From Chiral EFT Interactions to Nuclear Structure... and Back

Robert Roth
From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN, 3N,... interaction plus currents
From QCD to Nuclear Structure

Nuclear Structure

Unitary / Similarity Transformation

- adapt Hamiltonian to truncated low-energy model space
  - tame short-range correlations
  - improve convergence behavior
- transform Hamiltonian & observables consistently

NN+3N Interaction from Chiral EFT

Low-Energy QCD
Nuclear Structure

- Accurate solution of the many-body problem for light & intermediate masses (NCSM, CC,...)
- Controlled approximations for heavier nuclei (MBPT,...)
- All rely on truncated model spaces & benefit from unitary transformation

Low-Energy QCD

NN+3N Interaction from Chiral EFT

Unitary / Similarity Transformation

Exact & Approx. Many-Body Methods
Nuclear Interactions from Chiral EFT
Nuclear Interactions from Chiral EFT

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

- **variations:**
  - 3N at N2LO:
    modified cutoff or LECs, \(A=3,4\) refit

- **alternatives:**
  - consistent NN+3N at N2LO:
    Epelbaum, POUNDerS
  - consistent NN+3N at N3LO:
    LENPIC collaboration
  - \(\Delta\)-full chiral EFT, YN interaction,...
Similarity
Renormalization Group
continuous transformation driving Hamiltonian to band-diagonal form with respect to a uncorrelated 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 \(^3\text{H}\)
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

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

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

significant improvement of convergence behavior

Robert Roth – TU Darmstadt – 07/2013
Hamiltonian in A-Body Space

- evolution **induces** $n$-body contributions $H^{[n]}_\alpha$ to Hamiltonian

$$H_\alpha = H^{[1]}_\alpha + H^{[2]}_\alpha + H^{[3]}_\alpha + H^{[4]}_\alpha + H^{[5]}_\alpha + \ldots$$

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

- flow-parameter $\alpha$ provides **diagnostic tool** to assess neglected higher-order contributions

---

**SRG-Evolved Hamiltonians**

<table>
<thead>
<tr>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>NN&lt;sub&gt;only&lt;/sub&gt;</strong></td>
<td>use initial NN, keep evolved NN</td>
</tr>
<tr>
<td><strong>NN + 3N&lt;sub&gt;ind&lt;/sub&gt;</strong></td>
<td>use initial NN, keep evolved NN+3N</td>
</tr>
<tr>
<td><strong>NN + 3N&lt;sub&gt;full&lt;/sub&gt;</strong></td>
<td>use initial NN+3N, keep evolved NN+3N</td>
</tr>
<tr>
<td><strong>NN + 3N&lt;sub&gt;full&lt;/sub&gt; + 4N&lt;sub&gt;ind&lt;/sub&gt;</strong></td>
<td>use initial NN+3N, keep evolved NN+3N+4N</td>
</tr>
</tbody>
</table>
Importance Truncated
No-Core Shell Model
NCSM is one of the most powerful and universal ab initio many-body methods

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

- solve \textbf{large-scale eigenvalue problem} for a few extremal eigenvalues

- \textbf{all relevant observables} can be computed from the eigenstates

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

- adaptive \textbf{importance truncation} extends the range of NCSM by reducing the model space to physically relevant states

- we have developed a \textbf{parallelized IT-NCSM/NCSM code} capable of handling 3N matrix elements up to $E_{3\text{max}} = 16$
converged NCSM calculations essentially restricted to lower/mid p-shell

full \( N_{\text{max}} = 10 \) calculation for \(^{16}\text{O}\) 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

Roth, et al; PRL 107, 072501 (2011)

$E \ [\text{MeV}]$

$N_{\text{max}}$

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

Exp.

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

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

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

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

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

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

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

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

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

$\Lambda = 1.58 \text{ fm}^{-1}$
16O: Ground-State Energies

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

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

\( N_{\text{max}} \)

\( N_{\text{max}} \)

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

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

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

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

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

caused by long-range 2\( \pi \) terms (\( c_i \))

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
\((c_E \text{ refit to } ^4\text{He binding energy})\)

\[
\begin{align*}
\text{500 MeV} & \quad c_D = -0.2 \\
& \quad c_E = -0.205 \\
\text{450 MeV} & \quad c_D = -0.2 \\
& \quad c_E = -0.016 \\
\text{400 MeV} & \quad c_D = -0.2 \\
& \quad c_E = 0.098 \\
\text{350 MeV} & \quad c_D = -0.2 \\
& \quad c_E = 0.205 \\
\end{align*}
\]

\[\alpha = 0.04 \text{ fm}^4 \quad \Lambda = 2.24 \text{ fm}^{-1}\]
\[\alpha = 0.05 \text{ fm}^4 \quad \Lambda = 2.11 \text{ fm}^{-1}\]
\[\alpha = 0.0625 \text{ fm}^4 \quad \Lambda = 2.00 \text{ fm}^{-1}\]
\[\alpha = 0.88 \text{ fm}^{-1}\]

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 $E$ vs $N_{\text{max}}$ with various markers and parameters.](image)

- $\alpha = 0.04 \text{ fm}^4$
- $\alpha = 0.0625 \text{ fm}^4$
- $\alpha = 0.08 \text{ fm}^4$
- $\alpha = 0.16 \text{ fm}^4$

$h\Omega = 24\text{ MeV}$
$^{16}$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

$\hbar \Omega = 24\text{MeV}$

$E_{4\text{max}} = 6$

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

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

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

$\alpha = 0.16\text{ fm}^4$
\( ^{16}\text{O}: \) 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

Inclusion of explicit 4N is feasible (at least partially)

Effect of SRG-induced 4N as expected

\[ E \] [MeV]

\[ N_{\text{max}} \]

\[ \hat{h} \Omega = 24 \text{MeV} \]

\[ E_{m_{\text{max}}} = 6 \]

\[ \alpha = 0.04 \text{ fm}^4 \]

\[ \alpha = 0.0625 \text{ fm}^4 \]

\[ \alpha = 0.08 \text{ fm}^4 \]

\[ \alpha = 0.16 \text{ fm}^4 \]
Ab Initio IT-NCSM Calculations for p- and sd-Shell Nuclei
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)

\[ \text{NN+3N}_{\text{ind}} \]  
(chiral NN)

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

\[ A = \{12, 14, 16, 18, 20, 22, 24, 26\} \]

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

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

experiment

IT-NCSM

parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians
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

\[ \Lambda_{3N} = 400 \text{ MeV, } \alpha = 0.08 \text{ fm}^2, \quad E_{3 \text{ max}} = 14, \quad \text{Optimal } n \Omega \]

different many-body approaches using same NN+3N Hamiltonian give consistent results

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

Hergert et al., PRL 110, 242501 (2013)
Spectroscopy of Carbon Isotopes

Forssen et al., JPG 40, 055105 (2013); Roth et al., in prep.

\[ N_{\text{max}} \]

\[ E_x \, [\text{MeV}] \]

\[ \text{Exp.} \]

\[ 10^C \]

\[ 12^C \]

\[ 14^C \]

\[ 16^C \]

\[ 18^C \]

\[ 20^C \]

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

\[ \Lambda_{3N} = 400 \, \text{MeV} \]

\[ \alpha = 0.08 \, \text{fm}^4 \]

\[ \hbar \Omega = 16 \, \text{MeV} \]
Towards Consistent Chiral N3LO Hamiltonians
starting point: numerical 3N matrix elements in partial-wave Jacobi-momentum basis

- numerical partial-wave decomposition of Skibinski et al.
- ongoing collaborative effort to produce N2LO/N3LO matrix elements (LENPIC: Cracow, Bochum, Bonn, Jülich, Ohio SU, Iowa SU, Darmstadt)

interface: transformation into Jacobi-HO representation implemented and validated

- SRG evolution can be done in Jacobi-momentum or HO basis

first application: consistent NN+3N Hamiltonian at N2LO

- NN at N2LO: Epelbaum et al., cutoffs 450,…,600 MeV, phase-shift fit $\chi^2/\text{dat} \sim 10 \ (\sim 1)$ up to 300 MeV (100 MeV)
- 3N at N2LO: Epelbaum et al., cutoffs 450,…,600 MeV, nonlocal, fit to $a(nd)$ and $E(3H)$, included up to $J=7/2$
$^{12}$C: Consistent N2LO Hamiltonians

\[ N_{\text{max}} = 8, \quad \alpha = 0.08 \text{ fm}^4, \quad h\Omega = 16 \text{ MeV} \]
$^{12}\text{C}: \text{Consistent N2LO Hamiltonians}$

![Graph showing energy levels for different Hamiltonians](graph.png)

- **Standard** (N3LO+N2LO: 500 MeV)
- **POUNDerS** (N2LO+N2LO: 500/700 MeV, 450/500 MeV, 600/500 MeV, 550/600 MeV, 450/700 MeV)
- **Epelbaum** (N2LO+N2LO: 500 MeV)

Energy levels are labeled with quantum numbers:
- $2^+ 1$
- $2^+ 0$
- $4^+ 0$
- $4^+ 9$
- $1^+ 0$
- $0^+ 0$

Parameters used:
- $N_{\text{max}} = 8$
- $\alpha = 0.08 \text{ fm}^4$
- $h\Omega = 16 \text{ MeV}$

Robert Roth – TU Darmstadt – 07/2013
$^{12}$C: Consistent N2LO Hamiltonians

\[ N_{\text{max}} = 8, \quad \alpha = 0.08 \text{ fm}^4, \quad h\Omega = 16 \text{ MeV} \]
Ab Initio
Hyper-Nuclear Structure
Motivation: Hyper-Nuclear Structure

- precision data on hypernuclear ground states and spectroscopy exists
- ab initio few-body ($A \lesssim 4$) and phenomenological shell model or cluster calculations so far
- chiral EFT interactions including hyperons at LO,NLO are available (Haidenbauer, et al.)
- constrain YN & YY interaction by ab initio hypernuclear structure calculations
Ab Initio Toolbox

■ Hamiltonian from chiral EFT
  - NN+3N: standard chiral Hamiltonian (Entem&Machleidt, Navrátil)
  - YN: LO chiral interaction (Haidenbauer et al.), NLO is available

■ 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: $^7\Lambda\text{Li}$

$^6\text{Li}$

$^7\Lambda\text{Li}$

\(E_{\text{MeV}}\)

\(N_{\text{max}}\) \(\text{Exp.}\)

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

\(N_{\text{max}}\) \(\text{Exp.}\)

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

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

NN @ N3LO
Entem & Machleidt
\(\Lambda_{NN} = 500 \text{ MeV}\)

3N @ N2LO
Navratil
\(\Lambda_{3N} = 500 \text{ MeV}\)
triton fit

Jülich’04
Haidenbauer et al.
scatt. & hypertriton

Robert Roth – TU Darmstadt – 07/2013
Application: $^7_\Lambda\text{Li}$

$^6\text{Li}$

$^7\Lambda\text{Li}$

YN @ LO
$\Lambda_{YN} = 550$ MeV

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

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

YN @ LO
Haidenbauer et al.
$\Lambda_{YN} = 550$ MeV
scatt. & hypertriton

$\alpha = 0.08$ fm$^4$

$\hbar\Omega = 20$ MeV
Application: $^7_\Lambda$Li

$^6\text{Li}$

$^7\Lambda\text{Li}$

YN @ LO
$\Lambda_{YN} = 600$ MeV

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

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

YN @ LO
Haidenbauer et al.
$\Lambda_{YN} = 600$ MeV
scatt. & hypertriton

$\alpha = 0.08$ fm$^4$

$\hbar\Omega = 20$ MeV
Application: $^7_\Lambda Li$

\[ \text{NN @ N3LO} \]
Entem&Machleidt
\[ \Lambda_{NN} = 500 \text{ MeV} \]

\[ \text{3N @ N2LO} \]
Navratil
\[ \Lambda_{3N} = 500 \text{ MeV} \]
triton fit

\[ \text{YN @ LO} \]
Haidenbauer et al.
\[ \Lambda_{YN} = 650 \text{ MeV} \]
scatt. & hypertriton

\[ \alpha = 0.08 \text{ fm}^4 \]
\[ \hbar \Omega = 20 \text{ MeV} \]
Application: \( ^7_\Lambda\text{Li} \)

- \( ^6\text{Li} \)
- chiral YN @ LO
  \( \Lambda_{YN} = 700 \text{ MeV} \)

- \( ^7_\Lambda\text{Li} \)
  \( \Lambda_{NN} = 500 \text{ MeV} \)

- 3N @ N2LO
  \( \Lambda_{3N} = 500 \text{ MeV} \)
  triton fit

- YN @ LO
  Haidenbauer et al.
  \( \Lambda_{YN} = 700 \text{ MeV} \)
  scatt. & hypertriton

\[ \alpha = 0.08 \text{ fm}^4 \]
\[ h\Omega = 20 \text{ MeV} \]

hyper-nuclear structure sets tight constraints on YN interaction

start investigating sensitivity of spectra on YN input
New Horizons...

- **nuclear structure theory connected to QCD via chiral EFT**
  - chiral EFT as universal, controlled and improvable starting point
  - consistent and optimized interactions at N2LO, N3LO,...
  - consistent similarity transformation of Hamiltonian and observables

- **innovations in ab initio many-body theory**
  - consistent inclusion of 3N (and 4N) interactions
  - precision structure and spectroscopy in p- and sd-shell (IT-NCSM,...)
  - access to the medium-mass regime (CC, IM-SRG,...)
  - ab initio hyper-nuclear structure
  - bridge to reaction theory (NCSM/RGM, NCSMC)
  - uncertainty quantification, error propagation, feedback cycle

- **many exciting applications ahead...**
epilogue

thanks to my group & my collaborators

  Institut für Kernphysik, TU Darmstadt

- P. Navrátil
  TRIUMF Vancouver, Canada

- J. Vary, P. Maris
  Iowa State University, USA

- S. Quaglioni, G. Hupin
  LLNL Livermore, USA

- P. Piecuch
  Michigan State University, USA

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

- A. Kastakonstantinou
  University of Athens, Greece

- P. Papakonstantinou
  University of Athens, Greece

- H. Feldmeier, T. Neff
  GSI Helmholtzzentrum