Model independent computation of atomic nuclei: status and perspectives

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Aim: Bottom-up approach to nuclear structure

Purpose: Reliable predictions with error estimates.

Figure from A. Richter (2004)
How does the physics of nuclei impact the physical universe?
Ab-initio approaches to nuclear structure

Green’s function
Monte Carlo
No-core shell model
Lattice simulations
Virtually exact few-body methods …

Future aims

Other ab-initio methods for A≥16
UMOA (Fujii, Kamada, Suzuki)
Green’s function method (Barbieri)

Coupled-cluster method
Model independent description of $^4$He

$$\frac{d\hat{H}(s)}{ds} = \left[ \eta(s), \hat{H}(s) \right] \quad \text{with} \quad \eta(s) \equiv \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s)$$


- RG transformation of NN force induces NNN
- RG of NN and NNN independent of cutoff
- Small cutoff dependence $\rightarrow$ NNNN forces small

Nuclear forces from chiral effective field theory
[Weinberg; van Kolck; Epelbaum et al.; Entem & Machleidt; people@INT&UW, …]

Low energy constants from fit of NN data, A=3,4 nuclei, or light nuclei.
Fixing the low-energy constants of a chiral 3NF

Leading terms at order $N^2$LO [van Kolck (1994), Epelbaum et al (2002)]

- Long ($2\pi$)
- Intermediate ($\pi$)
- Short-range

$c$-terms (from pion-nucleon scattering) still with considerable uncertainties

Low-energy coefficients D and E of contact terms from $A>2$ nuclei

Figure 5. States dominated by p-shell configurations for $^{10}$B, $^{11}$B, $^{12}$C, and $^{13}$C calculated at $N_{\text{max}} = 6$ using $\hbar\Omega = 15$ MeV (14 MeV for $^{10}$B). Most of the eigenstates are isospin $T=0$ or $1/2$, the isospin label is explicitly shown only for states with $T=1$ or $3/2$. The excitation energy scales are in MeV.

Lattice simulations based on interactions from chiral effective field theory

Proton-neutron

\[ \delta(S_0) \text{ (degrees)} \]

\[ p_{CM} \text{ (MeV)} \]

Effort (1 MC trajectory) \( \sim V^{1.5} A^{1.7} \); \( <\text{Sign}> \sim \exp(-0.11A) \)

Toward medium-mass nuclei
Chiral $N^3$LO (500 MeV) by Entem & Machleidt, NN only

Binding energy per nucleon

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>CCSD</th>
<th>$\Lambda$-CCSD(T)</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^4$He</td>
<td>5.99</td>
<td>6.39</td>
<td>7.07</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>6.72</td>
<td>7.56</td>
<td>7.97</td>
</tr>
<tr>
<td>$^{40}$Ca</td>
<td>7.72</td>
<td>8.63</td>
<td>8.56</td>
</tr>
<tr>
<td>$^{48}$Ca</td>
<td>7.40</td>
<td>8.28</td>
<td>8.67</td>
</tr>
</tbody>
</table>


B/A=6.62 MeV (2 body clusters)
B/A=7.47 MeV (3 body clusters)

Chiral three-nucleon forces expected to yield 0.4MeV per nucleon?

Effort $\sim (A^2\Omega^4)^{2/3}$ ($j$-coupled scheme); $A^2\Omega^4$ ($m$ scheme)

[Hagen, TP, Dean, Hjorth-Jensen, Phys. Rev. Lett. 101, 092502 (2008)]
**Ab initio** description of proton halo state in $^{17}$F

- Continuum has to be treated properly
- Focus is on single-particle states
- Previous study: shell model in the continuum with $^{16}$O core
Bound states and resonances in $^{17}$F and $^{17}$O

Single-particle basis consists of bound, resonance and scattering states
- Gamow basis for $s_{1/2}$ $d_{5/2}$ and $d_{3/2}$ single-particle states
- Harmonic oscillator states for other partial waves

Computation of single-particle states via “Equation-of-motion CCSD”
- Excitation operator acting on closed-shell reference
- Here: superposition of one-particle and 2p-1h excitations

$$R_{\mu} = r^a a^\dagger_a + \frac{1}{2} r^a r^b a^\dagger_a a^\dagger_b a_j$$

$$[\overline{H}, R_{\mu}] |\phi_0\rangle = \omega_{\mu} R_{\mu} |\phi_0\rangle$$

- Gamow basis weakly dependent on oscillator frequency
- $d_{5/2}$ not bound; spin-orbit splitting too small
- $s_{1/2}$ proton halo state close to experiment

Variation of cutoff probes omitted short-range forces

- Proton-halo state ($s_{1/2}$) very weakly sensitive to variation of cutoff
- Spin-orbit splitting increases with decreasing cutoff

Ab initio description of nuclear reactions

[S. Quaglioni and P. Navrátil, PRL101, 092501 (2008); PRC79, 044606 (2009)]

\[
\int dr \ r^2 \left( \left\langle r' \ n \ \alpha \bigg| \hat{A}_1 (H - E) \hat{A}_1 \bigg| r \ n \ \alpha \right\rangle \ \left\langle r' \ d \ ^3H \ \alpha \bigg| \hat{A}_2 (H - E) \hat{A}_2 \bigg| r \ d \ ^3H \ \alpha \right\rangle \right) \left( \frac{g_1(r)}{r} \right) \left( \frac{g_2(r)}{r} \right) = 0
\]

Combination of no-core shell model and the resonating group method
Accurate nuclear Hamiltonian, consistent cluster wave functions
Correct asymptotic expansion, Pauli principle and translational invariance
[Slide courtesy of P. Navratil]
Main role of three-nucleon forces?

Monopole shifts from 3NF as density-dependent NN force. [A. Zuker, PRL 90, 42502 (2003)]

Contributions to binding of $^4$He. [Hagen, TP, Dean, Schwenk, Nogga, Wloch, Piecuch, PRC 76, 034302 (2007)]

$$\hat{H}_3 = \frac{1}{6} \sum_{ijk} \langle ijk||ijk \rangle + \frac{1}{2} \sum_{ijpq} \langle ijp||ijq \rangle \{\hat{a}^\dagger_p \hat{a}^\dagger_q \} + \frac{1}{4} \sum_{ipqrs} \langle ipq||irs \rangle \{\hat{a}^\dagger_p \hat{a}^\dagger_q \hat{a}_s \hat{a}_r \} + \hat{h}_3 ,$$

Error estimate due to CCSD approximation.
Is $^{28}\text{O}$ a bound nucleus?

**Experimental situation**

- “Last” stable oxygen isotope $^{24}\text{O}$
- $^{25}\text{O}$ unstable (Hoffman et al 2008)
- $^{26,28}\text{O}$ not seen in experiments
- $^{31}\text{F}$ exists (adding on proton shifts drip line by 6 neutrons!?)

Shell model (sd shell) with monopole corrections based on T=1/2 three-nucleon force predicts $^{24}\text{O}$ as last stable isotope of oxygen. [Otsuka, Suzuki, Holt, Schwenk, Akaishi, arXiv:0908.2607]
Neutron-rich oxygen isotopes from chiral NN forces

Chiral NN forces only: Too close to call. Theoretical uncertainties >> differences in binding energies.

Chiral potentials by Entem & Machleidt’s different from G-matrix-based interactions.

Ab-initio theory cannot rule out a stable $^{28}\text{O}$.

Three-body forces largest potential contribution that decides this question.

[G. Hagen, TP, D. J. Dean, M. Hjorth-Jensen, B. Velamur Asokan, PRC 80, 021306(R) (2009)]

No theoretical approach flawless yet. (No approach includes everything (continuum effects, 3NFs, no adjustments of interaction). Stay tuned …
Summary & Outlook

- Model independent description of atomic nuclei under way!
- Great progress in understanding effective interactions and their dependence on the resolution scale.
- Three-nucleon forces play a most exciting role
- Several complementary methods available that solve the nuclear many-body problem
- Improvements of algorithms, methods, and hardware enable progress
- Coupled cluster and SRG methods appear to scale up to selected heavy nuclei (\(^{78}\text{Ni},^{100}\text{Sn},^{132}\text{Sn},^{208}\text{Pb} \ldots\))
- Inclusion of continuum effects \(\rightarrow\) merger of structure and reactions; essential for computation of fragile halo states and weakly-bound nuclei

The next decade promises to be very exciting!