Ab-Initio Nuclear Structure beyond the p-Shell:
Interactions & Many-Body Techniques

Robert Roth
Institut für Kernphysik
Overview

■ Motivation

■ Unitarily Transformed Interactions
  • Unitary Correlation Operator Method
  • Similarity Renormalization Group

■ Computational Many-Body Methods
  • Testing UCOM & SRG in Nuclei: NCSM & HF+MBPT
  • Importance Truncated NCSM
Nuclear Structure

Low-Energy QCD
Nuclear Structure

- chiral EFT interactions: consistent NN & 3N interaction derived within $\chi$EFT
- traditional NN-interactions: Argonne V18, CD Bonn, ...
- reproduce experimental two-body data with high precision
- induce strong short-range central & tensor correlations
Nuclear Structure

- ‘exact’ solution of the many-body problem for light & intermediate masses (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
From QCD to Nuclear Structure

Nuclear Structure

Exact / Approx. Many-Body Tools

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 & deuteron)
  - generate new realistic int.

- need consistent effective interaction & effective operators

- unitary transformations most convenient
Nuclear Structure

- Exact / Approx. Many-Body Tools
- Modern Effective Interactions
- Realistic Nuclear Interactions
- Low-Energy QCD

I’m one of the MBT guys...

...and this is the stuff I’m trying to sell.
Unitarily Transformed Interactions

Unitary Correlation Operator Method (UCOM)

Correlation Operator

define a 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 to uncorrelated states (pre-diagonalization)

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

$$\langle \tilde{\psi} | O | \tilde{\psi}' \rangle = \langle \psi | C^\dagger O C | \psi' \rangle = \langle \psi | \tilde{O} | \psi' \rangle$$
Unitary Correlation Operator Method

explicit ansatz for unitary transformation operator motivated by the physics of short-range 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></td>
</tr>
<tr>
<td>$g_r = \frac{1}{2} [s(r) q_r + q_r s(r)]$</td>
<td></td>
</tr>
<tr>
<td>$q_r = \frac{1}{2} [\vec{r} \cdot \vec{q} + \vec{q} \cdot \vec{r}]$</td>
<td></td>
</tr>
<tr>
<td>$C = C_\Omega C_r = \exp\left(-i \sum_{i&lt;j} g_\Omega,ij \right) \exp\left(-i \sum_{i&lt;j} g_r,ij \right)$</td>
<td></td>
</tr>
<tr>
<td>- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair</td>
<td></td>
</tr>
<tr>
<td>$g_\Omega = \frac{3}{2} g(r)[(\vec{\sigma}<em>1 \cdot \vec{q}</em>\Omega)(\vec{\sigma}<em>2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}</em>\Omega)]$</td>
<td></td>
</tr>
<tr>
<td>$\vec{q}_\Omega = \vec{q} - \frac{\vec{r}}{r} q_r$</td>
<td></td>
</tr>
</tbody>
</table>

- $s(r)$ and $g(r)$ depend on & are optimized for initial potential
Correlated States: The Deuteron

- **Central Correlations**
  - $\langle r | \phi \rangle$
  - $\langle r | C_r \phi \rangle$
  - $\langle r | C_{\Omega} C_r \phi \rangle$

- **Tensor Correlations**
  - $s(r)$
  - $g(r)$

- $L = 0$ and $L = 2$

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

\[ ^3S_1 \]

\[ ^3S_1 - ^3D_1 \]

$V_{\text{AV18}}$

pre-diagonalization of Hamiltonian

$V_{\text{UCOM}}$
Unitarily Transformed Interactions

Similarity Renormalization Group (SRG)

flow evolution of the Hamiltonian to band-diagonal form with respect to uncorrelated many-body basis

Flow Equation for Hamiltonian

- evolution equation for Hamiltonian
  \[ \tilde{H}(\alpha) = C^\dagger(\alpha) H C(\alpha) \rightarrow \frac{d}{d\alpha} \tilde{H}(\alpha) = [\eta(\alpha), \tilde{H}(\alpha)] \]

- dynamical generator defined as commutator with the operator in whose eigenbasis \( H \) shall be diagonalized
  \[ \eta(\alpha) = \frac{2B}{2\mu} [\vec{q}^2, \tilde{H}(\alpha)] \]

UCOM vs. SRG

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

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

**strong off-diagonal contributions**

**short-range central & tensor correlations**

---

Argonne V18
SRG Evolution: The Deuteron

UCOM vs. SRG
extract the UCOM correlation functions $s(r)$ and $g(r)$ from the SRG evolved wavefunctions

$\tilde{\alpha} = 0.1000 \text{ fm}^4$
Computational Many-Body Methods

Testing UCOM & SRG Interactions in Nuclei
NCSM: $^4$He Convergence

$V_{\text{AV18}}$

$V_{\text{UCOM}}$

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

$V_{\text{AV18}}$

$V_{\text{UCOM}}$

omitted 3- & 4-body contributions
Correlated Hamiltonian in Many-Body Space

\[
\tilde{H} = C^\dagger \left( T + V_{NN} + V_{3N} \right) C
\]

\[
= \tilde{T}^{[1]} + \left( \tilde{T}^{[2]} + \tilde{V}_{NN}^{[2]} \right) + \left( \tilde{T}^{[3]} + \tilde{V}_{NN}^{[3]} + \tilde{V}_{3N}^{[3]} \right) + \cdots
\]

\[
= T + V_{UCOM} + V_{UCOM}^{[3]} + \cdots
\]

- **include full** \( V_{UCOM}^{[3]} \) consisting of genuine and induced 3N terms (very hard in UCOM, but Dick can do it in SRG)

- **replace** \( V_{UCOM}^{[3]} \) by phenomenological three-body force (easily tractable also for heavier nuclei)

- **minimize** \( V_{UCOM}^{[3]} \) by proper choice of unitary transformation (cheap calculation with a pure two-body interaction)
Three-Body Interactions — Tjon Line

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

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

- Change of $C_Ω$-correlator range results in shift along Tjon-line

This $V_{UCOM}$ requires minimal 3N interactions

Control the strength of the net 3N interaction through the parameters of the unitary transformation
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 $\alpha$

control the strength of the net 3N interaction through the parameters of the unitary transformation
$^{10}\text{B}$: Hallmark of a 3N Interaction?

![Graph showing $V_{\text{UCOM}}$ and experimental (Exp) values for different spin states (0+, 1+, 2+, 4+). The graph compares the calculated values with experimental data, highlighting the difference in energy ($E - E_{3^+}$) and focusing on the energy levels at $\hbar\Omega = 18\text{MeV}$. The graph includes markers for energy levels at $0\hbar\Omega$, $2\hbar\Omega$, $4\hbar\Omega$, $6\hbar\Omega$, and $8\hbar\Omega$, with experimental data points at $-62.1\text{MeV}$ and $-64.7\text{MeV}$. The graph illustrates the potential energy differences and the alignment between calculated and experimental values for the various spin states.]
\[ E - E_{3+} \]

Two-body \( V_{\text{UCOM}} \) fixed for \(^3\text{H}/^4\text{He}\) gives correct level ordering without any 3N interaction.
UCOM vs. SRG: $^4$He Convergence

$V_{UCOM}$ MIN, $I_9 = 0.09 \text{ fm}^3$

$V_{UCOM}$ SRG, $\bar{\alpha} = 0.04 \text{ fm}^4$

$V_{SRG}$ $\bar{\alpha} = 0.03 \text{ fm}^4$

UCOM & SRG show very similar convergence behavior in light nuclei

- $I_9$ or $\bar{\alpha}$ adjusted such that $^4$He binding energy is reproduced
UCOM vs. SRG: Hartree-Fock Systematics

UCOM & SRG generate (or require) very different 3N interactions

Robert Roth – TU Darmstadt – 03/2009
UCOM & simple 3N contact interaction gives good description of binding energies & radii

\[(E - E_{\text{exp}})/A \text{ [MeV]}\]

\[R_{\text{ch}} \text{ [fm]}\]

\begin{align*}
\text{HF} & : e_{\text{max}} = 10, 12, 14 \\
\text{HF+PT(2)} & : e_{\text{max}} = 10, 12, 14 \\
\text{UCOM} & : V_{\text{UCOM}} = \text{SRG, } \bar{\alpha} = 0.08 \text{ fm}^4 \\
\text{C} & = 1200 \text{ MeV fm}^6 \\
V_{\delta,3N} & : e_{3\text{max}} = 10
\end{align*}
Computational Many-Body Methods

Importance-Truncated No-Core Shell Model

Roth, Piecuch, Gour — arXiv: 0806.0333
Roth — arXiv: 0903.4605
Importance-Truncated NCSM

- converged NCSM calculations are 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 the relevant basis states using an a priori importance measure derived from MBPT

similar strategies have first been developed in quantum chemistry: configuration-selective multireference CI
given an initial approximation $|\psi_{\text{ref}}\rangle$ for the **target state** within a limited **reference space** $\mathcal{M}_{\text{ref}}$

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

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

$$\kappa_\nu = -\frac{\langle \Phi_\nu | H |\psi_{\text{ref}}\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

**construct importance-truncated space** $\mathcal{M}(\kappa_{\text{min}})$ spanned by basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$

**solve eigenvalue problem** in importance truncated space $\mathcal{M}(\kappa_{\text{min}})$ and obtain improved approximation of target state
Importance Truncation: Iterative Scheme

- non-zero importance measure $\kappa_\nu$ only for states which differ from $|\psi_{\text{ref}}\rangle$ by 2p2h excitation at most

**IT-NCSM[i]**
- simple iterative scheme for a single $N_{\text{max}}\hbar\Omega$ model space
  1. start with $|\psi_{\text{ref}}\rangle = |\Phi_0\rangle$
  2. construct importance truncated space containing up to 2p2h on top of $|\psi_{\text{ref}}\rangle$
  3. solve eigenvalue problem
  4. use dominant components of eigenstate ($|C_\nu| \geq C_{\text{min}}$) as new $|\psi_{\text{ref}}\rangle$, goto 1

**IT-NCSM(seq)**
- sequential update scheme for a set of $N_{\text{max}}\hbar\Omega$ spaces
  1. start with $N_{\text{max}} = 2$ eigenstate from full NCSM as initial $|\psi_{\text{ref}}\rangle$
  2. construct importance truncated space for $N_{\text{max}} + 2$
  3. solve eigenvalue problem
  4. use dominant components of eigenstate ($|C_\nu| \geq C_{\text{min}}$) as new $|\psi_{\text{ref}}\rangle$, goto 1

**full NCSM model space is recovered in the limit** $(\kappa_{\text{min}}, C_{\text{min}}) \rightarrow 0$ in IT-NCSM(seq) and IT-NCSM[$i_{\text{conv}}$]
Threshold Extrapolation

- all calculations done for a **sequence of importance thresholds** \( E(\kappa_{\text{min}}) \)

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

- **simultaneous extrapolation** of combined energy

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

to \( \kappa_{\text{min}} = 0 \) for set of \( \lambda \)-values

- all IT-NCSM energies shown are threshold extrapolated

\[ ^{16}\text{O}, \text{IT-NCSM(seq)} \]

\( \nu_{\text{UCOM}}, \hbar \Omega = 22 \text{ MeV}, N_{\text{max}} = 16 \)
$^4$He: Importance-Truncated NCSM

- **Iterative IT-NCSM$[i]$**: few iterations with $0\hbar\Omega$ determinant as initial reference
- **Reproduces exact NCSM result** for all $N_{\text{max}}$
- Reduction of basis by more than two orders of magnitude w/o loss of precision

![Graph showing $E$ and $D_{\text{max}}$ vs. $N_{\text{max}}$ for $^4$He](image)

- + full NCSM
- IT-NCSM$[1]$
- IT-NCSM$[2]$
- IT-NCSM$[3]$
$^4\text{He}$: Importance-Truncated NCSM

- **sequential IT-NCSM(seq):** single importance update using $(N_{\text{max}} - 2)\hbar\Omega$ eigenstate as reference.
- reproduces exact NCSM result for all $N_{\text{max}}$
- reduction of basis by more than two orders of magnitude w/o loss of precision

![Graph](image)

- + full NCSM
- IT-NCSM(seq)
$^4\text{He}$: Importance-Truncated NCSM

- reproduces exact NCSM result for all $\hbar\Omega$ and $N_{\text{max}}$
- importance truncation & threshold extrapolation is robust
- no center-of-mass contamination for any $N_{\text{max}}$ and $\hbar\Omega$

$E \ [\text{MeV}]$

$\hbar\Omega \ [\text{MeV}]$

$N_{\text{max}} = 4$

$V_{\text{UCOM}}$

$^4\text{He}$

+ full NCSM

● IT-NCSM(seq)
16O: Importance-Truncated NCSM

- Extrapolation $N_{\text{max}} \to \infty$ using five consecutive points

<table>
<thead>
<tr>
<th>$N_{\text{max}}$</th>
<th>$E_{\infty}$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>14...22</td>
<td>-133.1</td>
</tr>
<tr>
<td>12...20</td>
<td>-132.4</td>
</tr>
<tr>
<td>10...18</td>
<td>-130.8</td>
</tr>
<tr>
<td>experiment</td>
<td>-127.6</td>
</tr>
</tbody>
</table>

- Slow non-exponential convergence makes precise extrapolation difficult

- IT-NCSM(seq), $C_{\text{min}} = 0.0005$
- IT-NCSM(seq), $C_{\text{min}} = 0.0003$

Robert Roth – TU Darmstadt – 03/2009
$^{16}\text{O}$: Importance-Truncated NCSM

- SRG-evolved N3LO potential provides a much better convergence behavior.
- Nevertheless, $N_{\text{max}} \leq 8$ calculations are not sufficient.
- Non-exponential behavior observed with $V_{\text{UCOM}}$ is really due to interaction.

$V_{\text{SRG}}(\text{N3LO})$

$\lambda = 2.66 \text{ fm}^{-1}$

$\bar{\alpha} = 0.02 \text{ fm}^4$

$\hbar \Omega = 24 \text{ MeV}$

$D_{\text{max}}$

$E [\text{MeV}]$

$N_{\text{max}}$

+ full NCSM

$\bullet$ IT-NCSM(seq), $C_{\text{min}} = 0.0005$
$^{12}\text{C}$: IT-NCSM for Open-Shell Nuclei

- excellent agreement with full NCSM calculations
- IT-NCSM(seq) works just as well for non-magic / open-shell nuclei
- all calculations limited by available two-body matrix elements & CPU time only

$\nu_{\text{UCOM}} \hbar \Omega = 24 \text{ MeV}$

$D_{\text{max}}$ vs $N_{\text{max}}$

- full NCSM
- IT-NCSM(seq), $C_{\text{min}} = 0.0005$
- IT-NCSM(seq), $C_{\text{min}} = 0.0003$
$^{12}\text{C}$: IT-NCSM for Excited States

- **targeting ground & excited states** simultaneously via importance measure
- IT-NCSM(seq) can treat a ground state & few low-lying excited states on the same footing
- full access to spectroscopy

$V_{\text{SRG (N3LO)}}$

- $\lambda = 2.66 \text{ fm}^{-1}$
- $\bar{\alpha} = 0.02 \text{ fm}^4$
- $\hbar \Omega = 24 \text{ MeV}$

$D_{\text{max}}$

- IT-NCSM(seq), $C_{\text{min}} = 0.0005$
$^6$He & $^8$He: IT-NCSM for Open-Shell Nuclei

$^6$He
\[ V_{\text{UCOM}} \hbar \Omega = 24 \text{ MeV} \]

$^8$He
\[ V_{\text{UCOM}} \hbar \Omega = 24 \text{ MeV} \]
IT-NCSM: Pros and Cons

✔ **fulfills variational principle** & Hylleraas-Undheim theorem

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

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

✔ **open and closed-shell nuclei** with **ground and excited states** can be treated on the same footing

✔ **compatible with shell model**: compute any observable from wave functions in SM representation

✘ **only approximate size-extensivity** after threshold extrapolation in IT-NCSM(seq) or IT-NCSM[$i_{\text{conv}}$] – no explicit $npnh$ truncation

✘ computationally still demanding
Unitarily Transformed Interactions

- treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG,...
- phase-shift equivalent transformed interaction (e.g. $V_{UCOM}$) as universal input for...

Computational Many-Body Methods

- No-Core Shell Model,...
- Importance Truncated NCSM, Coupled Cluster Method,...
- Hartree-Fock plus MBPT, Padé Resummed MBPT, BHF, HFB, RPA, QRPA, Second RPA,...
- Fermionic Molecular Dynamics,...
thanks to my group & my collaborators

  Institut für Kernphysik, TU Darmstadt

- P. Navrátil
  Lawrence Livermore National Laboratory, USA

- P. Piecuch, J. Gour
  Michigan State University, USA

- H. Feldmeier, T. Neff,...
  Gesellschaft für Schwerionenforschung (GSI)