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
Nuclear Structure in the 21st Century

new frontiers in nuclear structure physics

Experiment

- fundamental astrophysical questions need nuclear input
- possibilities to investigate nuclei far off stability
- new nuclear structure facilities: RIA, FAIR@GSI,...

Theory

- improved understanding of fundamental degrees of freedom / QCD
- high-precision realistic nucleon-nucleon potentials
- \emph{ab initio} treatment of the many-body problem
Astrophysical Challenges
Theoretical Context

- finite nuclei
- few-nucleon systems
- nucleon-nucleon interaction
- hadron structure
- quarks & gluons
- deconfinement
Quantum Chromo Dynamics

Nuclear Structure

Theoretical Context

“solve” the quantum many-body problem with this interaction

“derive” a realistic nucleon-nucleon interaction from QCD
Realistic Nucleon-Nucleon Potentials
Nature of the NN-Interaction

- NN-interaction is **not fundamental**
- induced via mutual **polarization** of quark & gluon distributions
- analogous to **van der Waals** interaction between neutral atoms
- **short-ranged**: acts only if the nucleons overlap
- genuine **NNN-interaction** is important

\[ \rho_0^{-1/3} = 1.8 \text{fm} \]
How to Construct the NN-Potential?

- **QCD input**
  - symmetries
  - meson-exchange picture
  - chiral perturbation theory

- **short-range phenomenology**
  - ansatz for short-range behavior

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

\[ v(r) \]
\[ v(r) \tilde{L}^2 \]
\[ (S, T) \]
\[ (1, 0) \]
\[ (1, 1) \]
\[ (0, 0) \]
\[ (0, 1) \]
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 diagonalization of the Hamiltonian in a harmonic oscillator basis
Argonne v$_{18}$
With Illinois-2
GFMC Calculations
22 June 2004

12C results are preliminary.

[S. Pieper, private comm.]
Our Goal

nuclear structure calculations across the whole nuclear chart based on realistic NN-potentials

bound to simple Hilbert spaces for large particle numbers

need to deal with strong interaction-induced correlations
Correlations in Nuclei
What are Correlations?

\[ \text{correlations} = \text{everything beyond the independent particle picture} \]

- the quantum state of \( A \) independent (non-interacting) fermions is a **Slater determinant**

\[ |\psi\rangle = \mathcal{A}( |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_A\rangle) \]

- Slater determinants **cannot describe correlations** by definition
$M_S = 0$
\[ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \]

$M_S = \pm 1$
\[ |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle \]

- Spin-projected two-body density $\rho_{1,M_S}^{(2)}(\vec{r})$
- Uncorrelated two-body state
Deuteron: Manifestation of Correlations

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

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

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

Two-body density fully suppressed at small particle distances \(|\vec{r}|\)

**Central correlations**

Angular distribution depends strongly on relative spin orientation

**Tensor correlations**
Central Correlations

- strong repulsive core in central part of realistic interactions
- suppression of the probability density for finding two nucleons within the core region $\Rightarrow$ central correlations

can be described by “shifting” the nucleons out of the core region
Tensor Correlations

- analogy with dipole-dipole interaction
  \[ V_{\text{tensor}} \sim -\left( \frac{3 (\vec{\sigma}_1 \vec{r}) (\vec{\sigma}_2 \vec{r})}{r^2} - \vec{\sigma}_1 \vec{\sigma}_2 \right) \]

- couples the relative spatial orientation of two nucleons with their spin orientation → tensor correlations

can be described by “rotating” nucleons towards pole or equator depending on spin
Unitary Correlation Operator Method (UCOM)
Correlation Operator
introduce correlations by means of an unitary transformation with respect to the relative coordinates of all pairs

\[ C = \exp[-i \sum g_{ij}] \]

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

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

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

\[ \langle \tilde{\psi} | O | \tilde{\psi}' \rangle = \langle \psi | C^\dagger O C | \psi' \rangle = \langle \psi | \hat{O} | \psi' \rangle \]
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} [s(r) q_r + q_r s(r)] ]</td>
<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>
</tr>
<tr>
<td>[ q_r = \frac{1}{2} [\vec{r} \cdot \vec{q} + \vec{q} \cdot \vec{r}] ]</td>
<td>[ \vec{q}_\Omega = \vec{q} - \frac{\vec{r}}{r} q_r ]</td>
</tr>
</tbody>
</table>

\( s(r) \) and \( \vartheta(r) \) encapsulate the physics of short-range correlations
Correlated States

\[ \rho^{(2)}_{1, S_M}(\vec{r}) \]

**Central Correlations**

\[ s(r) \]

**Tensor Correlations**

\[ \vartheta(r) \]
Simplistic “Shell-Model” Calculation

- expectation values for harmonic osc. Slater determinant
- nuclei unbound without inclusion of correlations
- central and tensor correlations essential to obtain bound system
Application I:

Hartree-Fock Calculations
UCOM-Hartree-Fock Approach

- many-body state is a **Slater determinant** of single-particle states obtained by energy minimization
- **correlations cannot be described** by Hartree-Fock states
- bare realistic NN-potential leads to **unbound nuclei**
$E = A$ [MeV]

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

Correlated Argonne V18

$R_{ch}$ [fm]

- Experiment
- AV18$\alpha$
long-range correlations

**Ab Initio Strategy**

- improve many-body states such that long-range correlations are included
- many-body perturbation theory (MPT), configuration interaction (CI), coupled-cluster (CC),...
- many-body perturbation theory: second-order energy shift gives estimate for influence of long-range correlations

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

- preliminary

![Graph showing the comparison between experimental data and theoretical calculations for various isotopes. The graph plots the energy per nucleon (E/A) against atomic number (Z). The theoretical calculations are shown in blue and red, while the experimental data is indicated by black bars. The isotopes include \(^4\)He, \(^{16}\)O, \(^{34}\)Si, \(^{40}\)Ca, \(^{48}\)Ca, \(^{48}\)Ni, \(^{56}\)Ni, \(^{68}\)Ni, \(^{78}\)Ni, \(^{88}\)Sr, \(^{90}\)Zr, \(^{100}\)Sn, \(^{114}\)Sn, \(^{132}\)Sn, \(^{146}\)Gd, and \(^{208}\)Pb.]}
**Missing Pieces**

**long-range correlations**

**genuine three-body forces**

**three-body cluster contributions**

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**Pragmatic Approach**

- phenomenological two-body correction

\[ \delta V_{c+p+ls} = v_1(r) + \vec{q} v_{qq}(r) \vec{q} + v_{LS}(r) \vec{L} \cdot \vec{S} \]

- Gaussian radial dependencies with fixed ranges

- strengths used as fit parameters
  (fitted to \(^4\text{He}, \text{ }^{16}\text{O}, \text{ }^{24}\text{O}, \text{ }^{40}\text{Ca}, \text{ }^{48}\text{Ca}, \text{ }^{48}\text{Ni}, \text{ }^{90}\text{Zr})
Correlated Argonne V18 + Correction

![Graph showing E/A and R_ch as functions of atomic mass number]

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

Atoms: $^{4}\text{He}$, $^{16}\text{O}$, $^{34}\text{Si}$, $^{40}\text{Ca}$, $^{44}\text{Ca}$, $^{48}\text{Ni}$, $^{56}\text{Ni}$, $^{64}\text{Ni}$, $^{78}\text{Ni}$, $^{88}\text{Sr}$, $^{90}\text{Zr}$, $^{100}\text{Sn}$, $^{114}\text{Sn}$, $^{118}\text{Sn}$, $^{132}\text{Sn}$, $^{146}\text{Ni}$, $^{208}\text{Pb}$

- Black line: experiment
- Blue line: AV18$\alpha$
- Red line: AV18$\alpha$ + $\delta V_{c+p+ls}$
Charge Distributions

\[ \text{experiment} \quad \text{HF with AV18} \alpha + \delta V_{c+p+ls} \]
Application II

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

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

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

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

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

### Variation

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

### Diagonalization

in sub-space spanned by several non-orthogonal Slater determinants \( |Q_{i}\rangle \)
Intrinsic One-Body Density Distributions

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**
  - diagonalization within a set of different Slater determinants
Helium Isotopes: Energies & Radii

Binding energies

Matter & charge radii

He4  He5  He6  He7  He8

PAV\textsuperscript{π}
Multi-Config
Experiment
Helium Isotopes: Density Profiles

The graph shows the density profiles of helium isotopes $^4\text{He}$, $^6\text{He}$, and $^8\text{He}$, with $\rho(r)$ plotted against $r$ (in fermi). The profiles are labeled as total, neutron, and proton. Arrows indicate the presence of a neutron halo in these isotopes.
Structure of $^{12}$C

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

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

- exciting times for nuclear structure physics!
- realistic NN-potentials & *ab initio* calculations
- systematic schemes to derive effective (correlated / low-momentum) interactions
- innovative ways to treat the many-body problem

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

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