Towards
Ab Initio Nuclear Structure beyond the p-Shell

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Overview

■ Motivation

■ Modern Effective Interactions
  ● Unitary Correlation Operator Method
  ● Similarity Renormalization Group

■ Innovative Many-Body Methods
  ● No-Core Shell Model
  ● Importance Truncated NCSM

■ Perspectives
Nuclear Structure in the 21st Century

RIBF @ RIKEN, ...

NuSTAR @ FAIR, ...

nuclear astrophysics

nuclei far-off stability

exotic modes hyper-nuclei,...

predictive nuclear structure theory for exotic nuclei

bridging between low-energy QCD and nuclear structure theory
- chiral interactions: consistent NN & 3N interaction derived within $\chi$EFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental NN phase-shifts with high precision
- induce strong short-range central & tensor correlations
Nuclear Structure

- ‘exact’ solution of the many-body problem for light and intermediate masses (GFMC, NCSM, CC,...)
- controlled approximations for heavier nuclei (HF & MBPT,...)
- rely on restricted model spaces of tractable size
- not suitable for the description of short-range correlations

Realistic Nuclear Interactions

Low-Energy QCD

Exact / Approx. Many-Body Methods
Nuclear Structure

Exact / Approx. Many-Body Methods

Modern Effective Interactions

Realistic Nuclear Interactions

Low-Energy QCD

- adapt realistic potential to the available model space
  - tame short-range correlations
  - improve convergence behavior
- conserve experimentally constrained properties (phase shifts)
  - generate new realistic interaction
- need consistent effective interaction & effective operators
- unitary transformations most convenient
Modern Effective Interactions

Unitary Correlation Operator Method (UCOM)

**Correlation Operator**

define an unitary operator $C$ to describe the effect of short-range correlations

$$C = \exp[-i G] = \exp[-i \sum_{i<j} g_{ij}]$$

**Correlated States**

imprint short-range correlations onto uncorrelated many-body states

$$|\tilde{\psi}\rangle = C |\psi\rangle$$

**Correlated Operators**

adapt Hamiltonian and all other observables to uncorrelated many-body space

$$\tilde{O} = C^\dagger O C$$

$$\langle \tilde{\psi} | O | \tilde{\psi}' \rangle = \langle \psi | C^\dagger O C | \psi' \rangle = \langle \psi | \tilde{O} | \psi' \rangle$$
Deuteron: Manifestation of Correlations

- **exact deuteron solution** for Argonne V18 potential
  
  \[ \rho_{S=1, M_S=\pm 1}(\vec{r}) \]

- Short-range repulsion suppresses wavefunction at small distances \( r \)

- Central correlations

- Tensor interaction generates D-wave admixture in the ground state

- Tensor correlations

\[ \langle r | \phi_L \rangle \]

\[ L = 0 \]

\[ L = 2 \]

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

0 2 4 6 8
explicit ansatz for the correlation operator motivated by the **physics of short-range central and tensor correlations**

<table>
<thead>
<tr>
<th>Central Correlator $C_r$</th>
<th>Tensor Correlator $C_\Omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>radial distance-dependent shift in the relative coordinate of a nucleon pair</td>
<td>angular shift depending on the orientation of spin and relative coordinate of a nucleon pair</td>
</tr>
<tr>
<td>$g_r = \frac{1}{2} [s(r) q_r + q_r s(r)]$</td>
<td>$g_\Omega = \frac{3}{2} \vartheta(r) [(\vec{\sigma}<em>1 \cdot \vec{q}</em>\Omega)(\vec{\sigma}<em>2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}</em>\Omega)]$</td>
</tr>
<tr>
<td>$q_r = \frac{1}{2} [\vec{r} \cdot \vec{q} + \vec{q} \cdot \vec{r}]$</td>
<td>$\vec{q}_\Omega = \vec{q} - \frac{\vec{r}}{r} q_r$</td>
</tr>
</tbody>
</table>

- $s(r)$ and $\vartheta(r)$ for given potential determined by energy minimization in the two-body system (for each $S, T$)
Correlated States: The Deuteron

\[ \langle r | \phi \rangle \]

\[ \langle r | C_r | \phi \rangle \]

\[ \langle r | C \Omega C_r | \phi \rangle \]

\[ s(r) \]

\[ \vartheta(r) \]

Central correlations

Tensor correlations

Only short-range tensor correlations treated by \( C_\Omega \)
Correlated Interaction: $V_{UCOM}$

$^3S_1$

$^3S_1 - ^3D_1$

Pre-diagonalization of Hamiltonian

$V_{AV18}$

$V_{UCOM}$
Modern Effective Interactions

Similarity Renormalization Group (SRG)

unitary transformation of the Hamiltonian to a band-diagonal form with respect to a given uncorrelated many-body basis

### Flow Equation for Hamiltonian

- **evolution equation for Hamiltonian**

  \[ \tilde{H}(\alpha) = C^\dagger(\alpha) H C(\alpha) \quad \rightarrow \quad \frac{d}{d\alpha} \tilde{H}(\alpha) = [\eta(\alpha), \tilde{H}(\alpha)] \]

- **dynamical generator defined as commutator with the operator in whose eigenbasis \( H \) shall be diagonalized**

  \[ \eta(\alpha) = [T_{\text{int}}, \tilde{H}(\alpha)] = \frac{2B}{2\mu} [\tilde{q}^2, \tilde{H}(\alpha)] \]

- \( \eta(0) \) has the same structure as the UCOM generators \( g_r \) and \( g_\Omega \)
SRG Evolution: The Deuteron

\[ \langle r | \phi_{SRG}^L=0 \rangle \]

\[ \langle r | \phi_{SRG}^L=2 \rangle \]

strong off-diagonal contributions

short-range central & tensor correlations

SRG Evolution: The Deuteron

\[ V_{\text{SRG}}(q, q') \]

\[ \langle r \mid \phi_{\text{SRG}}^{L=0} \rangle \]

\[ \langle r \mid \phi_{\text{SRG}}^{L=2} \rangle \]

\[ \alpha = 0.1000 \text{ fm}^4 \]

suppression of off-diagonal contributions

elimination of short-range correlations
Exact Many-Body Methods

No-Core Shell Model

Roth & Navrátil — in preparation
No-Core Shell Model +
Matrix Elements of Correlated Realistic Interaction $V_{UCOM}$

- many-body state is expanded in Slater determinants of harmonic oscillator single-particle states
- large-scale diagonalization of Hamiltonian within a truncated model space ($N\hbar\omega$ truncation)
- assessment of short- and long-range correlations
- role of three-nucleon interactions
$^4\text{He}$: Convergence

$V_{\text{AV18}}$

$V_{\text{UCOM}}$

residual state-dependent long-range correlations
$^4$He: Convergence

**$V_{AV18}$**

**$V_{UCOM}$**

omitted three- and four-body contributions
Three-Body Interactions — Strategies

**Correlated Hamiltonian in Many-Body Space**

\[
\tilde{H} = C^\dagger (T + V_{NN} + V_{3N}) C \\
= \tilde{T}^{[1]} + (\tilde{T}^{[2]} + \tilde{V}^{[2]}_{NN}) + (\tilde{T}^{[3]} + \tilde{V}^{[3]}_{NN} + \tilde{V}^{[3]}_{3N}) + \cdots \\
= T + V_{UCOM} + V^{[3]}_{UCOM} + \cdots
\]

- strategies for treating the three-body contributions:
  1. **include full** $V^{[3]}_{UCOM}$ consisting of genuine and induced 3N terms
  2. **replace** $V^{[3]}_{UCOM}$ by phenomenological three-body force
  3. **minimize** $V^{[3]}_{UCOM}$ by proper choice of unitary transformation
Three-Body Interactions — Tjon Line

- Tjon-line: $E(^{4}\text{He})$ vs. $E(^{3}\text{H})$
- for phase-shift equivalent NN-interactions

![Graph showing $E(^{3}\text{H})$ vs. $E(^{4}\text{He})$ for various interactions such as AV18, Nijm II, Nijm I, and CD Bonn, with experimental data and calculated values $V_{NN} + V_{3N}$ indicated.]
Three-Body Interactions — Tjon Line

The graph illustrates the relationship between $E^{(4}\text{He)}$ and $E^{(3}\text{H)}$ for phase-shift equivalent NN-interactions. The graph shows that

- The Tjon-line: $E^{(4}\text{He)}$ vs. $E^{(3}\text{H)}$ for phase-shift equivalent NN-interactions.
- Change of $C_\Omega$-correlator range results in shift along Tjon-line.

By choosing a correlator with energies close to the experimental value, we can minimize the net three-body force.
Three-Body Interactions — Tjon Line

- **Tjon-line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions

- same behavior for the SRG interaction as function of $\alpha$

- minimize net three-body force by choosing correlator with energies close to experimental value

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10^B: Hallmark of a 3N Interaction?

\[ E - E_{3^+} \text{ [MeV]} \]

\[ V_{UCOM} \]

\[ \text{Exp} \]

\[ 4^+ \]

\[ 2^+ \]

\[ 0^+ \]

\[ 1^+ \]

\[ 3^+ \]

\[ \hbar \omega = 18 \text{MeV} \]

\[ h \omega = 18 \text{MeV} \]

$^{10}\text{B}$: Hallmark of a 3N Interaction?

$V_{\text{UCOM}}$ gives correct level ordering without any 3N interaction.
Exact Many-Body Methods

Importance Truncated No-Core Shell Model

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to p-shell
- full $6\hbar\omega$ calculation for $^{40}\text{Ca}$ presently not feasible (basis dimension $\sim 10^{10}$)

Importance Truncation
reduce NCSM space to relevant states using an a priori importance measure derived from MBPT
estimate a posteriori amplitude $C_\nu$ of shell model configuration $|\Phi_\nu\rangle$ via a priori perturbative weight $\kappa_\nu$ starting from a reference state $|\Psi_{\text{ref}}\rangle$:

$$\kappa_\nu = -\frac{\langle \Phi_\nu | H' | \Psi_{\text{ref}} \rangle}{E_\nu^{(0)} - E_{\text{ref}}^{(0)}}$$

iterative procedure for construction of importance truncated model space

![Graph showing amplitude $|C_\nu|$ vs. importance measure $|\kappa_\nu|$ for different model spaces: 1p1h, 2p2h, 3p3h, 4p4h.](image-url)
Benchmark: $^4$He

- reproduces exact NCSM result with an importance truncated basis that is 2 orders of magnitude smaller than the full $N_{\text{max}}\hbar\omega$ space
Benchmark: $^{16}$O

- excellent agreement with full NCSM calculation although configurations beyond 4p4h are not included
- dimension reduced by several orders of magnitude; possibility to go way beyond the domain of the full NCSM

$^{16}$O

$V_{UCOM}$

$h\omega = 20$ MeV

$\log_{10} D$

$N_{\text{max}}$

- full NCSM (Antoine)
- IT-NCSM 2p2h
- IT-NCSM 3p3h
- IT-NCSM 4p4h
Benchmark: $^{40}$Ca

$^{40}$Ca

$V_{UCOM}$

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

$^{40}$Ca

$V_{UCOM}$

$\hbar \omega = 17 \text{ MeV}$

- $16\hbar \omega$ calculations for $^{40}$Ca are feasible
- extrapolation of ground state energy ($3p3h$, $\hbar \omega = 17 \text{ MeV}$) yields

$$E_\infty \approx -316 \text{ MeV}$$

$$E_{\text{exp}} = -342.05 \text{ MeV}$$

+ full NCSM (Antoine)

- IT-NCSM 2p2h
- IT-NCSM 3p3h
- IT-NCSM 4p4h

Modern Effective Interactions

- Treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG, Lee-Suzuki,...
- Universal phase-shift equivalent correlated interaction $V_{UCOM}$

Innovative Many-Body Methods

- No-Core Shell Model,...
- Importance Truncated NCSM, Coupled Cluster Method,...
- Hartree-Fock plus MBPT, Padé Resummed MBPT, BHF, RPA,...

Unified description of nuclear structure across the whole nuclear chart is within reach
thanks to my group & my collaborators

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