Ab initio calculations of $^3\text{H}(d,n)^4\text{He}$ fusion

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Deuterium-Tritium fusion: a future energy source

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

Resonance at $E_{cm} = 48$ 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
Ab initio calculation of the Deuterium-Tritium fusion

- The $d^+\text{^3}H\rightarrow n^+\text{^4}He$ reaction
  - Many experimental cross section measurements

- Unresolved issues remain
  - Cross section dependence on polarization of the $d$ and $\text{^3}H$ nuclei less well known
  - Cross section modification due to the plasma environment (electron screening)
  - Mirror reaction $d^-\text{^3}He\rightarrow p^+\text{^4}He$ has larger uncertainties
  - Related reactions, i.e., $\text{^3}H(d,y)^5\text{He}$, $\text{^3}H(\text{^3}H,2n)^4\text{He}$, much less known, hard to measure

- From first principles or ab initio:
  - Nuclei as systems of nucleons interacting by nucleon-nucleon (and 3N) forces that describe accurately nucleon-nucleon (and $A=3$) systems

Ab initio theory can help shedding light on some of these issues: never attempted before!
Our many-body technique:

- **Combine** the *ab initio* no-core shell model (NCSM) with the resonating group method (RGM)

- **The NCSM:** An approach to the solution of the $A$-nucleon bound-state problem
  - Accurate nuclear Hamiltonian
  - Finite harmonic oscillator (HO) basis
    - Complete $N_{\text{max}}\Omega$ model space
  - Effective interaction due to the model space truncation
    - Similarity-Renormalization-Group evolved $NN(+NNN)$ potential
  - Short & medium range correlations
  - No continuum

- **The RGM:** A microscopic approach to the $A$-nucleon scattering of clusters
  - Nuclear Hamiltonian may be simplistic
  - Cluster wave functions may be simplified and inconsistent with the nuclear Hamiltonian
  - Long range correlations, relative motion of clusters

*Ab initio NCSM/RGM:* Combines the best of both approaches

**Accurate** nuclear Hamiltonian, **consistent** cluster wave functions

**Correct asymptotic expansion,** Pauli principle and translational invariance
The \textit{ab initio} NCSM/RGM in a snapshot

- Ansatz: \( \Psi^{(A)} = \sum \int d\vec{r} \phi_v(\vec{r}) \hat{A} \Phi^{(A-a,a)}_{\mu^\nu} \)

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

  \[ \sum \int d\vec{r} \left[ \mathcal{H}^{(A-a,a)}_{\mu^\nu}(\vec{r}', \vec{r}) - E \mathcal{N}^{(A-a,a)}_{\mu^\nu}(\vec{r}', \vec{r}) \right] \phi_v(\vec{r}) = 0 \]

  \[ \langle \Phi^{(A-a,a)}_{\mu^\nu} \left| \hat{A} H \hat{A} \right| \Phi^{(A-a,a)}_{\mu^\nu} \rangle \]
  \[ \langle \Phi^{(A-a,a)}_{\mu^\nu} \left| \hat{A}^2 \right| \Phi^{(A-a,a)}_{\mu^\nu} \rangle \]
  \[ \text{Hamiltonian kernel} \quad \text{Norm kernel} \]

- Many-body Schrödinger equation:

- \text{eigenstates of } H_{(A-a)} \text{ and } H_{(a)} \text{ in the } \text{ab initio} \text{ NCSM basis}

- Realistic nuclear Hamiltonian
Localized parts of kernels expanded in the HO basis

\[
\mathcal{N}_{\mu\ell',\nu\ell}^{(A-1,1)} (r', r) = \delta_{\mu\nu} \delta_{\ell\ell'} \frac{\delta(r' - r)}{r' r} (A - 1) \sum_{n'n} R_{n'\ell'}(r') \langle \Phi_{\mu\ell' n'n}^{(A-1,1)JT} | P_{A-1} | \Phi_{\nu\ell n}^{(A-1,1)JT} \rangle R_{n\ell}(r)
\]

\[
\langle \psi_{\mu_1}^{(A-1)} | a^+ a | \psi_{\nu_1}^{(A-1)} \rangle_{SD}
\]

Single-nucleon projectile: the norm kernel
Ab initio calculation of the $^3\text{H}(d,n)^4\text{He}$ fusion: Equations

\[ \int dr \ r^2 \left( \left\langle \frac{r'}{n} A_1 (H - E) \hat{A} \right| \varepsilon_n \right) \left( \left\langle \frac{r'}{n} A_2 (H - E) \hat{A} \right| \varepsilon_n \right) \left( \begin{array}{c} g_1(r) \\ g_2(r) \end{array} \right) = 0 \]
Solving the RGM equations

• The many-body problem has been reduced to a two-body problem!
  – Macroscopic degrees of freedom: nucleon clusters
  – Unknowns: relative wave function between the two clusters

• Non-local integral-differential coupled-channel equations:

\[
\left[ T_{rel}(r) + V_C(r) + E^{(A-a)}_{\alpha_1} + E^{(a)}_{\alpha_2} \right] u^{(A-a,a)}_\nu(r) + \sum_{a'v'} \int dr'r' W_{av,a'v'}(r,r') u^{(A-a',a')}_{v'}(r') = 0
\]

• Solve with R-matrix theory on Lagrange mesh imposing
  – Bound state boundary conditions ➔ eigenenergy + eigenfunction
  – Scattering state boundary conditions ➔ Scattering matrix
    • Phase shifts
    • Cross sections
    • ...

The R-matrix theory on Lagrange mesh is an elegant and powerful technique, particularly for calculations with non-local potentials
Input: \( NN \) interaction, \( ^2H, ^3H, ^3He, ^4He \) eigenstates

- Similarity-Renormalization-Group (SRG) evolved chiral \( N^3LO \) \( NN \) interaction
  - Accurate
  - Soft: Evolution parameter \( \Lambda \)
    - Study dependence on \( \Lambda \)
    - NNN interaction interaction effects for \( \Lambda=3,4,5 \) partly included for \( \Lambda\sim1.5 \text{ fm}^{-1} \)

- \( ^2H, ^3H, ^3He, ^4He \)
  - NCSM up to \( N_{\text{max}}=12 \): Sufficient for the selected NN potential with \( \Lambda=1.5 \text{ fm}^{-1} \)
  - Variational calculation
    - Optimal HO frequency from the ground-state minimum: Different for \( ^3H \) and \( ^4He \)
    - Select: \( \hbar\Omega=14 \text{ MeV} \)

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
\textbf{\( E_{\text{g.s.}} \) [MeV]} & \( ^2H \) & \( ^3H \) & \( ^3He \) & \( ^4He \) \\
\hline
\textbf{Calc.} & -2.20 & -8.27 & -7.53 & -28.22 \\
\hline
\textbf{\( \langle r_p^2 \rangle^{1/2} \) [fm]} & \( ^3H \) & \( ^3He \) & \( ^4He \) \\
\hline
\textbf{Calc.} & 1.64 & 1.81 & 1.49 \\
\textbf{Expt.} & 1.60 & 1.77 & 1.467(13) \\
\hline
\end{tabular}
\end{table}
**d+³H and n+⁴He elastic scattering: phase shifts**

- **d+³H elastic phase shifts:**
  - Resonance in the $^4S_{3/2}$ channel
  - Repulsive behavior in the $^2S_{1/2}$ channel → Pauli principle

- **n+⁴He elastic phase shifts:**
  - $d+³H$ channels produces slight increase of the $P$ phase shifts
  - Appearance of resonance in the $3/2^+$ $D$-wave, just above $d-³H$ threshold

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**The $d-³H$ fusion takes place through a transition of $d+³H$ is $S$-wave to $n+⁴He$ in $D$-wave:**

Importance of the **tensor force**
$^3\text{H}(d,n)^4\text{He}$ and $^3\text{He}(d,p)^4\text{He}$ cross sections

- NCSM/RGM:
  - $N_{\text{max}} = 13$
  - SRG-$N^3\text{LO}$ NN ($\Lambda=1.5$ fm$^{-1}$) potential
  - Only g.s. of $d$, $^3\text{H}$, $^4\text{He}$ included above

$$S(E) = E\sigma(E)\exp\left(\frac{2\pi Z_1Z_2e^2}{\hbar\sqrt{2mE}}\right)$$
The cross section improves with the inclusion of virtual breakup of the deuteron

- Deuteron weakly bound: easily gets polarized and easily breaks
- These effects included below the breakup threshold with continuum discretized by pseudo-states

First *ab initio* results for $d$-$^3$H and $d$-$^3$He fusion:
Very promising, correct physics, can become competitive with fitted evaluations …
\( ^3\text{H}(d,n)^4\text{He} \) cross section

- SRG-N\(^3\)LO (\(\Lambda=1.45 \text{ fm}^{-1}\)) NN potential
  - Position of the resonance matches experiment

S-factor narrower than the data
Resonance in the \(d^3\text{H}^4S_{1/2}\) partial wave
\(n^4\text{He}^2D_{3/2}\) decreasing, does not cross 90 degrees
### $^3\text{H}(d,n)^4\text{He}$ S-factors at $E_{\text{kin}}=0$

<table>
<thead>
<tr>
<th>$S(0)$ [MeV b]</th>
<th>$^3\text{H}(d,n)^4\text{He}$</th>
<th>$^3\text{He}(d,p)^4\text{He}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SRG-N$^3$LO $NN$</td>
<td>10 ± 0.5</td>
<td>6.0 ± 0.2</td>
</tr>
<tr>
<td>R-matrix data eval.</td>
<td>11.7 ± 0.2</td>
<td>5.9 ± 0.3</td>
</tr>
</tbody>
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- $\Lambda=1.45$ fm$^{-1}$ for $^3\text{H}(d,n)^4\text{He}$
- $\Lambda=1.5$ fm$^{-1}$ for $^3\text{H}(d,n)^4\text{He}$

$^3\text{He}(d,p)^4\text{He}$ in a good agreement with data evaluation

Strong electron screening in $^3\text{He}(d,p)^4\text{He}$ below 30 keV
Possibly some electron screening in $^3\text{H}(d,n)^4\text{He}$ below 10 keV

**Improvements:**
- Excitations of $^4\text{He}$; n-p-$^3\text{H}$ rather than d*, d”*
- Polarization of $^3\text{H}$; NNN interaction
Conclusions and Outlook

- With the NCSM/RGM approach we are extending the *ab initio* effort to describe low-energy reactions and weakly-bound systems

- The first $^7\text{Be}(p,\gamma)^8\text{B}$ *ab initio* S-factor calculation

- Deuteron-projectile results with SRG-N$^3$LO $NN$ potentials:
  - $d$-$^4\text{He}$ scattering
  - First *ab initio* study of $^3\text{H}(d,n)^4\text{He}$ & $^3\text{He}(d,p)^4\text{He}$ fusion

- Under way:
  - $^3\text{He}$-$^4\text{He}$ and $^3\text{He}$-$^3\text{He}$ scattering calculations
  - *Ab initio* NCSM with continuum (*NCSMC*)
  - Three-cluster NCSM/RGM and treatment of three-body continuum

- To do:
  - Inclusion of NNN force
  - Alpha clustering: $^4\text{He}$ projectile