New Horizons in Ab Initio Nuclear Structure Theory

Robert Roth
Ab Initio Nuclear Structure

Nuclear Structure Observables

Exact Solutions
solve nuclear many-body problem with converged truncations

Controlled Approx.
treat many-body problem with controlled & improvable approximations

Similarity Transformations
physics-conserving unitary transformation to adapt Hamiltonian to limited model space

Chiral EFT Hamiltonians
consistent NN,3N,... interactions & current operators

Chiral Effective Field Theory
based on relevant degrees of freedom & symmetries of QCD

Low-Energy Quantum Chromodynamics

Lattice QCD
quarks & gluon on a lattice

Lattice EFT
nucleons & pions on a lattice

Energy-Density Funct.
guided by chiral EFT

Robert Roth – TU Darmstadt – 05/2013
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**Nuclear Interactions from Chiral EFT**

- **chiral EFT background**: talks by Machleidt & Epelbaum

- **standard Hamiltonian**:
  - NN at N3LO: Entem & Machleidt, 500 MeV cutoff
  - 3N at N2LO: Navrátil, A=3 fit, 500 MeV cutoff

- **alternatives**:
  - modified 3N interaction at N2LO (cutoff, LECs)
  - consistent Hamiltonians at N2LO (NN: Epelbaum, POUNDERs-opt.)
  - consistent Hamiltonians at N3LO
  - $\Delta$-full chiral EFT, YN interaction,...

<table>
<thead>
<tr>
<th></th>
<th>NN</th>
<th>3N</th>
<th>4N</th>
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<td>LO</td>
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continuous transformation driving **Hamiltonian to band-diagonal form** with respect to a chosen basis

- **unitary transformation** of Hamiltonian:
  \[ H_\alpha = U_\alpha^\dagger H U_\alpha \]

- **evolution equations** for \( H_\alpha \) and \( U_\alpha \):
  \[ \frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \]

- **dynamic generator**: commutator with the operator in whose eigenbasis \( H_\alpha \) shall be diagonalized
  \[ \eta_\alpha = (2\mu)^2[T_{\text{int}}, H_\alpha] \]

simplicity and flexibility are great advantages of the SRG approach

solve SRG evolution equations using two-, three- & four-body matrix representation
SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

\[ \alpha = 0.000 \text{ fm}^4 \]
\[ \Lambda = \infty \text{ fm}^{-1} \]
\[ J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar \Omega = 28 \text{ MeV} \]

NCSM ground state \(^3\text{H}\)

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SRG Evolution in Three-Body Space

$\alpha = 0.320 \text{ fm}^4$

$\Lambda = 1.33 \text{ fm}^{-1}$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28 \text{ MeV}$

3B-Jacobi HO matrix elements

suppression of off-diagonal coupling $\hat{=} \text{ pre-diagonalization}$

NCSM ground state $^3\text{H}$

significant improvement of convergence behavior
evolution induces $n$-body contributions $H_{\alpha}^{[n]}$ to Hamiltonian

$$H_{\alpha} = H_{\alpha}^{[1]} + H_{\alpha}^{[2]} + H_{\alpha}^{[3]} + H_{\alpha}^{[4]} + \ldots$$

truncation of cluster series formally destroys unitarity and invariance of energy eigenvalues (independence of $\alpha$)

flow-parameter provides diagnostic tool to assess neglected higher-order contributions

SRG-Evolved Hamiltonians

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<tr>
<th>Type</th>
<th>Description</th>
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guided by chiral EFT
NCSM is one of the most powerful and universal exact ab-initio methods

- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\text{max}} \hbar \Omega$

- solve **large-scale eigenvalue problem** for a few extremal eigenvalues

- **all relevant observables** can be computed from the eigenstates

- range of applicability limited by **factorial growth** of basis with $N_{\text{max}} \& \Lambda$

- adaptive **importance truncation** extends the range of NCSM by reducing the model space to physically relevant states
converged NCSM calculations essentially restricted to lower/mid p-shell

full $N_{\text{max}} = 10$ calculation for $^{16}$O very difficult (basis dimension $> 10^{10}$)

**Importance Truncation**

reduce model space to the relevant basis states using an *a priori* importance measure derived from MBPT
$^4$He: Ground-State Energies

$NN_{\text{only}}$

$NN + 3N_{\text{ind}}$

$NN + 3N_{\text{full}}$

$h\Omega = 20 \text{ MeV}$

$E$ [MeV]

$N_{\text{max}}$

$\alpha = 0.04 \text{ fm}^4$

$\Lambda = 2.24 \text{ fm}^{-1}$

$\alpha = 0.05 \text{ fm}^4$

$\Lambda = 2.11 \text{ fm}^{-1}$

$\alpha = 0.0625 \text{ fm}^4$

$\Lambda = 2.00 \text{ fm}^{-1}$

$\alpha = 0.08 \text{ fm}^4$

$\Lambda = 1.88 \text{ fm}^{-1}$

$\alpha = 0.16 \text{ fm}^4$

$\Lambda = 1.58 \text{ fm}^{-1}$

Exp.
$^{12}\text{C: Ground-State Energies}$

$E [\text{MeV}]$ vs $N_{\text{max}}$

- $\hbar \Omega = 20 \text{ MeV}$
- $\alpha = 0.04 \text{ fm}^4$
- $\Lambda = 2.24 \text{ fm}^{-1}$
- $\alpha = 0.05 \text{ fm}^4$
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- $\alpha = 0.16 \text{ fm}^4$
- $\Lambda = 1.58 \text{ fm}^{-1}$

Exp.

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16\textsuperscript{O}: Ground-State Energies

\[ E_\text{NN only} \]

\[ E_\text{NN+3N_{ind}} \]

\[ E_\text{NN+3N_{full}} \]

\( h\Omega = 20 \text{ MeV} \)

\( N_{max} \)

\( E [\text{MeV}] \)

\( \alpha = 0.04 \text{ fm}^4 \)
\( \Lambda = 2.24 \text{ fm}^{-1} \)

\( \alpha = 0.05 \text{ fm}^4 \)
\( \Lambda = 2.11 \text{ fm}^{-1} \)

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\( \alpha = 0.16 \text{ fm}^4 \)
\( \Lambda = 1.58 \text{ fm}^{-1} \)

option 1: suppress induced 4N by modifying initial 3N

option 2: explicitly include induced 4N terms in IT-NCSM

clear signature of induced 4N originating from initial 3N

Roth, et al; PRL 107, 072501 (2011)
16O: Lowering the Initial 3N Cutoff

standard

reduced 3N cutoff

c_E refit to $^4$He binding energy

500 MeV

$c_D = -0.2$
$c_E = -0.205$

450 MeV

$c_D = -0.2$
$c_E = -0.016$

400 MeV

$c_D = -0.2$
$c_E = 0.098$

350 MeV

$c_D = -0.2$
$c_E = 0.205$

$\alpha = 0.04 \text{ fm}^4$
$\Lambda = 2.24 \text{ fm}^{-1}$

$\alpha = 0.05 \text{ fm}^4$
$\Lambda = 2.11 \text{ fm}^{-1}$

$\alpha = 0.0625 \text{ fm}^4$
$\Lambda = 2.00 \text{ fm}^{-1}$

$\alpha = 0.08 \text{ fm}^4$
$\Lambda = 1.88 \text{ fm}^{-1}$

lowering the initial 3N cutoff suppresses induced 4N terms
$^{16}O$: Explicit Inclusion of Induced $4N$

- induced $4N$ from SRG evolution in four-body Jacobi-HO
- transformation to $m$- or $JT$-scheme $4N$ matrix elements
- explicit $4N$ terms in IT-NCSM

![Graph showing energy levels as a function of $N_{\text{max}}$.](image)

- $E_{4\text{max}} = 6$
- $\hbar \Omega = 24\text{MeV}$

**Legend**

- $\text{NN+3N}_{\text{full}}$
- $\text{NN+3N}_{\text{full}}+4N_{\text{ind}}(0^+0)$

- $\alpha = 0.04 \text{ fm}^4$
- $\alpha = 0.0625 \text{ fm}^4$
- $\alpha = 0.08 \text{ fm}^4$
- $\alpha = 0.16 \text{ fm}^4$
16O: Explicit Inclusion of Induced 4N

- inclusion of explicit 4N is feasible (at least partially)
- effect of SRG-induced 4N as expected

- induced 4N from SRG evolution in four-body Jacobi-HO
- transformation to $m$- or $JT$-scheme 4N matrix elements
- explicit 4N terms in IT-NCSM

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$\frac{\hbar^2}{\Omega} = 24\,\text{MeV}$  
$E_{4\,\text{max}} = 6$
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Ground States of Oxygen Isotopes

$NN + 3N_{\text{ind}}$ (chiral NN)

$NN + 3N_{\text{full}}$ (chiral NN+3N)

$E_{\text{MeV}}$

$\Lambda_{3N} = 400 \text{ MeV}$, $\alpha = 0.08 \text{ fm}^4$, $E_{3\text{max}} = 14$, optimal $h\Omega$

Hergert et al., PRL (2013); arXiv:1302.7294
Ground States of Oxygen Isotopes

Hergert et al., PRL (2013); arXiv:1302.7294

\[ \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm} \]

Parameter-free ab initio calculations with full 3N interactions

Highlights predictive power of chiral NN+3N Hamiltonians
Ground States of Oxygen Isotopes

\[ \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad E_{3\text{max}} = 14, \quad \text{optimal } h\Omega \]
Ground States of Oxygen Isotopes

Different many-body approaches using the same NN+3N Hamiltonian give consistent results.

\( \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^2, \quad E_{3\text{max}} = 14, \quad \text{optimal } \Omega \)

Minor differences are understood (NO2B, \( E_{3\text{max}} \), ...)

\( \text{Hergert et al., PRL (2013); arXiv:1302.7294} \)
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Low-Energy Quantum Chromodynamics

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CC is one of the most efficient methods for the description of ground states of medium-mass or heavy closed-shell nuclei.

- Many-body state parametrized as **exponential wave operator** applied to single-determinant **reference state** $|\Phi_{\text{ref}}\rangle$

$$|\Psi_{\text{CC}}\rangle = \Omega |\Phi_{\text{ref}}\rangle = \exp(T_1 + T_2 + T_3 + \cdots + T_A) |\Phi_{\text{ref}}\rangle$$

- Truncation with respect to $n$-particle-$n$-hole **excitation operators** $T_n$

- Solve **non-linear system** of equations for the amplitudes in $T_1, T_2, T_3, \ldots$

- Extensions to near-closed-shell nuclei and excited states through **equations-of-motion methods**

- We have developed a parallelized CC code for **CCSD** and $\Lambda$-**CCSD(T)**
Inclusion of 3N Interactions

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- **premium option:** explicit 3N
  - extend coupled-cluster equations for explicit 3N interactions
  - CCSD-3B, Λ-CCSD(T)-3B are feasible, but much more expensive

- **low-cost option:** normal-ordered two-body approximation
  - write 3N interaction in normal-ordered form with respect to the actual A-body reference determinant (HF state)

\[
V_{3N} = \sum V^{3N}_{\ldots\ldots\ldots} a_0^\dagger a_0^\dagger a_\alpha a_\alpha a_\alpha
\]

\[
= W^{0B} + \sum W^{1B}_{\ldots\ldots\ldots} \{a_\alpha\} + \sum W^{2B}_{\ldots\ldots\ldots} \{a_\dagger a_\dagger a_\alpha a_\alpha\}
\]

\[
+ \sum W^{3B}_{\ldots\ldots\ldots\ldots\ldots\ldots\ldots} \{a_\dagger a_\dagger a_\dagger a_\alpha a_\alpha a_\alpha\}
\]

- discard normal-ordered three-body term and use two-body coupled-cluster formalism
CCSD with Explicit 3N Interactions

Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013)

\[ \text{NN+3N}_{\text{full}} \]

\[ E_{\text{MeV}} = \begin{align*}
16\text{O} & : h\Omega = 20 \text{ MeV} \\
24\text{O} & : h\Omega = 20 \text{ MeV} \\
40\text{Ca} & : h\Omega = 24 \text{ MeV} \\
48\text{Ca} & : h\Omega = 28 \text{ MeV}
\end{align*} \]

NO2B approximation reproduces explicit-3N results with better than 1% accuracy

\( \alpha = 0.02 \text{ fm}^4 \)
\( \alpha = 0.04 \text{ fm}^4 \)
\( \alpha = 0.08 \text{ fm}^4 \)

HF basis
\( E_{3\text{max}} = 12 \)
\( \Lambda_{3\text{N}} = 400 \text{ MeV} \)
Λ-CCSD(T) with NO2B Approximation

Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013)

**NN+3N**

- Experimental binding energies for Ca isotopes reproduced within 10%
- No parameter adjustments!

**Λ-CCSD(T)**

- α = 0.02 fm⁴
- α = 0.04 fm⁴
- α = 0.08 fm⁴

**CCSD**

- HF basis

**E₃ₓₐₓ** = 14

**Λ₃Ν** = 400 MeV

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Low-Energy Quantum Chromodynamics
Motivation: Hypernuclear Structure

- precision data on hypernuclear ground states and spectroscopy are available
- ab initio few-body ($A \lesssim 4$) and phenomenological shell model or cluster calculations so far
- chiral EFT interactions including hyperons are being constructed
- constrain YN & YY interaction by ab initio hypernuclear structure calculations
■ **Hamiltonian from chiral EFT**
  - NN+3N: standard chiral Hamiltonian (Entem&Machleidt, Navrátil)
  - YN: LO chiral interaction (Haidenbauer et al.), NLO in progress

■ **Similarity Renormalization Group**
  - consistent SRG-evolution of NN, 3N, YN interactions
  - using particle basis and including $\Lambda\Sigma$-coupling (larger matrices)
  - $\Lambda-\Sigma$ mass difference and $p\Sigma^\pm$ Coulomb included consistently

■ **Importance Truncated No-Core Shell Model**
  - include explicit ($p$, $n$, $\Lambda$, $\Sigma^+$, $\Sigma^0$, $\Sigma^-$) with physical masses
  - larger model spaces easily tractable with importance truncation
  - all $p$-shell single-$\Lambda$ hypernuclei are accessible
Application: $^7_\Lambda$Li

$^6\text{Li}$

$^7\Lambda\text{Li}$

Jülich’04

NN @ N3LO
Entem&Machleidt
$\Lambda_{NN} = 500$ MeV

3N @ N2LO
Navratil
$\Lambda_{3N} = 500$ MeV
triton fit

Jülich’04
Haidenbauer et al.
scatt. & hypertriton

$\alpha = 0.08 \text{ fm}^4$

$h\Omega = 20$ MeV

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**Application: $^7_\Lambda$Li**

- $^6\text{Li}$
- $^7\Lambda\text{Li}$

**Hypernuclear Structure**

Sets tight constraints on YN interaction.

**Start Investigating**

Sensitivity of spectra on YN input.

**NN @ N3LO**
- $\Lambda_{NN} = 500$ MeV
- Entem & Machleidt

**3N @ N2LO**
- $\Lambda_{3N} = 500$ MeV
- Navratil
- Triton fit

**YN @ LO**
- Haidenbauer et al.
- $\Lambda_{YN} = 700$ MeV
- Scatt. & hypertriton

$\alpha = 0.08 \text{ fm}^4$

$h\Omega = 20$ MeV
Conclusions
Conclusions

- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... propagate uncertainties & provide feedback

- consistent **inclusion of 3N & 4N interactions** in similarity transformations & many-body calculations
  - breakthrough in treatment of 3N & 4N matrix elements

- **innovations in many-body theory**: extended reach of exact methods & improved control over approximations
  - versatile toolbox for different observables & mass ranges

- many **exciting applications** ahead...
thanks to my group & my collaborators

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  Michigan State University, USA

- **H. Hergert**, K. Hebeler  
  Ohio State University, USA

- P. Papakonstantinou  
  IPN Orsay, F

- C. Forssén  
  Chalmers University, Sweden

- H. Feldmeier, T. Neff  
  GSI Helmholtzzentrum
Happy Birthday James !!!

...and many more happy & productive visits to Darmstadt