Ab Initio Nuclear Structure beyond the p-Shell

Robert Roth
Institut für Kernphysik
Technische Universität Darmstadt
Overview

- Motivation

- Modern Effective Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group

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

- Perspectives
From QCD to Nuclear Structure

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
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
From QCD to Nuclear Structure

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)

... also known as

Project ‘Bohrloch’

Deuteron: Manifestation of Correlations

**exact deuteron solution** for Argonne V18 potential

- $\langle r | \phi_L \rangle$
- $L = 0$
- $L = 2$

- short-range repulsion suppresses wavefunction at small distances $r$
- central correlations

- tensor interaction generates D-wave admixture in the ground state
- tensor correlations

Robert Roth – TU Darmstadt – 01/2008
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

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

$$\langle \tilde{\psi} | O | \tilde{\psi}' \rangle = \langle \psi | C^\dagger O C | \psi' \rangle = \langle \psi | \tilde{O} | \psi' \rangle$$
### Central Correlator $C_r$

- radial distance-dependent shift in the relative coordinate of a nucleon pair

\[
g_r = \frac{1}{2} [s(r) \mathbf{q}_r + \mathbf{q}_r s(r)]
\]

\[
\mathbf{q}_r = \frac{1}{2} [\mathbf{\bar{r}} \cdot \mathbf{\bar{q}} + \mathbf{\bar{q}} \cdot \mathbf{\bar{r}}]
\]

### Tensor Correlator $C_{\Omega}$

- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

\[
g_{\Omega} = \frac{3}{2} \vartheta(r) \left[ (\mathbf{\bar{\sigma}}_1 \cdot \mathbf{\bar{q}}_{\Omega}) (\mathbf{\bar{\sigma}}_2 \cdot \mathbf{\bar{r}}) + (\mathbf{\bar{r}} \leftrightarrow \mathbf{\bar{q}}_{\Omega}) \right]
\]

\[
\mathbf{\bar{q}}_{\Omega} = \mathbf{\bar{q}} - \frac{\mathbf{\bar{r}}}{r} \mathbf{q}_r
\]

- $s(r)$ and $\vartheta(r)$ for given potential determined by energy minimization in the two-body system (for each $S,T$)
korrelierte Wellenfunktion (Index ein Weglassen)

\[ r \chi(x) = \left( \frac{dR_-}{dx} \right)^{1/2} R_-(x) \Phi(R_-(x)) \]

\[
R_-(x) := R(Y(x) - 1) \quad \implies \begin{cases} 
R_-(R_+(r)) = r \\
R_+(R_-(x)) = x
\end{cases}
\]

\[
R'_-(x) := \frac{dR_-}{dx} = \frac{S(R_-(x))}{S(x)} \quad \implies \quad R'_-(x) = \frac{1}{R'_+(r)}
\]

\[
R'_+(r) := \frac{dR_+}{dr} = \frac{S(R_+(r))}{S(r)}
\]

Koordinatentransformation:

\[ r = R_-(x) \]
\[ x = R_+(r) \quad dx = R'_+(r) dr \quad \int\left| R'_+(r) \right| dr \]
Correlated States: The Deuteron

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

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

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

\[ L = 0 \]

\[ L = 2 \]

central correlations

tensor correlations

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

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

- **closed operator expression** for the correlated interaction $V_{\text{UCOM}}$ in two-body approximation
- correlated interaction and original NN-potential are **phase shift equivalent** by construction
- unitary transformation results in a **pre-diagonalization** of Hamiltonian (similar to renormalization group methods)
- operators of **all observables** (densities, transitions) have to be and can be **transformed consistently**
Correlated Interaction: $V_{\text{UCOM}}$

pre-diagonalization of Hamiltonian

$V_{\text{AV18}}$

$V_{\text{UCOM}}$

Robert Roth – TU Darmstadt – 01/2008
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
  \[ \eta(\alpha) = \frac{2B}{2\mu} [\vec{q}^2, \tilde{H}(\alpha)] \]

**UCOM vs. SRG**

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

Argonne V18

The diagram illustrates the evolution of the deuterium in the context of the SRG (Symanzik Reduction Group) approach, emphasizing strong off-diagonal contributions and short-range central & tensor correlations. The plots show the evolution of the $^3S_1$ and $^3D_1$ states, with a comparison to the Argonne V18 model.
SRG Evolution: The Deuteron

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

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

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

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

UCOM vs. SRG

extract the UCOM correlation functions \( s(r) \) and \( \vartheta(r) \) from the SRG evolved wavefunctions
Exact Many-Body Methods

No-Core Shell Model

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

$V_{AV18}$ and $V_{UCOM}$

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

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

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

$V_{AV18}$

$V_{UCOM}$

omitted three- and four-body contributions
Correlated Hamiltonian in Many-Body Space

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

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

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

- There is no ‘the three-body interaction’

- Phase-shift conserving unitary transformations can be used to convert between two- and three-body interactions

- We can try to minimize the net contribution of three-body terms, e.g., to the energies
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 $C_{\Omega}$-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**

- AV18
- Nijm II
- Nijm I
- CD Bonn

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

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

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

\[ E - E_{3+} \sim -62.1 -64.7 \]

\[ \hbar \omega = 18 \text{MeV} \]
$^{10}\text{B: Hallmark of a 3N Interaction?}$

$V_{UCOM}$ gives correct level ordering without any 3N interaction

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

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

Importance Truncated No-Core Shell Model

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

![Graph showing energy levels for $^{40}\text{Ca}$ with different NCSM calculations.](image)
Importance Truncation: General Idea

- start with $N_{\text{max}} \hbar \omega$ space of the NCSM
  
  \rightarrow \text{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 with $| \kappa_{\nu} | \geq \kappa_{\text{min}}$

  \rightarrow \text{contains 2p2h excitations w.r.t.} | \Psi_{\text{ref}} \rangle \text{ at most}

  \rightarrow \text{perturbative measure entails} \ N_{pN_{h}} \text{ hierarchy, i.e., higher-order} \ N_{pN_{h}} \text{ states only enter in higher orders of PT}
solve eigenvalue problem in importance truncated space
→ rigorous variational upper bound

iterative scheme: repeat construction of importance truncated model space using eigenstate as new $|\Psi_{\text{ref}}\rangle$
→ convergence to full $\mathcal{N}_{\text{max}}\hbar\omega$ space in the limit $\kappa_{\text{min}} \to 0$
→ convergence w.r.t. iterations implies approximate size extensivity

multiconfiguration PT can be used to directly correct for contribution of excluded configurations
$^4$He: Importance Truncated NCSM

- reproduces exact NCSM result for all $\hbar \omega$ and $N_{\text{max}}$
- importance truncation scheme and $\kappa_{\text{min}} \to 0$ extrapolation are reliable
- no center-of-mass contamination
- reduction of basis by up to two orders of magnitude

$^4$He

$V_{\text{UCOM}}$

$\hbar \omega = 34 \text{ MeV}$

![Graph showing energy $E$ vs. $N_{\text{max}}$ and log $D_{\text{max}}$ vs. $N_{\text{max}}$.]

$+$ full NCSM (Antoine)

- IT-NCSM(2p2h)
- IT-NCSM(4p4h)
$^{16}$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

---

$v_{UCOM} = 22$ MeV

$\hbar \omega = 22$ MeV

- full NCSM (Antoine)
  - IT-NCSM(2p2h)
  - IT-NCSM(4p4h)
$^{16}\text{O}$: Importance Truncated NCSM

- **perturbative correction** up to 6p6h on top of IT-NCSM(4p4h) eigenstate

- small contribution of configurations beyond 4p4h level

- extrapolation to $N_{\text{max}} \to \infty$

\[
E_{\text{IT-NCSM}(4p4h)} \approx -127.5 \pm 2 \text{ MeV}
\]

\[
E_{\text{IT-NCSM}(4p4h)+PT} \approx -128.5 \pm 2 \text{ MeV}
\]

\[
E_{\text{exp}} = -127.6 \text{ MeV}
\]

+ full NCSM (Antoine)

- IT-NCSM(2p2h)

- IT-NCSM(4p4h)

- IT-NCSM(4p4h)+MCPT(6p6h)
$^{16}\text{O}$ and $^{40}\text{Ca}$: Benchmark using $V_{\text{low}k}$

- Faster convergence with $V_{\text{low}k}$ but unrealistic binding energy
- Systematic deviation from coupled-cluster CCSD(T) results of Hagen, Dean, et al. [PRC 76, 044305 (2007)]
Direct Comparison: CC vs. IT-CI

- HF single-particle basis with truncation to 5,6,7,8 shells
- violation of translational invariance from the outset
- coupled-cluster calculation with non-perturbative triples correction: CR-CC(2,3)
- importance-truncated configuration interaction up to 4p4h plus multi-reference Davidson correction ($\lesssim 3$ MeV)

Diagram:
- $^{16}$O
- $V_{\text{UCOM}}$

Energy $E$ vs. $\hbar \omega$ [MeV]
- Solid symbols: CR-CC(2,3)
- Open symbols: IT-CI(4p4h)+MRD

CC by J. Gour & P. Piecuch (MSU)
■ **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,...
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, C. Barbieri,...
  Gesellschaft für Schwerionenforschung (GSI)

supported by the DFG through SFB 634
“Nuclear Structure, Nuclear Astrophysics and Fundamental Experiments...”
special thanks to

Hans Feldmeier

...for so many things