New Horizons in Nuclear Structure Theory

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Nuclear Structure in the 21st Century

- NuSTAR @ FAIR, ...
- RIBF @ RIKEN, ...
- Nuclear Astrophysics
- nuclei far-off stability
- exotic modes hyper-nuclei,...

predictive nuclear structure theory for exotic nuclei

bridging between low-energy QCD and nuclear structure theory

Modern Nuclear Structure Theory

Nuclear Structure

Ab Initio Approaches
Modern Eff. Interactions
Realistic Interactions
Density Functional Theory

Many-Body Approximations
Chiral EFT Interactions

Low-Energy QCD
Chiral EFT Interactions

- EFT for relevant degrees of freedom ($\pi, N$) based on symmetries of QCD (chiral symmetry)

- long-range pion dynamics treated explicitly

- unresolved short-range physics absorbed in contact terms

- low-energy constants fitted to experimental data ($NN, \pi N$)

- hierarchy of consistent NN & 3N (& 4N) interactions (including current operators)
**Realistic Potentials**
- generate strong correlations in many-body states
- short-range central & tensor correlations most important

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

**Modern Effective Interactions**
- adapt realistic potential to the available model space
  - tame short-range correlations
  - improve convergence behavior
- conserve experimentally constrained properties (phase shifts)

*can be viewed as realistic interactions*
Deuteron: Manifestation of Correlations

\[ \langle \mathbf{r} | \phi_L \rangle \]

- **exact deuteron solution** for Argonne V18 potential
- \( \rho_{S=1,M_S=\pm 1}(\mathbf{r}) \)
- \( \rho^{(2)}_{S=1,M_S=0}(\mathbf{r}) \)

- short-range repulsion suppresses wavefunction at small distances \( r \)
- central correlations
- tensor interaction generates D-wave admixture in the ground state
- tensor correlations
Modern Effective Interactions

Unitary Correlation Operator Method (UCOM)

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

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

$$\langle \tilde{\psi} | O | \tilde{\psi}' \rangle = \langle \psi | C^\dagger O C | \psi' \rangle = \langle \psi | \tilde{O} | \psi' \rangle$$
explicit ansatz for the correlation operator motivated by the **physics of short-range central and tensor correlations**

<table>
<thead>
<tr>
<th>Central Correlator ( C_r )</th>
<th>Tensor Correlator ( C_\Omega )</th>
</tr>
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<tbody>
<tr>
<td>■ <strong>radial distance-dependent shift</strong> in the relative coordinate of a nucleon pair</td>
<td></td>
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<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>
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<tr>
<td>■ <strong>angular shift depending on the orientation of spin and relative coordinate of a nucleon pair</strong></td>
<td></td>
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<tr>
<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>
<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 \( \vartheta(r) \) for given potential determined by energy minimization in the two-body system (for each \( S, T \)
Correlated States: The Deuteron

\[ \langle r \phi \rangle \]
\[ \langle r C_r \phi \rangle \]
\[ \langle r^2 \phi \rangle \]

\[ L = 0 \]
\[ L = 2 \]

\[ s(r) \]
\[ \varphi(r) \]

central correlations

tensor correlations

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

$V_{\text{UCOM}}$
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

\[
\eta(\alpha) \equiv \frac{1}{2\mu} \tilde{q}^2, \tilde{H}(\alpha)
\]

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

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

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

\[ 3S_1 - 3D_1 \]

\[ 3S_1 \]

\[ 2 \]

\[ r \] [fm]

\[ \langle r | \phi^L_{\text{SRG}} \rangle \]

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Argonne V18
SRG Evolution: The Deuteron

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

suppression of off-diagonal contributions

elimination of short-range correlations

Ab Initio Approaches

No-Core Shell Model

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

$V_{AV18}$

$V_{UCOM}$

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

**$V_{AV18}$**

**$V_{UCOM}$**

Omitted three- and four-body contributions
Three-Body Interactions — Tjon Line

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

![Graph](image_url)
Three-Body Interactions — Tjon Line

- **Tjon-line**: $E(\text{He}^4) \text{ vs. } E(\text{H}^3)$ 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

- CD Bonn
- AV18
- Nijm II
- Nijm I

[Graph showing $E(\text{He}^4)$ vs. $E(\text{H}^3)$ with experimental points and theoretical curves.]

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
$^{10}$B: Hallmark of a 3N Interaction?
$V_{UCOM}$ gives correct level ordering without any 3N interaction.
Ab Initio Approaches

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
$^4$He: Importance Truncated NCSM

- reproduces exact NCSM result with an importance truncated basis that is 2 orders of magnitude smaller than the full $N_{\text{max}}\hbar\omega$ space

$^4$He

$V_{\text{UCOM}}$

$\hbar\omega = 20 \text{ MeV}$

\[ \log_{10} D \]

\[ E \text{ [MeV]} \]

\[ N_{\text{max}} \]

- full NCSM (Antoine)
- IT-NCSM(2)
- IT-NCSM(3)
- IT-NCSM(4)
$^{16}$O: Importance Truncated NCSM

$^{16}$O

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

\[ h\omega = 20 \text{ MeV} \]

- excellent agreement with full NCSM calculation although dimension reduced by several orders of magnitude

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

\[ E_{\text{IT-NCSM(4)D}} = -127.9 \pm 2 \text{ MeV} \]

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

+ full NCSM (Antoine)

- IT-NCSM(2)

- IT-NCSM(3)

- IT-NCSM(4)

+ IT-NCSM(4) + Davidson
**40Ca: Importance Truncated NCSM**

- **16ℏω and more are feasible** for $^{40}$Ca in IT-NCSM(4)D
- Size of individual $npnh$-contributions depends on oscillator frequency
- Result consistent with experimental binding energy

Diagram:

- $^{40}$Ca
  - $V_{UCOM}$
  - $ℏω = 20$ MeV
  - $ℏω = 17$ MeV

- Full NCSM (Antoine)
- IT-NCSM(2)
- IT-NCSM(3)
- IT-NCSM(4)
- IT-NCSM(4) + Davidson
\( ^{16}\text{O}: \text{Coupled Cluster Method} \)

**CR-CC(2,3)**

- coupled-cluster calculation for \(^{16}\text{O}\) with \( V_{UCOM} \)
- including non-perturbative triples correction (completely renormalized CC)
- extrapolated ground-state energies

\[
E_{\text{CR-CC}(2,3)} = -126.9 \pm 5 \text{ MeV} \\
E_{\text{IT-NCSM}(4)D} = -127.9 \pm 2 \text{ MeV} \\
E_{\exp} = -127.6 \text{ MeV}
\]

calculations by J. Gour & P. Piecuch
■ Modern Effective Interactions
  ● treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG, Lee-Suzuki,...
  ● universal phase-shift equivalent correlated interaction $V_{UCOM}$

■ Innovative Many-Body Methods
  ● No-Core Shell Model, Importance Truncation, Coupled Cluster,...
  ● Hartree-Fock plus MBPT, Padé Resummed MBPT, RPA,...
  ● Fermionic Molecular Dynamics,...

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

  Institut für Kernphysik, TU Darmstadt

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