Exotic Nuclear Structures and Reactions in
Fermionic Molecular Dynamics

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Ryn, Poland
Overview

Fermionic Molecular Dynamics

Hoyle State in $^{12}$C

Helium Isotopes

Neon Isotopes, $^{17}$Ne 2 Proton Halo

Scattering $^{3}$He – $^{4}$He and
Radiative Capture $^{3}$He(α,γ)$^{7}$Be
Fermionic Molecular Dynamics (FMD)

Nucleon-Nucleon Interaction

FMD Wave Functions

Projection After Variation, Variation After Projection
Multiconfiguration
Microscopic Approach

**Aim**
- degrees of freedom: nucleons
- describe low energy properties of nuclear many-body system

In terms of a **Hamiltonian** $\hat{H} = \hat{T} + \hat{V}_{NN} + \hat{V}_{NNN}$ and **many-body states** $|\hat{\Psi}\rangle$

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

**Ingredients**

$\hat{H} = \text{Hamiltonian with realistic } NN\text{-potential } \hat{V}_{NN} \text{ and corresponding 3-body force } \hat{V}_{NNN}$

(phase shifts, deuteron, 3 and 4 nucleon systems)

$|\hat{\Psi}_n\rangle \in \text{many-body Hilbert space}$

$\langle r_1\sigma_1\tau_1, r_2\sigma_2\tau_2, \cdots, r_A\sigma_A\tau_A |\hat{\Psi}_n\rangle$ is terribly complicated for realistic interaction

main problem: short-range repulsive and tensor correlations induced by $\hat{V}_{NN}$
Argonne V18 \(( S = 1, \ T = 0 \) )

spins parallel or perpendicular to the relative distance vector

- strong repulsive core: nucleons can not get closer than \( \approx 0.5 \) fm
  - central correlations

- strong dependence on the orientation of the spins due to the tensor force
  - tensor correlations

the nuclear force will induce strong short-range correlations in the nuclear wave function
Effective two-body interaction

- short range repulsive and tensor correlations treated by UCOM

\[ \mathcal{H} \implies C^{-1} \mathcal{H} C = T + \mathcal{V}_{\text{UCOM}} + \ldots \]

- to account for medium-long ranged correlations missing in FMD Hilbert space
  add phenomenological two-body term \( \delta \mathcal{V} \) with central and spin-orbit part

- fit correction \( \delta \mathcal{V} \) to 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})

\[ \langle \delta \mathcal{V} \rangle \approx 15\% \langle \mathcal{V}_{\text{UCOM}} \rangle \]

- Same Hamiltonian \( \mathcal{H} = T + \mathcal{V}_{\text{UCOM}} + \delta \mathcal{V} \) for all nuclei
FMD Many-Body Hilbert Space

**Fermionic**
Slater determinant

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

antisymmetrized A-body state

**Molecular**

single-particle states

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

Gaussian wave-packets in phase-space, spin is free, isospin is fixed

**Dynamics in Hilbert space**

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

\[ \left| \Psi; J^\pi M \right\rangle = \sum_{aK} \Psi_{aK} \mathcal{P}_{MK}^{J^\pi} \mathcal{P}^{P=0} \left| Q^{(a)} \right\rangle \]

variational principle \( \Rightarrow Q^{(a)} = \{ q_v^{(a)}, v = 1 \cdots A \}, \Psi_{aK} \)
Perform Variation

**Minimization**

- minimize Hamiltonian expectation value 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
Projection to restore Symmetries

**Projection After Variation (PAV)**

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

\[ P^\pm = \frac{1}{2} \left( 1 \pm \Pi \right) \]
\[ P^J_{MK} = \frac{2J + 1}{8\pi^2} \int d^3\Omega \, D^{J*}_{MK}(\Omega) \, R(\Omega) \]
\[ P^P = \frac{1}{(2\pi)^3} \int d^3X \, \exp\{-i(P - \tilde{P}) \cdot X\} \]
\[ |Q^\pm; J^\pi M, K\rangle = P^\pm P^J_{MK} P^P=0 |Q\rangle \]

**Variation After Projection (VAP)**

- effect of projection can be large
- perform VAP (most time consuming)
- perform Variation after Parity Projection PAV\(\pi\)
- perform PAV\(\pi\) by applying **constraints** on radius, dipole moment, quadrupole moment or octupole moment and minimize the energy in the projected energy surface (GCM)

\[ |Q^\pm\rangle = \frac{1}{2} \left( 1 \pm \Pi \right) |Q\rangle \]
Multi-Configuration Mixing

» most general projected state for multi-configuration calculations

\[ |\Psi; J^\pi M\rangle = \sum_{aK} \Psi_{aK} P^{J\pi}_{MK} P^{P=0} |Q^{(a)}\rangle \]

» task: find a set of intrinsic states \( \{ |Q^{(a)}\rangle, a = 1, \ldots, N \} \) that describe the physical situation well

Multi-configuration calculations

\[ H |J^\pi M, n\rangle = E_n^{J^\pi} |J^\pi M, n\rangle \]

» diagonalize Hamiltonian in this set of non-orthogonal projected intrinsic states

\[ \sum_{bK'} \langle Q^{(a)} | H P^{J^\pi}_{KK'} P^{P=0} |Q^{(b)}\rangle \cdot c^n_{bK'} = E_n^{J^\pi} \sum_{bK'} \langle Q^{(a)} | P^{J^\pi}_{KK'} P^{P=0} |Q^{(b)}\rangle \cdot c^n_{bK'} \]

» energy levels \( E_n^{J^\pi} \) and eigenstates \( |J^\pi M, n\rangle \) describing nuclear many-body system

\[ |J^\pi M, n\rangle = \sum_{bK'} c^n_{bK'} P^{J^\pi}_{KK'} P^{P=0} |Q^{(b)}\rangle \]
Cluster States in $^{12}\text{C}$

Astrophysical Motivation

Structure

- Is the Hoyle state a $\alpha$-cluster state?
- Other excited $0^+$ and $2^+$ states

**Analyze wave functions in harmonic oscillator basis**
FMD - Variation, PAV$^\pi$, Multiconfig.

<table>
<thead>
<tr>
<th></th>
<th>$E$ [MeV]</th>
<th>$r_{charge}$ [fm]</th>
<th>$B(E2)$ [$e^2fm^4$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAV</td>
<td>-81.4</td>
<td>2.36</td>
<td>-</td>
</tr>
<tr>
<td>PAV$^\pi$</td>
<td>-88.5</td>
<td>2.51</td>
<td>36.3</td>
</tr>
<tr>
<td>Multiconfig(4)</td>
<td>-92.2</td>
<td>2.52</td>
<td>42.8</td>
</tr>
<tr>
<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>
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**

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

<table>
<thead>
<tr>
<th></th>
<th>Multiconfig</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E_b) [MeV]</td>
<td>92.4</td>
<td>92.2</td>
</tr>
<tr>
<td>(r_{charge}) [fm]</td>
<td>2.52</td>
<td>2.47</td>
</tr>
<tr>
<td>(B(E2)(0^+_1 \rightarrow 2^+_1) [e^2 fm^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_{rms}(0^+_1) [fm])</td>
<td>2.38</td>
<td></td>
</tr>
<tr>
<td>(r_{rms}(0^+_2) [fm])</td>
<td>3.42</td>
<td></td>
</tr>
<tr>
<td>(r_{rms}(0^+_3) [fm])</td>
<td>3.85</td>
<td></td>
</tr>
<tr>
<td>(r_{rms}(2^+_1) [fm])</td>
<td>2.44</td>
<td></td>
</tr>
<tr>
<td>(r_{rms}(2^+_2) [fm])</td>
<td>3.64</td>
<td></td>
</tr>
<tr>
<td>(r_{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>
</tbody>
</table>
**$^{12}\text{C}$ Hoyle State in Electron Scattering**

- calculate formfactors, center-of-mass treated properly, formfactor is an $A$-body operator

$$F(q) = \sum_{i} \langle \Psi_{a} | e^{iq(x_{i}-X)} | \Psi_{b} \rangle$$

- compare to experiment in Distorted Wave Born Approximation

- $\alpha$-cluster and "BEC" calculated with mod. Volkov interaction

"BEC" formfactors: Y. Funaki et al. EPJA 28(2006)259 and private communication

Cluster States in $^{12}\text{C}$

Harmonic Oscillator $N \hbar \Omega$ Excitations

Occupation probabilities of spaces with $N$ harmonic oscillator quanta

$$\text{Occ}(N) = \langle \Psi | \delta \left( \sum_{i=1}^{A} \left( \frac{H_{HO}^i}{\hbar \Omega} - \frac{3}{2} \right) - N \right) | \Psi \rangle$$
Helium Isotopes $^4\text{He} \rightarrow ^8\text{He}$

Structure
- Borromean behaviour
- Zero-point oscillation of soft dipole mode

Observables
- Charge radii
- Matter radii
- Proton, neutron densities
Helium Isotopes

**dipole and quadrupole constraints**

\[ |Q^\pm \rangle = \frac{1}{2} (1 \pm \Pi) |Q\rangle \]

\[\Rightarrow\] intrinsic densities of VAP\(\pi\) states

radial densities from multiconfiguration calculations
Helium Isotopes

Binding energies

Matter & Charge radii

Exp: Ozawa,Suzuki,Tanihata, NPA\textbf{A693}(2001)32; Raman,Nestor,Tikkanen, Atomic Data and Nucl. Data Tables \textbf{78}(2001)1

Helium Isotopes

**Binding energies**

- **He4**
- **He5**
- **He6**
- **He7**
- **He8**

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

**Matter & Charge radii**

- **He4**
- **He5**
- **He6**
- **He7**
- **He8**


\(^6\)He and \(^8\)He charge radius: P. Mueller et al, Phys. Rev. Lett. 99 (2007) 252501
Applications

$^{11}\text{Be}$ positive parity intruder

$^{10}\text{Be}$

$^{11}\text{Be}$ negative parity

$^{11}\text{Be}$ positive parity

$1/2^+$ state has a neutron halo
Neon Isotopes $^{17}\text{Ne} – ^{22}\text{Ne}$

Structure
- $s^2/d^2$ occupation in $^{17}\text{Ne}$ and $^{18}\text{Ne}$
- $^3\text{He}$ and $^4\text{He}$ cluster admixtures

Observables
- Charge Radii
- Matter Radii
- Is $^{17}\text{Ne}$ a Halo nucleus?
Intrinsic proton/neutron densities of dominant FMD state

- Variation after parity projection on positive and negative parity
- Crank strength of spin-orbit force, changes properties of single-particle orbits and their occupations
- “$s^2$” and “$d^2$” minima in $^{17,18}\text{Ne}$
- Explicit cluster configurations:
  - $^{17}\text{Ne}$: $^{14}\text{O}$$^3\text{He}$
  - $^{18}\text{Ne}$: $^{14}\text{O}$$^4\text{He}$
  - $^{19}\text{Ne}$: $^{16}\text{O}$$^3\text{He}$, $^{15}\text{O}$$^4\text{He}$
  - $^{20}\text{Ne}$: $^{16}\text{O}$$^4\text{He}$
  - $^{21}\text{Ne}$: “$^{17}\text{O}$”$^4\text{He}$
  - $^{22}\text{Ne}$: “$^{18}\text{O}$”$^4\text{He}$

$|Q^\pm\rangle$ minima
Neon Isotopes

Charge Radii

- charge radii of $^{17,18}$Ne depend strongly on $s^2/d^2$ occupations
- cluster admixtures responsible for large charge radii in $^{19-22}$Ne
- measurements of charge radii by COLLAPS@ISOLDE

W. Geithner, T. Neff, et al., submitted to PRL
Neon Isotopes

Separation Energies and Matter Radii

- Separation Energies

- Matter radii from interaction cross sections

- Good agreement with exception of $^{19}$Ne
Neon Isotopes

$^{17}$Ne Halo?

- proton skin $r_p - r_n = 0.45$ fm
- 40% probability to find a proton at $r > 5$ fm

<table>
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<th>FMD</th>
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<tbody>
<tr>
<td>$r_{ch}$ [fm]</td>
<td>3.03</td>
</tr>
<tr>
<td>$r_{mat}$ [fm]</td>
<td>2.75</td>
</tr>
<tr>
<td>$B(E2; \frac{1}{2}^- \rightarrow \frac{3}{2}^-)$ [e$^2$fm$^4$]</td>
<td>76.7</td>
</tr>
<tr>
<td>$B(E2; \frac{1}{2}^- \rightarrow \frac{5}{2}^-)$ [e$^2$fm$^4$]</td>
<td>119.8</td>
</tr>
<tr>
<td>occupancy $s^2$</td>
<td>40%</td>
</tr>
<tr>
<td>occupancy $d^2$</td>
<td>55%</td>
</tr>
</tbody>
</table>
Reactions

Program

- FMD Hilbert space should contain besides bound states, also resonances and scattering states
- Implement boundary conditions
- Phase shifts, capture cross section

$^3\text{He}(\alpha,\gamma)^7\text{Be}$ reaction
Localized FMD states can represent many-body scattering states

- asymptotic states product of “frozen” FMD states

\[ \langle A \mid ^3\text{He}, -D_i/2 \rangle \otimes \langle ^4\text{He}, +D_i/2 \rangle \]

- FMD states for compound system in the interaction region

\[ \langle ^7\text{Be} \rangle , \langle ^7\text{Be}^* \rangle \ldots \]

scattering state:

\[ \begin{align*}
\mid \text{interaction region} & + \ldots + \\ \\
\mid \text{asymptotic} & + \ldots + \\
\mid D_i & + \ldots \\
\end{align*} \]

Boundary conditions

- matching to the Coulomb solution of two point-like nuclei

- phase shifts for scattering or widths of resonances
boundary condition outgoing wave only, Gamov state

\[ \langle r \mid \Psi, [\ell \frac{1}{2}] J^\pi \rangle \xrightarrow{r \to \infty} i F_\ell(kr) + G_\ell(kr), \quad k = + \sqrt{2\mu Z} \]

complex eigenvalue \( Z = E - i \Gamma/2 \)

interaction slightly adjusted to give correct threshold
\[ \langle r \mid \Psi, [\ell \frac{1}{2}]J^\pi \rangle \xrightarrow{r \to \infty} F_\ell(kr) + \tan(\delta_\ell(k)) G_\ell(kr), \quad k = +\sqrt{2\mu E} \]

- boundary condition Coulomb scattering solutions
- phase shift \( \delta(E) \)

**non-resonant**

- \( ^3\text{He} - ^4\text{He} \) phase shifts

**resonant**

- frozen states only
Capture from $1/2^+$, $3/2^+$ and $5/2^+$ scattering states into $3/2^-$ and $1/2^-$ bound states

$^7$Be described by single PA$^\pi$ configuration (dashed line) or VAP configurations for $3/2^-$ and $1/2^-$ (dash dotted line) and additional $5/2^-$ and $7/2^-$ VAP configurations (solid line)

Interaction slightly adjusted to give correct threshold

New data
(LUNA, Seattle and Weizmann)

R-matrix fit to old data (—)
Descouvement et al. (2004)
Fermionic Molecular Dynamics, $V_{UCOM} + \delta V$

- Structure of light nuclei

- Halos and clustering, Hoyle state, borromean He isotopes, 2 proton halo energies, formfactors, radii, el. magn. & weak transitions, spectroscopic factors, . . .

- Resonances, scattering states, reactions
  phase shifts, cross sections, S-factors

Microscopic unified approach for nuclear structure and reactions
Thanks to my Collaborators

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- S. Bacca
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