Nuclear structure and dynamics from *ab initio* theory

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Outline

- Introduction to \textit{ab initio} No-Core Shell Model with Continuum (NCSMC)
- Polarized $^3\text{H}(d,n)^4\text{He}$ fusion
- $^{11}\text{Be}$ parity inversion in low-lying states, photo-dissociation
- Structure of the halo $sd$-shell nucleus $^{15}\text{C}$
First principles or *ab initio* nuclear theory

Quantum Chromodynamics (QCD)

Genuine *Ab Initio*
First principles or *ab initio* nuclear theory – what we do at present

- **Chiral Effective Field Theory** (parameters fitted to NN data)

- **Quantum Chromodynamics** (QCD)

- **Current ab initio** nuclear theory
  \[ H \Psi^{(A)} = E \Psi^{(A)} \]

- **Ab initio**
  - Degrees of freedom: Nucleons
  - All nucleons are active
  - Exact Pauli principle
  - Realistic inter-nucleon interactions
    - Accurate description of NN (and 3N) data
  - Controllable approximations
Conceptually simplest *ab initio* method: No-Core Shell Model (NCSM)

- Basis expansion method
  - Harmonic oscillator (HO) basis truncated in a particular way ($N_{\text{max}}$)
  - Why HO basis?
    - Lowest filled HO shells match magic numbers of light nuclei (2, 8, 20 – $^4$He, $^{16}$O, $^{40}$Ca)
    - Equivalent description in relative-coordinate and Slater determinant basis
- Short- and medium range correlations
- Bound-states, narrow resonances

\[ \Psi^A = \sum_{N=0}^{N_{\text{max}}} \sum_i C_{Ni} \Phi_{Ni}^{HO}(\eta_1, \eta_2, \ldots, \eta_{A-1}) \]

\[ \Psi_{SD}^A = \sum_{N=0}^{N_{\text{max}}} \sum_j C_{Nj} \Phi_{SDNj}^{HO}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = \Psi^A \varphi_{000}(\vec{R}_{CM}) \]
Extending no-core shell model beyond bound states

Include more many nucleon correlations...

\[ \Psi^A = \sum_{N=0}^{N_{\text{max}}} \sum_{i} c_{Ni} \Phi^A_{Ni} \]
Extending no-core shell model beyond bound states

Include more many nucleon correlations…

\[ \Psi^A = \sum_{N=0}^{N_{\text{max}}} \sum_i c_{Ni} \Phi_{Ni}^A \]

NCSM →

\[ (A-a) + \bar{r}_{A-a,a} + (a) \]

…using the Resonating Group Method (RGM) ideas

\[ a_{1\mu} + a_{2\mu} + a_{3\mu} = A \]

\[ \sum a_x \Psi^A = \Psi^A \]
Extending no-core shell model beyond bound states

Include more many nucleon correlations...

\[ \Psi^A = \sum_{N=0}^{N_{\text{max}}} \sum_i c_{Ni} \Phi^A_{Ni} \]

...using the Resonating Group Method (RGM) ideas

\[ a_1 + a_2 + a_3 = A \]
Coupled NCSMC equations

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

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

\[ E^{NCSM}_\lambda \delta_{\lambda\lambda'} \]

\[ H_{NCSM} \]

\[ h \]

\[ 1_{NCSM} \]

\[ g \]

\[ N_{RGM} \]

Solved by Microscopic R-matrix theory on a Lagrange mesh – efficient for coupled channels

Deuterium-Tritium fusion

- The $d^3\text{H} \rightarrow n^4\text{He}$ reaction
  - The most promising for the production of fusion energy in the near future
  - Used to achieve inertial-confinement (laser-induced) fusion at NIF, and magnetic-confinement fusion at ITER
  - With its mirror reaction, $^3\text{He}(d,p)^4\text{He}$, important for Big Bang nucleosynthesis

Resonance at $E_{\text{cm}}=48$ keV ($E_d=105$ keV) in the $J=3/2^+$ channel
Cross section at the peak: 4.88 b

17.64 MeV energy released:
14.1 MeV neutron and 3.5 MeV alpha
Harnessing fusion energy

The Deuterium-Tritium (DT) fusion

§ The fusion of deuterium (D) with tritium (T) is the most promising of the reactions that could power the thermonuclear reactors of the future.

§ While the DT fusion rate has been measured extensively, a fundamental understanding of the process is still missing.

§ Very little is known of how the polarization of the reactants’ spins affects the reaction.

\[
\begin{align*}
\sum (1/2^-) & \approx 1

\begin{align*}
1/2^- & \approx 1.5
\end{align*}
\]

FY: Faddeev-Yakubovsky method - Rimantas Lazauskas
n-\(^4\)He scattering and \(^3\)H+d fusion within NCSMC

\[ n-4\text{He} \quad \text{and} \quad d+3\text{H} \quad \text{fusion} \]

**n-\(^4\)He and d+\(^3\)H scattering phase-shifts**

- \(^4\text{He}+n \rightarrow 3\text{H}+d\)
- \(^4\text{He}+n\)\n
<table>
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<th>Energy [MeV]</th>
<th>(\delta) [deg]</th>
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<tr>
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<tr>
<td>15</td>
<td>90</td>
</tr>
<tr>
<td>20</td>
<td>120</td>
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**chiral N°3 LO NN**

NCSMC with SRG evolved NN+3Nind

FY with bare NN

FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

The \(d-3\text{H}\) fusion takes place through a transition of \(d+3\text{H}\) is S-wave to \(n+4\text{He}\) in D-wave:

Importance of the tensor and 3N force
The experimental peak at the center of mass energy of 49.7 keV corresponds to the enhancement from the 3/2$^+$ resonance of $^5$He with chiral NN+3N(500) interaction.
\[ ^3\text{H}(d,n)^4\text{He} \text{ with chiral NN+3N(500) interaction} \]

- While the DT fusion rate has been measured extensively, a fundamental understanding of the process is still missing.
- Very little is known experimentally of how the polarization of the reactants’ spins affects the reaction.

\[
\sigma_{unpol} = \sum_j \frac{2J+1}{(2I_D+1)(2I_T+1)} \sigma_j \\
\approx \frac{1}{3} \sigma_{\frac{1}{2}} + \frac{2}{3} \sigma_{\frac{3}{2}} \\
\sigma_{pol} \approx 1.5 \sigma_{unpol}
\]

Assuming the fusion proceeds only in S-wave with spins of D and T completely aligned: Polarized cross section 50% higher than unpolarized.
$^3\text{H}(\text{d,n})^4\text{He}$ with chiral NN+3N(500) interaction

**Polarized fusion**

\[
\frac{\partial \sigma_{\text{pol}}}{\partial \Omega_{\text{c.m.}}} (\theta_{\text{c.m.}}) = \frac{\partial \sigma_{\text{unpol}}}{\partial \Omega_{\text{c.m.}}} (\theta_{\text{c.m.}}) \left( 1 + \frac{1}{2} p_{zz} A_{zz}^{(b)} (\theta_{\text{c.m.}}) + \frac{3}{2} p_x q_x C_{x,x} (\theta_{\text{c.m.}}) \right)
\]

\[
\sigma_{\text{unpol}} = \sum_j \frac{2J+1}{(2J_D+1)(2J_T+1)} \sigma_J
\]

\[
\approx \frac{1}{3} \sigma_{\frac{1}{2}} + \frac{2}{3} \sigma_{\frac{3}{2}}
\]

\[
\sigma_{\text{pol}} \approx 1.5 \sigma_{\text{unpol}}
\]

NCSMC calculation demonstrates impact of partial waves with $l > 0$ as well as the contribution of $l = 0$ $J^p = \frac{1}{2}^+$ channel.
CHAPTER 1

**Polarized fusion**

\[
\frac{\partial \sigma_{\text{pol}}}{\partial \Omega_{\text{c.m.}}}(\theta_{\text{c.m.}}) = \frac{\partial \sigma_{\text{unpol}}}{\partial \Omega_{\text{c.m.}}}(\theta_{\text{c.m.}}) \left( 1 + \frac{1}{2} p_{zz} A_{zz}^{(b)}(\theta_{\text{c.m.}}) + \frac{3}{2} p_{xz} A_{xz}(\theta_{\text{c.m.}}) \right)
\]

For a realistic 80% polarization, reaction rate increases by ~32% or the same rate at ~45% lower temperature.
Neutron-rich halo nucleus $^{11}$Be

- $Z=4$, $N=7$
  - In the shell model picture g.s. expected to be $J^\pi=1/2^-$
  - $Z=6$, $N=7$ $^{13}$C and $Z=8$, $N=7$ $^{15}$O have $J^\pi=1/2^-$ g.s.
  - In reality, $^{11}$Be g.s. is $J^\pi=1/2^+$ - parity inversion
  - Very weakly bound: $E_{th}=-0.5$ MeV
  - Halo state – dominated by $^{10}$Be-$n$ in the S-wave
  - The 1/2$^-$ state also bound – only by 180 keV

- Can we describe $^{11}$Be in *ab initio* calculations?
  - Continuum must be included
  - Does the 3N interaction play a role in the parity inversion?
Structure of $^{11}\text{Be}$ from chiral NN+3N forces

- NCSMC calculations **including chiral 3N** ($N^3\text{LO NN}+N^2\text{LO 3NF400, NNLOsat}$)
  - $n^{10}\text{Be} + ^{11}\text{Be}$
    - $^{10}\text{Be}$: $0^+, 2^+$, $2^+$ NCSM eigenstates
    - $^{11}\text{Be}$: $\geq 6 \pi = -1$ and $\geq 3 \pi = +1$ NCSM eigenstates

$^{11}\text{Be}$ within NCSMC: Discrimination among chiral nuclear forces

- $^{10}\text{Be}(0^+)$
- $^{10}\text{Be}(2^+)$

$E_{\text{thr.}}$ [MeV] vs. $N_{\text{max}}$

- $N_{\text{CSM}}$ shows much better $N_{\text{max}}$ convergence
- $N_{\text{CSM}}$ tries to capture continuum effects via large $N_{\text{max}}$
- Drastic difference for the $1/2^+$ state right at threshold

References:
$^{11}\text{Be within NCSMC: Discrimination among chiral nuclear forces}$

$^{11}\text{Be}$ within NCSMC: Discrimination among chiral nuclear forces

![Graph showing energy levels for $^{11}\text{Be}$ with NCSMC and NCSM calculations compared to experimental data.](image)

$E_{\text{thr.}}$ [MeV]

- $^{11}\text{Be}$ (0$^+$)
- $^{11}\text{Be}$ (2$^+$)

NCSM shows much better $N_{\text{max}}$ convergence.

NCSM tries to capture continuum effects via large $N_{\text{max}}$.

Dramatic difference for the 1/2$^+$ state right at threshold.

$^{11}$Be within NCSMC: Discrimination among chiral nuclear forces

$^{11}$Be within NCSMC: Discrimination among chiral nuclear forces

Parity inversion

Photo-disassociation of $^{11}\text{Be}$

Halo structure

Cluster form factor

$$\langle r^{(f)}(r) \rangle = r \langle \Phi_{\nu r}^{(f)} | A | \psi_{J}^{(f)} \rangle$$

$$\psi_{J}^{(f)} = \left[ \left( |^{10}\text{Be} \alpha_{1}T_{1}^{n}T_{j}^{n} \rangle \right) | n_{2}^{+} T_{2}^{-} \rangle \right] Y_{\nu}(r) \delta(r-r_{0,1})$$

Bound to bound

<table>
<thead>
<tr>
<th></th>
<th>NCSM</th>
<th>NCSMC-phenom</th>
<th>Expt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B(\text{E1; } 1/2^+ \rightarrow 1/2^+)$ [e² fm²]</td>
<td>0.0005</td>
<td>0.117</td>
<td>0.102(2)</td>
</tr>
</tbody>
</table>

Bound to continuum

$\gamma^{+}^{11}\text{Be}(1/2^+) \rightarrow ^{10}\text{Be(g.s.)} + n$
NCSMC wave functions of $^{11}$Be used as input for other studies
Halo sd-shell nucleus $^{15}$C

- **Motivation:**
  - Halo $\frac{1}{2}^+$ S-wave and $5/2^+$ D-wave bound states
  - $^{14}$C(n,γ)$^{15}$C capture relevant for astrophysics

- Calculations in progress – all results preliminary
- NN chiral interaction – N$^3$LO Entem & Machleidt 2003, SRG evolved with $\lambda = 2.0$ fm$^{-1}$
- 3N chiral interaction – N$^2$LO with local/non-local regulator, SRG evolved with $\lambda = 2.0$ fm$^{-1}$
Halo sd-shell nucleus $^{15}\text{C}$

- NCSMC
  - $^{14}\text{C}$ ($^{14}\text{O}$) 0$^+$ and 2$^+$ eigenstates
  - $^{15}\text{C}$ ($^{15}\text{F}$) lowest 7 positive and 3 negative parity eigenstates

NCSMC-pheno

![Graphs showing energy levels and angular distributions for NCSMC-pheno calculations with $^{14}\text{C}$ and $^{15}\text{C}$ isotopes.](image)
**15C cluster form factors**

- **1/2⁺ S-wave and 5/2⁺ D-wave ANCs**
  - $C_{1/2^+} = 1.282 \text{ fm}^{-1/2}$ - compare to Moschini & Capel inferred from transfer data: $1.26(2) \text{ fm}^{-1/2}$
  - $C_{5/2^+} = 0.048 \text{ fm}^{-1/2}$
  - Spectroscopic factors: 0.96 for 1/2⁺ and 0.90 for 5/2⁺ - experiments 0.95(5) and 0.69, resp.
\(^{14}\text{C}(n,\gamma)^{15}\text{C} \) capture cross section


Relevant for
- Inhomogeneous Big Bang models
- Neutron induced CNO cycles
- Neutrino driven wind models for the r-process
- Validation of Coulomb dissociation method
Conclusions

- *Ab initio* calculations of nuclear structure and reactions becoming feasible beyond the lightest nuclei
  - Make connections between the low-energy QCD, many-body systems, and nuclear astrophysics

- Polarized DT fusion investigated within NCSMC
  - Sheds light on importance of \(/>0\) partial waves

- $^{11}$Be parity inversion explained with chiral NN+3N $N^2LO_{sat}$ interaction

- NCSMC calculations of $^{15}$C *sd*-shell halo nucleus in progress
  - Capture cross section, cluster form factors, ANCs
Thank you!

Merci!