Ab Initio Nuclear Structure for Light and Medium-Mass Nuclei

Sven Binder
INSTITUT FÜR KERNPHYSIK

TECHNISCHE UNIVERSITÄT DARMSTADT
Nature of the Nuclear Interaction

$\rho_0^{-1/3} = 1.8\text{fm}$
NN-interaction is **not fundamental**

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\[ \sim 1.6 \text{fm} \]
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- acts only if the nucleons overlap, i.e. at **short ranges**

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Nature of the Nuclear Interaction

- NN-interaction is **not fundamental**
- analogous to **van der Waals** interaction between neutral atoms
- induced via mutual **polarization** of quark & gluon distributions
- acts only if the nucleons overlap, i.e. at **short ranges**
- genuine **3N-interaction** is important

\[ \rho_0^{-1/3} = 1.8 \text{fm} \]
Nuclear Interactions from Chiral EFT
- low-energy **effective field theory**
  for relevant degrees of freedom \((\pi, N)\)
  based on symmetries of QCD
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- long-range **pion dynamics** explicitly
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- hierarchy of **consistent NN, 3N,… interactions** (plus currents)
Nuclear Interactions from Chiral EFT

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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
#### Nuclear Structure

<table>
<thead>
<tr>
<th>NN</th>
<th>3N</th>
<th>4N</th>
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</thead>
<tbody>
<tr>
<td>LO</td>
<td>X</td>
<td>—</td>
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<tr>
<td>NLO</td>
<td>H</td>
<td>—</td>
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<tr>
<td>N^2LO</td>
<td>—</td>
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<tr>
<td>N^3LO</td>
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- Derive consistent 2N & 3N forces from chiral EFT with nucleons and pions as DOF

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

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

Nuclear Structure

- Unitarily Transformed Hamiltonian
  - adapt Hamiltonian to truncated low-energy model space

NN+3N Interaction from Chiral EFT

Low-Energy QCD
From QCD to Nuclear Structure

Nuclear Structure

- Exact & Approx. Many-Body Methods
  - ab initio 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
Similarity Renormalization Group

Continuous transformation driving Hamiltonian to band-diagonal form with respect to a chosen basis

- **Unitary transformation** of Hamiltonian (and other observables)
  \[ \tilde{H}_\alpha = U_\alpha^\dagger H U_\alpha \]

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

- **Dynamic generator**: commutator with the operator in whose eigenbasis \( H \) shall be diagonalized
  \[ \eta_\alpha = (2\mu)^2 [T_{\text{int}}, \tilde{H}_\alpha] \]
**Similarity Renormalization Group**

Continuous transformation driving **Hamiltonian to band-diagonal form** with respect to a chosen basis.

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

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

Simplicity and flexibility are great advantages of the SRG approach.

Solve SRG evolution equations using two- & three-body matrix representation.
SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

chiral NN+3N
$N^3$LO + $N^2$LO, triton-fit, 500 MeV

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

NCSM ground state $^3$H

$E [\text{MeV}]$

$N_{\text{max}}$

$E' \rightarrow E \rightarrow 18 \rightarrow 20 \rightarrow 22 \rightarrow 24 \rightarrow 26 \rightarrow 28$

$(E, i')$

$(E, i)$

$0 \rightarrow 2 \rightarrow 4 \rightarrow 6 \rightarrow 8 \rightarrow 10 \rightarrow 12 \rightarrow 14 \rightarrow 16 \rightarrow 18 \rightarrow 20$
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

3B-Jacobi HO matrix elements

\[ \alpha = 0.010 \text{fm}^4 \]
\[ \Lambda = 3.16 \text{fm}^{-1} \]

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

NCSM ground state \(^3\)H
SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

\[ \alpha = 0.020 \text{ fm}^4 \]
\[ \Lambda = 2.66 \text{ fm}^{-1} \]

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

NCSM ground state \(^3\text{H}\)
SRG Evolution in Three-Body Space

\[ \alpha = 0.040 \text{ fm}^4 \]
\[ \Lambda = 2.24 \text{ fm}^{-1} \]

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

3B-Jacobi HO matrix elements

NCSM ground state \(^3\text{H}\)
SRG Evolution in Three-Body Space

\[ \alpha = 0.080 \text{ fm}^4 \]
\[ \Lambda = 1.88 \text{ fm}^{-1} \]

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

3B-Jacobi HO matrix elements

NCSM ground state $^3\text{H}$
SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

\[ \alpha = 0.160 \text{ fm}^4 \]
\[ \Lambda = 1.58 \text{ fm}^{-1} \]
\[ J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar \Omega = 28 \text{ MeV} \]

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 \(^3\text{H}\)
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

\[ E \rightarrow 18, 20, 22, 24, 26, 28 \]

\[ (E, \imath) \]

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

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

\[ 0 \rightarrow 2 \rightarrow 4 \rightarrow 6 \rightarrow 8 \rightarrow 10 \rightarrow 12 \rightarrow 14 \rightarrow 16 \rightarrow 18 \rightarrow 20 \]

\[ -8 \rightarrow -6 \rightarrow -4 \rightarrow -2 \rightarrow 0 \rightarrow 2 \]
Calculations in A-Body Space

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

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

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

Three 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 induced three-body terms

- **NN+3N-full**: start with NN+3N initial Hamiltonian and keep two- and all three-body terms
Calculations in A-Body Space

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

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

- truncation of cluster series inevitable — formally destroy $\alpha$-unitarity
  and invariance of energy eigenvalues (independence of $\alpha$)

$\alpha$-variation provides a diagnostic tool to assess
the contributions of omitted many-body interactions

Three SRG-Evolved Hamiltonians

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

- **NN+3N-full**: start with NN+3N initial Hamiltonian and keep two-
and all three-body terms
Importance-Truncated No-Core Shell Model

No-Core Shell Model — Basics

- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states (m-scheme)

$$|\psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\text{max}}\hbar\Omega$
No-Core Shell Model — Basics
\{ |i\rangle \}

\[ e_i = 2n_i + l_i \]
The No-Core Shell Model — Basics

\[\{ |i\rangle \}\]

\[e_i = 2n_i + l_i\]
No-Core Shell Model — Basics

\[ \{ |i\rangle \} \]

\[ e_i = 2n_i + l_i \]

\[ |\Phi_0\rangle \]

\[ |\Phi_v\rangle \]

\[ X_v = 3 \hbar \Omega \]
No-Core Shell Model — Basics

\( \{ |i\rangle \} \)

\( e_i = 2n_i + l_i \)

\( |\Phi_0\rangle \)

\( X_\nu = 3 \hbar \Omega \)

\( |\Phi_\mu\rangle \)

\( X_\mu = (2 + 3 + 5) \hbar \Omega \)
No-Core Shell Model — Basics

- model space:
  \[ \nu = \text{span}\left\{ |\Phi_\nu\rangle : X_\nu \leq N_{\text{max}} \hbar \Omega \right\} \]

- "low-energy part" of the many-body Hilbert space

- allows separation of center-of-mass and intrinsic degrees of freedom

\[
|\Phi_\nu\rangle \quad X_\nu = 3 \hbar \Omega
\]

\[
|\Phi_\mu\rangle \quad X_\mu = (2 + 3 + 5) \hbar \Omega
\]
No-Core Shell Model — Basics

- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states (m-scheme)

$$|\psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\text{max}} \hbar \Omega$

- numerical solution of **matrix eigenvalue problem** for the intrinsic Hamiltonian $H$ within truncated model space

$$H |\psi\rangle = E |\psi\rangle \rightarrow \begin{pmatrix} \vdots & \langle \Phi_\nu| H |\Phi_\mu\rangle & \vdots \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} C_\mu \\ \vdots \\ \vdots \end{pmatrix} = E \begin{pmatrix} C_\nu \\ \vdots \\ \vdots \end{pmatrix}$$

- model spaces of **up to $10^9$ basis states** are used routinely
Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full $10\hbar\Omega$ calculation for $^{16}\text{O}$ getting very difficult (basis dimension $> 10^{10}$)

![Graph showing energy levels for $^{16}\text{O}$ as a function of $N_{\text{max}}$. The graph indicates a linear decrease in energy with increasing $N_{\text{max}}$. Key points include:

- $E_{\text{NN-only}} = -110 \text{ MeV}$
- $\hbar\Omega = 20 \text{ MeV}$
- $\alpha = 0.04 \text{ fm}^4$]
Importance Truncated NCSM

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**Importance Truncation**

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

![Graph showing ground-state energies for $^4$He with different parameters.](image)

- $\hbar \Omega = 20$ MeV
- $N_{\text{max}}$ values range from 2 to 16, with a continuum limit at $\infty$.
- Various curves represent different values of $\alpha$ and $\Lambda$:
  - $\alpha = 0.04 \text{ fm}^4$, $\Lambda = 2.24 \text{ fm}^{-1}$
  - $\alpha = 0.05 \text{ fm}^4$, $\Lambda = 2.11 \text{ fm}^{-1}$
  - $\alpha = 0.0625 \text{ fm}^4$, $\Lambda = 2.00 \text{ fm}^{-1}$
  - $\alpha = 0.08 \text{ fm}^4$, $\Lambda = 1.88 \text{ fm}^{-1}$
  - $\alpha = 0.16 \text{ fm}^4$, $\Lambda = 1.58 \text{ fm}^{-1}$
$^4\text{He}: \text{Ground-State Energies}$

**NN only**

- **Strong $\alpha$-dependence:** induced 3N interactions

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

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

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

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$^4$He: Ground-State Energies

**NN only**

**NN+3N-induced**

![Plot of ground-state energies](image)

- **Strong $\alpha$-dependence:** induced 3N interactions

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

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

- $\alpha = 0.05 \text{ fm}^4$
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- $\Lambda = 1.88 \text{ fm}^{-1}$

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\[ ^4\text{He}: \text{Ground-State Energies} \]

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

\[ E \text{ [MeV]} \]
\[ \hbar \Omega = 20 \text{ MeV} \]

\[ N_{\text{max}} \]
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\[ \alpha = 0.16 \text{ fm}^4 \]
\[ \Lambda = 1.58 \text{ fm}^{-1} \]

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

**Exp.**
$^4$He: Ground-State Energies

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

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

$\hbar\Omega = 20$ MeV

**NN+3N-full**

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

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

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

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

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

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

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

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

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

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

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

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

- Exp.
$^6\text{Li}:\text{ Ground-State Energies}$

**NN only**

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

**NN+3N-induced**

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

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

**NN+3N-full**

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

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

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

**NN only**

- $\hbar \Omega = 20 \text{ MeV}$
- $N_{\text{max}}$ values: 2, 4, 6, 8, 10, 12, 14, $\infty$

**NN+3N-induced**

- $\alpha = 0.04 \text{ fm}^4$, $\Lambda = 2.24 \text{ fm}^{-1}$
- $\alpha = 0.05 \text{ fm}^4$, $\Lambda = 2.11 \text{ fm}^{-1}$
- $\alpha = 0.0625 \text{ fm}^4$, $\Lambda = 2.00 \text{ fm}^{-1}$
- $\alpha = 0.08 \text{ fm}^4$, $\Lambda = 1.88 \text{ fm}^{-1}$

**NN+3N-full**

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

**Exp.**

- $E$ in MeV, $N_{\text{max}}$ values: 2, 4, 6, 8, 10, 12, $\infty$
$^{16}\text{O}: \text{Ground-State Energies}$

**NN only**

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

**NN+3N-induced**

- $\alpha = 0.04 \text{ fm}^4$
- $\Lambda = 2.24 \text{ fm}^{-1}$
- $\alpha = 0.05 \text{ fm}^4$
- $\Lambda = 2.11 \text{ fm}^{-1}$
- $\alpha = 0.0625 \text{ fm}^4$
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- $\Lambda = 1.58 \text{ fm}^{-1}$

**NN+3N-full**

- Exp.
\[ O: \text{Ground-State Energies} \]

**NN only**

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

**NN+3N-induced**

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

**NN+3N-full**

- clear signature of induced 4N originating from initial 3N

caused by long-range \(2\pi\) terms \(c_i\)
$^{16}\text{O}: \text{Ground-State Energies}$

**NN only**

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

**NN+3N-induced**

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

- Exp.

---

3N interaction with 400 MeV cutoff, $c_E$ refitted to $^4\text{He}$ ground state
Spectroscopy of $^{12}$C

$E_x$ [MeV] vs $N_{max}$ for:
- **NN only**
- **NN+3N-induced**
- **NN+3N-full**

$\hbar \Omega = 16$ MeV

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

$\alpha = 0.08 \text{ fm}^4$
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Spectroscopy of $^{12}$C

$\hbar\Omega = 16$ MeV

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

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$\Lambda = 1.88 \text{ fm}^{-1}$
Spectroscopy of $^{12}\text{C}$

**NN only**

**NN+3N-induced**

**NN+3N-full**

$E_x$ [MeV]

$N_{\text{max}}$

$N_{\text{max}}$

$N_{\text{max}}$

$\hbar \Omega = 16 \text{ MeV}$

$^{12}\text{C}$

spectra largely insensitive to induced 4N

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

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

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

$\Lambda = 1.88 \text{ fm}^{-1}$
Normal-Ordered 3N Interaction

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avoid technical challenge of including explicit 3N interactions in many-body calculation
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avoid technical challenge of including explicit 3N interactions in many-body calculation

**idea:** write 3N interaction in normal-ordered form with respect to an $A$-body reference Slater-determinant ($0\hbar\Omega$ state)

\[
\hat{V}_{3N} = \sum V_{\cdots}^{3N} \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \hat{a}
\]

\[
= W_0^{0B} + \sum W_1^{1B} \{ \hat{a}^\dagger \hat{a} \} + \sum W_2^{2B} \{ \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \hat{a} \}
+ \sum W_3^{3B} \{ \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \hat{a} \}
\]
Normal-Ordered 3N Interaction

avoid technical challenge of including explicit 3N interactions in many-body calculation

**idea**: write 3N interaction in normal-ordered form with respect to an A-body reference Slater-determinant (0ℏΩ state)

\[
\hat{V}_{3N} = \sum_{\cdots\cdots} V_{\cdots\cdots亨} \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \hat{a} \\
= W^{0B} + \sum W^{1B} \{\hat{a}^\dagger \hat{a} \} + \sum W^{2B} \{\hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \}
+ \sum W^{3B} \{\hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \hat{a} \}
\]

**Normal-Ordering Approximation** (NO2B): discard residual 3B part \(W^{3B}\)
Benchmark of Normal-Ordered 3N

4He

16O

compare IT-NCSM results with explicit 3N to normal-ord. 3N truncated at the 2B level

$\alpha = 0.04 \text{ fm}^4$
$\alpha = 0.05 \text{ fm}^4$
$\alpha = 0.0625 \text{ fm}^4$
$\alpha = 0.08 \text{ fm}^4$
$\hbar \Omega = 20 \text{ MeV}$
Benchmark of Normal-Ordered 3N

- Compare IT-NCSM results with explicit 3N to normal-ord. 3N truncated at the 2B level
- Typical deviations up to 2% for $^4$He and 1% for $^{16}$O

**$^4$He**

- NN+3N-ind.
- NN+3N-full

**$^{16}$O**

- NN+3N-ind.
- NN+3N-full

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

- Explicit / NO2B
  - $\alpha = 0.04 \text{ fm}^4$
  - $\alpha = 0.05 \text{ fm}^4$
  - $\alpha = 0.0625 \text{ fm}^4$
  - $\alpha = 0.08 \text{ fm}^4$

$\hbar \Omega = 20 \text{ MeV}$
Coupled Cluster Method

Coupled Cluster Approach
Coupled Cluster Approach

- **exponential Ansatz** for wave operator

\[ |\psi\rangle = \hat{\Omega} |\Phi_0\rangle = e^{\hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots + \hat{T}_A} |\Phi_0\rangle \]
**Coupled Cluster Approach**

- **exponential Ansatz** for wave operator

\[
|\psi\rangle = \Omega|\Phi_0\rangle = e^{\hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots + \hat{T}_A}|\Phi_0\rangle
\]

- \(\hat{T}_n\): *npnh excitation* ("cluster") operators

\[
\hat{T}_n = \frac{1}{(n!)^2} \sum_{ijk...} t_{abc...} \{\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \cdots \hat{a}_k \hat{a}_j \hat{a}_i\}
\]
Coupled Cluster Approach

- **exponential Ansatz** for wave operator

\[ |\psi\rangle = \Omega |\phi_0\rangle = e^{\hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots + \hat{T}_A} |\phi_0\rangle \]

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- **similarity transformed** Schrödinger Eq.

\[ \hat{H} |\phi_0\rangle = \Delta E |\phi_0\rangle, \quad \hat{H} \equiv e^{-\hat{T}} \hat{H}_N e^{\hat{T}} \]
Coupled Cluster Approach

- **exponential Ansatz** for wave operator

\[ |\Psi\rangle = \Omega |\Phi_0\rangle = e^{\hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots + \hat{T}_A} |\Phi_0\rangle \]

- \( \hat{T}_n \): *npnh excitation* ("cluster") operators

\[
\hat{T}_n = \frac{1}{(n!)^2} \sum_{ijk\ldots} t_{abc\ldots} \{ \hat{a}_a \hat{a}_b \hat{a}_c \hat{c}_d \cdots \hat{a}_k \hat{a}_j \hat{a}_i \}
\]

- **similarity transformed** Schrödinger Eq.

\[
\hat{\mathcal{H}} |\Phi_0\rangle = \Delta E |\Phi_0\rangle, \quad \hat{\mathcal{H}} \equiv e^{-\hat{T}} \hat{H}_N e^{\hat{T}}
\]

- \( \hat{\mathcal{H}} \): non-Hermitian **effective Hamiltonian**
Coupled Cluster Approach
Coupled Cluster Approach

- **CCSD**: truncate $\hat{T}$ at 2p2h level, $\hat{T} = \hat{T}_1 + \hat{T}_2$
Coupled Cluster Approach

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**Coupled Cluster Approach**

- **CCSD**: truncate $\hat{T}$ at 2p2h level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

\[ |\Phi_0\rangle \quad \hat{T}_1 |\Phi_0\rangle \]
Coupled Cluster Approach

- **CCSD**: truncate $\hat{T}$ at 2p2h level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

| $|\Phi_0\rangle$ | $\hat{T}_1 |\Phi_0\rangle$ | $\hat{T}_2 |\Phi_0\rangle$ |
Coupled Cluster Approach

- **CCSD**: truncate $\hat{T}$ at 2p2h level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

\[ |\Phi_0\rangle \]
\[ \hat{T}_1 |\Phi_0\rangle \]
\[ \hat{T}_2 |\Phi_0\rangle \]
\[ \hat{T}_1 \hat{T}_2 \hat{T}_2 |\Phi_0\rangle \]
Coupled Cluster Approach

- **CCSD**: truncate $\hat{T}$ at 2p2h level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

  - higher excitations from products of lower-excitation operators

\[ |\Phi_0\rangle \]
\[ \hat{T}_1 |\Phi_0\rangle \]
\[ \hat{T}_2 |\Phi_0\rangle \]
Coupled Cluster Approach

- $|\Psi\rangle$ is parametrized by cluster operator amplitudes $t^a_i$, $t^{ab}_{ij}$
- avoid explicit expansion in **many-body basis** (particle number information carried by $|\Phi_0\rangle$)
- **polynomial**, rather than factorial, scaling with mass number $A$
- exploit **symmetries** (esp. spherical symmetry for closed-shell nuclei)

\[
\hat{T}_1 = \sum_{ai} t^a_i \left\{ \hat{a}_a^{\dagger} \otimes \hat{a}_i \right\}_0^{(0)}
\]
\[
\hat{T}_2 = \sum_{abij} \sum_J t^{ab}_{ij}(J) \left\{ \left\{ \hat{a}_a^{\dagger} \otimes \hat{a}_b^{\dagger} \right\}^{(J)} \otimes \left\{ \hat{a}_j \otimes \hat{a}_i \right\}^{(J)} \right\}_0^{(0)}
\]

- CC suited for **medium-mass** and **heavy regime**
\[ 16^O: \text{Coupled-Cluster with } 3N_{NO2B} \]

### NN only

- \( E \) vs. \( e_{max} \)
- Various curves for different parameters:
  - \( \alpha = 0.04 \text{ fm}^4 \)
  - \( \Lambda = 2.24 \text{ fm}^{-1} \)

### NN+3N-induced

- \( E \) vs. \( e_{max} \)
- Various curves for different parameters:
  - \( \alpha = 0.05 \text{ fm}^4 \)
  - \( \Lambda = 2.11 \text{ fm}^{-1} \)

### NN+3N-full

- \( E \) vs. \( e_{max} \)
- Various curves for different parameters:
  - \( \alpha = 0.0625 \text{ fm}^4 \)
  - \( \Lambda = 2.00 \text{ fm}^{-1} \)

### CCSD

- \( \hbar \Omega = 20 \text{ MeV} \)
- \( E_{3max} = 14 \)
- HO basis

- \( \alpha = 0.08 \text{ fm}^4 \)
- \( \Lambda = 1.88 \text{ fm}^{-1} \)
$^{16}\text{O}$: Coupled-Cluster with $3N_{NO2B}$

**NN only**

**NN+3N-induced**

**NN+3N-full**

$E$ [MeV] vs. $e_{\max}$

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

- **NN+3N-induced**
  - $\alpha = 0.05 \text{ fm}^4$
  - $\Lambda = 2.11 \text{ fm}^{-1}$

- **NN+3N-full**
  - $\alpha = 0.0625 \text{ fm}^4$
  - $\Lambda = 2.00 \text{ fm}^{-1}$
  - $\alpha = 0.08 \text{ fm}^4$
  - $\Lambda = 1.88 \text{ fm}^{-1}$

**CCSD**

3N interaction with 400 MeV cutoff, $c_E$ refitted to $^4\text{He}$ ground state

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

$e_{\max}$

Exp.
$^{48}$Ca: Coupled-Cluster with $3N_{NO2B}$

**NN only**

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

**NN+3N-induced**

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

**NN+3N-full**

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

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

$E_{3\text{max}} = 14$

HO basis

**CCSD**

Exp.
Coupled Cluster Method with Explicit 3N Interactions

CCSD with Explicit 3N Interaction

NN+3N induced

\[ E^{\text{NN+3N induced}} [\text{MeV}] \]

16\(^{16}\)O

\[ \hbar \Omega = 20 \text{ MeV} \]

exp

NN+3N full

\[ E^{\text{NN+3N full}} [\text{MeV}] \]

\[ 24\(^{24}\)O \]

\[ \hbar \Omega = 20 \text{ MeV} \]

exp

CCSD

3B / NO2B

\[ \alpha = 0.02 \text{ fm}^4 \]

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

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

HF basis

\[ E_{3\text{ max}} = 12 \]
CCSD with Explicit 3N Interaction

**NN+3N induced**

- **40Ca**
  - $\hbar \Omega = 24$ MeV
  - $E_{3 \text{max}} = 12$

**NN+3N full**

- **48Ca**
  - $\hbar \Omega = 28$ MeV
  - $E_{3 \text{max}} = 12$

**Graph Details**

- **Energy** $E$ [MeV]
- **e$_{\text{max}}$**
- **Comparison**
  - **CCSD**
  - **3B / NO2B**
  - **HF basis**
  - Symbols:
    - $\alpha = 0.02 \text{ fm}^4$
    - $\alpha = 0.04 \text{ fm}^4$
    - $\alpha = 0.08 \text{ fm}^4$

**Additional Information**

- *NN* + 3N induced interaction
- *NN* + 3N full interaction
- Experimental data (exp)
$E_{3\text{max}}$ truncation

- full $\hat{V}_{3B}$ matrix too large to handle

- $E_{3\text{max}}$ truncation: use $\hat{V}_{3B}$ matrix elements $\langle pqr|\hat{V}_{3B}|stu \rangle$ with

  $$e_p + e_q + e_r \leq E_{3\text{max}} \lor e_s + e_t + e_u \leq E_{3\text{max}}$$

  $$e_p = 2n_p + l_p$$

- current limits:

  $$E_{3\text{max}} \leq \begin{cases} 
  12 & : \text{CC, explicit 3N} \\
  14, \ldots & : \text{NCSM, explicit 3N} \\
  14, \ldots & : \text{CC,NCSM NO2B} 
  \end{cases}$$

- storage

- availability
$E_{3\text{max}}$ Dependence (CCSD$_{\text{NO2B}}$)

- $E_{3\text{max}}$ not significant for **soft** interactions

- **harder interactions**: up to 2% change in g.s. energies for $E_{3\text{max}} = 12 \rightarrow 14$

- $\alpha$-dependence for **NN+3N induced reduced** for larger $E_{3\text{max}}$

- $\alpha$-dependence for **NN+3N full enhanced** for larger $E_{3\text{max}}$

---

- $\alpha = 0.02 \text{ fm}^4$, $\Lambda = 2.66 \text{ fm}^{-1}$
- $\alpha = 0.04 \text{ fm}^4$, $\Lambda = 2.24 \text{ fm}^{-1}$
- $\alpha = 0.08 \text{ fm}^4$, $\Lambda = 1.88 \text{ fm}^{-1}$
ΛCCSD(T) - Improving upon CCSD
CCSD(T) - Improving upon CCSD

- CCSDT, i.e., $\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3$, expensive
CCSD(T) - Improving upon CCSD

- CCSDT, i.e., $\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3$, **expensive**

- solution of the Coupled Cluster $\Lambda$ equations give **a posteriori** fourth order correction to CC energy functional

$$\mathcal{E} = \langle \Phi_0 | (1 + \Lambda) \hat{H} | \Phi_0 \rangle_C$$

due to triples excitations

$$\delta E_{\text{CCSD(T)}} = \frac{1}{(3!)^2} \sum_{abc} \tilde{\lambda}_{ijk} \frac{1}{\epsilon_{ijk}} \tilde{\tau}_{abc}$$
\[ \Lambda_{\text{CCSD}(T)}_{\text{NO2B}} \]

**NN+3N induced**

\begin{align*}
\text{\textit{40Ca}} & \quad \hbar \Omega = 24 \text{ MeV} \\
\text{\textit{48Ca}} & \quad \hbar \Omega = 28 \text{ MeV}
\end{align*}

![Graph showing energy levels for NN+3N induced and full calculations with various alpha values and E_{max} configurations.](image)

**NN+3N full**

HF basis

\[ E_{3\text{max}} = 12 \]
\( \Lambda \text{CCSD(T)}_{\text{NO2B}} \)

**NN+3N induced**

<table>
<thead>
<tr>
<th>40Ca</th>
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<td>E_{\text{exp}} [MeV]</td>
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- \( \Lambda \text{CCSD(T)} / \text{CCSD} \)
  - \( \alpha = 0.02 \text{ fm}^4 \)
  - \( \alpha = 0.04 \text{ fm}^4 \)
  - \( \alpha = 0.08 \text{ fm}^4 \)

**NN+3N full**

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- \( \Lambda \text{CCSD(T)} / \text{CCSD} \)
  - \( \alpha = 0.02 \text{ fm}^4 \)
  - \( \alpha = 0.04 \text{ fm}^4 \)
  - \( \alpha = 0.08 \text{ fm}^4 \)

HF basis
CCSD\textsubscript{NO2B} vs. ΛCCSD(T)\textsubscript{NO2B}

- inclusion of **triples excitations mandatory** (up to 6 % more binding for heavier nuclei)

- cluster truncation works better for **softer interactions**

- $\alpha = 0.02 \text{ fm}^4$ results not necessarily closer to **exact result** than $\alpha = 0.08 \text{ fm}^4$

- $\Rightarrow$ calculations with **bare** 3N interaction suffer from cluster truncation and $E_{3\text{max}}$ cut

\[\alpha = 0.02 \text{ fm}^4, \Lambda = 2.66 \text{ fm}^{-1}\]
\[\alpha = 0.04 \text{ fm}^4, \Lambda = 2.24 \text{ fm}^{-1}\]
\[\alpha = 0.08 \text{ fm}^4, \Lambda = 1.88 \text{ fm}^{-1}\]
Goal: Heavy Nuclei

Current $E_{3\text{max}}$ limits do not allow for reasonable calculations beyond $A \geq 60$
Conclusions

■ new era of **ab-initio nuclear structure theory** connected to QCD via chiral EFT

■ consistent **inclusion of 3N interactions** in similarity transformations & many-body calculations

■ normal-ordering approximation as **efficient and accurate way** to include 3N interactions

■ many-body calculations extended to the **medium-mass** regime
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  Institut für Kernphysik, TU Darmstadt

- **P. Navrátil**
  TRIUMF Vancouver, Canada

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

- S. Quaglioni
  LLNL Livermore, USA

- P. Piecuch
  Michigan State University, USA

- H. Hergert
  Ohio State University, USA

- P. Papakonstantinou
  IPN Orsay, F

- C. Forssén
  Chalmers University, Sweden

- H. Feldmeier, T. Neff
  GSI Helmholtzzentrum