From the NN Interaction to Nuclear Structure and Reactions

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Overview

Nucleon Nucleon Interaction
- Central and Tensor correlations
- Correlated Interaction in momentum space
- Operator representation of correlated interaction

Fermionic Molecular Dynamics
Improving the Many-Body State
- PAV, VAP and Multiconfiguration

Applications
- Helium, Lithium, Beryllium, Carbon isotopes, \(^{12}\text{C}\)
- Reactions
The Nucleon-Nucleon Interaction

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

Effective Interactions

- with effective interactions many properties of nuclear systems like energies, radii, spectra can be described successfully
- many-body states used with effective interactions can not describe the short-range correlations induced by realistic interactions

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

does not connect to higher momenta and can be used directly in simple model spaces (mean-field, shell-model)

derive effective interaction from realistic interaction

by explicitly including correlations with unitary correlation operator $\mathcal{C}$

Ansatz
Central and Tensor Correlations

\[ \tilde{c} = c_\Omega c_r \]

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

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

\[ \tilde{c}_r = \exp \left\{ -i \frac{S}{2} \left[ \mathbf{p}_r \cdot \mathbf{s}(r) + \mathbf{s}(r) \cdot \mathbf{p}_r \right] \right\} \]

\[ \tilde{c}_\Omega = \exp \left\{ -i \frac{\vartheta}{3} \left[ \frac{3}{2} \left( \mathbf{\sigma}_1 \cdot \mathbf{p}_\Omega \right) \cdot \mathbf{r} + \frac{3}{2} \left( \mathbf{\sigma}_1 \cdot \mathbf{r} \right) \cdot \left( \mathbf{\sigma}_2 \cdot \mathbf{p}_\Omega \right) \right] \right\} \]

- Central Correlations
  - \( \tilde{c}_r = \exp \left\{ -i \frac{S}{2} \left[ \mathbf{p}_r \cdot \mathbf{s}(r) + \mathbf{s}(r) \cdot \mathbf{p}_r \right] \right\} \)
  - probability density shifted out of the repulsive core

- Tensor Correlations
  - \( \tilde{c}_\Omega = \exp \left\{ -i \frac{\vartheta}{3} \left[ \frac{3}{2} \left( \mathbf{\sigma}_1 \cdot \mathbf{p}_\Omega \right) \cdot \mathbf{r} + \frac{3}{2} \left( \mathbf{\sigma}_1 \cdot \mathbf{r} \right) \cdot \left( \mathbf{\sigma}_2 \cdot \mathbf{p}_\Omega \right) \right] \right\} \)
  - tensor force admixes other angular momenta
Central and Tensor Correlations

Central Correlations

\[ \zeta_r = \exp \left\{-\frac{i}{2} \left[ p_r s(r) + s(r) p_r \right] \right\} \]

\( \Rightarrow \) probability density shifted out of the repulsive core

Tensor Correlations

\[ \zeta_\Omega = \exp \left\{-i \vartheta(r) \left[ \frac{3}{2} (\sigma_1 \cdot p_\Omega)(\sigma_2 \cdot r) + \frac{3}{2} (\sigma_1 \cdot r)(\sigma_2 \cdot p_\Omega) \right] \right\} \]

\( \Rightarrow \) tensor force admixes other angular momenta

\[ p = p_r + p_\Omega \]

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

**Correlated Realistic Interaction \( V_{UCOM} \)**

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

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

- both central and tensor correlations are essential for binding

![Diagram showing two-body densities](image-url)

![Graph showing energies](image-url)
\[ \langle klm \big| \hat{H}^{[2]} \big| k'l'm' \rangle = i^{l''-l} M \int d^3x \ Y_{lm}^* (\hat{x}) j_l(kx) \langle x \big| \hat{H}^{[2]} \big| x \rangle j_{l'}(k'x) Y_{l'm'} (\hat{x}) \]

\[ \langle k \big| \hat{H}^{[2]} \big| k \rangle, \langle k \big| V \big| k \rangle \] [fm]

\[ k \] [fm\(^{-1}\)]

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

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

- **unique effective potential** – identical to \( V_{\text{lowk}} \)
- Kuo, Schwenk, Bogner

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

Off-diagonal Matrix Elements
AV18 Interaction in Momentum Space

Off-diagonal Matrix Elements

- Bare potential
- Correlated interaction
AV18 Interaction in Momentum Space

Off-diagonal Matrix elements

“pre-diagonalization”: correlated interaction no longer connects to high momenta

bare potential

correlated interaction
\( \tilde{c}^t (T + V) \tilde{c} = T \)

\[
+ \sum_{ST} \hat{V}^{ST}_c (r) + \frac{1}{2} (p_r^2 \hat{V}^{ST}_{p^2} (r) + \hat{V}^{ST}_{p^2} (r) p_r^2) + \hat{V}^{ST}_{p^2} (r) l^2 \\
+ \sum_T \hat{V}^T_{lss} (r) \mathbf{l} \cdot \mathbf{s} + \hat{V}^T_{p l s} (r) l^2 \mathbf{l} \cdot \mathbf{s} \\
+ \sum_T \hat{V}^T_l (r) S_{12} (r, r) + \hat{V}^T_{tcp} (r) p_r S_{12} (r, p) + \hat{V}^T_{pl} (r) S_{12} (l, 1) + \\
\hat{V}^T_{lcp l p} (r) S_{12} (p, p) + \hat{V}^T_{p l c p} (r) l^2 S_{12} (p, p)
\]

- one-body kinetic energy
- **central** potentials
- **spin-orbit** potentials
- **tensor** potentials

- bulk of tensor force mapped onto central part of correlated interaction
- long-range part of tensor force up to now omitted, matrix elements recently implemented
Fermionic Molecular Dynamics

Fermionic
Slater determinant
\[
|Q\rangle = \mathcal{A}(|q_1\rangle \otimes \cdots \otimes |q_A\rangle)
\]
\[\Rightarrow\]
antisymmetrized A-body state

Molecular
single-particle states
\[
\langle x | q \rangle = \sum_i c_i \exp\left\{-\frac{(x - b_i)^2}{2a_i}\right\} \otimes |\chi_i^\uparrow, \chi_i^\downarrow\rangle \otimes |\xi\rangle
\]
\[\Rightarrow\]
Gaussian wave-packets in phase-space, spin is free, isospin is fixed

Dynamics
Time-dependent variational principle
\[
\delta \int dt \frac{\langle Q | \frac{d}{dt} - \hat{H} | Q \rangle}{\langle Q | Q \rangle} = 0
\]
Minimization

- minimize Hamiltonian 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

*intrinsically deformed nuclei*
Effective two-body interaction

- correlated two-body interaction is lacking three-body correlations and genuine three-body forces
- (tensor parts of correlated interaction are omitted)
- simulate missing parts by momentum-dependent central and (isospin-dependent) spin-orbit two-body correction term
- fit correction term to binding energies and radii of “closed-shell” nuclei ($^4$He, $^{16}$O, $^{40}$Ca), ($^{24}$O, $^{34}$Si, $^{48}$Ca)
- altogether about a 15% correction to the ab-initio potential

Projected tetrahedral configurations are about 6 MeV lower in energy than “closed-shell” configurations
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FMD Nuclear Chart

Variation

1 Gaussian per single-particle state

2 Gaussians per single-particle state
How to improve?

**Projection After Variation (PAV)**
- mean-field may break symmetries of Hamiltonian
- restore inversion and rotational symmetry by parity and angular-momentum projection $P_{MK}^{J\pi}$

**Variation After Projection (VAP)**
- effect of projection can be large
- perform Variation after Parity Projection
- 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
  $$\left\{\left|Q^{(a)}\right\rangle, \ a = 1, \ldots, N\right\}$$

\[ P_{MK}^{J\pi} = \frac{2J + 1}{8\pi^2} \int d^3\Omega\ D_{MK}^{J\pi}(\Omega)^* R(\Omega) \]

\[ \sum_{K'} \left\langle Q | H P_{KK'}^{J\pi} | Q \right\rangle \cdot c_{K'} = E_K^{J\pi} \sum_{K'} \left\langle Q | P_{KK'}^{J\pi} | Q \right\rangle \cdot c_{K'} \]
How to improve?

Projection After Variation (PAV)

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

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Multiconfiguration Calculations

- diagonalize Hamiltonian in a set of projected intrinsic states
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  \{|Q^{(a)}\rangle, \quad a = 1, \ldots, N\}
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\[
\begin{align*}
P_{\sim MK}^J &= \frac{2J + 1}{8\pi^2} \int d^3\Omega \ D_{MK}^J \ast (\Omega) \ R(\Omega) \\
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\end{align*}
\]

PAV\textsuperscript{\textpi} procedure

- Variation after Parity Projection using interaction with no, half and full spin-orbit correction term
- calculate projected energy with full spin-orbit correction term
- select configuration with lowest projected energy

Multiconfig procedure

- Constrained Variation for a set of values
- VAP result given by configuration with lowest projected energy
- perform multiconfiguration calculations with VAP state and all other constrained configurations
- select configuration that lowers energy the most
- select next configuration
How to improve?

**Projection After Variation (PAV)**

- mean-field may break symmetries of Hamiltonian
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**Multiconfiguration Calculations**

- diagonalize Hamiltonian in a set of projected intrinsic states $\{ |Q^{(a)}\rangle, \; a = 1, \ldots, N \}$

**Center-of-Mass Projection**

- decouple center-of-mass and internal motion

**PAV**

\[
P_{MK}^{J\pi} = \frac{2J + 1}{8\pi^2} \int d^3\Omega \; D_{MK}^{l}(\Omega)^\star R(\Omega)
\]

\[
\sum_{K'} \langle Q | H P_{KK'}^{l} | Q \rangle \cdot c_{K'} = E_{K}^{l} \sum_{K'} \langle Q | P_{KK'}^{l} | Q \rangle \cdot c_{K'}
\]

**PAV** procedure

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Helium Isotopes

dipole and quadrupole constraints

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

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

- **Binding energies**
  - Various states and binding energies for He4, He5, He6, He7, and He8 isotopes.
  - Red lines indicate PAV\(^\pi\) results, blue lines for Multiconfig, and black lines for Experiment.

- **Matter & charge radii**
  - Comparative analysis of matter and charge radii for the same isotopes as in binding energies.

**Key Elements**:
- He4, He5, He6, He7, He8
- Binding energies in MeV
- Matter & charge radii in fm
- Various nuclear states and configurations are denoted.
Helium Isotopes

**Binding energies**

- **PAV**
- **Multiconfig**
- **Experiment**

**Matter & charge radii**

Zero-point oscillations of the soft-dipole mode essential for description of binding energies and radii
Lithium Isotopes

quadrupole constraints

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

Binding energies

Matter & Charge radii
Lithium Isotopes

Binding energies

-20  -25  -30  -35  -40  -45
\[ \text{MeV} \]

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

Matter & Charge radii

-2.2  -2.4  -2.6  -2.8  -3.0  -3.2  -3.4
\[ \text{fm} \]

$^{10}\text{Li}$ and $^{11}\text{Li}$ are very delicate, should be treated as projected $^9\text{Li}$-core plus neutrons
Lithium Isotopes with cm-projection

**Binding energies**

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

**Magnetic moments**

**Quadrupole moments**

with cm-projection
Beryllium Isotopes

intrinsic densities of $V^{\pi}$ states

cluster structure evolves with addition of neutrons
Beryllium Isotopes

quadrupole constraints

Binding energies

Matter & charge radii

Be7  Be8  Be9  Be10  Be11  Be12  Be13  Be14

PAV\(^*\)  Multiconf  Exp
Beryllium Isotopes

quadrupole constraints

![Graph showing binding energies and matter & charge radii for beryllium isotopes.]

- Binding energies:
  - Be7, Be8, Be9, Be10, Be11, Be12, Be13, Be14
  - Strong $\alpha + ^3\text{He}$ and $\alpha + \alpha$ cluster contributions
  - Borromean system

- Matter & charge radii:
  - Positive parity state coming down

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Carbon Isotopes

intrinisc densities of $V_\pi$ states
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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<tr>
<td>V/PAV</td>
<td>81.4</td>
<td>2.36</td>
<td>-</td>
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<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>
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<tr>
<td>Multiconfig</td>
<td>92.2</td>
<td>2.52</td>
<td>42.8</td>
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<tr>
<td>Experiment</td>
<td>92.2</td>
<td>2.47</td>
<td>39.7 ± 3.3</td>
</tr>
</tbody>
</table>
\( ^{12}C \) – excited 0\(^+ \) and 2\(^+ \) states

quadrupole and octupole constraints

\( 0_2^+ \) state

\( |\langle \cdot | 0_2^+ \rangle| = 0.76 \quad |\langle \cdot | 0_2^+ \rangle| = 0.71 \quad |\langle \cdot | 0_2^+ \rangle| = 0.50 \)

\( 0_3^+ \) state

\( |\langle \cdot | 0_3^+ \rangle| = 0.69 \quad |\langle \cdot | 0_3^+ \rangle| = 0.65 \quad |\langle \cdot | 0_3^+ \rangle| = 0.44 \)

<table>
<thead>
<tr>
<th>\</th>
<th>Multiconfig</th>
<th>Experiment</th>
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<tbody>
<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>
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<td>( r_{\text{rms}}(0_1^+) ) [fm] \</td>
<td>2.38</td>
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<td>( r_{\text{rms}}(0_2^+) ) [fm] \</td>
<td>3.42</td>
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<td>( r_{\text{rms}}(0_3^+) ) [fm] \</td>
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<td>( r_{\text{rms}}(2_1^+) ) [fm] \</td>
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<td>( r_{\text{rms}}(2_2^+) ) [fm] \</td>
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<td>( r_{\text{rms}}(2_3^+) ) [fm] \</td>
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<tr>
<td>( Q(2_1^+) ) [efm^2] \</td>
<td>5.85</td>
<td></td>
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<tr>
<td>( Q(2_2^+) ) [efm^2] \</td>
<td>-23.65</td>
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<tr>
<td>( Q(2_3^+) ) [efm^2] \</td>
<td>5.89</td>
<td></td>
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\[ \mathbf{R}-\text{matrix approach} \]

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 \( V_{\text{UCOM}} \) as effective interaction

Brink-type many-body states

\[
\left| \Psi_J^I(M,J)(R) \right> = \mathcal{P}_M^I \left| \Psi(R) \right>
\]

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

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

**Todo**

- include adiabatic configurations in the interaction region, get groundstate band
- use projected tetrahedral \( ^{16}\text{O} \) for asymptotic states
- multichannel calculations
Summary & Outlook

Summary

» consistent many-body approach for conventional and exotic nuclei
» FMD basis is flexible enough to describe clustering, shell effects and halos, Neff, Feldmeier, Nuc. Phys. A738 (2004) 357
» importance of VAP and multiconfiguration calculations
» binding energies and radii well described

Experimental data taken from:

- INDC(HUN)-033
- Raman, Nestor, Tikkanen, Atomic Data and Nuclear Data Tables 78 (2001) 1
Summary

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Outlook

- systematic study of light nuclei
- other observables: momentum distributions, spectroscopic factors, two-body densities, electromagnetic and weak transitions
- investigate effects of center of mass projection
- investigate effects of long range part of tensor force
- Resonances, elastic scattering, microscopic derivation of nucleus-nucleus potentials, transfer reactions, ...