Towards Nuclear Structure from Consistent Chiral NN+3N Interactions

Robert Roth
Nuclear Structure Theory — Wish List

- nuclear structure & reactions as low-energy effective theory based on QCD
- robust & quantitative predictions for nuclei far-off stability
- controlled & improvable many-body approaches
- theoretical toolbox for all masses and observables
Ab Initio Nuclear Structure

Nuclear Structure Observables

Exact Ab-Initio Solutions
- few-body, no-core shell model, etc.

Approx. Many-Body Methods
- controlled & improvable schemes

Similarity Transformations
- physics-conserving transform. of observables

Chiral Interactions
- consistent & improvable NN, 3N,... interactions

Chiral Effective Field Theory
- systematic low-energy effective theory of QCD

Energy-Density-Functional Theory
- guided by chiral EFT

Low-Energy Quantum Chromodynamics

Nuclear Lattice Sim.
- chiral EFT on lattice

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PREDICTION

VALIDATION

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Low-Energy Quantum Chromodynamics
Nuclear Interactions from Chiral EFT

- **low-energy effective field theory** for relevant degrees of freedom ($\pi, N$) based on symmetries of QCD
- **long-range pion dynamics** explicitly
- short-range physics absorbed in **contact terms**, low-energy constants fitted to experiment ($NN, \pi N, ...$)
- hierarchy of **consistent NN, 3N,... interactions** (plus currents)
- **many ongoing developments**
  - 3N interaction at $N^3$LO
  - explicit inclusion of $\Delta$-resonance
  - formal issues: power counting, renormalization, cutoff choice,...

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<th>3N</th>
<th>4N</th>
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Why Similarity Transformations?

Argonne V18

\( J^\pi = 1^+, T = 0 \)

deuteron wave-function

strong coupling of low- and high-momentum modes

strong short-range correlations in many-body states
Why Similarity Transformations?

chiral N³LO
Entem & Machleidt, 500 MeV

$J^\pi = 1^+, T = 0$

momentum-space matrix elements

deuteron wave-function

Similarity Renormalization Group

**unitary transformation** of Hamiltonian \( \tilde{H}_\alpha = U_\alpha U_\alpha^\dagger H U_\alpha \)

**evolution equations** for \( \tilde{H}_\alpha \) and \( U_\alpha \) depending on generator \( \eta_\alpha \):

\[
\frac{d}{d\alpha} \tilde{H}_\alpha = \left[ \eta_\alpha, \tilde{H}_\alpha \right]
\]

\[
\frac{d}{d\alpha} U_\alpha = -U_\alpha \eta_\alpha
\]

**dynamic generator**: commutator with the operator in whose eigenbasis \( H \) shall be diagonalized

\[
\eta_\alpha = (2\mu)^2 \left[ T_{\text{int}}, \tilde{H}_\alpha \right]
\]

simplicity and flexibility are great advantages of the SRG approach

other transformation approaches (UCOM, \( V_{\text{low}k} \)) follow as special cases

continuous transformation driving Hamiltonian to band-diagonal form with respect to a chosen basis
SRG Evolution of Matrix Elements

- Convert Fock-space operator equations into **coupled evolution equations for matrix elements** in \( n \)-body Hilbert space.

- \( n = 2 \): use **antisym. relative \( LS \)-coupled two-body states**
  - momentum space: \( |q(LS)JT\rangle \)
  - harmonic oscillator: \( |n(LS)JT\rangle \)

- System of **coupled evolution equations** for each \( J^{\pi}ST \)-block

\[
\frac{d}{d\alpha} \langle n(LS)JT | \tilde{H}_\alpha | n'(L'S)JT \rangle = (2\mu)^2 \sum_{n''L''} \sum_{n'''L'''} \left[ \langle nL... | T_{\text{int}} | n''L''... \rangle \langle n''L''... | \tilde{H}_\alpha | n'''L'''... \rangle \langle n'''L'''... | \tilde{H}_\alpha | n'L'... \rangle - 2\langle nL... | \tilde{H}_\alpha | n''L''... \rangle \langle n''L''... | T_{\text{int}} | n'''L'''... \rangle \langle n'''L'''... | \tilde{H}_\alpha | n'L'... \rangle + \langle nL... | \tilde{H}_\alpha | n''L''... \rangle \langle n''L''... | \tilde{H}_\alpha | n'''L'''... \rangle \langle n'''L'''... | T_{\text{int}} | n'L'... \rangle \right]
\]

SRG Evolution in Two-Body Space

\[ \alpha = 0.000 \text{ fm}^4 \]
\[ \Lambda = \infty \text{ fm}^{-1} \]
\[ J^{\pi} = 1^+, T = 0 \]

\[ \Lambda = \infty \text{ fm}^{-1} \]

Deuteron wave-function

\[ \phi_L(r) [\text{arb. units}] \]

\[ r [\text{fm}] \]

\[ L = 0 \]
\[ L = 2 \]
\[ \alpha = 0.320 \text{ fm}^4 \]
\[ \Lambda = 1.33 \text{ fm}^{-1} \]
\[ J^\pi = 1^+, T = 0 \]

suppression of off-diagonal coupling \( \hat{=} \) pre-diagonalization

elimination of short-range correlations
SRG Evolution of Matrix Elements

- convert Fock-space operator equations into **coupled evolution equations for matrix elements** in $n$-body Hilbert space

- $n = 3$: use antisym. Jacobi-coordinate three-body states
  - harmonic oscillator: $|Ei^\pi T\rangle$

- system of **coupled evolution equations** for each $J^\pi T$-block

$$\frac{d}{d\alpha}\langle Ei^\pi T|\hat{H}_\alpha|E'i^'J^\pi T\rangle = (2\mu)^2 \sum_{E''i''}^{E_{SRG}} \sum_{E'''i'''}^{E_{SRG}} \left[ \langle Ei...|T_{int}|E''i''...\rangle \langle E''i''...|\hat{H}_\alpha|E'''i'''...\rangle \langle E'''i'''...|\hat{H}_\alpha|E'i'...\rangle 
- 2\langle Ei...|\hat{H}_\alpha|E''i''...\rangle \langle E''i''...|T_{int}|E'''i'''...\rangle \langle E'''i'''...|\hat{H}_\alpha|E'i'...\rangle 
+ \langle Ei...|\hat{H}_\alpha|E''i''...\rangle \langle E''i''...|\hat{H}_\alpha|E'''i'''...\rangle \langle E'''i'''...|T_{int}|E'i'...\rangle \right]$$

- we use $E_{SRG} = 40$ for $J \leq 5/2$ and ramp down to 24 in steps of 4 (sufficient to converge the intermediate sums for $\hbar\Omega \gtrsim 16$ MeV)
SRG Evolution in Three-Body Space

$\alpha = 0.000 \text{ fm}^4$

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

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

3B-Jacobi HO matrix elements

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

suppression of off-diagonal coupling
\( \hat{=} \) pre-diagonalization

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

significant improvement of convergence behavior

**Calculations in A-Body Space**

- **cluster decomposition**: decompose evolved Hamiltonian from 2B/3B space into irreducible $n$-body contributions $\tilde{H}_\alpha^{[n]}$

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

- **cluster truncation**: can construct cluster-orders up to $n = 3$ from evolution in 2B and 3B space, have to discard $n > 3$

  - only the **full evolution in A-body space** is formally unitary and conserves A-body energy eigenvalues (independent of $\alpha$)
  
  - $\alpha$-dependence of eigenvalues of the Hamiltonian measures impact of the omitted induced many-body interactions

  $\alpha$-variation provides a **diagnostic tool** to assess the omitted induced many-body interactions
1. **Computation of initial 2B/3B-Jacobi HO matrix elements of chiral NN+3N interactions**
   - We use Petr Navratil’s ManyEff code for computing 3B-Jacobi matrix elements and corresponding CFPs.

2. **SRG evolution in 2B/3B space and cluster decomposition**
   - Efficient implementation using adaptive ODE solver & BLAS; largest block takes a few hours on single node.

3. **Transformation of 2B/3B Jacobi HO matrix elements into JT-coupled representation**
   - Formulated transformation directly into JT-coupled scheme; highly efficient implementation; can handle $E_{3,\text{max}} = 16$ in JT-coupled scheme.

4. **Data management and on-the-fly decoupling in many-body codes**
   - Invented optimized storage scheme for fast on-the-fly decoupling; can keep all matrix elements up to $E_{3,\text{max}} = 16$ in memory.
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No-Core Shell Model (NCSM)

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 $N_{\text{max}} \& A$

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

- we have developed a parallelized IT-NCSM/NCSM code capable of handling 3N matrix elements up to $E_{3\text{max}} = 16$
Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full 10 or 12ℏΩ calculation for 16O not really feasible (basis dimension > 10^{10})

**Importance Truncation**
reduce model space to the relevant basis states using an a priori importance measure derived from MBPT

![Graph showing energy levels for 16O with IT-NCSM and full NCSM calculations.](image-url)
Importance Truncation: General Idea

- given an initial approximation $|\Psi_{\text{ref}}^{(m)}\rangle$ for the target states

- **measure the importance** of individual basis state $|\Phi_\nu\rangle$ via first-order multiconfigurational perturbation theory

$$k_\nu^{(m)} = -\frac{\langle \Phi_\nu | H | \Psi_{\text{ref}}^{(m)} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

- construct **importance truncated space** spanned by basis states with $|k_\nu^{(m)}| \geq k_{\text{min}}$ and solve eigenvalue problem

- **sequential scheme**: construct next $N_{\text{max}}$ using previous eigenstates as reference

- **a posteriori** **threshold extrapolation** and perturbative correction used to recover contributions from discarded basis states

  for $k_{\text{min}} \to 0$ the full NCSM model space and thus the exact solution is recovered
Threshold Extrapolation

- do calculations for a sequence of importance thresholds $\kappa_{\text{min}}$
- observables show smooth threshold dependence
- systematic approach to the full NCSM limit
- use a posteriori extrapolation $\kappa_{\text{min}} \to 0$ of observables to account for effect of excluded configurations

**Graphical Representation**

- $H_{\text{int}}$ for $^{16}\text{O}$
  - SRG(N3LO)
  - $\alpha = 0.04 \text{ fm}^4$
  - $\hbar \Omega = 20 \text{ MeV}$
  - $N_{\text{max}} = 8$

- $H_{\text{cm}}$
- $J$

**Axes**
- $\kappa_{\text{min}} \ [10^{-5}]$
- [MeV]

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Low-Energy Quantum Chromodynamics
A Tale of Three Hamiltonians

**Initial Hamiltonian**

- **NN**: chiral interaction at N$^3$LO (Entem & Machleidt, 500 MeV)
- **3N**: chiral interaction at N$^2$LO ($c_D$, $c_E$ from $^3$H binding & half-life)

**SRG-Evolved Hamiltonians**

- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and three-body terms
- **NN+3N-full**: start with NN+3N initial Hamiltonian and keep two- and three-body terms

\[\alpha\text{-variation provides a diagnostic tool to assess the contributions of omitted many-body interactions}\]
**4He: Ground-State Energies**

**NN only**
- **strong $\alpha$-dependence:** induced 3N interactions

- $\hbar\Omega = 20$ MeV

**NN+3N-induced**
- **no $\alpha$-dependence:** no induced 4N interactions

**NN+3N-full**
- **no $\alpha$-dependence:** no induced 4N interactions

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

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

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

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

- $\alpha = 0.16 \text{ fm}^4$
  - $\Lambda = 1.58 \text{ fm}^{-1}$
$^6\text{Li}: \text{Ground-State Energies}$

**NN only**

$E [\text{MeV}]$

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

$N_{\text{max}}$

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

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

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

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**NN+3N-induced**

**NN+3N-full**

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

**NN only**

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

**NN+3N-induced**

- Inclusion of initial 3N interaction results in induced 4N terms

**NN+3N-full**

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

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

- $\alpha = 0.0625 \text{ fm}^4$
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- $\alpha = 0.16 \text{ fm}^4$
- $\Lambda = 1.58 \text{ fm}^{-1}$

- Exp.
\textbf{16O: Ground-State Energies}

\begin{align*}
\hbar \Omega &= 20 \text{ MeV} \\
E_{\text{NN only}}(N_{\text{max}}) &= \cdots \\
E_{\text{NN+3N-induced}}(N_{\text{max}}) &= \cdots \\
E_{\text{NN+3N-full}}(N_{\text{max}}) &= \cdots \\
\end{align*}

\begin{align*}
\alpha &= 0.04 \text{ fm}^4 \\
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\end{align*}

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\end{align*}

\begin{align*}
\alpha &= 0.16 \text{ fm}^4 \\
\Lambda &= 1.58 \text{ fm}^{-1} \\
\end{align*}

$^{16}$O: Energy vs. Flow Parameter

- **initial NN Hamiltonian**
  - induced 3N interactions are significant
  - no indication of induced 4N
  - NN+3N-induced unitarily equivalent to initial NN

- **initial NN+3N Hamiltonian**
  - induced 4N interactions are sizable in upper p-shell
  - generated by long-range $2\pi$ terms of initial 3N interaction
  - design modified SRG generator to suppress induced 4N
$^6\text{Li}$: Excitation Energies

**NN only**

- $\alpha = 0.04 \text{ fm}^4$
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**NN+3N-induced**

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$h\Omega = 20 \text{ MeV}$
Spectroscopy of $^{12}$C

IT-NCSM gives access to complete spectroscopy of p- and sd-shell nuclei starting from chiral NN+3N interactions
Spectroscopy of $^{12}$C

- IT-NCSM gives access to complete spectroscopy of p- and sd-shell nuclei starting from chiral NN+3N interactions

- Spectra largely insensitive to induced 4N interactions
Spectroscopy of $^{16}$C

Recent experiments (Petri et al.) confirm $B(E2)$ pattern obtained in the NN+3N-full calculation

<table>
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<tr>
<th>$E_x$ [MeV]</th>
<th>$N_{max}$</th>
<th>Exp.</th>
<th>$B(E2)$ [rel. units]</th>
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<th>NN+3N-ind.</th>
<th>NN+3N-full</th>
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Conclusions
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- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... some issues remain

- consistent **inclusion of 3N interactions** in similarity transformations & many-body calculations
  - breakthrough in computation & handling of 3N 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...
Epilogue

thank you to my group & my collaborators

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