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

nuclei far-off stability

hyper-nuclei,...

Nuclear Astrophysics

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 Potential

\[ v(r) \]

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

\( (S, T) \)

- (1, 0)
- (1, 1)
- (0, 0)
- (0, 1)

\[ v(r) S_{12} \]

\[ v(r) (\hat{L} \cdot \hat{S}) \]

\[ v(r) (\hat{L} \cdot \hat{S})^2 \]
Argonne v18
With Illinois-2
GFMC Calculations
22 June 2004

“exact” numerical solution of interacting A-nucleon problem

[S. Pieper, private comm.]

12C results are preliminary.
Modern Nuclear Structure Theory

Nuclear Structure

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

Low-Energy QCD
Modern Nuclear Structure Theory

Nuclear Structure

Many-Body Methods

Effective Interactions

Density Functional Models

Realistic NN-Potentials

Chiral Interactions

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)
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

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

\[ G^\dagger = G \]

\[ C^\dagger C = 1 \]

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

\[ C = C_\Omega C_r \]

<table>
<thead>
<tr>
<th>Central Correlator ( C_r )</th>
<th>Tensor Correlator ( 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} \left[ s(r) q_r + q_r s(r) \right] ]</td>
<td>[ g_\Omega = \frac{3}{2} \vartheta(r) \left[ (\vec{\sigma}<em>1 \cdot \vec{q}</em>\Omega)(\vec{\sigma}<em>2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}</em>\Omega) \right] ]</td>
</tr>
<tr>
<td>[ q_r = \frac{1}{2} \left[ \vec{r} \cdot \vec{q} + \vec{q} \cdot \vec{r} \right] ]</td>
<td>[ \vec{q}_\Omega = \vec{q} - \frac{\vec{r}}{r} q_r ]</td>
</tr>
</tbody>
</table>

\( s(r) \) and \( \vartheta(r) \) for given potential determined in the two-body system
Correlated States: The Deuteron

\[ \langle r \phi \rangle \]

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

\[ \langle r | C_0 C_r \phi \rangle \]

\[ L = 0 \]

\[ L = 2 \]

\[ s(r) \]

\[ \vartheta(r) \]

central correlations

tensor correlations

constraint on range of tensor correlator
Correlated Interaction — $V_{UCOM}$

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

- **Closed operator expression** for the correlated interaction $V_{UCOM}$ 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** $V_{low-k}$.
Simplistic “Shell-Model” Calculation

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

![Graph showing energy per nucleon (E/A) for various nuclei: 4He, 16O, 48Ca, 90Zr, 132Sn, 208Pb. The graph includes labels for central and tensor correlations.]
Application I

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

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

NCSM code by Petr Navrátil [PRC 61, 044001 (2000)]
$^4\text{He}$: 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
Tjon-Line and Correlator Range

-8.6 -8.4 -8.2 -8.0 -7.8 -7.6

\( E(3H) \) [MeV]

-30

-29

-28

-27

-26

-25

-24

\( E(4\text{He}) \) vs. \( E(3\text{H}) \)

for phase-shift equivalent NN-interactions

-8.6 -8.4 -8.2 -8.0 -7.8 -7.6

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

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

Exp.

AV18

Nijm II

Nijm I

CD Bonn

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

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

![Diagram](image-url)
large-scale NCSM calculations throughout the p-shell in progress (with and w/o Lee-Suzuki transformation)
10B: Benchmarking $V_{\text{UCOM}}$

- Large-scale NCSM calculations throughout the p-shell in progress (with and w/o Lee-Suzuki transformation)

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

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
- correlations cannot be described by Hartree-Fock states
- starting point for **improved many-body calculations**: MBPT, RPA, SM/CI, CC,...
Hartree-Fock with $V_{\text{UCOM}}$

![Graph showing the comparison between experimental and Hartree-Fock (HF) results for various isotopes.](image)

- Long-range correlations are missing.

**Axes:**
- $E/A$ [MeV]
- $R_{ch}$ [fm]

**Isotopes:**
- $^4\text{He}$, $^{16}\text{O}$, $^{24}\text{O}$, $^{34}\text{Si}$, $^{40}\text{Ca}$, $^{48}\text{Ca}$, $^{48}\text{Ni}$, $^{56}\text{Ni}$, $^{68}\text{Ni}$, $^{78}\text{Ni}$, $^{88}\text{Sr}$, $^{90}\text{Zr}$, $^{100}\text{Sn}$, $^{114}\text{Sn}$, $^{132}\text{Sn}$, $^{146}\text{Gd}$, $^{208}\text{Pb}$
Perturbation Theory with $V_{UCOM}$

- Long-range correlations are easily tractable within PT, SM/CI, 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)
UCOM-FMD Approach

**Gaussian Single-Particle States**

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

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

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

**Slater Determinant**

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

**Correlated Hamiltonian**

\[
\tilde{H} = T + V_{UCOM} + \delta V_{c+p+ls}
\]

**Variation**

\[
\frac{\langle Q|\tilde{H} - T_{cm}|Q\rangle}{\langle Q|Q\rangle} \rightarrow \min
\]

**Projection**

restoration of rotational and inversion symmetry

PAV / VAP

**Multi-Configuration**

mixing of several intrinsic configurations

GCM
Intrinsic One-Body Density Distributions

\[ \rho(\vec{x}) [\rho_0] \]

\( ^4\text{He} \quad ^{16}\text{O} \quad ^{40}\text{Ca} \)

\( ^9\text{Be} \)

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

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

\begin{center}
\begin{tabular}{lcc}
\hline
 & Multi-Config & Experiment \\
\hline
$E$ [MeV] & 92.4 & 92.2 \\
$R_{\text{ch}}$ [fm] & 2.52 & 2.47 \\
$B(E2, 0_1^+ \rightarrow 2_1^+)$ [$e^2$ fm$^4$] & 42.9 & 39.7 ± 3.3 \\
$M(E0, 0_1^+ \rightarrow 0_2^+)$ [fm$^2$] & 5.67 & 5.5 ± 0.2 \\
\hline
\end{tabular}
\end{center}

$\langle |0_2^+\rangle \rangle = 0.76$

$\langle |0_2^+\rangle \rangle = 0.71$

$\langle |0_2^+\rangle \rangle = 0.50$
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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