Ab initio reactions of nucleons on light nuclei

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The \textit{ab initio} NCSM/RGM in a snapshot

- Ansatz: \( \Psi^{(A)} = \sum \int d\vec{r} \phi_{\nu}(\vec{r}) \hat{A} \Phi_{\nu \vec{r}}^{(A-a,a)} \)

- Many-body Schrödinger equation:

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

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

- Non-local integro-differential coupled-channel equations:

\[ [\hat{T}_{\text{rel}}(r) + \hat{V}_C(r) - (E - E_{\nu})] u_{\nu}(r) + \sum_{\nu} \int dr' r' W_{\nu \nu}(r, r') u_{\nu}(r') = 0 \]

Fully implemented for \textit{nucleon-nucleus} basis. Work on \textit{deuteron-nucleus} basis under way.
NCSM/RGM *ab initio* calculation of $n^{-3}H$ and $p^{-3}He$ phase shifts

- NCSM/RGM calculations with $n^{+3}H$(g.s.) and $p^{+3}He$(g.s.), respectively.
- $\chi$EFT $N^3$LO NN potential: convergence reached with two-body effective interaction
- Benchmark with Alt, Grassberger and Sandhas (AGS) results [PRC75, 014005(2007)]
  - What is missing? - $n^{+3}H$(ex), $^2n$+d, $p^{-3}He$(ex), $^2p$+d configurations

The omission of three-nucleon partial waves with $1/2 < J \leq 5/2$ leads to effects of comparable magnitude on the AGS results. Need to include target excited states!
$n^{-4}\text{He} \& p^{-4}\text{He}$ phase shifts from accurate NN interactions

- $^{-4}\text{He}$ states: g.s., 0$^+$
- Reasonable agreement with experiment for $^2S_{1/2}$, $^2P_{1/2}$, $^2D_{3/2}$ channels
- Coulomb under control

Insufficient spin-orbit strength: $^2P_{3/2}$ underestimated $\rightarrow$ NNN needed

CD-Bonn the best description of $^2S_{1/2}$ phase shifts
First ever *ab initio* calculation of $A_y$ in for a $A=5$ system. *Strict test of inter-nucleon interactions.*


### NCSM/RGM *ab initio* calculation of $n+^7\text{Li}$ scattering

**$^7\text{Li}$**
- Full NCSM up to $N_{\text{max}}=10$ (12 possible)
- IT-NCSM up to $N_{\text{max}}=18$
  - Convergence of both ground and excited states

**$^8\text{Li}$**
- NCSM predicts unobserved low-lying $0^+$ and $2^+$ states
- NCSM/RGM with $^7\text{Li}$ $3/2^-$ and $1/2^-$ bound states included
- Up to $N_{\text{max}}=14$ so far ($\hbar\Omega=20$ MeV used)
  - Moderate changes from $N_{\text{max}}=6$ to $N_{\text{max}}=14$
- Bound states
  - $2^+$ state bound by 1.07 MeV (expt 2.03 MeV)
  - $1^+$ state bound by 0.18 MeV (expt 1.05 MeV)

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![Graph](https://via.placeholder.com/150)

**$^7\text{Li}$**

**$^7\text{Li}$**

**$^8\text{Li}$**

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**PRC 73, 065801 (2006)**
NCSM/RGM \textit{ab initio} calculation of $n+^7\text{Li}$ scattering

- $^7\text{Li}$ 3/2$^-$ and 1/2$^-$ bound states included
- SRG-$N^3\text{LO}$ NN interaction with $\Lambda=2.02$ fm$^{-1}$
  - Up to $N_{\text{max}}=14$ so far (h$\Omega=20$ MeV used)
  - Moderate changes from $N_{\text{max}}=6$ to $N_{\text{max}}=14$
  - $2^+$ and $1^+$ states bound
  - Other states unbound

\begin{align*}
4.652 & \quad 7^2 \text{Li} \\
2.467 & \quad ^4\text{He}+t \\
0.47761 & \quad j=\frac{3}{2}; T=\frac{1}{2}
\end{align*}

\begin{align*}
3.21 & \quad 1^+ \text{Li} \\
2.255 & \quad 3^+ \text{Li} \\
0.9808 & \quad ^8\text{Li}
\end{align*}

- S-wave scattering length
  - Expt: $a_{01}=0.87(7)$ fm
  - $a_{02}=-3.63(5)$ fm
  - Calc: $a_{01}=1.31$ fm
  - $a_{02}=-0.18$ fm

Qualitative agreement with experiment. Calculated broad $1^+$ resonance, predicted narrow $0^+$ resonance. The $3^+$ resonance not seen when $^7\text{Li}$ 7/2$^-$ state not included.
NCSM/RGM *ab initio* calculation of \( n + ^7\text{Li} \) scattering

- \(^7\text{Li} 3/2^-, 1/2^-\) and \( 7/2^-\) states included
- Result for \( N_{\text{max}}=8 \) shown
- \( 2^+ \) and \( 1^+ \) states bound (slightly more)
- \( 0^+ \) and \( 1^+ \) resonances not affected
- \( 3^+ \) and \( 2^+ \) resonances appear
- Improvement of S-wave scattering length

\[
\begin{align*}
\text{Expt: } a_{01} &= 0.87(7) \text{ fm} \\
a_{02} &= -3.63(5) \text{ fm} \\
\text{Calc: } a_{01} &= 0.73 \text{ fm} \\
a_{02} &= -1.42 \text{ fm}
\end{align*}
\]

Good match of bound states and narrow resonances with the \(^8\text{Li} \) NCSM result. Predicted narrow \( 0^+ \) and \( 2^+ \) resonance. Seen at recent \( p + ^7\text{Be} \) FSU experiment.
Nucleon-$^{12}\text{C}$ scattering with SRG-$N^3\text{LO}$ NN potential

- $^{12}\text{C}$
  - Full NCSM up to $N_{\text{max}}=8$
  - IT NCSM up to $N_{\text{max}}=18(!)$
    - Perfect agreement for both the $0^+$ ground- and $2^+$ excited state up to $N_{\text{max}}=8$
    - Convergence of the IT-NCSM
      - $\hbar\omega=24$ MeV used
  - $^{13}\text{N}$, $^{13}\text{C}$ within the NCSM
    - $1/2^+$ state too high by $\sim 6$ MeV
- $^{13}\text{N}$, $^{13}\text{C}$ within the NCSM/RGM
  - up $N_{\text{max}}=16$ with $^{12}\text{C}$ g.s. and $2^+$ included
  - $^{13}\text{C}$:
    - $1/2^-$ bound by $5.34$ MeV (expt $4.95$ MeV)
    - $3/2^-$ bound by $2.23$ MeV (expt $1.27$ MeV)
    - $1/2^+$ bound by $0.03$ MeV (expt $1.86$ MeV)
      - Excitation energy $5.31$ MeV (expt $3.09$ MeV)

Excitation energy of the $1/2^+$ state drops by $4$ MeV when $n-^{12}\text{C}$ long-range correlations included
**$p$-$^{12}C$ scattering with SRG-N$^3$LO NN potential**

- Experiments with a polarized proton target under way
- NCSM/RGM up $N_{\text{max}}=16$
  - $^{12}C$ g.s. and $2^+$ included
  - $1/2^-$ state bound by 2.9 MeV
    - $^{13}N$ ground state
  - Other states unbound
  - $1/2^+$ resonance at ~1.2 MeV
  - $5/2^+$ resonance
  - Good stability: Moderate changes from $N_{\text{max}}=6$ to $N_{\text{max}}=16$
  - Minimal difference between $N_{\text{max}}=14$ and $N_{\text{max}}=16$

Qualitative agreement with experiment
The deuteron projectile: Norm kernel

\[ \langle 1, \ldots, A-2 | r' \rangle (A-1, A) \begin{aligned} 1 & - 2( A - 2 ) \hat{P}_{A-2, A-1} + \frac{1}{2} (A - 2)(A - 3) \hat{P}_{A-2, A-1} \hat{P}_{A-3, A-1} \end{aligned} \begin{aligned} \mu, \ell' & - 2(A-2) \times \end{aligned} \begin{aligned} v, \ell \end{aligned} (A-2) (2) + (A-2)(A-3)/2 \times \begin{aligned} \langle (A-2) | r \rangle (A-1, A) \end{aligned} \]

\[ SD \left\langle \psi_{\mu_1}^{(A-2)} | a^+ a^+ a a \psi_{\nu_1}^{(A-2)} \right\rangle_{SD} \]
The deuteron projectile: Hamiltonian kernel

\[
\begin{align*}
-2(A - 2)(A - 3) & V_{A-1,A-3} \hat{P}_{A-2,A-1} \\
\end{align*}
\]
$d$-$\alpha$ scattering: Progress so far

- Norm kernel coded
- Hamiltonian kernel partially coded
  - Term with three-body density in progress
- Convergence reached for $d$-$\alpha$ norm kernel (physics - Pauli principle)
Toward the first \textit{ab initio} description of the Deuterium-Tritium fusion

- Solve the many-body Schrödinger equation in the Hilbert space spanned by the RGM basis states:

\[ \int dr \ r^2 \left\langle r' \ \alpha \ \frac{\hat{A}_1 (H - E)}{A_1} \ \alpha \ r \ \alpha \ r_n \ \frac{\hat{A}_2 (H - E)}{A_2} \ T \ D \right| \left( g_1 (r) \ \frac{r_r}{r} \right) = 0 \]

- Progress so far: Norm kernels calculated

The D+T norm kernel:
(a) diagrammatic representation of the “direct” and “exchange” components; exchange components for the spin-parity-isospin (b) 1/2+1/2 and (c) 3/2+1/2 channels
FY09 accomplishments

- Development of *ab initio* many-body reaction theory by merging the NCSM and the RGM (P. Navratil and S. Quaglioni)
  - Results with NN potentials used by UNEDF collaboration
    - $n^{-7}$Li with SRG-N$^3$LO using the importance-truncated NCSM
    - $p^{-12}$C with SRG-N$^3$LO using the importance-truncated NCSM
    - $n^{-16}$O with SRG-N$^3$LO using the importance-truncated NCSM
    - Collaboration with R. Roth (TU Darmstadt)
  - Deuteron-nucleus scattering under development

- Development of the TRDENS transition density code
  - Distribution of two-body density structure over groups of processors

- Similarity-renormalization-group evolution of NN+NNN interactions
  - Collaboration with D. Furnstahl (OSU) and E. Jurgenson (OSU)

- $A=14$ nuclei with chiral EFT NN+NNN up to $N_{\text{max}}=8$
  - Transformation of NNN to SD basis up to $N_{\text{max}}=8$
  - Collaboration with J. Vary, P. Maris, H. Nam, E. Ormand and D. Dean
Publications relevant to UNEDF in 2008/2009


- S. Quaglioni, P. Navratil, *Ab initio many-body calculations of n-3H, n-4He, p-3He, 4He, and n-10Be scattering*, PHYSICAL REVIEW LETTERS 101, 092501 (2008)

Future plan

- The rest of Year 3
  - Complete \textit{n-7Li} calculations
  - Begin \textit{n-8He} investigation
  - Continue work on deuteron-nucleus formalism (supported by LDRD)

- Year 4
  - \textit{n-8He}, \textit{n-9Li} calculations
  - Development of \textit{3H} and \textit{3He} – nucleus formalism (supported by LDRD)
  - Development of the coupling of NCSM/RGM and NCSM $\rightarrow$ NCSMC
  - Similarity-renormalization-group evolution of NN+NNN interactions
    - Application to \textit{p}-shell nuclei (supported by DOE/SC/NP)
  - Further development of importance-truncation NCSM scheme

- Year 5
  - High profile science: Capture reactions - $^3\text{He}(\alpha,\gamma)^7\text{Be}$

- Computational challenges:
  - \textit{n-body} density \((n>2)\) calculations
    - Distribution of structure allocation, parallelization