Overview

■ Motivation

■ Nuclear Interactions from QCD

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

■ Computational Many-Body Methods
  • No-Core Shell Model
  • Importance Truncated NCSM
Nuclear Structure in the 21st Century

NuSTAR & friends @ FAIR

nuclear astrophysics

nuclei far-off stability

exotic modes hyper-nuclei,...

reliable nuclear structure theory for exotic nuclei

bridging between low-energy QCD and nuclear structure theory
Theoretical Context

- finite nuclei
- few-nucleon systems
- nucleon-nucleon interaction
- hadron structure
- quarks & gluons
- deconfinement
Theoretical Context

How to solve the quantum many-body problem?

How to derive the nuclear interaction from QCD?

Quantum Chromo Dynamics

Nuclear Structure
Nuclear Interactions from QCD
Nature of the Nuclear Interaction

- NN-interaction is not fundamental

- analogous to van der Waals interaction between neutral atoms

- induced via mutual polarization of quark & gluon distributions

- acts only if the nucleons overlap, i.e. at short ranges

- genuine 3N-interaction is important

\[ \rho_0^{-1/3} = 1.8 \text{fm} \]
Nuclear Interaction from Lattice QCD

- first steps towards construction of a nuclear interaction through lattice QCD simulations
- compute relative two-nucleon wavefunction on the lattice
- invert Schrödinger equation to obtain local ‘effective’ two-nucleon potential
- schematic results so far (unphysical quark masses, S-wave interactions only,...)
**Nuclear Interaction from Chiral EFT**

- **EFT for relevant degrees of freedom** \( (\pi,N) \) based on symmetries of QCD
- long-range **pion dynamics** treated explicitly
- short-range physics absorbed in **contact terms**
- low-energy constants fitted to experimental data \( (NN, \pi N) \)
- hierarchy of **consistent NN, 3N,... interactions** (including current operators)

<table>
<thead>
<tr>
<th></th>
<th>2N forces</th>
<th>3N forces</th>
<th>4N forces</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO ( (Q_0^0) )</td>
<td><img src="image1" alt="Diagram" /></td>
<td><img src="image2" alt="Diagram" /></td>
<td><img src="image3" alt="Diagram" /></td>
</tr>
<tr>
<td>NLO ( (Q_0^1) )</td>
<td><img src="image4" alt="Diagram" /></td>
<td><img src="image5" alt="Diagram" /></td>
<td><img src="image6" alt="Diagram" /></td>
</tr>
<tr>
<td>N^2LO ( (Q_0^2) )</td>
<td><img src="image7" alt="Diagram" /></td>
<td><img src="image8" alt="Diagram" /></td>
<td><img src="image9" alt="Diagram" /></td>
</tr>
<tr>
<td>N^3LO ( (Q_0^3) )</td>
<td><img src="image10" alt="Diagram" /></td>
<td><img src="image11" alt="Diagram" /></td>
<td><img src="image12" alt="Diagram" /></td>
</tr>
</tbody>
</table>

Meißner, NPA 751 (2005) 149c
Realistic NN-Interactions

- **QCD ingredients**
  - chiral effective field theory
  - meson-exchange theory

- **short-range phenomenology**
  - contact terms or parameterization of short-range potential

- **experimental two-body data**
  - scattering phase-shifts & deuteron properties reproduced with high precision

- **supplementary 3N interaction**
  - adjusted to spectra of light nuclei

- Argonne V18
- CD Bonn
- Nijmegen I/II
- Chiral N3LO
- Argonne V18 + Illinois 2
- Chiral N3LO + N2LO
Argonne V18 Potential
Similarity Transformed Interactions
Why Transformed Interactions?

**Realistic Interactions**
- generate strong correlations in many-body states
- short-range central & tensor correlations most important

**Many-Body Methods**
- rely on truncated many-nucleon Hilbert spaces
- not capable of describing short-range correlations
- extreme: Hartree-Fock based on single Slater determinant

**Similarity Transformation**
- adapt realistic potential to the available model space
- conserve experimentally constrained properties (phase shifts)
What are Correlations?

- The quantum state of $A$ independent (non-interacting) fermions is a **Slater determinant**

$$|\psi\rangle = \mathcal{A} \ (|\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_A\rangle)$$

- Any two-body interaction induces correlations which cannot be described by a single Slater determinant
Deuteron: Manifestation of Correlations

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

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

\[ \rho^{(2)}_{S=1,M_S=0}(\vec{r}) \]

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

- Tensor interaction generates \( L=2 \) admixture to ground state

- **Central correlations**

- **Tensor correlations**
Similarity Transformed Interactions

Unitary Correlation Operator Method (UCOM)

Correlation Operator

define a unitary operator \( C \) to describe the effect of short-range correlations

\[
C = \exp[-i G] = \exp[-i \sum \limits_{i<j} g_{ij}]
\]

Correlated States

imprint short-range correlations onto uncorrelated many-body states

\[
\tilde{\psi} = C |\psi\rangle
\]

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><strong>Central Correlator</strong> $C_r$</th>
<th><strong>Tensor Correlator</strong> $C_\Omega$</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>$g_\Omega = \frac{3}{2} \vartheta(r) [(\vec{\sigma}<em>1 \cdot \vec{q}</em>\Omega)(\vec{\sigma}<em>2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}</em>\Omega)]$</td>
</tr>
<tr>
<td>$q_r = \frac{1}{2} [\vec{r} \cdot \vec{q} + \vec{q} \cdot \vec{r}]$</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 $\vartheta(r)$ are optimized for the initial potential
Correlated States: The Deuteron

\[ L = 0 \]

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

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

\[ \langle r | C_{\Omega} r \phi \rangle \]

Central correlations

Tensor correlations

Only short-range tensor correlations treated by \( C_\Omega \)

Robert Roth – TU Darmstadt – 07/2008
Correlated Interaction: \( V_{\text{UCOM}} \)

\[ \begin{align*}
\mathcal{S}_1 & \quad \mathcal{S}_1 - \mathcal{D}_1 \\
q\left[ \text{fm}^{-1} \right] & q\left[ \text{fm}^{-1} \right] \\
q'\left[ \text{fm}^{-1} \right] & q'\left[ \text{fm}^{-1} \right]
\end{align*} \]

\( V_{\text{AV18}} \)

pre-diagonalization of Hamiltonian

\( V_{\text{UCOM}} \)
Similarity 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
  \[ \eta(\alpha) = \frac{2B}{\mu} [\tilde{q}^2, \tilde{H}(\alpha)] \]

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

Robert Roth – TU Darmstadt – 07/2008
SRG Evolution: The Deuteron

\[ \alpha = 0.0004 \text{fm}^4 \]
SRG Evolution: The Deuteron

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

\[ \alpha = 0.0010 \text{ fm}^4 \]

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

\[ \langle r | \phi_{\text{SRG}}^{L=2} \rangle \]
\[ \alpha = 0.0020 \text{ fm}^4 \]
SRG Evolution: The Deuteron

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

\[ \alpha = 0.0040 \text{ fm}^4 \]
SRG Evolution: The Deuteron

\[ \alpha = 0.0100 \text{ fm}^4 \]
SRG Evolution: The Deuteron

\[ \alpha = 0.0200 \text{ fm}^4 \]
SRG Evolution: The Deuteron

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

\[ \alpha = 0.0400 \text{ fm}^4 \]
SRG Evolution: The Deuteron

\[
\alpha = 0.1000 \text{fm}^4
\]
SRG Evolution: The Deuteron

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

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

suppression of off-diagonal contributions

elimination of short-range correlations

Robert Roth – TU Darmstadt – 07/2008
SRG Evolution: The Deuteron

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

**UCOM vs. SRG**

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

No-Core Shell Model

Roth & Navrátil — in preparation
Basics of the No-Core Shell Model

- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states

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

- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\text{max}} \hbar \omega$

with increasing model space size more and more correlations can be described by the model space facilitates systematic study of short- and long-range correlations
$^4$He: Convergence

$V_{AV18}$

$V_{UCOM}$

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

**$V_{AV18}$**

- $N_{\text{max}}$
- $\hbar \omega [\text{MeV}]$
- $E [\text{MeV}]$
- $E_{AV18}$

**$V_{UCOM}$**

- $\hbar \omega [\text{MeV}]$
- $E [\text{MeV}]$

*omitted 3- & 4-body contributions*
Tjon-Line and Correlator Range

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

- **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

**this \( V_{\text{UCOM}} \) is used in the following**

**minimize net 3N interaction** by choosing correlator close to experimental point

\[ AV18 \]

\[ \text{Nijm II} \]

\[ \text{Nijm I} \]

\[ \text{CD Bonn} \]

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

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

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

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

Exp

- $4^+$
- $2^+$
- $0^+$
- $1^+$
- $3^+$

-62.1 -64.7
$^{10}$B: Hallmark of a 3N Interaction?

$V_{\text{UCOM}}$ 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 $^{40}\text{Ca}$ 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
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
$^4\text{He}$: 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

\[ V_{\text{UCOM}} \]
\[ \hbar \omega = 40 \text{ MeV} \]
$^{16}$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

\[ V_{\text{UCOM}} \bar{\hbar}\omega = 22 \text{ MeV} \]

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

- full NCSM
- IT-NCSM(1 iter, 2p2h)
- IT-NCSM(2 iter, 4p4h)
\[ ^{16}\text{O}: \text{Importance Truncated NCSM} \]

\[ V_{\text{UCOM}} \quad \hbar \omega = 22 \text{ MeV} \]

- Extrapolation to \( N_{\text{max}} \rightarrow \infty \)

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

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

- 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)
- dramatic reduction of basis dimension
- rough extrapolation $N_{\text{max}} \rightarrow \infty$ is consistent with experimental binding energy

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

- full NCSM
- IT-NCSM(1 iter, 2p2h)
- IT-NCSM(2 iter, 4p4h)
- IT-NCSM(2 iter, 4p4h) + MRD
Computational Many-Body Methods

Other Options...
similarity transformed interactions (e.g. $V_{UCOM}$) provide universal input for various many-body methods

- exact few-body methods
- coupled-cluster method
- Hartree-Fock & many-body perturbation theory
- RPA & Second-RPA
- FMD with projection & configuration mixing
- NCSM + Resonating Group Method
Hartree-Fock with $V_{UCOM}$

- Long-range correlations are missing

![Graph showing the comparison between experimental and Hartree-Fock (HF) results for various isotopes, highlighting the absence of long-range correlations in the Hartree-Fock calculations.](image)
Perturbation Theory with $V_{UCOM}$

Long-range correlations are perturbative

Indications for presence of residual 3N interaction ??
Conclusions

- three steps from QCD to the nuclear chart
  - QCD-based nuclear interactions
  - similarity 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

  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,...
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