Ab initio Nuclear Reactions

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Physical and Life Sciences/Physics

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Ab initio Reactions: NCSM/RGM

Team:
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LLNL effort:
  • UNEDF – Year 5:
    - Benchmark n-$^8$He, and n-$^9$Li scattering.
    - Investigate p-$^7$Be scattering and capture reactions.
    - Investigate $^3$He-$^4$He scattering and capture reactions.
    - Use two-, three-, and four-body transition densities for A=3,4 nuclei.
    - Development of three-body transition density calculation for A>4.
  • LDRD
    - Develop formalism for a=2,3,4 clusters in the RGM formalism
    - Code Hamiltonian and Norm kernels for a=2,3,4 clusters with NN
    - Primary goal is to get to $^{12}$C($\alpha,\gamma$)$^{16}$O
    - Ambitious goal, will get to a=3 clusters this year
Ab initio Reactions: NCSM/RGM

- FY11 UNEDF DOE/NP budget decreased by 50%
  - Effort on ab initio reactions was decreased to zero on UNEDF
    - Due to commitment to post-doctoral employees in other efforts

- Reduction will be restored, and deliverables will be rethought

- Still operating under CR rules
  - Funding received in pro-rated amounts quarterly
  - Currently, only 42% of the reduced budget has been received
    - Affects subcontract to SDSU
**Ab initio** NCSM/RGM Formalism

- **Ab initio** calculations for reactions and clustering in nuclei
- Constructs integration kernels (≈ projectile-target potentials) starting from
  - NCSM wave functions
  - NN(+NNN) interactions
- Solves:
  \[
  \sum \int d\vec{r} \left[ \mathcal{H}_{\mu\nu}^{(A-a,a)}(\vec{r}',\vec{r}) - E\mathcal{N}_{\mu\nu}^{(A-a,a)}(\vec{r}',\vec{r}) \right] \phi_\nu(\vec{r}) = 0
  \]

The Resonating Group Method correctly accounts for:
1) the interaction (Hamiltonian kernel) and the Pauli principle (Norm kernel) between clusters and 2) all the available channels

Ultimate Goal: \(3\alpha \rightarrow ^{12}\text{C}\) and \(^{12}\text{C}(\alpha,\gamma)^{16}\text{O}\)
Accurate evaluations and uncertainties for nuclear astrophysics and fusion diagnostic

- The elastic $n^{-3}H$ cross section for 14 MeV neutrons, important for understanding how the fuel is assembled in an implosion at NIF, was not known precisely enough.
- Nuclear theory was asked to help.
- Delivered evaluated data with required 5% uncertainty and successfully compared to measurements using an Inertial Confinement Facility.

- $T(T,2n)^4He$ also important
  - Requires 3-body cluster states

*Ab initio* theory reduces uncertainty due to conflicting data ($\bullet$, $\circ$, $\Delta$, $\triangle$, $\triangledown$ )

Navrátil et al., LLNL-TR-423504, LLNL-TR-435981, arXiv.1009.3965
Reactions important for solar astrophysics


- The $^7\text{Be}(p,\gamma)^8\text{B}$ is the final step in the nucleosynthetic chain leading to $^8\text{B}$
- $\sim10\%$ error in latest $S_{17}(0)$: dominated by uncertainty in theoretical models
- NCSM/RGM results with largest realistic model space
  - SRG-$N^3\text{LO}$ NN potential ($\lambda = 1.86 \text{ fm}^{-1}$)
  - $N_{\text{max}} = 10$
  - $p^+^7\text{Be}(\text{g.s., } 1/2^-, 7/2^-, 5/2_1^-, 5/2_2^-)$
- Sep. energy: 136 keV (Expt. 137 keV)
- $S_{17}(0) = 19.4 \text{ eV b}$ on the lower side of, but consistent with latest evaluation
- Run time: $\sim150,000 \text{ CPU hrs}$

**$^7\text{Be}(p,\gamma)^8\text{B}$ astrophysical S-factor**

$$\sigma(E) = \frac{S(E)}{E} \exp\left(\frac{-2\pi Z_e^2 e^2}{h\sqrt{2mE}}\right)$$

*Ab initio* theory predicts simultaneously both normalization and shape of $S_{17}$. 
Reactions important for solar astrophysics

- Remaining uncertainties
- Larger $N_{\text{max}}$
  - $N_{\text{max}} = 10,12$ calculations with 3 lowest $^7$Be eigenstates very close
  - $N_{\text{max}} = 10$ reasonable HO model space
- Higher $^7$Be eigenstates
  - $N_{\text{max}} = 8$ with 8 lowest $^7$Be eigenstates
  - Influence of $7/2^-$ could be significant
  - But: $N_{\text{max}} = 8$ is not sufficient!
  - $N_{\text{max}} = 10$, with 8 $^7$Be eigenstates presently out of reach
- $\pm 0.7$ eV b uncertainty on $S_{17}(0)$
- NNN force (SRG-induce + “real”) still missing

$^7$Be($p,\gamma)^8$B astrophysical S-factor

$\sigma(E) = \frac{S(E)}{E} \exp\left(\frac{-2\pi Z_Z e^2}{\hbar \sqrt{2mE}}\right)$

Ab initio theory predicts simultaneously both normalization and shape of $S_{17}$. 
Reactions with clusters – LDRD -> SciDAC-3

- NCSM/RGM results for $d(^{3}\text{He},p)^{4}\text{He}$
  - SRG-$N^{3}$LO NN potential ($\lambda = 1.5 \text{ fm}^{-1}$)
  - Approx. treatment of virtual breakup:
    Include multiple excited deuteron pseudo-states
- Data curve up and deviate from theoretical results at low energy due to laboratory electron-screening.
- Run time: $\sim 100,000 \text{ CPU hrs}$

**Fundamental description still requires:**
1) NNN force (SRG-induced + “real”)
2) 3-body cluster states & solution of 3-body scattering problem

**$^{3}\text{He}(d,p)^{4}\text{He}$ astrophysical S-factor**

\[
s(E) = \frac{S(E)}{E} \exp\left(\frac{-2nZ_{1}Z_{2}e^{2}}{h\sqrt{2mE}}\right)
\]

- $d^{3}\text{He} \rightarrow p^{4}\text{He}$

Excited $d$ pseudo-states in both $^{3}S_{1}$-$^{3}D_{1}$ and $^{3}D_{2}$ channels

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NSCM/RGM in the future

- Couple NCSM/RGM \((A-a,a)\) basis with NCSM \(A\)-body eigenstates (NCSMC)

\[
\Psi^{(A)}_{\text{NCSMC}} = \sum_{\lambda} c^{(A)}_{\lambda} \left| A \lambda J^\pi T \right> + \sum_{a,\nu} \int d\vec{r} \; \varphi^{(A-a,a)}_{\nu} (\vec{r}) \; \hat{A}^{(A-a,a)} \left| \Phi^{(A-a,a)}_{\nu} \right>
\]

- Solve:

\[
\begin{pmatrix}
H & h \\
h & \mathcal{H}
\end{pmatrix}
\begin{pmatrix}
c \\
\varphi
\end{pmatrix} =
\begin{pmatrix}
1 & g \\
g & \mathcal{N}
\end{pmatrix}
\begin{pmatrix}
c \\
\varphi
\end{pmatrix}
\]

- First step, \(A + (A-1,1)\) formalism, under development by S. Baroni & P. Navratil
- Develop the NCSMC formalism with \(a > 1\)
- Consistent treatment of bound and continuum states
- Three-body final states \(T(T,2n)^4\text{He}\)
Activities with restoration

- Benchmark n-$^8$He, and n-$^9$Li scattering.
- Investigate p-$^7$Be scattering and capture reactions.
- Investigate $^3$He-$^4$He scattering and capture reactions.
  - Use two-, three-, and four-body transition densities for A=3,4 nuclei.
  - Development of three-body transition density calculation for A>4.
- Include NNN interaction for n+A and p+A systems