Many-body interactions and nuclear structure at the limits of stability

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Outline

Introduction

Some key intellectual issues

Many-body approaches to nuclei

Summary and perspectives
People

Oslo
Elise Bergli, Andreas Ekström, Torgeir Engeland, Gustav Jansen, Øyvind Jensen, Simen Kvaal, MHJ and Eivind Osnes

Oak Ridge National Lab and University of Tennessee, Knoxville
David J. Dean, Gaute Hagen, Witek Nazarewicz and Thomas Papenbrock

Michigan State University
Alex B. Brown and Angelo Signoracci

Advanced Science Research center and Tokyo and Aizu Universities,
Takaharu Otsuka, Michio Honma, Takahiro Misuzaki, Toshio Suzuki, Koshiroh Tsukiyama, Naofumi Tsunoda, Yutaka Utsuno

Codes
Codes at http://www.fys.uio.no/compphys/software.html
Selected questions from QCD to the nuclear many-body problem

▶ How to derive the in medium nucleon-nucleon interaction from basic principles?
▶ How does the nuclear force depend on the proton-to-neutron ratio?
▶ What are the limits for the existence of nuclei?
▶ How can collective phenomena be explained from individual motion?
▶ Shape transitions in nuclei?

**Multiscale Physics:** The many scales pose a severe challenge to *ab initio* descriptions of nuclear systems.
To address these questions one needs a credible theory

We wish to understand the limits of stability of nuclear matter. Which correlations drive the physics towards the driplines?

Requirements to theory

- It should be fully microscopic and start with present two- and three-body interactions derived from e.g., effective field theory;
- It can be improved upon systematically, e.g., by inclusion of three-body interactions and more complicated correlations;
- It allows for description of both closed-shell systems and valence systems;
- For nuclear systems where shell-model studies are the only feasible ones, viz., a small model space requiring an effective interaction, one should be able to derive effective two and three-body (and more complicated) equations and interactions for the shell model;
Aims, motivations and challenges

Requirements to theory

- It can be used to generate excited spectra for nuclei where many shells are involved (It is hard for the traditional shell model to go beyond one major shell. The inclusion of several shells may imply the need of complex effective interactions needed in studies of weakly bound systems);
- Nuclear structure results should be used in marrying microscopic many-body results with reaction studies;
- Need to link ab initio methods with density functional theories. Possible road to multiscale physics; and
- Need to develop link with time-dependent theories.
Key intellectual issues

1. Can we understand the link between Lattice QCD and Effective field theories?

2. Can we link the cutoff of the interaction with a specific model-space size? That is, can we link many-body theories with effective field theories? All interactions have a cutoff $\Lambda$ ($\Lambda \sim 500 – 700$ MeV). A cutoff produces always missing many-body physics (intruder states etc).

3. Can we provide proper error estimates (single-particle basis truncation and truncations in number of excitations)?

4. Do we understand how many-body forces evolve as we add more and more particles?

5. Can we extract information about correlations beyond the independent particle model?
Why do we stress these requirements? We’d like to extract some simple physics messages.

Otsuka et al, PRL 104, 012501 (2010)

The monopole term is defined as

$$\bar{V}_{abab} = \frac{\sum_J (2J + 1) \langle (ab)J|V|(ab)J \rangle}{\sum_J (2J + 1)}$$

where \( ab \) are single-particle orbits and \( J \) is the total angular momentum and \( \langle (ab)J|V|(ab)J \rangle \) is the antisymmetrized two-body matrix element. It can be parameterized in terms of simple central part (gaussian) plus a tensor part (important for understanding shell evolution).

Single-particle energies

$$\epsilon_a = t_a + \sum_J \sum_h (2J + 1) \langle (ah)J|V|(ah)J \rangle$$
Evolution of quasiparticle states in terms of the monopole part
Ground state of $^{101}$Sn, Darby et al, PRL105, 2010

- Shell-model calculation with $^{88}$Sr as core.
  MBPT to third order.
- Ground state of $^{101}$Sn is $7/2^+$
- Core-polarization and tensor force crucial
- One crucial matrix element $\langle (0g_{7/2})^2 J = 0 | V | (0g_{7/2})^2 J = 0 \rangle$
How large a model space do we need?

Example: $^{16}\text{O}$

For $^{16}\text{O}$, one can show that a nucleon-nucleon interaction with momentum cutoff $\Lambda = 600$ MeV requires a model-space based on approx 28380 single-particle states. The total number of Slater determinants, with no restrictions on energy excitations, is

$\binom{28380}{8} \times \binom{28380}{8} \approx 10^{62}$. 

Any direct diagonalization method in such a huge basis is simply impossible. One possible approach is to introduce a smaller model space with a pertinent effective interaction.

**Need effective interactions or smarter methods for doing ab initio calculations.** See JPG 37, 064035, for examples and further discussion.
Coupled Cluster summary

Wavefunction:

$$|\psi\rangle \simeq |\psi_{CC}\rangle = e^{\hat{T}} |\Phi_0\rangle \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$

$$\hat{T}_n = \left(\frac{1}{n!}\right)^2 \sum_{i_1,i_2,\ldots,i_n} t_{i_1i_2\ldots i_n} a^{\dagger}_{i_1} a_{i_2} \ldots a^{\dagger}_{i_n} a_{i_1} \ldots a_{i_2} a_{i_1}.$$  

Energy equation:

$$E_{CC} = \langle \Phi_0 | \bar{H} | \Phi_0 \rangle, \quad \bar{H} = e^{-\hat{T}} \hat{H} e^{\hat{T}} - \langle \Phi_0 | \hat{H} | \Phi_0 \rangle$$

Amplitude equations:

$$0 = \langle \Phi_{i_1\ldots i_n}^{a_1\ldots a_n} | \bar{H} | \Phi_0 \rangle$$
How reliable is Coupled-cluster theory?

Application to quantum dots

Circular quantum dots, comparison between Coupled-cluster theory and Diffusion Monte Carlo

1. Simple Hamiltonian, no three-body or more complicated many-body forces, hope is that missing many-body physics is negligible
2. Harmonic oscillator basis, two dimensions
4. Truncation in terms of many-body excitations such as 1p-1h, 2p-2h, 3p-3h can only be justified \textit{a posteriori}. No proper error estimates.
How reliable is coupled cluster theory?

The Hamiltonian for quantum dots

The one-body part of our Hamiltonian becomes

$$\hat{H}_0 = \sum_{i=1}^{N} \left( -\frac{1}{2} \nabla_i^2 + \frac{\omega^2}{2} r_i^2 \right),$$

whereas the interacting part is (in our work as a renormalized one)

$$\hat{V} = \sum_{i<j}^{N} \frac{1}{|r_i - r_j|}.$$

The unperturbed part of the Hamiltonian yields the single-particle energies

$$\epsilon = \omega \left( 2n + |m| + 1 \right).$$

Gives rise to magic numbers 2, 6, 12, 20, 30...
How reliable is Coupled-cluster theory?

Application to quantum dots, 12 electrons, ground state in a.u.

Pedersen, Hagen, MHJ, Kvaal and Pederiva, arXiv:1009.4833

<table>
<thead>
<tr>
<th>(\omega)</th>
<th>(R)</th>
<th>(E_{HF})</th>
<th>CCSD</th>
<th>CCSD(T)</th>
<th>(\Lambda)-CCSD(T)</th>
<th>DMC</th>
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<tbody>
<tr>
<td>0.28</td>
<td>16</td>
<td>26.4410</td>
<td>25.7081</td>
<td>25.6346</td>
<td>25.6456</td>
<td>25.6356 ± 0.001</td>
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<tr>
<td></td>
<td>18</td>
<td>26.4551</td>
<td>25.7085</td>
<td>25.6334</td>
<td>25.6446</td>
<td></td>
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<tr>
<td></td>
<td>20</td>
<td>26.4659</td>
<td>25.7089</td>
<td>25.6324</td>
<td>25.6439</td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>16</td>
<td>40.0922</td>
<td>39.2195</td>
<td>39.1543</td>
<td>39.1615</td>
<td>39.159 ± 0.001</td>
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<tr>
<td></td>
<td>18</td>
<td>40.1080</td>
<td>39.2194</td>
<td>39.1527</td>
<td>39.1601</td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>40.1202</td>
<td>39.2194</td>
<td>39.1516</td>
<td>39.1591</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>16</td>
<td>66.7686</td>
<td>65.7430</td>
<td>65.6926</td>
<td>65.6963</td>
<td>65.700 ± 0.001</td>
</tr>
<tr>
<td></td>
<td>18</td>
<td>66.7867</td>
<td>65.7417</td>
<td>65.6903</td>
<td>65.6941</td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>66.8006</td>
<td>65.7409</td>
<td>65.6886</td>
<td>65.6924</td>
<td></td>
</tr>
</tbody>
</table>
How reliable is Coupled-cluster theory?

Role of correlation energy

Pedersen, Hagen, MHJ, Kvaal and Pederiva, arXiv:1009.4833

<table>
<thead>
<tr>
<th>$\omega$ = 0.28</th>
<th>$\omega$ = 0.5</th>
<th>$\omega$ = 1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$\Delta E_2$</td>
<td>$\Delta E_3$</td>
</tr>
<tr>
<td>6</td>
<td>93%</td>
<td>99%</td>
</tr>
<tr>
<td>12</td>
<td>91%</td>
<td>99%</td>
</tr>
<tr>
<td>20</td>
<td>90%</td>
<td>99%</td>
</tr>
</tbody>
</table>

Percentage of correlation energy at the CCSD level ($\Delta E_2$) and at the $\Lambda$-CCSD(T) level ($\Delta E_3$), for different number of electrons $N$ and values of the confining harmonic potential $\omega$. 
Relative error as function of number of shells $R$ for 12 electrons and $\hbar \omega = 0.5$ a.u.

Calculations with and without renormalized Coulomb interaction. The log of the relative error $\epsilon$ is plotted.
Petit quantum dot summary

- Essentially no missing many-body physics, in nuclear physics this is a problem
- Even for small $\omega$ excellent agreements. Need to test for even smaller values where correlations become increasingly important
- Correlations beyond Hartree-Fock level become small for larger systems (ground state properties). Mean-field a good starting point, as in large nuclei.
$^4$He “bare” chiral interactions ($N^3$LO with $\Lambda = 500$ MeV), quality of results, G. Hagen et al, PRC 82, 034330 (2010)
Nucleons and Pions as effective degrees of freedom only. Chiral perturbation theory for different orders ($\nu$) of the expansion in terms of momentum/pion mass.

<table>
<thead>
<tr>
<th>Chiral order</th>
<th>2N force</th>
<th>3N force</th>
<th>4N force</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu = 0$</td>
<td>$V_{1\pi} + V_{\text{cont}}$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$\nu = 1$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$\nu = 2$</td>
<td>$V_{1\pi} + V_{2\pi} + V_{\text{cont}}$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$\nu = 3$</td>
<td>$V_{1\pi} + V_{2\pi}$</td>
<td>$V_{2\pi} + V_{1\pi, \text{cont}} + V_{\text{cont}}$</td>
<td>$-$</td>
</tr>
<tr>
<td>$\nu = 4$</td>
<td>$V_{1\pi} + V_{2\pi} + V_{3\pi} + V_{\text{cont}}$</td>
<td>More three-body</td>
<td>four-body force</td>
</tr>
</tbody>
</table>

At order $\nu = 4$ one should include four-body forces in many-body calculations!
$^{40}$Ca “bare” chiral interactions ($N^3$LO with $\Lambda = 500$ MeV), quality of results, G. Hagen et al., PRC 82, 034330 (2010)
$^{48}\text{Ca}$ “bare” chiral interactions ($N^3\text{LO}$ with $\Lambda = 500$ MeV), quality of results, G. Hagen et al, PRC \textbf{82}, 034330 (2010)
Oxygen Isotopes

Several experiments worldwide

- The oxygen isotopes are the heaviest isotopes for which the drip line is well established.
- Two out of four stable even-even isotopes exhibit a doubly magic nature, namely $^{22}\text{O}$ ($Z = 8$, $N = 14$) and $^{24}\text{O}$ ($Z = 8$, $N = 16$).
- The structure of these two doubly magic nuclei is assumed to be governed by the evolution of the $1s_{1/2}$ and $0d_{5/2}$ one-quasiparticle states.
- The isotopes $^{25}\text{O}$, $^{26}\text{O}$, $^{27}\text{O}$, and $^{28}\text{O}$ are outside the drip line, since the $0d_{3/2}$ orbit is not bound.
- *Can we extract information about correlations beyond the independent particle model?*
$^{28}$O with two different chiral interactions, Hagen et al., Phys. Rev. C\textbf{80}, 021306 (2009), need data on $^{28}$O
More to the picture than meets the eye! Otsuka et al., PRL 105, (2010)

- $N^3$LO with $\Lambda = 500$ MeV interaction
- Berggren basis and realistic nucleon-nucleon interactions (GHF)
- Standard harmonic oscillator basis with Hartree-Fock calculation (OHF)
- 17 oscillator shells plus 30 Woods-Saxon Berggren states for each of the $s_{1/2}$, $d_{5/2}$, and $d_{3/2}$ states
Role of possible missing many-body physics

- $s_{1/2}$ state is a halo state ($r_{\text{rms}} = 5.333$ fm), no influence from short-range effects.
- $1/2^+$ halo state is dominated by long-ranged forces.
- Spin-orbit splitting between the $3/2^+$ and $5/2^+$ states increases with decreasing cutoff.
Spectroscopic factors for $^{24}\text{O}$, Ø. Jensen \textit{et al}, PRC \textbf{83}, 021305(R) (2011)

\begin{equation}
S_{A-1}^A(lj) = \left| O_{A-1}^A(lj; r) \right|^2 ,
\end{equation}

\begin{equation}
O_{A-1}^A(lj; r) = \sum_n \int \langle A - 1 | \tilde{a}_{nlj} | A \rangle \phi_{nlj}(r). \end{equation}

Here, $O_{A-1}^A(lj; r)$ is the radial overlap function of the many-body wavefunctions for the two independent systems with $A$ and $A - 1$ particles respectively. The double bar denotes a reduced matrix element, and the integral-sum over $n$ represents both the sum over the discrete spectrum and an integral over the corresponding continuum part of the spectrum.
Spectroscopic factors for $^{24}$O, Ø. Jensen et al, PRC 83, 021305(R) (2011)

- N$^3$LO with $\Lambda = 500$ MeV interaction, CCSD calculation
- Bergren basis (GHF) and Harmonic oscillator basis (OHF)
- Spectroscopic factors for neutron $d_{5/2}$ and $s_{1/2}$
- 17 oscillator shells plus 30 Woods-Saxon Berggren states for each of the $s_{1/2}$, $d_{5/2}$, and $d_{3/2}$ states
Spectroscopic factors from Gade et al, PRC 77, 044306 (2008). Can we understand these quenchings?

- Reduction of measured nucleon knock-out cross sections relative to theoretical
- Plotted as function of separation energies of the two nucleon species
- Results from heavy-ion induced one-\(\pi\) and one-\(\nu\) knock-out reactions and electron-induced proton removal from stable nuclei.
- Only expt uncertainties included

- Simple model for $^5\text{He}+n \rightarrow ^6\text{He}$
- Single-particle energies obtained using complex basis
- Vary the binding energy (and thereby separation energy) of $p_{3/2}$ state
- Cusp in SF due to coupling to scattering states
Spectroscopic factors for $^{14}$O, $^{16}$O, $^{22}$O, $^{24}$O and $^{28}$O, Ø. Jensen et al, in preparation

- $N^3$LO with $\Lambda = 500$ MeV interaction, CCSD calculation
- Spectroscopic factors for proton $p_{3/2}$ and $p_{1/2}$
- Quenching due to coupling to scattering states
- Different from standard scenario (long-range, short-range+tensor correlations)
Radial overlaps for $^{14}\text{O}$, $^{16}\text{O}$, $^{22}\text{O}$, $^{24}\text{O}$ and $^{28}\text{O}$, $\emptyset$. Jensen et al., in preparation

- Radial overlap ratios wrt $^{16}\text{O}$ for proton $p_{1/2}$.
- Downward dip at larger radii due to more bound $p_{1/2}$ states with increasing $A$.
- For $^{14}\text{O}$ the $p_{1/2}$ proton is less bound with respect to $^{16}\text{O}$, resulting in a bend upward.
SFs and separation energies $^{14}\text{O}$, $^{16}\text{O}$, $^{22}\text{O}$, $^{24}\text{O}$ and $^{28}\text{O}$, Ø. Jensen et al, in preparation

- SFs for $p_{1/2}$ as function of separation energies
- When large differences in separation energies, large quenchings for protons
- Neutrons are weakly bound and less quenched.
Many-body correlations Ø. Jensen et al, in preparation.
SF for $p_{1/2}$ as function of various cutoffs for $^{24}\text{O}$

- $\text{N}^3\text{LO}$ interaction evolved to a lower momentum cutoff $\lambda$.
- Case 1: SFs using a mean-field HF solution for the $A$ and $A-1$ nuclei.
- Case 2: HF for $A$ nucleus and 2p1h for $A-1$ nucleus.
- Case 3: full calculation.
SF summary

- Quenching of spectroscopic factors for deficient nucleon species due to coupling to scattering states.
- Need experimental data.
- New interesting cases with large proton/neutron asymmetries where we can run calculations: $^{24}$S (last bound), $^{30}$S, $^{32}$S (data) and $^{36}$S; and $^{22}$Si, $^{28}$Si, $^{30}$Si and $^{34}$Si (data).
- Preliminary: last bound protons ($d_{3/2}$) in calcium isotopes up to $^{60}$Ca show small quenching. Is it the centrifugal barrier?
- More speculations: do we see these quenchings due to the continuum only for light systems (low $l$-values)?
Summary and perspectives. Where are we now?

- We can compute with a given Hamiltonian reliable energies for $A \pm 1$ and $A \pm 2$ nuclei (two-particle attached/removed). This means we can do all oxygen isotopes except $^{19}$O. Need data beyond $^{24}$O.

- We can provide spectroscopic factors, see Jensen et al., Phys. Rev. C 82, 014310 (2010)

- Not yet: three-body interactions in the Hamiltonian.

- Can study the evolution of many-body forces as we increase the number of valence nucleons. Experiment can constrain our missing correlations beyond two-body interactions.

- We can therefore extract the $A$-dependence of such correlations and their isospin dependence.

- We can understand the $A$-dependence of spin-orbit partners! But need data to constrain missing many-body physics. Theory can be used to extract simple information on say various components of the nuclear force.