The Unitary Correlation Operator Method

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From QCD to Nuclear Structure

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

Quantum Chromo Dynamics
Nuclear Structure
better resolution / more fundamental
From QCD to Nuclear Structure

- Quantum Chromo Dynamics
- Nuclear Structure

Better resolution / more fundamental

Solve the interacting nuclear many-body problem

Construct realistic nucleon-nucleon interaction from 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
Potential and Proton Size

proton charge radius $\sqrt{\langle r^2 \rangle_e} = (0.81 \cdots 0.86) \text{ fm}$

Proton Charge Distribution and $S=0$, $T=1$ Potential

- proton size not small compared to interaction range
- half-density overlap at maximum attraction, overlap of tails at average NN-distance in nuclear matter
- $V_{NN}$ not elementary
  more like atom-atom potential
- expect three-body forces
Describe basic properties of nuclear many-body system in terms of a realistic nucleon-nucleon interaction $H$ and a many-body state $|\hat{\Psi}\rangle$

$$\langle \vec{r}_1, \vec{\sigma}_1, \tau_1 ; \vec{r}_2, \vec{\sigma}_2, \tau_2 ; \ldots ; \vec{r}_A, \vec{\sigma}_A, \tau_A | \hat{\Psi} \rangle$$

degrees of freedom: $\vec{r}$ cm position, $\vec{\sigma}$ spin, $\tau$ isospin of each nucleon

▶ solve many-body problem

$$\hat{H} |\hat{\Psi}_n\rangle = E_n |\hat{\Psi}_n\rangle$$

▶ Exact solutions for spectra and transitions

$A = 2, 3, 4$  Fadeev, Yakubowski, Hyperspherical harmonics, …

$A \lesssim 12$  no-core SM, GFMC (for bound states only)

$A \gtrsim 12$  numerical effort beyond today’s computer
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Exact many-body state $|\hat{\Psi}_n\rangle$ is terribly complicated for realistic NN-interaction.

WHY?
Introduction

- Short Range Central and Tensor Correlations
- Unitary Correlation Operator Method
  - realistic $\Rightarrow$ correlated Hamiltonian
- Applications:
  - No-Core Shell Model
  - Hartree Fock & Pertubation
    - (Fermionic Molecular Dynamics)
- Summary and Outlook
Realistic $NN$-potential

$V_{NN}(\vec{r}_{12}, \vec{p}_{12} = 0, \vec{\sigma}_1, \vec{\sigma}_2, T = 0)$

- $V_{NN}$ repulsive at small distances
  - $\sim$ strong short-range central correlations
    nucleons cannot get closer than $\approx 0.6$ fm

- $V_{NN}$ depends strongly on orientation of $\vec{\sigma}_1, \vec{\sigma}_2$ with respect to $\vec{r}_{12}$
  - $\sim$ tensor correlations
    protons and neutrons want to align their spins with $\vec{r}_{12}$

Problem:
Slater determinants cannot describe these correlations
Realistic $NN$-potential

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**Problem:**
Slater determinants cannot describe these correlations

**Solution:** include short-range correlations by unitary transformation (UCOM)

$$\left| \tilde{\Psi} \right\rangle = C \left| \Psi \right\rangle = C_\Omega C_r \left| \Psi \right\rangle$$

- $C_r$ central correlator shifts nucleons out of repulsive core
- $C_\Omega$ tensor correlator aligns spins along $\vec{r}_{12}$
The Correlation Operator Method (UCOM) introduces short-range correlations by means of a unitary transformation with respect to the relative coordinates of all pairs.

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

\[ \mathcal{G}^\dagger = \mathcal{G} \]
\[ \mathcal{C}^\dagger \mathcal{C} = 1 \]

Correlated States
\[ |\hat{\Psi}\rangle = \mathcal{C} |\Psi\rangle \]

Correlated Operators
\[ \hat{O} = \mathcal{C}^{-1} \hat{O} \mathcal{C} \]

\[ \langle \hat{\Psi} | \hat{O} | \hat{\Psi}' \rangle = \langle \Psi | \mathcal{C}^{-1} \hat{O} \mathcal{C} | \Psi' \rangle = \langle \Psi | \hat{O} | \Psi' \rangle \]
Two-Body Correlations

- two-body generator

\[ \zeta = e^{-i\tilde{G}}, \quad G = \sum_{i<j} g_{ij} \]

Cluster Expansion

correlated operators \( \hat{A} = C^\dagger A C \) are no longer operators with definite particle number

- decompose correlated operator into irreducible \( k \)-body operators

\[ \hat{A} = \hat{A}^{[1]} + \hat{A}^{[2]} + \hat{A}^{[3]} + \ldots \]

Two-Body Approximation

\[ \tilde{T}^{C2} = \tilde{T}^{[1]} + \tilde{T}^{[2]}, \quad \tilde{V}^{C2} = \tilde{V}^{[2]} \]

- correlation range should be smaller than mean distance of nucleons

Correlator \( \zeta \)

should conserve translational, rotational and Galilei invariance

cluster decomposition principle should be fulfilled

Spin-Isospin Dependence

nuclear interaction strongly depends on spin and isospin

\[ \nu = \sum_{s,t} \nu_{ST} \Pi_{ST} \]

- different correlations in the respective channels

\[ g = \sum_{s,t} g_{ST} \Pi_{ST} \]

- correlated interaction in two-body space

\[ \hat{\nu} = \sum_{s,t} (e^{ig_{ST}} \nu_{ST} e^{-ig_{ST}}) \Pi_{ST} \]
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 superposition of few Slater determinants

\[ V_{01}(r) \text{ [MeV]} \]

\[ \rho^{(2)}_{SD}(r) \text{ [fm}^{-3}] \]

\[ C \sim r \]

“shift the nucleons out of the core region”
Radial shift

- correlator shifts nucleons out of core
- radial shift generated by radial momentum $p_r$

$$\zeta_r = \exp \left[ -i G_r \right] = \exp \left[ -i \sum_{i<j} g_{r,ij} \right]$$

$$g_r = \frac{1}{2} \left\{ s(r)p_r + p_rs(r) \right\}, \quad p_r \Rightarrow \frac{1}{i} \left( \frac{1}{r} + \frac{\partial}{\partial r} \right)$$

Correlated 2-body wave function

$$\langle \vec{X}, \vec{r} | e^{-ig_r} | \Phi \rangle = \frac{R_-(r)}{r} \sqrt{R'_-(r)} \langle \vec{X}, R_-(r)\hat{r} | \Phi \rangle$$

$e^{-ig_r}$ acts only on relative distance $r$, not on orientation $\hat{r}$, not on c.m. $\vec{X}$, nor on spins

Correlation function

use correlation function $R_{\pm}(r)$ instead of shift function $s(r)$

$$\int_r^{R_+(r)} \frac{d\xi}{s(\xi)} = \pm 1, \quad R_{\pm}(r) \approx r \pm s(r)$$

Correlated operators

$$e^{+ig_r} V(r) e^{-ig_r} = V(R_+(r))$$

$$e^{+ig_r} (\vec{r} \times \vec{p}) e^{-ig_r} = (\vec{r} \times \vec{p})$$
Centrally Correlated Hamiltonian

\[ \hat{t}^{[1]} = t \]

\[ \hat{t}^{[2]} = c_r^\dagger(t_1 + t_2)c_r - (t_1 + t_2) \]

\[ \Rightarrow \frac{1}{2} \left[ p_r^2 \frac{1}{2\mu_r(r)} + \frac{1}{2\hat{\mu}_r(r)p_r^2} \right] + \frac{1}{2\hat{\mu}_\Omega(r)} \frac{l^2}{r^2} \]

\[ + \frac{1}{2\mu} \left( \frac{7R''_+(r)^2}{4R'_+(r)^4} - \frac{R'''_+(r)}{2R'_+(r)^3} \right) \]

Potential

\[ \hat{v}^c \Rightarrow v^c(R_+(r)) \]

\[ \hat{v}^b \Rightarrow v^b(R_+(r)) \hat{l} \cdot \hat{s} \]

\[ \hat{v}^f \Rightarrow v^f(R_+(r)) s_{12}(\hat{r}, \hat{r}) \]
Tensor Correlations

- analogy with dipole-dipole interaction
  \[ V_{\text{tensor}} \sim -\left[ 3 (\vec{\sigma}_1 \hat{r})(\vec{\sigma}_2 \hat{r}) - \vec{\sigma}_1 \vec{\sigma}_2 \right] \]
  
- couples the relative spatial orientation \( \hat{r} \) of two nucleons with their spin orientations
  ➤ tensor correlations
  
- cannot be described by single or superposition of few Slater determinants

\[ \sim \Omega \]

"rotate nucleons towards poles or equator depending on spin orientation"
Angular shift

- Correlator shifts nucleons to attractive regions

Angular shift generated by $\vec{p}_\Omega = \vec{p} - p_r \hat{r}$

$$Z_\Omega = \exp \left[ -i G_\Omega \right] = \exp \left[ -i \sum_{i<j} g_{\Omega,ij} \right]$$

$$g_{\Omega} = \theta(r) \frac{3}{2} \left( \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) \left( \vec{r}_1 \cdot \vec{r}_2 \right) + \left( \vec{\sigma}_1 \cdot \vec{r}_2 \right) \left( \vec{\sigma}_2 \cdot \vec{p}_\Omega \right)$$

Correlated 2-body wave function (LS - coupled)

$$\langle r | \zeta_\Omega | \varphi; (J, 1)J \rangle = \varphi(r) | (J, 1)J \rangle$$

$$\langle r | \zeta_\Omega | \varphi; (J - 1, 1)J \rangle = \cos \left( \theta^{(J)}(r) \right) \varphi(r) | (J - 1, 1)J \rangle + \sin \left( \theta^{(J)}(r) \right) \varphi(r) | (J + 1, 1)J \rangle$$

Correlation function

$$\theta^{(J)}(r) = 3 \sqrt{J(J+1)} \theta(r)$$

tensor correlator admixes $L = 2$ to $L = 0$, etc.

Correlated operators

Central interactions

$$\text{invariant}$$

$$e^{+ig_\Omega} V(r) e^{-ig_\Omega} = V(r)$$

Correlated tensor:

$$e^{+ig_\Omega} s_{12}(\hat{r}, \hat{\mathbf{p}}) e^{-ig_\Omega} =$$

$$e^{-3\theta(r)} s_{12}(\hat{\mathbf{r}}, \hat{\mathbf{r}})$$

tensor

$$+ 2 \left( 1 - e^{-3\theta(r)} \right) (3 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)$$

central

$$+ 6 \left( 1 - e^{-3\theta(r)} \right) \vec{l} \cdot \vec{s}$$

spin-orbit

$$+ \ldots$$

small terms

Correlated States: The Deuteron

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

\( L = 0 \)

\( r \) [fm]

0 0.05 0.1 0.15

0 1 2 3 4 5
Correlated States: The Deuteron

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

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

\[ s(r) \]

Central correlations
Correlated States: The Deuteron

\[ \langle r \phi \rangle \]

\[ \langle r C_{C} \phi \rangle \]

\[ \langle r C_{\Delta C} \phi \rangle \]

\[ L = 0 \]

\[ s(r) \]

\[ \vartheta(r) \]

constraint on range of tensor correlator

central correlations

tensor correlations

Central and Tensor Correlators

\[ C = \tilde{C}_\Omega \tilde{C}_r \]

**Central Correlator** \( \tilde{C}_r = \exp\left[-i \sum_{i<j} g_{r,ij} \right] \)
- radial distance-dependent shift in the relative coordinate of a nucleon pair
  \[ g_r = \frac{1}{2} s(r) p_r + p_r s(r) \]
  \[ p_r = \frac{1}{2} \left( \vec{r} \cdot \vec{p} + \vec{p} \cdot \frac{\vec{r}}{r} \right) \]

**Tensor Correlator** \( \tilde{C}_\Omega = \exp\left[-i \sum_{i<j} g_{\Omega,ij} \right] \)
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair
  \[ g_\Omega = \frac{3}{2} \theta(r) \left( \vec{\sigma}_1 \cdot \vec{p}_\Omega \right) \left( \vec{\sigma}_2 \cdot \vec{r} \right) + (\vec{r} \leftrightarrow \vec{p}_\Omega) \]
  \[ \vec{p}_\Omega = \vec{p} - \frac{\vec{r}}{r} p_r \]

\( s(r) \) and \( \theta(r) \)
for given potential determined in the two-body system
Central Correlations

- determine $s(r)$ and $\vartheta(r)$ in each spin-isospin channel by minimizing the energy in the two-body system

$$\min_{s(r), \vartheta(r)} \langle \phi_{\text{trial}}^{ST} | C_r^+ C_{\Omega}^+ H C_{\Omega} C_r | \phi_{\text{trial}}^{ST} \rangle$$

- correlation functions depend only weakly on the trial wave function
- range of $s(r), \vartheta(r)$ greater mean distance of nucleons $\Rightarrow$ large 3-body terms $\hat{T}^{[3]} + \hat{V}^{[3]}$
- restrict the range of the tensor correlations in the $S = 1, T = 0$ channel (parameter $I_\vartheta = \int dr \ r^2 \vartheta(r)$)

Tensor Correlations

Momentum-Space Matrix Elements

\[ \langle q (LS)_{JT} | V_{\text{bare}} | q' (L'S)_{JT} \rangle \]

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

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

pre-diagonalisation of Hamiltonian

AV18
Interaction in Momentum Space

\[ \langle klm | \hat{H}^{[2]} | k'lm' \rangle = i^{\ell'-\ell} M \int d^3 x \int d^3 x' Y_{lm}^*(\hat{x}) j_{\ell}(kx) \langle \hat{x} | \hat{H}^{[2]} | \hat{x}' \rangle j_{\ell'}(k'x') Y_{l'm'}(\hat{x}') \]

**1S_0 channel**

- Uncorrelated
- Correlated

**3S_1 channel**

Unique effective potential – identical to \( V_{\text{lowk}} \)

Achim Schwenk, et al nucl-th/0108041

\( V_{\text{lowk}} \) Cutoff \( \Lambda = 1.0 - 2.0 \text{ fm}^{-1} \)
Comparison with $V_{\text{low-k}}$


[Graph showing interactions]
• expectation value of Hamiltonian (with AV18) for Slater determinant of harmonic oscillator states

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

\begin{align*}
4^\text{He} & \quad 1^6\text{O} & \quad 4^8\text{Ca} & \quad 9^0\text{Zr} & \quad 13^2\text{Sn} & \quad 20^8\text{Pb}
\end{align*}

central & tensor correlations essential to obtain bound nuclei
correlations induce high-momentum components
contributions of tensor correlations very big
different correlator ranges relevant especially at the fermi surface
Application I

No-Core Shell Model
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)

estimate of short- and long-range correlations

NCSM code by Petr Navrátil [PRC 61, 044001 (2000)]
$^4\text{He: Convergence}$

$V_{AV18}$

$V_{UCOM}$

Residual state-dependent long-range correlations
$^4\text{He}: \text{Convergence}$

$V_{AV18}$

$V_{UCOM}$

Omitted three- and four-body contributions
- **Tjon-line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions.
• **Tjon-line**: $E^{(4)}\text{He}$ vs. $E^{(3)}\text{H}$ for phase-shift equivalent NN-interactions

• change of $\mathcal{C}_\Omega$-correlator range results in shift along Tjon-line

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minimise net three-body force by choosing correlator with energies close to experimental value
- **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 for p-Shell Nuclei

systematic NCSM study throughout p-shell in progress

$\hbar \omega = 26$ MeV

$V_{\text{UCOM}}$ and $V_{\text{UCOM}} + \text{Lee-Suzuki}$ calculations by Petr Navratil

$E_0$ [MeV] vs. $N_{\text{max}}$

$E^*$ [MeV]

Exp Chiral

$8\hbar \omega$, $10\hbar \omega$, $12\hbar \omega$, $12\hbar \omega$
large-scale NCSM calculations throughout the p-shell in progress (with Lee-Suzuki transformation)
large-scale NCSM calculations throughout the p-shell in progress (with Lee-Suzuki transformation)

$\nu_{UCOM}$ gives correct level ordering without any NNN interaction

calculations by Petr Navrátil – preliminary
Application II:

Hartree-Fock & Beyond
Standard Hartree-Fock

+ Matrix Elements of Correlated
Realistic NN-Interaction \( V_{\text{UCOM}} \)

- 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 $V_{\text{UCOM}}$

-8
-6
-4
-2
0
-2
-4
-6
-8
40 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

$E/A$ [MeV]

$R_{ch}$ [fm]

long-range correlations are missing

Perturbation Theory with $V_{\text{UCOM}}$

long-range correlations are perturbative
easily tractable within PT, SM/CI, CC, RPA,...

indications for presence of residual three-body force

Summary

- **Unitary Correlation Operator Method**
  treats short range repulsive and tensor correlations
  \[ C = C_r C_\Omega \]

- **UCOM** defines phase-equivalent correlated interaction \( V_{UCOM} \)
  for many-body methods with low-k Hilbert spaces: HF, shell model, FMD
  \( V_{UCOM} \) virtually independent on realistic starting \( V_{NN} \)

- Range of tensor correlator \( C_\Omega \) adjusted to minimize irreducible 3-body forces

- No-core shell model calculations for light nuclei
  \( V_{UCOM} \) produces effects attributed to 3N forces belonging to chiral NN or AV18

- Hartree Fock + 2nd order perturbation for nuclei up to \(^{208}\text{Pb}\)
  indication for necessity of 3N forces for \( V_{UCOM} \)

Outlook

- Improve \( s(r), \vartheta(r) \)
- 3N force for \( V_{UCOM} \)?
- Test many-body states with correlated observables \( C^\dagger A C \)
  el. magn. transitions & moments, \( \beta \)-decay etc.
Anwendung 2

Fermionic Molecular Dynamics
**Fermionic**

Slater determinant

\[ |Q\rangle = \mathcal{A}\left(|q_1\rangle \otimes \cdots \otimes |q_A\rangle\right) \]

\(\Rightarrow\) antisymmetrized A-body state

**Molecular**

single-particle states

\[ \langle \vec{x}|q\rangle = \sum_i c_i \exp\left\{-\frac{(\vec{x} - \vec{b}_i)^2}{2a_i}\right\} \otimes |\chi_i\rangle \otimes |\xi\rangle \]

\(\Rightarrow\) Gaussian wave-packets in phase-space, spin is free, isospin is fixed

**Dynamics in Hilbert space**

spanned by one or several non-orthogonal \(|Q^{(a)}\rangle\)

\[ |\Psi\rangle = \sum_a \psi_a |Q^{(a)}\rangle \]

variational principle \(\rightarrow\) \(Q^{(a)} = \{ q^{(a)}_v, v = 1 \cdots A \}, \psi_a \)

\(\Rightarrow\) Hilbert space contains shell-model, clusters, halos
Effective Correction to the Interaction

**Effective two-body interaction**

- correlated two-body interaction $\hat{H} = \hat{C}^\dagger \hat{H} \hat{C}$ is lacking three-body forces

- instead of three-body force use additional **momentum-dependent** and **spin-orbit** two-body correction term

- fit correction term to binding energies and radii of “closed-shell” nuclei

- altogether a **15%** correction to the *ab-initio* two-body potential

$^{16}\text{O}$ and $^{40}\text{Ca}$ are not “closed shell” nuclei!
### Radius and Quadrupole Moment as Generator Coordinates

<table>
<thead>
<tr>
<th></th>
<th>( r_{\text{charge}} ) [fm]</th>
<th>( Q ) [fm(^2)]</th>
<th>( B(E2) ) [e(^2)fm(^4)]</th>
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<tr>
<td>PAV</td>
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<td>-6.25</td>
<td>9.31</td>
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<td>VAP</td>
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<td>-8.02</td>
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<tr>
<td>Multiconfig</td>
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### Energies

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<td>Variation</td>
<td>4(^+) -40.6</td>
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<tr>
<td>PAV</td>
<td>4(^+) -41.0</td>
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<tr>
<td>VAP</td>
<td>4(^+) -47.7</td>
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<tr>
<td>Multiconf</td>
<td>4(^+) -54.8</td>
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<tr>
<td>Exp</td>
<td>4(^+) -53.5</td>
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</table>

FMD - Variation, PAV$^\pi$, Multiconfig.

<table>
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<tr>
<th></th>
<th>$E$ [MeV]</th>
<th>$r_{\text{charge}}$ [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>
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<td>PAV$^\pi$</td>
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<td>2.51</td>
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<tr>
<td>Multiconfig(4)</td>
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<td>Multiconfig(14)</td>
<td>-92.4</td>
<td>2.52</td>
<td>42.9</td>
</tr>
<tr>
<td>Exp</td>
<td>-92.2</td>
<td>2.47</td>
<td>39.7 ± 3.3</td>
</tr>
</tbody>
</table>

$^{12}\text{C}$

Structure of the Carbon – Hoyle State

\[
\begin{align*}
\langle \psi_0^+ \rangle &= 0.76 \\
\langle \psi_{0_2}^+ \rangle &= 0.71 \\
\langle \psi_{0_2}^+ \rangle &= 0.50
\end{align*}
\]
Helium Isotopes

\[ \text{soft-dipole mode} \]

neutrons are oscillating against \( \alpha \)-core
Helium Isotopes

![Graph showing binding energies and matter radii for He4, He5, He6, He7, and He8 isotopes. The graph includes data from Ozawa, Suzuki, Tanihata, NPA 693 (2001) 32; Raman, Nestor, Tikkanen, Atomic Data and Nucl. Data Tables 78 (2001) 1.](image-url)
Helium Isotopes

Beryllium Isotopes

Cluster structure changes with addition of neutrons
**Beryllium Isotopes**

**Binding energies**

- Binding energies for Be isotopes are shown with different nuclear states, such as $0^+$, $1/2^+$, and $3/2^-$.
- The plot includes data points for Be7 to Be14 isotopes.

**Matter radii**

- Matter radii are depicted for the same isotopes, showing the experimental (Exp) and theoretical (PAV, Multiconf) values.
- The radii are given in femtometers (fm).

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Exp: Ozawa, Suzuki, Tanihata, NPA 693 (2001) 32; Raman, Nestor, Tikkanen, Atomic Data and Nucl. Data Tables 78 (2001) 1

Mikroskopische Kern-Kern-Potentiale

- Vielteilchenzustände: Fermionische Molekulardynamik (FMD)
- Effektive $^\text{NN}$-Wechselwirkung: abgeleitet von der realistischen Argonne-V18 $^\text{NN}$-Wechselwirkung (UCOM)

![Diagram showing mass densities for different isotopes of oxygen](image)

$^{}_{16}\text{O}$ - $^{}_{16}\text{O}$

$^{}_{22}\text{O}$ - $^{}_{22}\text{O}$

$^{}_{24}\text{O}$ - $^{}_{24}\text{O}$
Astrophysikalischer S-Faktor

\[ S(E) = \sigma_{\text{fusion}}(E) \, E \, e^{2\pi \eta} \]

\( \eta = \) Sommerfeld-Parameter
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

7Be Phase Shift 7/2− Resonance

\[ J^\pi = 7/2^- \]

Multiconfiguration \(^3\text{He}\)

- Experimental data
- 30 frozen + \(^7\text{Be} \) PAV\( ^\pi \)
- 30 frozen configurations

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

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

\[ \gamma \text{ resonance} \]

wave function large in interior

PAV\( ^\pi \) state essential

$^7\text{Be}$ Phase Shift $5/2^-$ Resonance

Zusammenfassung und Ausblick

**Neue Ära der Kernstruktur**

- **Unitary Correlation Operator Method** beschreibt kurzreichweitige radiale und tensorielle Korrelationen

- **UCOM** erzeugt ab-initio korrelierte Wechselwirkung $\hat{H}$
  für Vielteilchenmethoden wie HF, Shalenmodell, FMD

- Observablen müssen und können auch korreliert werden

- no-core Schalenmodell Rechnungen für leichte Kerne

- **FMD** Rechnungen mit demselben $\hat{H}^{C2} + \hat{H}^{corr}$ für $3 \leq A \leq 60$

- Ein mikroskopisches Modell für:
  Bindungsenergien, Radien, Spektren, Übergänge,
  Kontinuum, Resonanzen, Reaktionen

**Ausblick**

- ”ab initio” Idee weiter verfolgen → Vorhersagekraft

- Vorhersagen für viele exotische leichte Kerne (vor Messung)

- Korrelierte Übergänge: M1, $\beta$-Zerfall, quenching

- Ab-initio korrelierte WW in HF, RPA oder ähnlichem für $A > 60$

- Langreichweitige Tensorkorr. – 3-Teilchenkräfte

- ...
Epilogue

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

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How to improve?

Projection After Variation (PAV)

- mean-field may break symmetries of Hamiltonian
- restore reflection and rotational symmetry by parity and angular-momentum projection $P_{MK}^{J\pi}$

\[
\sum_{K'} \langle Q | HP_{KK'}^{J\pi} | Q \rangle c_{K'} = E_{K}^{J\pi} \sum_{K'} \langle Q | P_{KK'}^{J\pi} | Q \rangle c_{K'}
\]

Variation After Projection (VAP)

- effect of projection can be large
- perform VAP applying constraints on radius, dipole moment, quadrupole moment or octupole moment and minimize the energy in the projected energy surface

Multiconfiguration Calculations

- diagonalize Hamiltonian in a set of projected intrinsic states

\[
\left\{ P_{KK'}^{J\pi} | Q^{(a)} \rangle, \quad a = 1, \cdots, N \right\}
\]
Two-Body Correlations

- two-body generator

\[ \tilde{C} = e^{-i\tilde{G}}, \quad G = \sum_{i<j} g_{ij} \]

Cluster Expansion

correlated operators \( \hat{A} = \tilde{C}^\dagger \tilde{A} \tilde{C} \) are no longer operators with definite particle number

- decompose correlated operator into irreducible \( k \)-body operators

\[ \hat{A} = \hat{A}^{[1]} + \hat{A}^{[2]} + \hat{A}^{[3]} + \cdots \]

Two-Body Approximation

\[ \hat{T}^{C2} = \hat{T}^{[1]} + \hat{T}^{[2]}, \quad \hat{V}^{C2} = \hat{V}^{[2]} \]

- correlation range should be smaller than mean distance of nucleons (to avoid 3-body terms)

Correlator \( \tilde{C} \) should conserve translational, rotational and Galilei invariance short ranged

Two-Body Correlations

**two-body generator**

\[ C = e^{-iG}, \quad G = \sum_{i<j} g_{ij} \]

Cluster Expansion

correlated operators \( \hat{A} = C^\dagger AC \) are no longer operators with definite particle number

**decompose correlated operator into irreducible \( k \)-body operators**

\[ \hat{A} = \hat{A}^{[1]} + \hat{A}^{[2]} + \hat{A}^{[3]} + \cdots \]

Two-Body Approximation

\[ \hat{T}^{C2} = \hat{T}^{[1]} + \hat{T}^{[2]}, \quad \hat{V}^{C2} = \hat{V}^{[2]} \]

Correlator \( \mathcal{C} \)

should conserve translational, rotational and Galilei invariance short ranged

Spin-Isospin Dependence

nuclear interaction strongly depends on spin and isospin

\[ v = \sum_{S,T} v_{ST} \Pi_{ST} \]

**different correlations in the respective channels**

\[ g = \sum_{S,T} g_{ST} \Pi_{ST} \]

**correlated interaction in two-body space**

\[ \hat{V} = \sum_{S,T} (e^{ig_{ST}} v_{ST} e^{-ig_{ST}}) \Pi_{ST} \]
Radial and Tensor Correlations

\[ C = C_\Omega C_r \]
\[ = e^{-iG_\Omega} e^{-iG_r} \]

\[ \vec{p} = \vec{p}_r + \vec{p}_\Omega \]
\[ \vec{p}_r = \frac{1}{2} \left[ \frac{\vec{r}}{r} \left( \vec{r} \vec{p} \right) + \left( \vec{p} \frac{\vec{r}}{r} \right) \frac{\vec{r}}{r} \right], \quad \vec{p}_\Omega = \frac{1}{2r} \left[ \vec{l} \times \frac{\vec{r}}{r} - \frac{\vec{r}}{r} \times \vec{l} \right] \]

Radial Correlator

\[ G_r = \frac{1}{2} \{ p_r s(r) + s(r) p_r \} \]

● probability density shifted out of the repulsive core

\[ S = 0, \quad T = 1 \]

Manfred Ristig, Z. Physik 199 (1967) 325

Radial Correlator

\[ G_r = \frac{1}{2} \{ p_r s(r) + s(r) p_r \} \]

- probability density shifted out of the repulsive core

\[ S = 0, \ T = 1 \]

Tensor Correlations

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

- tensor force admixes other angular momenta

\[ S = 1, \ T = 0 \]
Radial and Tensor Correlations

\[ C = C_\Omega C_r = e^{-iG_\Omega} e^{-iG_r} \]

\[ \tilde{p} = \tilde{p}_r + \tilde{p}_\Omega \]

\[ \tilde{p}_r = \frac{1}{2} \left\{ \frac{\tilde{r}}{r} \left( \frac{\tilde{r}}{r} \tilde{p} \right) + \left( \frac{\tilde{p}}{r} \right) \frac{\tilde{r}}{r} \right\}, \quad \tilde{p}_\Omega = \frac{1}{2r} \left[ \hat{l} \times \frac{\tilde{r}}{r} - \frac{\tilde{r}}{r} \times \hat{l} \right] \]

Radial Correlator

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

- probability density shifted out of the repulsive core

\[ S = 0, \quad T = 1 \]

Tensor Correlations

\[ \hat{\rho}(\Omega)(\sigma_2 \cdot \tilde{r}) + (\sigma_1 \cdot \tilde{r})(\sigma_2 \cdot \tilde{p}_\Omega) \]

- tensor force admixes other angular momenta

Manfred Ristig Z.Physik 199 (1967) 325
Quasi-exact calculations for light nuclei possible

exact result from PRC64 (2001) 044001

- use no-core shell model code from Petr Navratil (LLNL)
- neglected 3-body correlated terms same order as genuine 3N interactions
- more investigations needed

test of two-body approximation

E [MeV] vs. $\hbar \Omega$ [MeV] for $^4$He

MTV Interaction
No-Core Shell Model Calculations

{\[ ^3\text{He} \]}

- correlated
- bare

exact results from PRC52 (1995) 2885

{\[ ^4\text{He} \]}

- correlated
- bare

- use no-core shell model code from Pétr Navratil (LLNL)

correlations induce high-momentum components
contributions of tensor correlations very big
different correlator ranges relevant especially at the fermi surface
\[ \langle klm | \hat{H}^{[2]} | k' l' m' \rangle = i^{l''-l} M \int d^3 x \int d^3 x' Y_{lm}^*(\hat{x}) j_l(kx) \langle \hat{x} | \hat{H}^{[2]} | \hat{x}' \rangle j_{l'}(k'x') Y_{l'm'}(\hat{x}') \]

1\text{S}_0 \text{ channel}

3\text{S}_1 \text{ channel}

\[ \langle k \mid \hat{H}^{[2]} \mid k \rangle, \langle k \mid V \mid k \rangle [\text{fm}] \]

\[ \langle k \mid \hat{H}^{[2]} \mid k \rangle, \langle k \mid V \mid k \rangle [\text{fm}] \]

\[ k [\text{fm}^{-1}] \]

\[ k [\text{fm}^{-1}] \]

unique effective potential – identical to \( V_{\text{lowk}} \)

Achim Schwenk, et. al nucl-th/0108041

\[ V_{\text{lowk}} \text{ Cutoff } \Lambda = 1.0 - 2.0 \text{ fm}^{-1} \]
AV18 Interaction in Momentum Space

Off-diagonal Matrix Elements

"pre-diagonalization"

bare potential

correlated interaction
Increasing range of tensor correlator

$^3$He

$^4$He

$^{11}\text{B} \ (^{3}\text{He}, t) \ ^{11}\text{C} – \text{Gamov-Teller transitions}$

transition: $C^{-1}_\Omega \sigma \tau_+ C_\Omega$
up to now only: $\sigma \tau_+$

NCSM: Navrátil, Ormand
no core shell model with 3-body force, PRC 68(2003)
third $3/2^-$ missing

FMD with configuration mixing

Exp.: Y. Fujita, P. von Brentano et al.
Variation

\begin{tabular}{ccc}
\hline
$E_b$ [MeV] & $r_{charge}$ [fm] & $r_{matter}$ [fm] \\
\hline
PAV 1g & 99.1 & 2.52 & 2.88 \\
PAV & 105.0 & 2.49 & 2.60 \\
Exp & 110.8 & 2.70 ± 0.03 & 2.76 ± 0.06 \\
\hline
\end{tabular}

\begin{tabular}{ccc}
\hline
$E_{2+}$ [MeV] & $B(E2)$ [$e^2fm^4$] \\
\hline
PAV & 1.29 & 4.6 \\
Exp & 1.77 & 3.15 ± 0.95 \\
Global Best Fit$^1$ & 1.77 & 82 ± 14 \\
\hline
\end{tabular}

$^1$ Raman et al, Atomic Data and Nuclear Data Tables 78 (2001) 1

calculated B(E2) consistent with anomalously long lifetime of $2^+$ state measured at RIKEN
Imai et al, PRL in print


Nuclear Chart

FMD, Variation

1 Gaussian per single-particle state

correlated $AV18 + \tilde{H}^{corr}$
FMD, Variation
Nuclear Chart

Three-Nucleon Interactions from Few- to Many-Body Systems
March 12-16, 2007 at TRIUMF

1 Gaussian per single-particle state

2 Gaussians per single-particle state

(E - E_{exp}) / A [MeV]

correlated AV18 + \tilde{\hat{H}}_{corr}
Nuclear Degrees of Freedom

quarks

heavy nuclei

few nucleons

nucleon QCD

few-body systems free NN force

many-body systems effective NN force

Nuclear Degrees of Freedom

Three-Nucleon Interactions from Few- to Many-Body Systems

March 12-16, 2007 at TRIUMF

cm-coordinates and spins

⃗r_i
⃗σ_i
⃗r_j
⃗σ_j

few nucleons

quarks

 gluons

nucleon
QCD

few-body systems
free NN force

many-body systems
effective NN force