Shells, Clusters, and Halos

within Fermionic Molecular Dynamics

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Nuclear Degrees of Freedom
Realistic NN Potential

- describes phase shifts and deuteron properties
- central, spin-orbit, tensor, momentum dependent

\[ V_{NN}(r_{12}, p_{12}, \sigma_1, \sigma_2, \tau_1, \tau_2) \]

e.g.
- chiral effective field theory (pion exchange & contact terms)
- Bonn potential (pion & heavier meson exchange)
- Argonne potential (pion exchange & phenomenological short range terms)

NN scattering data

\[ ^2S+1_LJ \]
Potential and Proton Size

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

Proton charge radius $\sqrt{\langle r^2 \rangle_e} = (0.81 \cdots 0.86)$ fm
describe basic properties of nuclear many-body system
in terms of a realistic nucleon-nucleon interaction $H = \tilde{T} + \tilde{V}_{NN}$ and a many-body state $|\hat{\Psi}\rangle$

\[
\langle r_1, \sigma_1, \tau_1; r_2, \sigma_2, \tau_2; \ldots; r_A, \sigma_A, \tau_A |\hat{\Psi}\rangle
\]

 Aim

solve

\[
\tilde{H} |\hat{\Psi}_n\rangle = E_n |\hat{\Psi}_n\rangle
\]

by means of Green Function Monte Carlo Method (GFMC)
describe basic properties of nuclear many-body system
in terms of a realistic nucleon-nucleon interaction $\hat{H} = \hat{T} + \hat{V}_{NN}$ and a many-body state $|\hat{\Psi}\rangle$

$$\langle r_1, \sigma_1, \tau_1; r_2, \sigma_2, \tau_2; \ldots; r_A, \sigma_A, \tau_A |\hat{\Psi}\rangle$$

**Aim**

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

by means of Green Function Monte Carlo Method (GFMC)

GFMC result:

$|\hat{\Psi}_n\rangle$ is terribly complicated for a realistic NN-interaction.

WHY?
Radial Correlations

BECAUSE 1.) realistic interactions have short-range repulsion

- probability density of nucleons in the repulsive core strongly suppressed

\[ r = |\mathbf{r}_1 - \mathbf{r}_2| \]

potential & two-body density of $^4\text{He}$ in $S=0$, $T=1$ channel

- correlations in the relative distance of nucleons cannot be described by Slater determinants (product of single-particle states)
BECAUSE 2) tensor interaction is an essential component in any realistic interaction ➤ exchange of pions

✗ without tensor force no bound nuclei!

tensor operator

\[ s_{12} \left( \frac{\mathbf{r}}{r}, \frac{\mathbf{r}'}{r'} \right) = 3 \left( \sigma_1 \cdot \frac{\mathbf{r}}{r} \right) \left( \sigma_2 \cdot \frac{\mathbf{r}}{r} \right) - (\sigma_1 \cdot \sigma_2) \]
couples spins and the relative spatial orientation of nucleons

✗ correlations between the orientation of the spins and the relative orientation of nucleons cannot be described by Slater determinant

**Deuteron** \( S = 1, T = 0 \)
deuteron has \( L = 2 \) admixture due to tensor force

\[ \langle r \left| \hat{d} \right\rangle = \frac{\hat{u}(r)}{r} \left| L = 0 \right\rangle + \frac{\hat{w}(r)}{r} \left| L = 2 \right\rangle \]

\[ \hat{u}(r) \quad \hat{w}(r) \]

\[ \frac{1}{\sqrt{2}} \left( \left| \uparrow \downarrow \right\rangle + \left| \downarrow \uparrow \right\rangle \right) \]
Where is the problem?

- Unitary Correlation Operator Method
  realistic → correlated Hamiltonian

- Many-body states taken from Fermionic Molecular Dynamics
- Spin projektion, Configuration mixing

- Summary and Outlook
Unitary Transformation

**Unitary Transformation**

Transform eigenvalue problem

\[ \hat{H} | \hat{\Psi}_n \rangle = E_n | \hat{\Psi}_n \rangle \]

with the unitary operator \( \tilde{C} \)

\[ | \hat{\Psi}_n \rangle = \tilde{C} | \Psi_n \rangle, \quad \tilde{C}^{-1} = \tilde{C}^\dagger \]

Into the equivalent eigenvalue problem

\[ \tilde{\hat{H}} | \Psi_n \rangle = (\tilde{C}^\dagger \tilde{H} \tilde{C}) | \Psi_n \rangle = E_n | \Psi_n \rangle \]

**“pre-diagonalization”**

Include typical effects common to all states

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**Nuclear System**

The nuclear system has different scales:

- Long range (low momenta) – can be described by mean-field (Slater determinant)
- Short-range (high momenta) – cannot be described by mean-field

Include short-range correlations by unitary transformation

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Unitary correlator admixes components from outside the model space \( | \Psi_n \rangle \)

Does not project on model space
Two-Body Correlations

- two-body generator

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

Cluster Expansion

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

- decompose correlated operator into irreducible k-body operators

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

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)
Radial and Tensor Correlations

\[ C = C_\Omega C_r \]
\[ = e^{-i G_\Omega} e^{-i G_r} \]

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

Radial Correlations

\[ g_r = \frac{1}{2} \{ \text{probability density shifted out of the repulsive core} \} \]

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

\[ C = C_\Omega C_r \]
\[ = e^{-i G_\Omega} e^{-i G_r} \]

**Radial Correlator**

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

- probability density shifted out of the repulsive core

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

\[ v_c(r) \]

\[ \rho^{(2)}(r) \]

\[ [\text{fm}^{-3}] \]

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

**Tensor Correlations**

\[ g_\Omega = \frac{3}{2} \left\{ (\sigma_1 \cdot p_\Omega)(\sigma_2 \cdot r) + (\sigma_1 \cdot r)(\sigma_2 \cdot p_\Omega) \right\} \]

- tensor force admixes other angular momenta

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

\[ v^c(r) \]

\[ \rho^{(2)}(r) \]

\[ [\text{fm}^{-3}] \]

\[ r \; [\text{fm}] \]
Radial and Tensor Correlations

\[ C = C_\Omega C_r = e^{-i G_\Omega} e^{-i G_r} \]

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

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

### Radial Correlator

\[ g_r = \frac{1}{2} \{ \tilde{\rho}_r s(\mathbf{r}) + s(\mathbf{r}) \tilde{\rho}_r \} \]

- probability density shifted out of the repulsive core

### Tensor Correlations

\[ \rho^{(2)}(r) = (\mathbf{\sigma}_2 \cdot \mathbf{r}) + (\mathbf{\sigma}_1 \cdot \mathbf{r})(\mathbf{\sigma}_2 \cdot \mathbf{p}_\Omega) \]

- tensor force admixes other angular momenta

\[ \tilde{\rho}_r^{(2)}(r) = \rho^{(2)}(r) \]

\[ v_c(r) = v^c(r) \]

\[ v_t(r) = v_t(r) \]

\[ \hat{\rho}_L(2)(r) = \hat{\rho}_L(2)(r) \]

\[ \hat{\rho}_{L=0}(2)(r) = \hat{\rho}_{L=0}(2)(r) \]

\[ \hat{\rho}_{L=2}(2)(r) = \hat{\rho}_{L=2}(2)(r) \]
Correlations in Nuclei

\[ \rho_{S,T}^{(2)}(r_1 - r_2) \quad S = 1, M_S = 1, T = 0 \]

- radial correlator shifts density out of the repulsive core
- tensor correlator aligns density with spin orientation

- both radial and tensor correlations are essential for binding
Fermionic Molecular Dynamics

Fermionic
Slater determinants

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

\[ \text{antisymmetrized } A\text{-body state} \]

Molecular
Gaussian wave packets for single-particle states

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

Dynamics
Variational principle

\[ \delta \int dt \frac{\langle Q | C^\dagger \left[ i \frac{d}{dt} - H \right] C | Q \rangle}{\langle Q | Q \rangle} = 0 \]

Interaction

\[ \hat{H}^{\text{eff}} = \hat{H}^{C^2} + \hat{H}^{\text{corr}} \]

\[ \hat{H}^{C^2} = \left[ C^\dagger H C \right]^{C^2} \]

\[ \hat{H}^{\text{corr}} \text{ – correlated ab-initio interaction in two-body approximation} \]

\[ \hat{H}^{\text{corr}} \text{ – momentum and spin-orbit two-body correction adjusted on doubly magic nuclei} \]

\[ \textbullet \text{ corrects for missing 3-body correlations and genuine 3-body forces} \]

\[ \text{strength } \approx 15\% \text{ of ab-initio potential} \]

Variation

minimize \( \langle Q | \hat{H}^{\text{eff}} | Q \rangle \) by variation of the parameters of the single-particle states
FMD, Variation
Nuclear Chart

1 Gaussian per single-particle state

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

Nuclear Chart

1 Gaussian per single-particle state

correlated $\Delta V18 + \hat{H}_{corr}$

2 Gaussians per single-particle state
Selected nuclei - one-body density of intrinsic states

\[ \rho^{(1)}(r) \] 

\begin{align*}
\text{He}^4 & \quad \text{C}^{12} & \quad \text{O}^{16} \\
\text{Ne}^{20} & \quad \text{Mg}^{24} & \quad \text{Ca}^{40}
\end{align*}

spherical nuclei

intrinsically deformed nuclei
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 $P^{J^z}_{MK}$

$$\sum_{K'} \langle Q | H P^{J^z}_{KK'} | Q \rangle \cdot c_{K'} = E^J_K \sum_{K'} \langle Q | P^{J^z}_{KK'} | Q \rangle \cdot c_{K'}$$

**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

$$\left\{ P^{J^z}_{KK'} | Q^{(a)} \rangle, \quad a = 1, \ldots, N \right\}$$
Radius and Quadrupole Moment as Generator Coordinates

<table>
<thead>
<tr>
<th></th>
<th>$r_{charge}$ [fm]</th>
<th>$Q$ [fm$^2$]</th>
<th>$B(E2)$ [$e^2$fm$^4$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAV</td>
<td>2.39</td>
<td>-6.25</td>
<td>9.31</td>
</tr>
<tr>
<td>VAP</td>
<td>2.49</td>
<td>-8.02</td>
<td>15.36</td>
</tr>
<tr>
<td>Multiconfig</td>
<td>2.74</td>
<td>-11.88</td>
<td>30.39</td>
</tr>
</tbody>
</table>

$8^Be$
12C

### Energies and Radii

<table>
<thead>
<tr>
<th></th>
<th>$E_b$ [MeV]</th>
<th>$r_{charge}$ [fm]</th>
<th>$B(E2)$ [$e^2fm^4$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>V/PAV</td>
<td>84.7</td>
<td>2.33</td>
<td>-</td>
</tr>
<tr>
<td>VAP</td>
<td>91.9</td>
<td>2.38</td>
<td>24.7</td>
</tr>
<tr>
<td>Multiconfig</td>
<td>93.4</td>
<td>2.50</td>
<td>40.0</td>
</tr>
<tr>
<td>Exp</td>
<td>92.2</td>
<td>2.47</td>
<td>39.7 ± 3.3</td>
</tr>
</tbody>
</table>

### Energy Levels

- **VAP**
  - $0^+_1$
  - $3^-_1$

- **Multiconfig**
  - $0^+_2$
  - $0^+_3$
  - $0^+_4$

- **Exp**
  - $0^+_1$
  - $0^+_2$
  - $0^+_3$
  - $1^-$
  - $2^-$
He Isotopes - Variation After Projection (VAP)

\[ y \text{ [fm]} \]
\[ x \text{ [fm]} \]
\[ r \text{ [fm]} \]
\[ \rho(r) \]
He Isotopes - Variation After Projection (VAP)
He Isotopes - Variation After Projection (VAP)
He Isotopes - Variation After Projection (VAP)

\[ \rho(r) = \rho_0 \]

\[ 4 \text{ He} \]

\[ 6 \text{ He} \]

\[ 7 \text{ He} \]

\[ 8 \text{ He} \]

\[ \text{quadrupole} \]

\[ \text{dipole} \]
He Isotopes - PAV, VAP, Multiconfig

ground state energies

-25.0
-26.0
-27.0
-28.0
-29.0
-30.0
-31.0
-32.0

[MeV]

4He 5He 6He 7He 8He

PAV VAP Multiconf Experiment

quadrupole
dipole
\[ E_b \text{ [MeV]} \quad r_{\text{charge}} \text{ [fm]} \quad r_{\text{matter}} \text{ [fm]} \]

<table>
<thead>
<tr>
<th></th>
<th>( E_b )</th>
<th>( r_{\text{charge}} )</th>
<th>( r_{\text{matter}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAV 1g</td>
<td>99.1</td>
<td>2.52</td>
<td>2.88</td>
</tr>
<tr>
<td>PAV</td>
<td>105.0</td>
<td>2.49</td>
<td>2.60</td>
</tr>
<tr>
<td>Exp</td>
<td>110.8</td>
<td>2.70 ± 0.03</td>
<td>2.76 ± 0.06</td>
</tr>
</tbody>
</table>

\[ E_{2^+} \text{ [MeV]} \quad B(E2) \text{ [e}^2\text{fm}^4] \]

<table>
<thead>
<tr>
<th></th>
<th>( E_{2^+} )</th>
<th>( B(E2) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAV</td>
<td>1.29</td>
<td>4.6</td>
</tr>
<tr>
<td>Exp</td>
<td>1.77</td>
<td>3.15 ± 0.95</td>
</tr>
<tr>
<td>Global Best Fit(^1)</td>
<td>1.77</td>
<td>82 ± 14</td>
</tr>
</tbody>
</table>

\(^1\) Raman \emph{et al}, Atomic Data and Nuclear Data Tables 78 (2001) 1

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\( \Rightarrow \) calculated \( B(E2) \) consistent with anomalously long lifetime of \( 2^+ \) state measured at RIKEN

Imai \emph{et al}, PRL in print
FMD

Be Isotopes - Proton, Neutron Densities
Summary and Outlook

**Unitary Correlation Operator Method**
- describes short ranged central and tensor correlations

**UCOM** provides ab-initio correlated interaction $\hat{H}^{C2}$
- for many-body methods like HF, shell model, FMD

**Observables must and can be correlated as well**
- Feldmeier, Neff, Roth, Schnack, NP A632 (1998) 61
- Neff, Feldmeier, NP A713 (2003), 311

**FMD** Calculations with the same $\hat{H}^{C2} + \hat{H}^{corr}$ for $3 \leq A \leq 60$

**Projection, configuration mixing** → masses, radii, spectra, transitions

**Outlook**
- Predictions for many exotic light nuclei (before measurement)
- Correlated transitions: M1, $\beta$-decay, quenching
- Resonances, width of many-body states
- Ab-initio correlated interaction in HF, RPA or similar for $A > 60$
- Long ranged tensor correlations. – 3-body forces – $\hat{H}^{corr}$

Dr. T. Neff, A. Cribeiro, Prof. R. Roth, H. Hergert
GFMC calculations

![Diagram showing energy levels of various nuclei and reaction channels.](image)

Wiringa, Pieper, PRL 89 (2002) 182501

- genuine three-body forces (IL2) needed for description of real nuclei
MTV Interaction
No-Core Shell Model Calculations

$^3\text{He}$

- Correlated
- Bare

$^4\text{He}$

- Correlated
- Bare

Exact results from PRC52 (1995) 2885

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

Only radial correlations
Nucleon Momentum Distributions

Other Observables

Bonn-A

\[
\hat{n}(k) / A = A \left[ \text{fm}^3 \right] 
\]

Argonne V18

\[
\hat{n}(k) / A = A \left[ \text{fm}^3 \right] 
\]

- correlations induce high-momentum components
- contributions of tensor correlations very big
- different correlator ranges relevant especially at the fermi surface
Interaction in Momentum Space

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

1\(S_0\) channel

- Uncorrelated
- Correlated

3\(S_1\) channel

- Unique effective potential – identical to \(V_{\text{lowk}}\)
  Kuo, Schwenk, nucl-th/0108041

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

Off-diagonal Matrix Elements

\[
\langle \frac{1}{2} S_0; k \mid V \mid \frac{1}{2} S_0; k' \rangle
\]

bare potential

\[
\langle \frac{3}{2} S_1; k \mid V \mid \frac{3}{2} D_1; k' \rangle
\]

correlated interaction

\[
\langle \frac{1}{2} S_0; k \mid \hat{H}^{[2]} \mid \frac{1}{2} S_0; k' \rangle
\]

\[
\langle \frac{3}{2} S_1; k \mid \hat{H}^{[2]} \mid \frac{3}{2} D_1; k' \rangle
\]
Increasing range of tensor correlator

\( ^3\text{He} \)

\( ^4\text{He} \)

CCT/CHICSi/GSI - May 25, 2004
$^{11}\text{B}$ ($^{3}\text{He}, t$) $^{11}\text{C}$ – Gamov-Teller transitions

transition: $\sigma \cdot \tau_+$

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 Bretano et al. to be published
Silizium - Einteilchendichte des intrinsischen Zustands

Variation → rund

Erdnuss lokales Minimum vor Projektion ca. 5 MeV höher als rund

Ufo vor Projektion ca. 10 MeV höher als rund