Toward Realistic Calculations of Light-Ion Fusion Reactions

INT “Structure of light Nuclei”
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Guillaume Hupin

Collaborators:
S. Quaglioni (LLNL)
P. Navrátil (TRIUMF, LLNL)
R. Roth (TU Darmstadt)
J. Langhammer (TU Darmstadt)
W. Horiuchi (Hokkaido Univ.)
From nucleons to nuclei to fusion reactions

- **Objective:**
  
  *Address static and dynamical properties of light ions and describe fusion reactions.*

- **Ingredients**
  
  - High-precision nuclear interaction, two- plus three-nucleon, derived from the Chiral Effective Field Theory (EFT) and softened by the Similarity Renormalization Group technique.

- **Recipe**
  
  - Solve the Schrödinger equation.
  - Address structural properties. (bound states, narrow resonances)
    - *Ab initio* many-body approaches ($A \leq \sim 16$); No-Core Shell Model (NCSM)
  - Address dynamical properties. (scattering, reactions)
    - Extend No-Core Shell-Model with the Resonating Group Method (RGM)
Some of the building block of our universe are driven by fusion processes: nucleosynthesis, stellar evolution ...

Nuclear astrophysics community relies on accurate fusion reactions observables.

Turn out to be experimentally challenging:

- Low rates: Coulomb repulsion + Low energy (quantum tunneling effects).
- Projectile and target are not fully ionized in a lab. This leads to laboratory electron screening

A fundamental theory is needed to enhance predictive capability of stellar modeling
**Ab initio NCSM/RGM Formalism for binary clusters**


- Starts from:
  \[ \Psi^{(A)}_{RGM} = \sum_{\nu} \int d \vec{r} \, g_{\nu}(\vec{r}) \, \hat{A}_{\nu} | \Phi^{(A-a,a)}_{v_{\vec{r}}} \rangle \]

  - **Relative wave function** (unknown)
  - **Channel basis**

- **Schrödinger equation on channel basis:**
  \[ H \Psi^{(A)}_{RGM} = E \Psi^{(A)}_{RGM} \sum_{\nu} \int d \vec{r} \left[ H_{v'v}(\vec{r}', \vec{r}) - E \, N_{v'v}(\vec{r}', \vec{r}) \right] g_{\nu}(\vec{r}) = 0 \]

  - **Hamiltonian kernel**
  - **Norm (overlap) kernel**

- Constructs integration kernels (≈ projectile-target potentials) starting from:
  - Underlying (realistic) interactions among nucleons
  - NCSM *ab initio* wave functions

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**RGM accounts for:** 1) nucleon-nucleon interaction (Hamiltonian kernel), 2) Pauli principle (Norm kernel) between clusters and 3) center of mass motion of cluster; NCSM accounts for: internal structure of clusters

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Navrátil and Quaglioni, PRL 101, (2008)
Navrátil and Quaglioni, PRL 108, (2012)
**Ab initio NCSM/RGM Formalism for binary clusters**

a few details

\[
|\Psi_{J^T}\rangle = \sum_v \int \frac{g_v^{J^T}(r)}{r} \hat{A}_v \left[ \langle A - a | \alpha_1 I_1^{\pi_1} T_1 | a \alpha_2 I_2^{\pi_2} T_2 \rangle \right]^{(sT)} Y_\ell (\hat{r}_{A-a,a}) \frac{\delta(r - r_{A-a,a})}{rr_{A-a,a}} r^2 dr
\]

Relative wave functions subject to the boundary/scattering asymptotic solution within R-matrix theory

We use the closure properties of HO radial wave function

\[
\delta(r - r_{A-a,a}) = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})
\]

We defined the RGM model space such that \(n < N_{\text{max}}\), this expansion is good for localized parts of the integration kernels.

Since we are using NCSM wave functions, it is convenient to introduce Jacobi channel states in the HO space

\[
|\Phi_{vn}^{J^T}\rangle = \left[ \langle A - a | \alpha_1 I_1^{\pi_1} T_1 | a \alpha_2 I_2^{\pi_2} T_2 \rangle \right]^{(sT)} Y_\ell (\hat{r}_{A-a,a}) R_{n\ell}(r_{A-a,a})
\]

The coordinate space channel states are given by

\[
|\Phi_{vr}^{J^T}\rangle = \sum_n R_{n\ell}(r) |\Phi_{vn}^{J^T}\rangle
\]
Matrix elements of translationally invariant operators

- Translational invariance is preserved (exactly!) also with SD cluster basis

\[
\begin{align*}
\langle \Phi_{fSD}^{(A-a',a')} | \hat{O}_{t.i.} | \Phi_{iSD}^{(A-a,a)} \rangle_{SD} &= \sum_{i_R f_R} M_{iSD fSD} i_R f_R \langle \Phi_{f_R}^{(A-a',a')} | \hat{O}_{t.i.} | \Phi_{i_R}^{(A-a,a)} \rangle_{SD} \\
\end{align*}
\]

What we calculate in the “SD” channel basis

- Observables calculated in the translationally invariant basis

Advantage: can use powerful second quantization techniques

\[
\begin{align*}
\langle \Phi_{v'n'}^{(A-a',a')} | \hat{O}_{t.i.} | \Phi_{vn}^{(A-a,a)} \rangle_{SD} \propto \langle \psi_{\alpha_1}^{(A-a')} | a^+ \rangle \langle a \psi_{\alpha_1}^{(A-a)} \rangle_{SD}, \quad SD \langle \psi_{\alpha_1}^{(A-a')} | a^+ a a^+ a a \psi_{\alpha_1}^{(A-a)} \rangle_{SD}, \ldots
\end{align*}
\]
Matrix elements of translationally invariant operators

Then the SD channel states are defined such that the eigenstates of the heaviest of the two clusters (target) are described by a SD wave function:

\[
\left| \Phi_{vn}^{J^\pi T} \right\rangle_{SD} = \left| A - a \, \alpha_1 I_1^T_1 \right\rangle_{SD} \left| a \, \alpha_2 I_2^T_2 \right\rangle^{(sT)} Y_\ell \left( \hat{R}_{c.m.}^{(a)} \right) R_{n\ell} \left( \hat{R}_{c.m.}^{(a)} \right)
\]

\[
\left| A - a \, \alpha_1 I_1^T_1 \right\rangle \varphi_{00} \left( \hat{R}_{c.m.}^{(A-a)} \right)
\]

Vector proportional to the c.m. coordinate of the \( A-a \) nucleons

In the case of the nucleon-nucleus system we can applied the following basis change

\[
\left| \Phi_{vn}^{J^\pi T} \right\rangle_{SD} = \sum_j \hat{S}^j \left( -1 \right)^{I_1 + J + j} \begin{pmatrix} I_1 & 1/2 & s \\ \ell & J & j \end{pmatrix} \left| A - 1 \, \alpha_1 I_1^T_1 \right\rangle \varphi_{n\ell j} \frac{1}{2} \left( \vec{r}_A \sigma A T_A \right) \left( J^\pi T \right)
\]

This basis is convenient to express the kernels with the help of second quantization.
Effective interaction using SRG technique

1. From Quantum Chromo Dynamic (QCD), derive the bare nuclear (NN+NNN) interaction as an expansion selecting relevant degrees of freedom with the Chiral EFT.

2. Evolve (1) to extract a low-energy effective interaction using the SRG technique. This greatly improves the convergence of Many Body calculations.

3. Solve the non-relativistic Schrödinger equation with evolved two- plus three-(“induced” + “real”) interactions.
Convergence properties

Analysis of model space dependence

Expanding the size in the HO space.

Expanding the size in the RGM space.

Static DoF (gs+excited states)

Analysis of the inclusion of $^4$He lowest eigenstate

Scattering phase-shift of n-$^4$He system as a function of Nmax, for $V_{\text{low}k}$ and chiral EFT N3LO

Expanding the size in the RGM space.

Scattering phase-shift of n-$^4$He system sensitivity study of the inclusion of the first six excited states of $^4$He.
Convergence properties

Analysis of model space dependence

Expanding the size in the HO space.

Expanding the size in the RGM space.

Scattering phase-shifts of d-\(^4\)He system

Sensitivity study of the inclusion of deuterium pseudo excited states.

Sensitivity study of the number deuterium pseudo excited states.

Scattering phase-shift of n-\(^4\)He system as a function of Nmax, for \(V_{\text{low}k}\) and chiral EFT N3LO

\[ N = 1 \]
\[ N = 0 \]
Ab initio many-body calculation of the $^7\text{Be}(p,\gamma)^8\text{B}$ radiative capture

The $^7\text{Be}(p,\gamma)^8\text{B}$ is the final step in the nucleosynthetic chain leading to $^8\text{B}$ and one of the main inputs of the standard model of solar neutrinos

- ~10% error in latest $S_{17}(0)$: dominated by uncertainty in theoretical models
- NCSM/RGM results with largest realistic model space ($N_{\text{max}} = 10$):
  - $p+^7\text{Be}(\text{g.s., } 1/2^-, 7/2^-, 5/2_1^-, 5/2_2^-)$
  - Siegert’s E1 transition operator
- Parameter $\lambda$ of SRG NN interaction chosen to reproduce separation energy: 136 keV (Expt. 137 keV)
- $S_{17}(0) = 19.4(7)$ eVb on the lower side of, but consistent with latest evaluation

Astrophysical S-factor:
Ab initio many-body calculations of the $^3\text{H}(d,n)^4\text{He}$ and $^3\text{He}(d,p)^4\text{He}$ fusion


Calculated S-factors converge with the inclusion of the virtual breakup of the deuterium, obtained by means of excited $^3S_1-^3D_1 (d^*)$ and $^3D_2 (d''*)$ pseudo-states.

Evidence of incomplete model (nuclear force) compared to beam-target measurements.

Incomplete nuclear interaction: requires NNN force (SRG-induced + “real”)

$\sigma(E) = \frac{S(E)}{E} \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2mE}}\right)$
Including the NNN force into the NCSM/RGM approach

- Three-nucleon interaction derives from the underlying QCD theory.
- NNN force is fundamentally important.
- NNN-force components arise also from the SRG evolution of the NN interaction.

Example of NNN effects

Without NNN force g.s. has wrong spin.


Goal of this work

Up to now

Induced forces

NNN-induced interaction needs to be accounted in order to preserve the unitarity

Chiral EFT interaction

NN bare

NNN bare
Including the NNN force into the NCSM/RGM approach
nucleon-nucleus formalism

\[ \langle \Phi_{\nu' \nu}^{T} | \hat{A}_{\nu} V^{NNN} \hat{A}_{\nu} | \Phi_{\nu \nu}^{T} \rangle = \left\langle \frac{(A-1)}{r'} (a' = 1) \right| V^{NNN} \left( 1 - \sum_{i=1}^{A-1} \hat{P}_{i A} \right) (a = 1) \right\rangle \]

\[ V^{NNN}_{\nu' \nu} (r, r') = \sum_{n'n'} R_{nn'}(r') R_{nl}(r) \left[ \frac{(A-1)(A-2)}{2} \langle \Phi_{n'n'}^{T} | V_{A-2A-1A} (1 - 2P_{A-1A}) | \Phi_{nl}^{T} \rangle \right] \]

Direct potential:

\[ \propto_{SD} \langle \psi^{(A-1)}_{\alpha_i} | a_i^+ a_j^+ a_l a_k | \psi^{(A-1)}_{\alpha_i} \rangle_{SD} \]

\[ - \frac{(A-1)(A-2)(A-3)}{2} \langle \Phi_{n'n'}^{T} | P_{A-1A} V_{A-3A-2A-1} | \Phi_{nl}^{T} \rangle . \]

Exchange potential:

\[ \propto_{SD} \langle \psi^{(A-1)}_{\alpha_i} | a_h^+ a_i^+ a_j^+ a_m a_l a_k | \psi^{(A-1)}_{\alpha_i} \rangle_{SD} \]
Including the NNN force into the NCSM/RGM approach
nucleon-nucleus formalism

Exchange potential:

\[
\alpha \left\langle SD \left| \psi_{\alpha}^{(A-1)} | a_h^+ a_i^+ a_j^+ a_m a_l a_k \right| \psi_{\alpha}^{(A-1)} \right\rangle_{SD}
\]

\[
\alpha \left\langle SD \left| \psi_{\alpha}^{(A-1)} \left| \left( a_h^+ a_i^+ \right)^{h'} a_j^+ \right| \left( a_m a_l \right)^{h} a_k \right| \psi_{\alpha}^{(A-1)} \right\rangle_{SD}
\]

\[
\frac{1}{(A-1)(A-2)(A-3)} \sum_{j_0 j'_0 t'_0 t_0} \sum_{n_{\alpha l_j a} n_{\alpha l_j a} n_{\alpha l_j a} n_{\alpha l_j a}} \sum_{K J_0 \tau T_0} \sum_{n_{b \alpha l_j a} n_{b \alpha l_j a}} \hat{\tau} \hat{K} \hat{J}_0 \hat{T}_0 \hat{g}' \hat{t}'
\]

\[
\left\{ I_1 K I'_1 \right\} \left\{ j' K j \right\} \left\{ j' J_0 \right\} \left\{ g' J_0 \right\} \left( -1 \right)^{j'_a + j'_b - j'_0 + j' + K + I_1 + J} \left( -1 \right)^{3/2 - t'_0 + j' + \tau + T_1 + T}
\]

\[
\left\langle \left( n_{\alpha l_j a} n_{\alpha l_j a} n_{\alpha l_j a} n_{\alpha l_j a} \right) J_0 T_0 \left| V_{A-3 A-2 A-1} \left( n_{\alpha l_j a} n_{\alpha l_j a} n_{\alpha l_j a} n_{\alpha l_j a} \right) J_0 T_0 \right\rangle
\]

\[
\left\langle SD \left| A - 1 \alpha'_1 I'_1 T'_1 \right| \left| \left( a_n l_j a_{n_l b} l_{j'} a_{n_l a} l_{j a} \right) J'_0 t'_0 \left| g' t' \right| \left( a_{n_l a} l_{j a} a_{n_l b} l_{j b} \right) J_0 T_0 \right. \right\rangle \left. \right| A - 1 \alpha_1 I_1 T_1 \right\rangle_{SD}
\]

We use NNN matrix elements in the JT-coupled basis

The matrix elements of the three-body density become quickly too large to be stored.
Including the NNN force into the NCSM/RGM approach
nucleon-nucleus formalism

Exchange potential:

\[ \alpha_{SD} \left\langle \psi_{\alpha_i}^{(A-1)} \left| \begin{array}{c} a_h^+ a_i^+ a_j^+ a_m a_l a_k \\ \psi_{\alpha_i}^{(A-1)} \end{array} \right\rangle_{SD} \right. \]

\[ \alpha_{SD} \left\langle \psi_{\alpha_i}^{(A-1)} \left| \left( a_h^+ a_i^+ \right)^{g'} a_j^+ \right\rangle_{SD} \left\langle \psi_{\beta}^{(A-4)} \left| \left( a_m a_l \right)^{g} a_k \right\rangle_{SD} \right. \]

\[ \frac{1}{(A-1)(A-2)(A-3)} \sum_{j_0j_1t_0t_1} \sum_{n_a l a_j a} \sum_{n_b l b j_b} \sum_{g' t_g} \hat{J}_0 \hat{T}_0 \hat{g}' \hat{t}_g \left\{ \begin{array}{ccc} I'_\beta & g' & I'_1 \\ J_0 & j'_0 & j'_1 \\ J_1 & j & J \end{array} \right\} \left\{ \begin{array}{ccc} T_\beta & t'_g & T'_1 \\ T_0 & t'_0 & 1/2 \\ T_1 & 1/2 & T \end{array} \right\} \]

\[ (-1)^{j'_0 + j_0 + g' + I_\beta - I_1 + j} ( -1 )^{3/2 + T_0 + t'_0 + T_\beta - T_1} \left\langle \left[ \left( n'_a l'_a j'_a; n'_b l'_b j'_b \right) J'_0 T'_0 \right] V_{A-3 A-2 A-1} \left[ \left( n_a l a_j a; n_b l b j_b \right) J_0 T_0 \right] \right. \]

\[ \left\langle A - 1 \alpha'_1 I'_1 T'_1 \left| \left( a_{n l j}^+ (a_{n'_b l'_b j'_b}^+ a_{n'_a l'_a j'_a}^+) J'_0 t'_0 \right) g' t'_g \right| \left| A - 4 \alpha_\beta I_\beta T_\beta \right\rangle_{SD} \]

\[ \left\langle A - 4 \alpha_\beta I_\beta T_\beta \left| \left( a_{n a l a j a}^+ \tilde{a}_{n a l a j a}^+ J_0 t_0 \tilde{a}_{n b l b j b} \right) J_0 T_0 \right| \left| A - 1 \alpha_1 I_1 T_1 \right\rangle_{SD} \]

We introduce a closure relationship

These amplitudes can be stored

But only for light nuclei...
Including the NNN force into the NCSM/RGM approach
nucleon-nucleus formalism

Exchange potential:

\[ \propto \langle \psi_{\alpha_i}^{(A-1)} | a_h^+ a_i^+ a_m^+ a_k | \psi_{\alpha_i}^{(A-1)} \rangle_{SD} \]

Coming back to NCSM

\[
\frac{1}{(A-1)(A-2)(A-3)} \sum_{n_a l_a j_a} \sum_{n_b l_b j_b} \sum_{n'_a l'_a j'_a} \sum_{n''_a l''_a j''_a} \sum_{M_1 M_1'} \sum_{M_1 M_1' M_1''} C^{JM}_{I_1 I_1'} C^{JM}_{I_1 M_1} C^{TM}_{I_1 M_1} \frac{1}{2 m_{I_1}} \frac{1}{2 m_{I_1'}} \frac{1}{2 m_{I_1''}}
\]

\[
\langle n'_a l'_a j'_a : n'_b l'_b j'_b : n''_a l''_a j''_a | V_{A-3A-2A-1} | n_{\alpha l_{\alpha j_{\alpha}}} : n_{a l_{a j_{a}}} : n_{b l_{b j_{b}}} \rangle
\]

\[
\langle SD | \left( A - 1 \alpha_{I_1}^I M_1 M_1 T_1 M_1' \right) a_{n l_j}^+ a_{n b l_j}^+ a_{n a l_{a j_{a}}}^+ a_{n a l_{a j_{a}}} a_{n a l_{a j_{a}}} a_{n b l_{b j_{b}}} a_{n b l_{b j_{b}}} a_{n a l_{a j_{a}}} | A - 1 \alpha_{I_1}^I M_1 M_1 T_1 M_1' \rangle_{SD} \}
\]

The M-scheme NCSM is a promising path to perform the calculation of the kernels

No Information is stored
N-$^4$He scattering with NN+NNN interactions

G. Hupin, J. Langhammer, S. Quaglioni, P. Navrátil, R. Roth, work in progress

Convergence pattern is similar to the NN case.

Also needed: exploration of the λ SRG and ℏω parameters (ongoing).

Convergence of the phase shifts when accounting for $^4$He excited states.
N-\(^{4}\)He scattering with NN+NNN interactions

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Convergence pattern seems to be similar to the NN case.

A systematic exploration of the Nmax and # of target eigenstates is ongoing.

From an earlier calculation with the Lee-Suzuki at N3LO we know that the resonances are sensitive to the inclusion of the first six excited states of \(^{4}\)He.
N-$^4$He scattering with NN+NNN interactions

G. Hupin, J. Langhammer, S. Quaglioni, P. Navrátil, R. Roth, work in progress

NNN case: convergence with respect to the many body space, first excited states

Convergence pattern seems to be similar to the NN case. A systematic exploration of the Nmax and # of target eigenstates is ongoing.

From an earlier calculation with the Lee-Suzuki at N3LO we know that the resonances are sensitive to the inclusion of the first six excited states of $^4$He.

Expanding the size in the RGM space.

Convergence of the phase shifts when accounting for $^4$He excited states.

Navrátil and Quaglioni, PRC83 044609, (2011)
N-\(^4\)He scattering: NN versus NNN interactions, first results

G. Hupin, J. Langhammer, S. Quaglioni, P. Navrátil, R. Roth, work in progress

The largest splitting between \(P\) waves is obtained with NN +NNN.
The NN only agrees better than the full NN interaction (NN +NNN-ind).
Static DoF should be explored.

Comparison between NN, NN +NNN-ind and NN+NNN at N\(_{\text{max}}\)=11

Now only with ground state!
N-$^4$He scattering: NN versus NNN interactions, first results
G. Hupin, J. Langhammer, S. Quaglioni, P. Navrátil, R. Roth, work in progress

The largest splitting between $P$ waves is obtained with NN +NNN. The NN only agrees better than the full NN interaction (NN +NNN-ind). Static DoF should be explored.

Comparison between NN, NN +NNN-ind and NN+NNN at Nmax=13
Including the NNN force into the NCSM/RGM approach
deuteron-nucleus formalism

\[
\left\langle \Phi_{v'r'}^{J^\pi T} \left| \hat{A}_v, V_{NNN} \hat{A}_v \right| \Phi_{vr}^{J^\pi T} \right\rangle = \left\langle \Phi_{r'}^{(A-2)} \left| V_{NNN} \left(1 - \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{i,k} + \sum_{i<j=1}^{A-2} \hat{P}_{i,A-1} \hat{P}_{j,A} \right) \right| \Phi_{r}^{(A-2)} \right\rangle
\]

Direct

\begin{align*}
(a) & \quad (b) & \quad (c) & \quad (d) \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
\end{align*}

Exchange

\begin{align*}
(e) & \quad (f) & \quad (g) & \quad (h) \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
\end{align*}

Up to four body density
$^4\text{He}(d,d)^4\text{He}$ with SRG-evolved chiral NN+NNN force

G. Hupin, S. Quaglioni, P. Navratil, work in progress

**Phase shifts with $\lambda = 2$ fm$^{-1}$**

- NN+NNN
- NN only

$N_{\text{max}} = 8$

$d(g.s.) + ^4\text{He}(g.s.)$ scattering phase shifts for SRG-NN+NNN potential with $\lambda=2$ fm$^{-1}$.

**Phase shifts with $\lambda = 1.5$ fm$^{-1}$**

$N_{\text{max}} = 12 d(g.s.,^3S_1-^3D_1,^3D_2,^3D_3-^3G_3) + ^4\text{He}(g.s.)$ SRG-N$^3$LO NN potential with $\lambda=1.5$ fm$^{-1}$.

Preliminary results in a small model space and with only $d$ and $^4\text{He}$ g.s., look promising.
Conclusions and Outlook

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

- Ability to describe:
  - Nucleon-nucleus collisions
  - Deuterium-nucleus collisions
  - \((d,N)\) transfer reactions
  - \(^3\text{H}\)- and \(^3\text{He}\)-nucleus collisions

- Recent results with SRG-N\(^3\)LO NN pot.:
  - \(^3\text{H}(n,n)^3\text{H}\), \(^4\text{He}(d,d)^4\text{He}\), \(^3\text{H}(d,n)^4\text{He}\),
  - \(^3\text{He}(d,p)^4\text{He}\), \(^7\text{Be}(p,\gamma)^8\text{B}\)

- Work in progress
  - Inclusion of NNN force in nucleon-nucleus formalism: applications to \(N^+^4\text{He}\)
  - Calculation of \(^4\text{He}+p \rightarrow ^4\text{He}+p+\gamma\) bremsstrahlung process

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Thanks to my collaborators:

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- W. Horiuchi (Hokkaido Univ.)