Ab Initio Nuclear Structure Theory: Beyond the Ordinary

Robert Roth
Overview

- **Ab Initio Toolbox**
  - Similarity Renormalization Group
  - No-Core Shell Model
  - Medium-Mass Methods

- **Beyond the Ordinary**
  - Hypernuclei
    - Merging NCSM & IM-SRG
    - Sensitivity & Correlations
Ab Initio Toolbox
Ab Initio Nuclear Structure - Tools

Nuclear Structure & Reaction Observables

Many-Body Solution: NCSM, CC, IM-SRG,...

Pre-Processing: Similarity Renorm. Group

Chiral EFT: Interactions & Operators

• systematic and improvable input for all ab initio calculations
• only “selected” chiral interactions used in nuclear structure so far
• next-generation chiral EFT interactions give opportunity to quantify uncertainties

Low-Energy QCD
Ab Initio Nuclear Structure - Tools

Nuclear Structure & Reaction Observables

Many-Body Solution: NCSM, CC, IM-SRG,...

Pre-Processing: Similarity Renorm. Group

Chiral EFT: Interactions & Operators

• drastically improves convergence of many-body calculation
• induces many-body interactions that can be sizeable
• challenge: include or suppress induced many-body contributions

Low-Energy QCD
Ab Initio Nuclear Structure - Tools

- Nuclear Structure & Reaction Observables
  - Many-Body Solution: NCSM, CC, IM-SRG,...
  - Pre-Processing: Similarity Renorm. Group
  - Chiral EFT: Interactions & Operators

- Low-Energy QCD

- Different many-body methods for different mass regions and different observables
- Present frontiers: continuum & open-shell medium-mass nuclei
Chiral EFT for Nuclear Interactions

Weinberg, van Kolck, Machleidt, Entem, Meissner, Epelbaum, Krebs,...

- **NN**
  - LO: $XH$
  - NLO: $\ldots$
  - N2LO: $\ldots$
  - N3LO: $\ldots$
  - N4LO: $\ldots$

- **3N**
  - LO: —
  - NLO: —
  - N2LO: $\ldots$
  - N3LO: $\ldots$
  - N4LO: $\ldots$

- **4N**
  - LO: —
  - NLO: —
  - N2LO: —
  - N3LO: $\ldots$
  - N4LO: $\ldots$

**standard interaction:**

- NN @ N3LO (Entem&Machleidt, cutoff 500 MeV)
- 3N @ N2LO (local, cutoff 400 or 500 MeV)
# Chiral EFT for Nuclear Interactions

**LENPIC interactions:**

- consistent family of interactions from LO to N4LO with semilocal regulators

## NN

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<tr>
<th>LO</th>
<th>NLO</th>
<th>N2LO</th>
<th>N3LO</th>
<th>N4LO</th>
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## 3N

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## 4N

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<th>N2LO</th>
<th>N3LO</th>
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*Weinberg, van Kolck, Machleidt, Entem, Meissner, Epelbaum, Krebs,...*
Similarity Renormalization Group

- **continuous unitary transformation driving Hamiltonian towards diagonal form**

- **unitary transformation via flow equation**
  \[
  H_\alpha = U_\alpha^\dagger H_0 U_\alpha \rightarrow \frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha]
  \]

- **dynamic generator determines physics of transformation**
  \[
  \eta_\alpha = (2\mu)^2 \left[ T_{\text{int}}, H_\alpha \right]
  \]

- **solve flow equation using matrix representation in two- and three-body space**

- **flow parameter \( \alpha \) determines how far to go**
Need to truncate evolved Hamiltonian:

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

Variation of flow parameter provides diagnostic for omitted many-body terms.

Truncations used in the following:

- **NN+3N**
  - Use initial NN, keep evolved NN+3N

- **NN+3N**
  - Use initial NN+3N, keep evolved NN+3N

**pro:** Improves convergence of many-body calculations.

**con:** Induces many-body interactions.
No-Core Shell Model

NCSM-type approaches are the most powerful and universal ab initio methods for the p- and lower sd-shell

- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\text{max}}\hbar\Omega$
NCSM-type approaches are the most powerful and universal ab initio methods for the p- and lower sd-shell

- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\text{max}}\hbar\Omega$
  - convergence of observables w.r.t. $N_{\text{max}}$ is the only limitation and source of uncertainty

- **Importance-Truncated NCSM**: reduce NCSM model space to physically relevant basis states and extrapolate to full space a posteriori
  - increases the range of applicability of NCSM significantly

- **NCSM with Continuum**: merge NCSM for description of clusters with Resonating Group Method for description of their relative motion
  - explicitly includes continuum degrees of freedom

*(tomorrow’s talk by Petr Navrátil)*
Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)

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

Hergert et al., PRL 110, 242501 (2013)

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

parameter-free ab initio calculations with explicit chiral 3N interactions

highlights predictive power of chiral NN+3N interactions
Spectra of Oxygen Isotopes


\[ \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad \hbar \Omega = 16 \text{ MeV} \]
Medium-Mass Methods

advent of novel ab initio approaches targeting the ground state of medium-mass nuclei very efficiently

- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian
Medium-Mass Methods

- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian

- **In-Medium Similarity Renormalisation Group**: decouple many-body reference state from particle-hole excitations by SRG transformation
  - normal-ordered A-body Hamiltonian truncated at the two-body level
  - open and closed-shell nuclei can be targeted directly

- **Coupled-Cluster Theory**: ground-state is parametrised by exponential wave operator acting on single-determinant reference state
  - truncation at doubles level (CCSD) with corrections for triples contributions
  - directly applicable for closed-shell nuclei, equations-of-motion methods for open-shell

Advent of novel ab initio approaches targeting the ground-state of medium-mass nuclei very efficiently

*Tsukiyama, Bogner, Schwenk, Hergert,...*

*Hagen, Papenbrock, Dean, Piecuch, Binder,...*
Ground States of Oxygen Isotopes

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

\[ \text{experiment} \]

\[ \text{IT-NCSM} \]

Hergert et al., PRL 110, 242501 (2013)
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

Hergert et al., PRL 110, 242501 (2013)

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

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

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

\[ A \text{O} \]

different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations
systematic multi-reference IM-SRG study of even Ca and Ni isotopes

excellent agreement with best available coupled-cluster results

chiral 3N interaction changes behavior at and beyond \( ^{54}\text{Ca} \)

\( \Lambda_{3N} = 400 \text{ MeV} \)
\( \alpha = 0.04 \text{ fm}^4 (\bigcirc) \)
\( = 0.08 \text{ fm}^4 (\bullet) \)

\( E_{3\text{max}} = 14, 16 \)
Open-Shell Medium-Mass Nuclei

- two-neutron separation energies hide overall energy shift
- compares well to updated Gor'kov-GF results
- chiral 3N interaction predicts flat "drip-region" from $^{56}\text{Ca}$ to $^{60}\text{Ca}$

$S_{2n}$ [MeV] vs. $A$

- $\Lambda_{3N} = 400$ MeV
- $\Lambda_{3N} = 350$ MeV

$E_{3m}$ max = 14, 16

,parametric

$\alpha = 0.04\text{ fm}^4 (\bigcirc)$
$0.08\text{ fm}^4 (\bullet)$

Hergert et al., PRC 90, 041302(R) (2014)
Beyond the Ordinary:

Hypernuclei

with

Roland Wirth
Ab Initio Hypernuclear Structure

- precise data on ground states & spectroscopy of hypernuclei
- ab initio few-body and phenomenological shell or cluster model calculations done so far
- chiral YN & YY interactions at (N)LO are available

constrain YN interactions with hypernuclear spectroscopy

time to transfer ab initio toolbox to hypernuclei
Ab Initio Hypernuclear Structure

- Lattice QCD can be a game changer in hypernuclear physics
- Extract YN & YY phase shifts from Lattice QCD, possibly also YNN
- Compute light hypernuclei directly on the lattice

Lattice data to determine YN, YY, YNN interactions

Structure theory for consistency check and access to heavier hypernuclei
Ab Initio Toolbox for Hypernuclei

- 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 ΛΣ-coupling (larger matrices)
  - Λ-Σ mass difference and ρΣ± Coulomb included consistently

- Importance Truncated No-Core Shell Model
  - include explicit (p, n, Λ, Σ+, Σ0, Σ−) with physical masses
  - larger model spaces easily tractable with importance truncation
  - all p-shell single-Λ hypernuclei are accessible
Application: $^7\Lambda$Li

**IT-NCSM**

- **chiral NN+3N**
  - Standard
  - N3LO+N2LO
  - $\Lambda_{3N}=500$ MeV
  - $\alpha=0.08$ fm$^4$

- **chiral YN**
  - LO
  - $\Lambda_{YN}=700$ MeV
  - $\alpha=0.08$ fm$^4$

$\hbar\Omega=20$ MeV

---

**NN+3N**

$^6\text{Li}$

$^7\Lambda\text{Li}$

**YN**

Bare YN
Application: $^7\Lambda$Li

\[\begin{align*}
\text{NN+3N}_{\text{full}} & \quad \text{YN} & \quad \text{YN+YNN}_{\text{ind}} \\
\end{align*}\]

$^6\Lambda$Li

\[\begin{align*}
\text{IT-NCSM} & \\
\text{chiral NN+3N} & \text{standard} \quad \text{N3LO+N2LO} \\
\Lambda_{3N} &= 500 \text{ MeV} \\
\alpha &= 0.08 \text{ fm}^4 \\
\text{chiral YN} & \text{LO} \\
\Lambda_{YN} &= 700 \text{ MeV} \\
\alpha &= 0.08 \text{ fm}^4 \\
\hbar\Omega &= 20 \text{ MeV}
\end{align*}\]
Application: $^7\Lambda\text{Li}$

IT-NCSM

chiral NN+3N
standard
N3LO+N2LO
$\Lambda_{3N}=500$ MeV
$\alpha=0.08$ fm$^4$

chiral YN
LO
$\Lambda_{YN}=700$ MeV
$\alpha=0.08$ fm$^4$

$\Lambda$ binding energy and induced $\Lambda NN$ interaction of the same order
Application: $^9\Lambda$Be

$^{8}\text{Be}$

$^{9}\Lambda$Be

$^{9}\Lambda$Be

NN+3N\text{full}

YN

YN+YN\text{ind}

IT-NCSM

chiral NN+3N

standard

N3LO+N2LO

$\Lambda_{3N}=500 \text{ MeV}$

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

chiral YN

LO

$\Lambda_{YN}=700 \text{ MeV}$

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

$\hbar \Omega=20 \text{ MeV}$
Application: $^{13}_\Lambda C$

**IT-NCSM**

- **chiral NN+3N**
  - Standard
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  - LO
  - $\Lambda_{YN}=700$ MeV
  - $\alpha=0.08$ fm$^4$

- $\hbar\Omega=20$ MeV
Induced YNN Interactions

- **induced YNN interactions** are surprisingly large in light hypernuclei

\[ V_{\text{YNN}_{\text{ind}},\alpha} \sim 0.80 \ |B_{\Lambda}| \]
\[ V_{\text{YNN}_{\text{ind}},\alpha} \sim 0.40 \ |V_{\text{YN},\alpha}| \]
\[ V_{\text{NNN}_{\text{ind}},\alpha} \sim 0.07 \ |V_{\text{NN},\alpha}| \]

...something to do with \( \Lambda-\Sigma \) conversion?
Suppression of $\Lambda$-$\Sigma$ Conversion

- design SRG-generator that **suppresses the $\Lambda$-$\Sigma$ conversion** exclusively
- $\Sigma$ admixture in the wave functions eliminated or “integrated out”
- same large induced YNN interactions as in standard SRG
Suppression of $\Lambda$-$\Sigma$ Conversion

Origin of the Induced Terms — Wegner SRG

Two-body evolution suppresses $\Lambda$-$\Sigma$ conversion

Mechanism for inducing $YNN$?

$\uppi$- $\upupsilon$ conversion

Induced $YNN$ terms driven by suppression of $\Lambda$-$\Sigma$ conversion?

SRG evolves full coupled-channel theory to effective $\Lambda$-only theory

full theory with explicit $\Sigma$ degrees of freedom

does not include any initial $YNN$ interaction

effective $\Lambda$-only theory, $\Sigma$ fully decoupled

Strong repulsive $\Lambda NN$ interaction is induced

[Diagram showing the transition from full theory to effective $\Lambda$-only theory]
Implications for the Hyperon Puzzle

- Neutron stars reach densities, where hyperon production should be energetically favorable
- Including explicit $\Lambda$s with $\Lambda N$ interaction softens EOS - does not support $2M_\odot$ neutron star
- Possible phenomenological fix: include strongly repulsive $\Lambda NN$ interaction

Lonardoni et al.; PRL 114, 092301 (2014)
Recent Example: AFDMC

- **Auxiliary Field Diffusion Monte Carlo** calculations for hypernuclei and homogeneous matter

- **only include Λ degrees of freedom** explicitly with phenomenological ΛN and ΛNN interactions fitted to hypernuclei

- strongly repulsive ΛNN interaction shifts onset of Λ production to larger densities and **increases maximum neutron-star mass**

![Graph showing E vs. ρ and M vs. R with annotations for PNMs and ΛN + ΛNN interactions.](Lonardoni et al.; PRL 114, 092301 (2014))
How do the binding energies of hypernuclei look like with AFDMC?

- in ab initio theory with Λ and Σ degrees of freedom there is no need for strong initial YNN interactions...
- ... and there is no hyperon puzzle!
Epilogue

- thanks to my group and my collaborators

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