## Toward Realistic Calculations of Light-lon Fusion Reactions

INT "Structure of light Nuclei"

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### (RGM)

### 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  $\leq$  ~16); No-Core Shell Model (NCSM)
  - Address dynamical properties. (scattering, reactions)
    - Extend No-Core Shell-Model with the Resonating Group Method











### 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:

0.1 Relative Energy (MeV)

- 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

S. Quaglioni and P. Navrátil, Phys. Rev. Lett. 101, 092501 (2008); Phys. Rev. C 79, 044606 (2009)



- Constructs integration kernels (~ projectile-target potentials) star
  - Underlying (realistic) interactions among nucleons
  - NCSM *ab initio* wave functions

Navrátil and Quaglioni, PRL 101, (2008) Navrátil and Quaglioni, PRL 108, (2012)

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



## Ab initio NCSM/RGM Formalism for binary clusters a few details

$$\left|\Psi^{J^{\pi}T}\right\rangle = \sum_{v} \int \underbrace{g_{v}^{J^{\pi}T}(r)}_{r} \hat{A}_{v} \left[ \left( \left| A - a \; \alpha_{1} I_{1}^{\pi_{1}} T_{1} \right\rangle \right| a \; \alpha_{2} I_{2}^{\pi_{2}} T_{2} \right) \right]^{(sT)} Y_{\ell}(\hat{r}_{A-a,a}) \right]^{(J^{\pi}T)} \frac{\delta(r - r_{A-a,a})}{rr_{A-a,a}} r^{2} dr$$

 $\Phi_{vr}^{J^{\pi}T}$ 

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

(Jacobi) channel basis

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<sub>max</sub>, this expansion is good for localized parts of the integration kernels.

 $\left|\Phi_{vr}^{J^{\pi}T}\right\rangle = \sum R_{n\ell}(r) \left|\Phi_{vn}^{J^{\pi}T}\right\rangle$ 

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

$$\left| \Phi_{vn}^{J^{\pi}T} \right\rangle = \left[ \left( \left| A - a \; \alpha_{1} I_{1}^{\pi_{1}} T_{1} \right\rangle \left| a \; \alpha_{2} I_{2}^{\pi_{2}} T_{2} \right\rangle \right)^{(sT)} Y_{\ell}(\hat{r}_{A-a,a}) \right]^{(J^{\pi}T)} R_{n\ell}(r_{A-a,a})$$

The coordinate space channel states are given by

### Matrix elements of translationally invariant operators

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

$${}_{SD} \left\langle \Phi_{f_{SD}}^{(A-a',a')} \left| \hat{O}_{t.i.} \right| \Phi_{i_{SD}}^{(A-a,a)} \right\rangle_{SD} = \sum_{i_R f_R} M_{i_{SD} f_{SD}, i_R f_R} \left\langle \Phi_{f_R}^{(A-a',a')} \left| \hat{O}_{t.i.} \right| \Phi_{i_R}^{(A-a,a)} \right\rangle$$



Advantage: can use powerful second quantization techniques

$$\sum_{SD} \left\langle \Phi_{v'n'}^{(A-a',a')} \left| \hat{O}_{t.i.} \right| \Phi_{vn}^{(A-a,a)} \right\rangle_{SD} \propto \sum_{SD} \left\langle \psi_{\alpha_1'}^{(A-a')} \left| a^* a \right| \psi_{\alpha_1}^{(A-a)} \right\rangle_{SD}, \quad SD \left\langle \psi_{\alpha_1'}^{(A-a')} \left| a^* a^* a a \right| \psi_{\alpha_1}^{(A-a)} \right\rangle_{SD}, \quad \cdots$$



### 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:

$$\begin{split} \left| \Phi_{\nu n}^{J^{\pi}T} \right\rangle_{SD} &= \begin{bmatrix} \left( \left| A - a \; \alpha_1 I_1^{\pi_1} T_1 \right\rangle_{SD} \middle| a \; \alpha_2 I_2^{\pi_2} T_2 \right) \right)^{(sT)} Y_{\ell} \left( \hat{R}_{c.m.}^{(a)} \right) \\ \left| A - a \; \alpha_1 I_1^{\pi_1} T_1 \right\rangle \varphi_{00} \left( \vec{R}_{c.m.}^{(A-a)} \right) \\ \text{Vector proportional to the c.m. coordinate of the A-a nucleons} \\ \text{Vector proportional to the c.m. coordinate of the A-a nucleons} \\ \text{the case of the nucleon-nucleus system we can plied the following basis change} \\ \left| \Phi_{\nu n}^{J^{\pi}T} \right\rangle_{SD} &= \sum_{j} \; \hat{sj} \; (-1)^{I_1 + J + j} \left\{ \begin{array}{c} I_1 \; \frac{1}{2} \; s \\ \ell \; J \; j \end{array} \right\} \\ \text{asis is convenient to express the s with the help of second ation.} \\ \times \left[ \left| A - 1 \; \alpha_1 I_1^{\pi_1} T_1 \right\rangle \; \varphi_{n\ell j \frac{1}{2}} \left( \vec{r}_A \sigma_A \tau_A \right) \right]^{(J^{\pi}T)} \\ \end{split}$$

This basis is convenient to express the kernels with the help of second quantization.

In

ap



### 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.

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k' (fm<sup>-1</sup>)

k (fm<sup>-1</sup>)

### **Convergence properties**

S. Quaglioni and P. Navrátil, Phys. Rev. Lett. 101, 092501 (2008); Phys. Rev. C 79, 044606 (2009)





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### Ab initio many-body calculation of the ${}^{7}Be(p, \gamma){}^{8}B$ radiative capture

P. Navrátil, R. Roth, and S. Quaglioni, Phys. Lett. B704, 379 (2011)



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

- ~10% error in latest S<sub>17</sub>(0): dominated by uncertainty in theoretical models
- NCSM/RGM results with largest realistic model space (N<sub>max</sub> = 10):
  - p+<sup>7</sup>Be(g.s., 1/2<sup>-</sup>, 7/2<sup>-</sup>, 5/2<sub>1</sub><sup>-</sup>, 5/2<sub>2</sub><sup>-</sup>)
  - Siegert's E1 transition operator
- Parameter λ of SRG NN interaction chosen to reproduce separation energy: 136 keV (Expt. 137 keV)
- S<sub>17</sub>(0) = 19.4(7) eVb on the lower side of, but consistent with latest evaluation



normalization and shape of  $S_{17}$ 

### Astrophysical S-factor:

$$\sigma(E) = \frac{S(E)}{E} \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2mE}}\right)$$



# Ab initio many-body calculations of the ${}^{3}H(d,n){}^{4}He$ and ${}^{3}He(d,p){}^{4}He$ fusion

P. Navrátil, S. Quaglioni, PRL 108, 042503 (2012)



(SRG-induced + "real")

Calculated S-factors converge with the inclusion of the virtual breakup of the deuterium, obtained by means of excited  ${}^{3}S_{1}-{}^{3}D_{1}$  ( $d^{*}$ ) and  ${}^{3}D_{2}$  ( $d^{**}$ ) pseudostates.





## 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.



R. Roth, J. Langhammer, A. Calci, S. Binder, and P. Navratil, PRL 107, 072501 (2011).



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



$$\left\langle \Phi_{\nu'r'}^{J^{\pi}T} \left| \hat{A}_{\nu'} V^{NNN} \hat{A}_{\nu} \right| \Phi_{\nu r}^{J^{\pi}T} \right\rangle = \left\langle \begin{array}{c} \begin{pmatrix} (A-1) \\ r' \end{pmatrix} \\ r' \end{pmatrix} \left| V^{NNN} \left( 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \right) \right| \begin{pmatrix} (A-1) \\ (a=1) \end{pmatrix} \right\rangle$$

$$\mathcal{V}_{\nu'\nu}^{NNN}(r,r') = \sum_{(a)} R_{n'l'}(r')R_{nl}(r) \left[ \underbrace{(A-1)(A-2)}{2} \left\langle \Phi_{\nu'n'}^{J^{\pi}T} | V_{A-2A-1A}(1-2P_{A-1A}) | \Phi_{\nu n}^{J^{\pi}T} \right\rangle \right]$$

$$\underbrace{\mathsf{Direct potential:}}_{(a)} \qquad \underbrace{\mathsf{Direct potential:}}_{SD} \left\langle \psi_{\alpha_{1}}^{(A-1)} \left| a_{i}^{*}a_{j}^{*}a_{l}a_{k} \right| \psi_{\alpha_{1}}^{(A-1)} \right\rangle_{SD} - \underbrace{(A-1)(A-2)(A-3)}_{2} \left\langle \Phi_{\nu'n'}^{J^{\pi}T} | P_{A-1A}V_{A-3A-2A-1} | \Phi_{\nu n}^{J^{\pi}T} \right\rangle \right].$$

$$\underbrace{\mathsf{Exchange potential:}}_{(c)} \qquad \underbrace{\mathsf{Exchange potential:}}_{SD} \left\langle \psi_{\alpha_{1}}^{(A-1)} \left| a_{h}^{*}a_{i}^{*}a_{m}a_{l}a_{k} \right| \psi_{\alpha_{1}}^{(A-1)} \right\rangle_{SD}$$

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We use NNN matrix elements in the JTcoupled basis

The matrix elements of the three-body density become quickly too large to be stored





Exchange potential: 
$$\propto \int_{SD} \left\langle \psi_{\alpha_{1}^{\prime}}^{(A-1)} \middle| a_{h}^{*} a_{i}^{*} a_{j}^{*} a_{m} a_{l} a_{k} \middle| \psi_{\alpha_{1}}^{(A-1)} \right\rangle_{SD}$$
Coming back to NCSM

$$\frac{1}{(A-1)(A-2)(A-3)} \sum_{\substack{n_a l_a j_a \\ n_b l_b j_b \\ n'_a l'_a j'_a \\ m'_b l_b j_b \\ n'_a l'_a j'_a \\ m'_a l'_a j'_a \\ m'_b l'_b j'_b \\ m'_a l'_a j'_a \\ m'_b l'_b j'_b \\ m'_b l'_b \\ m'_b \\ m'_b l'_b \\ m'_b \\ m'_b$$



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





### **N-4He 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  $\lambda$  SRG and  $\hbar\omega$  parameters (ongoing).



### N-<sup>4</sup>He scattering with NN+NNN interactions

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





Navrátil and Quaglioni, PRC83

044609, (2011)

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



### N-<sup>4</sup>He scattering with NN+NNN interactions

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

Expanding the size in the Heerci RGM space. 60 Static DoF (qs+excited states) 30 [geb] NNN case: convergence with respect to the  $\sim$ many body space, first excited states 120× × ×  $^{2}P_{3/2}$ -30 90 60 -60 30 [deg]  ${}^{2}D_{3/2}$ 0  $\sim$ 0 NN+NN, Nmax=11  $g.s.,0^+,0^-$ -30  $g.s.,0^+$  ${}^{1}S_{1/2}$ g.s. Expt -60 n+<sup>4</sup>He -90 ×× 124 8 160  $E_{kin}$  [MeV] Convergence of the phase shifts when accounting for <sup>4</sup>He excited states.



Navrátil and Quaglioni, PRC83

044609, (2011)

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



## N-<sup>4</sup>He scattering: NN versus NNN interactions, first results

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





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$$\left\langle \Phi_{v'r'}^{J^{\pi}T} \left| \hat{A}_{v'} V^{NNN} \hat{A}_{v} \right| \Phi_{vr}^{J^{\pi}T} \right\rangle = \left\langle \begin{array}{c} (A-2) \\ (A-2) \\ r'(a=2) \end{array} \right| V^{NNN} \left( 1 - \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{i,k} + \sum_{i< j=1}^{A-2} \hat{P}_{i,A-1} \hat{P}_{j,A} \right) \right| \begin{pmatrix} (A-2) \\ (a=2) \end{pmatrix} \rangle$$



## <sup>4</sup>He(*d*,*d*)<sup>4</sup>He with SRG-evolved chiral NN+NNN force

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





### **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
  - <sup>3</sup>H- and <sup>3</sup>He-nucleus collisions
- Recent results with SRG-N<sup>3</sup>LO NN pot.:
  - <sup>3</sup>H(n,n)<sup>3</sup>H, <sup>4</sup>He(d,d)<sup>4</sup>He, <sup>3</sup>H(d,n)<sup>4</sup>He,
     <sup>3</sup>He(d,p)<sup>4</sup>He, <sup>7</sup>Be(p,γ)<sup>8</sup>B
- Work in progress
  - Inclusion of NNN force in nucleon-nucleus formalism: applications to *N*+<sup>4</sup>He
  - Calculation of  ${}^{4}\text{He}+p \rightarrow {}^{4}\text{He}+p+\gamma$  bremsstrahlung process

### Thanks to my collaborators:

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