### Toward Realistic Description of Low energy Fusion for Astrophysics: Application to N-<sup>4</sup>He and d-<sup>4</sup>He Scattering

International Workshop XLI on Gross Properties of Nuclei and Nuclear Excitations: "Astrophysics and Nuclear Structure"

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#### Lawrence Livermore National Laboratory

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#### **Guillaume Hupin**

### **From Stars to Nuclei**



Evolution of stars: birth, main sequence and death

The sun 💿



Н	73.46%
Не	24.85%
0	0.77%
С	0.29%
Fe	0.16%



## Fusion processes play an important role in determining the evolution of our universe: nucleosynthesis, stellar evolution ...



- What powers stars ?
- How long does a star live ?

Nuclear astrophysics community relies on accurate fusion reactions observables among others.

Challenging for both experiment and theory:

- Low rates: Coulomb repulsion between target and projectile + low energy (quantum tunneling effects).
- Projectile and target are not fully ionized in a lab. This leads to laboratory electron screening
- Fundamental theory is still missing







### Some words about the ingredients of an *ab initio* calculation

#### A high precision nuclear Hamiltonian



The nuclear interaction has a strong repulsive core.

This makes nuclear structure calculation converge slowly.

#### ...and also NNN interaction



We need a NNN interaction to achieve a high-precision.

This is ~100 times numerically costlier.



### **Status of nuclear reaction models**

- Ab initio nuclear reactions lagging behind structure calculations
  - Exact reaction calculations for very light systems A=3,4
    - Faddeev / Faddev-Yacubovsky
    - Alt-Grassberger-Sandhas
    - Hyperspherical Harmonics, ...



 Now trying to incorporate continuum effects in methods for light nuclei to describe reactions



Nuclear scattering is sensitive to NNN interaction which plays an important role in the spin-orbit physic



### Why is it *hard* to model nuclear reactions?

If we used Harmonic oscillator states...



... inbound and outbound waves cannot be described by <u>finite</u> number of basis states



For more information on boundary conditions and R-matrix see P. Descouvemont, D. Baye Rep. Prog. Phys. 73 (2010)



## From nucleons to nuclear reactions



• Objective:

Address static and dynamical properties of light ions and describe fusion reactions.

- Ingredients
  - High-precision nuclear interaction, two- plus three-nucleon, derived within the Chiral Effective Field Theory (EFT).
- Recipe
  - Solve the many-body Schrödinger equation.
  - Address structural properties. (bound states, narrow resonances)
    - Ab initio many-body approaches (A ≤ ~16); No-Core Shell Model (NCSM)
  - Address dynamical properties. (scattering, reactions)
    - Extend No-Core Shell-Model with the Resonating Group Method (RGM)





### 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)



Schrödinger equation on channel basis:

RGM accounts for: 1) interaction (Hamiltonian kernel), 2) Pauli principle (Norm kernel) between clusters and NCSM accounts for: internal structure of clusters



### Matrix elements of translationally invariant operators

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

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



Advantage: can use powerful second quantization techniques

$$\sum_{SD} \left\langle \Phi_{\nu'n'}^{(A-a',a')} \left| \hat{O}_{t.i.} \right| \Phi_{\nu n}^{(A-a,a)} \right\rangle_{SD} \propto \sum_{SD} \left\langle \psi_{\alpha'_1}^{(A-a')} \left| a^+ a \right| \psi_{\alpha_1}^{(A-a)} \right\rangle_{SD}, \quad SD \left\langle \psi_{\alpha'_1}^{(A-a')} \left| a^+ a^+ a a \right| \psi_{\alpha_1}^{(A-a)} \right\rangle_{SD}, \quad \cdots$$



### Going around the hard core problem

E. Jurgenson, Navrátil, R. J. Furnstahl Phys. Rev. Lett. 103 (2009)

In configuration interaction methods we need to soften interaction to address the hard core We use the Similarity-Renormalization-Group (SRG) method





Flow parameter









## Demonstrated capability to describe binary-cluster reactions starting from NN interactions

☑ Nucleon-nucleus collisions

- ✓ n-<sup>3</sup>H, p-<sup>3</sup>He, N-<sup>4</sup>He, n-<sup>10</sup>Be scattering with N<sup>3</sup>LO NN (mod. Lee-Suzuki eff. Int.)
- Nucleon scattering on <sup>3</sup>H, <sup>3,4</sup>He,<sup>7</sup>Li,<sup>7</sup>Be,<sup>12</sup>C,<sup>16</sup>O with SRG-N<sup>3</sup>LO
- ✓ <sup>7</sup>Be(p,γ)<sup>8</sup>B radiative capture with SRG-N<sup>3</sup>LO

☑ Deuterium-nucleus collisions

 ✓ d-<sup>4</sup>He scattering and <sup>6</sup>Li structure with SRG-N<sup>3</sup>LO

✓ <sup>3</sup>H(d,n)<sup>4</sup>He and <sup>3</sup>He(d,p)<sup>4</sup>He reactions with SRG-N<sup>3</sup>LO









# 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)



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.

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



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

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

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

$$\overset{(a)}{=} \frac{(A-1)(A-2)(A-3)}{2} \left\langle \Phi_{\alpha_{1}'}^{J^{\pi}T} | P_{A-1A}V_{A-3A-2A-1} | \Phi_{\nu n}^{J^{\pi}T} \right\rangle \right] .$$

$$\overset{(a)}{=} \frac{(A-1)(A-2)(A-3)}{2} \left\langle \Phi_{\nu'n'}^{J^{\pi}T} | P_{A-1A}V_{A-3A-2A-1} | \Phi_{\nu n}^{J^{\pi}T} \right\rangle \right] .$$

$$\overset{(a)}{=} \frac{(A-1)(A-2)(A-3)}{2} \left\langle \Phi_{\nu'n'}^{J^{\pi}T} | P_{A-1A}V_{A-3A-2A-1} | \Phi_{\nu n}^{J^{\pi}T} \right\rangle \right] .$$

$$\overset{(a)}{=} \frac{(A-1)(A-2)(A-3)}{2} \left\langle \Phi_{\nu'n'}^{J^{\pi}T} | P_{A-1A}V_{A-3A-2A-1} | \Phi_{\nu n}^{J^{\pi}T} \right\rangle \int_{SD} SD$$



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# We are following two ways of handling the three-body density

$$\begin{cases} I_{\beta} g' I'_{1} \\ J_{0} j'_{0} f'_{0} g' I'_{1} \\ J_{0} j'_{0} f'_{0} f'_{$$

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# We are following two ways of handling the three-body density





### n-<sup>4</sup>He scattering: study of the model space convergence





- Calculations are done using the chiral EFT interaction at N<sup>3</sup>LO for the NN and N<sup>2</sup>LO for the NNN.
- For this study, we take  $\hbar\omega=20$
- The SRG flow parameter is  $\lambda$ =2.0
- Convergence pattern is good.



### n-<sup>4</sup>He scattering: study of the RGM convergence in the NNN case

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





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



### n-<sup>4</sup>He scattering: study of the RGM convergence in the NN case

P. Navrátil and S. Quaglioni, Phys. Rev. C 83 044609, (2011)





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





### n-<sup>4</sup>He scattering: NN+NNN with the first three excited states





### **Preliminary results for the lambda dependence**





### **Cross section and p-4He scattering**

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









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### Including the NNN force into the NCSM/RGM approach deuteron-nucleus formalism

$$\left\langle \Phi_{\nu r}^{rT} \left| \hat{A}_{\nu} V^{NNN} \hat{A}_{\nu} \right| \Phi_{\nu r}^{rT} \right\rangle = \left\langle \underbrace{\left\langle A - 2 \right\rangle}_{r(a=2)} \right\rangle V^{NNN} \left( 1 - \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{i,k} + \sum_{i < j=1}^{A-2} \hat{P}_{i,A-1} \hat{P}_{j,A} \right) \left| \underbrace{\left\langle A - 2 \right\rangle}_{(a=2)} \right\rangle$$
Direct
$$\left\langle \underbrace{\left\langle A - 2 \right\rangle}_{(a=2)} \right\rangle \left\langle A - 2 \right\rangle}_{(a=2)} \left\langle A - 2 \right\rangle_{(a=2)} \left\langle A - 2 \right\rangle}_{(a=2)} \left\langle A - 2 \right\rangle_{(a=2)} \left\langle A - 2 \right\rangle_{(a=2)} \right\rangle$$

$$\left\langle A - 2 \right\rangle_{(a=2)} \left\langle A - 2 \right\rangle_{(a=2)} \left\langle A - 2 \right\rangle_{(a=2)} \left\langle A - 2 \right\rangle_{(a=2)} \right\rangle$$
Exchange
$$\left\langle A - 2 \right\rangle_{(a=2)} \left\langle A - 2 \right\rangle_{(a=2)}$$

### <sup>4</sup>He(*d*,*d*)<sup>4</sup>He with NN+NNN interaction

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





Preliminary results in a small model space and with only d and <sup>4</sup>He g.s., look promising



### <sup>4</sup>He(*d*,*d*)<sup>4</sup>He with NN-only

S. Quaglioni and P. Navratil





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



### **Conclusions and Outlook**



Evolution of stars, birth, main sequence, death

- We are extending the *ab initio* NCSM/RGM approach to describe low-energy reactions with two- and three-nucleon interactions.
- We are able to describe:
  - Nucleon-nucleus collisions with NN+NNN interaction
  - Deuterium-nucleus collisions with NN+NNN interaction
- Work in progress
  - The present NNN force is "incomplete", need to go to N<sup>3</sup>LO
  - Before definite conclusion
    - Study of  $\lambda$  dependence
    - $\quad Study \ of \ \hbar \omega \ dependence$
  - Scattering of heavier target



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

$$\left|\Psi^{J^{\pi}T}\right\rangle = \sum_{v} \int \underbrace{g_{v}^{J^{\pi}T}(r)}_{r} \hat{A}_{v} \left[ \left( \left| A - a \; \alpha_{1} I_{1}^{\pi_{1}} T_{1} \right\rangle \right| a \; \alpha_{2} I_{2}^{\pi_{2}} T_{2} \right) \right]^{(sT)} Y_{\ell}(\hat{r}_{A-a,a}) \right]^{(J^{\pi}T)} \frac{\delta(r - r_{A-a,a})}{rr_{A-a,a}} r^{2} dr$$
Relative wave functions subject to the boundary/scattering asymptotic solution within R-matrix theory  $\left| \Phi_{vr}^{J^{\pi}T} \right\rangle$  (Jacobi) channel basis

We use the closure properties of HO radial wave function

$$\delta(r-r_{A-a,a}) = \sum_{n} R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

solution within R-matrix theory

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

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

The coordinate space channel states are given by



### 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:

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

a



### 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<sup>-</sup>, 5/2<sup>-</sup>)
  - Siegert's E1 transition operator
- Parameter λ 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:

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

