Current status and challenges of ab-initio computations of nuclei

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INT workshop on “Nuclear Physics from Lattice QCD”

INT, May 5th, 2016
Computing “real nuclei” from “pseudo EFT” interactions

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Outline

- Challenges and status of ab initio computations of nuclei
- Accurate binding energies and radii from a chiral interaction
- The neutron radius and dipole polarizability of $^{48}$Ca
- Unexpected large charge radii of $^{52}$Ca questions its magicity
- Structure of $^{78}$Ni from first principles computations
- Role of continuum on shell structure of neutron-rich calcium isotopes
Trend in realistic ab-initio calculations

Explosion of many-body methods (Coupled clusters, Green’s function Monte Carlo, In-Medium SRG, Lattice EFT, MCSM, No-Core Shell Model, Self-Consistent Green’s Function, UMOA, ...)

Application of ideas from EFT and renormalization group (V_{low-k}, Similarity Renormalization Group, ...)

Computational capabilities exceed accuracy of available interactions

Reach of ab-initio computations of nuclei

Nuclei for which ab-initio computations have been attempted

H. Hergert et al, Physics Reports 621, 165-222 (2016)
### Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]

<table>
<thead>
<tr>
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<th>LO $O\left(\frac{Q}{\Lambda}\right)$</th>
<th>NLO $O\left(\frac{Q^2}{\Lambda^2}\right)$</th>
<th>$O\left(\frac{Q^3}{\Lambda^3}\right)$</th>
<th>$O\left(\frac{Q^4}{\Lambda^4}\right)$</th>
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<td>4N</td>
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- developing higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard et al 2007; Krebs et al 2012; Hebeler et al 2015; …]
- local / non-local formulations [Gezerlis et al 2013/2014]
- propagation of uncertainties on horizon [Navarro Perez 2014, Carlsson et al 2015]
- different optimization protocols [Ekström et al 2013]
- Improved understanding and handling via renormalization group transformations [Bogner et al 2003; Bogner et al 2007]
- Problem: Not RG invariant. Different power counting schemes underway
Oxygen chain with interactions from chiral EFT

Different methods agree within uncertainties
The challenge is now with the interactions

Nuclear saturation is finely tuned

- A 4% change in the binding energy of $^4$He yields a 15% change in $^{16}$O [B. Carlsson, A. Ekström, C. Forssén et al., PRX 6, 011019 (2016)].
- Regulator dependence in saturation properties of nuclear matter
- Not possible to simultaneously describe nuclear matter light nuclei by only adjusting $c_E$ and $c_D$ of 3NF

G. Hagen et al., PRC 89 014319 (2013)
Accurate nuclear binding energies and radii from a chiral interaction

- Chiral interactions have failed at describing both binding energies and radii of nuclei
- Predictive power does not go together with large extrapolations
- Nuclear saturation may be viewed as an emergent property
Accurate nuclear binding energies and radii from a chiral interaction

Solution: Simultaneous optimization of NN and 3NFs
Include charge radii and binding energies of $^3\text{H}$, $^3,^4\text{He}$, $^{14}\text{C}$, $^{16}\text{O}$ in the optimization ($\text{NNLO}_{\text{sat}}$)


Not new: GFMC with AV18 and Illinois-7 are fit to 23 levels in nuclei with $A < 10$
Electric charge distributions have been a long-standing problem for *ab initio* theory.

\[
BE(\text{Th}) = 404(3) \text{ MeV} \\
BE(\text{Exp}) = 416 \text{ MeV}
\]

\[
R_{Ch} (\text{Th}) = 3.48(3) \text{ fm} \\
R_{Ch, \text{Exp}} = 3.477(2) \text{ fm}
\]
Nuclear matter from NNLO\textsubscript{sat}


- Interactions from Hebeler \textit{et al} not constrained by heavier nuclei.
- They reproduce binding energy and radii of few-body systems
- Non-local regulators in the 3NF important for saturation

Hagen et al (2014); Carbone et al (2013); Coraggio et al 2014;

K. Hebeler \textit{et al} 
PRC 83, 031301 2011
What is the neutron skin of $^{48}$Ca

**Neutron skin** = Difference between radii of neutron and proton distributions

Relates atomic nuclei to neutron stars via neutron EOS

Correlated quantity: dipole polarizability

Model-independent measurement possible via parity-violating electron scattering (P-REX/C-REX at JLab)
Neutron radius and skin of $^{48}$Ca

- Neutron skin significantly smaller than in DFT
- Neutron skin almost independent of the employed Hamiltonian
- Our prediction is consistent with existing data


Uncertainty estimates from family of chiral interactions.

DFT:
SkM*, SkP, Sly4, SV-min, UNEDF0, and UNEDF1

$R_{\text{skin}}$ (fm) vs $R_{\text{p}}$ (fm) vs $R_{n}$ (fm)
Neutron radii and dipole polarizabilities

Brown, PRL 2000, Piekarewicz & Horowitz, PRL 2001; Furnstahl, NPA 2002; Reinhard & Nazarewicz, PRC 2010; Piekarewicz et al., PRC 2012; Horowitz et al, PRC 2012; ...

\[ \alpha_D: ^{208}\text{Pb} \text{ by Tamii et al, PRL 2011; } ^{68}\text{Ni} \text{ by Rossi et al, PRL 2013; } ^{120}\text{Sn} \text{ by Hashimoto et al. (2015); } ^{48}\text{Ca} \text{ coming soon ...} \]

\[ R_n: ^{208}\text{Pb} \text{ by Abrahanyan et al, PRL 2012; Tarbert et al, PRL 2013; } ^{48}\text{Ca} \text{ planned ...} \]
Dipole polarizability of $^{48}$Ca


DFT results are consistent and within band of ab-initio results

Data being analyzed by Osaka-Darmstadt collaboration

$\alpha_D$ (fm$^3$)

$^{40}$Ca

$R_p$ (fm)

Ab-initio prediction: $2.19 \lesssim \alpha_D \lesssim 2.60$ fm$^3$
Large charge radii questions magicity of $^{52}$Ca

doi:10.1038/nphys3645

- Charge radii of $^{49,51,52}$Ca, obtained from laser spectroscopy experiments at ISOLDE, CERN
- Unexpected large charge radius questions the magicity of $^{52}$Ca
- Theoretical models all underestimate the charge radius
- Ab-initio calculations reproduce the trend of charge radii
Structure of $^{78}$Ni from first principles

A high $2^+$ energy in $^{78}$Ni indicates that this nucleus is doubly magic.

A measurement of this state has been made at RIBF, RIKEN.
R. Taniuchi et al., in preparation

- From an observed correlation we predict the $2^+$ excited state in $^{78}$Ni using the experimental data for the $2^+$ state in $^{48}$Ca.
- Similar correlations have been observed in other nuclei, e.g. Tjon line in light nuclei.

G. Hagen, G. R. Jansen, and T. Papenbrock
arXiv (2016)
$4^+ / 2^+ = 1.2$ is consistent with $^{78}\text{Ni}$ being a doubly magic nucleus.

- Continuum impacts level ordering in $^{79}\text{Ni}$
- Dripline is beyond $^{80}\text{Ni}$
Role of continuum on unbound states in calcium isotopes


1.8/2.0 (EM)
K. Hebeler et al,
PRC 83, 031301 (2011)
Summary

• Exciting times in nuclear theory:
  ➢ explosion of many-body solvers
  ➢ many new developments regarding interactions and currents

• NNLO$_{\text{sat}}$ a pragmatic approach to the problem of nuclear saturation

• Neutron skin, dipole polarizability in $^{48}$Ca, and charge radii of neutron-rich calciums

• Structure of neutron-rich $^{78}$Ni suggest it is doubly magic
  ➢ predictions for soon-to-be measured quantities
  ➢ charge radii in neutron-rich calcium isotopes not well understood

• How to address the problem of finetuned interactions, regulator dependencies and saturation in nuclei?

• Explore new power counting schemes?

• Computation of heavy nuclei from Hamiltonian based methods

• Propagation of uncertainties from the interaction to the nuclear many-body problem on the horizon

• Quantifying systematic uncertainties associated with truncations in ab-initio methods is still a challenge