Ab-Initio Nuclear Structure beyond the p-Shell:

Interactions & Many-Body Techniques

Robert Roth
Institut für Kernphysik

TECHNISCHE UNIVERSITAT DARMSTADT
Overview

■ Motivation

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

■ Computational Many-Body Methods
  • No-Core Shell Model
  • Importance Truncated NCSM
Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

- 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

- Low-Energy QCD
  - Realistic Nuclear Interactions
  - Modern Effective Interactions
    - 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
    - adapt realistic potential to the available model space
    - conserve experimentally constrained properties (phase shifts & deuteron)
    - need consistent effective interaction & effective operators
    - unitary transformations most convenient
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)

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

$$\langle \tilde{\psi} | O | \tilde{\psi}' \rangle = \langle \psi | C^\dagger O C | \psi' \rangle = \langle \psi | \tilde{O} | \psi' \rangle$$
An explicit ansatz for unitary transformation operator motivated by the physics of short-range correlations.

**Central Correlator** $C_r$

- Radial distance-dependent shift in the relative coordinate of a nucleon pair
  
  $$g_r = \frac{1}{2} [s(r) q_r + q_r s(r)]$$
  
  $$q_r = \frac{1}{2} [\frac{r}{r} \cdot \bar{q} + \bar{q} \cdot \frac{r}{r}]$$

**Tensor Correlator** $C_\Omega$

- Angular shift depending on the orientation of spin and relative coordinate of a nucleon pair
  
  $$g_\Omega = \frac{3}{2} \vartheta(r)[(\vec{\sigma}_1 \cdot \vec{q}_\Omega)(\vec{\sigma}_2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}_\Omega)]$$
  
  $$\vec{q}_\Omega = \vec{q} - \frac{r}{r} q_r$$

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

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

\[ L = 0 \]

\[
\begin{align*}
\langle r | \phi \rangle & = \text{central correlations} \\
\langle r | C_r \phi \rangle & = \text{central correlations} \\
\langle r | C_\Omega C_r \phi \rangle & = \text{only short-range tensor correlations treated by } C_\Omega
\end{align*}
\]
Correlated Interaction: $V_{UCOM}$

$^3S_1$  

$^3S_1 - ^3D_1$

$V_{AV18}$

pre-diagonalization of Hamiltonian

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

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

**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

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

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

\[ \langle r | \phi_{\text{SRG}}^{L=2} \rangle \]
SRG Evolution: The Deuteron

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

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

Suppression of off-diagonal contributions

Elimination of short-range correlations

Robert Roth – TU Darmstadt – 02/2009
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

No-Core Shell Model

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

$V_{\text{AV18}}$

$V_{\text{UCOM}}$

$E$ [MeV]

$E_{\text{AV18}}$

$N_{\text{max}}$

$\hbar \omega$ [MeV]

$\hbar \omega$ [MeV]

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

$V_{\text{AV18}}$

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

$V_{\text{UCOM}}$

$E$ [MeV] vs. $\hbar\omega$ [MeV], $E_{\text{UCOM}}$ vs. $\hbar\omega$ [MeV]

omitted 3- & 4-body contributions
Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

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

- **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

- AV18
- Nijm II
- Nijm I
- CD Bonn
- Exp.
- $V_{NN} + V_{3N}$
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

---

\[ E(3\text{H}) \text{ [MeV]} \]

\[ E(4\text{He}) \text{ [MeV]} \]

- AV18
- Nijm II
- Nijm I
- CD Bonn

**this $V_{UCOM}$ is used in the following**

---

Robert Roth – TU Darmstadt – 02/2009
$^{10}$B: Hallmark of a 3N Interaction?
$^{10}\text{B}: \text{ Hallmark of a 3N Interaction?}$

$V_{UCOM}$ 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
Importance-Truncated NCSM

- converged NCSM calculations are essentially restricted to p-shell
- full $6\hbar\omega$ calculation for $^{40}$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**

![Graph showing energy levels of $^{40}$Ca]
Importance Truncation: General Idea

- 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
Iterative Scheme: IT-NCSM[i]

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

- simple **iterative construction** of importance truncated model space:
  1. start with $|\psi_{\text{ref}}\rangle = |\Phi_0\rangle$
  2. construct model space of states with $|\kappa_\nu| \geq \kappa_{\text{min}}$
  3. solve eigenvalue problem
  4. use dominant components of eigenstate as new $|\psi_{\text{ref}}\rangle$, goto 1

- need $n/2$ iterations to recover full space with npnp excitations in the limit $\kappa_{\text{min}} \to 0$
**Sequential Scheme: IT-NCSM(seq)**

- **special property of** $N_{\text{max}}\hbar\omega$ **space**: step from $N_{\text{max}}$ to $N_{\text{max}} + 2$ requires 2p2h excitations at most
  - combine importance update with increase of $N_{\text{max}}$ by 2

- **sequential calculation** for set of $N_{\text{max}}\hbar\omega$ spaces:
  1. complete NCSM calculation for $N_{\text{max}} = 0$ or 2 to obtain $|\Psi_{\text{ref}}\rangle$
  2. construct importance-truncated space with $N_{\text{max}} + 2$ of states with $|\kappa_\nu| \geq \kappa_{\text{min}}$
  3. solve eigenvalue problem
  4. use dominant components of eigenstate as new $|\Psi_{\text{ref}}\rangle$, goto 1

- **only one importance update** for each value of $N_{\text{max}}$ needed to recover full space in the limit $\kappa_{\text{min}} \to 0$
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.
$^4$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 energy levels and $D_{\text{max}}$ vs. $N_{\text{max}}$ for $^4$He](image)

**Legend**:
- $+$: full NCSM
- ■: IT-NCSM[1]
- ●: IT-NCSM[2]
- ●: IT-NCSM[3]
$^4$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 showing energy levels and occupation numbers](image-url)

- full NCSM
- IT-NCSM(seq)
4He: 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

$E [\text{MeV}]$

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

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

Robert Roth – TU Darmstadt – 02/2009
$^{16}\text{O}: \text{Importance-Truncated NCSM}$

- Extrapolation to $N_{\text{max}} \to \infty$
  \[ E_{\text{IT-NCSM(seq)}} = -133(3) \text{ MeV} \]
  \[ E_{\text{exp}} = -127.6 \text{ MeV} \]

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

- Slow non-exponential convergence makes precise extrapolation difficult

**Graph:**
- $E$ 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

\[ V_{\text{UCOM}} \bar{\hbar}\omega = 24 \text{ MeV} \]
$^{12}\text{C}$: 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 CPU-time only

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

- $D_{\text{max}}$ vs $N_{\text{max}}$
- $E$ vs $N$

$C_{\text{min}} = 0.0005$, $C_{\text{min}} = 0.0003$
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
**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)