From Shell-Structure to Clusters and Halos

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Overview

Nucleon Nucleon Interaction
- Central and Tensor correlations
- Correlated Interaction
- \textit{ab initio} calculations

Fermionic Molecular Dynamics
- PAV, VAP and Multiconfiguration

Applications
- Helium, Lithium, Beryllium, Carbon isotopes, $^{12}\text{C}$

Outlook
- Molecular resonances, nucleus nucleus potentials
- Spectroscopic amplitudes and spectroscopic factors
Realistic Interactions

- reproduce scattering data and deuteron properties
- meson-exchange (Bonn), phenomenological (Argonne), $\chi$-PT
- repulsive core and tensor force induce strong short-range correlations in many-body state
- directly used only in Few-body Models and GFMC

Effective Interactions

- with effective interactions many properties of nuclear systems like energies, radii, spectra can be described successfully with simple many-body wave functions (HF, shell model, microscopic cluster models)
- in the No-Core Shell Model the Lee-Suzuki transformation is used to derive an effective interaction from realistic interactions

**Ansatz**

derive **effective interaction** from **realistic interaction**

by explicitly including correlations with **unitary correlation operator** $\mathcal{C}$ formulated in coordinate space

correlated interaction

$$\tilde{H} = \mathcal{C}^\dagger H \mathcal{C}$$

is evaluated in two-body approximation of cluster expansion
Realistic Interactions

- reproduce scattering data and deuteron properties
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Correlator $\mathcal{C}$

conserves translational, rotational and Galilei invariance

is of finite range and preserves the phase shifts
Central and Tensor Correlations

\[ C = C_\Omega C_r \]

**Central Correlations**

\[ C_r = \exp \left\{ -\frac{i}{2} \left[ \hat{p}_r s(r) + s(r) \hat{p}_r \right] \right\} \]

- probability density shifted out of the repulsive core

**Tensor Correlations**

\[ C_\Omega = \exp \left\{ -i \delta(r) \left[ \frac{3}{2} (\sigma_1 \cdot \hat{p}_\Omega)(\sigma_2 \cdot \hat{r}) + \frac{3}{2} (\sigma_1 \cdot \hat{r})(\sigma_2 \cdot \hat{p}_\Omega) \right] \right\} \]

- tensor force admixes other angular momenta

### Diagrams

**S = 0, T = 1**

- \( \rho^{(2)}(r) \)
- \( \rho'(r) \)
- \( V(r) \)

**S = 1, T = 0**

- \( \hat{\rho}^{(2)}(r) \)
- \( \hat{\rho}'(r) \)
- \( \hat{V}(r) \)
Central and Tensor Correlations

Central Correlations
\[ \zeta_r = \exp \left\{ -\frac{i}{2} \{ p_s(r) + s(r)p_r \} \right\} \]
probability density shifted out of the repulsive core

Tensor Correlations
\[ \zeta_\Omega = \exp \left\{ -i \vartheta(r) \left[ \frac{3}{2} (\sigma_1 \cdot \Omega)(\sigma_2 \cdot r) + \frac{3}{2} (\sigma_1 \cdot r)(\sigma_2 \cdot \Omega) \right] \right\} \]
tensor force admixes other angular momenta

\[ p_r = \frac{1}{2} \left\{ \frac{r}{r} (\vec{r} \cdot p) + \left( \frac{p_r^2}{r^2} \right) \frac{\vec{r}}{r^2} \right\}, \quad p_\Omega = \frac{1}{2\pi} \left\{ \vec{1} \times \frac{\vec{r}}{r^2} - \frac{\vec{r}}{r^2} \times \vec{1} \right\} \]
Correlated Two-Body Densities and Energies

\[ \rho_{S,\ell}^{(2)}(\mathbf{r}_1 - \mathbf{r}_2) \quad S = 1, M_S = 1, T = 0 \]

**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

Correlated AV18 Interaction in Momentum Space

Off-diagonal Matrix Elements

- correlated interaction is more attractive at low momenta
- off-diagonal matrix elements connecting low- and high-momentum states are strongly reduced
- correlated interaction is similar to $V_{\text{low } k}$
  Bogner, Kuo, Schwenk,

No-Core Shell Model Calculations

Tjon Line

fix range of tensor correlations in the 3- and 4-body system to reproduce observed binding energies for this range three-body forces and three-body contributions of the correlated interaction cancel mostly.
ab initio Many-Body calculations

Hartree-Fock plus Many-body Perturbation theory for spherical nuclei

Additional attraction mainly by medium to long range tensor forces appears to be a global effect.

working on No-Core Shell Model calculations using Antoine and Oxbash
Operator Representation of $V_{UCOM}$

\[ \zeta^T(T + V)\zeta = T \]

\[ + \sum_{ST} \hat{V}^{ST}_c(r) + \frac{1}{2}(p_r^2 \hat{V}^{ST}_{p^2}(r) + \hat{V}^{ST}_{p^2}(r)p_r^2) + \hat{V}^{ST}_{p^2}(r)\mathbf{l}^2 \]

\[ + \sum_T \hat{V}^T_{ls}(r)\mathbf{l} \cdot \mathbf{s} + \hat{V}^T_{P\Omega l}(r)\mathbf{l}^2\mathbf{1} \cdot \mathbf{s} \]

\[ + \sum_T \hat{V}^T_{t}(r)S_{12}(r, r) + \hat{V}^T_{tr\Omega}(r)p_r S_{12}(r, p\Omega) + \hat{V}^T_{tl\Omega}(r)S_{12}(l, 1) + \]

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

- bulk of tensor force mapped onto central part of correlated interaction
- tensor correlations also change the spin-orbit part of the interaction

Fermionic Molecular Dynamics

**Fermionic**
Slater determinant

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

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

**Molecular**

single-particle states

\[ \langle x | q \rangle = \sum_i c_i \exp \left\{ -\frac{(x - b_i)^2}{2a_i} \right\} \otimes |\chi_{i}^{\uparrow}, \chi_{i}^{\downarrow}\rangle \otimes |\xi\rangle \]

\[ \Rightarrow \text{Gaussian wave-packets in phase-space, spin is free, isospin is fixed} \]

width of wave-packet is a variational parameter

superposition of two wave-packets helps especially for halo nuclei

**Dynamics**

Time-dependent variational principle

\[ \delta \int dt \frac{\langle Q | \frac{d}{dt} \hat{H} | Q \rangle}{\langle Q | Q \rangle} = 0 \]

Perform Variation

Minimization

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

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

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

Spherical nuclei

Intrinsically deformed nuclei
**Effective two-body interaction**

- FMD model space can’t describe correlations induced by medium-ranged tensor forces
- simulate by *momentum-dependend* central and (isospin-dependend) *spin-orbit* two-body correction term
- fit correction term to binding energies and radii of “closed-shell” nuclei \((^4\text{He}, ^{16}\text{O}, ^{40}\text{Ca}), (^{24}\text{O}, ^{34}\text{Si}, ^{48}\text{Ca})\)
- develop a new correction term that is fixed in 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

\[(E - E_{\text{exp}})/A \text{ [MeV]}\]
How to improve?

Projection After Variation (PAV)

- mean-field may break symmetries of Hamiltonian
- restore inversion, translational and rotational symmetry by projection on parity, linear momentum and angular-momentum

Variation After Projection (VAP)

- effect of projection can be large
- perform Variation after Parity Projection VAP\(\Pi\)
- perform VAP by 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

\[ \sum_{K'b} \braket{Q^{(a)}}{H\mathcal{P}^{0}_{KK'}\mathcal{P}^{P=0}}{Q^{(b)}} \cdot \zeta^{(i)}_{K'b} = \]

\[ E^{(i)} \sum_{K'b} \braket{Q^{(a)}}{\mathcal{P}^{P=0}}{Q^{(b)}} \cdot \zeta^{(i)}_{K'b} \]
Helium Isotopes

dipole and quadrupole constraints

intrinsic nucleon densities of VAP states
radial densities from multiconfiguration calculations
Helium Isotopes

Binding energies

Matter & charge radii

Helium Isotopes

![Graph showing binding energies and radii for helium isotopes.]

- **Binding energies**
  - PAV\(^\pi\)
  - Multiconfig
  - Experiment

- **Matter & charge radii**
  - Important zero-point oscillations of the soft-dipole mode for describing binding energies and radii.

- **Notation**:
  - He\(^4\)
  - He\(^5\)
  - He\(^6\)
  - He\(^7\)
  - He\(^8\)

- **Remarks**:
  - Zero-point oscillations are essential for the description of binding energies and radii.

- **References**:

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Lithium Isotopes

quadrupole constraints

intrinsic densities of $V^\pi$ states
Lithium Isotopes

with cm-projection

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**Binding energies**

![Graph showing binding energies for different lithium isotopes with various spin states, including \( ^{3/2} \), \( ^{1/2} \), and \( ^{1} \).]

**Matter & Charge radii**

![Graph showing matter and charge radii for different lithium isotopes, with charge radii shifted by 0.5 fm.]

Lithium Isotopes

 Binding energies

 strong $\alpha + d$ and $\alpha + t$ cluster contributions

 Matter & Charge radii

 $\alpha$ and $d$ contributions

 $\alpha$ and $t$ contributions

 $^9$Li-core plus neutrons


Lithium Isotopes

with cm-projection

**Binding energies**

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

**Magnetic moments**

- $\mu_N$

**Quadrupole moments**

- $e^2 fm^4$

Isotopes:
- Li5
- Li6
- Li7
- Li8
- Li9
- Li10
- Li11

**Binding energies**

- $^{2+}$
- $^{3/2-}$

**Magnetic moments**

- $^{1+}$
- $^{2+}$

**Quadrupole moments**

- $^{1+}$
- $^{3/2-}$

**Notes:**
- Lithium isotopes and their respective binding energies, magnetic moments, and quadrupole moments are shown with projections for $P_{AV}^s$, Multiconf, and Exp.
- The diagram highlights the strong contributions of $\alpha + d$ and $\alpha + t$ clusters in the binding energies.
Beryllium Isotopes

Intrinsic densities of $V^{\pi}$ states evolve with addition of neutrons.
Beryllium Isotopes

quadrupole constraints

Binding energies

Matter & charge radii

[MeV]

[fm]

2.2
2.4
2.6
2.8
3.0
3.2
3.4

Be7
Be8
Be9
Be10
Be11
Be12
Be13
Be14

20
Beryllium Isotopes

quadrupole constraints

Binding energies

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

borromean system

Matter & charge radii

positive parity state coming down

PAV$^*$
Multiconf
Exp

Be7
Be8
Be9
Be10
Be11
Be12
Be13
Be14

[MeV]

[fm]

2.2
2.4
2.6
2.8
3.0
3.2
3.4

3/2$^-$
3/2$^-$

0$^+$
0$^+$

3/2$^-$
3/2$^-$

1/2$^+$
1/2$^+$

0$^+$
0$^+$

1/2$^-$
1/2$^-$

0$^+$
0$^+$

1/2$^+$
1/2$^+$

0$^+$
0$^+$

Positive parity state

Matter & charge radii

Strong $\alpha + ^3\text{He}$ and $\alpha + \alpha$ cluster contributions

Borromean system

Be7
Be8
Be9
Be10
Be11
Be12
Be13
Be14
Carbon Isotopes

 intrinsic densities of $\nu$ states

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Cluster vs. Shell structure

$^{12}\text{C}$

**radius and octupole constraints**

<table>
<thead>
<tr>
<th></th>
<th>$E_b$ [MeV]</th>
<th>$r_{\text{charge}}$ [fm]</th>
<th>$B(E2) [e^2\text{fm}^4]$</th>
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</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>
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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>
</tr>
<tr>
<td>Multiconfig</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>

**Variation**

$^{12}\text{C}$

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**Diagram:**
- Graph showing radial and octupole constraints for $^{12}\text{C}$.
- Table comparing $E_b$, $r_{\text{charge}}$, and $B(E2)$ for different configurations.
- Graph illustrating energy levels and states for $^{12}\text{C}$.

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12C – excited 0\(^+\) and 2\(^+\) states

**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**

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

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<th>Multiconfig</th>
<th>Experiment</th>
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<tr>
<td>(E_b) [MeV]</td>
<td>92.4</td>
<td>92.2</td>
</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^+_1 \rightarrow 0^+_2) [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>
<td></td>
</tr>
<tr>
<td>(r_{\text{rms}}(2^+_1)) [fm]</td>
<td>2.44</td>
<td></td>
</tr>
<tr>
<td>(r_{\text{rms}}(2^+_2)) [fm]</td>
<td>3.64</td>
<td></td>
</tr>
<tr>
<td>(r_{\text{rms}}(2^+_3)) [fm]</td>
<td>3.63</td>
<td></td>
</tr>
<tr>
<td>(Q(2^+_1)) [efm^2]</td>
<td>5.85</td>
<td></td>
</tr>
<tr>
<td>(Q(2^+_2)) [efm^2]</td>
<td>-23.65</td>
<td></td>
</tr>
<tr>
<td>(Q(2^+_3)) [efm^2]</td>
<td>5.89</td>
<td></td>
</tr>
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</table>

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Microscopic R-matrix approach

- divide Hilbert space into interaction region and asymptotic region
- solve the many-body Schrödinger equation in the interaction region
- match to boundary conditions defined in the asymptotic region
- FMD states can be used like in a microscopic cluster model
- use $V_{UCOM}$ as effective interaction

Brink-type many-body states

$$\left| \Psi_{J,M}^{J}(R) \right\rangle = P_{J-M|0}^{J} \left| \Psi(R) \right\rangle$$

$$\left| \Psi(R) \right\rangle = \mathcal{A}\left\{ \left| ^{16}\text{O}; \frac{1}{2}R \right\rangle \left| ^{16}\text{O}; -\frac{1}{2}R \right\rangle \right\}$$

- transform into RGM wave functions in asymptotic region
- apply Gamov boundary conditions (purely outgoing Coulomb wave) to calculate resonance properties

Todo

- deformed $^{32}\text{S}$ configurations in the interaction region to describe the groundstate band
- include other channels
Outlook

Microscopic Nucleus-Nucleus Potentials

- use GCM wave function

\[
\left| \Psi_M^{J} (\mathbf{R}) \right\rangle = P_{J0}^{l} \mathcal{A} \left\langle \left| x^{16}O; \frac{1}{2}\mathbf{R} \right\rangle \left| x^{16}O; -\frac{1}{2}\mathbf{R} \right\rangle \right
\]

- 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-factors

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

- fusion cross sections for neutron rich isotopes are of interest for pycnonuclear reactions in the crust of neutron stars
Spectroscopic information

- Single nucleon spectroscopic amplitudes and spectroscopic factors
- Cluster spectroscopic amplitudes and spectroscopic factors
- Non-orthogonality of cluster configurations properly treated

Graphs showing:
- Single nucleon spectroscopic amplitudes and spectroscopic factors
- Cluster spectroscopic amplitudes and spectroscopic factors
- Non-orthogonality of cluster configurations properly treated

Graphs with data points for different configurations and oscillator constants.
Summary & Outlook

Summary

- consistent many-body approach for conventional and exotic nuclei
- FMD basis is flexible enough to describe clustering, shell effects and halos
- same effective NN interaction based on realistic interaction used for all nuclei
- importance of VAP and multiconfiguration calculations
- binding energies and radii well described
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consistent many-body approach for conventional and exotic nuclei
FMD basis is flexible enough to describe clustering, shell effects and halos
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importance of VAP and multiconfiguration calculations
binding energies and radii well described

Outlook

systematic study of light nuclei in the \( p \)- and \( sd \)-shell
other observables: formfactors, momentum distributions, spectroscopic factors, two-body densities, electromagnetic and weak transitions
molecular resonances, microscopic nucleus-nucleus potentials, transfer reactions, . . .
compare to No-Core Shell Model calculations (using the same effective interaction)