Ab Initio Nuclear Structure from Chiral NN+3N Hamiltonians

Robert Roth
From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD
Nuclear Structure

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

NN+3N Interaction from Chiral EFT

Unitary / Similarity Transformation

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

Low-Energy QCD
Nuclear Structure

Exact & Approx. Many-Body Methods

- 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

Unitary / Similarity Transformation

NN+3N Interaction from Chiral EFT

Low-Energy QCD
How can we extend current ab-initio methods to describe open-shell and deformed nuclei?

How can we include the effects of three-nucleon forces in a computationally efficient manner?

How can we describe the onset of pairing in nuclei within various ab-initio frameworks?

Benchmarking and accuracy: can we develop reliable theoretical error estimates?

How can we bridge structure and reactions in a consistent fashion?

How can we generate reliable predictions for the drip-lines?
Nuclear Interactions from Chiral EFT
**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 ($NN, \pi N, \ldots$).
- Hierarchy of **consistent NN, 3N, … interactions** (plus currents).
- Many **ongoing developments**
  - 3N interaction at N3LO, N4LO, …
  - Explicit inclusion of $\Delta$-resonance
  - $YN$- & $YY$-interactions
  - Formal issues: power counting, renormalization, cutoff choice, …

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Chiral NN+3N Hamiltonians

- **standard Hamiltonian:**
  - NN at N3LO: Entem / Machleidt, 500 MeV cutoff
  - 3N at N2LO: Navrátil, local, 500 MeV cutoff, fit to $T_{1/2}(^3\text{H})$ and $E(^3\text{H}, ^3\text{He})$

- **standard Hamiltonian with modified 3N:**
  - NN at N3LO: Entem / Machleidt, 500 MeV cutoff
  - 3N at N2LO: Navrátil, local, with modified LECs and cutoffs, refit to $E(^4\text{He})$

- **consistent N2LO Hamiltonian:**
  - NN at N2LO: Epelbaum et al., 450,...,600 MeV cutoff
  - 3N at N2LO: Epelbaum et al., nonlocal, 450,...,600 MeV cutoff

- **consistent N3LO Hamiltonian:**
  - coming soon...
Similarity
Renormalization Group

Roth, Calci, Langhammer, Binder — in preparation (2013)
Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
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 \( U_\alpha \):
  \[ \frac{d}{d\alpha} \tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha] \]

- **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.

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 $^3\text{H}$
\[ \alpha = 0.320 \text{ fm}^4 \]
\[ \Lambda = 1.33 \text{ fm}^{-1} \]
\[ J^{\pi} = \frac{1}{2}^+, T = \frac{1}{2}, \hbar \Omega = 28 \text{ MeV} \]

**SRG Evolution in Three-Body Space**

3B-Jacobi HO matrix elements

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

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

significant improvement of convergence behavior
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 destroys unitarity and invariance of energy eigenvalues (independence of $\alpha$)

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

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

1. Initial 3B-Jacobi HO matrix elements of chiral 3N interactions
   - Direct computation using Petr Navratil’s ManyEff code (N2LO)
   - Conversion of partial-wave decomposed moment-space matrix elements of Epelbaum et al. (N2LO, N3LO,...)

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

3. Transformation of 2B/3B Jacobi HO matrix elements into JT-coupled representation
   - Transform 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
   - Optimized storage scheme for fast on-the-fly decoupling; can keep all matrix elements up to $E_3^{\text{max}} = 16$ in memory; suitable for GPUs
Importance Truncated No-Core Shell Model

Roth, Calci, Langhammer, Binder — in preparation (2013)
Navrátil, Roth, Quaglioni — Phys. Rev. C 82, 034609 (2010)
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
Importance Truncated NCSM

- Converged NCSM calculations essentially restricted to lower/mid p-shell.
- Full $N_{\text{max}}$ calculation for $^{16}\text{O}$ very difficult ($\text{basis dimension}>10^10$).
- Similar strategies have first been developed and applied in quantum chemistry:
  - Configuration-selective multireference CI

**Importance Truncation**

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

![Graph showing energy levels for $^{16}\text{O}$](image)

- $E [\text{MeV}]$ vs. $N_{\text{max}}$ for $^{16}\text{O}$.
- NN-only $\alpha = 0.04 \text{ fm}^4$.
- $\hbar \Omega = 20 \text{ MeV}$.

Buenker & Peyerimhoff (1974);
Huron, Malrieu & Rancurel (1973);
and others...
**Importance Truncation: Basic Idea**

- **Starting point**: approximation $|\Psi_{\text{ref},m}\rangle$ for the **target states** within a limited reference space $\mathcal{M}_{\text{ref}}$

  $$|\Psi_{\text{ref},m}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C^{(\text{ref},m)}_{\nu} |\Phi_{\nu}\rangle$$

- **Measure the importance** of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

  $$(\Phi_{\nu}| H |\Psi_{\text{ref},m})$$

  importance measure only probes 2p2h excitations on top of $\mathcal{M}_{\text{ref}}$ for a two-body Hamiltonian

- **Construct importance-truncated space** $\mathcal{M}_{\text{IT}}(\kappa_{\text{min}})$ from all basis states with $|\kappa_{\nu}(m)| \geq \kappa_{\text{min}}$ for any $m$

- **Solve eigenvalue problem** in $\mathcal{M}_{\text{IT}}(\kappa_{\text{min}})$ and obtain improved approximation of target state

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- **property of** $N_{\text{max}}$-truncated space: step from $N_{\text{max}}$ to $N_{\text{max}} + 2$ requires $2p2h$ excitations at most

- **sequential calculation** for a range of $N_{\text{max}}\hbar\Omega$ spaces:
  
  1. do full NCSM calculations up to a convenient $N_{\text{max}}$
  2. use components of eigenstates with $|C^{(m)}_{\nu}| \geq C_{\text{min}}$ as initial $|\Psi_{\text{ref},m}\rangle$
  3. consider all states $|\Phi_{\nu}\rangle \not\in \mathcal{M}_{\text{ref}}$ from an $N_{\text{max}} + 2$ space and add those with $|\kappa^{(m)}_{\nu}| \geq \kappa_{\text{min}}$ to importance-truncated space $\mathcal{M}_{\text{IT}}$
  4. solve eigenvalue problem in $\mathcal{M}_{\text{IT}}$
  5. use components of eigenstate
  6. goto 1

*full NCSM space is recovered* in the limit $(\kappa_{\text{min}}, C_{\text{min}}) \to 0$
Threshold Extrapolation

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

- Repeat calculations for a sequence of importance thresholds $\kappa_{\text{min}}$

- Observables show smooth threshold dependence and systematically approach the full NCSM limit

- Use a posteriori extrapolation $\kappa_{\text{min}} \rightarrow 0$ of observables to account for effect of excluded configurations
Constrained Threshold Extrapolation

\[ E_\lambda(\kappa_{\text{min}}) = E(\kappa_{\text{min}}) + \lambda \Delta_{\text{excl}}(\kappa_{\text{min}}) \]

for free: importance selection gives perturbative energy correction \( \Delta_{\text{excl}}(\kappa_{\text{min}}) \) accounting for excluded states

\[ \kappa_{\text{min}} \to 0 \]

Parameter \( \lambda \) defining a family of energy sequences

proposed by Buenker & Peyerimhoff (1975): “Energy Extrapolation in CI Calculations”

Simultaneous extrapolation for family of \( \lambda \)-values with constraint \( E_\lambda(0) = E_{\text{extrap}} \)
Uncertainty Quantification in the IT-NCSM
### Importance Truncation

- use sequence of \((C_{\text{min}}, \kappa_{\text{min}})\)-truncated model spaces
- extrapolate to \(\kappa_{\text{min}} \to 0\) using polynomial ansatz or more refined constrained extrapolation scheme
- uncertainty estimate derived from extrapolation protocol
- **systematic uncertainty** absent in full NCSM

### Model-Space Truncation

- use sequence of \(N_{\text{max}}\)-truncated model spaces
- extrapolate to \(N_{\text{max}} \to \infty\) using exponential ansatz or more elaborate extrapolation schemes
- uncertainty estimate derived from extrapolation protocol
- same **extrapolation uncertainties** as in full NCSM
Comment on $C_{\text{min}}$ Truncation

- truncation of reference state to components with $|C_{\nu}| \geq C_{\text{min}}$
- technical reason: importance selection phase scales with $(\dim M_{\text{ref}})^2$
- typically $C_{\text{min}} = 2 \times 10^{-4}$

Practically no influence on threshold extrapolated energies.

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Protocol: Simple $\kappa_{\text{min}}$ Extrapolation

- perform IT-NCSM calculations for range of $\kappa_{\text{min}}$-values, typically $\kappa_{\text{min}} = 3, 3.5, ..., 10 \times 10^{-5}$
- extrapolation $\kappa_{\text{min}} \to 0$ using polynomial $P_p(\kappa_{\text{min}})$ fit to full $\kappa_{\text{min}}$-set, typically of order $p = 3$
- generate uncertainty band from set of alternative extrapolations
  - $P_{p-1}$ and $P_{p+1}$ extrapolations using full $\kappa_{\text{min}}$-range
  - $P_p$ extrapolations with lowest and lowest two $\kappa_{\text{min}}$-points dropped
- quote standard deviation as nominal uncertainty
Protocol: Constrained $\kappa_{\text{min}}$ Extrapolation

- select a few $\lambda$-values to get symmetrical approach towards common $E_{\text{extrap}} = E_{\lambda}(\kappa_{\text{min}} = 0)$

- constrained simultaneous extrapolation $\kappa_{\text{min}} \to 0$ using polynomial $P_p(\kappa_{\text{min}})$, typically of order $p = 3$

- generate uncertainty band from set of constrained extrapolations
  - $P_{p-1}$ and $P_{p+1}$ extrapolations using full $\kappa_{\text{min}}$-range
  - $P_p$ extrapolations with lowest and lowest two $\kappa_{\text{min}}$-points dropped
  - $P_p$ extrapolations with smallest and largest $\lambda$-set dropped

- std. deviation gives uncertainty

$^{16}$O

NN-only, $\alpha = 0.04 \text{ fm}^4$

$\hbar\Omega = 20 \text{ MeV}$, $N_{\text{max}} = 12$
Characterization of SRG-Evolved NN+3N Hamiltonians

Roth, Calci, Langhammer, Binder — in preparation (2013)
$^4\text{He}: \text{Ground-State Energies}$

**NN only**

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

**NN+3N-induced**

- $N_{\text{max}} = 2, 4, 6, 8, 10, 12, 14, \infty$
- $\alpha = 0.04 \text{ fm}^4$
- $\Lambda = 2.24 \text{ fm}^{-1}$
- $\alpha = 0.05 \text{ fm}^4$
- $\Lambda = 2.11 \text{ fm}^{-1}$
- $\alpha = 0.0625 \text{ fm}^4$
- $\Lambda = 2.00 \text{ fm}^{-1}$
- $\alpha = 0.08 \text{ fm}^4$
- $\Lambda = 1.88 \text{ fm}^{-1}$
- $\alpha = 0.16 \text{ fm}^4$
- $\Lambda = 1.58 \text{ fm}^{-1}$

**NN+3N-full**

- $N_{\text{max}} = 2, 4, 6, 8, 10, 12, 14, \infty$
- $\alpha = 0.04 \text{ fm}^4$
- $\Lambda = 2.24 \text{ fm}^{-1}$
- $\alpha = 0.05 \text{ fm}^4$
- $\Lambda = 2.11 \text{ fm}^{-1}$
- $\alpha = 0.0625 \text{ fm}^4$
- $\Lambda = 2.00 \text{ fm}^{-1}$
- $\alpha = 0.16 \text{ fm}^4$
- $\Lambda = 1.58 \text{ fm}^{-1}$

Exp.
\( ^{12}\text{C}: \text{Ground-State Energies} \)

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

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

**NN only**

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

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

\[ 2, 4, 6, 8, 10, 12, 14, \infty \]

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

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

**NN+3N-induced**

\[ \alpha = 0.05 \text{ fm}^4 \]

\[ \Lambda = 2.11 \text{ fm}^{-1} \]

**NN+3N-full**

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

\[ \Lambda = 2.00 \text{ fm}^{-1} \]

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

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

\[ \alpha = 0.16 \text{ fm}^4 \]

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

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

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

**NN only**

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

**NN+3N-induced**

**NN+3N-full**

in progress: explicit inclusion of induced 4N ($\rightarrow$ A. Calci)

clear signature of induced 4N originating from initial 3N

- $\alpha = 0.04\, \text{fm}^4$
  $\Lambda = 2.24\, \text{fm}^{-1}$
- $\alpha = 0.05\, \text{fm}^4$
  $\Lambda = 2.11\, \text{fm}^{-1}$
- $\alpha = 0.0625\, \text{fm}^4$
  $\Lambda = 2.00\, \text{fm}^{-1}$
- $\alpha = 0.08\, \text{fm}^4$
  $\Lambda = 1.88\, \text{fm}^{-1}$
- $\alpha = 0.16\, \text{fm}^4$
  $\Lambda = 1.58\, \text{fm}^{-1}$
16O: Lowering the Initial 3N Cutoff

Standard

\[ c_D = -0.2 \]
\[ c_E = -0.205 \]

Reduced 3N cutoff (\( c_E \) refit to \(^4\)He binding energy)

500 MeV

\[ c_D = -0.2 \]
\[ c_E = -0.016 \]

450 MeV

\[ c_D = -0.2 \]
\[ c_E = -0.098 \]

400 MeV

\[ c_D = -0.2 \]
\[ c_E = 0.205 \]

350 MeV

\[ c_D = -0.2 \]
\[ c_E = 0.205 \]

Lowering the initial 3N cutoff suppresses induced 4N terms

\[ \alpha = 0.04 \text{ fm}^4 \]
\[ \Lambda = 2.24 \text{ fm}^{-1} \]
\[ \alpha = 0.05 \text{ fm}^4 \]
\[ \Lambda = 2.11 \text{ fm}^{-1} \]
\[ \alpha = 0.0625 \text{ fm}^4 \]
\[ \Lambda = 2.00 \text{ fm}^{-1} \]
\[ \alpha = 0.08 \text{ fm}^4 \]
\[ \Lambda = 1.88 \text{ fm}^{-1} \]
\[ n\Omega = 20 \text{ MeV} \]
Spectroscopy of $^{12}\text{C}$

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

$\hbar\Omega = 16\text{ MeV}$
Spectroscopy of $^{12}$C

$^{12}$C

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

spectra largely insensitive to induced 4N

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

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

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

$\Lambda = 1.88 \text{ fm}^{-1}$
Ab Initio IT-NCSM Calculations for p- and sd-Shell Nuclei
Spectroscopy of Carbon Isotopes

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

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

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

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Spectroscopy of Carbon Isotopes

\[
B(E2, 2^{+} \rightarrow 0^{+}) \quad [e^{2}\text{fm}^4]
\]

- **10^C**
  - NEW EXPERIMENT
  - ANL, McCutchan et al.

- **12^C**
  - \( B(E2, 2^{+}_{1} \rightarrow 0^{+}_{\text{gs}}) \)
  - \( B(E2, 2^{+}_{2} \rightarrow 0^{+}_{\text{gs}}) \)

- **14^C**
  - \( B(E2, 2^{+}_{1} \rightarrow 0^{+}_{\text{gs}}) \)
  - \( B(E2, 2^{+}_{2} \rightarrow 0^{+}_{\text{gs}}) \)

- **16^C**
  - NEW EXPERIMENT
  - NSCL, Petri et al.

- **18^C**
  - NEW EXPERIMENT
  - NSCL, Voss et al.

- **20^C**
  - \( \Lambda_{3N} = 400 \text{ MeV} \)
  - \( \alpha = 0.08 \text{ fm}^4 \)
  - \( \hbar\Omega = 16 \text{ MeV} \)
Ground States of Oxygen Isotopes

Hergert, Binder, Calci, Langhammer, Roth; arXiv:1302.7294

NN+3N-induced (chiral NN)

$\Lambda_{3N} = 400\text{ MeV}, \alpha = 0.08\text{ fm}^4, E_{3\text{ max}} = 14, \text{ optimal } \hbar\Omega$

NN+3N-full (chiral NN+3N)
Ground States of Oxygen Isotopes

Hergert, Binder, Calci, Langhammer, Roth; arXiv:1302.7294

**NN+3N-induced**
(chiral NN)

**NN+3N-full**
(chiral NN+3N)

- $\Lambda_{3N} = 400$ MeV, $\hbar\Omega$

- Parameter-free ab initio calculations with full 3N interactions

- Highlights predictive power of chiral NN+3N Hamiltonians
Ground States of Oxygen Isotopes

$\Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad E_{3\max} = 14, \quad \text{optimal } \hbar\Omega$
Ground States of Oxygen Isotopes

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

\[ \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}, \quad E_{3 \text{ max}} = 1, \quad \text{optimal } \hbar \Omega \]

Hergert, Binder, Calci, Langhammer, Roth; arXiv:1302.7294
Multi-Reference Normal-Ordering Approximation
Motivation: Normal Ordering

- circumvent **formal extension of many-body method** to include explicit 3N interactions
- avoid the **increase of computational cost** caused by inclusion of explicit 3N interactions
- **normal-ordered two-body approximation** works very well for closed-shell systems (→ S. Binder)
- can we do the same for **open-shell nuclei**?
Normal Ordering of 3N Interaction

- **starting point**: three-body operator in second-quantized form with respect to the zero-body vacuum $|0\rangle$

\[
V_{3N} = \frac{1}{36} \sum_{abc, \bar{a}\bar{b}\bar{c}} V_{\bar{a}b\bar{c}}^{abc} A_{\bar{a}b\bar{c}}^{abc}
\]

\[
V_{\bar{a}b\bar{c}}^{abc} = \langle abc|V_{3N}|\bar{a}\bar{b}\bar{c}\rangle \\
A_{\bar{a}b\bar{c}}^{abc} = \alpha_{a}^{\dagger} \alpha_{b}^{\dagger} \alpha_{c}^{\dagger} \alpha_{\bar{a}} \alpha_{\bar{b}} \alpha_{\bar{c}}
\]

- **single-reference normal ordering**: assume reference state $|\Phi_{SR}\rangle$ given by a single Slater determinant
  - standard toolbox: Wick theorem, contractions, etc.

- **multi-reference normal ordering**: assume reference state $|\Phi_{MR}\rangle$ given by a superposition of Slater determinants
  - generalized Wick theorem and n-tupel contractions proposed by Mukherjee & Kutzelnigg (1997)
■ **three-body operator in normal-ordered form** with respect to multi-reference state $|\Phi_{MR}\rangle$

$$V_{3N} = W + \sum_{c,\tilde{c}} W^c_{\tilde{c}} \tilde{A}^c_{\tilde{c}} + \frac{1}{4} \sum_{bc,\tilde{b}c} W^{bc}_{\tilde{b}c} \tilde{A}^{bc}_{\tilde{b}c} + \frac{1}{36} \sum_{abc,\tilde{a}b\tilde{c}} W^{abc}_{\tilde{a}b\tilde{c}} \tilde{A}^{abc}_{\tilde{a}b\tilde{c}}$$

where $\tilde{A}^{\ldots\ldots}$ indicates multi-reference normal ordered string of creation and annihilation operators (abstract concept)

■ matrix elements of **normal-ordered n-body contributions** involve one-, two- and three-body density matrices for $|\Phi_{MR}\rangle$

$$W = \frac{1}{36} \sum_{abc,\tilde{a}b\tilde{c}} V^{abc}_{\tilde{a}b\tilde{c}} \rho^{abc}_{\tilde{a}b\tilde{c}}$$

$$W^c_{\tilde{c}} = \frac{1}{4} \sum_{ab,\tilde{a}b} V^{abc}_{\tilde{a}b\tilde{c}} \rho^{ab}_{\tilde{a}b}$$

$$W^{bc}_{\tilde{b}c} = \sum_{a,\tilde{a}} V^{abc}_{\tilde{a}b\tilde{c}} \rho^{a}_{\tilde{a}}$$

$$W^{abc}_{\tilde{a}b\tilde{c}} = V^{abc}_{\tilde{a}b\tilde{c}}$$
discard normal-ordered three-body contribution to define the
normal-ordered two-body (NO2B) approximation

\[ V_{\text{NO2B}} = W + \sum_{c, \tilde{c}} W_c^{\tilde{c}} \tilde{A}_c^{\tilde{c}} + \frac{1}{4} \sum_{bc, \tilde{b}, \tilde{c}} W_{bc}^{\tilde{b} \tilde{c}} \tilde{A}_{bc}^{\tilde{b} \tilde{c}} \]

converted back into vacuum normal order with respect to \(|0\rangle\)

\[ V_{\text{NO2B}} = \tilde{V} + \sum_{c, \tilde{c}} \tilde{V}_c^{\tilde{c}} A_c^{\tilde{c}} + \frac{1}{4} \sum_{bc, \tilde{b}, \tilde{c}} \tilde{V}_{bc}^{\tilde{b} \tilde{c}} A_{bc}^{\tilde{b} \tilde{c}} \]

with new matrix elements

\[ \tilde{V} = \frac{1}{36} \sum_{abc, \tilde{a}, \tilde{b}, \tilde{c}} V_{\tilde{a} \tilde{b} \tilde{c}}^{abc} \left( \rho_{\tilde{a} \tilde{b} \tilde{c}}^{abc} - 18 \rho_{\tilde{a}}^{a} \rho_{\tilde{b} \tilde{c}}^{bc} + 36 \rho_{\tilde{a}}^{a} \rho_{\tilde{b}}^{b} \rho_{\tilde{c}}^{c} \right) \]

\[ \tilde{V}_{\tilde{c}}^{c} = \frac{1}{4} \sum_{ab, \tilde{a} \tilde{b}} V_{\tilde{a} \tilde{b} \tilde{c}}^{abc} \left( \rho_{\tilde{a} \tilde{b}}^{ab} - 4 \rho_{\tilde{a}}^{a} \rho_{\tilde{b}}^{b} \right) \]

\[ \tilde{V}_{\tilde{b} \tilde{c}}^{bc} = \sum_{a, \tilde{a}} V_{\tilde{a} \tilde{b} \tilde{c}}^{abc} \rho_{\tilde{a}}^{a} \]
Single-Reference Normal Ordering

- **single-reference normal ordering** is recovered by pugging in density matrices for a single Slater-determinant

\[
\begin{align*}
\rho^a_{\bar{a}} & = n_a \delta^a_{\bar{a}} \\
\rho^{ab}_{\bar{a} \bar{b}} & = \rho^a_{\bar{a}} \rho^b_{\bar{b}} - \rho^b_{\bar{a}} \rho^a_{\bar{b}} \\
\rho^{abc}_{\bar{a} \bar{b} \bar{c}} & = \ldots
\end{align*}
\]

- three-body operator in **single-reference NO2B approximation** converted back into vacuum representation

\[
V_{\text{NO2B}} = \tilde{V} + \sum_{c, \bar{c}} \tilde{V}^c_{\bar{c}} A^c_{\bar{c}} + \frac{1}{4} \sum_{bc, \bar{b} \bar{c}} \tilde{V}^{bc}_{\bar{b} \bar{c}} A^{bc}_{\bar{b} \bar{c}}
\]

with simplified matrix elements

\[
\begin{align*}
\tilde{V} & = \frac{1}{6} \sum_{abc} V^{abc}_{abc} n_a n_b n_c \\
\tilde{V}^c_{\bar{c}} & = -\frac{1}{2} \sum_{ab} V^{abc}_{ab\bar{c}} n_a n_b \\
\tilde{V}^{bc}_{\bar{b} \bar{c}} & = \sum_{a} V^{abc}_{ab\bar{c}} n_a
\end{align*}
\]
IT-NCSM with MR-NO2B Approximation

1. perform NCSM with explicit 3N interaction for small $N_{\text{max}}$
   - ground state defines the reference state $|\Phi_{\text{MR}}\rangle$
   - no explicit information on excited states enters

2. compute zero-, one- and two-body matrix elements of MR-NO2B approximation
   - density matrices for $|\Phi_{\text{MR}}\rangle$ can be precomputed and stored
   - three-body density matrix is not need explicitly

3. perform NCSM or IT-NCSM calculation up to large $N_{\text{max}}$ using MR-NO2B approximation
   - same computational cost as a simple NN-only calculation
   - larger model spaces become accessible
Benchmark: $^6\text{Li}$

$^6\text{Li}$

$\Lambda_{3N} = 500\ \text{MeV}$

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

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

explicit 3N
Benchmark: $^6\text{Li}$

NN+3N-induced

$E$ [MeV]

NN+3N-full

$E_x$ [MeV]

$\Lambda_{3N} = 500$ MeV
$\alpha = 0.08$ fm$^4$
$\hbar\Omega = 20$ MeV

Explicit 3N

$^6\text{Li}$

MR-NO2B

$N_{\text{max}}^\text{ref} = 2, 4, 6$
Benchmark: $^{12}$C

MR-NO2B approximation works surprisingly well for ground states as well as excited states

MR-NO2B approximation is robust with respect to variations of the reference state, i.e. $N_{\text{ref max}}^{\text{ref}}$

$\Lambda_{3N} = 500$ MeV
$\alpha = 0.08$ fm$^4$
$\hbar \Omega = 20$ MeV

MR-NO2B
$N_{\text{ref max}}^{\text{ref}} = 2, 4$
Challenge: $^{10}\text{B}$

$\Lambda_{3N} = 500 \text{ MeV}$

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

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

$N_{\text{ref}}^{\text{max}} = 2, 4$

$10\text{B}$
Reflections
Questions I

- How can we extend current ab-initio methods to describe open-shell and deformed nuclei?
  - IT-NCSM describes open and closed-shell nuclei on the same footing
  - MR-IM-SRG is a true open-shell approach for medium/heavy masses (→ H. Hergert), others are following

- How can we include the effects of three-nucleon forces in a computationally efficient manner?
  - explicit 3N interactions are used in IT-NCSM very efficiently
  - CCSD and ΛCCSD(T) is available with explicit 3N (→ S. Binder)
  - single- and multi-reference normal ordering provide robust approximations at reduced cost
  - this does not imply that any kind of ‘summation over the third particle’ is accurate
Questions II

■ How can we describe the onset of pairing in nuclei within various ab-initio frameworks?
  • any ab initio approach for open shells has to describe pairing

■ Can we develop reliable theoretical error estimates?
  • defining element of any ab initio approach
  • uncertainty quantification case by case within the many-body approach, not just guessing
  • uncertainty quantification also necessary for the chiral EFT inputs

■ How can we bridge structure and reactions in a consistent fashion?
  • NCSM/RGM and NCSMC with 3N are on their way (→ P. Navratil)

■ How can we generate reliable predictions for the drip-lines?
  • simply do all of the above...
Epilogue

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