New Frontiers in Nuclear Structure Theory

From Realistic Interactions to the Nuclear Chart

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Overview

- Motivation

- Modern Effective Interactions
  - Correlations & Unitary Correlation Operator Method

- Applications
  - No Core Shell Model
  - Hartree-Fock & Beyond
  - Fermionic Molecular Dynamics
Nuclear Structure in the 21st Century

- RISING, AGATA, REX-ISOLDE, ...
- NUSTAR @ FAIR
- Nuclear Astrophysics
- nuclei far-off stability
- hyper-nuclei,...

Reliable nuclear structure theory for exotic nuclei

Bridging between low-energy QCD and nuclear structure theory
Modern Nuclear Structure Theory

Nuclear Structure

- ab initio Approaches
- Many-Body Methods
- Effective Interactions
- Density Functional Models
- Realistic NN-Potentials
- Chiral Interactions

Low-Energy QCD
Realistic NN-Potentials

- QCD motivated
  - symmetries, meson-exchange picture
  - chiral effective field theory

- short-range phenomenology
  - short-range parametrisation or contact terms

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

- supplementary three-nucleon force
  - 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

\[ v(r) \quad v(r) \bar{L}^2 \]

\[ (S, T) \]
- (1, 0)
- (1, 1)
- (0, 0)
- (0, 1)

\[ v(r) S_{12} \quad v(r) (\bar{L} \cdot \bar{S}) \quad v(r) (\bar{L} \cdot \bar{S})^2 \]

\[ [\text{MeV}] \quad [\text{MeV}] \quad [\text{MeV}] \]

\[ r [\text{fm}] \quad r [\text{fm}] \quad r [\text{fm}] \]
Ab initio Methods: GFMC

Argonne v18
With Illinois-2
GFMC Calculations
22 June 2004

“exact” numerical solution of interacting $A$-nucleon problem

[S. Pieper, private comm.]

$^{12}$C results are preliminary.

Robert Roth – TU Darmstadt – 03/2006
Modern Nuclear Structure Theory

Nuclear Structure

-ab initio Approaches

Many-Body Methods

Effective Interactions

Density Functional Models

Realistic NN-Potentials

Chiral Interactions

Low-Energy QCD
Modern Nuclear Structure Theory

Nuclear Structure

- Many-Body Methods
- Effective Interactions
- Density Functional Models
- Realistic NN-Potentials
- Chiral Interactions
- \textit{ab initio} Approaches

Low-Energy QCD
Why Effective Interactions?

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

Many-Body Methods
- rely on truncated many-nucleon Hilbert spaces for $A > 12$
- 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
- conserve experimentally constrained properties (phase shifts)
Deuteron: Manifestation of Correlations

\[ MS = 0 \]
\[ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \]

\[ MS = \pm 1 \]
\[ |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle \]

- Spin-projected two-body density \( \rho_{1,MS}^{(2)}(\vec{r}) \)
- Exact deuteron solution for Argonne V18 potential

- Two-body density fully suppressed at small particle distances \( |\vec{r}| \)
- Angular distribution depends strongly on relative spin orientation

Central correlations

Tensor correlations
Unitary Correlation Operator Method (UCOM)
Correlation Operator
introduce short-range correlations by means of a unitary transformation with respect to the relative coordinates of all pairs

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

\[ G^\dagger = G \]
\[ C^\dagger C = 1 \]

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

Correlated Operators
\[ \tilde{O} = C^\dagger O C \]

\[ \langle \tilde{\psi} | O | \tilde{\psi}' \rangle = \langle \psi | C^\dagger O C | \psi' \rangle = \langle \psi | \tilde{O} | \psi' \rangle \]
Central and Tensor Correlators

\[ C = C_\Omega C_r \]

### Central Correlator \( C_r \)
- radial distance-dependent shift in the relative coordinate of a nucleon pair

\[
\begin{align*}
g_r &= \frac{1}{2} \left[ s(r) q_r + q_r s(r) \right] \\
q_r &= \frac{1}{2} \left[ \frac{\vec{r}}{r} \cdot \vec{q} + \vec{q} \cdot \frac{\vec{r}}{r} \right]
\end{align*}
\]

### Tensor Correlator \( C_\Omega \)
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

\[
\begin{align*}
g_\Omega &= \frac{3}{2} \vartheta(r) \left[ (\vec{\sigma}_1 \cdot \vec{q}_\Omega)(\vec{\sigma}_2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}_\Omega) \right] \\
\vec{q}_\Omega &= \vec{q} - \frac{\vec{r}}{r} q_r
\end{align*}
\]

\( s(r) \) and \( \vartheta(r) \) describe the physics of short-range correlations.
- $s(r)$ 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

\[
s(r) \quad \text{and} \quad \vartheta(r)
\]

\[
\begin{align*}
(s, t) &= (0, 0) & (s, t) &= (1, 0) \\
(s, t) &= (0, 1) & (s, t) &= (1, 1)
\end{align*}
\]
Correlated States: The Deuteron

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

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

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

\[ L = 0 \]

\[ L = 2 \]

central correlations

tensor correlations

constraint on range of tensor correlator

\[ s(r) \]

\[ \vartheta(r) \]

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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-diagonalisation** of Hamiltonian
- momentum-space matrix elements of correlated interaction are **similar to** $V_{\text{low} - k}$
Correlated Interaction — $V_{UCOM}$

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

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

$$(\vec{L} \cdot \vec{S}), \; S_{12}(\vec{r}, \vec{r}), \; S_{12}(\vec{L}, \vec{L}),$$

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

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

- $C_r$-transformation evaluated directly
- $C_\Omega$-transformation through Baker-Campell-Hausdorff expansion
- $\tilde{v}_p(r)$ uniquely determined by bare potential and correlation functions
Momentum-Space Matrix Elements

\[ ^3S_1 \]

\[ ^3S_1 \rightarrow ^3D_1 \]

V_{AV18}

pre-diagonalisation of Hamiltonian

V_{UCOM}

AV18

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Simplistic “Shell-Model” Calculation

- expectation value of Hamiltonian (with AV18) for Slater determinant of harmonic oscillator states

![Graph with nuclei and energy levels](image)

- Central & tensor correlations essential to obtain bound nuclei
Application I

No-Core Shell Model
No-Core Shell Model
+ Matrix Elements of Correlated Realistic NN-Interaction $V_{\text{UCOM}}$

- many-body state is expanded in Slater determinants of harmonic oscillator single-particle states
- large scale diagonalisation of Hamiltonian within a truncated model space ($\mathcal{N}\hbar\omega$ truncation)
- assessment of short- and long-range correlations

NCSM code by Petr Navrátil [PRC 61, 044001 (2000)]
$^4\text{He}: \text{Convergence}$

- $V_{AV18}$
- $V_{UCOM}$

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

$V_{\text{AV18}}$

$V_{\text{UCOM}}$

Mismatched three- and four-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: $E(\text{^4He})$ vs. $E(\text{^3H})$ for phase-shift equivalent NN-interactions
- Change of $C_\Omega$-correlator range results in shift along Tjon-line
- Minimise net three-body force by choosing correlator with energies close to experimental value

\[
\begin{align*}
E(\text{^4He}) & \text{ vs. } E(\text{^3H}) \\
\text{AV18} & \quad \text{Nijm II} \\
\text{Nijm I} &
\end{align*}
\]

\[
\begin{align*}
\text{Exp.} & \quad \text{CD Bonn} \\
V_{\text{UCOM}}(\text{AV18}) &
\end{align*}
\]

- $V_{\text{UCOM}}$ is used in the following

\[
\begin{align*}
E(\text{^4He}) & \text{ vs. } E(\text{^3H}) \\
\text{AV18} & \quad \text{Nijm II} \\
\text{Nijm I} &
\end{align*}
\]
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

minimise net three-body force by choosing correlator with energies close to experimental value
systematic NCSM calculations throughout p-shell in progress (with and without Lee-Suzuki transformation)
$^{10}\text{B}: \text{Benchmark for } V_{\text{UCOM}}$

Calculations by Petr Navrátil – preliminary
$^{10}$B: Benchmark for $V_{\text{UCOM}}$

$V_{\text{UCOM}}$ gives correct level ordering without any NNN interaction

$E - E_c$ calculations by Petr Navrátil – preliminary
Application II:

Hartree-Fock & Beyond
Standard Hartree-Fock +

Matrix Elements of Correlated Realistic NN-Interaction $V_{\text{UCOM}}$

- many-body state is a **Slater determinant** of single-particle states expanded in oscillator basis ($\sim$12 major shells)

- **correlations cannot be described** by Hartree-Fock states

- starting point for **improved many-body calculations**: MBPT, RPA, SM/CI, CC,...
Hartree-Fock with $V_{UCOM}$

- Long-range correlations are missing.
long-range correlations are perturbative within PT, SM/Cl, CC, RPA,...

indications for presence of residual three-body force
Outlook: UCOM + RPA

- **ERPA/SRPA**: long-range correlations
- **HFB**: pairing with realistic interactions
- Effect of simple three-nucleon forces
Application III

Fermionic Molecular Dynamics (FMD)
Gaussian Single-Particle States

\[ |q\rangle = \sum_{\nu=1}^{n} c_{\nu} |a_{\nu}, \vec{b}_{\nu}\rangle \otimes |\chi_{\nu}\rangle \otimes |m_{t}\rangle \]

\[ \langle \vec{x}|a_{\nu}, \vec{b}_{\nu}\rangle = \exp \left[ -\frac{(\vec{x} - \vec{b}_{\nu})^2}{2 a_{\nu}} \right] \]

- \(a_{\nu}\) : complex width
- \(\chi_{\nu}\) : spin orientation
- \(\vec{b}_{\nu}\) : mean position & momentum

Slater Determinant

\[ |Q\rangle = \mathcal{A} ( |q_{1}\rangle \otimes |q_{2}\rangle \otimes \cdots \otimes |q_{A}\rangle ) \]

Correlated Hamiltonian

\[ \tilde{H} = T + V_{\text{UCOM}} + \delta V_{c+p+ls} \]
Intrinsic One-Body Density Distributions

capable of describing spherical shell-model as well as intrinsically deformed and $\alpha$-cluster states
Intrinsic Shapes of $^{12}\text{C}$

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<tr>
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<th>intrinsic</th>
<th>projected</th>
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<td>$\langle H \rangle$</td>
<td>-81.4</td>
<td>-81.5</td>
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<td>$\langle T \rangle$</td>
<td>212.1</td>
<td>212.1</td>
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<tr>
<td>$\langle V_{ls} \rangle$</td>
<td>-39.8</td>
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<td>-88.5</td>
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<td>$\langle T \rangle$</td>
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<td>186.1</td>
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<td>$\langle V_{ls} \rangle$</td>
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<td>$\langle H \rangle$</td>
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<td>$\langle T \rangle$</td>
<td>182.8</td>
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<td>$\langle V_{ls} \rangle$</td>
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<td>$\langle V_{ls} \rangle$</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td>$\sqrt{\langle r^2 \rangle}$</td>
<td>2.44</td>
<td>2.42</td>
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## Structure of $^{12}$C

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<tr>
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<th>$E$ [MeV]</th>
<th>$R_{ch}$ [fm]</th>
<th>$B(E2)$ [$e^2\text{fm}^4$]</th>
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<td>V/PAV</td>
<td>81.4</td>
<td>2.36</td>
<td>-</td>
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<td>VAP $\alpha$-cluster</td>
<td>79.1</td>
<td>2.70</td>
<td>76.9</td>
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<td>PAV$^\pi$</td>
<td>88.5</td>
<td>2.51</td>
<td>36.3</td>
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<td>VAP</td>
<td>89.2</td>
<td>2.42</td>
<td>26.8</td>
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<tr>
<td>Multi-Config</td>
<td>92.2</td>
<td>2.52</td>
<td>42.8</td>
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<tr>
<td>Experiment</td>
<td>92.2</td>
<td>2.47</td>
<td>$39.7 \pm 3.3$</td>
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</table>
Structure of $^{12}\text{C}$ — Hoyle State

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<tr>
<th>$E$ [MeV]</th>
<th>Multi-Config</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_{\text{ch}} \text{[fm]}$</td>
<td>$2.52$</td>
<td>$2.47$</td>
</tr>
<tr>
<td>$B(E2, 0_1^+ \to 2_1^+)$ $[e^2 \text{fm}^4]$</td>
<td>$42.9$</td>
<td>$39.7 \pm 3.3$</td>
</tr>
<tr>
<td>$M(E0, 0_1^+ \to 0_2^+)$ $[\text{fm}^2]$</td>
<td>$5.67$</td>
<td>$5.5 \pm 0.2$</td>
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Outlook: Resonances & Scattering in FMD

- collective coordinate representation as tool for the description of continuum states in FMD

First steps towards fully microscopic and consistent description of structure and reactions
Conclusions

- **Unitary Correlation Operator Method (UCOM)**
  - explicit description of short-range central and tensor correlations
  - universal phase-shift equivalent correlated interaction $V_{UCOM}$

- **Innovative Many-Body Methods**
  - No-Core Shell Model
  - Hartree-Fock, MBPT, SM/CI, CC, RPA, ERPA, SRPA,...
  - Fermionic Molecular Dynamics

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

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