Three-cluster dynamics within an ab initio framework

Universality in Few-Body Systems:
Theoretical Challenges and New Directions

INT 14-1

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Outline

- Introduction
- Microscopic three-cluster problem
- Formalism for the (A-2)+1+1 mass partition
- Applications to $^6$He
- Conclusions
- Outlook
Our goal is to develop a fundamental theory for the description of thermonuclear reactions and exotic nuclei.
Theory needed because fusion reactions are difficult or impossible to measure at astrophysical energies

- The nuclear fusion process operates mainly by tunneling through the Coulomb barrier
  - Extremely low rates
  
  \[ \sigma(E) = \frac{S(E)}{E} \exp \left( -\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2mE}} \right) \]

- Projectiles and targets are not fully ionized
  - Electron screening can mask “bare” nuclear cross section
Developing such a fundamental theory is extremely complicated and a longstanding goal of nuclear theory

*Ab initio* many-body calculations:

- A (all active) point-like nucleons
- Nuclear two- and three-body (NN+NNN) forces guided by Quantum Chromodynamics (QCD)
- Unitary transformation to soften bare Hamiltonian: e.g., Similarity Renormalization Group (SRG)

Efficient theoretical framework and High Performance Computing (HPC)
Our starting point is a method to describe static properties of light nuclei from first principles

- Ab initio no-core shell model (NCSM) approach

\[ N = N_{\text{max}} + 1 \]
\[ N = 1 \]
\[ N = 0 \]
\[ N = \max + 1 \]
\[ \Delta E = N_{\text{max}} \hbar \Omega \]

Helped to point out the fundamental importance of three-nucleon (NNN) forces in structure calculations.

PRL 99, 042501 (2007)
We extended this approach by adding the dynamics between nuclei with the resonating-group method (RGM).

- NCSM/RGM approach

  Ab initio NCSM wave functions of the nuclei

  NN interactions

  Pioneered ab initio calculations of light-nuclei fusion reactions
We are now working to complete this picture

- Extended NCSM/RGM to include:
  1) NNN force in reactions
  2) States of the compound nucleus
  3) Three-cluster states in the continuum

This talk
1) Importance of the NNN force in reactions

Elastic scattering of neutrons on $^4$He

This work sets the stage for a truly accurate prediction of the $d+^3$H$\rightarrow^4$He+n fusion from QCD-based NN+NNN forces

6 billion NNN matrix elements!
2) Importance of states of the compound system

G. Hupin, S. Quaglioni, and P. Navratil, in progress

Six-body correlations important also for binding energy (~1 MeV)
3) We want to describe also systems for which the lowest threshold for particle decay is of the 3-body nature

- Exotic nuclei, (Borromean halos, dripline nuclei)
  - $^6$He ($= ^4$He + n + n )
  - $^6$Be ($= \alpha + p + p$ )
  - $^{11}$Li ($= ^9$Li + n + n )
  - $^{14}$Be ($= ^{12}$Be + n + n )
  - …

- Constituents do not bind in pairs!

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Microscopic three-cluster problem

- Starts from:

\[
\Psi^{(A)} = \sum_v \iint \! d\tilde{x} \, d\tilde{y} \ G_v(\tilde{x}, \tilde{y}) \ \hat{A}_v \left| \Phi_{v\tilde{x}\tilde{y}} \rightangle
\]

- Projects \((H - E)\Psi^{(A)} = 0\) onto the channel basis:

\[
\sum_v \iint \! d\tilde{x} \, d\tilde{y} \ \left[ H_{v'v}(\tilde{x}', \tilde{y}', \tilde{x}, \tilde{y}) - E \ N_{v'v}(\tilde{x}', \tilde{y}', \tilde{x}, \tilde{y}) \right] \ G_v(\tilde{x}, \tilde{y}) = 0
\]

\[
\langle \Phi_{v'x'\tilde{y}'} | \hat{A}_v H \hat{A}_v | \Phi_{v\tilde{x}\tilde{y}} \rangle \quad \text{Hamiltonian kernel}
\]

\[
\langle \Phi_{v'x'\tilde{y}'} | \hat{A}_v^2 \hat{A}_v | \Phi_{v\tilde{x}\tilde{y}} \rangle \quad \text{Norm or Overlap kernel}
\]
This can be turned into a set of coupled-channels Schrödinger equations for the hyperradial motion

- Hyperspherical Harmonic (HH) functions form a natural basis:

\[
|\Phi_{\nu \tilde{x} \tilde{y}}\rangle = \sum_K \phi_{K x y}^* (\alpha) |\Phi_{\nu K \rho}\rangle
\]

- Then, with orthogonalization and projection over \(\phi_{K' x' y'} (\alpha')\):

\[
\sum_{\nu K} \int \rho^5 \left[ N^{-1/2} H N^{-1/2} \right]_{\nu'\nu} (\rho', \rho) \frac{u_{K\nu}(\rho)}{\rho^{5/2}} = E \frac{u_{K'\nu'}(\rho')}{\rho'^{5/2}}
\]

\[
\left[ N^{1/2} G \right]_{\nu} (x, y) = \rho^{-5/2} \sum_{K} u_{\nu K}(\rho) \phi_{K x y} (\alpha)
\]
These equations can be solved using R-matrix theory

Expansion on a basis

Internal region
\( (\rho \leq a) \)

\[ u_{Kv}(\rho) = \sum_n c_n^{Kv} f_n(\rho) \]

External region
\( (\rho > a) \)

Bound state asymptotic behavior

\[ u_{Kv}(\rho) = C_{Kv} \sqrt{k \rho} \ K_{K+2}(k \rho) \]

Scattering state asymptotic behavior

\[ u_{Kv}(\rho) = A_{Kv} \left[ H^-_{K}(k \rho) \ \delta_{vv'} \delta_{KK'} - S_{\nu K,\nu' K}^+ \ H^+_{K}(k \rho) \right] \]
4He+n+n within the NCSM/RGM

- Accurate soft NN interaction: SRG-evolved chiral N3LO potential with Λ=1.5 fm⁻¹
  - Fits NN data with high accuracy
  - But: misses both chiral initial and SRG-induced NNN force
  - Fortuitously: two effects mostly compensate each other for very light systems

- 4He ab initio wave function obtained within the NCSM

\[ H^{(A-2)} \psi_{\beta_i}^{(A-2)}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{A-2}) = E_{\beta_i}^{(A-2)} \psi_{\beta_i}^{(A-2)}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{A-2}) \]

  - Large expansions in A-body harmonic oscillator (HO) basis
  - Preserves: 1) Pauli principle, and 2) translational invariance
  - Can include NNN interactions
  - 4He binding energy close to experiment: 28.22 MeV (expt.: 28.3 MeV)

- Fully antisymmetric channel states:

\[ \hat{A}_v = \sqrt{\frac{(A-2)!}{2!}} \left[ 1 - \sum_{j=1}^{A-2} \sum_{k=A-1}^{A} \hat{p}_{j,k} + \sum_{i<j=1}^{A-2} \hat{p}_{i,A-1} \hat{P}_{j,A} \right] \frac{1 - \hat{p}_{A-1,A}}{\sqrt{2}} \]
The formalism is general for (A-2)+1+1 mass partitions
Norm or overlap kernel (Pauli principle)

\[
N_{\nu'\nu}(x',y',x,y) = \frac{1}{2} \left[ 1 - (-1)^{\ell_x + \ell_{x'} + S_{23} + T_{23}} \right] x' x \left[ 1 - (-1)^{\ell_x + S_{23} + T_{23}} \right] y' y \\
\delta_{\nu'\nu} \frac{\delta(x' - x)}{x'} \frac{\delta(y' - y)}{y'} \\
-2(A-2) \sum_{n_x,n_{x'},n_y} R_{n_x}^{\ell_x}(x') R_{n_y}^{\ell_y}(y') \langle \Phi_{\nu' n_{x'}, n_{y}} | P_{A-2,A} | \Phi_{\nu n_x, n_y} \rangle R_{n_x}^{\ell_x}(x) R_{n_y}^{\ell_y}(y) \\
+ \frac{(A-2)(A-3)}{2} \sum_{n_x,n_{x'},n_y} R_{n_x}^{\ell_x}(x') R_{n_y}^{\ell_y}(y') \langle \Phi_{\nu' n_{x'}, n_{y}} | P_{A-3,A-1} P_{A-2,A} | \Phi_{\nu n_x, n_y} \rangle R_{n_x}^{\ell_x}(x) R_{n_y}^{\ell_y}(y)
\]
The formalism is general for \((A-2)+1+1\) mass partitions

Norm or overlap kernel (Pauli principle)

\[
\langle \psi_\mu | a^+ a | \psi_\nu \rangle
\]

\[
\langle \psi_\mu | a^+ a^+ a | \psi_\nu \rangle
\]

\[
\left( \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{i,k} + \sum_{i<j=1}^{A-2} \hat{P}_{i,A-1} \hat{P}_{j,A} \right) \left( 1 - \hat{P}_{A-1,A} \right)
\]

Matrix element \(\langle \hat{A}_v^2 - 1 \rangle\) over three-cluster states:

\( ^4\text{He} \)

\[
- 2(A-2) \times \quad + (A-2)(A-3)/2 \times
\]

\[
\langle \psi_{\mu_1}^{(A-2)} | a^+ a | \psi_{\nu_1}^{(A-2)} \rangle_{\text{SD}}
\]

\[
\langle \psi_{\mu_1}^{(A-2)} | a^+ a^+ a a | \psi_{\nu_1}^{(A-2)} \rangle_{\text{SD}}
\]
The formalism is general for \((A-2)+1+1\) mass partitions

Hamiltonian kernel (nucleon-nucleon-target potentials)

\[
\left\langle \psi_{\mu_1}^{(A-2)} \left| a^+ a \left| \psi_{\nu_1}^{(A-2)} \right\rangle_{SD} \right.ight.
\]

\[
= V(x') N_{\nu_1, \nu_2} (x', y', x, y) +
\]

\[
\left\langle \psi_{\mu_1}^{(A-2)} \left| a^+ a^+ a a \left| \psi_{\nu_1}^{(A-2)} \right\rangle_{SD} \right. \right.
\]

\[
\left\langle \psi_{\mu_1}^{(A-2)} \left| a^+ a^+ a a \left| \psi_{\nu_1}^{(A-2)} \right\rangle_{SD} \right. \right.
\]

\[
\left\langle \psi_{\mu_1}^{(A-2)} \left| a^+ a^+ a a \left| \psi_{\nu_1}^{(A-2)} \right\rangle_{SD} \right. \right.
\]
Part of the interaction kernel is localized only in $x, x'$

$$
\langle y' x' | V_{A-1A} \left( 1 - \hat{P}_{A-1,A} \right) | x y \rangle
$$

$$
\propto \sum_{n_x} R_{n_x^L} (x') R_{n_x^L} (x) \langle n_x^L | n_x^L \delta_{s_{23} T_{23}} V | n_x^L \rangle
$$

$$
\times (1 - (-1)^{\ell_x + s_{23} + T_{23}}) \delta(y' - y) \frac{y'y}{y'y}
$$

Extended-size HO expansion

$$
N_{\text{ext}} \gg N_{\text{max}}
$$

$$
\approx \sum_{n_y} R_{n_y^L} (y') R_{n_y^L} (y)
$$
Results for $^6$He ground state

6-body diagonalization vs $^4$He(g.s)+n+n calculation

- Differences between NCSM 6-body and NCSM/RGM $^4$He(g.s.)+n+n results due to core polarization
- Contrary to NCSM, NCSM/RGM wave function has appropriate asymptotic behavior

\[
\chi_\nu(x,y) = \frac{1}{\rho^{5/2}} \sum_K u_{\nu K}(\rho) \phi_{\nu K}^{\pi J}(\alpha)
\]
Other convergence tests

- HH expansion
- Extended-size HO expansion

\[ \chi_{\nu}(x, y) = \frac{1}{\rho^{5/2}} \sum_{K} u_{\nu K}(\rho) \phi_{K}^{\ell_x \ell_y}(\alpha) \]

\[ \left\langle V_{A-1A} \left(1 - \hat{P}_{A-1A}\right) \right\rangle \propto \sum_{n_y} R_{n_x \ell_y}(y') R_{n_x \ell_y}(y) \]
Probability density of $^6$He ground state

$J^\pi = 0^+$
$(\ell_x = \ell_y = S = 0)$

$J^\pi = 0^+$
$(\ell_x = \ell_y = S = 1)$
Probability density of $^6\text{He}$ ground state

$J^\pi = 0^+$

($\ell_x = \ell_y = S = 0$)
Results for $^4\text{He}(\text{g.s.})+n+n$ continuum

C. Romero-Redondo, S. Quaglioni, and P. Navratil, in progress

Scattering phase shifts

Energy spectrum of states

$\Gamma = \frac{2}{d\delta(E)/dE}_{E=E_R}$
Convergence with respect to HO model space size
Other convergence tests

- HH expansion

$$\chi_\nu(x, y) = \frac{1}{\rho^{5/2}} \sum_{K} u_{vK}(\rho) \phi_{K}^{\ell_x, \ell_y}(\alpha)$$
Other convergence tests

- Extended-size HO expansion

\[ \langle V_{A-1A} (1 - \hat{P}_{A-1A}) \rangle \propto \sum_{n_y} R_{n_y \ell_y}(y') R_{n_y \ell_y}(y) \]

- Sizable effects only when neutrons are in \(^1\text{S}_0\) partial wave (strong attraction)
Conclusions

- We are building an efficient ab initio theory including the continuum
  - NCSM eigenstates $\rightarrow$ short- to medium-range A-body structure
  - NCSM/RGM cluster states $\rightarrow$ scattering physics of the system

- We map the many-body problem into a few-cluster problem
  - The Pauli exclusion principle is treated exactly
  - Inter-cluster interactions arise from underlying nuclear Hamiltonian

- First ab initio description of three-cluster dynamics
  - $^4\text{He}+n+n$ bound and continuum states
  - Good qualitative description of the low-lying spectrum of $^6\text{He}$
Outlook

- For a complete picture we need to:
  - Run calculations with NNN forces (codes are ready)
  - Introduce core excitations by coupling to NCSM A-body eigenstates

- Future applications of three-cluster formalism
  - Calculations of radii, electric dipole transitions
  - Other systems: $^5\text{H} (^3\text{H} + n + n)$, $^{11}\text{Li} (= ^9\text{Li} + n + n)$, $^{12}\text{Be} (= ^{10}\text{Be} + n + n)$

- Ultimate goal: binary & ternary light-nucleus fusion reactions
  - Transfer reactions: $^3\text{H}(^3\text{H}, 2n)^4\text{He}$