Unitarily Transformed Interactions for Ab-Initio Nuclear Structure
Overview

■ Motivation

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

■ Computational Many-Body Methods
  • No-Core Shell Model
  • Importance Truncated NCSM & CI
  • Coupled-Cluster Method
From QCD to Nuclear Structure

Nuclear Structure

Realistic Nuclear Interactions

- 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

Low-Energy QCD
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

Exact / Approx. Many-Body Tools
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
Unitarily Transformed Interactions

Unitary Correlation Operator Method (UCOM)

Deuteron: Manifestation of Correlations

- **Exact deuteron solution** for Argonne V18 potential
  \[ \rho^{(2)}_{S=1, M_S=\pm 1}(\vec{r}) \]

- Short-range repulsion suppresses wave function at small distances \( r \)
- Central correlations
- Tensor interaction generates \( L=2 \) admixture to ground state
- Tensor correlations

\[ \langle r \mid \phi_L \rangle \]

\( r \) [fm]

\( L = 0 \)

\( L = 2 \)
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>
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</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} \theta(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} [\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>

\[ C = C_\Omega C_r = \exp(-i \sum_{i<j} g_\Omega,ij) \exp(-i \sum_{i<j} g_r,ij) \]

- \( s(r) \) and \( \theta(r) \) depend on & are optimized for initial potential

Robert Roth – TU Darmstadt – 02/2009
Correlated States: The Deuteron

$L = 0$

$\langle r | \phi \rangle$

$\langle r | C_r \phi \rangle$

$\langle r | C_\Omega C_r \phi \rangle$

Central correlations

Tensor correlations

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

$^{3}S_{1}$

$^{3}S_{1} - ^{3}D_{1}$

$V_{\text{AV18}}$

pre-diagonalization of Hamiltonian

$V_{\text{UCOM}}$
Correlated Interaction: $V_{\text{UCOM}}$

$$V_{\text{UCOM}} = \sum_p \frac{1}{2} [\tilde{\nu}_p(r) O_p + O_p \tilde{\nu}_p(r)]$$

$$O = \{1, (\bar{\sigma}_1 \cdot \bar{\sigma}_2), \bar{q}^2, \bar{q}^2(\bar{\sigma}_1 \cdot \bar{\sigma}_2), \bar{l}^2, \bar{l}^2(\bar{\sigma}_1 \cdot \bar{\sigma}_2),$$

$$\bar{\sigma}_2, \bar{q}_2, \bar{q}_2(\bar{\sigma}_1 \cdot \bar{\sigma}_2), \bar{q}_r, S_{12}(\bar{r}, \bar{r}), S_{12}(\bar{l}, \bar{l}),$$

$$\bar{S}_{12}(\bar{q}_\Omega, \bar{q}_\Omega), q_r S_{12}(\bar{r}, \bar{q}_\Omega), \bar{l}^2(\bar{l} \cdot \bar{q}),$$

$$\bar{l}^2 \bar{S}_{12}(\bar{q}_\Omega, \bar{q}_\Omega), \ldots \} \otimes \{1, (\bar{\tau}_1 \cdot \bar{\tau}_2)\}$$

- $C_r$-transformation evaluated directly
- $C_\Omega$-transformation through Baker-Campell-Hausdorff expansion
- $\tilde{\nu}_p(r)$ determined by bare potential and correlation functions
Optimal Correlation Functions

- $s(r)$ and $\vartheta(r)$ determined by two-body **energy minimisation**
- constraint on range of the tensor correlators $\vartheta(r)$ to isolate state independent **short-range correlations**

\[ s(r) \]

\[ \vartheta(r) \]

![Graphs of $s(r)$ and $\vartheta(r)$ for different $(S, T)$ values](image-url)
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
  \[ \tilde{H}(\alpha) = C^\dagger(\alpha) H C(\alpha) \quad \rightarrow \quad \frac{d}{d\alpha} \tilde{H}(\alpha) = [\eta(\alpha), \tilde{H}(\alpha)] \]

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

UCOM vs. SRG

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

Argonne V18

Strong off-diagonal contributions

Short-range central & tensor correlations
SRG Evolution: The Deuteron

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

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

suppression of off-diagonal contributions

elimination of short-range correlations
SRG Evolution: The Deuteron

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

\[ \bar{\alpha} = 0.1000 \text{ fm}^4 \]
SRG-Generated UCOM Correlators: AV18

- determine UCOM correlators from SRG-evolved two-body wave functions via

$$\left| \Phi_{\text{SRG}}^{(0)} \right\rangle \equiv C \left| \Phi_{\text{SRG}}^{\tilde{\alpha}} \right\rangle$$

![Graphical representation](image)
oscillatory behavior of wave function leads to long-range correlators

- cutoff artifact?

\[ S = 1, T = 0 \]
Computational Many-Body Methods

No-Core Shell Model

Roth & Navrátil — in preparation
$^4\text{He}$: Convergence

$V_{\text{AV18}}$

$V_{\text{UCOM}}$

Residual long-range correlations

$E_{\text{AV18}}$

$\hbar \omega$ [MeV]

$E$ [MeV]
$^{4}\text{He}$: Convergence

**$V_{\text{AV18}}$**

**$V_{\text{UCOM}}$**

$N_{\text{max}}$

$E_{\text{AV18}}$

$E_{\text{UCOM}}$

- Omitted 3- & 4-body contributions

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Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

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

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

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

- **include full** \( V^{[3]}_{UCOM} \) consisting of genuine and induced 3N terms
  (not really feasible beyond lightest isotopes)

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

- **minimize** \( V^{[3]}_{UCOM} \) by proper choice of unitary transformation
  (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

The graph shows the comparison between $E(4\text{He})$ and $E(3\text{H})$ for different NN-interactions, including AV18, Nijm II, Nijm I, CD Bonn, and experimental values. The graph highlights the Tjon-line as a line of equality between the two energies for 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 $C_\Omega$-correlator range results in shift along Tjon-line

minimize net 3N interaction by choosing correlator close to experimental point
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 $3N$ interaction by choosing correlator close to experimental point
$V_{\text{UCOM}}$  
MIN, $I_9 = 0.09 \text{ fm}^3$

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

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

UCOM & SRG show very similar convergence behavior in light nuclei

$E$ [MeV]

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

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

$R_{ch}$ [fm]

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

$V_{UCOM}$

MIN, $I_\theta = 0.09$ fm$^3$

$V_{SRG}$

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

$\bar{\alpha} = 0.03$ fm$^4$
$^{10}$B: Hallmark of a 3N Interaction?

$V_{UCOM}$

$E - E_{3^+}$ [MeV]

-2 -1 0 1 2 3 4 5 6 7

$\hbar \omega = 18 \text{MeV}$

Exp

4+

2+

0+

1+

3+

-62.1 -64.7
**10B: Hallmark of a 3N Interaction?**

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

Importance-Truncated No-Core Shell Model

Roth, Piecuch, Gour — arXiv: 0806.0333
Roth — in preparation
- 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 important 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

measure the importance of individual basis state \( |\Phi_\nu\rangle \) via first-order multiconfigurational perturbation theory

\[
\kappa_\nu = -\frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}
\]

construct importance-truncated space spanned by basis states with \( |\kappa_\nu| \geq \kappa_{\text{min}} \) and solve eigenvalue problem

iterative scheme: repeat construction of importance-truncated model space using eigenstate as improved reference \( |\Psi_{\text{ref}}\rangle \)

threshold extrapolations and perturbative corrections can be used to account for discarded basis states
$^4$He: Importance-Truncated NCSM

- **iterative IT-NCSM($i$)** shows very fast convergence
- 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 $E$ vs. $N_{\text{max}}$ and $D_{\text{max}}$ vs. $N_{\text{max}}$ for $^4$He.](image)

- $\hbar \omega = 40$ MeV
- $V_{\text{UCOM}}$

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$^4\text{He}$: Importance-Truncated NCSM

- **sequential IT-NCSM(seq)** provides same results as IT-NCSM(3) with just one update per $N_{\text{max}}$
- reproduces exact NCSM result for all $N_{\text{max}}$
- reduction of basis by more than two orders of magnitude w/o loss of precision

\[ V_{\text{UCOM}} \hbar \omega = 40 \text{ MeV} \]

\[ D_{\text{max}} \]

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$^4$He: Importance-Truncated NCSM

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

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

- full NCSM
- IT-NCSM(seq)
$^{16}\text{O}$: Importance-Truncated NCSM

- IT-NCSM(seq) provides **excellent agreement with full NCSM calculation**
- Dimension reduced by several orders of magnitude
- Possibility to go **way beyond** the domain of the full NCSM

$V_{UCOM}$

$\hbar \omega = 22 \text{ MeV}$

Graph showing:
- $E$ [MeV] vs. $N_{\text{max}}$
- $D_{\text{max}}$ vs. $N_{\text{max}}$

Legend:
- + full NCSM
- IT-NCSM(seq), $C_{\text{min}} = 0.0005$
- IT-NCSM(seq), $C_{\text{min}} = 0.0003$
$^6$He & $^8$He: IT-NCSM for Open-Shell Nuclei

$^6$He

$V_{UCOM} \hbar \omega = 24$ MeV

$^8$He

$V_{UCOM} \hbar \omega = 24$ MeV

$E$ [MeV]

$D_{max}$

$N_{max}$
12C: 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 CPU-time only

\[ V_{UCOM} \]  
\[ \hbar \omega = 24 \text{ MeV} \]

\[ 10^3 \quad 10^4 \quad 10^5 \quad 10^6 \quad 10^7 \quad 10^8 \quad 10^9 \]

\[ N_{max} \]

\[ D_{max} \]

- full NCSM
- IT-NCSM(seq), \( C_{min} = 0.0005 \)
- IT-NCSM(seq), \( C_{min} = 0.0003 \)
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 $\kappa_{\text{min}} \to 0$ 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: excited states and angular-momentum projection via Lanczos, eigenstates in shell-model representation, computation of observables

✘ computationally still demanding
Perspectives

- three steps from QCD to the nuclear chart
  - QCD-based nuclear interactions
  - unitarily transformed interactions (UCOM, SRG,...)
  - computational many-body methods
- exciting new developments in all three sectors
- alternative route using density functional methods

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

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