Nuclear Structure based on Correlated Realistic NN-Interactions

Robert Roth
Institut für Kernphysik, TU Darmstadt

INT Program
“Nuclear Structure Near the Limits of Stability”
Seattle, 2005
Our Aim

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

- Argonne V18, CD Bonn, Nijmegen,...
- reproduce experimental scattering data and deuteron properties with high accuracy

\[ v(r) L^2 \]

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

\[ v(r) (L \cdot S) \]

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

**AV18**

- \((S, T) = (1, 0)\)
- \((1, 1)\)
- \((0, 0)\)
- \((0, 1)\)
Realistic NN-Potentials

- several realistic NN-potentials are available
  - Argonne V18, CD Bonn, Nijmegen,...
  - reproduce experimental scattering data and deuteron properties with high accuracy

- need to be supplemented by a three-nucleon potential
  - NNN-potential depends on NN-potential
  - present NNN-potentials are purely phenomenological
  - very promising developments in chiral effective field theories towards a consistent NN + NNN-potential
Ab Initio Many-Body Calculations

Argonne v18
With Illinois-2
GFMC Calculations
22 June 2004

Energy (MeV)

12C results are preliminary.

[S. Pieper, private comm.]
Our Aim

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
Overview

- Correlations in Nuclei
- Unitary Correlation Operator Method (UCOM)
- UCOM + No-Core Shell Model
- UCOM + Hartree-Fock
- UCOM + Fermionic Molecular Dynamics
Correlations in Nuclei
Deuteron: Manifestation of Correlations

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

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

- 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**
Central Correlations

**Strong repulsive core in central part of realistic interactions**

- Suppression of the probability density for finding two nucleons within the core region → **central correlations**

- Cannot be described by single or superpos. of few Slater determinants

"Shift the nucleons out of the core region"
Tensor Correlations

\[ V_{\text{tensor}} \sim -\left(3 \left(\hat{\sigma}_1 \cdot \vec{r} \right) \left(\hat{\sigma}_2 \cdot \vec{r} \right) \frac{1}{r^2} - \hat{\sigma}_1 \cdot \hat{\sigma}_2 \right) \]

- analogy with dipole-dipole interaction
- couples the relative spatial orientation of two nucleons with their spin orientation → tensor correlations
- cannot be described by single or superpos. of few Slater determinants

“rotate nucleons towards poles or equator depending on spin orientation”
Unitary Correlation Operator Method (UCOM)
Correlation Operator

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

\[ C = \exp[-i G] = \exp[-i \sum_{i<j} g_{ij}] \]
\[ g = g(\vec{r}, \vec{q}; \vec{\sigma}_1, \vec{\sigma}_2, \vec{\tau}_1, \vec{\tau}_2) \]

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

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

\[ C = C_\Omega C_r \]

### Central Correlator \( C_r \)
- **Radial distance-dependent shift** in the relative coordinate of a nucleon pair

\[
\begin{align*}
g_r &= \frac{1}{2} [s(r) q_r + q_r s(r)] \\
q_r &= \frac{1}{2} \left[ \frac{\vec{r}}{r} \cdot \vec{q} + \vec{q} \cdot \frac{\vec{r}}{r} \right]
\end{align*}
\]

### Tensor Correlator \( C_\Omega \)
- **Angular shift depending on the orientation of spin and relative coordinate of a nucleon pair**

\[
\begin{align*}
g_\Omega &= \frac{3}{2} \vartheta(r) \left[ (\vec{\sigma}_1 \cdot \vec{d}_\Omega) (\vec{\sigma}_2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{d}_\Omega) \right] \\
\vec{d}_\Omega &= \vec{q} - \frac{\vec{r}}{r} q_r
\end{align*}
\]

\( s(r) \) 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**
Correlated States

Central correlation functions for different $L$ values:
- $L = 0$
- $L = 2$

Tensor correlation functions $s(r)$ and $\vartheta(r)$ as a function of $r$ [fm].
Correlated Operators

Cluster Expansion
\[ \tilde{O} = C^\dagger O C = \tilde{O}^{[1]} + \tilde{O}^{[2]} + \tilde{O}^{[3]} + \ldots \]

Cluster Decomposition Principle
If the correlation range is small compared to the mean particle distance, then higher orders are small.

Two-Body Approx.
\[ \tilde{O}^{C^2} = \tilde{O}^{[1]} + \tilde{O}^{[2]} \]

Operators of all observables can be and have to be correlated consistently.
Correlated NN-Potential — $V_{UCOM}$

\[ \tilde{H}^{C2} = \tilde{T}^{[1]} + \tilde{T}^{[2]} + \tilde{V}^{[2]} = T + V_{UCOM} \]

- **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** $V_{low-k}$
Momentum-Space Matrix Elements

\[ q = \left[ \text{fm}^{-1} \right] \]

- \( ^3S_1 \)
- \( ^3S_1 - ^3D_1 \)

\[ q' = \left[ \text{fm}^{-1} \right] \]

\[ V_{\text{bare}} \]

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

AV18

pre-diagonalisation of Hamiltonian
Comparison with $V_{\text{low}k}$
Simplistic “Shell-Model” Calculation

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

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

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

No-Core Shell Model
convergence dramatically improved compared to bare interaction

assessment of the importance of long-range correlations

direct evaluation of omitted higher-order contributions

Jacobi-NCSM code by Petr Navrátil without Lee-Suzuki

[PRC 61, 044001 (2000)]
$^4$He: Convergence

$V_{\text{bare}}$

$V_{\text{UCOM}}$

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

$V_{\text{bare}}$

$V_{\text{UCOM}}$

Omitted higher-order cluster contributions
Tjon-Line and Correlator Range

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

- change in correlator range results in shift along Tjon-line

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

---

**Figure:**

- This correlator is used in the following

- Experimental data

- $V_{\text{UCOM}}(\text{AV18})$

- $V_{\text{NN}} + V_{\text{NNN}}$

- $I_\theta$ [fm$^3$]

- $0.03$

- $0.04$

- $0.05$

- $0.12$
Application II

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

- single-particle states expanded in a spherical oscillator basis
- truncation in $n$, $l$, and/or $N = 2n + l$ (typically $N_{\text{max}} = 8...14$)
- Coulomb interaction included exactly
- formulated with intrinsic kinetic energy $T_{\text{int}} = T - T_{\text{cm}}$ to eliminate center of mass contributions
Missing Pieces

- long-range correlations
- genuine three-body forces
- three-body cluster contributions

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

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

![Graph showing energy levels for different nuclei](image)

- **$N_{max} = 12$**
- **4He, 16O, 24O, 34Si, 40Ca, 48Ca, 48Ni, 56Ni, 68Ni, 78Ni, 88Sr, 90Zr, 100Sn, 114Sn, 132Sn, 146Gd, 208Pb**

- **experiment**
  - **HF**
  - **HF+PT2**
  - **HF+PT2+PT3**
Long-Range Correlations: MBPT

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

\[ A_{\text{O}} \]

\[ A_{\text{Ni}} \]

\[ A_{\text{Sn}} \]

HF
HF+PT2
experiment
Beyond Hartree-Fock
- residual long-range correlations are **perturbative**
- mostly long-range **tensor correlations**
- easily tractable within MBPT, CI, CC,...

Net Three-Body Force
- small effect on binding energies for all masses
- cancellation does not work for all observables
- construct simple effective three-body force
long-range correlations

genuine three-body forces

three-body cluster contributions

**Pragmatic Approach**

- phenomenological two-body correction

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

- Gaussian radial dependencies with fixed ranges

- strengths used as fit parameters (3 parameters)
Correlated Argonne V18 + Correction

\[ E = A \begin{bmatrix} \text{MeV} \end{bmatrix} \]

The diagram shows the energy \( E/A \) and radius \( R_{ch} \) for various isotopes, comparing experimental data and calculations with \( V_{UCOM} \) and \( V_{UCOM} + \delta V_{c+p+ls} \).
Charge Distributions

- **16O**
- **48Ca**
- **90Zr**
- **40Ca**
- **88Sr**
- **208Pb**

**Graphs:**
- **0.02**
- **0.04**
- **0.06**
- **0.08**
- **0.1**

**Axes:**
- **r [fm]**

**Legend:**
- **experiment**
- **HF with \( V_{UCOM} + \delta V_{c+p+ls} \)**
Application III

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

**Gaussian Single-Particle States**

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

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

- \(a_{\nu}\): 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**

\[
\tilde{H}_{\text{int}} = T_{\text{int}} + V_{\text{UCOM}} \left[ + \delta V_{c+p+ls} \right]
\]

**Variation**

\[
\frac{\langle Q | \tilde{H}_{\text{int}} | Q \rangle}{\langle Q | Q \rangle} \rightarrow \min
\]

**Diagonalisation**

in sub-space spanned by several non-orthogonal Slater determinants \(|Q_i\rangle\)
\[ \langle q_k, q_l | G(r) S_{12}(\vec{q}_\Omega, \vec{q}_\Omega) | q_m, q_n \rangle = \gamma_{klmn}^2 R_{km} R_{ln} G_{klmn} \{ \]

\[ s_{12}(\vec{\rho}_{klmn} \times \vec{\pi}_{klmn}, \vec{\rho}_{klmn} \times \vec{\pi}_{klmn}) (5\alpha_{klmn} + \gamma_{klmn} \vec{\rho}_{klmn}^2) + \]

\[ s_{12}(\vec{\pi}_{klmn}, \vec{\pi}_{klmn}) (9\alpha_{klmn}^2 + 13\alpha_{klmn}\gamma_{klmn} \vec{\rho}_{klmn}^2 + 2\gamma_{klmn}^2 \vec{\rho}_{klmn}^4) - \]

\[ s_{12}(\vec{\pi}_{klmn}, \vec{\rho}_{klmn}) \left( \frac{9}{2} \alpha_{klmn} \beta_{klmn} + 16\alpha_{klmn}\gamma_{klmn}(\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn}) + \right) \]

\[ \frac{5}{2} \gamma_{klmn} \beta_{klmn} \vec{\rho}_{klmn}^2 + 4\gamma_{klmn}^2 (\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn}) \vec{\rho}_{klmn}^2 \right) + \]

\[ s_{12}(\vec{\rho}_{klmn}, \vec{\rho}_{klmn}) \left( \frac{21}{4} \gamma_{klmn}(\theta_{klmn} - \alpha_{klmn}\lambda_{klmn}) + \frac{9}{4} \theta_{klmn} - \frac{9}{2} + \right) \]

\[ 2\gamma_{klmn}^2 (\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn})^2 + 4\gamma_{klmn} \beta_{klmn}(\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn}) - \]

\[ \frac{3}{4} \gamma_{klmn} \left( \frac{\theta_{klmn}}{\alpha_{klmn} + \kappa} + \gamma_{klmn}\lambda_{klmn} \right) \vec{\rho}_{klmn}^2 \right) \} \]
Variation: Chart of Nuclei

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

\[ \rho^{(1)}(\vec{x}) \]

able 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
Results for p-Shell Nuclei
Helium Isotopes: Densities

Multi-Config
radial density profiles

PAV\(_\pi\)
intrinsic densities
Lithium Isotopes: Intrinsic Densities

PAV$^\pi$

intrinsic densities
Lithium Isotopes: Energies & Radii

**Binding energies**

- Strong $\alpha + d$ and $\alpha + t$ cluster contributions

**Matter & Charge radii**

- Very delicate; treat as projected $^9$Li-core plus neutrons
Lithium Isotopes: Moments

Magnetic moments

Quadrupole moments
Carbon Isotopes: Intrinsic Densities

PAV\(^\pi\)
intrinsic densities
Carbon Isotopes: Energies & Radii

Binding energies

Matter & charge radii

PAV
Multiconf
Exp

C10 C11 C12 C13 C14 C15 C16 C17 C18 C19 C20

[MeV]

[fm]
### Intrinsic Shapes of $^{12}$C

<table>
<thead>
<tr>
<th></th>
<th>Intrinsic</th>
<th>Projected</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\langle H \rangle$</td>
<td>-81.4</td>
<td>-81.5</td>
</tr>
<tr>
<td>$\langle T \rangle$</td>
<td>212.1</td>
<td>212.1</td>
</tr>
<tr>
<td>$\langle V_{ls} \rangle$</td>
<td>-39.8</td>
<td>-40.2</td>
</tr>
<tr>
<td>$\sqrt{\langle r^2 \rangle}$</td>
<td>2.22</td>
<td>2.22</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Intrinsic</th>
<th>Projected</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\langle H \rangle$</td>
<td>-77.0</td>
<td>-88.5</td>
</tr>
<tr>
<td>$\langle T \rangle$</td>
<td>189.2</td>
<td>186.1</td>
</tr>
<tr>
<td>$\langle V_{ls} \rangle$</td>
<td>-12.0</td>
<td>-17.1</td>
</tr>
<tr>
<td>$\sqrt{\langle r^2 \rangle}$</td>
<td>2.40</td>
<td>2.37</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Intrinsic</th>
<th>Projected</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\langle H \rangle$</td>
<td>-74.1</td>
<td>-85.5</td>
</tr>
<tr>
<td>$\langle T \rangle$</td>
<td>182.8</td>
<td>179.0</td>
</tr>
<tr>
<td>$\langle V_{ls} \rangle$</td>
<td>-5.8</td>
<td>-8.0</td>
</tr>
<tr>
<td>$\sqrt{\langle r^2 \rangle}$</td>
<td>2.45</td>
<td>2.42</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Intrinsic</th>
<th>Projected</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\langle H \rangle$</td>
<td>-57.0</td>
<td>-75.9</td>
</tr>
<tr>
<td>$\langle T \rangle$</td>
<td>213.9</td>
<td>201.4</td>
</tr>
<tr>
<td>$\langle V_{ls} \rangle$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$\sqrt{\langle r^2 \rangle}$</td>
<td>2.44</td>
<td>2.42</td>
</tr>
</tbody>
</table>
Structure of $^{12}$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 $^{12}$C — Hoyle State

<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>$B(E2, 0^+_1 \rightarrow 2^+_1)$ [$e^2$ fm$^4$]</td>
<td>42.9</td>
<td>39.7 ± 3.3</td>
</tr>
<tr>
<td>$M(E0, 0^+_1 \rightarrow 0^+_2)$ [fm$^2$]</td>
<td>5.67</td>
<td>5.5 ± 0.2</td>
</tr>
</tbody>
</table>

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

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

$\langle \left| 0^+_2 \right\rangle \rangle = 0.50$
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**
  - access to nuclei across the whole nuclear chart
  - basis for improved many-body calculations: MBPT, CI, CC, RPA,...

- **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  
    Institut für Kernphysik, TU Darmstadt

  - 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...”