CCM and the Nuclear Many-Body Problem

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Outline

1. Introduction
2. Coupled Cluster Method
   - Coupled Cluster Method: Basics
   - Coupled Cluster Method: Ideas
3. Our work
   - Past
   - Current
4. Outlook

Motivation

- CCM$\leftrightarrow$Manchester
- Revival of CCM in NP (David Dean/Morten Hjorth-Jensen/Piotr Piecuch)
- Earlier Michaila and Heisenberg
- Did some work on it ourselves: PDRA left after a year.
- Rethinking our approach
- Old work by Kümmel, Lührmann and Zabolitsky
- Is it reliable?
- Apologies, no answer yet :-).

CCM

Basics

- Efficient parametrisation of wave function, $|\Psi\rangle = e^S|\Phi_0\rangle$.
- The operator S is creation only, $S = \sum_I s_I C_I^\dagger$
- Very natural in configuration space!
- Underlying bi-variational principle.

Problems

- Fails for hard-core forces
- Converges slowly even for “modern” forces.
- Requires G-matrix + CCM

One slide CCM

- $S = \sum_I s_I C_I^\dagger$
- $\tilde{S} = \sum \tilde{s}_I C_I$
- $C_I|\Phi_0\rangle = 0$
- $O(\{s\},\{\tilde{s}\}) = \langle\Phi_0|\tilde{S}e^{-S}\hat{O}e^{S}|\Phi_0\rangle$
- $\delta H(\{s\},\{\tilde{s}\}) = 0$ gives s_I^{eq}, $\tilde{s}_I^{eq}$.
- Note $E = \langle\Phi_0|e^{-S}He^{S}|\Phi_0\rangle$, $0 = \langle\Phi_0|C_I e^{-S}He^{S}|\Phi_0\rangle$.
- TDV $\delta(H - i\partial_t)(\{s\},\{\tilde{s}\}) = 0$ gives excited states.
- Also (for “free”) Helmann-Feynman theorem and canonical variables.

CCM as in Quantum Chemistry

Why popular in QChem?

- Deal accurately with weak residual force.
- CCM equations are “easy”:
- $\langle \Phi | C_I e^{-S} H e^{S} | \Phi \rangle$ is a finite polynomial in s_I; can be evaluated using matrix algebra.
- Diagrammatics; excited states; links to resummed PT.
- Very high accuracy required.
- Implemented in “foolproof” codes such as Gaussian and Gamess.
- It works...

Mihaila and Heisenberg

PRC **61** 054309; PRL **84** 1403; PRC **60** 054303; PRC **59** 1440

- Use bare nuclear force (Argonne V18) with quantum chemistry approach.

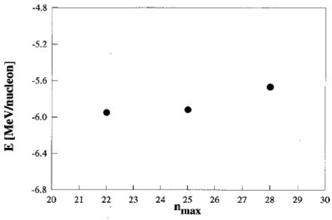


FIG. 2. Dependence of the binding energy on the n_{max} cutoff for $l_{\mathrm{max}}=11$.

- Has it converged? Probably not! Needs $\geq 100\hbar\omega$...

Dean/Hjorth-Jensen/Piecuch/...

EPJA **25** 485; JPG **31** S1291; PRL **94** 212501; NPA **742** 299C; PRC **69** 054320; PRL **92** 132501

- Use G matrix or LS to smooth the nuclear force, and be able to work in a small (largish $\simeq 10\hbar\omega$) model space

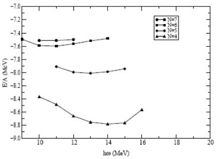


Figure 4. Dependence of the ground-state energy of ^{16}O on $\hbar\omega$ as a function of increasing model space.

- Good convergence? Looks like it!
- Problem: need for effective operators.

Shell model?

Too many reference to include; search for Navratil, Barrett, ...

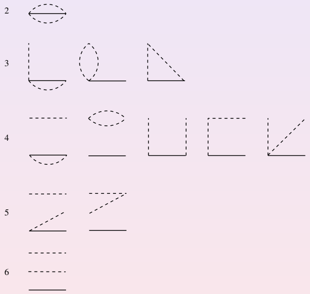
- The work by Barrett/.... on the no-core shell model has great similarities.
- Removal of CM excitations based on reproduction of CM.
- In complete spaces can decompose as $\Phi(x_1, .., x_n) = \Phi(\{x_{ij}\})\phi_n(R)$. $n \neq 0$: Rather inefficient, and main limiting factor.
- Effective interaction theory hard to understand.
- Lee Suzuki: Yes and no!
- Still, great overlap with CCM in LS method

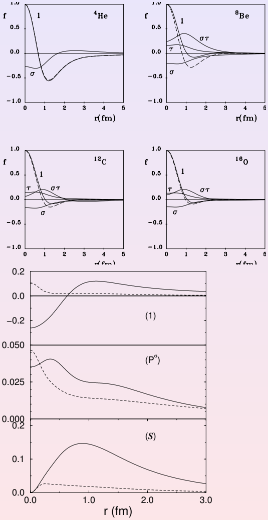
Coordinate space

- We have been following a different route, directly using coordinate space.
- See PLB **480** 61; JPG **25** 945; NPA **643** 243; NPA **609** 218 and older references.
- Inspired by CCM–in various guises.
- Technology uses
  - Monte-Carlo integration
  - Gaussian seminals

TICI2

- Linearise a translationally invariant form of CCM
- TICI2$\longrightarrow$ translates neatly into coordinate space
- $$\langle\{r\}|\Phi\rangle = (1+\sum_k\sum_{i<j} f_k(r_{ij})O^k)$$
  $$\langle\{r\}|\Phi_{ho}\rangle$$
- Lacks full screening.
- Correlates nicely for V4

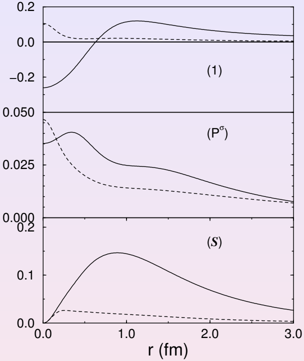




Interaction	Nucleus	$-E$	α
Gogny/V6	^{4}He	27.36	0.70
	^{8}Be	40.79	0.58
	^{12}C	73.37	0.61
	^{16}O	128.68	0.64
SSC/V6	^{4}He	24.12	0.68
	^{8}Be	25.98	0.54
	^{12}C	39.64	0.54
	^{16}O	63.55	0.55
AV14/V6	^{4}He	14.77	0.59
	^{8}Be	9.26	0.43
	^{12}C	10.50	0.41
	^{16}O	14.97	0.40
AV18/V6	^{4}He	15.40	0.61
	^{8}Be	11.13	0.47
	^{12}C	14.96	0.46
	^{16}O	23.76	0.46

J-TICI2

- Jastrow correlations used for hard-core forces $\Phi = \prod_{i<j} g(r_{ij})\Phi_0$.
- Most easily done in coordinate space
- Hybrid method: Jastrow+TICI2 $\Phi = (1 + \sum_k \sum_{ij} f^k(r_{ij})O^k) \prod_{i<j} g(r_{ij})\Phi_0$.
- has full screening!
- but is much more involved calculation (can't go beyond ^{16}O)



	TICI2	J-TICI2	VMC	GFMC
Gogny/V6	27.36	27.58	27.71 ± 0.06	
SSC/V6	24.12	26.74	29.20 ± 0.12	
AV14/V6	14.77	20.37	23.24 ± 0.08	24.79 ± 0.20
AV18/V6	15.40	21.08	24.80 ± 0.09	
Reid-V6	5.67	22.70	27.82 ± 0.12	28.30 ± 0.12

TICC2

- Can we do CCM directly in coordinate space.
- In some sense, but orthogonality of functions is different from orthogonality in configuration space.
- Works for some QFTs.
- Wavefunction $\exp(\sum_{i<j} f_k(r_{ij} O_k)|\Phi(r)\rangle$
- Results for central f ($O = 1$) published
- Have some results for more general f.
- Gets expensive!

Back to the past...

Look at Kümmel *et al* (Phys Rep, 1978)

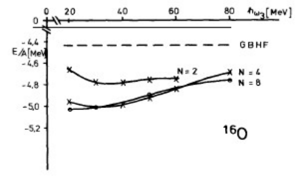


Fig. 3. Same as fig. 2, for ^{16}O.

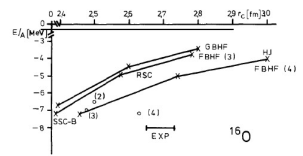


Fig. 5. Same as fig. 4 for ^{16}O.

CCM and hard core truncations

- The technique used in these calculations is a mixture between configuration space and coordinate space.
- Designed originally for hardcore forces.
- You pay a price...
- But even in 1976 claimed full convergence...
- Can we trust that?

Elements of the technology

- Diagrammatically, CCM contains terms where the potential is not fully screened.
- Such terms are infinite for hard core forces
- They are removed by other terms that are equally infinite.
- This suggests large cancellations for strong-core forces!
- If we neglect those terms that are infinite at certain order of truncation, we still have a systematic expansion.
- It is not trivial to define such terms.
- Most naturally done in terms of subsystem amplitudes.

Elements of the technology II

- The idea is to express e.g. the two body amplitudes $\chi^{\Lambda}_{n_1 l_1, n_2 l_2}$ as $\chi^{\Lambda}_{NL;l}(r_{12})$.
- Must start from Harm osc. reference state.
- This transformation requires large numbers of Brody-Moshinsky brackets.
- Truncate severely on CM *NL* (correct for NM).
- potential acts as a (non-local) operator on r_{12}
- Allows for momentum, but not for energy dependence.
- Did CM truncation converge?
- How can we check this?
- included 3 and some 4-body terms–convergence?

Requirements

- Develop a code.
- Don't worry about efficiency yet!
- Work with local forces first
- Be able to check convergence
- Don't need effective operators!
- Expect first version to be ready in a couple of months.

Efficiency

- I don’t understand how they could do these calculations in 3 minutes in 1976
- Will be glad if we can do them that quickly today!
- Not the main goal obviously.
- Don’t worry about CM–all techniques used by Navratil are possible.
- Can we really deal with non-localities as well as I think?
- Don’t we require matrix representation of the force?

Other potential improvements

Hard-core CCM is one truncation within a class. Alternatively, we could use the “super subN” calculations, where we do not set unknown terms to zero, but make a smart approximation for those terms, e.g., one that satisfies hard core BCs.
Much more difficult, but potentially promising.

Outlook

- We are working on a program to do this again!
- Test to destruction.
- But work directly from nuclear force, no intermediate (Lee-Suzuki, ...) technology.
- Goal to produce an “easy to use” code.
- Thanks to Ray Bishop, Rafa Guardiola, Jesus Navarro, Toni Puente, Inyaki Moliner, Michaela Portesi, Sarmistha Banik, Massi Alvioli.