Ab Initio Nuclear Structure

with

SRG-Evolved NN plus 3N Interactions

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Nuclear Structure

- Chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- Provides consistent NN & 3N interaction plus currents
  - In the following:
    - NN at $N^3$LO (Entem & Machleidt, 500 MeV)
    - 3N at $N^2$LO (low-energy constants $c_D$ & $c_E$ from triton fit)
Nuclear Structure

**Unitarily Transformed Hamiltonian**
- adapt Hamiltonian to truncated low-energy model space
  - tame short-range correlations
  - improve convergence behavior
- transform Hamiltonian & observables consistently
- conserve experimentally constrained few-body properties

**NN+3N Interaction from Chiral EFT**

**Low-Energy QCD**
From QCD to Nuclear Structure

Nuclear Structure

- Exact & Approx. Many-Body Methods
  - ‘exact’ solution of the many-body problem for light & intermediate masses (NCSM, CC,...)
  - controlled approximations for heavier nuclei (HF & MBPT,...)
  - all rely on restricted model spaces & benefit from unitary transformation

- Unitarily Transformed Hamiltonian

- NN+3N Interaction from Chiral EFT

- Low-Energy QCD
From QCD to Nuclear Structure

Nuclear Structure

- Exact & Approx. Many-Body Methods
- Unitarily Transformed Hamiltonian
- NN+3N Interaction from Chiral EFT

Low-Energy QCD

Focus on consistent inclusion of chiral 3N interaction
Evolution of Nuclear Many-Body Forces with the Similarity Renormalization Group

E. D. Jurgenson, P. Navrátil, and R. J. Furnstahl

$^3\text{H}$

\begin{align*}
N^3\text{LO (500 MeV)}
\end{align*}

\begin{align*}
\text{NN (+ NNN-induced)}
\end{align*}

\begin{align*}
\text{NN + NNN}
\end{align*}

$^4\text{He}$

\begin{align*}
N^3\text{LO (500 MeV)}
\end{align*}

\begin{align*}
\text{NN + NNN}
\end{align*}
Overview

- Unitarily Transformed NN+3N Hamiltonians
  - Similarity Renormalization Group
  - consistent transformation of chiral NN+3N interactions

- Exact Ab-Initio Calculations
  - Importance-Truncated NCSM
  - test of SRG-transformed chiral NN+3N interactions throughout the p-shell

- Approximate Many-Body Methods
  - Hartree-Fock & Perturbation Theory
  - ground-state systematics throughout the nuclear chart using SRG-transformed chiral NN+3N interactions
Unitarily Transformed NN+3N Hamiltonians

Similarity Renormalization Group

Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
evolution of the Hamiltonian to band-diagonal form with respect to uncorrelated many-body basis

- **unitary transformation** of Hamiltonian:
  \[ \tilde{H}_\alpha = U_\alpha \dagger H U_\alpha \]

- **evolution equations** for \( \tilde{H}_\alpha \) and \( U_\alpha \) depending on generator \( \eta_\alpha \)
  \[
  \frac{d}{d\alpha} \tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha] \\
  \frac{d}{d\alpha} U_\alpha = -U_\alpha \eta_\alpha
  \]

- **dynamic generator**: commutator with the operator in whose eigenbasis \( H \) shall be diagonalized
  \[ \eta_\alpha = (2\mu)^2 [T_{\text{int}}, \tilde{H}_\alpha] \]
SRG Evolution of Matrix Elements

- represent operator equation in \textit{n-body Jacobi HO basis} \(|EiJ^\pi T\)
  
  \(n = 2\): relative LS-coupled HO states: \(|E(\text{LS})J^\pi T\)
  
  \(n = 3\): antisymmetrized Jacobi-coordinate HO states: \(|EiJ^\pi T\)

- system of \textbf{coupled evolution equations} for each \((J^\pi T)\)-block

\[
\frac{d}{d\alpha} \langle EiJ^\pi T | \tilde{H}_\alpha | E'iJ^\pi T \rangle = (2\mu)^2 \sum_{E''} E_{\text{SRG}} \sum_{i''} E_{\text{SRG}} \left[ \langle EiJ^\pi T | T_{\text{int}} | E''i''J^\pi T \rangle \langle E''i''J^\pi T | \tilde{H}_\alpha | E'jJ^\pi T \rangle 
- 2 \langle EiJ^\pi T | \tilde{H}_\alpha | E''i''J^\pi T \rangle \langle E''i''J^\pi T | T_{\text{int}} | E'jJ^\pi T \rangle \langle E'jJ^\pi T | \tilde{H}_\alpha | E'iJ^\pi T \rangle 
+ \langle EiJ^\pi T | \tilde{H}_\alpha | E''i''J^\pi T \rangle \langle E''i''J^\pi T | \tilde{H}_\alpha | E'jJ^\pi T \rangle \langle E'jJ^\pi T | T_{\text{int}} | E'iJ^\pi T \rangle \right]
\]

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

\( \alpha = 0.00 \text{ fm}^4 \)
\( \Lambda = \infty \text{ fm}^{-1} \)

\( J^{\pi} = 1^+, T = 0, \hbar \Omega = 28 \text{ MeV} \)

2B-Jacobi HO matrix elements

momentum space \( ^3S_1 \)
SRG Evolution in Two-Body Space

\[ \alpha = 0.32 \text{ fm}^4 \]
\[ \Lambda = 1.33 \text{ fm}^{-1} \]
\[ J^{\pi} = 1^+, T = 0, \hbar\Omega = 28 \text{ MeV} \]

2B-Jacobi HO matrix elements

momentum space \( ^3S_1 \)
\[ \alpha = 0.00 \text{ fm}^4 \]
\[ \Lambda = \infty \text{ fm}^{-1} \]
\[ J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar \Omega = 28 \text{ MeV} \]
$\alpha = 0.32 \text{ fm}^4$

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

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

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

3B-Jacobi HO matrix elements

$E$, $\hbar \Omega = 28 \text{ MeV}$
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** conserves A-body energy eigenvalues and, thus, independent of $\alpha$
  
  - $\alpha$-dependence of eigenvalues of the truncated Hamiltonian measures impact of omitted many-body interactions

  $\alpha$-variation provides a **diagnostic tool** to assess the contributions of omitted 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; 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
Exact Ab Initio Calculations

Importance Truncated NCSM

NCSM is one of the most powerful and universal exact ab initio methods

- compute low-lying eigenvalues of the Hamiltonian in a **model space of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\text{max}}\hbar\Omega$

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

- range of applicability limited by **factorial growth** of Slater-determinant basis with $N_{\text{max}}$ and $A$

- 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 $E_{3\text{max}} = 16$
Converged NCSM calculations essentially restricted to lower/mid p-shell.

Full 10 or 12ℏΩ calculation for $^{16}$O not really feasible (basis dimension $> 10^{10}$).

**Importance Truncation**

Reduce NCSM space to the relevant basis states using an *a priori* importance measure derived from MBPT.
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

\[
\kappa^{(m)}_\nu = -\frac{\langle \Phi_\nu | H | \psi_{\text{ref}}^{(m)} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}
\]

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

- **sequential scheme**: construct importance truncated space for next $N_{\text{max}}$ using previous eigenstates as reference $|\psi_{\text{ref}}^{(m)}\rangle$

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

IT-NCSM with SRG-Evolved Chiral NN+3N Interactions
**A Tale of Three Hamiltonians**

- **NN only**: start with NN-only initial Hamiltonian and evolve in two-body space

\[
\hat{H}^{\text{NN-only}}_{\alpha} = T_{\text{int}} + \tilde{T}_{\text{int,}\alpha}^{[2]} + \tilde{V}_{\text{NN,}\alpha}^{[2]}
\]

- **NN+3N-induced**: start with NN-only initial Hamiltonian and evolve in three-body space

\[
\hat{H}^{\text{NN+3N-induced}}_{\alpha} = T_{\text{int}} + \tilde{T}_{\text{int,}\alpha}^{[2]} + \tilde{V}_{\text{NN,}\alpha}^{[2]} + \tilde{T}_{\text{int,}\alpha}^{[3]} + \tilde{V}_{\text{NN,}\alpha}^{[3]}
\]

- **NN+3N-full**: start with NN+3N initial Hamiltonian and evolve in three-body space

\[
\hat{H}^{\text{NN+3N-full}}_{\alpha} = T_{\text{int}} + \tilde{T}_{\text{int,}\alpha}^{[2]} + \tilde{V}_{\text{NN,}\alpha}^{[2]} + \tilde{T}_{\text{int,}\alpha}^{[3]} + \tilde{V}_{\text{NN,}\alpha}^{[3]}
\]

\(\alpha\)-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions.
$^4$He: Ground-State Energies

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

$h\Omega = 20$ MeV

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

- $\alpha = 0.04\,\text{fm}^4$, $\Lambda = 2.24\,\text{fm}^{-1}$
- $\alpha = 0.05\,\text{fm}^4$, $\Lambda = 2.11\,\text{fm}^{-1}$
- $\alpha = 0.0625\,\text{fm}^4$, $\Lambda = 2.00\,\text{fm}^{-1}$
- $\alpha = 0.08\,\text{fm}^4$, $\Lambda = 1.88\,\text{fm}^{-1}$
- $\alpha = 0.16\,\text{fm}^4$, $\Lambda = 1.58\,\text{fm}^{-1}$
\[ \hbar \Omega = 20 \text{ MeV} \]

\[ \alpha = 0.04 \text{ fm}^4 \quad \Lambda = 2.24 \text{ fm}^{-1} \]
\[ \alpha = 0.05 \text{ fm}^4 \quad \Lambda = 2.11 \text{ fm}^{-1} \]
\[ \alpha = 0.0625 \text{ fm}^4 \quad \Lambda = 2.00 \text{ fm}^{-1} \]
\[ \alpha = 0.08 \text{ fm}^4 \quad \Lambda = 1.88 \text{ fm}^{-1} \]
\[ \alpha = 0.16 \text{ fm}^4 \quad \Lambda = 1.58 \text{ fm}^{-1} \]
$^{12}$C: Ground-State Energies

**NN only**

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

**NN+3N-induced**

- **no $\alpha$-dependence:**
  - no induced 4N contrib.

**NN+3N-full**

- **some $\alpha$-dependence:**
  - induced 4N interactions

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

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

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

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

- $\alpha = 0.16 \text{ fm}^4$
  - $\Lambda = 1.58 \text{ fm}^{-1}$
16O: Ground-State Energies

**NN only**

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

**NN+3N-induced**

- no $\alpha$-dependence:
  - no induced 4N contrib.

**NN+3N-full**

- sizable $\alpha$-dependence:
  - induced 4N interactions

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

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

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

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

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

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

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

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

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

$\Lambda = 1.58\text{ fm}^{-1}$
$^{16}O$: Energy vs. Flow Parameter

- **NN only**: strong $\alpha$-dependence $\Rightarrow$ significant induced 3N contributions

- **NN+3N-induced**: no $\alpha$-dependence $\Rightarrow$ all relevant induced terms from initial NN captured at 3N level

- **NN+3N-full**: sizable $\alpha$-dependence $\Rightarrow$ additional induced terms caused by initial 3N appear at 4N level

$h\Omega = 20$ MeV
$^{16}\text{O}$ & $^4\text{He}$: Energy vs. Flow Parameter

\begin{align*}
\hbar\Omega &= 20 \text{ MeV} \\
E_\infty &\text{ [MeV]}
\end{align*}

- $^{16}\text{O}$
- $^4\text{He}$

- $\hbar\Omega = 20 \text{ MeV}$
- $E_\infty$ [MeV]

- $0$ to $0.16$ [$\alpha$ [fm$^4$]]
$^6\text{Li}$: Excitation Energies

NN only

NN+3N-induced

NN+3N-full

$E_x$ [MeV] vs. $N_{\text{max}}$

$h\Omega = 20$ MeV

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

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

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

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

$\alpha = 0.15 \text{ fm}^4$
$\Lambda = 1.58 \text{ fm}^{-1}$
$^{12}\text{C}$: Excitation Energies

**NN only**

- $E_x [\text{MeV}]$

- $N_{\text{max}}$

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

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

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

**NN+3N-induced**

- $E_x [\text{MeV}]$

- $N_{\text{max}}$

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

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

**NN+3N-full**

- $E_x [\text{MeV}]$

- $N_{\text{max}}$

- $\alpha = 0.16 \text{ fm}^4$
  - $\Lambda = 1.58 \text{ fm}^{-1}$
$^{12}$C: Spectroscopy

- spectroscopy of heavy Carbon isotopes (e.g., $^{16}$C, $^{18}$C) next...

\[ \hbar \Omega = 20 \text{ MeV} \]
\[ \alpha = 0.08 \text{ fm}^4 \]
\[ \Lambda = 1.88 \text{ fm}^{-1} \]
Conclusions
Conclusions

- ab initio nuclear structure calculations with consistently SRG-evolved chiral NN+3N interactions
  - consistent SRG evolution up to the 3N level
  - efficient transformation and management of JT-coupled 3N matrix elements
  - IT-NCSM with full 3N interactions up to $N_{\text{max}} = 12 \ (14)$ for all p-shell nuclei (and lower sd-shell)

- indications that induced 4N contributions resulting from initial 3N interaction become significant beyond mid-p-shell

- use modified SRG generators to suppress induced 4N contributions from the outset

- many exciting applications ahead...
Epilogue

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