Modern 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
  - Random Phase Approximation & Beyond
  - Fermionic Molecular Dynamics
Nuclear Structure in the 21st Century

NUSTAR @ FAIR
RIBF @ RIKEN

Nuclear Astrophysics

NUSTAR @ FAIR
RIBF @ RIKEN

nuclei far-off stability

SPIRAL2 @ GANIL
HIE-ISOLDE @ CERN

hyper-nuclei,...

reliable nuclear structure theory for exotic nuclei

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

Nuclear Structure

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

\[ v(r) \]

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

\[ (S, T) \]

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

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

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

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

\[
\begin{array}{c}
0 & 1 & 2 \\
[0, 100] & [0, 100] & [0, 100] \\
\text{[MeV]} & \text{[fm]} & \text{[fm]}
\end{array}
\]
$M_S = 0$
\[ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \]

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

- spin-projected two-body density $\rho^{(2)}_{1,M_S}(\vec{r})$
- 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
Ab initio Methods: GFMC

Argonne v$_{18}$
With Illinois-2
GFMC Calculations
22 June 2004

"exact" numerical solution of interacting $A$-nucleon problem

$^{12}$C results are preliminary.

[S. Pieper, private comm.]
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
Modern Nuclear Structure Theory

Nuclear Structure

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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

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

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

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

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

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

**Tensor Correlator** \( C_\Omega \)

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

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

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

\( s(r) \) and \( \vartheta(r) \)

for given potential determined in the two-body system
Correlated States: The Deuteron

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

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

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

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

Central correlations

Tensor correlations

Only short-range tensor correlations treated by \( C_\Omega \)
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.

- Momentum-space matrix elements of correlated interaction are **similar to** $V_{\text{low-k}}$.

- Operators of **all observables** (densities, transitions) have to be and can be **transformed consistently**.
Simplistic “Shell-Model” Calculation

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

![Graph showing expectation values for different nuclei](image)

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

No-Core Shell Model

in collaboration with
Petr Navrátil (LLNL)
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
$^{4}\text{He}: \text{Convergence}$

Diagrams showing the energy levels $E$ as a function of the angular momentum $\hbar \omega$ for $V_{AV18}$ and $V_{UCOM}$ potentials. The diagrams illustrate 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

Tjon-line: $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions
Tjon-Line and Correlator Range

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

**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

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

Exp. $V_{UCOM}(\text{AV18})$
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
$^6\text{Li}$ : NCSM throughout the p-Shell

$^6\text{Li}$

$\hbar \omega = 26 \text{MeV}$

E$^*$ [MeV]

$E$ [MeV]

systematic NCSM studies throughout p-shell with $V_{UCOM}$ (+ Lee-Suzuki transformation)

$^{10}\text{B: Hallmark of a 3N Interaction?}$

\[ V_{\text{UCOM}} \]

$E - E_{3^+}$ [MeV]

$E_{3^+} = -62.1$ MeV

$E_{4^+} = -64.7$ MeV

$\hbar \omega = 18$ MeV

$0^+, 2^+, 4^+, 6^+, 8^+$
$^{10}\text{B}: \text{ Hallmark of a 3N Interaction?}$

$V_{\text{UCOM}}$ gives correct level ordering without any 3N interaction
NCSM

- converged calculations essentially restricted to p-shell
- $6\hbar\omega$ calculation for $^{40}\text{Ca}$ presently not feasible ($\sim 10^{10}$ states)

Importance Sampling NCSM

- diagonalization in space of important many-body configurations
- a priori importance measure given by perturbation theory

\begin{align*}
V_{\text{UCOM}}, \hbar\omega &= 14 \text{ MeV} \\
E_{\text{MeV}} \quad \nu = 0 & \quad \nu = 2 & \quad \nu = 4 & \quad \nu = 6 & \quad \nu = 8 & \quad \nu = 10 & \quad \nu = 12
\end{align*}
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 ($\sim 13$ 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

![Graph showing energy per particle (E/A) and charge radius ($R_{ch}$) for different isotopes.]

- $^4$He, $^{16}$O, $^{24}$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, $^{208}$Pb

- Experiment (black line) and Hartree-Fock (HF, blue circles)
long-range correlations are perturbative easily tractable within PT, SM/CI, CC, RPA,...

indications for presence of residual three-body force
**RPA, ERPA & SRPA**

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

- **Fully self-consistent RPA** based on the Hartree-Fock orbits using the same $V_{UCOM}$
  - recovering sum rules with high precision, spurious center-of-mass mode fully decoupled at $\sim 10$ keV

- **Extended-RPA and Second-RPA** to include effects of ground state correlations and complex configurations
Isoscalar Giant Monopole

prediction for ISGMR in good agreement with experiment

incompressibility resulting from $V_{UCOM}$ is reasonable
Centroid energies systematically too large

Effective mass too small & single-particle spectra too wide

Indication for long-range ground state correlations & three-nucleon force
Outlook: RPA with Three-Body Forces

- long-range tensor correlator & repulsive three-body contact interaction

- systematic improvement of
  - rms-radii
  - single-particle spectra
  - strength distributions

- standard $V_{UCOM}$

- $V_{UCOM}$ with long-range tensor & three-body contact interaction
Application IV

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

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

Correlated Hamiltonian

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

Variation

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

Projection

restoration of rotational and inversion symmetry
PAV / VAP

Multi-Configuration

mixing of several intrinsic configurations
GCM
capable of describing spherical shell-model as well as intrinsically deformed and $\alpha$-cluster states
Structure of $^{12}$C

<table>
<thead>
<tr>
<th></th>
<th>$E$ [MeV]</th>
<th>$R_{ch}$ [fm]</th>
<th>$B(E2)$ [$e^2$ fm$^4$]</th>
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<tbody>
<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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<tr>
<td>PAV$\pi$</td>
<td>88.5</td>
<td>2.51</td>
<td>36.3</td>
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<tr>
<td>VAP</td>
<td>89.2</td>
<td>2.42</td>
<td>26.8</td>
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<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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Structure of $^{12}\text{C} — \text{Hoyle State}$

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

\[3\text{He}-\alpha\] Frozen+PAV\(^{\pi}\]

\[\delta(E) [\text{deg}]\]

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

\[\text{FMD Exp. Frozen Frozen+PAV}^{\pi} \text{ Exp.}\]

\[\begin{array}{c|cc}
\text{3 He+}\alpha & \text{3 He+}\alpha \\
\hline
\text{FMD} & \text{Exp.} \\
\end{array}\]
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
Epilogue

- thanks to my group & my collaborators
  
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    NSCL, Michigan State University
  
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