Ab Initio Nuclear Structure Theory
with Chiral NN plus 3N Interactions

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From QCD to Nuclear Structure

Nuclear Structure

NN+3N Interaction from Chiral EFT

- 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)

Low-Energy QCD
From QCD to Nuclear Structure

Nuclear Structure

Unitarily Transformed Hamiltonian

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

NN+3N Interaction from Chiral EFT

- transform Hamiltonian & observables consistently

Low-Energy QCD

- conserve experimentally constrained few-body properties
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

Importance Truncated No-Core Shell Model with NN+3N

Similarity Renormalization Group with NN+3N

Focus on consistent inclusion of chiral 3N interaction
Unitarily Transformed Hamiltonian

Similarity
Renormalization Group

Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
Similarity Renormalization Group

- **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
  \[ \eta_\alpha = (2\mu)^2 [T_{\text{int}}, \tilde{H}_\alpha] \]
continuous transformation driving Hamiltonian to band-diagonal form with respect to a chosen basis

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

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

simplicity and flexibility are great advantages of the SRG approach
SRG Evolution of Matrix Elements

- represent operator equation in **antisym.** \( n \)-body Jacobi basis
  - \( n = 2 \): momentum space \(|q(LS)JT\rangle\) or harmonic oscillator \(|E(LS)J^\pi T\rangle\)
  - \( n = 3 \): harmonic oscillator Jacobi states \(|EiJ^\pi T\rangle\)

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

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

- 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

chiral NN
Entem & Machleidt. N3LO, 500 MeV

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

deuteron wave-function

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

\[ L = 0 \quad L = 2 \]
SRG Evolution in Two-Body Space

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

momentum-space matrix elements

\[ ^3S_1 \]
\[ ^3S_1 - ^3D_1 \]

deuteron wave-function

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

\[ r \text{ [fm]} \]
SRG Evolution in Two-Body Space

\[ \alpha = 0.002 \text{ fm}^4 \]
\[ \Lambda = 4.73 \text{ fm}^{-1} \]
\[ J^\pi = 1^+, T = 0 \]

momentum-space matrix elements

\[ ^3S_1 \]
\[ ^3S_1 - ^3D_1 \]

deuteron wave-function

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

\( L = 0 \)
\( L = 2 \)

\[ r \text{ [fm]} \]
SRG Evolution in Two-Body Space

\[ \alpha = 0.005 \text{ fm}^4 \]
\[ \Lambda = 3.76 \text{ fm}^{-1} \]
\[ J^\pi = 1^+, T = 0 \]

momentum-space matrix elements

\[ {}^3S_1 \]

\[ {}^3S_1 - {}^3D_1 \]

deuteron wave-function

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

L = 0

L = 2
SRG Evolution in Two-Body Space

\[ \alpha = 0.010 \text{ fm}^4 \]
\[ \Lambda = 3.16 \text{ fm}^{-1} \]
\[ J^\pi = 1^+, T = 0 \]

deuteron wave-function

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

- Blue: \( L = 0 \)
- Red: \( L = 2 \)
SRG Evolution in Two-Body Space

\[ \alpha = 0.020 \text{ fm}^4 \]
\[ \Lambda = 2.66 \text{ fm}^{-1} \]
\[ J^\pi = 1^+, T = 0 \]

momentum-space matrix elements

\[ ^3S_1 \]

\[ ^3S_1 - ^3D_1 \]

deuteron wave-function

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

\[ L = 0 \]
\[ L = 2 \]
SRG Evolution in Two-Body Space

\[ \alpha = 0.040 \text{ fm}^4 \]
\[ \Lambda = 2.24 \text{ fm}^{-1} \]
\[ J^\pi = 1^+, T = 0 \]

Deuteron wave-function

\[ \phi_L(r) \text{ [arb. units]} \]
SRG Evolution in Two-Body Space

\[ \alpha = 0.080 \text{ fm}^4 \]
\[ \Lambda = 1.88 \text{ fm}^{-1} \]
\[ J^\pi = 1^+, T = 0 \]

momentum-space matrix elements

\[ ^3S_1 \]
\[ ^3S_1 - ^3D_1 \]

deuteron wave-function

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

\[ L = 0 \quad L = 2 \]
SRG Evolution in Two-Body Space

\[ \alpha = 0.160 \text{ fm}^4 \]

\[ \Lambda = 1.58 \text{ fm}^{-1} \]

\[ j^\pi = 1^+, T = 0 \]

deuteron wave-function

\[ \phi_L(r) \text{ [arb. units]} \]
SRG Evolution in Two-Body Space

\[ \alpha = 0.320 \, \text{fm}^4 \]

\[ \Lambda = 1.33 \, \text{fm}^{-1} \]

\[ J^\pi = 1^+, T = 0 \]

momentum-space matrix elements

\[ ^3S_1 \]

\[ ^3S_1 - ^3D_1 \]

deuteron wave-function

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

- \( L = 0 \)
- \( L = 2 \)
SRG Evolution in Two-Body Space

\[ \alpha = 0.320 \text{ fm}^4 \]

\[ \Lambda = 1.33 \text{ fm}^{-1} \]

\[ J^\pi = 1^+, T = 0 \]

deuteron wave-function

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

elimination of short-range correlations
SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

chiral NN+3N
\( N^3\text{LO} + N^2\text{LO}, \text{triton-fit, 500 MeV} \)

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

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

3B-Jacobi HO matrix elements

\( \alpha = 0.000 \text{ fm}^4 \)
\( \Lambda = \infty \text{ fm}^{-1} \)

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

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

\[ \begin{array}{ccccccccc}
0 & 2 & 4 & 6 & 8 & 10 & 12 & 14 & 16 & 18 & 20 \\
\hline \\
E [\text{MeV}] & -8 & -6 & -4 & -2 & 0 & 2 \\
\end{array} \]
SRG Evolution in Three-Body Space

\[ \alpha = 0.010 \text{ fm}^4 \]
\[ \Lambda = 3.16 \text{ fm}^{-1} \]
\[ J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar \Omega = 28 \text{ MeV} \]

3B-Jacobi HO matrix elements

NCSM ground state $^3\text{H}$
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$\alpha = 0.020 \text{ fm}^4$

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3B-Jacobi HO matrix elements

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

3B-Jacobi HO matrix elements

\[ \alpha = 0.040 \text{ fm}^4 \]
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NCSM ground state \(^3\text{H}\)
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\[ \alpha = 0.080 \text{ fm}^4 \]
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\[ \alpha = 0.160 \text{ fm}^4 \]
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3B-Jacobi HO matrix elements

NCSM ground state \(^3\text{H}\)
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NCSM ground state \(^3\text{H}\)
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3B-Jacobi HO matrix elements

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

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

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 **cluster-truncated Hamiltonian** measures impact of discarded induced many-body terms
**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 Hamiltonian measures impact of omitted induced many-body interactions

*\(\alpha\)-variation provides a diagnostic tool to assess the omitted induced many-body interactions*
Sounds easy, but...

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
Exact Many-Body Methods

Importance Truncated NCSM

NCSM is one of the most powerful and universal ab initio many-body 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 $\Lambda$

- 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 \(^{16}\text{O}\) not really feasible (basis dimension > \(10^{10}\))

![Graph showing energy levels vs. \(N_{\text{max}}\) for \(^{16}\text{O}\) with NN-only interaction, \(\alpha = 0.04 \text{ fm}^4\), \(\hbar\Omega = 20 \text{ MeV}\).]
Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full 10 or 12$\hbar\Omega$ calculation for $^{16}$O 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
### A Tale of Three Hamiltonians

#### Initial Hamiltonian

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

#### 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
### 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-live)

#### 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

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions
\( \alpha = 0.04 \text{ fm}^4 \quad \Lambda = 2.24 \text{ fm}^{-1} \)
\( \alpha = 0.05 \text{ fm}^4 \quad \Lambda = 2.11 \text{ fm}^{-1} \)
\( \alpha = 0.0625 \text{ fm}^4 \quad \Lambda = 2.00 \text{ fm}^{-1} \)
\( \alpha = 0.08 \text{ fm}^4 \quad \Lambda = 1.88 \text{ fm}^{-1} \)
\( \alpha = 0.16 \text{ fm}^4 \quad \Lambda = 1.58 \text{ fm}^{-1} \)
\( ^4\text{He}: \text{Ground-State Energies} \)

**NN only**

- strong \( \alpha \)-dependence: induced 3N interactions

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

\[
\begin{align*}
\alpha &= 0.04 \text{ fm}^4 & \Lambda &= 2.24 \text{ fm}^{-1} \\
\alpha &= 0.05 \text{ fm}^4 & \Lambda &= 2.11 \text{ fm}^{-1} \\
\alpha &= 0.0625 \text{ fm}^4 & \Lambda &= 2.00 \text{ fm}^{-1} \\
\alpha &= 0.08 \text{ fm}^4 & \Lambda &= 1.88 \text{ fm}^{-1} \\
\alpha &= 0.16 \text{ fm}^4 & \Lambda &= 1.58 \text{ fm}^{-1}
\end{align*}
\]
$^4$He: Ground-State Energies

**NN only**

- Strong $\alpha$-dependence: induced 3N interactions
- $\hbar \Omega = 20$ MeV

**NN+3N-induced**

- $\alpha = 0.04$ 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

**NN+3N-induced**

- no $\alpha$-dependence: no induced 4N interactions

---

$E [\text{MeV}]$

$N_{\text{max}}$

---

α = 0.04 fm$^4$

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

α = 0.05 fm$^4$

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

α = 0.0625 fm$^4$

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

α = 0.08 fm$^4$

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

α = 0.16 fm$^4$

$\Lambda = 1.58 \text{ fm}^{-1}$

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

Exp.
$^4$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

**NN+3N-full**

- Exp.

---

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

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

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

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

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

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

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

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

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

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

- **NN only**
  - strong $\alpha$-dependence:
    - induced 3N interactions
  - $\hbar \Omega = 20 \text{ MeV}$

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

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

 Parameters:
- $\alpha = 0.04 \text{ fm}^4$
  - $\Lambda = 2.24 \text{ fm}^{-1}$
- $\alpha = 0.05 \text{ fm}^4$
  - $\Lambda = 2.11 \text{ fm}^{-1}$
- $\alpha = 0.0625 \text{ fm}^4$
  - $\Lambda = 2.00 \text{ fm}^{-1}$
- $\alpha = 0.08 \text{ fm}^4$
  - $\Lambda = 1.88 \text{ fm}^{-1}$
- $\alpha = 0.16 \text{ fm}^4$
  - $\Lambda = 1.58 \text{ fm}^{-1}$
$^6$Li: Ground-State Energies

### NN only

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

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

### NN+3N-induced

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

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

### NN+3N-full

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

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

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

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

### NN only

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

### NN+3N-induced

### NN+3N-full
$^{12}\text{C}$: Ground-State Energies

**NN only**

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

**NN+3N-induced**

- World Record

**NN+3N-full**

- World Record

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

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

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

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

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

**NN only**

- $E [\text{MeV}]$
- $N_{\text{max}}$
- $\hbar\Omega = 20 \text{ MeV}$

**NN+3N-induced**

- $E [\text{MeV}]$
- $N_{\text{max}}$
- $\text{Exp.}$

**NN+3N-full**

- $E [\text{MeV}]$
- $N_{\text{max}}$
- $\text{Exp.}$

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

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

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

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

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

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

**NN only**
- $\hbar \Omega = 20$ MeV

**NN+3N-induced**
- $\alpha = 0.04$ fm$^4$
- $\Lambda = 2.24$ fm$^{-1}$

**NN+3N-full**
- $\alpha = 0.16$ fm$^4$
- $\Lambda = 1.58$ fm$^{-1}$

Graphs show the energy $E$ in MeV as a function of $N_{\text{max}}$ for different values of $\alpha$ and $\Lambda$. Legend includes symbols and their corresponding parameters.


$^{16}$O: Ground-State Energies

**NN only**

- $E_{\text{NN only}}$ vs. $N_{\text{max}}$
- $\hbar \Omega = 20 \text{ MeV}$

**NN+3N-induced**

- $E_{\text{NN+3N-induced}}$ vs. $N_{\text{max}}$
- Inclusion of initial 3N interaction results in induced 4N terms

**NN+3N-full**

- $E_{\text{NN+3N-full}}$ vs. $N_{\text{max}}$

Parameters:

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

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

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

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

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

**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**

- $\alpha = 0.0625 \text{ fm}^4$
- $\Lambda = 2.00 \text{ fm}^{-1}$
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- $\Lambda = 1.88 \text{ fm}^{-1}$
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$\hbar \Omega = 20 \text{ MeV}$
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.
IT-NCSM gives access to complete spectroscopy of p- and sd-shell nuclei starting from chiral NN+3N interactions.
Spectroscopy of $^{16}\text{C}$

**NN only**

- $E_x$ vs $N_{\text{max}}$
- $\hbar\Omega = 16 \text{ MeV}$
- $\alpha = 0.08 \text{ fm}^4$

**NN+3N-induced**

- $E_x$ vs $N_{\text{max}}$

**NN+3N-full**

- $E_x$ vs $N_{\text{max}}$

Preliminary
Spectroscopy of $^{16}$C

NN only  | NN+3N-induced | NN+3N-full
---|---|---
2$^+$ → 0$^+$ | 1 | 1 | 1
2$^+$ → 0$^+$ | 0.97 | 0.75 | 0.11
2$^+$ → 2$^+$ | 1.27 | 1.69 | 0.65
3$^+$ → 2$^+$ | 0.34 | 0.31 | 0.02
4$^+$ → 2$^+$ | 0.91 | 0.69 | 0.80

$\hbar \Omega = 1$  
$\alpha = 0.08\ fm^{-1}$
Spectroscopy of $^{16}$C

**Table:**

<table>
<thead>
<tr>
<th>$B(E2)$ [rel. units]</th>
<th>NN only</th>
<th>NN+3N-induced</th>
<th>NN+3N-full</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^+_1 \rightarrow 0^+_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$2^+_2 \rightarrow 0^+_1$</td>
<td>0.97</td>
<td>0.75</td>
<td>0.11</td>
</tr>
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<td>0.80</td>
</tr>
</tbody>
</table>

Recent experiments (Petri et al.) confirm $B(E2)$ pattern obtained in the NN+3N-full calculation.
Where do we go from here?

- beyond the lightest nuclei, **SRG-induced 4N contributions** affect the absolute energies, but not the excitation energies

- with the inclusion of the leading 3N interaction we already obtain a **very reasonable description** of spectra (and ground states)

**SRG Transformation**

- Which parts of the initial 3N cause the induced 4N contributions?

- Can we find alternative SRG generators with suppressed induced 4N?

**Chiral NN+3N Interactions**

- How sensitive is the spectroscopy on specifics of the 3N interaction (cutoff, $c_i$’s) ?

- How does the inclusion of the subleading 3N terms affect the picture?
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- How does the inclusion of the subleading 3N terms affect the picture?

**first answers in Joachim Langhammer’s talk on Friday...**
Sensitivity on Initial $3N$ — $^{16}O$

Modified 3N interaction with shifted $c_i$

- Standard 3N
- $\tilde{N}_{\text{max}} = 2$
- $\tilde{N}_{\text{max}} = 4$
- $\tilde{N}_{\text{max}} = 6$
- $\tilde{N}_{\text{max}} = 8$
- $\tilde{N}_{\text{max}} = 10$
- $\tilde{N}_{\text{max}} = 12$
- $\tilde{N}_{\text{max}} = 14$

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

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

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

400 MeV cutoff
Sensitivity on Initial 3N — $^{12}\text{C}$

**standard 3N**

- $\hbar \Omega = 20 \text{ MeV}$
- $\alpha = 0.08 \text{ fm}^4$

**modified 3N interaction with shifted $c_i$**

- 400 MeV cutoff

---

**Graphs:**

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

Legend:

- $0^+1$
- $2^+1$
- $2^+0$
- $1^+1$
- $4^+0$
- $1^+0$
- $2^+0$
- $0^+0$
- $0^+0$
- $0^+0$

---

**Text:**

- Modified 3N interaction with shifted $c_i$
- 400 MeV cutoff
- All NN+3N-full

---

**Equation:**

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

$\alpha = 0.08 \text{ fm}^4$
Sensitivity on Initial 3N — $^{12}\text{C}$

Standard 3N

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Modified 3N interaction with shifted $c_i$

- All NN+3N-full

400 MeV cutoff

spectra of $A \geq 10$ nuclei are a very sensitive benchmark for chiral 3N interactions
Conclusions
Conclusions

- 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

Thanks to my group & my collaborators

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  TRIUMF Vancouver, Canada

- **S. Quaglioni**
  LLNL Livermore, USA

- **H. Hergert, P. Piecuch**
  Michigan State University, USA

- **C. Forssén**
  Chalmers University, Sweden

- **H. Feldmeier, T. Neff,**...
  GSI Helmholtzzentrum
Supplements
Importance Truncation: General Idea

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

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

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

- 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 $|\psi^{(m)}_{\text{ref}}\rangle$

- a posteriori **threshold extrapolation** and **perturbative correction** used to recover contributions from discarded basis states
Importance Truncation: General Idea

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- **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 $\kappa_{\text{min}} \to 0$ 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 $\kappa_{\text{min}} \rightarrow 0$ of observables to account for effect of excluded configurations.

- SRG(N3LO) $\alpha = 0.04 \, \text{fm}^4$, $\hbar \Omega = 20 \, \text{MeV}$, $N_{\text{max}} = 8$.

- $^{16}\text{O}$ calculations for a sequence of importance thresholds $\kappa_{\text{min}}$. 

- Systematic approach to the full NCSM limit.
Constrained Threshold Extrapolation

- estimate energy contribution of excluded states perturbatively \( \Delta_{\text{excl}}(\kappa_{\text{min}}) \)

- simultaneous fit of combined energy
  \[
  E_\lambda(\kappa_{\text{min}}) = E_{\text{int}}(\kappa_{\text{min}}) + \lambda \Delta_{\text{excl}}(\kappa_{\text{min}})
  \]
  for set of \( \lambda \)-values with the constraint \( E_\lambda(0) = E_{\text{extrap}} \)

- robust threshold extrapolation with error bars determined by variation of fit function
Origin of SRG-Induced 4N Terms

\begin{align*}
\text{std. 3N} & \quad c_D = 0 \\
\text{16O} & \quad \hbar\Omega = 20 \text{ MeV} \\
c_E = 0 & \quad c_i = 0
\end{align*}

- set $c_D$, $c_E$, or $c_i$ to zero and refit $c_D$ or $c_E$ to get triton ground-state energy
- $\alpha$-dependence changes only if the $c_i$ terms are switched off

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

$\alpha = 0.16 \text{ fm}^4 \quad \Lambda = 1.58 \text{ fm}^{-1}$
Origin of SRG-Induced 4N Terms

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$16O$

$\hbar \Omega = 20$ MeV

Long-range $2\pi$ terms of initial 3N are the origin of SRG-induced 4N

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

$\alpha = 0.16$ fm$^4$, $\Lambda = 1.58$ fm$^{-1}$
Sensitivity on 3N Cutoff: $^{16}$O

- Reduce 3N cutoff to 400 MeV and refit $c_E$ to reproduce the $^4$He ground-state energy.
- Strong impact on $\alpha$-dependence and absolute ground-state energy.

![Graph showing sensitivity of 3N cutoff on $^{16}$O](image)

- $\hbar \Omega = 20$ MeV
- $N_{\text{max}}$ range from 2 to 14
- $E$ as a function of $N_{\text{max}}$ for standard 3N and 3N cutoff 400 MeV

Parameters:

- $\alpha = 0.08 \text{ fm}^4$
- $\Lambda = 1.88 \text{ fm}^{-1}$
- $\alpha = 0.16 \text{ fm}^4$
- $\Lambda = 1.58 \text{ fm}^{-1}$
Sensitivity on $c_i$ Shift: $^{16}$O

- Include shifts of $c_i$ values from $N^3$LO terms and refit $c_E$ to reproduce the $^4$He ground-state energy.

- Sizable impact on $\alpha$-dependence and absolute ground-state energy.

**standard 3N**

- $\hbar \Omega = 20$ MeV

**shifted $c_i$**

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

- $\alpha = 0.16$ fm$^4$
- $\Lambda = 1.58$ fm$^{-1}$
Sensitivity on $c_3$ & $c_4$: $^{16}\text{O}$

**standard 3N**

- $c_4 = 5.4 \rightarrow 3.4$
- $c_3 = -3.2 \rightarrow -4.7$

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

- $\alpha = 0.08 \text{ fm}^4$
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- $\alpha = 0.16 \text{ fm}^4$
- $\Lambda = 1.58 \text{ fm}^{-1}$
Sensitivity on 3N Cutoff: $^{12}$C

- Significant improvement of $1^+0$ energy and of overall agreement

**standard 3N**

**3N cutoff 400 MeV**

$\hbar \Omega = 20$ MeV

$\alpha = 0.08 \text{ fm}^4$
Sensitivity on $c_i$ Shift: $^{12}$C

- slight improvement of $1^+0$ energy and of over-all agreement
Sensitivity on $c_i$ Shift: $^{12}$C

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spectra of $A \geq 10$ nuclei are a very sensitive benchmark for chiral 3N interactions.
Sensitivity on $c_3$ & $c_4$: $^{12}$C

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