Ab initio calculations for exotic nuclei

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1. Exotic structure of $^9$He from the no-core shell model with continuum
   - Motivation
   - Basic features of the NCSMC
   - Results for $^9$He

2. Microscopic optical potentials with nonlocal ab initio densities for intermediate energies
   - Results for stable nuclei
   - Results for $^6$He and $^8$He
1. Exotic structure of $^9$He
Neutron-rich nuclei

- **Theory**
  - Importance of many-body forces at extreme neutron excesses
  - Challenge to our current computational techniques

- **Experiment**
  - Difficult to produce in sufficient quantities
  - Challenging to analyze
The He isotopic chain

- One of the few chains accessible to both detailed theoretical and experimental studies
Motivations

The He isotopic chain

- One of the few chains accessible to both detailed theoretical and experimental studies

- $^9\text{He}$ system
  - Characterized by $N/Z = 3.5$
  - One of the most neutron extreme systems studied so far
The He isotopic chain

- One of the few chains accessible to both detailed theoretical and experimental studies

- $^9$He system
  - Characterized by $N/Z = 3.5$
  - One of the most neutron extreme systems studied so far
  - Possible candidate for a positive parity ground state

Famous example: $^{11}$Be
Controversial experimental situation

- No bound state
- Most experiments see a $1/2^-$ resonance at $\sim 1$ MeV
- Is there a $1/2^+$ resonance? Is the ground state $1/2^+$ or $1/2^-$?
  - $a_0 \sim -10$ fm (Chen et al.)
  - $a_0 \sim -3$ fm (Al Falou, et al.)
- Any higher-lying resonances?
- Recent $^8$He(p,p) measurement at TRIUMF by Rogachev: PLB **754** (2016) 323
  Found no T=5/2 resonances

From talk by Nigel Orr at ECT* (2013)
Two long-standing problems affect the physics of the $^9$He system

1. The existence of the $1/2^+$ state

2. The width of the $1/2^-$ state
   - Experimentally ~ 0.1 MeV
   - Theoretically ~ 1 MeV
Low-energy QCD

Nuclear structure and reactions
From QCD to nuclei

Low-energy QCD

NN+3N interactions from chiral EFT

...or accurate meson-exchange potentials

Nuclear structure and reactions
From QCD to nuclei

Low-energy QCD

NN+3N interactions from chiral EFT

Unitary/similarity transformations

...or accurate meson-exchange potentials

SRG Softens NN, induces 3N

\[ H |\Psi\rangle = E |\Psi\rangle \]

Nuclear structure and reactions
From QCD to nuclei

Low-energy QCD

NN+3N interactions from chiral EFT

Unitary/similarity transformations

Many-Body methods

Nuclear structure and reactions

...or accurate meson-exchange potentials

SRG
Softens NN, induces 3N

NCSM, NCSMC, CCM, IM-SRG, SCGF, GFMC, HH, Nuclear Lattice EFT...

\[ H \left| \Psi \right\rangle = E \left| \Psi \right\rangle \]
**Ab initio** no-core shell model

- Short- and medium range correlations
- Bound-states, narrow resonances

\[
\Psi^{(A)} = \sum_{\lambda} c_\lambda |^{(A)} \text{core shell model}, \lambda \rangle
\]
• \textit{Ab initio} no-core shell model
  – Short- and medium range correlations
  – Bound-states, narrow resonances

• …with resonating group method
  – Bound & scattering states, reactions
  – Cluster dynamics, long-range correlations

\[
\Psi^{(A)} = \sum_{\nu} \int d\vec{r} \; \gamma_{\nu}(\vec{r}) \; \hat{A}_{\nu}\left(\begin{array}{c}
\vec{r} \\
(A-a), \nu
\end{array}\right)
\]

Unknowns
• **Ab initio** no-core shell model
  – Short- and medium range correlations
  – Bound-states, narrow resonances

• ...with resonating group method
  – Bound & scattering states, reactions
  – Cluster dynamics, long-range correlations

• Most efficient: *ab initio* no-core shell model with continuum

\[ \Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| (A) , \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| (A-a) , (a) , \nu \right\rangle \]
• NCSMC calculations with several interactions
  – $N^2\text{LO}_{\text{sat}}$ NN + 3N
  – NN $N^3\text{LO}$ + 3N $N^2\text{LO}$
  – SRG-$N^4\text{LO}500$ NN

• Calculations with SRG-$N^4\text{LO}500$ NN
  – $^9\text{He} \sim (^{9}\text{He})_{\text{NCSM}} + (n^{8}\text{He})_{\text{NCSM/RGM}}$
    • $^8\text{He}$: 0$^+$ and 2$^+$ NCSM eigenstates
    • $^9\text{He}$: 4 negative-parity NCSM eigenstates
      6 positive-parity NCSM eigenstates

  – Importance of large $N_{\text{max}}$ basis:
    • SRG-$N^4\text{LO}500$ NN with $\lambda=2.4$ fm$^{-1}$
      up to $N_{\text{max}} = 11$ with $^9\text{He}$ NCSM (m-scheme basis of 350 million)
Phase shift convergence with SRG-N^4LO500 NN
\( \lambda = 2.4 \text{ fm}^{-1} \)

Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin,
PRC 97, 034314 (2018)
Phase shift convergence with SRG-\(N^4\)LO500 NN
\(\lambda = 2.4 \text{ fm}^{-1}\)

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Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC 97, 034314 (2018)
Phase shifts with SRG-N^4LO500 NN \( \lambda = 2.4 \text{ fm}^{-1} \)

Energy spectrum

No bound state

Two resonances in the \( ^2P_{1/2} \) and \( ^6P_{3/2} \) channels

No resonance in the \( ^2S_{1/2} \) state

Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC 97, 034314 (2018)
Structure of unbound $^9\text{He}$

Eigenphase shifts with SRG-N$^4$LO500 NN $\lambda=2.4$ fm$^{-1}$

Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC 97, 034314 (2018)

Summary

Robust results for $1/2^-$ ($\sim 1$ MeV) and $3/2^-$ ($\sim 4$ MeV) P-wave resonances (3/2$^-$ resonance in n-$^8\text{He}(2^+)$ channel)

$1/2^+$ S-wave with vanishing scattering length: $a_s = 0 \sim -1$ fm

No evidence for other higher lying resonances

<table>
<thead>
<tr>
<th>$J^\pi$</th>
<th>NCSMC</th>
<th>NCSMC-pheno</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1/2^-$</td>
<td>$E_R = 0.69$</td>
<td>$\Gamma = 0.83$</td>
</tr>
<tr>
<td>$3/2^-$</td>
<td>$E_R = 4.70$</td>
<td>$\Gamma = 0.74$</td>
</tr>
</tbody>
</table>
2. Microscopic optical potentials for intermediate energies
The first-order optical potential

• The elastic nucleon-nucleus scattering amplitude

\[ T_{el}(k', k; E) = U(k', k; E) + \int d^3p \frac{U(k', p; E) T_{el}(p, k; E)}{E - E(p) + i\epsilon} \]

• The first-order optical potential
  – Obtained from the multiple scattering theory
  – Impulse approximation

\[ U(q, K; E) = \sum_{\alpha=n,p} \int d^3P \eta(P, q, K) t_{p\alpha} \left[ q, \frac{1}{2} \left( \frac{A + 1}{A} K - P \right) ; E \right] \times \rho_{\alpha} \left( P - \frac{A - 1}{2A} q, P + \frac{A - 1}{2A} q \right) \]
• Extension of: Navratil, PRC 70, 014317 (2004)

• Non-local nuclear density operator

\[ \rho_{op} = \sum_{i=1}^{A} \delta(r - r_i) \delta(r' - r'_i) \]

• The matrix elements between a general initial and final state are obtained from the NCSM in the Cartesian coordinate single-particle Slater determinant basis

• Removal of the COM component is required
  – Enabled by the factorization of the Slater determinant and Jacobi eigenstates
Non-local densities

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)
Scattering observables – Stable nuclei

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)

FF from local density

\[ \rho_\alpha(q) = 4\pi \int_0^\infty dr r^2 j_0(qr) \rho_\alpha(r) \]

Navratil, PRC 70, 014317 (2004)

Factorized optical potential

\[ U(q, K; E) \sim \sum_{\alpha=n,p} t_{p\alpha} \left[ q, \frac{A + 1}{2A} K; E \right] \rho_\alpha(q) \]
Scattering observables – Stable nuclei

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)

Good description of differential cross sections

Reproduction of the general trend of the $A_y$
Scattering observables – Stable nuclei

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)

(a) 100 MeV $^{16}$O (p,p)$^{16}$O

(b) 135 MeV $^{16}$O (p,p)$^{16}$O

(c) 200 MeV $^{16}$O (p,p)$^{16}$O

NN-$N^4$LO(500)+3Nlnl

$N_{\text{max}} = 8 \quad \lambda_{\text{SRG}} = 2.0 \text{ fm}^{-1}$

$A_y$

NN-$N^4$LO(500)+3Nlnl

$N_{\text{max}} = 8 \quad \lambda_{\text{SRG}} = 2.0 \text{ fm}^{-1}$

(a) 100 MeV $^{16}$O (p,p)$^{16}$O

(b) 135 MeV $^{16}$O (p,p)$^{16}$O

(c) 200 MeV $^{16}$O (p,p)$^{16}$O

$\sigma/d\Omega \text{ [mb}/\text{sr} \text{]}$
Scattering observables – Halo nuclei

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)

\[ \text{NN-N}^4\text{LO(500)}+3\text{Nlnl} \]
\[ N_{\text{max}} = 12 \quad \lambda_{\text{SRG}} = 2.0 \text{ fm}^{-1} \]

(a) 71 MeV 6\text{He (p,p)}^6\text{He}

(b) 71 MeV 6\text{He (p,p)}^6\text{He}

Reasonable description of the differential cross section
• Investigation of the $^9$He structure with the inclusion of the three-nucleon interaction
  – Introducing a controlled approximation for the 3N terms

• Calculation of the p+$^8$He scattering process
  – New TRIUMF experiment for $^8$He(p,p) reaction

• Improvement of optical potential
  – Inclusion of the three-nucleon interaction
  – Inclusion of medium effects

• Calculation of the (e,e’p) quasi-elastic reactions with microscopic nonlocal optical potentials
Backup Slides
Coupled NCSMC equations

\[ H \Psi^{(A)} = E \Psi^{(A)} \]

\[ \Psi^{(A)} = \sum_{\lambda} c_{\lambda} \langle A | \lambda, \lambda \rangle + \sum_{\nu} \int d\vec{r} \; \gamma_{\nu}(\vec{r}) \; \hat{A}_{\nu} \left| \vec{r} \right\rangle \langle A - a | (a), \nu \rangle \]

E^{NCSM}_\lambda \quad \delta_{\lambda \lambda'}

\[
\begin{pmatrix}
H_{NCSM} & h \\
\hline
h & H_{RGM}
\end{pmatrix}
\begin{pmatrix}
C \\
\gamma
\end{pmatrix}
= E
\begin{pmatrix}
1_{NCSM} & g \\
\hline
g & N_{RGM}
\end{pmatrix}
\begin{pmatrix}
C \\
\gamma
\end{pmatrix}
\]

Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic R-matrix on Lagrange mesh
Separation into “internal” and “external” regions at the channel radius $a$

**Internal region**

$$u_c(r) = \sum_n A_{cn} f_n(r)$$

**External region**

$$u_c(r) \sim v_c^{-\frac{1}{2}} \left[ \delta c_i I_c(k_c r) - U_{c} O_c(k_c r) \right]$$

- This is achieved through the Bloch operator:
  $$L_c = \frac{\hbar^2}{2\mu_c} \delta(r-a) \left( \frac{d}{dr} - \frac{B_c}{r} \right)$$

- System of Bloch-Schrödinger equations:

$$\left[ \hat{T}_{\text{rel}}(r) + L_c + \hat{V}_{\text{Coul}}(r) - (E - E_c) \right] u_c(r) + \sum_{c'} \int dr' r' W_{cc'}(r,r') u_{c'}(r') = L_c u_c(r)$$

- **Internal region**: expansion on Lagrange square-integrable basis

$$u_c(r) = \sum_n A_{cn} f_n(r)$$

- **External region**: asymptotic form for large $r'$

$$u_c(r) \sim C_c W(k_c r) \quad \text{or} \quad u_c(r) \sim v_c^{-\frac{1}{2}} \left[ \delta c_i I_c(k_c r) - U_{c} O_c(k_c r) \right]$$

**Scattering matrix**

**Bound state**

**Scattering state**
6\textsuperscript{He} and 8\textsuperscript{He} NCSM ground-state energies

\[ \lambda_{\text{SRG}} = 2.4 \text{ fm}^{-1} \]

\[ N^4\text{LO} (\Lambda = 500 \text{ MeV}) \]

Minimum at \( \hbar \Omega = 20 \text{ MeV} \)

Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC 97, 034314 (2018)
Energy extrapolation

\[ E(N_{\text{max}}) = E_\infty + ae^{-bN_{\text{max}}} \]

NCSM ground-state energies

\[ \lambda_{\text{SRG}} = 2.4 \text{ fm}^{-1} \]

\[ h\Omega = 20 \text{ MeV} \]

\[ N^{4}\text{LO} (\Lambda = 500 \text{ MeV}) \]

\begin{table}
\begin{tabular}{|c|c|c|c|}
\hline
 & \( ^4\text{He} \) & \( ^6\text{He} \) & \( ^8\text{He} \) \\
\hline
NCSM & -28.36 & -28.9(2) & -30.1(3) \\
Expt & -28.30 & -29.27 & -31.41 \\
\hline
\end{tabular}
\end{table}

Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC 97, 034314 (2018)
\[ ^{8}\text{He} \text{ NCSM excitation energies} \]

\[ E_x (2^+) \text{ [MeV]} \]

\[ \text{N}^{4}\text{LO} (\Lambda = 500 \text{ MeV}) \]
\[ \lambda_{\text{SRG}} = 2.4 \text{ fm}^{-1} \]
\[ \hbar\Omega = 20 \text{ MeV} \]

\[ ^{8}\text{He} \text{ 2}^+ \text{ state} \]

Experimentally unbound

Important for subsequent NCSMC calculations

<table>
<thead>
<tr>
<th>( N_{\text{max}} )</th>
<th>( E_x (2^+) \text{ [MeV]} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>4.67</td>
</tr>
<tr>
<td>10</td>
<td>4.22</td>
</tr>
</tbody>
</table>
• Translationally invariant non-local densities

\[ \langle A\lambda_j J_j M_j | \rho_{op}^{trinv} (\vec{r} - \vec{R}, \vec{r}' - \vec{R}) | A\lambda_i J_i M_i \rangle \]

\[ = \left( \frac{A}{A - 1} \right)^{\frac{3}{2}} \sum_{\hat{j}_f} \frac{1}{\hat{i}_f} (J_i M_i K k | J_f M_f) \]

\[ \times (M^K)^{-1}_{n_l n'_l n_{11} n_{12} n_{21} n_{22}} \left( Y_l^* (\vec{r} - \vec{R}) Y_{l'}^* (\vec{r}' - \vec{R}) \right)^{(K)} \]

\[ \times R_{n,l} \left( \sqrt{\frac{A}{A - 1}} |\vec{r} - \vec{R}| \right) R_{n',l'} \left( \sqrt{\frac{A}{A - 1}} |\vec{r}' - \vec{R}| \right) \]

\[ \times (-1)^{l_1 + l_2 + K + j_2 - \frac{1}{2}} \hat{j}_1 \hat{j}_2 \left\{ \begin{array}{ccc} j_1 & j_2 & K \\ l_2 & l_1 & \frac{1}{2} \end{array} \right\} \]

\[ \times SD \langle A\lambda_f J_f || (a_{n_1, l_1, j_1}^\dagger \tilde{a}_{n_2, l_2, j_2})^{(K)} || A\lambda_i J_i \rangle SD \]
• Translationally invariant non-local densities

\[
\langle A\lambda_j J_j M_j | \rho_{op}^{\text{trinv}}(\vec{r} - \vec{R}, \vec{r}' - \vec{R}) | A\lambda_i J_i M_i \rangle \\
= \left( \frac{A}{A-1} \right)^{\frac{3}{2}} \sum_{J_f} \frac{1}{J_f} (J_i M_i K k | J_f M_f) \\
\times (M^K)^{-1}_{nln'l',n_1l_1n_2l_2} \left( Y_l^*(\vec{r} - \vec{R}) Y_{l'}^*(\vec{r}' - \vec{R}) \right)_k \\
\times R_{n,l} \left( \sqrt{\frac{A}{A-1}} | \vec{r} - \vec{R} | \right) R_{n',l'} \left( \sqrt{\frac{A}{A-1}} | \vec{r}' - \vec{R} | \right) \\
\times (-1)^{l_1+l_2+K+j_2-\frac{1}{2}} \hat{j}_1 \hat{j}_2 \left\{ \begin{array}{ccc} j_1 & j_2 & \frac{K}{2} \\ l_2 & l_1 & \frac{1}{2} \end{array} \right\} \\
\times SD \langle A\lambda_f J_f || (a_{n_1,l_1,j_1}^\dagger \tilde{a}_{n_2,l_2,j_2}^{(K)}) || A\lambda_i J_i \rangle_{SD}
\]

• Ground-state density for even-even nuclei

\[
\rho(\vec{r}, \vec{r}') = \sum_l \rho_l(\vec{r}, \vec{r}') (-1)^l \frac{\sqrt{2l+1}}{4\pi} P_l(\cos \omega)
\]
• Translationally invariant non-local densities

\[
\langle A\lambda_j J_j M_j | \rho_{op}^{trinv}(\vec{r} - \vec{R}, \vec{r}' - \vec{R}) | A\lambda_i J_i M_i \rangle
\]

\[
= \left( \frac{A}{A-1} \right)^{3/2} \sum_{\hat{j}_f} \frac{1}{\hat{j}_f} (J_i M_i K k | J_f M_f )
\]

\[
\times (M^K)^{-1}_{nln'l',n_1l_1n_2l_2} \left( Y^*_l(\vec{r} - \vec{R}) Y_{l'}^*(\vec{r}' - \vec{R}) \right)(K)
\]

\[
\times R_{n,l}(\sqrt{\frac{A}{A-1}}|\vec{r} - \vec{R}|) R_{n',l'}(\sqrt{\frac{A}{A-1}}|\vec{r}' - \vec{R}|)
\]

\[
\times (-1)^{l_1+l_2+K+j_2-\frac{1}{2}} \hat{j}_1 \hat{j}_2 \left\{ \begin{array}{ccc} j_1 & j_2 & K \\ l_2 & l_1 & \frac{1}{2} \end{array} \right\}
\]

\[
\times SD \langle A\lambda_f J_f || (a_{n_1,l_1,j_1}^\dagger \tilde{a}_{n_2,l_2,j_2})(K) || A\lambda_i J_i \rangle_{SD}
\]

• Ground-state density for even-even nuclei

\[
\rho(r, r') = \sum_l \rho_l(r, r') (-1)^l \frac{\sqrt{2l + 1}}{4\pi} P_l(\cos \omega)
\]
Form factors (FF)

FF from local density

\[
\rho_\alpha(q) = 4\pi \int_0^\infty dr r^2 j_0(qr) \rho_\alpha(r)
\]

PRC 70, 014317 (2004)

FF from non-local density

\[
\rho_\alpha(q) = \int d^3P \rho_\alpha \left( P - \frac{A - 1}{2A} q, P + \frac{A - 1}{2A} q \right)
\]

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)
Scattering observables – Stable nuclei

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)

\[
\rho_\alpha(q) = \int dP \, \rho_\alpha \left(P - \frac{A-1}{2A} q, P + \frac{A-1}{2A} q\right) U(q, K; E) \sim \sum_{\alpha=n,p} t_{p\alpha} \left[q, \frac{A+1}{2A} K; E\right] \rho_\alpha(q)
\]

FF from nonlocal density

Factorized optical potential
Scattering observables – Consistency

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)

\[ \frac{d\sigma}{d\Omega_{\text{lab}}} \text{ [mb/sr]} \]

- \text{NN-N}^4\text{LO(500)+3Nind} - N_{\text{max}} = 14, \lambda_{\text{SRG}} = 2.0 \text{ fm}^{-1}
- \text{NN-N}^4\text{LO(500)+3Nlnl} - N_{\text{max}} = 14, \lambda_{\text{SRG}} = 2.0 \text{ fm}^{-1}
- \text{NN-N}^4\text{LO(500)} - N_{\text{max}} = 18

\[ ^4\text{He (p,p)} ^4\text{He} \]

200 MeV

\[ \theta_{\text{lab}} \text{ [deg]} \]
Scattering observables – Stable nuclei

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)

NN-N^4LO(500)+3Nlnl

(a) 72 MeV

\( ^4\text{He} \ (p,p) \ ^4\text{He} \)

(b) 156 MeV

\( ^4\text{He} \ (p,p) \ ^4\text{He} \)

\( d\sigma/d\Omega \ [\text{mb/sr}] \)

\( N_{\text{max}} = 14 \quad \lambda_{\text{SRG}} = 2.0 \text{ fm}^{-1} \)

\( d\sigma/d\Omega \ [\text{mb/sr}] \)

\( A_y \)

\( 72 \text{ MeV} \)

\( ^4\text{He} \ (p,p) \ ^4\text{He} \)

\( 200 \text{ MeV} \)

\( ^4\text{He} \ (p,p) \ ^4\text{He} \)
Comparison with RMF

Gennari, Vorabbi, Calci, Navratil, PRC 97, 034619 (2018)

Shift with respect the RMF results