Overview

- Motivation

- Correlated Realistic NN-Potentials
  - 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, SPIRAL2

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
Modern Nuclear Structure Theory
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
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.]

12C results are preliminary.

Modern Nuclear Structure Theory

Nuclear Structure

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

Low-Energy QCD
Modern Nuclear Structure Theory

Nuclear Structure

- Many-Body Methods
- Effective Interactions
- Density Functional Models
- Realistic 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 larger $A$
- 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 spaces
- 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

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

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

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 Correlator $C_r$

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

\[
g_r = \frac{1}{2} \left[ s(r) \ q_r + q_r \ s(r) \right]
\]

\[
q_r = \frac{1}{2} \left[ \vec{r} \cdot \vec{q} + \vec{q} \cdot \vec{r} \right]
\]

### Tensor Correlator $C_\Omega$

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

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

\[
\vec{q}_\Omega = \vec{q} - \frac{\vec{r}}{r} q_r
\]

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

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

\[ \langle r \phi \rangle \]

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

\[ \langle r \mid C \Omega C_r \mid \phi \rangle \]

\[ L = 0 \]

\[ L = 2 \]

\[ s(r) \]

\[ \theta(r) \]

central correlations

tensor correlations

constraint on range of tensor correlator
\[ \tilde{H} = T + V_{\text{UCOM}} + V_{\text{UCOM}}^{[3]} + \cdots \]

- **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* $V_{\text{low} - k}$
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 Navrátíl [PRC 61, 044001 (2000)]
$^4\text{He: Convergence}$

$V_{AV18}$

$V_{UCOM}$

residual state-dependent long-range correlations
$^4$He: Convergence

**$V_{AV18}$**

**$V_{UCOM}$**

omitted 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

- AV18
- Nijm II
- Nijm I
- CD Bonn
- Exp.
- XXX + 3-body

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

$E$ ($^4\text{He}$) [MeV]
**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 $V_{\text{UCOM}}$ is used in the following.

- $V_{\text{UCOM}}(\text{AV18})$
- CD Bonn
- Exp.

**Graph Details**

- $E^{(4}\text{He})$ vs. $E^{(3}\text{H})$ [MeV]
- $E^{(3}\text{H})$ [MeV]
- $E^{(4}\text{He})$ vs. $E^{(3}\text{H})$ [MeV]
- $V_{\text{UCOM}}(\text{AV18})$
- increasing $C_\Omega$-range

**Interactions**

- AV18
- Nijm II
- Nijm I
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
**10B: Benchmarking $V_{\text{UCOM}}$**

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

![Graph](attachment:image.png)

calculated by Petr Navrátil – preliminary
large-scale NCSM calculations throughout the p-shell in progress (with and w/o Lee-Suzuki transformation)

$V_{UCOM}$ gives correct level ordering without any NNN interaction
Application II:

Hartree-Fock & Beyond
Standard Hartree-Fock +
Matrix Elements of Correlated 
Realistic NN-Interaction $V_{UCOM}$

- 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 $V_{UCOM}$

The graph shows the comparison between experimental and Hartree-Fock (HF) calculations for various isotopes. The graph plots $E/A$ [MeV] and $R_{ch}$ [fm] against the atomic number $Z$.

Long-range correlations are missing

- $E/A$ [MeV] values are shown on the y-axis.
- $R_{ch}$ [fm] values are shown on the x-axis.
- The black bars represent experimental data, while the blue dots represent the HF calculations.
- The isotopes plotted include $^4\text{He}$, $^{16}\text{O}$, $^{24}\text{O}$, $^{34}\text{Si}$, $^{40}\text{Ca}$, $^{48}\text{Ni}$, $^{56}\text{Ni}$, $^{68}\text{Ni}$, $^{78}\text{Ni}$, $^{88}\text{Sr}$, $^{90}\text{Zr}$, $^{100}\text{Sn}$, $^{114}\text{Sn}$, $^{132}\text{Sn}$, $^{146}\text{Gd}$, and $^{208}\text{Pb}$.
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

Graphs showing the results for different isotopes and the impact of various parameters on the nuclear forces.
Application III

Fermionic Molecular Dynamics (FMD)
**Gaussian Single-Particle States**

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

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

- \( a_{\nu} \): complex width
- \( \chi_{\nu} \): spin orientation
- \( \vec{b}_{\nu} \): 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**

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

** Variation**

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

**Projection**

restoration of rotational and inversion symmetry (PAV / VAP)

**Multi-Configuration**

mixing of several intrinsic configurations (GCM)
Intrinsic One-Body Density Distributions

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

\(4\)He, \(16\)O, \(40\)Ca 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>
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<tr>
<td>V/PAV</td>
<td>81.4</td>
<td>2.36</td>
<td>-</td>
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<tr>
<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>
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<td>VAP</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 ± 3.3</td>
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</table>
Structure of $^{12}\text{C} — \text{Hoyle State}$

<table>
<thead>
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<th>Multi-Config</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ [MeV]</td>
<td>92.4</td>
<td>92.2</td>
</tr>
<tr>
<td>$R_{\text{ch}}$ [fm]</td>
<td>2.52</td>
<td>2.47</td>
</tr>
<tr>
<td>$B(E2, 0^+_1 \rightarrow 2^+_1)$ [$e^2 \text{fm}^4$]</td>
<td>42.9</td>
<td>39.7 ± 3.3</td>
</tr>
<tr>
<td>$M(E0, 0^+_1 \rightarrow 0^+_2)$ [$\text{fm}^2$]</td>
<td>5.67</td>
<td>5.5 ± 0.2</td>
</tr>
</tbody>
</table>

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

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

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