Ab Initio Nuclear Structure beyond the p-Shell

Importance Truncated No-Core Shell Model

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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

Low-Energy QCD
Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

- 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
From QCD to Nuclear Structure

Nuclear Structure

- Exact / Approx. Many-Body Methods
  - ‘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
Nuclear Structure

- Exact / Approx. Many-Body Methods
  - 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
  - provide consistent effective interaction & effective operators
  - unitary transformations most convenient

- Modern Effective Interactions

- Realistic Nuclear Interactions

- Low-Energy QCD
Modern Effective Interactions

Unitary Correlation Operator Method (UCOM)

Deuteron: Manifestation of Correlations

- **exact deuteron solution** for Argonne V18 potential

\[ \rho_{S=1, M_S=\pm 1}^{(2)}(\vec{r}) \]

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

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

- Central correlations

- Tensor correlations

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

\( r \) [fm]

\( L = 0 \)

\( L = 2 \)
**Unitary Correlation Operator Method**

Explicit ansatz for unitary transformation operator *motivated by the physics of short-range central & 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>$g_\Omega = \frac{3}{2} \vartheta(r) \left[ (\vec{\sigma}<em>1 \cdot \vec{q}</em>\Omega)(\vec{\sigma}<em>2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}</em>\Omega) \right]$</td>
</tr>
<tr>
<td>$q_r = \frac{1}{2} [\frac{\vec{r}}{r} \cdot \vec{q} + \vec{q} \cdot \frac{\vec{r}}{r}]$</td>
<td>$\vec{q}_\Omega = \vec{q} - \frac{\vec{r}}{r} \ q_r$</td>
</tr>
</tbody>
</table>

$C = C_\Omega C_r = \exp \left( -i \sum_{i<j} g_{\Omega,ij} \right) \exp \left( -i \sum_{i<j} g_{r,ij} \right)$

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

\[ \langle r \mid \phi \rangle \]

\[ \langle r \mid \phi \rangle \]

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

\[ \langle r \mid C_{\Omega} C_r \phi \rangle \]

- Central correlations
- Tensor correlations

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

$3S_1$  
$3S_1 - 3D_1$

$V_{AV18}$

pre-diagonalization of Hamiltonian

$V_{UCOM}$
Modern Effective Interactions

Similarity Renormalization Group (SRG)

Roth, Reinhardt, Hergert — arXiv:0802.4239
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
  \[
  \eta(\alpha) \equiv \frac{2B}{2\mu} [\vec{q}^2, \tilde{H}(\alpha)]
  \]

**UCOM vs. SRG**

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

\[ \langle r \left| \phi^{L=0}_{\text{SRG}} \right\rangle \]

\[ \langle r \left| \phi^{L=2}_{\text{SRG}} \right\rangle \]

strong off-diagonal contributions

short-range central & tensor correlations

Argonne V18

Robert Roth – TU Darmstadt – 04/2008
SRG Evolution: The Deuteron

UCOM vs. SRG

extract the UCOM correlation functions \( s(r) \) and \( \vartheta(r) \) from the SRG evolved wavefunctions

\[ \alpha = 0.1000 \text{ fm}^4 \]
Exact Many-Body Methods

No-Core Shell Model

Roth & Navrátil — in preparation
Many-body state is expanded in Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states

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

$N_{\text{max}} \hbar \omega$ model space: truncate basis of Slater determinants with respect to number of oscillator quanta (unperturbed excitation energy)

With increasing model space size more and more correlations can be described by the shell model states.

Facilitates systematic study of short- and long-range correlations.
$^4$He: Convergence

\[ V_{\text{AV18}} \]

\[ V_{\text{UCOM}} \]

$E_{\text{AV18}}$ vs. $\hbar \omega$ [MeV]

$E$ vs. $\hbar \omega$ [MeV]

residual state-dependent long-range correlations
$^4\text{He}: \text{Convergence}$

**$V_{AV18}$**

**$V_{UCOM}$**

Omitted three- and four-body contributions
Three-Body Interactions — Tjon Line

\[ E(4\text{He}) \text{ vs. } E(3\text{H}) \]

Tjon-line: for phase-shift equivalent NN-interactions

\[ E(4\text{He}) \text{ vs. } E(3\text{H}) \]
Three-Body Interactions — Tjon Line

- 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

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

This $V_{\text{UCOM}}$ is used in the following

$E(^4\text{He})$ [MeV] vs. $E(^3\text{H})$ [MeV]

- AV18
- Nijm II
- Nijm I
- CD Bonn
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
$^{10}$B: Hallmark of a 3N Interaction?

\[ \nu_{UCOM} \]

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

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

\[ 0\hbar \omega \quad 2\hbar \omega \quad 4\hbar \omega \quad 6\hbar \omega \quad 8\hbar \omega \]

\[ \text{Exp} \]

\[ \begin{align*}
4^+ & : \quad -62.1 \\
2^+ & : \quad -64.7
\end{align*} \]
$^{10}\text{B: Hallmark of a 3N Interaction?}$

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

Importance Truncated No-Core Shell Model

Roth, Piecuch, Gour — in preparation
Roth — in preparation
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
Importance Truncation: General Idea

- start with $\mathcal{N}_{\text{max}} \hbar \omega$ space of the NCSM
  - separation of intrinsic and center-of-mass component of state

- **importance measure**: identify important basis states $|\Phi_\nu\rangle$ via first-order multiconfigurational perturbation theory
  \[
  \kappa_\nu = -\frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}
  \]

- **importance truncation**: starting from approximation $|\Psi_{\text{ref}}\rangle$ of target state, construct importance truncated space spanned by basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$
  - contains 2p2h excitations with respect to $|\Psi_{\text{ref}}\rangle$ at most
  - perturbative measure entails $\mathcal{N}p\mathcal{N}h$ hierarchy, i.e., higher-order $\mathcal{N}p\mathcal{N}h$ states only enter in higher orders of PT

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Importance Truncation: General Idea

- solve **eigenvalue problem** in importance truncated space
  - rigorous variational upper bound

- **iterative scheme**: repeat construction of importance truncated model space using eigenstate as improved reference $|\Psi_{\text{ref}}\rangle$
  - recovers full $\mathcal{N}_{\text{max}}\hbar\omega$ space after $A/2$ iterations in the limit $\kappa_{\text{min}} \to 0$
  - typically 2 or 3 iterations to convergence

- **threshold extrapolation**: constrained extrapolation $\kappa_{\text{min}} \to 0$ of energies recovers contribution of excluded configurations

- **perturbative estimates** and **Davidson corrections** for the contribution of the next iteration also possible
importance measure $\kappa_\nu$ provides **reliable a priori estimate** of the a posteriori amplitude $C_\nu$ obtained from diagonalization.

$1^6$O
$V_{UCOM}$
$\hbar\Omega = 22$ MeV
$N_{max} = 6$
Technicalities: Threshold Extrapolation

- **smooth** $\kappa_{\text{min}}$-dependence allows for robust extrapolation
- include perturbative estimate of excluded configurations for simultaneous constrained extrapolation $\kappa_{\text{min}} \rightarrow 0$

$\mathcal{N}_{\text{max}} = 6$

$\mathcal{N}_{\text{max}} = 10$

$\mathcal{N}_{\text{max}} = 14$

$\mathcal{N}_{\text{max}} = 18$

$E_{\text{[MeV]}}$ vs. $\kappa_{\text{min}} \left[ 10^{-5} \right]$

$^{16}\text{O}$

$V_{\text{UCOM}}$

$\hbar \Omega = 22 \text{ MeV}$
$^4\text{He}$: Importance Truncated NCSM

- reproduces exact NCSM result for all $\hbar \omega$ and $N_{\text{max}}$
- importance measure and threshold extrapolation are reliable
- no center-of-mass contamination of states

\[ E \text{ [MeV]} \quad \hbar \Omega \text{ [MeV]} \]

- $^4\text{He}$
- $V_{\text{UCOM}}$
- $N_{\text{max}} = 4$

- full NCSM
- IT-NCSM (2 iter, 4p4h)
4\textsuperscript{He}: Importance Truncated NCSM

- reproduces exact NCSM result for all $\hbar \omega$ and $N_{\text{max}}$
- iterations converge very fast
- reduction of basis by more than two orders of magnitude w/o loss of precision
- saturation of IT-NCSM dimension indicates convergence

$V_{\text{UCOM}} = 40 \text{ MeV}$

$\hbar \Omega = 40 \text{ MeV}$
$^{16}$O: Importance Truncated NCSM

- 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

![Graph showing energy (E) and maximum dimension ($D_{max}$) vs. maximum nucleon number ($N_{max}$)]
$^{16}\text{O}$: Importance of Truncated NCSM

- Extrapolation to $N_{\text{max}} \to \infty$
  \[ E_{\text{IT-NCSM}(2 \text{ iter})} \approx -129 \pm 1 \text{ MeV} \]
  \[ E_{\text{IT-NCSM}(2 \text{ iter})+\text{MRD}} \approx -130 \pm 1 \text{ MeV} \]
  \[ E_{\exp} = -127.6 \text{ MeV} \]

- $V_{\text{UCOM}}$ predicts reasonable binding energies also for heavier nuclei

**Diagram**: Graph showing the energy $E$ in MeV as a function of $N_{\text{max}}$. The graph includes different symbols representing different calculations and configurations.

- Full NCSM
- IT-NCSM(1 iter, 2p2h)
- IT-NCSM(2 iter, 4p4h)
- IT-NCSM(2 iter, 4p4h) + MRD
$^{40}$Ca: Importance Truncated NCSM

- 16\hbar\Omega and more are feasible for $^{40}$Ca in IT-NCSM(2 iter)
- size of individual $N_p N_h$-contributions depends on $\hbar\Omega$
- result consistent with experimental binding energy

For $^{40}$Ca, $V_{UCOM}$:

- $\hbar\Omega = 20$ MeV
- $\hbar\Omega = 17$ MeV

Graph showing the variation of $E$ [MeV] with $N_{\text{max}}$.
Direct Comparison: CC vs. IT-CI

- **CR-CC vs. IT-CI:**
  - good agreement for all $\hbar \Omega$ and models spaces
  - lack of strict size extensivity in the IT-CI is irrelevant

- **CR-CC/IT-CI vs. IT-NCSM:**
  - CC/CI seems to tend to a lower binding energy than IT-NCSM
  - CC/CI suffer from center-of-mass contamination

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in collaboration with J. Gour & P. Piecuch (MSU)
IT-NCSM: Pros and Cons

✔ rigorously fulfills variational principle and Hylleraas-Undheim theorem

✔ no sizable center-of-mass contamination induced by IT in $N_{\text{max}} \hbar \Omega$ space

✔ constrained threshold extrapolation $\kappa_{\text{min}} \rightarrow 0$ recovers contribution of excluded configurations efficiently and accurately

✔ perturbative correction and Davidson correction for perturbative energy correction can be used

✔ compatible with shell-model: excited states and angular-momentum projection via Lanczos, eigenstates in shell-model representation, computation of observables

✘ only approximate size-extensivity if working with few iterations

✘ computationally still demanding
Modern Effective Interactions

- treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG, Lee-Suzuki,...
- phase-shift equivalent correlated interaction $V_{UCOM}$ which is soft and requires minimal three-body forces
- universal input for...

Innovative Many-Body Methods

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