Nuclear Structure with Correlated Realistic NN-Interactions

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Overview

Unitary Correlation Operator Method
- Central and Tensor correlations
- Correlated Interaction
- *ab initio* calculations

Fermionic Molecular Dynamics
- PAV, VAP and Multiconfiguration
- Helium, Beryllium, Carbon isotopes, $^{12}$C
- Resonances and Scattering States
Realistic and Effective Nucleon-Nucleon Interactions

Realistic Interactions

- reproduce scattering data and deutron properties
- meson-exchange (Bonn), phenomenological (AV18), $\chi$-PT (Idaho)
- **repulsive core** and **tensor force** induce **strong short-range correlations**
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Effective Interactions

- phenomenological effective interactions describe many properties of nuclear systems like energies, radii, spectra successfully using simple many-body wave functions (HF, shell model, microscopic cluster models)
- No-Core Shell Model uses Lee-Suzuki transformation in oscillator basis
- $G$-matrix and $V_{lowk}$ derive effective interaction in momentum space
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Our approach

- derive effective interaction from realistic interaction by explicitly including correlations with unitary correlation operator $\hat{C}$ formulated in coordinate space
- correlated (effective) interaction

$$\hat{H} = \hat{C}^\dagger \hat{H} \hat{C}$$
**Correlation Operator**

- induce short-range (two-body) central and tensor correlations into the many-body state

\[
\mathcal{C} = \mathcal{C}_\Omega \mathcal{C}_r = \exp[-i \sum_{i<j} g_{\Omega,ij}] \exp[-i \sum_{i<j} g_{r,ij}] \quad , \quad \mathcal{C}^\dagger \mathcal{C} = 1
\]

- correlation operator should conserve the symmetries of the Hamiltonian and should be of finite-range, **phase shift equivalent** to bare interaction by construction

**Correlated Operators**

- correlated operators will have contributions in higher cluster orders

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

- two-body approximation: correlation range should be small compared to mean particle distance

**Correlated Interaction**

\[
\mathcal{C}^\dagger (\mathcal{T} + \mathcal{V}) \mathcal{C} = \mathcal{T} + \mathcal{V}_{\text{UCOM}} + \mathcal{V}^{[3]}_{\text{UCOM}} + \ldots
\]
Central Correlations

- radial distance-dependent shift in the relative coordinate of each nucleon pair

\[ g_r = \frac{1}{2} \left[ p_r s(r) + s(r) p_r \right], \quad p_r = \frac{1}{2} [\mathbf{p} \cdot \mathbf{r} + \mathbf{r} \cdot \mathbf{p}] \]

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

\[ p_r = \frac{1}{2} [\mathbf{p} \cdot \mathbf{r} + \mathbf{r} \cdot \mathbf{p}] \]

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

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

\[ V^{c}(r) \]

\[ S = 0, T = 1 \]
• **angular shift in the relative coordinate** of each nucleon pair depending on the orientation of the spins

\[
\varrho_{\Omega} = \varrho(r)\left[\frac{3}{2}(\sigma_1 \cdot p_\Omega)(\sigma_2 \cdot r) + \frac{3}{2}(\sigma_1 \cdot r)(\sigma_2 \cdot p_\Omega)\right], \quad p_\Omega = p - r p_r
\]

\[S = 1, T = 0\]
Determine Correlation Functions

Central Correlations

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

$$\min_{s(r),\vartheta(r)} \langle \phi_{\text{trial}}^{ST} \mid C_r^+ \tilde{C}_\Omega H \tilde{C} \Omega C_r \mid \phi_{\text{trial}}^{ST} \rangle$$

- correlation functions depend only weakly on the trial wave function

- restrict the range of the tensor correlations in the $S = 1, T = 0$ channel (parameter $I_\vartheta$)

Tensor Correlations
Correlated Two-Body Densities and Energies

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

- central correlator \(C_r\) shifts density out of the repulsive core
- tensor correlator \(C_\Omega\) aligns density with spin orientation

both central and tensor correlations are essential for binding

\[ \langle T \rangle \]
\[ \langle H \rangle \]
\[ \langle V \rangle \]

Correlated Interaction in Momentum Space

$^3S_1$ bare

$^3S_1 - ^3D_1$ bare

correlated interaction is more attractive at low momenta

$^3S_1$ correlated

$^3S_1 - ^3D_1$ correlated

off-diagonal matrix elements connecting low- and high-momentum states are strongly reduced

Correlated AV18 Interaction in Momentum Space

Bogner, Kuo, Schwenk, Phys. Rept. 386 (2003) 1
use Jacobi-coordinate NCSM code by Petr Navrátil for $^3$He and $^4$He (don’t use Lee-Suzuki transformation)

- dramatically **improved convergence** compared to bare interaction

- **does not converge to exact result for bare interaction** due to omitted higher order terms $V^{[3]}_{UCOM}$, ...

- study the effect of higher order contributions as a function of tensor correlation range $I_8$. 
• choose tensor correlation range \( I_\vartheta = 0.09 \) such that need for three-body forces is minimized

**different perspective**: don't try to reproduce the results of the bare interaction but consider \( V_{\text{UCOM}} \) as a realistic potential to describe experiment
HF and MBPT calculations

Additional attraction mainly by medium to long range tensor forces

Long-range correlations appear to be perturbative

Spherical Hartree-Fock in 12 $\hbar\omega$ harmonic oscillator basis
• NCSM calculations with “bare” $V_{UCOM}$ and Lee-Suzuki effective interaction derived from $V_{UCOM}$ show consistent convergence pattern

• Binding energy close to experiment

• Spectra with $V_{UCOM}$ are of similar quality than with other modern NN forces
• correct level ordering without three-body forces
• binding energy close to experiment

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

calculations by Petr Navrátil
Fermionic Molecular Dynamics

Fermionic

Slater determinant

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

- antisymmetrized \( A \)-body state

Molecular

single-particle states

\[ \left< x \left| q \right> = \sum_i c_i \exp \left\{ -\frac{(x - b_i)^2}{2a_i} \right\} \otimes \left| \chi^{\uparrow}_i, \chi^{\downarrow}_i \right> \otimes \left| \xi \right> \]

- Gaussian wave-packets in phase-space (complex parameter \( b_i \) encodes mean position and mean momentum), spin is free, isospin is fixed
- width \( a_i \) is an independent variational parameter for each wave packet
- superposition of two wave packets for each single particle state
Perform Variation

Minimization

- minimize Hamiltonian expectation value with respect to all single-particle parameters $q_k$

$$
\min_{\{q_k\}} \frac{\langle Q | \hat{H} - T_{cm} | Q \rangle}{\langle Q | Q \rangle}
$$

- this is a Hartree-Fock calculation in our particular single-particle basis
- the mean-field may break the symmetries of the Hamiltonian

16O  40Ca  20Ne  27Al

spherical nuclei  intrinsically deformed nuclei
\[ \tilde{C}^\dagger (T + V) \tilde{C} = \tilde{T} \]

- **one-body kinetic energy**

\[ + \sum_{ST} \hat{V}^{ST}_c (r) + \frac{1}{2} \left( p_{\tilde{r}}^2 \hat{V}^{ST}_{p^2} (r) + \hat{V}^{ST}_{p^2} (r) p_{\tilde{r}}^2 \right) + \hat{V}^{ST}_p (r) \tilde{l}^2 \]

- **central potentials**

\[ + \sum_{T} \hat{V}^T_{ls} (r) \tilde{l} \cdot \tilde{s} + \hat{V}^T_{p^2ls} (r) \tilde{l}^2 \tilde{l} \cdot \tilde{s} \]

- **spin-orbit potentials**

\[ + \sum_{T} \hat{V}^T_i (r) S_{12} (r, r) + \hat{V}^T_{trp\Omega} (r) p_r S_{12} (r, p\Omega) + \hat{V}^T_{ll} (r) S_{12} (l, l) + \]

\[ \hat{V}^T_{lp\Omega p\Omega} (r) S_{12} (p\Omega, p\Omega) + \hat{V}^T_{p^2lp\Omega p\Omega} (r) \tilde{l}^2 S_{12} (p\Omega, p\Omega) \]

- **tensor potentials**

**bulk of tensor force mapped onto central part of correlated interaction**

**tensor correlations also change the spin-orbit part of the interaction**

\[ \text{Nucl. Phys. A745 (2004) 3} \]
Effective two-body interaction

- FMD model space can’t describe correlations induced by residual medium-long ranged tensor forces
- use longer ranged tensor correlator to partly account for that
- add phenomenological two-body correction term with a momentum-dependend central and (isospin-dependend) spin-orbit part
- fit correction term to binding energies and radii of “closed-shell” nuclei ($^4$He, $^{16}$O, $^{40}$Ca), ($^{24}$O, $^{34}$Si, $^{48}$Ca)

-> develop a new correction term that is checked against (small scale) No-Core Shell Model calculations

Projected tetrahedral configurations are about 6 MeV lower in energy than “closed-shell” configurations
1 Gaussian per single-particle state
PAV, VAP and Multiconfiguration

Projection After Variation (PAV)
- mean-field may break symmetries of Hamiltonian
- restore inversion, translational and rotational symmetry by projection on parity, linear and angular momentum

\[ P^p = \frac{1}{(2\pi)^3} \int d^3X \exp\{-i(P - P) \cdot X\} \]

Variation After Projection (VAP)
- effect of projection can be large
- perform Variation after Parity Projection \( \text{VAP}^\pi \)
- perform VAP in GCM sense by applying constraints on radius, dipole moment, quadrupole moment or octupole moment and minimize the energy in the projected energy surface

▶ investigate “real” VAP

Multiconfiguration Calculations
- diagonalize Hamiltonian in a set of projected intrinsic states

\[ \sum_{K'b} \langle Q^{(a)} | H_{KK'}^{\pi} P^{P=0} | Q^{(b)} \rangle \cdot c_{K'b}^{(i)} = \]

\[ E_{J}^{\pi} \sum_{K'b} \langle Q^{(a)} | P_{KK'}^{J} P^{P=0} | Q^{(b)} \rangle \cdot c_{K'b}^{(i)} \]
- intrinsic nucleon densities of VAP states
- radial densities from multiconfiguration calculations
Helium Isotopes

Binding energies

Matter & charge radii

Beryllium Isotopes

- intrinsic densities of $V_{\pi}$ states

cluster structure evolves with addition of neutrons
Beryllium Isotopes

quadrupole constraints

Binding energies

Matter & charge radii
Beryllium Isotopes

quadrupole constraints

Binding energies

\[ \begin{align*}
\text{Be}_7 &: 2.2 \\
\text{Be}_8 &: 2.4 \\
\text{Be}_9 &: 2.6 \\
\text{Be}_{10} &: 2.8 \\
\text{Be}_{11} &: 3.0 \\
\text{Be}_{12} &: 3.2 \\
\text{Be}_{13} &: 3.4 \\
\text{Be}_{14} &: 3.6
\end{align*} \]

\[ \text{[MeV]} \]

strong \( \alpha + {^3}\text{He} \) and \( \alpha + \alpha \) cluster contributions

borromean system

Matter & charge radii

\[ \text{[fm]} \]

positive parity state coming down
Carbon Isotopes

- intrinsic densities of $V^\pi$ states
Cluster vs. Shell structure

$^{12}$C

radius and octupole constraints

<table>
<thead>
<tr>
<th>$E_b$ [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>
</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>Multiconfig</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>

$V^\pi/PAV^\pi$

Multi-config
excited $0^+$ and $2^+$ states

$^{12}\text{C}$

quadrupole and octupole constraints

$0^+_2$ state

$\langle \cdot | 0^+_2 \rangle = 0.76$ $\langle \cdot | 0^+_2 \rangle = 0.71$ $\langle \cdot | 0^+_2 \rangle = 0.50$

$0^+_3$ state

$\langle \cdot | 0^+_3 \rangle = 0.69$ $\langle \cdot | 0^+_3 \rangle = 0.65$ $\langle \cdot | 0^+_3 \rangle = 0.44$

<table>
<thead>
<tr>
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<th>Experiment</th>
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</tr>
<tr>
<td>$r_{\text{charge}}$ [fm]</td>
<td>2.52</td>
<td>2.47</td>
</tr>
<tr>
<td>$B(E2) (0^+_1 \rightarrow 2^+_1)$ [e^2fm^4]</td>
<td>42.9</td>
<td>39.7 ± 3.3</td>
</tr>
<tr>
<td>$M(E0) (0^+_2 \rightarrow 0^+_3)$ [fm^2]</td>
<td>5.67</td>
<td>5.5 ± 0.2</td>
</tr>
<tr>
<td>$r_{\text{rms}} (0^+_1)$ [fm]</td>
<td>2.38</td>
<td></td>
</tr>
<tr>
<td>$r_{\text{rms}} (0^+_2)$ [fm]</td>
<td>3.42</td>
<td></td>
</tr>
<tr>
<td>$r_{\text{rms}} (0^+_3)$ [fm]</td>
<td>3.85</td>
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<td>$r_{\text{rms}} (2^+_1)$ [fm]</td>
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<tr>
<td>$r_{\text{rms}} (2^+_2)$ [fm]</td>
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<tr>
<td>$r_{\text{rms}} (2^+_3)$ [fm]</td>
<td>3.63</td>
<td></td>
</tr>
<tr>
<td>$Q(2^+_1)$ [e_fm^2]</td>
<td>5.85</td>
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<tr>
<td>$Q(2^+_2)$ [e_fm^2]</td>
<td>-23.65</td>
<td></td>
</tr>
<tr>
<td>$Q(2^+_3)$ [e_fm^2]</td>
<td>5.89</td>
<td></td>
</tr>
</tbody>
</table>
Aim: Microscopic description of $^3\text{He}(\alpha,\gamma)^7\text{Be}$

- GCM states with FMD states for $^3\text{He}$ and $^4\text{He}$ like in a microscopic cluster model for the description of the asymptotic behaviour
- use FMD states for $^7\text{Be}$ in the interaction region

Matching to the asymptotic solution

- for scattering and resonance states we have to implement boundary conditions by matching to the Coulomb solution of two point-like nuclei
- in the GCM Slater determinants the relative motion of the clusters, the internal wave functions of the clusters and the center-of-mass wave function are entangled
- if the widths of all Gaussians are equal the relative motion of the two nuclei and the center of mass wave function can be given analytically
- in the FMD we use a projection on total linear momentum to get rid of the center of mass problem and introduce a collective variable representation to access the relative wave function
Size measure

- Operator $\tilde{B}$ measures the size of the system
  
  $$\tilde{B} = \frac{1}{A^2} \sum_{i<j} (\tilde{x}(i) - \tilde{x}(j))^2$$

- Diagonalize in the space of the cluster configurations, eigenvalues relate to relative distance in the asymptotic region
  
  $$\tilde{B} |\beta\rangle = |\beta\rangle \Rightarrow \beta(r) = \frac{A_1 A_2}{A^2} r^2 + \beta_1 + \beta_2$$

- Evaluate $\langle \beta | [H, B]^s | \Psi\rangle$ in many-body and two-body world to get boundary conditions

- Match to outgoing Coulomb (Resonances) or Coulomb scattering solutions and solve non-linear eigenvalue problem
first steps towards microscopic and consistent description of structure and reactions
Microscopic Nucleus-Nucleus Potentials

- use GCM wave function

\[ | \Psi_J^M(R) \rangle = p_J^M \mathcal{A} \left( | x\text{O}; \frac{1}{2} R \rangle | x\text{O}; -\frac{1}{2} R \rangle \right) \]

- transform into RGM wave function to get rid of center-of-mass

- fit a local equivalent potential to the RGM potential surface (diagonalize the RGM norm kernel)

- solve two-body Schrödinger equation for all \( l \) with Incoming Wave Boundary Condition

- calculate and sum the penetration probabilities to calculate the fusion cross section

\[ S(E) = \sigma(E) E e^{2\pi\eta} \]

**Pycnonuclear reactions** in the crust of neutron stars
Summary

Unitary Correlation Operator Method

- explicit description of short-range central and tensor correlations
- phase-shift equivalent correlated interaction $V_{\text{UCOM}}$
- $V_{\text{UCOM}}$ used in HF+MBPT and first NCSM calculations

Fermionic Molecular Dynamics

- Structure of light nuclei
- Halos and clustering
- First steps in calculating resonances, scattering states and reactions
• A. Cribeiro, **H. Feldmeier**, K. Langanke  
  GSI Darmstadt

• H. Hergert, N. Paar, P. Papakonstantinou, **R. Roth**  
  Institut für Kernphysik, TU Darmstadt

• B.A. Brown  
  NSCL, Michigan State University