The Coupled Cluster Method and Nuclear Physics

Niels Walet

School of Physics and Astronomy
University of Manchester

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Outline

1. Introduction
2. The Nuclear Force
   - Symmetries
   - Phase-Shift Equivalence
   - The complexity of modern forces
   - The need for three-body forces
3. Many Body techniques
   - Model space reductions
   - Many body techniques
4. Coupled Cluster Method
   - Basics
   - Coupled Cluster Method: Ideas
   - Valencia/Manchester
   - Hard-Core Truncations
5. Summary

Outline

Introduction

- Talks falls a apart in a few pieces
- Will start with a discussion of the nuclear force
- Continue on to nuclear many-body physics
- Meant to be introductory
- Stop me if I am unclear, or speed me up if I am belabouring the obvious

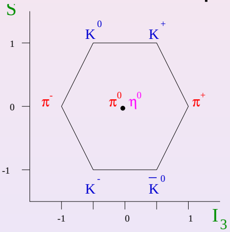
The Nuclear Force

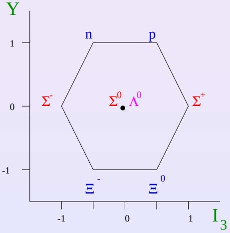
- Some of what I discuss is open to interpretation–everything is my own view!
- I am a sceptic as regards the use of $V_{\text{low }k}$: I may be in a minority!
- I borrowed liberally from talks by Ruprecht Machleidt, Gaute Hagen, and others.
- There is a beautiful synthesis in the work of Suzuki and Okamoto, which has had a strong influence on my thinking.
- There is a long history, and much recent activity.
- Undoubtedly I will only scratch the surface.

Neutrons and Protons, Quarks, etc.

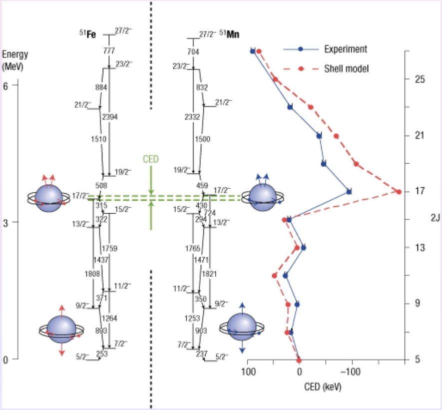
- Nucleons (neutrons, protons, . . .) and mesons (pions, rho mesons, ...) are not fundamental particles!
- Quantum-ChromoDynamics (QCD) is the fundamental theory, but not very useful at low energies due to confinement.
- Work with nucleons and mesons anyway.
- Isospin symmetry: Neutrons and protons two partners of an isospin doublet; pions triplet.
- Different isospin projection: Different charge.
- Isospin broken by Coulomb force, as well as explicitly (proton mass differs from neutron mass).

Fundamental multiplets





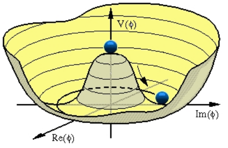
Even in finite nuclei



D. D. Warner, M. A. Bentley and P. Van Isacker

Nature Physics ***2****, 311 - 318 (2006)*

Chiral Symmetry

- If quarks are massless, there is a chiral symmetry (left-handed quarks behave the same as right-handed ones)
- This symmetry is spontaneously broken $SU_L(2) \times SU_R(2) \to SU_V(2) \times SU_A(2) \to SU_V(2)$.
- 

  original at http://www.fys.uio.no/ farido/higgs-mecanisme.gif
- Goldstone boson: pion
- Realised approximately in nature:
  - u and d quarks are almost massless
  - $m_\pi \approx 138\ \text{MeV}/c^2 \ll$ smaller than any other scale.
  - Long-range physics: pions. Cf. Coulomb force.

Channel description

- Nucleon (p, p and n, p) scattering analysed in partial waves ("channels")
- Channels ${}^{2S+1}L_T$ (e.g., ${}^3S_0$), $L+S+T = \text{odd}$
- Channels couple: tensor force (spin 2 tensor times orbital angular momentum tensor)
- Changes L by up to 0 or 2 units
- Central part attractive, but tensor force binds deuteron. ${}^3S_0$ and ${}^3D_0$ coupled channels ($J=1, T=0$)
- Resonance in ${}^1S_1$ channel ($J=0, T=1$)
- Excitation of internal degrees of freedom around 300 MeV, Δ is a broad $N\pi$ resonance peaked at 1232 MeV.

Determination of forces

- Phase-shift databases: gather all experimental data, and do phase-shift analysis on them
- Historically 2 (Nijmegen and Virginia); I don't know current status
- Fit a potential to phase shifts and deuteron binding energy.
- To fit a potential we need a model
- Most historical models based on meson exchanges.
- Field theoretically an OK idea, but requires substantial phenomenology for short range.
- There is a great freedom in choice of short range behaviour.

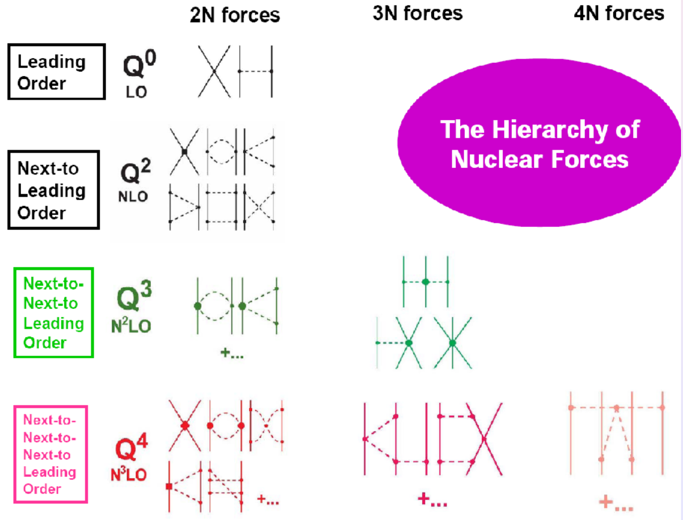
Determination of forces 2

- Full MEC is quantum field theory $\rightarrow$ we get highly non-local potentials
- Some techniques (e.g., GFMC) require a local potential.
- Many different choices.
  - Reid (local, infinite core),
  - Argonne family (local, strong core)
  - Bonn: start from mesons, leads to energy dependent potential
  - Idaho: Start from modern ideas, non-local.
- Fit quality $\chi^2/\mathrm{DOF} \approx 1$.

Heavy Baryon Chiral Perturbation Theory

- This is firmly rooted in Weinberg's ideas on chiral (pion-nucleon) Lagrangians
- The key notion is that if we only knew broken chiral symmetry, we can set up a non-renormalizble effective field theory in the relevant degrees of freedom.
- There is a power-counting, in momentum transfers and pion masses.
- Systematic expansion, but at each order in quantum loops we need to remove additional infinities.
- Need for counter terms: contact (zero-range) terms.
- Such a model induces many-body forces.
- Any physical model that excludes fundamental nucleonic excitations (e.g., Δ's) has many-body forces.

Chiral forces



application

- Contact forces troublesome (back to hard core)
- Soften the hard-core in a phenomenological way
- Cut-off on short-range pion exchange
- Quite effective!

χ^2/datum for the reproduction of the 1999 np database

Energy range (MeV)	# of data	Idaho N^3LO (500–600)	Bochum/Juelich N^3LO (600/700–450/500)	Argonne V18
0–100	1058	1.0–1.1	1.0–1.1	0.95
100–190	501	1.1–1.2	1.3–1.8	1.10
190–290	843	1.2–1.4	2.8–20.0	1.11
0–290	2402	1.1–1.3	1.7–7.9	1.04

Phase-shift equivalence, 3-body forces

- There is a problem that many extremely different potentials give equivalent results for phase shifts and deuteron binding energy.
- Nuclear binding is linked to the off-shell behaviour of the potentials: poorly determined by phase shifts.
- Almost all require 3-body forces to even do $A = 3$ right (A_y puzzle)
- One can show that there are ways to trade-off off-shell behaviour vs. 3-body forces [Birse et al]
- But much information in nuclear forces above $E_{CM} = 300$ MeV is irrelevant anyway.
- Renormalise: Full T matrix [Birse et al] or "half on-shell".

$V_{\text{low }k}$

- see Bogner, Schwenk, Kuo and Brown nucl-th/0111042
- Approach to derive phase shift equivalent potentials
- Lippmann-Schwinger in partial waves

$$T(k',k,\omega) = V_{NN}(k,k') + \frac{2}{\pi}\mathscr{P}\int_0^\infty V_{NN}(k,p)\frac{p^2dp}{\omega - p^2}T(p,k,\omega).$$

- Define P and Q projectors, $P+Q=1$, $PQ=0$.
- $P = \dfrac{2}{\pi}\displaystyle\int_0^\Lambda \langle k|\,k^2dk\,|k\rangle.$
- No potential such that

$$T(k',k,\omega) = V_{NN}^{\Lambda}(k,k') + \frac{2}{\pi}\mathscr{P}\int_0^{\Lambda} V_{NN}^{\Lambda}(k,p)\frac{p^2dp}{\omega - p^2}T(p,k,\omega).$$

- But can use “half on shell”, for $\omega = k^2$
- Captures known many-body techniques (for two-body problem).

example

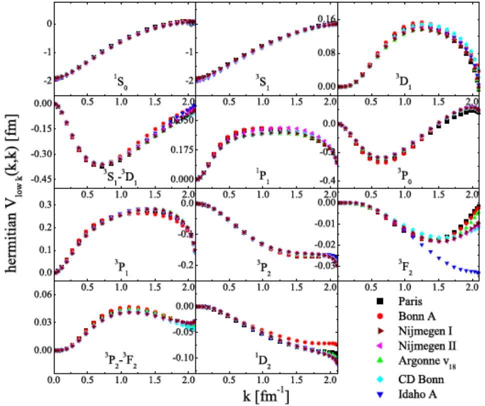


Fig. A.1. Diagonal momentum-space matrix elements of the hermitian $\overline{V}_{\text{low k}}$ obtained from the different potential models for a cutoff $\Lambda = 2.1\,\text{fm}^{-1}$. Results are shown for the partial waves $J \leqslant 4$.

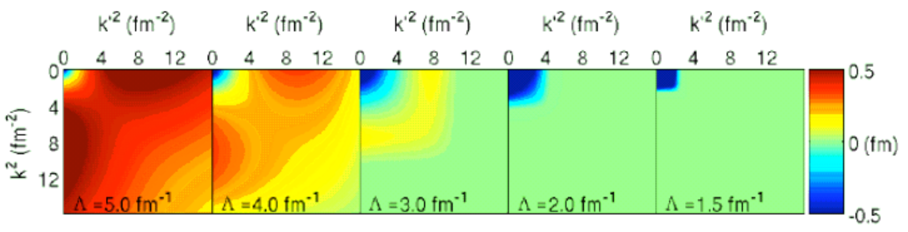
Bogner et al, Phys. Rep. ***386*** *(2003), 1-27*

Argonne

- The Argonne potential (AV18) Contains 18 different operators, 14 isospin symmetric.
- There are 7 $T = 0$ and 7 $T = 1$.
- Each of these are 2 central operators, the two-body spin-orbit one, the tensor force and 3 higher order terms.
- Repulsive core of about 1 GeV.
- Usually applied with Urbana 3-body forces (with parameters linked to few nucleonic systems and nuclear matter).

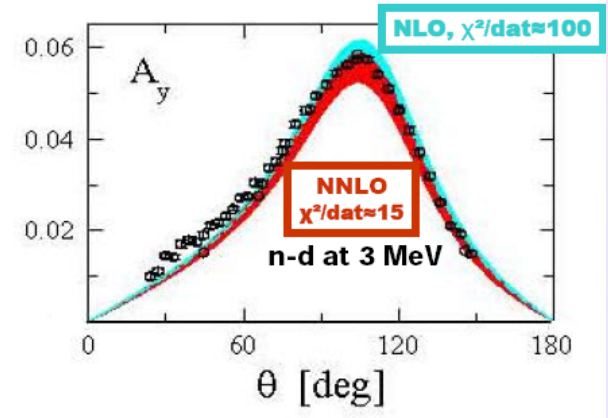
$V_{\mathrm{low}\ k}$

Sketch $V_{\mathrm{low}\ k}$ vs Λ



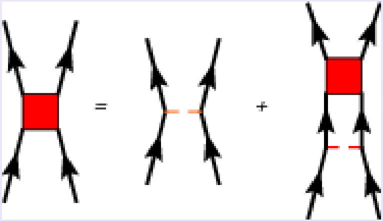
Polarised scattering for $A = 3$

Polarised neutron scattering of deuterium is a known problem for two body forces; even for NNLO 3-body forces not gone.



Ladder sums

- We can't apply even standard mean field theory for finite nuclei.
- One solution is to resum an infinite set of diagrams.
- The standard choice is the Bethe-Galitskii *G*-matrix, the sum of all ladder diagrams
- Gives the Brueckner-Bethe Hartree-Fock theory



Lee-Suzuki et al

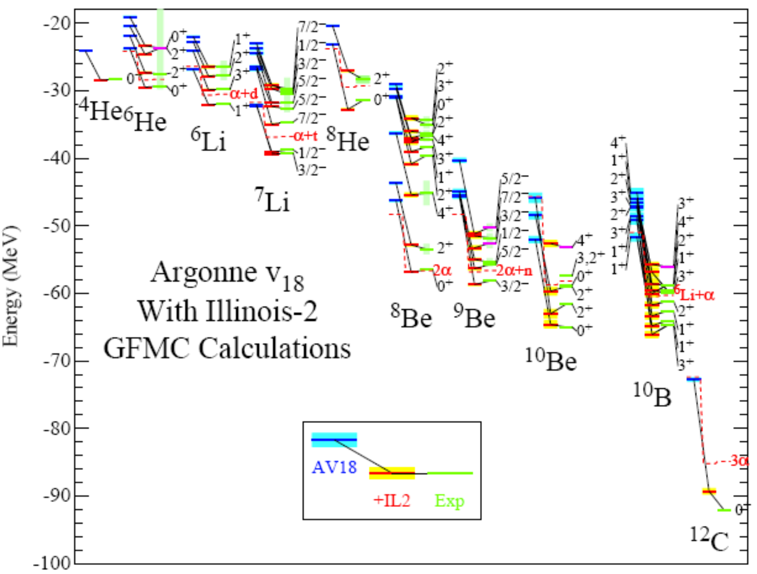
- Similar to $V_{\text{low }k}$, but in medium.
- All of the Feshbach-Löwdin form
- Lee-Suzuki is the original method to calculate an interaction adapted to a model space.
- Closely linked to the Unitary Model Operator Approach of Suzuki and Okamoto.
- Alternative is the Unitary Correlation Operator Method of Roth et al.
- Big weakness: Calculation of effective operators is required.
- But!!! that supposes we know the observables that go with a given interaction

Few Body

There are specialised techniques for few-body systems

- 3-body: Faddeev equations
- 4-body: Faddeev-Yakubovsky equations
- Hyperspherical Harmonics calculations ($A \leq 10$)
- Stochastic Variational Techniques
- Green's function Monte Carlo (local forces!)
- All agree for ^{4}He with AV8' force.

GFMC


Energy (MeV)
Argonne v18
With Illinois-2
GFMC Calculations
4He
6He
6Li
7Li
8He
8Be
9Be
10Be
10B
12C
α+d
α+t
2α
2α+n
6Li+α
3α
AV18
+IL2
Exp

Shell Model=CI

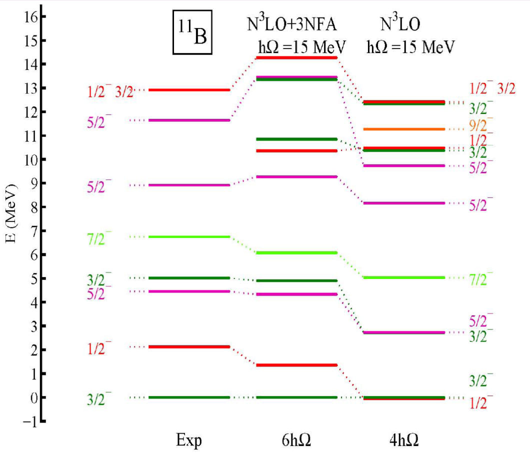
- Shell model has a long history in nuclear physics
- Goes back to Mayer and Jenssen in the late 40s
- Shell structure like harmonic oscillator one
- Caused by the average effect of other nucleons
- Often work in a few shells, and perform full CI
- Breaks translational invariance.
- Requires a fit of the interaction
- In heavier nuclei pairing near Fermi surface important
- Nuclei are superfluids!...

Translationally invariant Shell model

Too many references to include; search for Navratil, Barrett, Vary, ...

- The work on the no-core shell model has had great success.
- Removal of CoM excitations based on complete Harm oscillator space for CoM.
- In complete spaces of Harmonic oscillator states decompose $\Phi(x_1,..,x_n) = \Phi(\{x_{ij}\})\phi_n(R)$. $n \neq 0$:
- Rather inefficient due to excitation of CoM
- Effective interaction theory required
- Many different techniques.
- Mature technology.

Shell model with NNLO and N3LO



CCM

Basics

- Efficient parametrisation of wave function, in terms of unlinked excitations, $|\Psi\rangle = e^S|\Phi_0\rangle$ (Bocchum notation)
- 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

- $S = \sum_I s_I C_I^\dagger$
- $\tilde{S} = \sum \tilde{s}_I C_I$
- $C_I|\Phi_0\rangle = 0$
- $O(\{s\},\{\tilde{s}\}) = \langle\Phi_0|(1+\tilde{S})e^{-S}\hat{O}e^{S}|\Phi_0\rangle$
- $\delta H(\{s\},\{\tilde{s}\}) = 0$ 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 (EOMCCM).
- Also (for “free”) Helmann-Feynman theorem and canonical variables.
- Usual assumption $\langle\Phi_0|C_I C_J^\dagger|\Phi_0\rangle = \delta_{IJ}$.

CCM as in Quantum Chemistry

Why popular in QChem?

- Deals 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...

History

- Coester and Kümmel, 1950s
- Bocchum group, 1970s
- Valencia/Manchester group; 80s and 90s
- Mihaila/Heisenberg: 90s
- ORNL/Oslo/MSU: current
- Manchester: current

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.

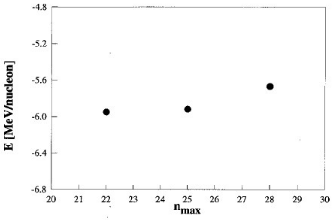


FIG. 2. Dependence of the binding energy on the n_{max} cutoff for $l_{max} = 11$.

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

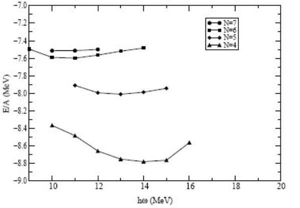
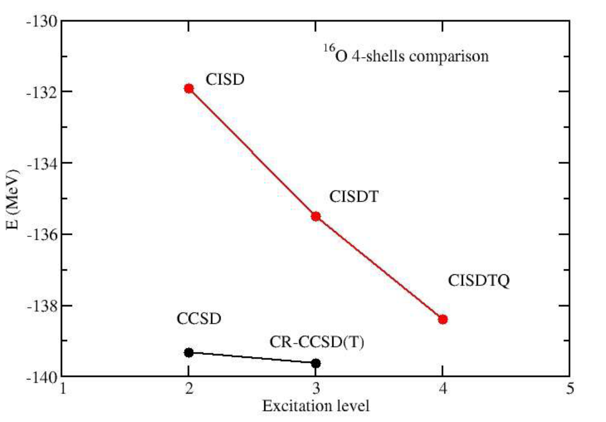


Figure 4. Dependence of the ground-state energy of ^{16}O on $\hbar\omega$ as a function of increasing model space.

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

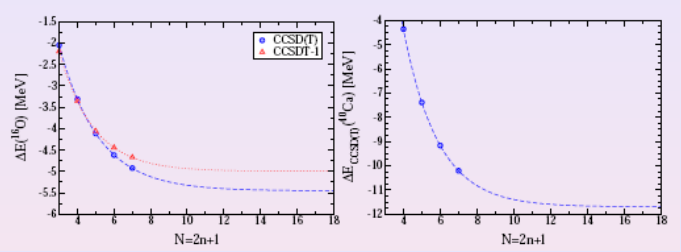
Wins over shell model?



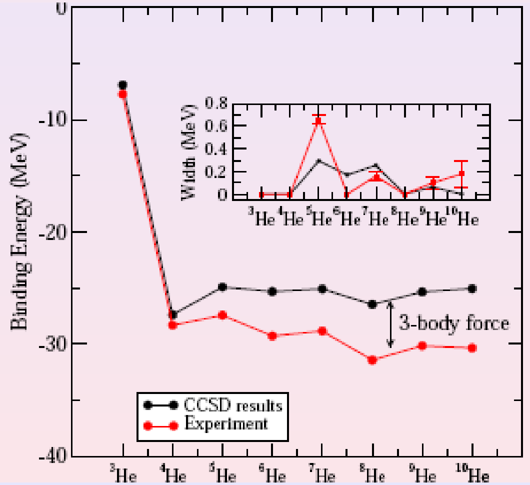
Kowalski, PRL 92 (2004) 132501.

+Hagen: using $V_{\text{low }k}$

- More recently have started using $V_{\text{low }k}$.
- Is soft enough to directly go into calculations
- How about cut-off on wave functions?
- Effective operators?
- J coupling rather than m scheme.



+Hagen: using complex scaling



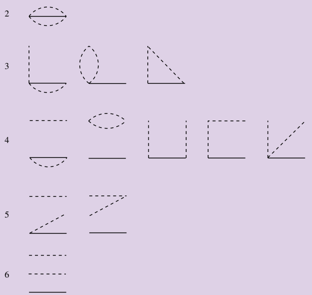
Coordinate space

- 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

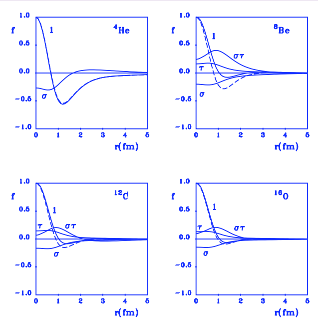
TICI2

- Linearise a translationally invariant form of CCM
- TICI2$\rightarrow$ 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

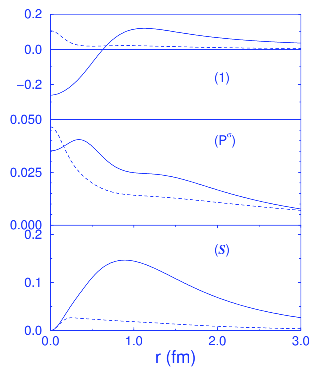
diagrams



V4



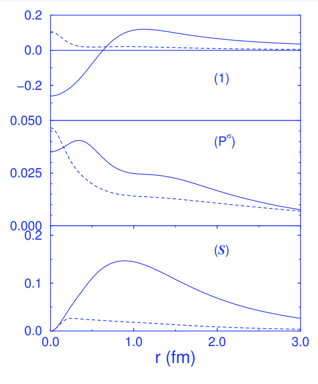
V6



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
- Most easily done in coordinate space
- Hybrid method: Jastrow+TICI2
- 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)

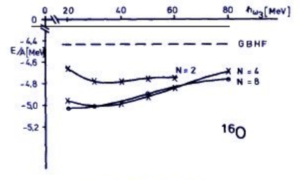


Fig. 3. Same as fig. 2, for ^{16}O.

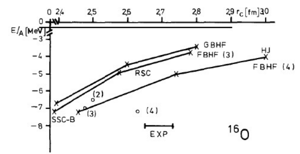


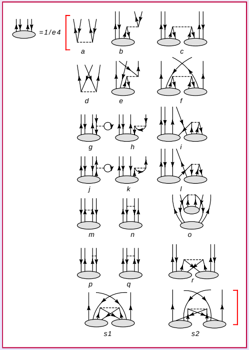
Fig. 5. Same as fig. 4 for ^{16}O.

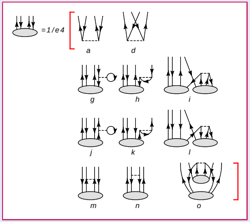
CCM and hard core truncations

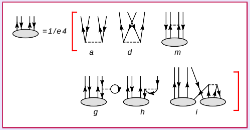
- The technique used in these calculations is a mixture between configuration space and coordinate space.
- Designed originally for hardcore forces.
- You pay a price...
- But even in 1976 claimed full convergence...
- Can we trust that?

Hard-core truncations

Look at nuclear matter (SUB2=doubles); full Goldstone diagrams (Bishop and Lührmann), and remove “unscreened terms”

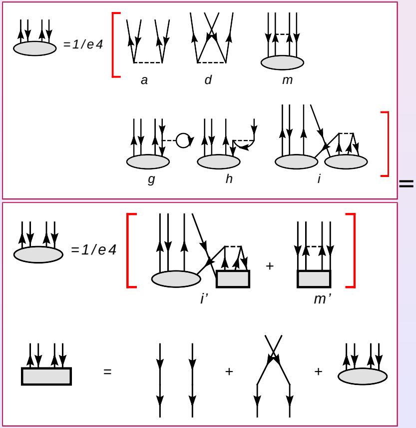




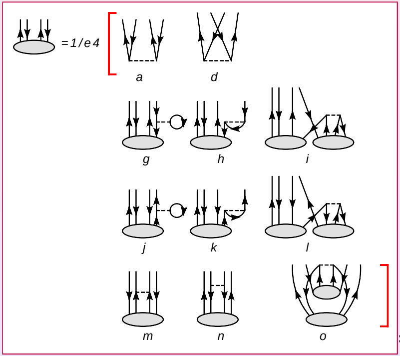


Bethe Goldstone

pp ladders only

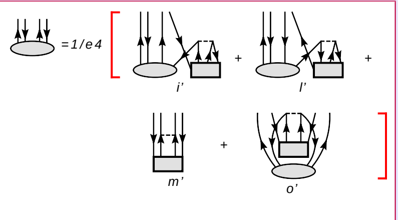


Bethe Goldstone 2



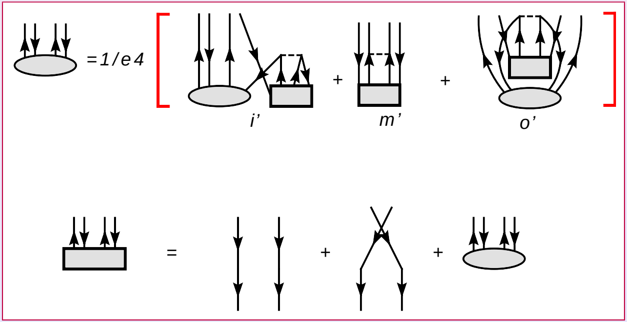
pp, *hh*, and mixed leadders:

=



Bocchum

The Bocchum choice, intermediate, with bare particle energies. Strongly Influenced by Brandow.



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.

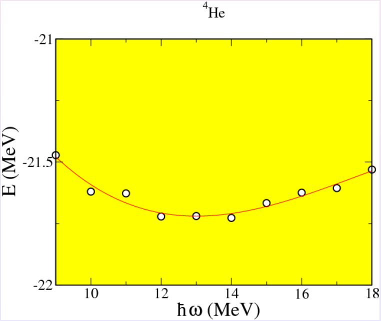
Elements of the technology II

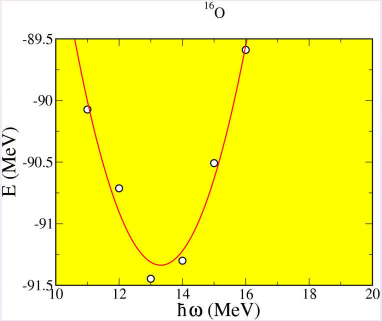
- The idea is to express e.g. the two body amplitudes $\chi^{\Lambda}_{n_1 l_1, n_2 l_2}$ as $\chi^{\Lambda}_{NL;l}(r_{12})$.
- Must start from Harm osc. reference state.
- This transformation requires large numbers of Brody-Moschinsky brackets.
- Truncate severely on CM *NL* (correct for NM).
- potential acts as a (non-local) operator on r_{12}
- Allows for momentum, but not for energy dependence.
- Did CM truncation converge?
- Translational invariance well dealt with
- Bocchum truncation founded on MBT in that era–want to do things systematically.
- Normal SD only contained in HC SUB4.

Requirements

- We have redone some of the Bocchum calculations
- Can be done efficiently in J coupling
- Work with local forces for now
- Be able to check convergence
- Don't need effective operators!
- Find the standard result (very tentatively) for ^{4}He, we have $E = -22.$ MeV for HC SUB2, $E = -28$ MeV for HC SUB3 using AV14 (slight overbinding).

HC SUB2


^{4}He
-21
-21.5
-22
10
12
14
16
18
E (MeV)
ħω (MeV)


^{16}O
-89.5
-90
-90.5
-91
-91.5
10
12
14
16
18
20
E (MeV)
ħω (MeV)

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.
- Work with relative Hamiltonian–all techniques very similar to those use in no-core shell model.
- 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 (based on factorisable approximation to next order).

Equations derived for bosons. An early version used by Bishop and Lührmann in the electron gas.

Much more difficult, but potentially promising.

CCM in Nuclear Physics

- CCM in Nuclear Physics is alive and well.
- For $V_{\mathrm{low}\ k}$ the many-body method of choice.
- Use as test on UNEDF.
- Potentially useful for other “soft forces”.
- The Bocchum CCM is alive and well
- Should look at “real” chiral forces, with contact terms.