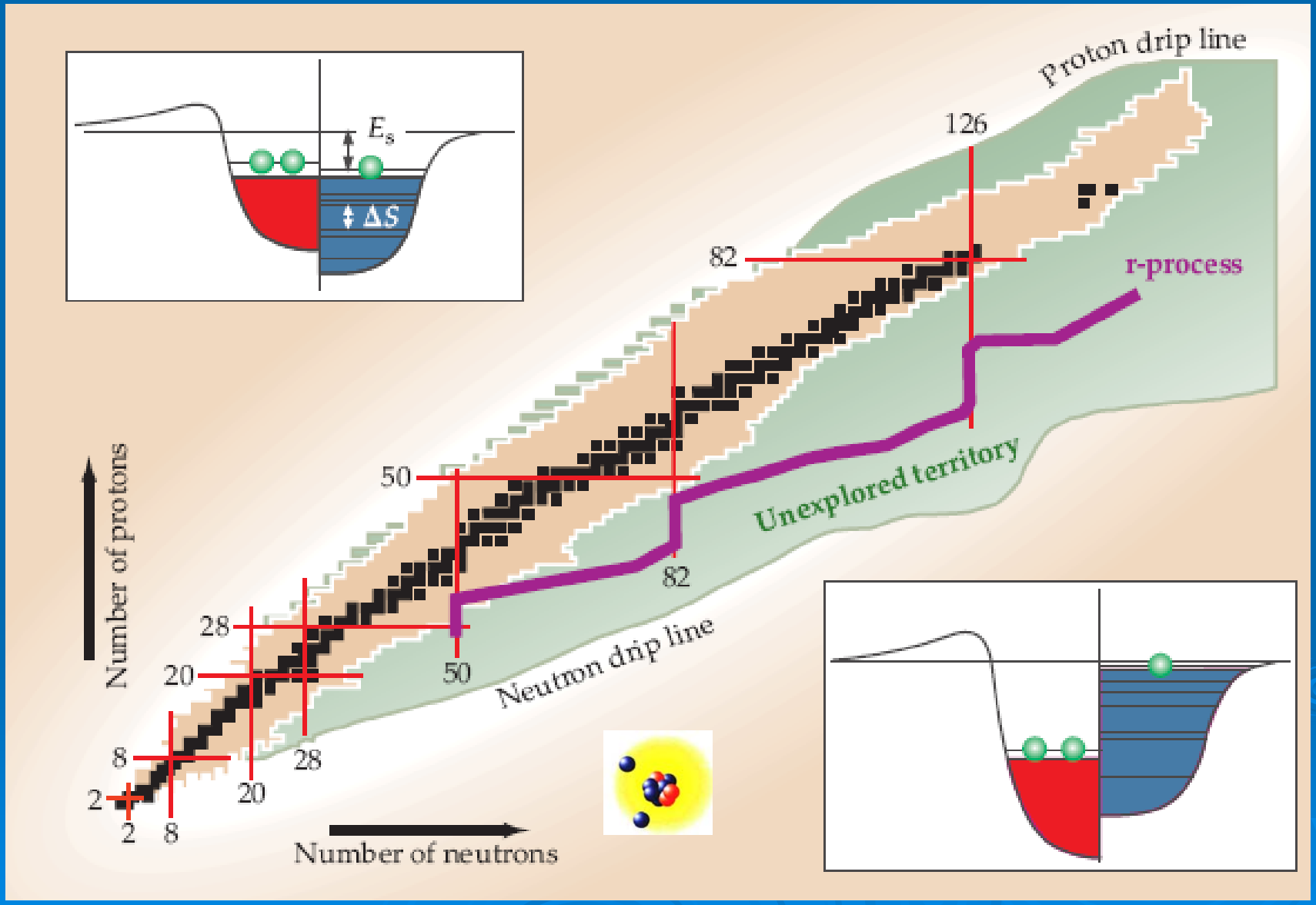


"[C]ountries throughout the world are aggressively pursuing rare-isotope science, often as their highest priority in nuclear science, attesting to the significance accorded internationally to this exciting area of research"
NAS RISAC Report

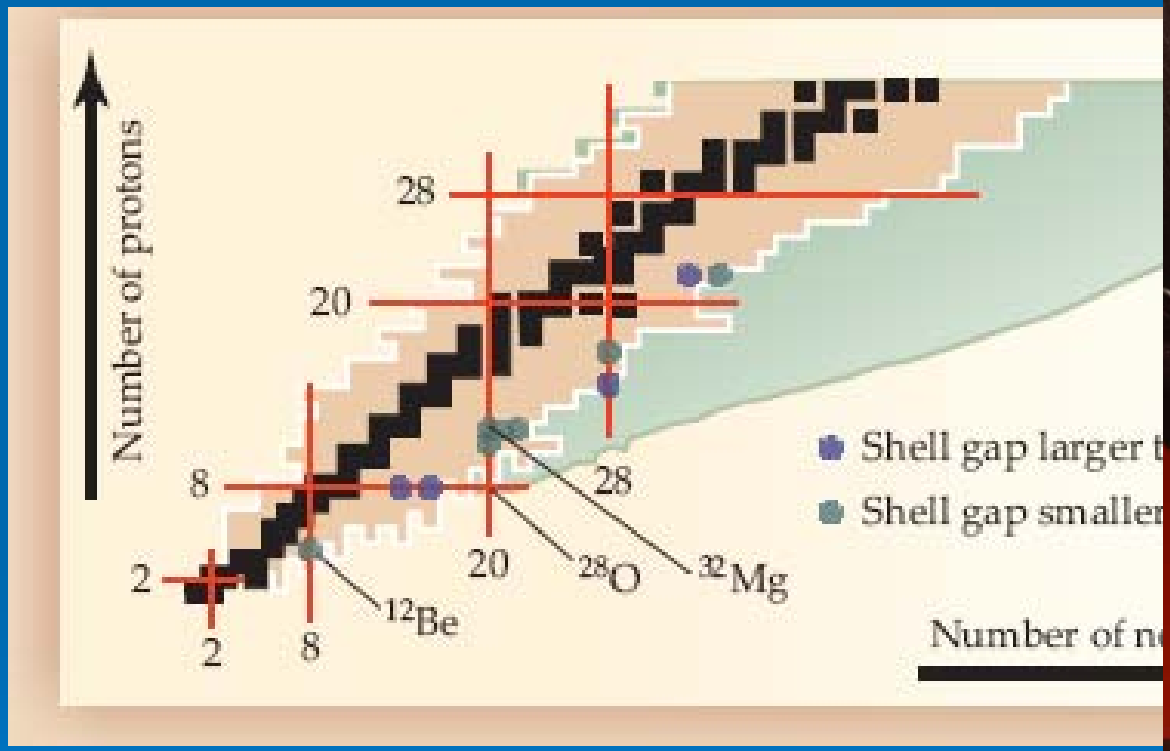


Future U.S. FRIB based on a heavy-ion linac driver a high priority.

The changing landscape of nuclei

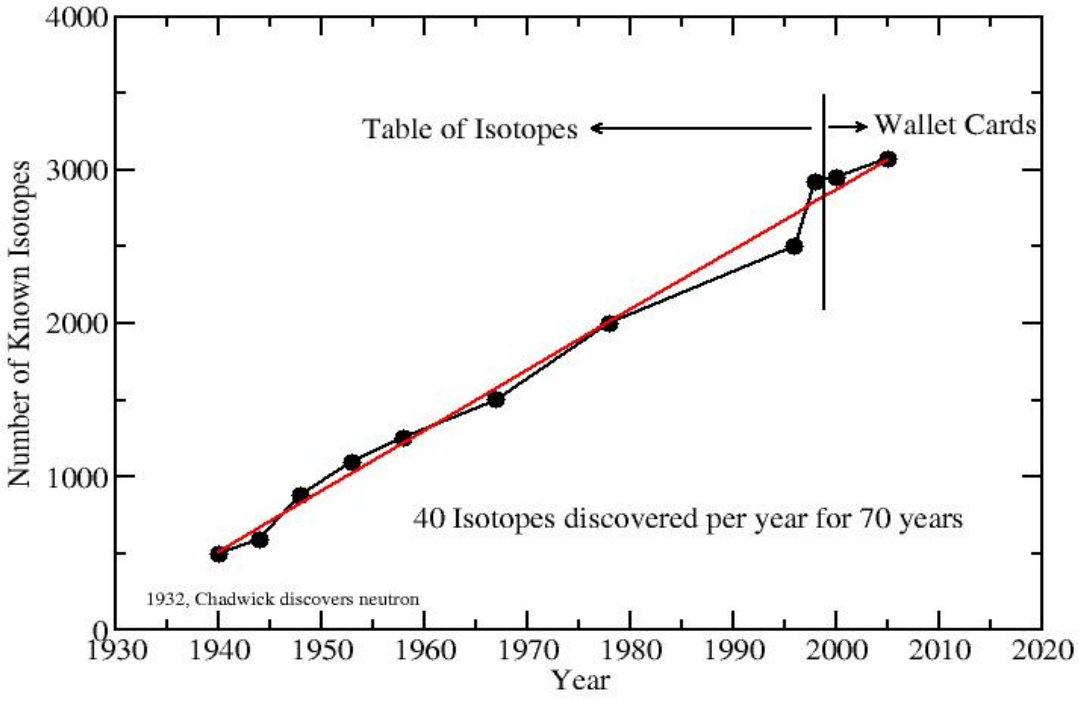


Changing shell gaps: one of the challenges



Why do theory at all?

Nuclear Discovery: 60 years



- Discovery of new nuclei a rather slow process
- Increasingly costly
- Probably will not reach ALL nuclei that are relevant even with FRIB
- Probably cannot measure all relevant nuclear properties
- Points to need for robust, predictive theory with quantifiable error bars

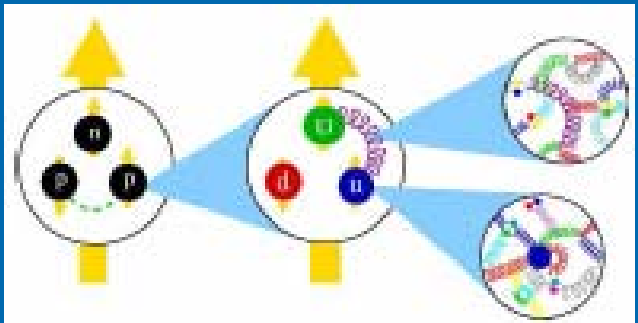
The challenge of theory for nuclei

"The first, the basic approach, is to study the elementary particles, their properties and mutual interaction. Thus one hopes to obtain knowledge of the nuclear forces. If the forces are known, one should, in principle, be able to calculate deductively the properties of individual nuclei. Only after this has been accomplished can one say that one completely understands nuclear structure….The other approach is that of the experimentalist and consists in obtaining by direct experimentation as many data as possible for individual nuclei. One hopes in this way to find regularities and correlations which give a clue to the structure of the nucleus….The shell model, although proposed by theoreticians, really corresponds to the experimentalist's approach."
–M. Goeppert-Mayer, Nobel Lecture

Two ways of doing business (I will focus primarily on the first):

- **QCD → NN (and NNN) forces → calculate → predict → experiment**
- **Experiment → effective forces → calculate → predict**
- **Progress involves feedback…**

Effective Field Theory



Interplay between nucleonic and sub-nucleonic (quarks and gluons) degrees of freedom in few-body nuclear systems

It's pretty complicated inside a nucleon!!

Starting point is an effective chiral πN Lagrangian:

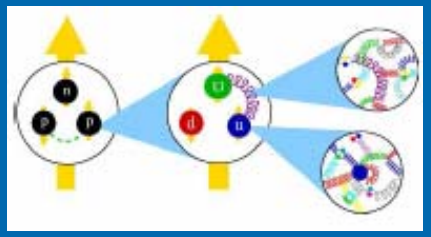
$$L_{\pi N} = L_{\pi N}^{(1)} + L_{\pi N}^{(2)} + L_{\pi N}^{(3)} + \cdots$$

- **Obeys QCD symmetries (spin, isospin, chiral symmetry)**
- **Develops a low-momentum interaction suitable for nuclei**
- **?Should some day be connected directly to QCD?**

$$L_{\pi N}^{(1)} = \overline{N}\left(iD_0 - \frac{g_A}{2}\vec{\sigma}\bullet\vec{u} \right)N \approx \overline{N}\left[i\partial_0 - \frac{1}{4f_\pi^2}\tau\bullet(\pi\times\partial_0\pi) - \frac{g_A}{2f_\pi}\tau\bullet(\vec{\sigma}\bullet\nabla)\pi \right]N + \cdots$$

Progress on the interaction: Effective Field Theory

Thus one hopes to obtain knowledge of the nuclear forces. If the forces are known… (MGM)



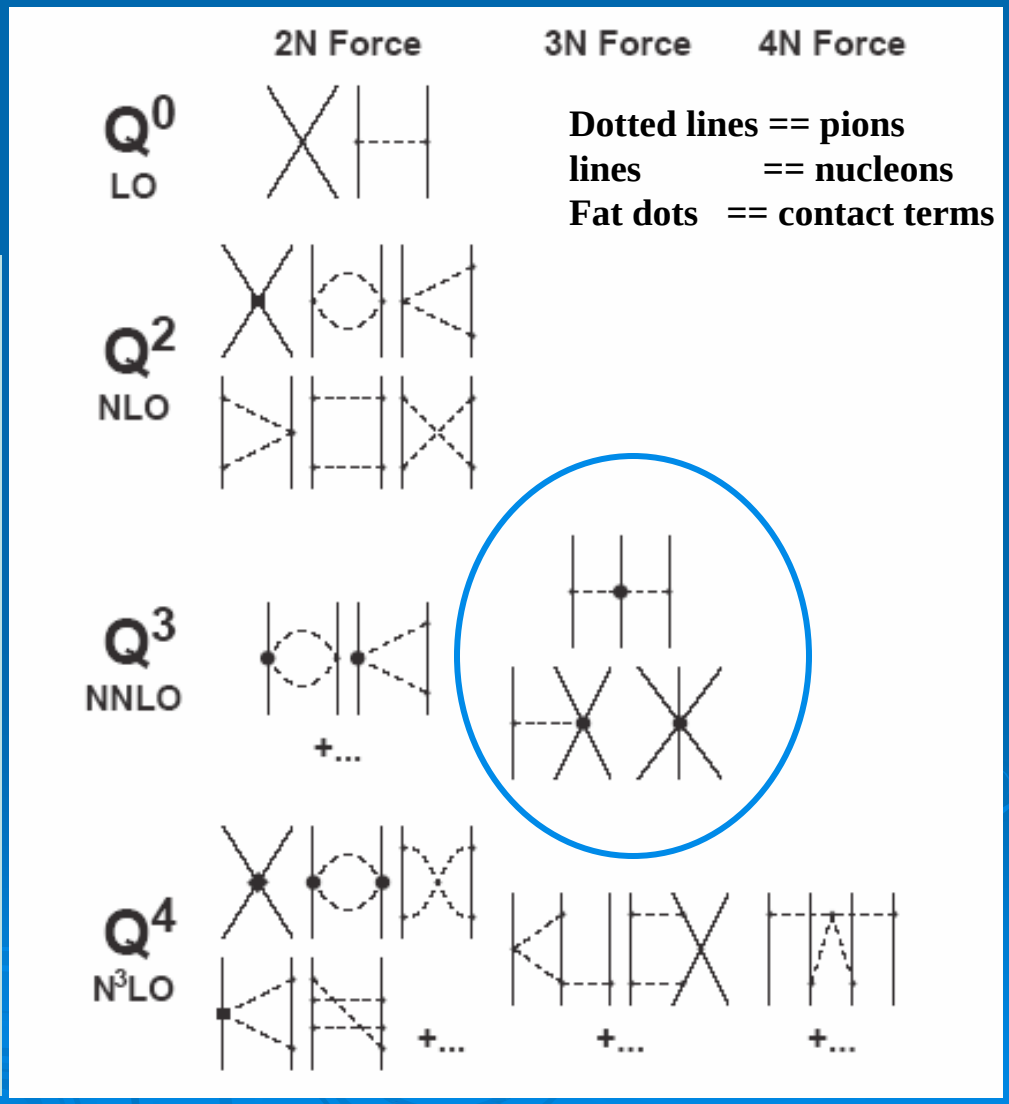
Effective Lagrangian → obeys QCD symmetries (spin, isospin, chiral symmetry breaking)

Lagrangian
→ infinite sum of Feynman diagrams.

Invoke power counting:
Expand in $O(Q/\Lambda_{QCD})$
Weinberg, Ordonez, Ray, van Kolck

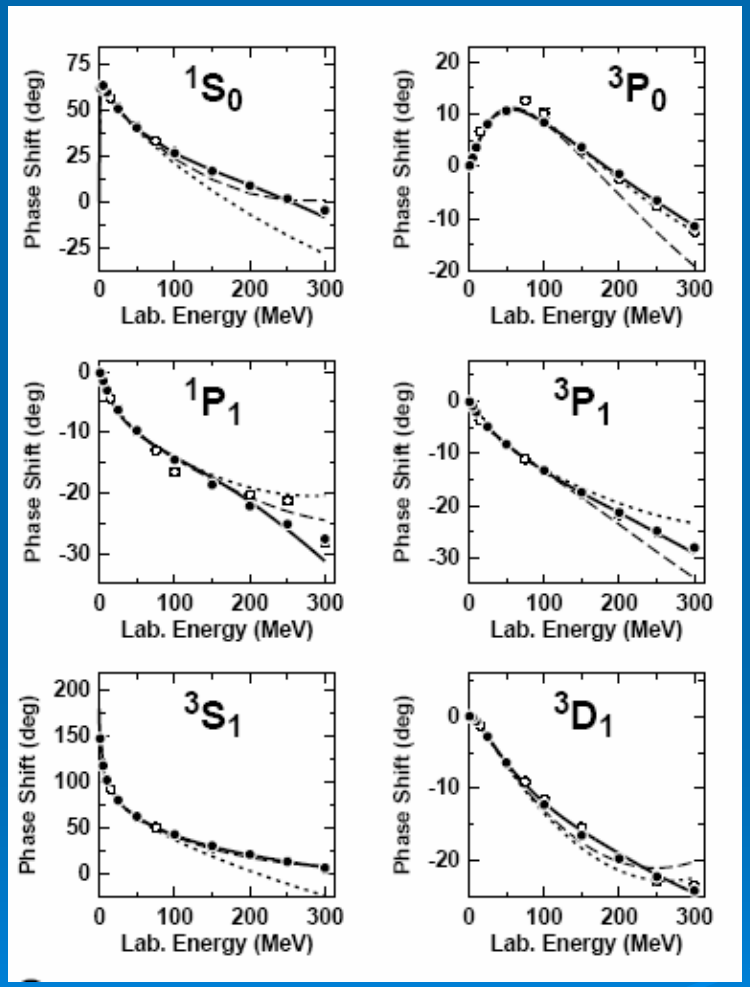
NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

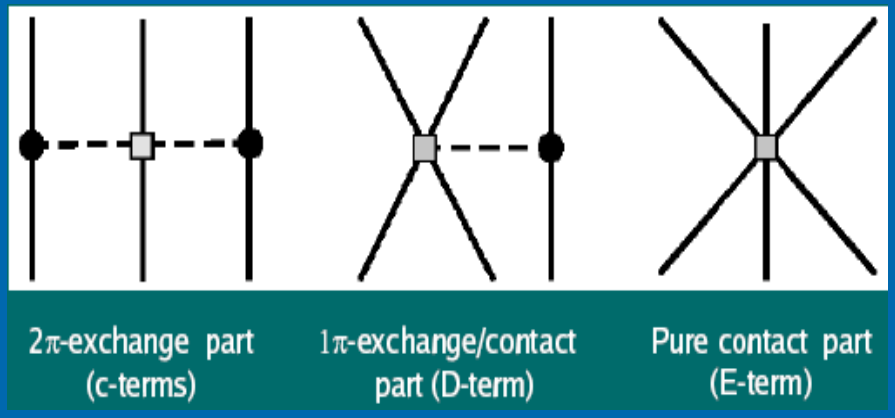
3-body (and higher) forces are inevitable.

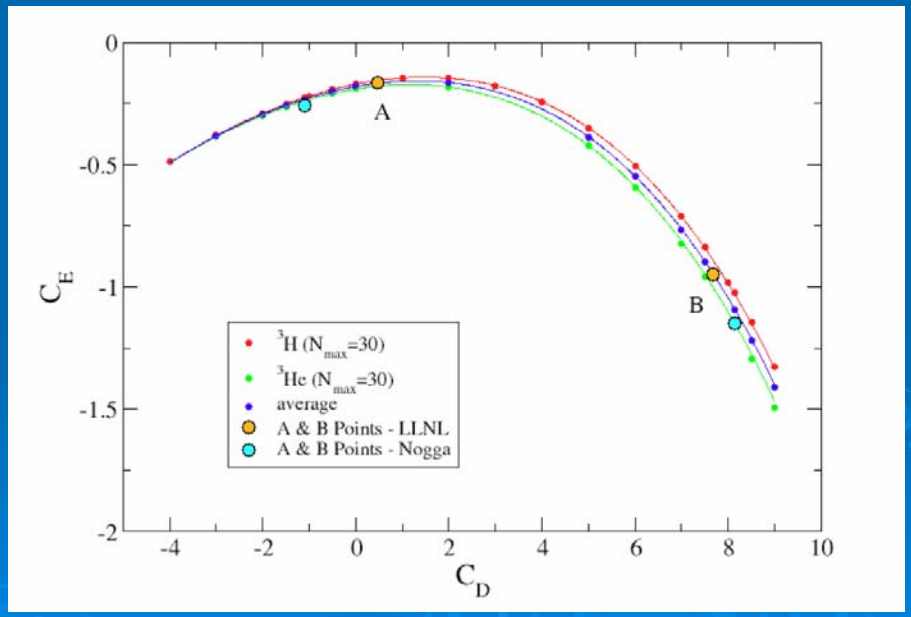


Effective field theory potentials bring a 3-body force

"…the force should be chosen on the basis of NN experiments (and possibly subsidiary experimental evidence…) (Bethe)





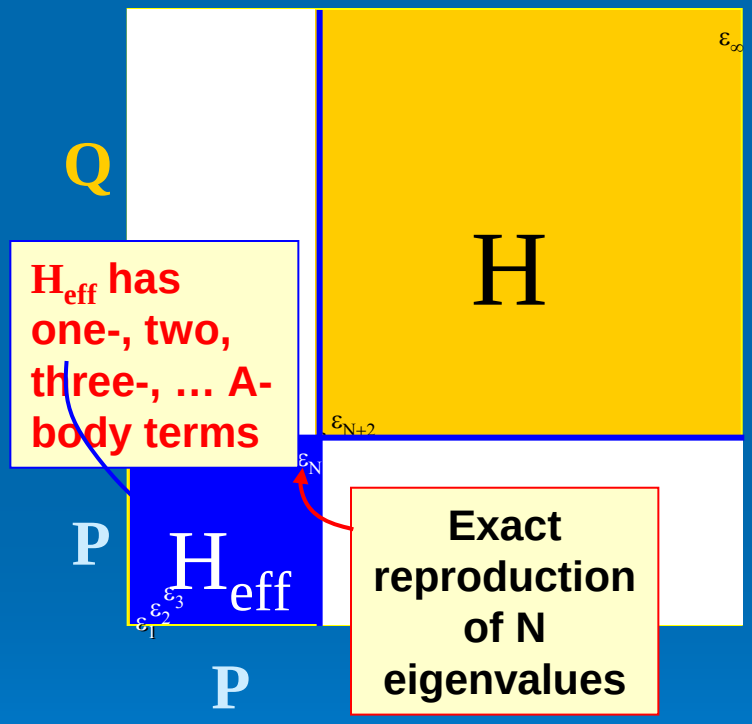


dashed → NLO
dot → N²LO
solid → N³LO

Challenge: Deliver the best NN and NNN interactions with their roots in QCD (eventually from LQCD, see Ishii, Aoki and Hatsuda, arXiv:nucl-th/0611096)

Progress: Embracing renormalization

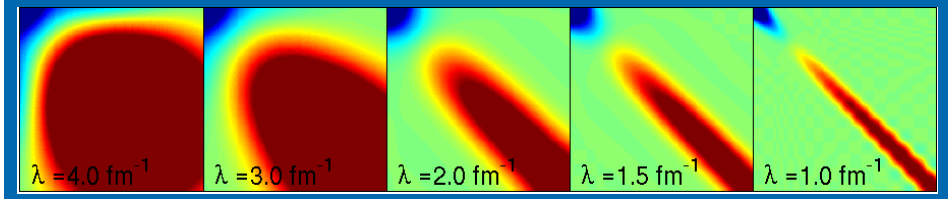
Project H into large basis;
Perform Lee-Suzuki (NCSM)
Use Heff as 2-(+3) body interaction



Recovers Bare A-body in large space
Requires addition of 3-body force for experimental binding (adjust to He-4)
Challenge: slow convergence

$$\frac{d}{d\Lambda} V^{\Lambda}_{\mathrm{low}\,k}(k',k) = \frac{2}{\pi} \frac{V^{\Lambda}_{\mathrm{low}\,k}(k',\Lambda)\, T^{\Lambda}(\Lambda,k;\Lambda^2)}{1-(k/\Lambda)^2}$$

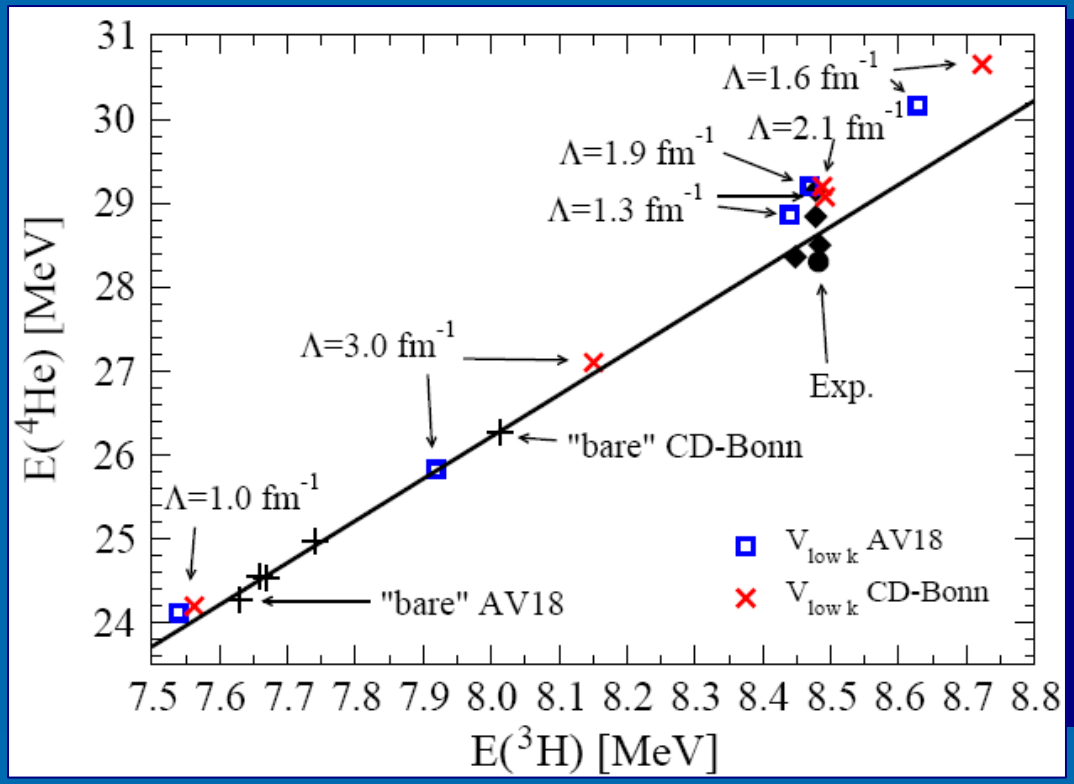
- **Renormalize at a momentum cutoff Λ**
- **Project onto oscillator basis**
- **Preserves phase shifts to the cutoff**
- **"reasonable" convergence**



Challenges:
- **Does not recover bare result**
- **Requires 3-body force for experimental binding**
  …adjust to He-4
- **Λ-independence**

Schwenk, Bogner, Furnstahl,…

Interaction: $V_{low\text{-}k}$ from Av18 + chiral 3NF



As cutoff Λ is varied, motion along Tjon line.

Addition of Λ-dependent three-nucleon force yields agreement with experiment.

Three-nucleon force perturbative at cutoff Λ=1.9 fm^{-1} *for these nuclei.*

A. Nogga, S. K. Bogner, and A. Schwenk, Phys. Rev. C 70 (2004) 061002.

	^{3}H					^{4}He				
Λ [fm^{-1}]	T	$V_{low\,k}$	c-terms	D-term	E-term	T	$V_{low\,k}$	c-terms	D-term	E-term
1.0	21.06	−28.62	0.02	0.11	−1.06	38.11	−62.18	0.10	0.54	−4.87
1.3	25.71	−34.14	0.01	1.39	−1.46	50.14	−78.86	0.19	8.08	−7.83
1.6	28.45	−37.04	−0.11	0.55	−0.32	57.01	−86.82	−0.14	3.61	−1.94
1.9	30.25	−38.66	−0.48	−0.50	0.90	60.84	−89.50	−1.83	−3.48	5.68
2.5(a)	33.30	−40.94	−2.22	−0.11	1.49	67.56	−90.97	−11.06	−0.41	6.62
2.5(b)	33.51	−41.29	−2.26	−1.42	2.97	68.03	−92.86	−11.22	−8.67	16.45
3.0($*$)	36.98	−43.91	−4.49	−0.73	3.67	78.77	−99.03	−22.82	−2.63	16.95

From the interaction to solving the nuclear many-body problem

Begin with a NN (+3N) Hamiltonian

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

Bare (GFMC) (Local only, Av18 plus adjusted 3-body)

Basis expansion (explore forces)

Basis expansions:

- **Determine the appropriate basis**
- **Generate H_{eff} in that basis**
- **Use many-body technique to solve problem**

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

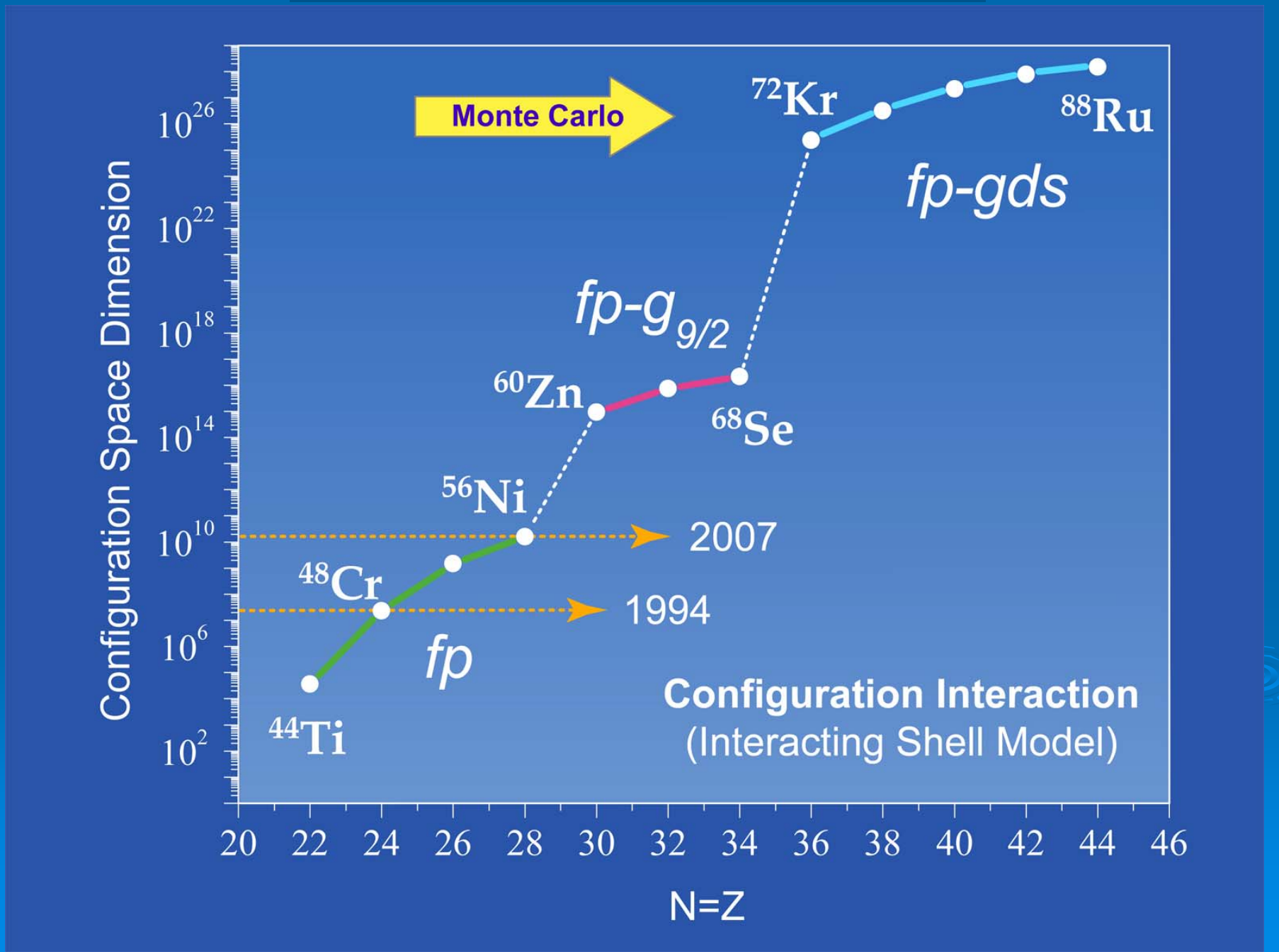
Oscillator single-particle basis states

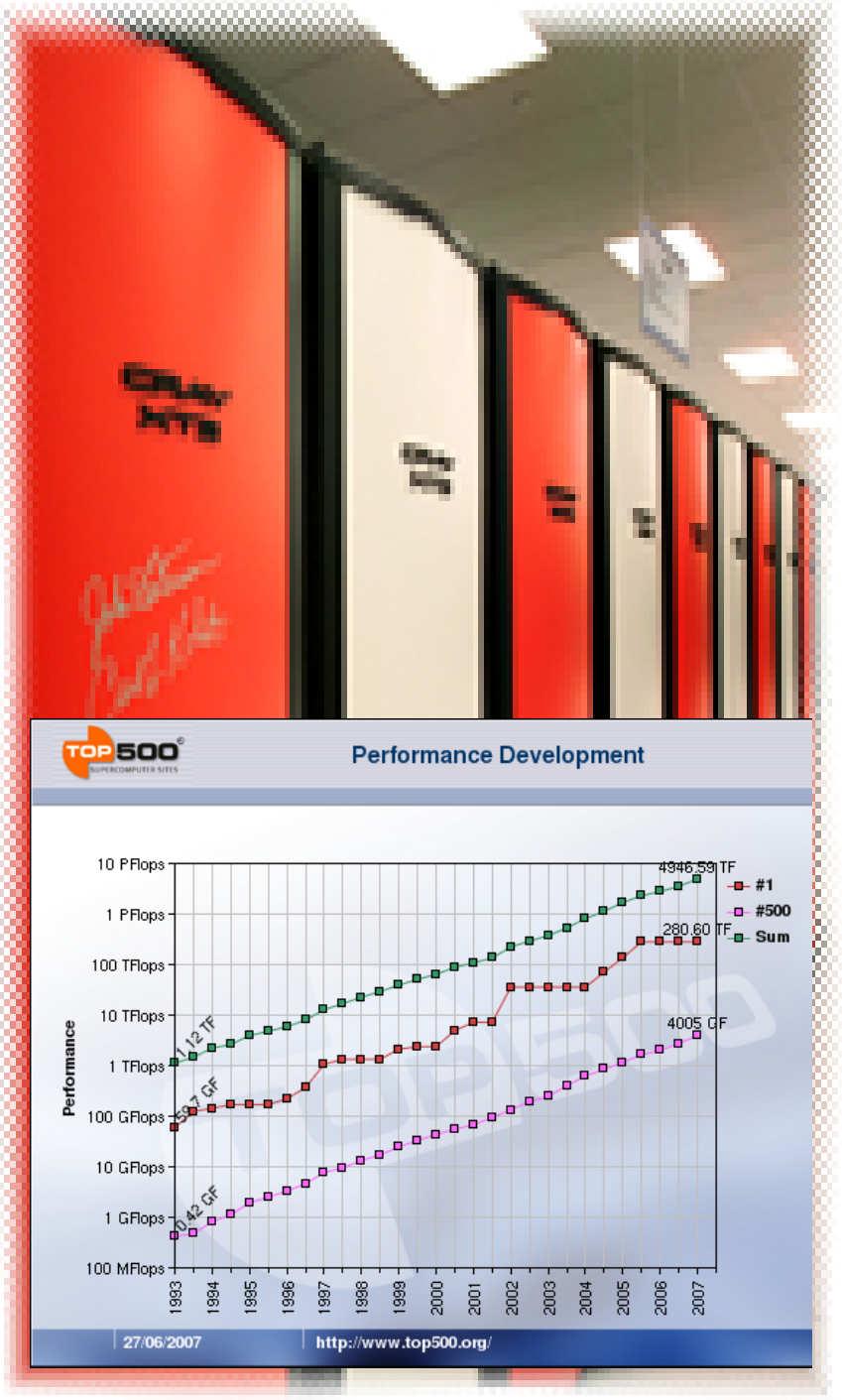
Many-body basis states

Substantial progress in many-body developments

- **GFMC; AFDMC**
- **No Core shell model (not a model)**
- **Coupled-cluster theory**
- **UCOM,…**
- **AFMC**

Exponential scaling of shell model





"…be able to calculate deductively the properties of individual nuclei"

- Computation absolutely essential
- "Moore's law" power law in raw computing power: 2 year doubling time.
- Petascale: 3 years
- Exascale: 10 years

- Challenge: develop algorithms that will effectively utilize both core speed and memory to attack nuclear problems.

- Measure of success: predictive nuclear theory in medium-mass nuclei (to mass 100).

Coupled Cluster Theory: ab initio in medium mass nuclei

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

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

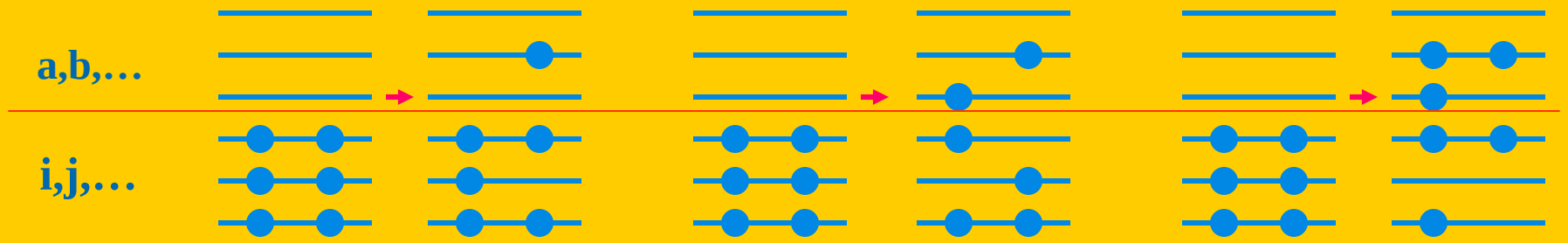
$$\langle \Phi_{ij\cdots}^{ab\cdots} | \exp(-T) H \exp(T) | \Phi \rangle = \langle \Phi_{ij\cdots}^{ab\cdots} | \bar{H} | \Phi \rangle = 0$$

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

The many-body wave function in cluster amplitudes

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

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



$m_A = N$, exact theory;

$m_A < N$, approximate theory

$m_A = 2 \quad T = T_1 + T_2 \qquad CCSD \qquad n_o^2 n_u^4 \left(n_o^2 n_u^2\right)$

$m_A = 3 \quad T = T_1 + T_2 + T_3 \qquad CCSDT \qquad n_o^3 n_u^5 \left(n_o^3 n_u^3\right)$

Important (technical) detail: normal-ordered Hamiltonian

The Hamiltonian is normal-ordered w.r.t. the vacuum state |Φ>.

$$\begin{aligned}\hat{H} &= \sum_{pq} \varepsilon_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{4} \sum_{pqrs} \langle pr||sr\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s \\ &= \sum_i \varepsilon_{ii} + \frac{1}{2} \sum_{ij} \langle ij||ij\rangle \\ &+ \sum_{ij} \left(\varepsilon_{pq} + \sum_i \langle pi||qi\rangle \right) \{\hat{a}_p^\dagger \hat{a}_q\} + \frac{1}{4} \sum_{pqrs} \langle pq||sr\rangle \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s\}\end{aligned}$$

Similarly, the Hamiltonian of the 3NF becomes

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

Vacuum energy and density-dependent one-body terms

Density-dependent two-body terms

$$\hat{h}_3 \equiv \frac{1}{36} \sum_{pqrstu} \langle pqr||stu\rangle \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger \hat{a}_u \hat{a}_t \hat{a}_s\}$$

Residual three-body terms

Note: 1. The form of the Hamiltonian is different for each nucleus under consideration.

2. Normal-ordering necessary for evaluation of similarity-transformed Hamiltonian.

3. “Density-dependend” terms are coherent sums over two- and three-body matrix elements.

View of the CC equations from 10,000 feet

$$He^{T}\left|\Phi\right\rangle = E_0 e^{T}\left|\Phi\right\rangle$$

$$e^{-T}He^{T}\left|\Phi\right\rangle = E_0 e^{-T}e^{T}\left|\Phi\right\rangle = E_0\left|\Phi\right\rangle = \overline{H}\left|\Phi\right\rangle$$

$$\overline{H} = e^{-T}He^{T} = \left(He^{T}\right)_C$$

$$\overline{H} = H + [H,T] + \frac{1}{2}[[H,T],T] + \frac{1}{6}[[[H,T],T],T] + \frac{1}{24}[[[[H,T],T],T],T]$$

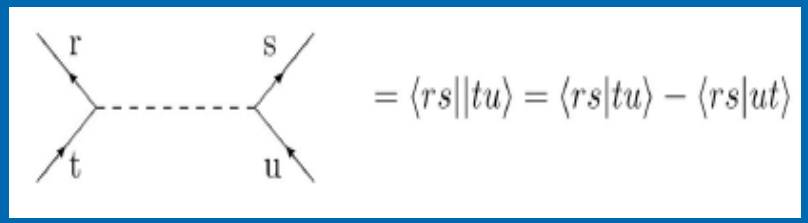
Finite series in T.

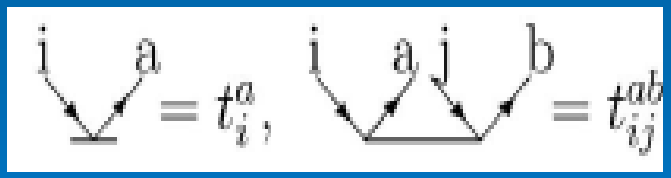
$$\left\langle \Phi_{i_1 i_2 \ldots i_k}^{a_1 a_2 \ldots a_k} \left| \left(H_N e^{T^{(A)}}\right)_C \right| \Phi \right\rangle = 0, \quad k = 1,\ldots,m_A$$

$$E_0 = \left\langle \Phi \left| H \right| \Phi \right\rangle + \left\langle \Phi \left| \left(H_N e^{T^{(A)}}\right)_C \right| \Phi \right\rangle = \left\langle \Phi \left| \left[H_N \left(T_1 + T_2 + \frac{1}{2}T_1^{\,2} \right) \right]_C \right| \Phi \right\rangle$$

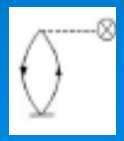
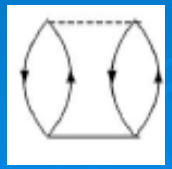
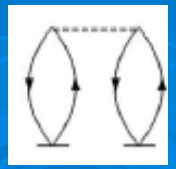
A word on diagrams in CC theory

$$E_0 = \langle \Phi | H | \Phi \rangle + \left\langle \Phi \left| \left(H_N e^{T^{(A)}} \right)_C \right| \Phi \right\rangle = \left\langle \Phi \left| \left[H_N \left(T_1 + T_2 + \frac{1}{2} T_1^2 \right) \right]_C \right| \Phi \right\rangle$$





- sign determined by number of hole-lines and loops $(-1)^{h+l}$
- $1/2^m$ for equivalent lines (originating in one vertex but ending in another)
- 1/2 for each equivalent pair vertex

$E_{CCSD} = E_0 +$  +  + 

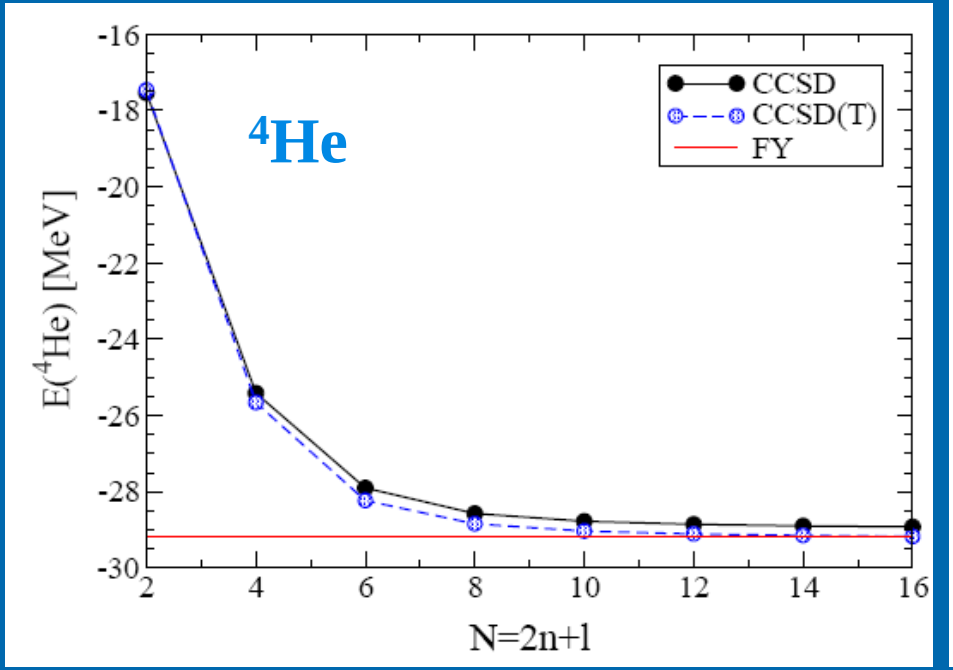
$$= \sum_{ia} f_{ia} t_i^a + \frac{1}{2} \sum_{aibj} \langle ij \| ab \rangle t_i^a t_j^b + \frac{1}{4} \sum_{aibj} \langle ij \| ab \rangle t_{ij}^{ab}$$

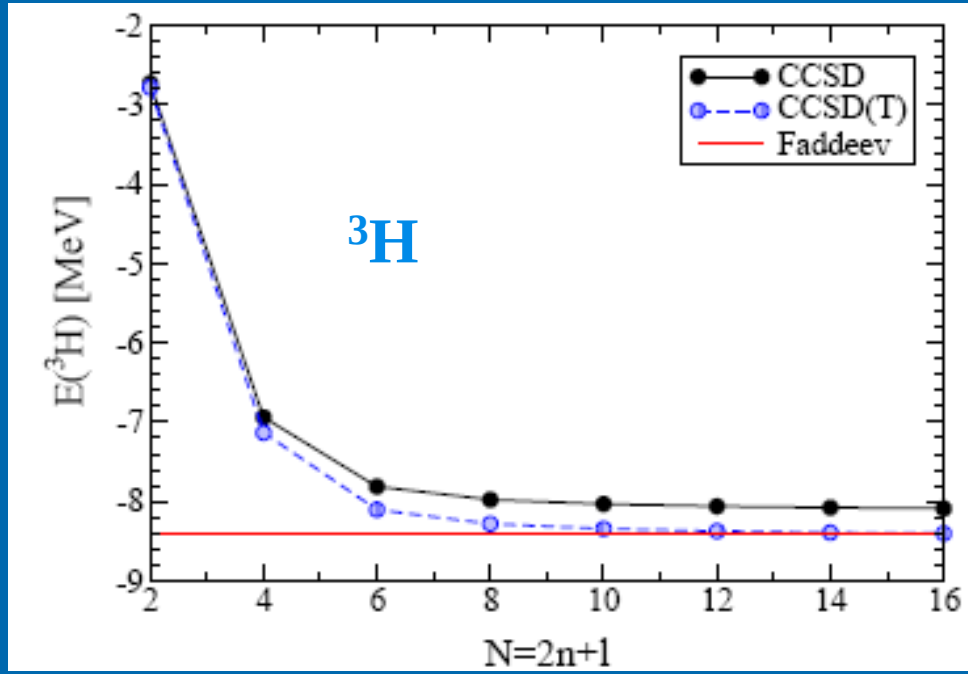
Physical/technical roadmap

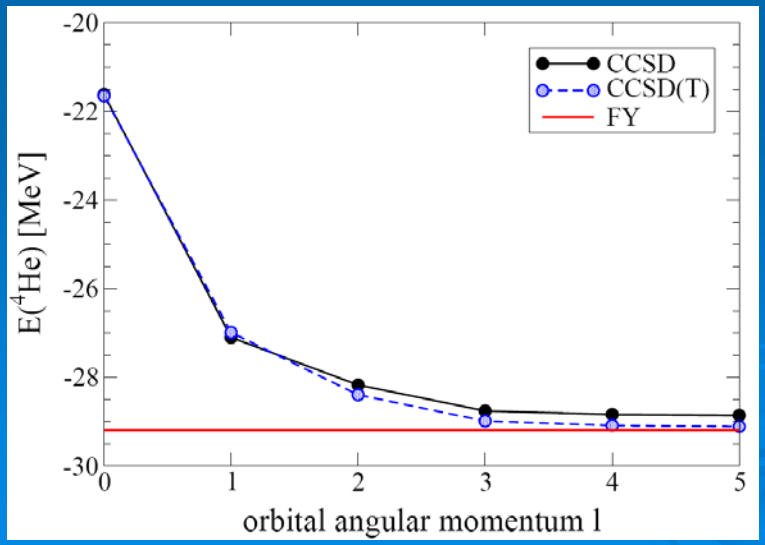
Ground state correlations:	**CCSD**
Triples corrections:	**CCSD(T)**
Excited States (up to 2p-2h):	**EOM-CCSD**
A+/-1 systems	**EOM-CCSD(A+/-1)**
Properties	**Left eigenvalue problem**
Resonances:	**Complex-CCSD**
Full triples:	**CCSDT-1,2,3,4**
3-body interaction:	**H3-CCSD**
Triples corrections	**H3-CCSD(T)**

NOTE: In the earliest work (2004-2005); we used $H=T+G(\omega)$
We now (all 2007 papers) use $H=T-T_{cm}+V$
$\langle H_{cm} \rangle$ very small in large spaces, and must extrapolate to zero in infinite space (very small means < 0.2 MeV)

CC vs Faddeev-Yakubowsky benchmarks met for ^{4}He



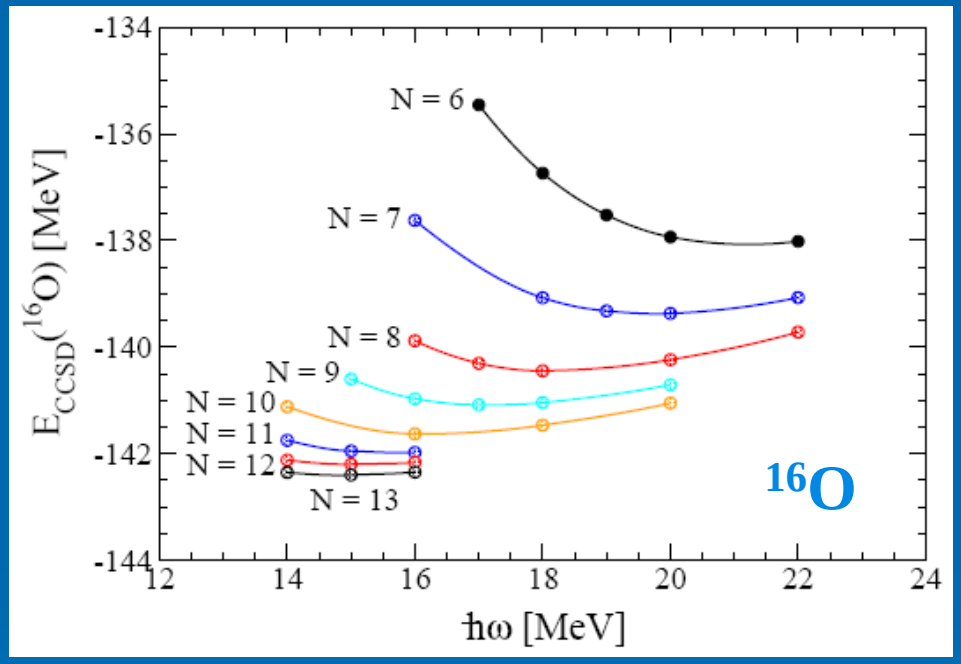


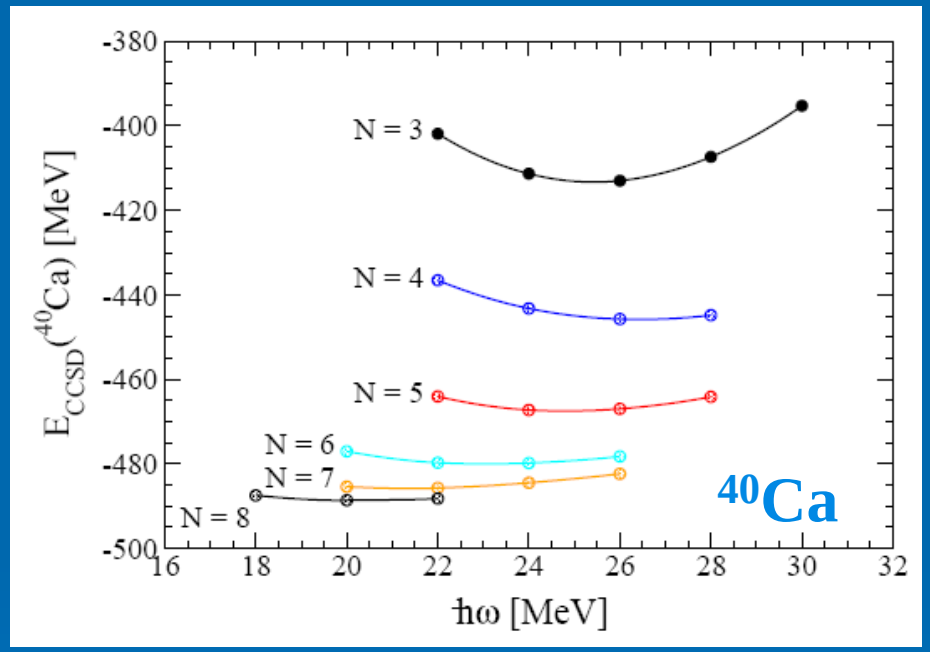


All interactions: AV18 at Λ=1.9 (He) and 2.1 (O,Ca) fm^{-1}

Hagen, Dean, Hjorth-Jensen, Papenbrock, Schwenk, arXiv:0707.1516; PRC 76, 044305 (2007)

Behavior of CCSD as function of model space
Medium mass nuclei

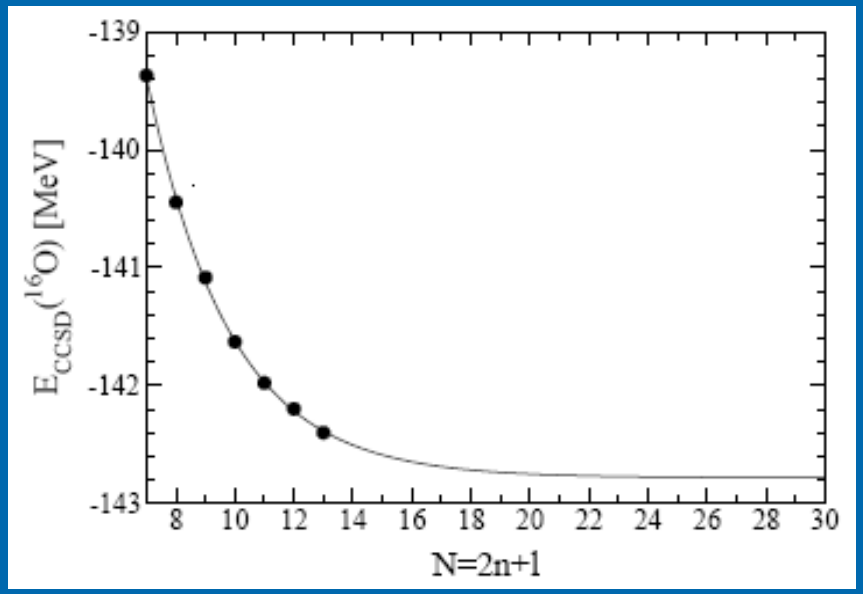




- Converging energy
- Decreasing hw dependence

N=8:
10^{63} many-body basis states

CCSD exponential fall off with basis size

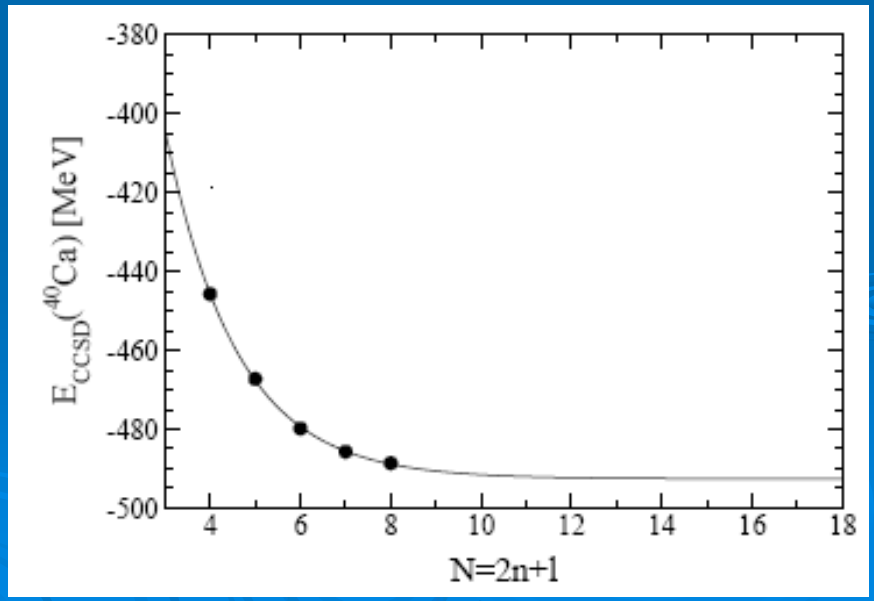


$$E_{CCSD,\infty}\left({}^{16}\mathrm{O}\right) = -142.78\ \mathrm{MeV}$$
$$E_{CCSD}\left({}^{16}\mathrm{O}\right) = -142.40\ \mathrm{MeV}$$

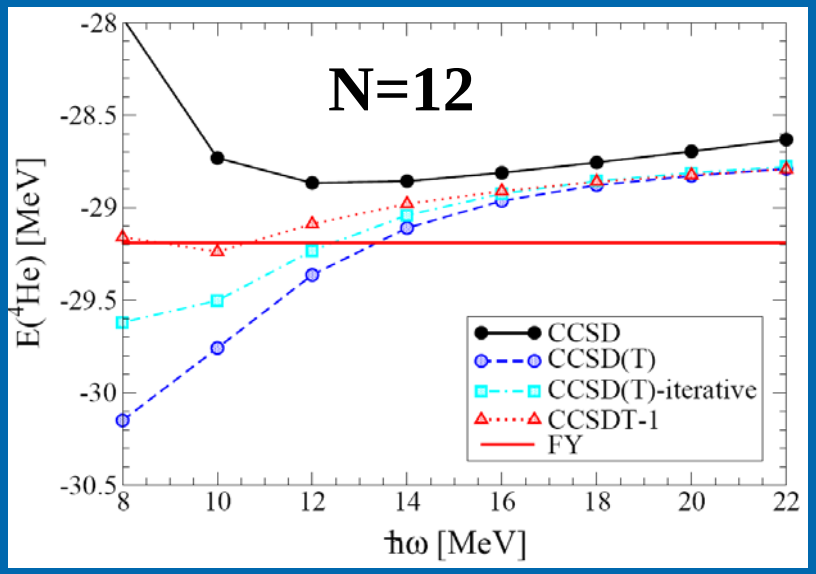
Nearly converged in model space

$$E_{CCSD,\infty}\left({}^{40}\mathrm{Ca}\right) = -492.6\ \mathrm{MeV}$$
$$E_{CCSD}\left({}^{40}\mathrm{Ca}\right) = -488.6\ \mathrm{MeV}$$

Less than 1% in ^{40}Ca

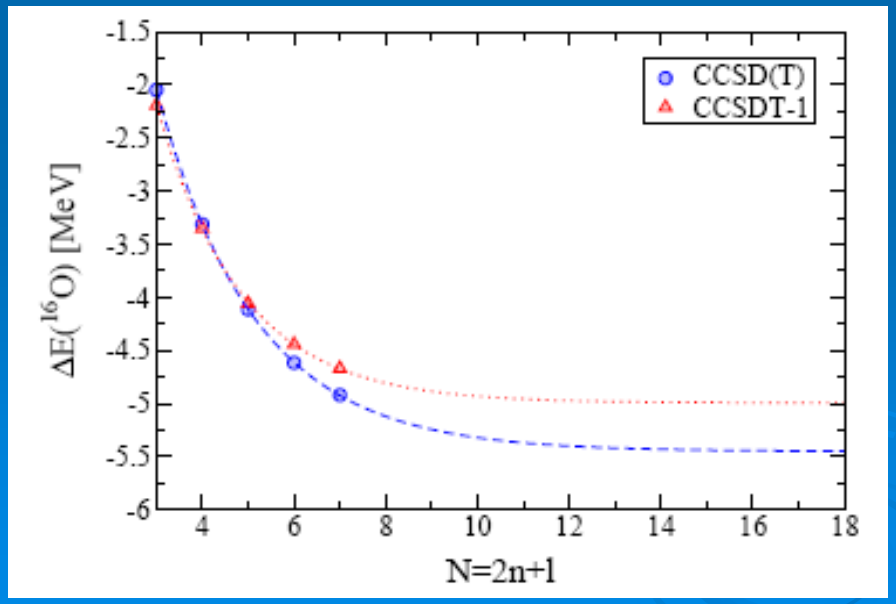


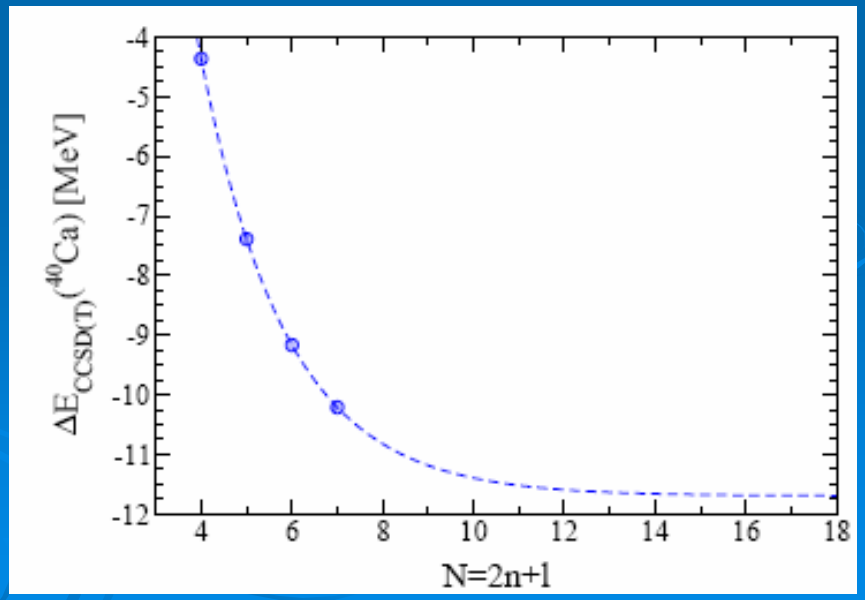
Triples corrections implemented



$$
\begin{aligned}
&\text{CCSDT-1} && 0 = \langle \phi_{ijk}^{abc} | \left(\hat{F}\hat{T}_3 + \hat{H}\hat{T}_2 \right)_c | \phi \rangle \,, \\
&\text{CCSDT-2} && 0 = \langle \phi_{ijk}^{abc} | \left(\hat{F}\hat{T}_3 + \hat{H}\hat{T}_2 + \hat{H}\hat{T}_2^2/2 \right)_c | \phi \rangle \,, \\
&\text{CCSDT-3} && 0 = \langle \phi_{ijk}^{abc} | \left(\hat{F}\hat{T}_3 + \hat{H} e^{\hat{T}_1+\hat{T}_2} \right)_c | \phi \rangle \,, \\
&\text{CCSDT} && 0 = \langle \phi_{ijk}^{abc} | \left(\hat{H} e^{\hat{T}_1+\hat{T}_2+\hat{T}_3} \right)_c | \phi \rangle \,. \qquad (8)
\end{aligned}
$$

Computational check:
If CCSD(T) and CCSDT-1
are not diverging with hω, then okay.





Bottom line for these studies

Convergence demonstrated:

- **Model space**
- **hw**
- **cluster size**

Error estimate: **<< 1%** **< 1%** **1%**

	^{4}He	^{16}O	^{40}Ca
E_0	-11.8	-60.2	-347.5
ΔE_{CCSD}	-17.1	-82.6	-143.7
$\Delta E_{\mathrm{CCSD(T)}}$	-0.3	-5.4	-11.7
$E_{\mathrm{CCSD(T)}}$	-29.2	-148.2	-502.9
exact (FY)	-29.19(5)		

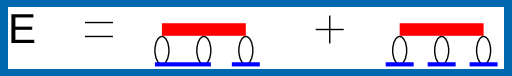
Everybody gets E_0. So the real measure of change should be in the correlation energy (Δ above), not the total.

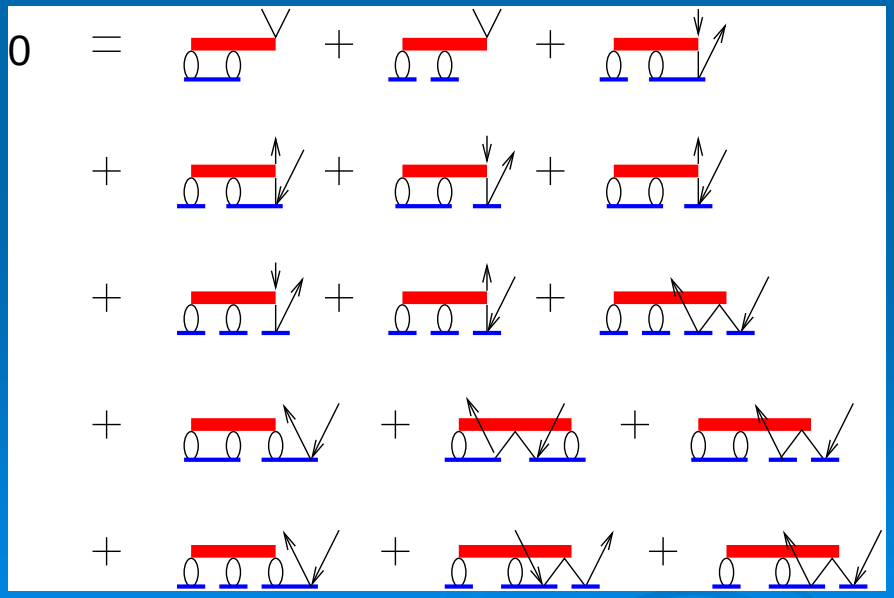
Coupled-cluster theory with 3NF

Why only CCSD and not CCSDT ?

Expect that CCSD approximation is valid for three-nucleon force: density-dependent 2-body terms dominant.

CCSD with TNF as expensive as CCSDT with NN force.





Energy and 1p-1h equation as examples.

Factorization of diagrams very useful!

1p-1h: 15 diagrams

2p-2h: 51 diagrams

1p-1h cluster amplitude in factorized form

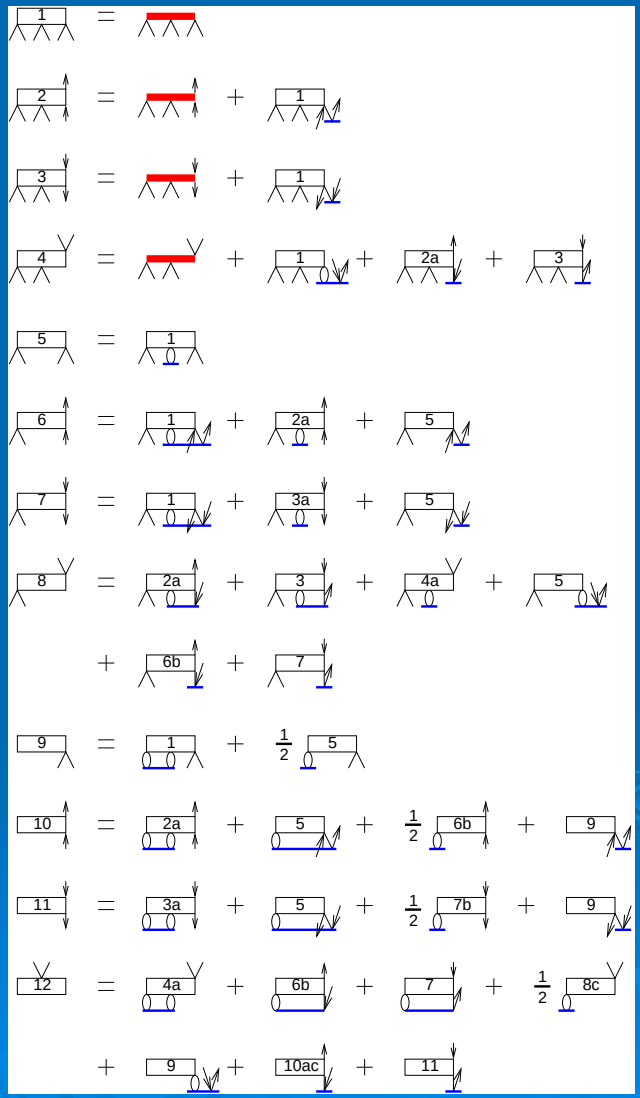
Correction to *1p-1h* equation:

$$
\begin{aligned}
0 \;=\; & \frac{1}{4}\sum_{ckdl}\langle kla||cdi\rangle t^{cd}_{kl} + \sum_{cke} I(6\mathrm{b})^{ka}_{ce} t^{ce}_{ki} \\
& - \sum_{ckm} I(7)^{km}_{ci} t^{ca}_{km} + \frac{1}{2}\sum_{kc} I(8\mathrm{c})^{ka}_{ci} t^{c}_{k} + \sum_{ck} I(9)^{k}_{c} t^{ca}_{ki} \\
& + \sum_{e} I(10\mathrm{ac})^{a}_{e} t^{e}_{i} - \sum_{m} I(11)^{m}_{i} t^{a}_{m}.
\end{aligned}
$$

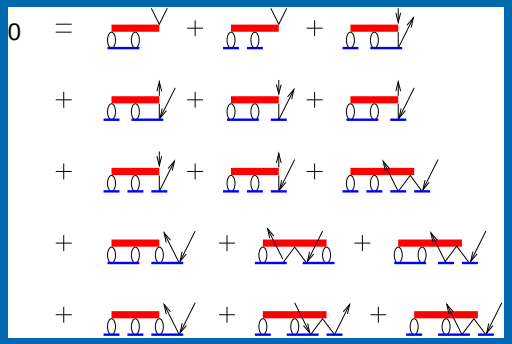
Intermediates:

$$
\begin{aligned}
I(5)^{km}_{ce} &= \frac{1}{4}\sum_{dl}\langle klm||cde\rangle t^{d}_{l}, \\
I(6\mathrm{b})^{ka}_{ce} &= \frac{1}{2}\sum_{dl}\langle kla||cde\rangle t^{d}_{l}, \\
I(7\mathrm{b})^{km}_{ci} &= \frac{1}{2}\sum_{dl}\langle klm||cdi\rangle t^{d}_{l}, \\
I(7)^{km}_{ci} &= \frac{1}{4}\sum_{lde}\langle klm||cde\rangle t^{de}_{li} + I(7\mathrm{b})^{km}_{ci} + 2\sum_{e} I(5)^{km}_{ce} t^{e}_{i}, \\
I(8\mathrm{c})^{ka}_{ci} &= \sum_{dl}\langle kla||cdi\rangle t^{d}_{l}, \\
I(9)^{k}_{c} &= \frac{1}{4}\sum_{delm}\langle klm||cde\rangle t^{de}_{lm} + 2\sum_{em} I(5)^{km}_{ce} t^{e}_{m}, \\
I(10\mathrm{ac})^{a}_{e} &= \frac{1}{4}\sum_{ckdl}\langle kla||cde\rangle t^{cd}_{kl} + \sum_{kc} I(6\mathrm{b})^{ka}_{ce} t^{c}_{k}, \\
I(11)^{m}_{i} &= \frac{1}{4}\sum_{ckdl}\langle klm||cdi\rangle t^{cd}_{kl} + 2\sum_{kce} I(5)^{km}_{ce} t^{ce}_{ki} \\
&\quad + \sum_{kc} I(7\mathrm{b})^{km}_{ci} t^{c}_{k} + \sum_{c} I(9)^{m}_{c} t^{c}_{i}.
\end{aligned}
$$

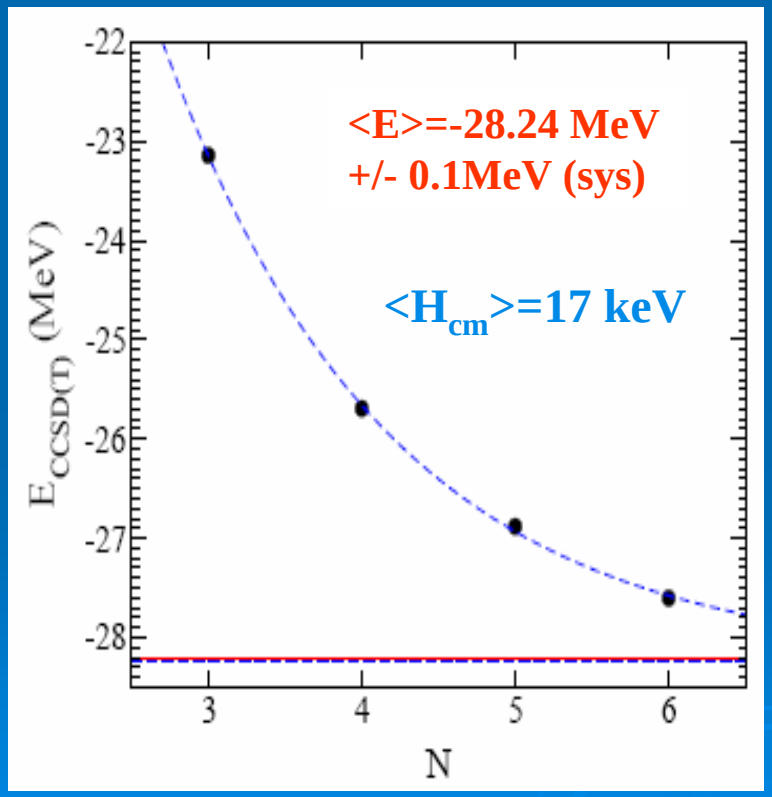
Factorized diagrams:

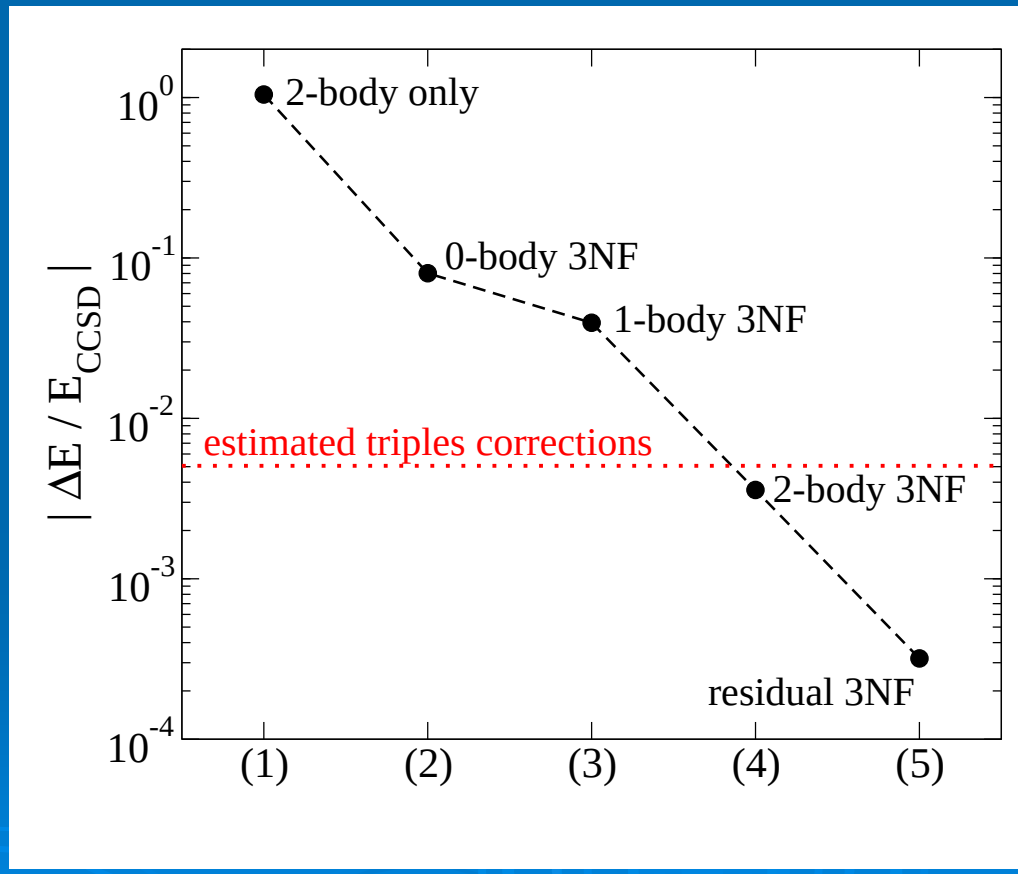


Benchmark: inclusion of full TNF in CCSD: F-Y comparisons in ^{4}He



Solution at CCSD and CCSD(T) levels involve roughly 67 more diagrams…..

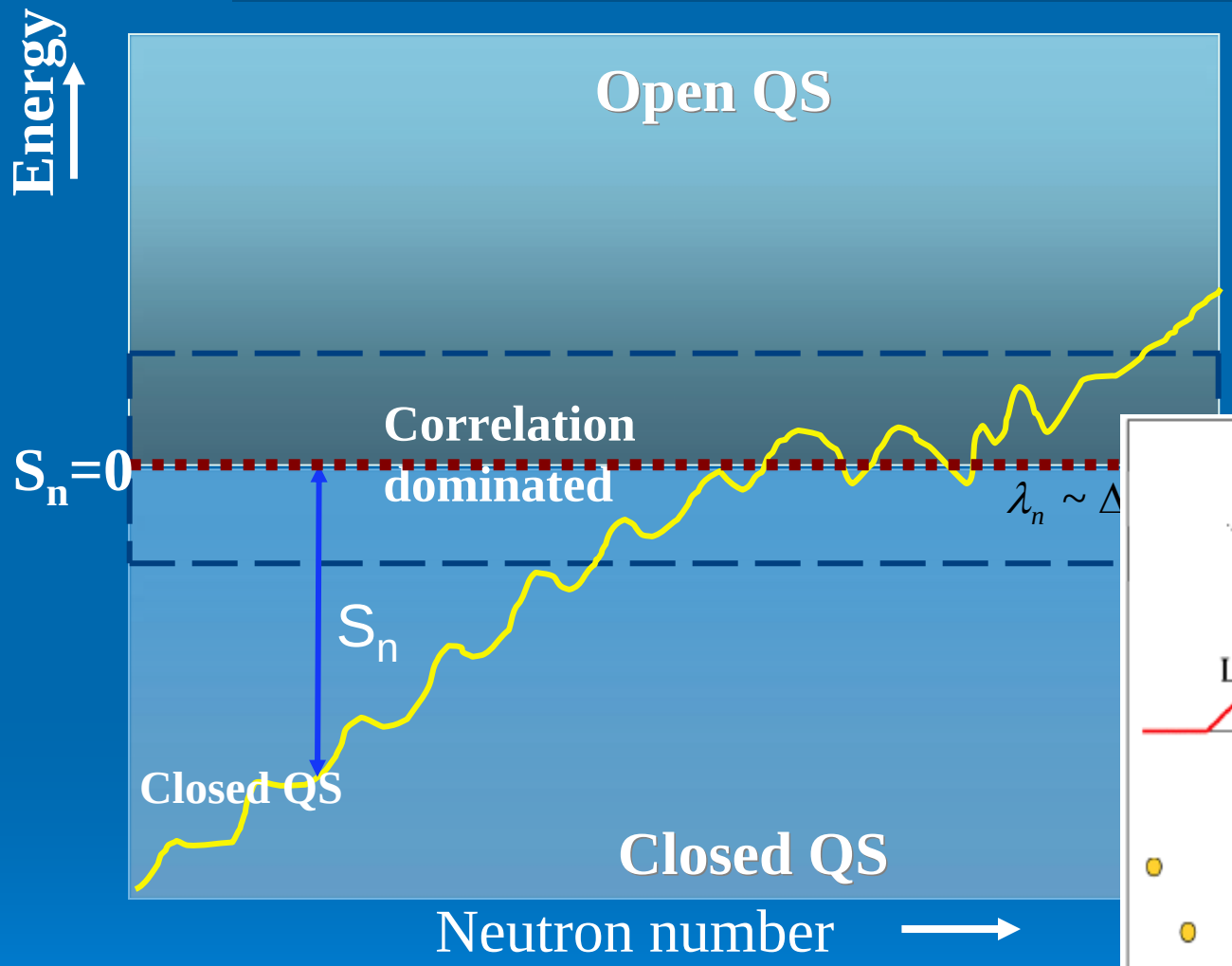




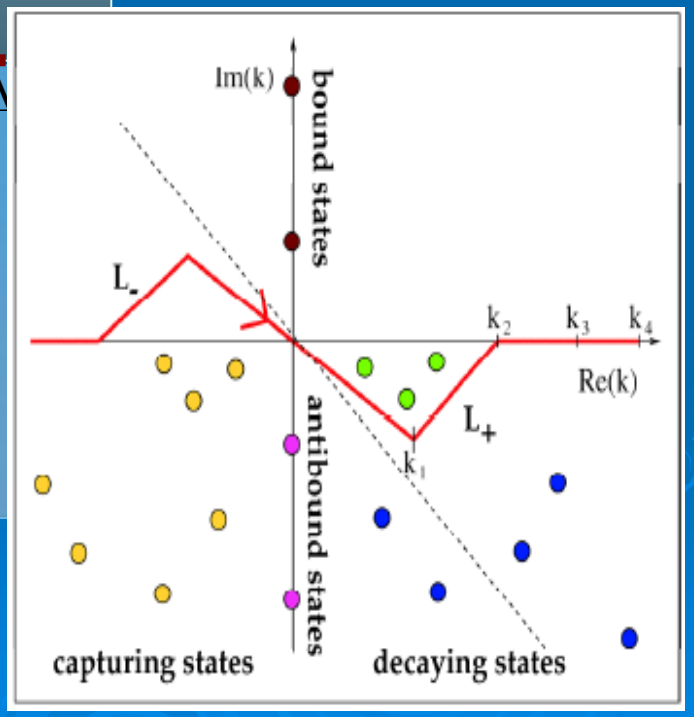
3-body force, or just its density dependent terms?

Hagen, Papenbrock, Dean, Schwenk, Nogga, Wloch, Piecuch
arXiv:0704.3439; PRC76, 034302 (2007)

Progress: Coupling of nuclear structure and reaction theory (microscopic treatment of open channels)



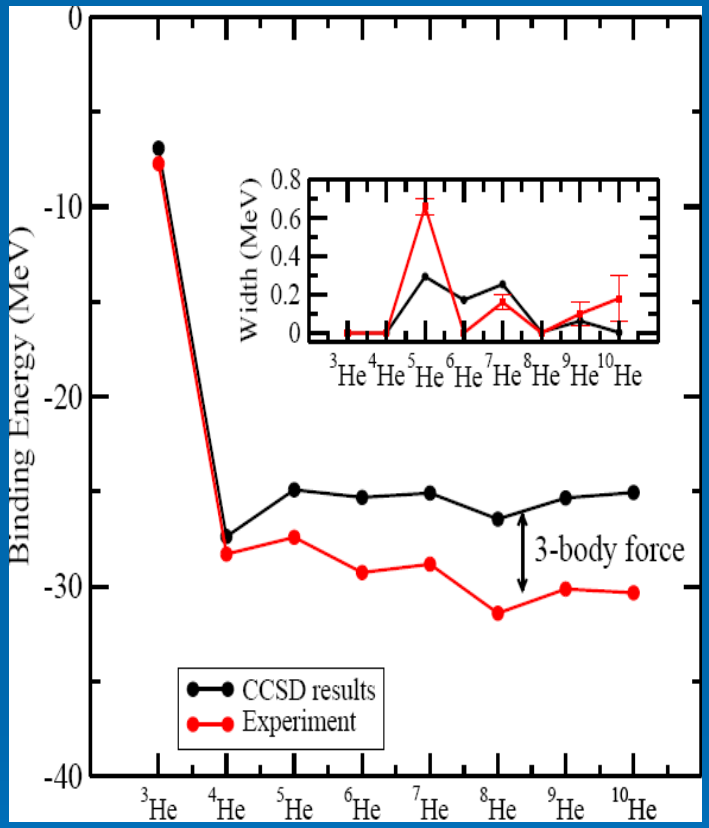
Important interdisciplinary aspects…(see recent ECT* workshop on subject)



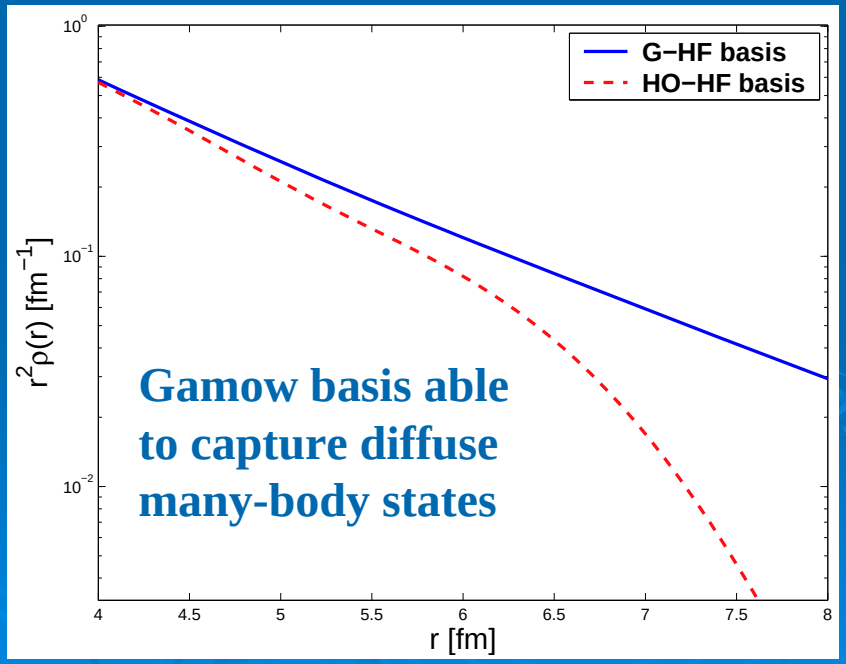
Introduction of
Continuum basis states (Gamow, Berggren)
→Continuum shell models
(many including: Michel, Rotureau, Volya, Ploszajczak, Liotta, Nazarewicz,…)

Progress: ab initio weakly bound and unbound nuclei

N^{3}LO V_{lowk} (λ=1.9 fm^{-1})



Single-particle basis includes bound, resonant, non-resonant continuum, and scattering states
ENORMOUS SPACES….almost 1k orbitals.
10^{22} many-body basis states in ^{10}He



^{6}He gs spin

Naïve filling	**=1.4**
CCSD	**=0.6**
CCSD(T)	**=0.6**
CCSDT-1,2,3	**=0.2**
CCSDT	**=0.04**

Which result is more accurate?

	^{16}O	^{40}Ca
CCSD(T)	-148.2	-502.9
NCSM (4p4h/3p3h)	-137.8	-461.8

PRL99, 095201 (2007)
"In this Letter, we have shown the first converged NCSM calculations for the ground state of 40Ca with two different realistic NN interactions."

(now -471.8 with some 4p-4h, so probably not really converged.

Truncated NCSM	Coupled-cluster approach
Model space restricted to np-nh excitations	Similarity transform with 2p-2h clusters
3p3h truncation level; 4p4h excitations only in small model space	CCSD + triples correction at large model space
Truncation not size extensive	***Size extensive***

The Description of Collective Motions in Terms of Many-Body Perturbation Theory

J. Hubbard

Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, Vol. 240, No. 1223. (Jul. 16, 1957), pp. 539-560.

3. The linked-cluster expansion

The linked-cluster expansion was first suggested by Brueckner (1955) and has been proved by Goldstone (1957) using the diagrammatic method of analysis of the perturbation series. The necessity for this result arises because the ordinary perturbation series for the energy, including that derived above, contain terms which diverge more strongly than N, the number of particles in the system, as $N \to \infty$. Such terms can have no physical significance and must cancel out against each other: we should, therefore, be able to eliminate them from the series, which is done in the linked-cluster expansion. This elimination will be carried out easily and naturally in this section using the diagrammatic analysis.

The unlinked terms diverge (or scale) more strongly than N. They are unphysical.

PHYSICAL REVIEW VOLUME 100, NUMBER 1 OCTOBER 1, 1955

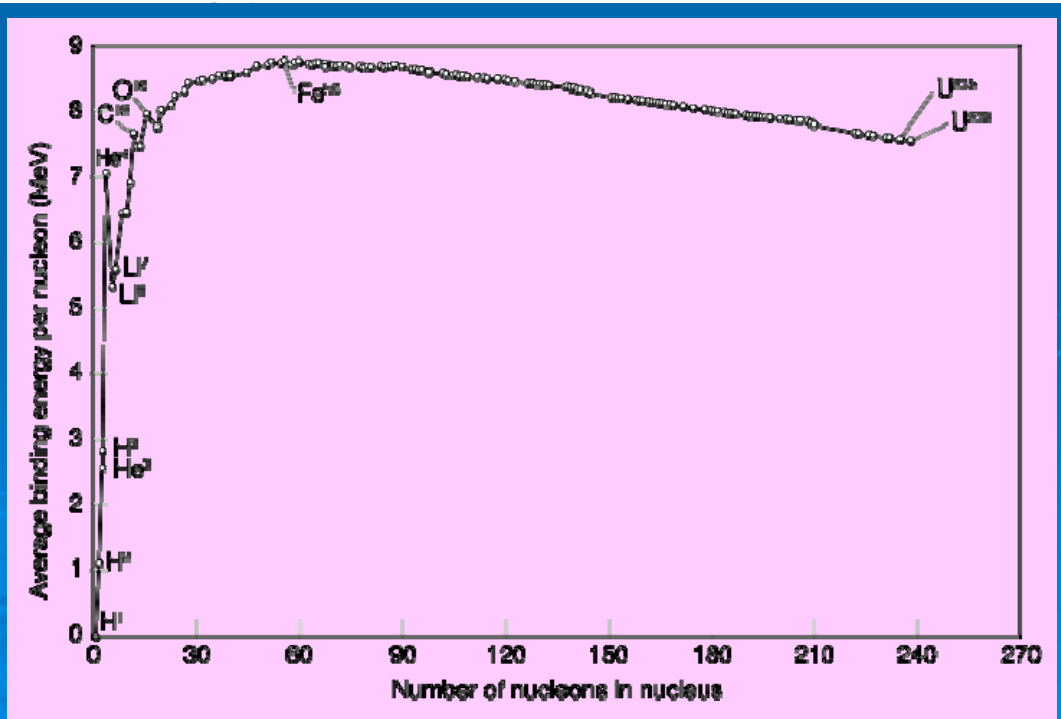
Many-Body Problem for Strongly Interacting Particles. II. Linked Cluster Expansion*

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

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.

Implication: BE ~ A
(approximately true for nuclei!!)

BE/A ~ -8 MeV



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}

Beginning of our involvement:

Dean & Hjorth-Jensen, 2004; Kowalski et al, 2004,

Wloch et al 2005, Gour et al 2006; Hagen et al 2007a, 2007b

Useful References

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

Bartlett, Ann. Rev. Phys. Chem. 32, 359 (1981); Bartlett, RMP (2007)

The beginning of coupled-cluster theory

1.C

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

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.

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** **"Mean field"**

Hamiltonian diagonalization (Barrett et al.)

- **Detailed spectroscopic information available**
- **Wave functions calculated and stored**
- **Dimension of problem increases dramatically with the number of active particles (combinatorial growth).**
- **Disconnected diagrams enter if truncated**

Relationship between shell model and CC amplitudes

$$B_1 = T_1$$

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

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

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

$$\ldots$$

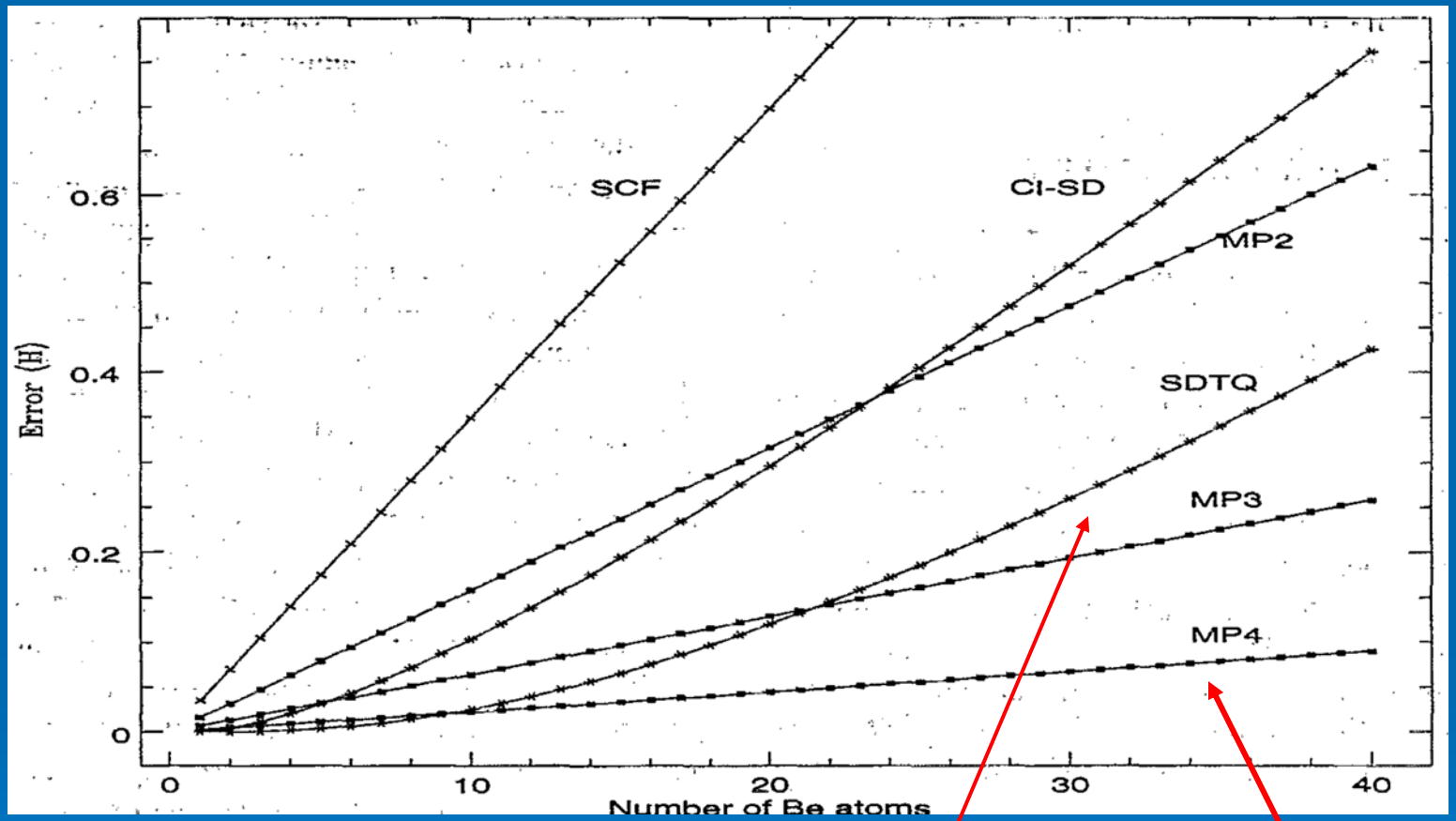
CCSD

CCSDT

“Disconnected quadruples”

“Connected quadruples”

Non linear scaling of the error in size-nonextensive methods

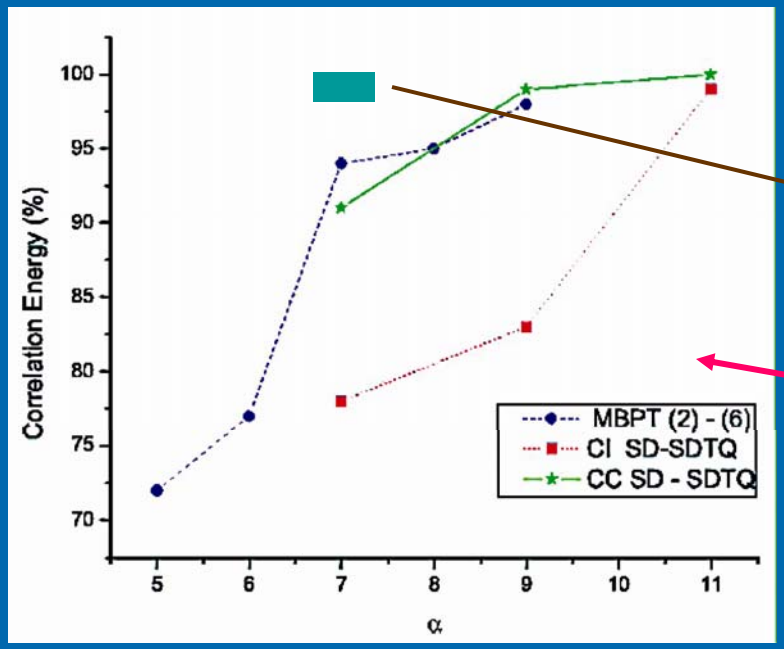


[Duch and Diercksen, J. Chem. Phys. 101 (1994) 3018]

Size extensive

Not size extensive

Comparisons with other many-body techniques

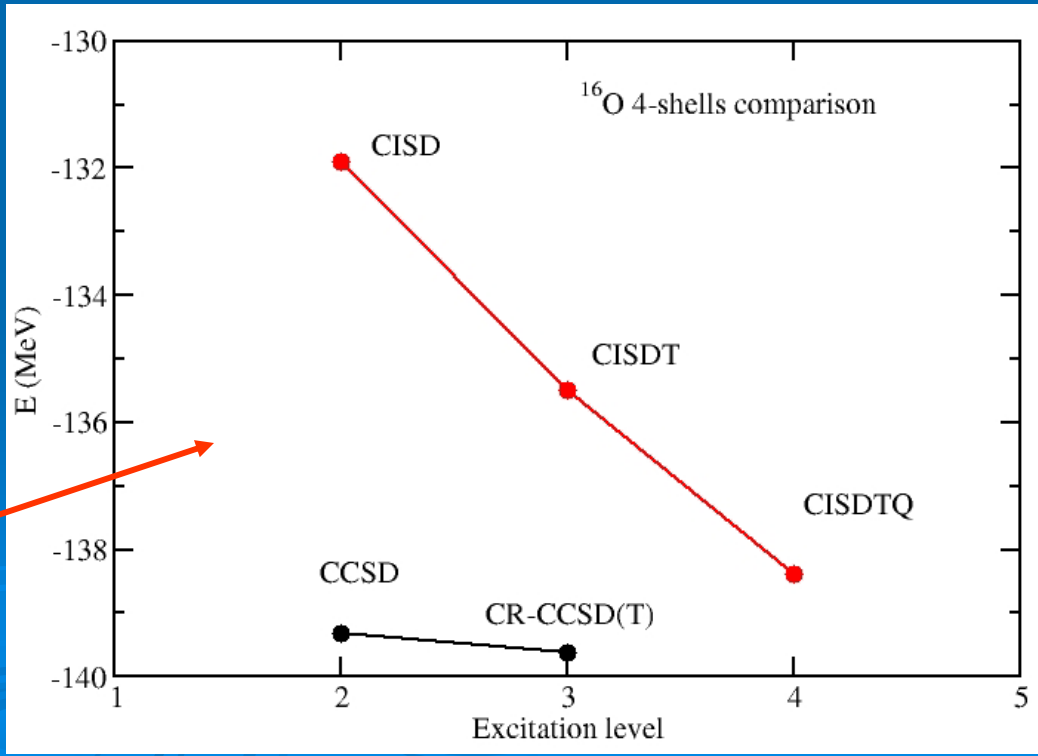


MBPT(4)	$O(n^3N^4)$
CCSD	$O(n^2N^4)N_{it}$
CCSD(T)	$O(n^2N^4)N_{it}+O(n^3N^4)$
CISDTQ	$O(n^4N^6)N_{it}$

Quantum chemistry example (Bartlett, RMP)

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

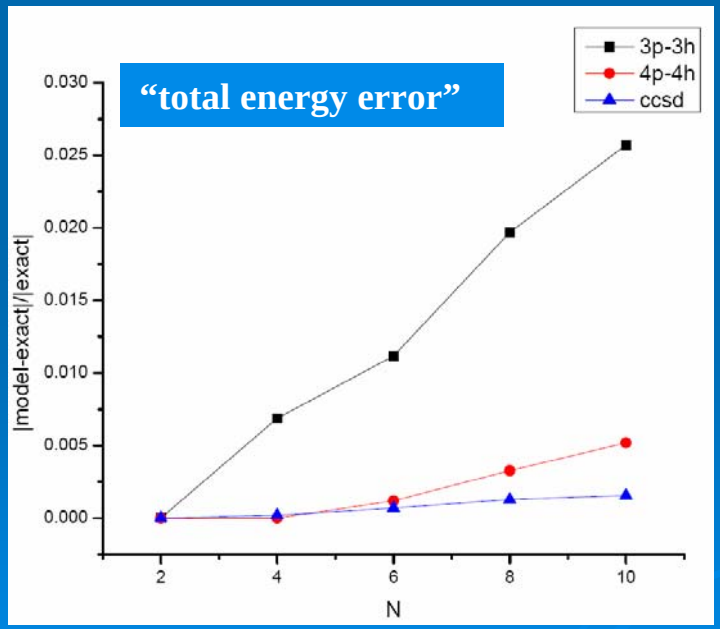
$$n^{\alpha_n} N^{\alpha_N} N_{it}^{\alpha_{it}}$$



Nuclear Example (Kowalski et al PRL 2004).

CC is size extensive; truncated CI is not

- s states (from n=0 to n=9).
- spe's starting at 0,2,4,6,8,10,..
- V = -1.0*pairing + 0.5*(-1+2*rand)
- Error in total energy (N=40)
  - 3p-3h 14.5% (5.8% N=16)
  - 4p-4h 4%
  - CCSD 0.85%



^{56}Ni fp-shell example (16 valence particles)
Exact is Caurier et al PRC 59, 2039 (1999)

	Etot	Ecorr	%error (Ecorr)	%error (Etot)
E0	-68.34	0.00		
2p-2h	-73.65	-5.31	47.77	6.18
3p-3h	-74.20	-5.86	42.30	5.48
4p-4h	-76.86	-8.52	16.14	2.09
5p-5h	-77.49	-9.15	9.94	1.29
Exact	-78.50	-10.16	0.00	0.00

Enormous errors in the correlation energy at 3p-3h

Indicates the near linear growth in error that one can expect in truncated CI calcs as one adds particles.

Truncated CI == disconnected diagrams
Known problem of CI in chemistry
See also excellent analysis in Horoi et al PRL (2007)
(CI vs CC analysis – same conclusion!)

Dean, et al….

Conclusions

- The quantum many-body problem is everywhere; its solution is one of the great intellectual challenges of our day
- Moving toward a PREDICTIVE capability in nuclei.
- Exciting physics probing drip-line properties
  - Life time predictions; diffuse nuclear systems; diffuse pairing; nucleosynthesis; bb-decay?
- What do we have now?
  - CCSD; CCSD(T)
  - EOM-CCSD L and R; one-body densities; A+/-1 EOM
  - V3-CCSD
  - Continuum CCSD
- What are the challenges?
  - Scale up (at 1000 processors now, need to go to 10k+)
  - Sparse vs dense matrix algorithm (speed vs memory)
  - Time dependence?
  - Multi reference
  - Calculating an effective interaction within CC approaches?
  - Physics: O-chain, Ni doubly magic; 11Li; Sn chain; light ion fusion….

What's the vision II?

- We need to work on hard problems.
- Benchmarking, while necessary, is not visionary.
- Can we move from post-diction to prediction?
  - What will it take?
  - Are we able to partner with other communities to do it?
  - Is our Hamiltonian good enough?
- Can we see through the maze of challenges to a solution?
- Are we too risk adverse?