New Frontiers in Nuclear Structure Theory

From Realistic Interactions to the Nuclear Chart

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Overview

■ Motivation
  ● Nucleon-Nucleon Interactions
  ● Solving the Many-Body Problem

■ Correlations & Unitary Correlation Operator Method

■ Applications
  ● No Core Shell Model
  ● Hartree-Fock and beyond
  ● Fermionic Molecular Dynamics
<table>
<thead>
<tr>
<th>Experiment</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>■ fundamental astrophysical questions need nuclear input</td>
<td>■ improved understanding of fundamental degrees of freedom / QCD</td>
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<tr>
<td>■ possibilities to investigate nuclei far off stability</td>
<td>■ high-precision realistic nucleon-nucleon potentials</td>
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<td>■ new nuclear structure facilities: FAIR@GSI, RIA,...</td>
<td>■ <em>ab initio</em> treatment of the many-body problem</td>
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</table>
Theoretical Context

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

Quantum Chromo Dynamics

Towards better resolution / more fundamental

Nuclear Structure

“solve” the interacting nuclear many-body problem

“construct” realistic nucleon-nucleon interaction from QCD
Realistic Nucleon-Nucleon Potentials
How to Construct the NN-Potential?

- **QCD input**
  - symmetries
  - meson-exchange picture
  - chiral effective field theory

- **short-range phenomenology**
  - ansatz for short-range behaviour

- **experimental two-body data**
  - scattering phase-shifts & deuteron properties
  - reproduced with $\chi^2/\text{datum} \approx 1$
Argonne V18 Potential

\[ v(r) \]

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

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

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

\[ v(r) (\vec{L} \cdot \vec{S})^2 \]

\[(S, T)\]

- \((1, 0)\)
- \((1, 1)\)
- \((0, 0)\)
- \((0, 1)\)
Nuclear Many-Body Problem
Ab initio Calculations

solve the quantum many-body problem for \( A \) nucleons interacting via a realistic NN-potential

- exact numerical solution possible for small systems at an enormous computational cost

- **Green’s Function Monte Carlo**: Monte Carlo sampling of the \( A \)-body wave function in coordinate space; imaginary time cooling

- **No-Core Shell Model**: large-scale diagonalisation of the Hamiltonian in a harmonic oscillator basis
Green’s Function Monte Carlo

Argonne v18
With Illinois-2
GFMC Calculations
22 June 2004

[560x147]12C results are preliminary.

[S. Pieper, private comm.]
Our Goal

nuclear structure calculations across the **whole nuclear chart** based on **realistic NN-potentials** and as close as possible to an **ab initio** treatment

bound to **simple Hilbert spaces** for large particle numbers

need to deal with strong **interaction-induced correlations**
Deuteron: Manifestation of Correlations

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

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

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

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

Diagram: Two 3D representations showing the difference in central and tensor correlations for the deuteron.
Unitary Correlation Operator Method (UCOM)
Unitary Correlation Operator Method

**Correlation Operator**

Introduce correlations by means of an unitary transformation with respect to the relative coordinates of all pairs

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

\[ g = g(\vec{r}, \vec{q}; \vec{\sigma}_1, \vec{\sigma}_2, \vec{\tau}_1, \vec{\tau}_2) \]

\[ G^\dagger = G \]

\[ C^\dagger C = 1 \]

**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>
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<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>
</tbody>
</table>

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

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

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

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

\( s(r) \) and \( \vartheta(r) \) encapsulate the physics of short-range correlations
Optimal Correlation Functions

- $s(r)$ 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**

![Graphs of $s(r)$ and $\vartheta(r)$ for different $(S, T)$ values](image-url)
Correlated States

\[ \rho_{1,S_M}(\vec{r}) \]

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

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

\[ \langle r \phi \rangle \]

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

\[ = L = 0 \]

\[ = L = 2 \]

\[ r \ [\text{fm}] \]

\[ 0 \ 0.05 \ 0.1 \ 0.15 \]

\[ 0 \ 0.05 \ 0.1 \ 0.15 \]

\[ 0 \ 0.05 \ 0.1 \ 0.15 \]

\[ 0 \ 0.05 \ 0.1 \ 0.15 \]

\[ 0 \ 0.05 \ 0.1 \ 0.15 \]

\[ 0 \ 0.05 \ 0.1 \ 0.15 \]

\[ s(r) \]

\[ \vartheta(r) \]

\[ r \ [\text{fm}] \]

\[ 0 \ 0.02 \ 0.04 \ 0.06 \]

\[ 0.02 \ 0.04 \ 0.06 \ 0.08 \]

\[ r \ [\text{fm}] \]

\[ 0 \ 1 \ 2 \ 3 \ 4 \]

\[ 0 \ 0.05 \ 0.1 \ 0.15 \ 0.2 \]

\[ 0 \ 0.05 \ 0.1 \ 0.15 \ 0.2 \]

central correlations

tensor correlations
Correlated NN-Potential — $V_{UCOM}$

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

- **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** $V_{\text{low-}k}$
Simplistic “Shell-Model” Calculation

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

![Graph of energy per nucleon (E/A) for various nuclei (4He, 16O, 48Ca, 90Zr, 132Sn, 208Pb) showing energy levels.]

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 $V_{UCOM}$

- 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)]
$^4\text{He}: \text{Convergence}$

**$V_{\text{bare}}$**

**$V_{\text{UCOM}}$**

$E [\text{MeV}]$ vs $\hbar \omega [\text{MeV}]$ for different $N_{\text{max}}$ values:

- $E_{\text{AV18}}$ (horizontal line)
- Residual state-dependent long-range correlations indicated

Graphs show energy levels for different Hamiltonians, with $N_{\text{max}}$ varying from 0 to 4.
\[ \begin{align*} 
\rho(\omega) &= \frac{4}{\pi} \frac{\omega}{(\omega^2 + \omega_0^2)^2} \\
\rho_{V_{\text{bare}}} &= \rho_{V_{\text{UCOM}}} \\
N_{\text{max}} &= 0, 2, 4 \\
E_{\text{AV18}} &= \begin{cases} 
-20 & \text{for } N_{\text{max}} = 0 \\
-30 & \text{for } N_{\text{max}} = 2, 4 
\end{cases} \\
E &= \begin{cases} 
\begin{array}{c}
0 \\
20 \\
40 \\
60 \\
\end{array} 
\text{for } N_{\text{max}} = 0 \\
\begin{array}{c}
-20 \\
-30 \\
-40 \\
-50 \\
\end{array} 
\text{for } N_{\text{max}} = 2, 4 
\end{cases} \\
E_{\text{UCOM}} &= \begin{array}{c}
0 \\
20 \\
40 \\
60 \\
\end{array} 
\text{for } N_{\text{max}} = 0 \\
\begin{array}{c}
-20 \\
-30 \\
-40 \\
-50 \\
\end{array} 
\text{for } N_{\text{max}} = 2, 4 
\end{align*} \]
Tjon-Line and Correlator Range

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

for phase-shift equivalent NN-interactions

- AV18
- Nijm II
- Nijm I
- CD Bonn

Exp.

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

- **Tjon-line**: $E(\text{He}^4)$ vs. $E(\text{He}^3)$ for phase-shift equivalent NN-interactions
- Change in $C_\Omega$-correlator range results in shift along Tjon-line

Choose correlator with energies close to experimental value, i.e., **minimise net three-body force**

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 in $C_\Omega$-correlator range results in shift along Tjon-line

choose correlator with energies close to experimental value, i.e., 
**minimise net three-body force**
$^6\text{Li}$: NCSM for p-Shell Nuclei

Systematic NCSM study throughout p-shell in progress

Calculations by Petr Navratil
Application II:

Hartree-Fock Calculations
many-body state is a **Slater determinant** of single-particle states expanded in oscillator basis

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

bare realistic NN-potential leads to **unbound nuclei**
Hartree-Fock with Correlated AV18

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

\[ R_{ch} \text{ [fm]} \]

- \( ^{4}\text{He} \)
- \( ^{16}\text{O} \)
- \( ^{34}\text{Si} \)
- \( ^{40}\text{Ca} \)
- \( ^{48}\text{Ni} \)
- \( ^{56}\text{Ni} \)
- \( ^{68}\text{Ni} \)
- \( ^{78}\text{Ni} \)
- \( ^{88}\text{Sr} \)
- \( ^{90}\text{Zr} \)
- \( ^{100}\text{Sn} \)
- \( ^{114}\text{Sn} \)
- \( ^{132}\text{Sn} \)
- \( ^{146}\text{Gd} \)
- \( ^{208}\text{Pb} \)

- experiment
- \( V_{\text{UCOM}} \)
Beyond Hartree-Fock

- improve many-body states such that long-range correlations are included
- many-body perturbation theory (MBPT), configuration interaction (CI), coupled-cluster (CC),...
**Long-Range Correlations: MBPT**

- **many-body perturbation theory**: second-order energy shift gives estimate for influence of long-range correlations

\[
\Delta E^{(2)} = -\frac{1}{4} \sum_{i,j}^{\text{occu.}} \sum_{a,b}^{\text{unoccu.}} |\langle \phi_a \phi_b | T_{\text{int}} + V_{\text{UCOM}} | \phi_i \phi_j \rangle|^2 \frac{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}
\]

![Plot showing energy levels for various isotopes.](image-url)
Long-Range Correlations: MBPT

E/A [MeV]

A_O

A_Ni

A_Sn

HF
HF+PT2
experiment
Missing Pieces

**Beyond Hartree-Fock**
- residual long-range correlations are **perturbative**
- mostly long-range **tensor correlations**
- easily tractable within MBPT, SM/CI, CC, ...

**Residual Three-Body Force**
- small effect on binding energies for all masses
- cancellation does not work for all observables
- simple effective three-body force feasible
Outlook: UCOM + RPA

\[ R(\text{fm}^4/\text{MeV}) \]

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

\[ ^{16}\text{O} \]

\[ ^{40}\text{Ca} \]

\[ ^{48}\text{Ca} \]

\[ ^{90}\text{Zr} \]

\[ ^{132}\text{Sn} \]

\[ ^{208}\text{Pb} \]

Drozdz et al.

EXP.
Application III

Fermionic Molecular Dynamics (FMD)
**UCOM-FMD Approach**

**Gaussian Single-Particle States**

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

\[ \langle \vec{x}|a_\nu, \vec{b}_\nu\rangle = \exp \left[ -\frac{1}{2} \frac{(\vec{x} - \vec{b}_\nu)^2}{a_\nu} \right] \]

\( a_\nu \): 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**

\[ \tilde{H} = T + V_{UCOM} + \delta V_{c+p+ls} \]
### Variation: Chart of Nuclei

#### Chemical Elements

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<th>N</th>
<th>2</th>
<th>4</th>
<th>6</th>
<th>8</th>
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<th>12</th>
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</table>

### Energy Deviation

The chart shows the energy deviation from the experimental values for each isotope. The color scale ranges from -0.5 (blue) to 1.5 (red), indicating the deviation from the expected value. The deviation is normalized by the atomic mass (A) of the isotope.

- **Single Gaussian per nucleon**
- **Two Gaussians per nucleon**

The deviation is given by:

\[
\frac{(E - E_{\text{exp}})}{A} \quad \text{[MeV]}
\]
Intrinsic One-Body Density Distributions

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

\[ ^4\text{He} \]
\[ ^{16}\text{O} \]
\[ ^{40}\text{Ca} \]
\[ ^9\text{Be} \]

capable of describing spherical shell-model as well as intrinsically deformed and \( \alpha \)-cluster states
Beyond Simple Variation

- **Projection after Variation (PAV)**
  - restore inversion and rotational symmetry by angular momentum projection

- **Variation after Projection (VAP)**
  - find energy minimum within parameter space of parity and angular momentum projected states
  - implementation via generator coordinate method (constraints on multipole moments)

- **Multi-Configuration**
  - diagonalisation within a set of different Slater determinants
### Intrinsic Shapes of $^{12}\text{C}$

<table>
<thead>
<tr>
<th></th>
<th>intrinsic</th>
<th>projected</th>
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<tbody>
<tr>
<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>
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<td>-40.2</td>
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<tr>
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<td>2.22</td>
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<tr>
<td>$\langle V_{ls} \rangle$</td>
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<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

<table>
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<tr>
<th></th>
<th>$E$ [MeV]</th>
<th>$R_{ch}$ [fm]</th>
<th>$B(E2)$ [$e^2$ 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>
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<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} — $ Hoyle State

![Graph showing the structure of $^{12}\text{C}$]

<table>
<thead>
<tr>
<th>Multi-Config (4)</th>
<th>Multi-Config (14)</th>
<th>Experiment</th>
</tr>
</thead>
</table>

\[ \langle 0^+ | 0^+ \rangle = 0.76 \]

\[ \langle 0^+ | 0^+ \rangle = 0.71 \]

\[ \langle 0^+ | 0^+ \rangle = 0.50 \]

<table>
<thead>
<tr>
<th></th>
<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>$R_{ch}$ [fm]</td>
<td>2.52</td>
<td>2.47</td>
</tr>
<tr>
<td>$B(E2, 0_1^+ \rightarrow 2_1^+)$ [e² fm⁴]</td>
<td>42.9</td>
<td>39.7 ± 3.3</td>
</tr>
<tr>
<td>$M(E0, 0_1^+ \rightarrow 0_2^+)$ [fm²]</td>
<td>5.67</td>
<td>5.5 ± 0.2</td>
</tr>
</tbody>
</table>
Summary

- **Unitary Correlation Operator Method (UCOM)**
  - short-range central and tensor correlations treated explicitly
  - long-range correlations have to be accounted for by model space

- **Correlated Realistic NN-Potential** $V_{UCOM}$
  - low-momentum / phase-shift equivalent / operator representation
  - robust starting point for all kinds of many-body calculations
Summary

- **UCOM + No-Core Shell Model**
  - dramatically improved convergence
  - tool to assess long-range correlations & higher-order contributions

- **UCOM + Hartree-Fock / RPA**
  - ground states & excitations across the whole nuclear chart
  - basis for improved many-body calculations: MBPT, SM/CI, CC,...

- **UCOM + Fermionic Molecular Dynamics**
  - clustering and intrinsic deformations in p- and sd-shell
  - projection / multi-config provide detailed structure information
Epilogue

- **thanks to my group & my collaborators**

  - H. Hergert, N. Paar, P. Papakonstantinou, A. Zapp
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  - T. Neff
    NSCL, Michigan State University

  - H. Feldmeier
    Gesellschaft für Schwerionenforschung (GSI)

supported by the DFG through SFB 634
“Nuclear Structure, Nuclear Astrophysics and Fundamental Experiments...”