Ab-Initio Light-Ion Reactions with Chiral Two- and Three-Body Interactions.

Progress in *Ab-Initio* Techniques in Nuclear Physic

Vancouver, February 22th 2013.

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LLNL-PRES-622652

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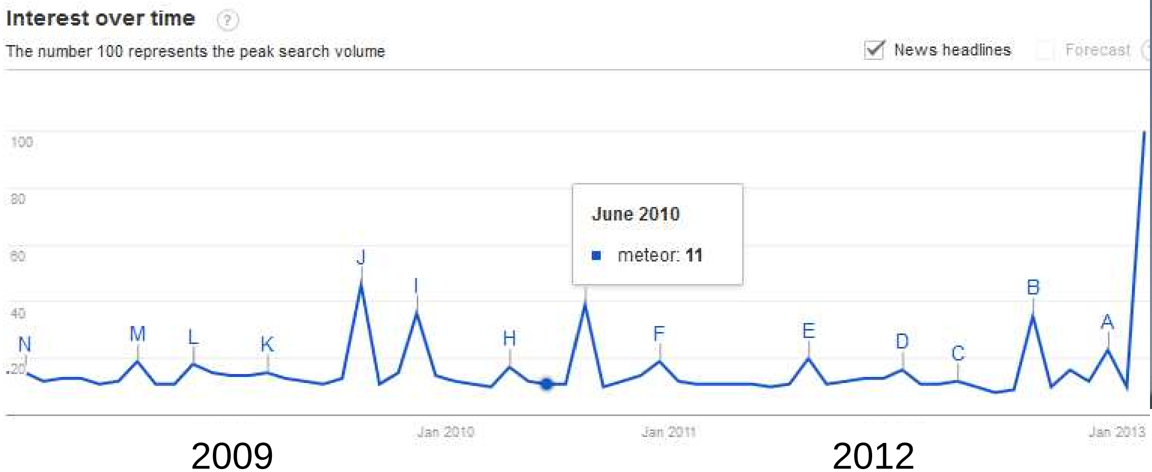
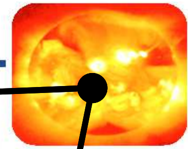
✓ Astrophysics motivations

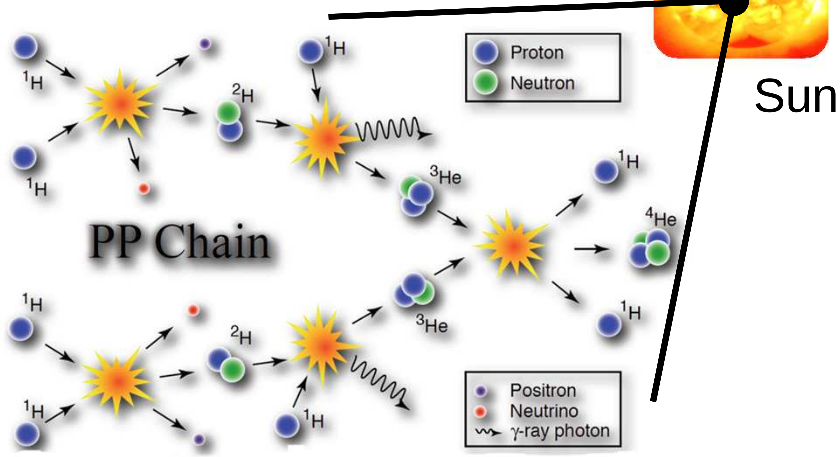


Russia, 1 week and a day ago

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 ?
- …



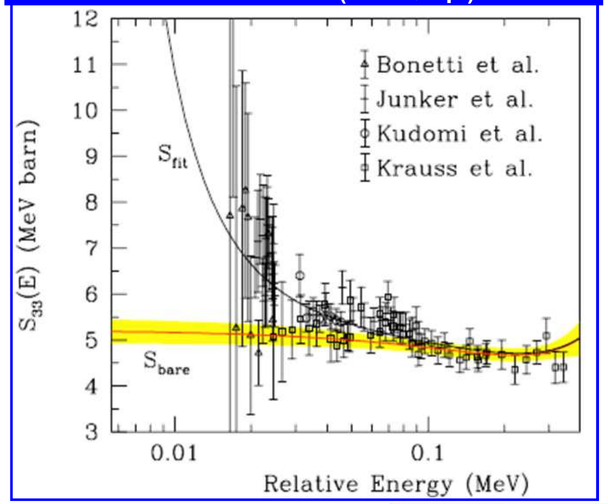


Nuclear astrophysics community relies on accurate fusion reactions observables among others.

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

S-factor for $^3He(^3He,2p)^4He$

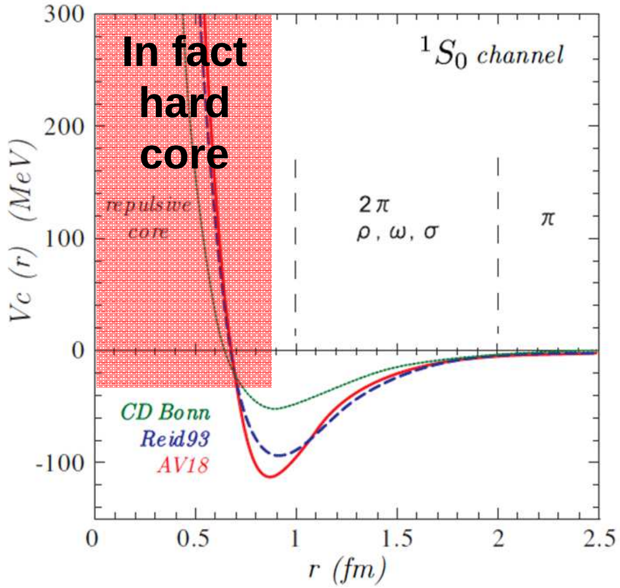


$$\sigma(E)=\frac{S(E)}{E}\exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar\sqrt{2mE}}\right)$$

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

A high precision nuclear Hamiltonian

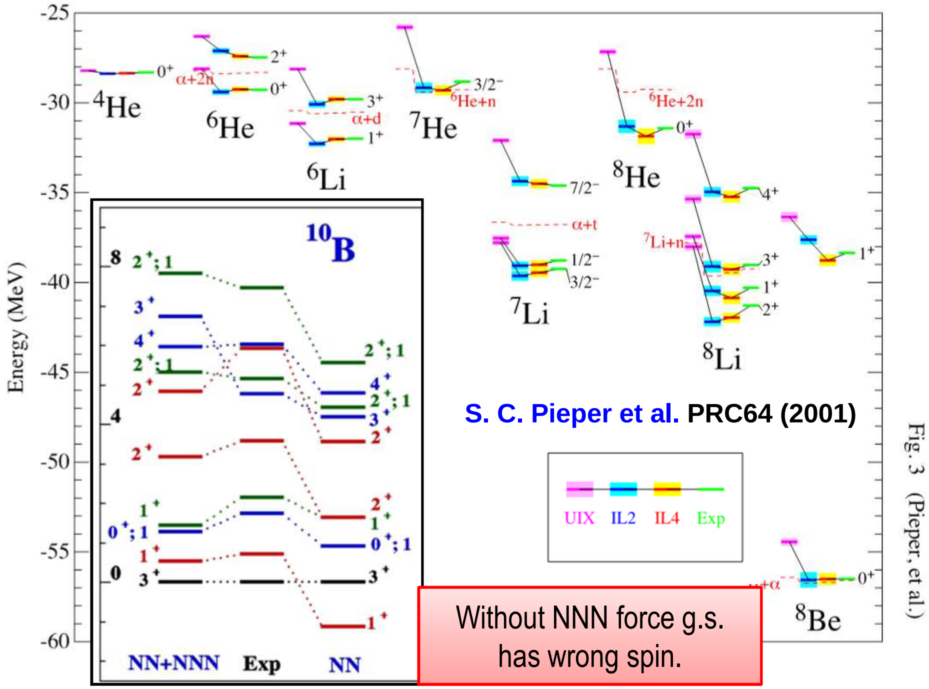
We have a NN interaction…



N. Ishii et al. PRL99 (2007)

The nuclear interaction has a strong repulsive core.
This makes nuclear structure calculation converge slowly.

…and also NNN interaction



S. C. Pieper et al. PRC64 (2001)

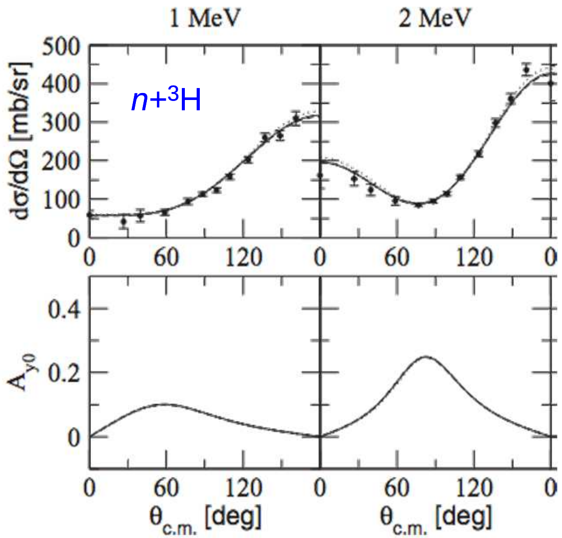
Without NNN force g.s. has wrong spin.

P. Navrátil et al. PRL 99 (2007)

We need a NNN interaction to achieve a high-precision.
This is ~100 times numerically costlier.

Status of nuclear reaction models

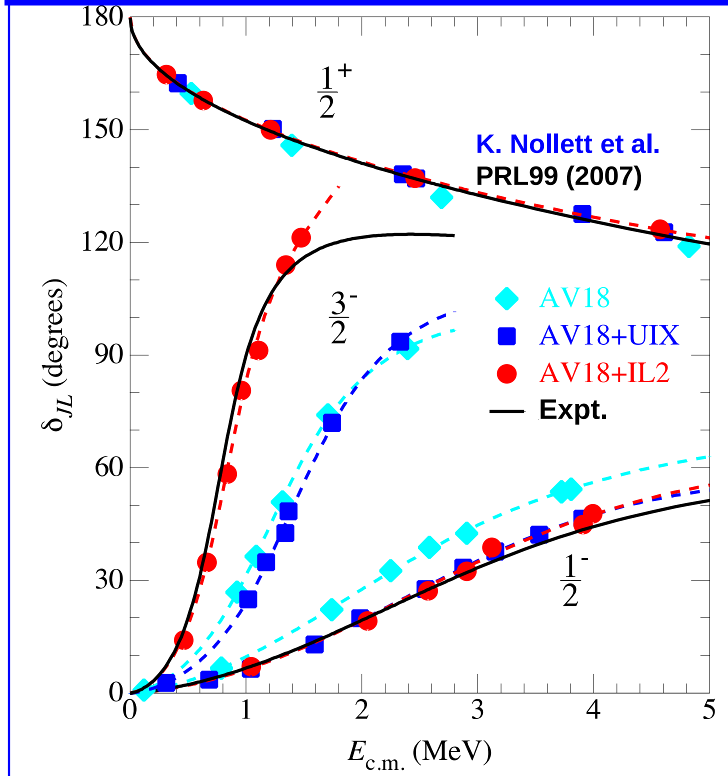
- *Ab initio* nuclear reactions lagging behind structure calculations
  - Exact reaction calculations for very light systems ***A*=3,4**
    - Faddeev / Faddev-Yacubovsky
    - Alt-Grassberger-Sandhas
    - Hyperspherical Harmonics, …



M. Viviani at al.
PRC84 (2011)

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

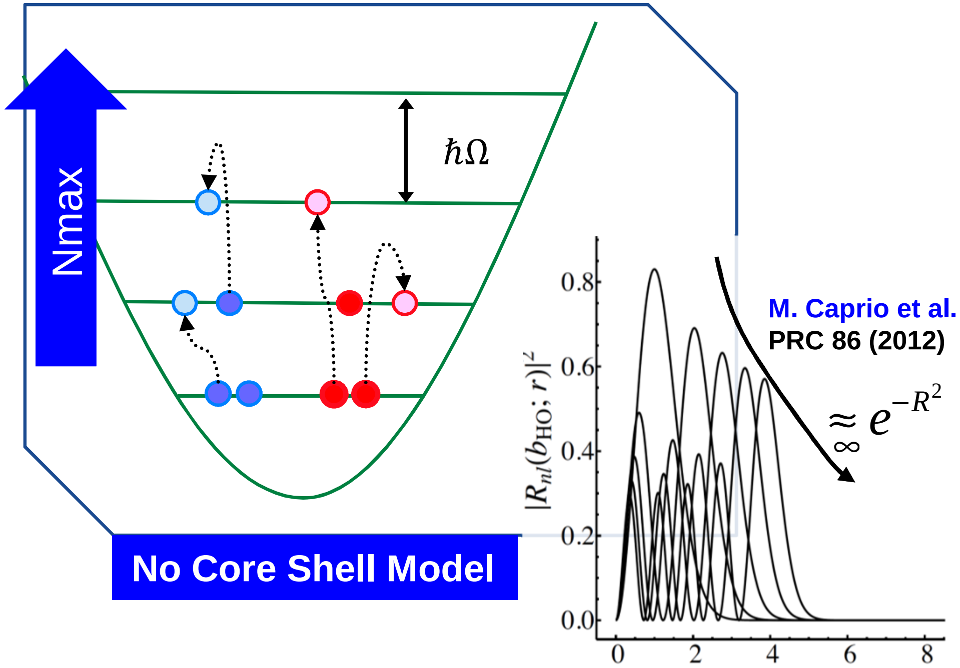
n-α phase-shifts in QMC calculation with/without NNN interaction



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

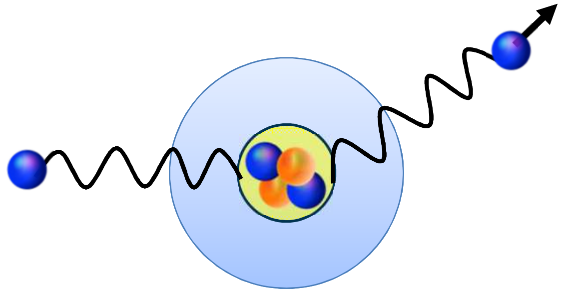
Why is it *hard* to model nuclear reactions?

If we used Harmonic oscillator states…



$$\Psi^{(A)} = \sum_{N=N_{\min}}^{N_{\max}} c_N \Phi_N^{HO}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A)$$

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

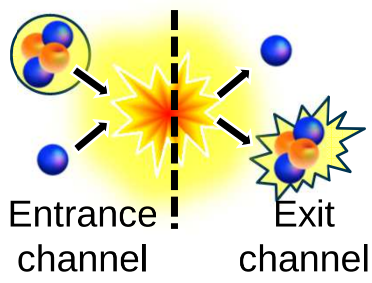


For more information on boundary conditions and R-matrix see
P. Descouvemont, D. Baye *Rep.Prog.Phys.*73 (2010)

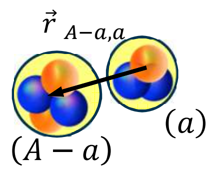
Ab initio NCSM/RGM: formalism for binary clusters

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

Ex: n-^{4}He scattering



- Starts from:



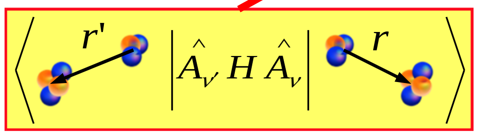
$$\Psi^{(A)}_{RGM} = \sum_{\nu} \int d\vec{r}\, g_\nu(\vec{r})\, \hat{A}_\nu \left| \Phi^{(A-a,a)}_{\nu\vec{r}} \right\rangle$$

$$\psi^{(A-a)}_{\alpha_1} \psi^{(a)}_{\alpha_2} \delta(\vec{r} - \vec{r}_{A-a,a})$$

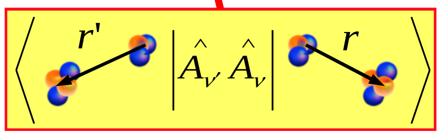
Relative wave function (unknown) — Antisymmetrizer — Channel basis

- Schrödinger equation on channel basis:

$$H\Psi^{(A)}_{RGM} = E\Psi^{(A)}_{RGM} \Rightarrow \sum_{\nu} \int d\vec{r} \left[H_{\nu'\nu}(\vec{r}\,',\vec{r}) - E\, N_{\nu'\nu}(\vec{r}\,',\vec{r}) \right] g_\nu(\vec{r}) = 0$$



Hamiltonian kernel



Norm (overlap) kernel

$\propto$ NCSM densities

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

Ab initio NCSM/RGM: formalism for binary clusters

Few details

$$\left|\Psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi T)} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}} r^2 dr$$

Constrained by the asymptotic scattering solution

$\left|\Phi_{\nu r}^{J^\pi T}\right\rangle$ (Jacobi) channel basis

- We use the closure properties of HO radial wave function

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

This defines the RGM model space (Ok for localized parts of the kernels)

- We introduce Jacobi channel states in the HO space

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

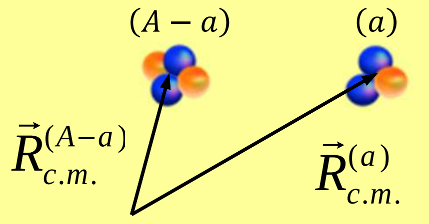
- The coordinate space channel states are given by $\left|\Phi_{\nu r}^{J^\pi T}\right\rangle = \sum_n R_{n\ell}(r) \left|\Phi_{\nu n}^{J^\pi T}\right\rangle$

Matrix elements of translationally invariant operators

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

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

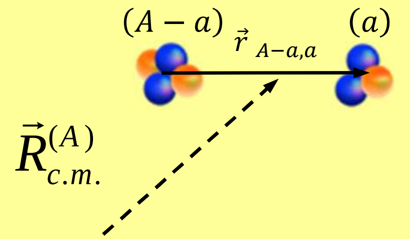
What we calculate in the "SD" channel basis



$$ \left|\psi^{(A-a)}_{\alpha_1}\right\rangle_{SD} \left|\psi^{(a)}_{\alpha_2}\right\rangle \varphi_{n\ell}(\vec{R}^{(a)}_{c.m.}) $$

Matrix inversion

Observables calculated in the translationally invariant basis



$$ \left|\psi^{(A-a)}_{\alpha_1}\right\rangle \left|\psi^{(a)}_{\alpha_2}\right\rangle \varphi_{n\ell}(\vec{r}_{A-a,a}) $$

- Advantage: can use powerful second quantization techniques

$$ {}_{SD}\left\langle \Phi^{(A-a',a')}_{\nu'n'} \middle| \hat{O}_{t.i.} \middle| \Phi^{(A-a,a)}_{\nu n} \right\rangle_{SD} \propto {}_{SD}\left\langle \psi^{(A-a')}_{\alpha_1'} \middle| a^+ a \middle| \psi^{(A-a)}_{\alpha_1} \right\rangle_{SD}, \; {}_{SD}\left\langle \psi^{(A-a')}_{\alpha_1'} \middle| a^+ a^+ a a \middle| \psi^{(A-a)}_{\alpha_1} \right\rangle_{SD}, \; \cdots $$

In practice, we made use of second quantization

More insights

1. New basis: Slater Determinant channel basis

   ➢ The target (A>a nucleons) described by a Slater Determinant

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle_{SD} \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell\left(\hat{R}^{(a)}_{c.m.}\right)\right]^{(J^\pi T)} R_{n\ell}\left(R^{(a)}_{c.m.}\right)$$

$$\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \varphi_{00}\left(\vec{R}^{(A-a)}_{c.m.}\right)$$

Vector proportional to the c.m. coordinate of the *A*-*a* nucleons

Vector proportional to the c.m. coordinate of the *a* nucleons

2. With a basis change, we can recover a simple expression

$$|\Phi^{J^\pi T}_{\nu n}\rangle_{\rm SD} = \sum_j \hat{s}\hat{j}\ (-1)^{I_1+J+j} \left\{ \begin{array}{ccc} I_1 & \frac{1}{2} & s \\ \ell & J & j \end{array} \right\}$$

$$\times \left[|A{-}1\,\alpha_1 I_1^{\pi_1} T_1\rangle_{\rm SD}\, \varphi_{n\ell j\frac{1}{2}}(\vec{r}_A \sigma_A \tau_A) \right]^{(J^\pi T)}$$

Then, the kernels can be calculated with the help of the second quantization

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

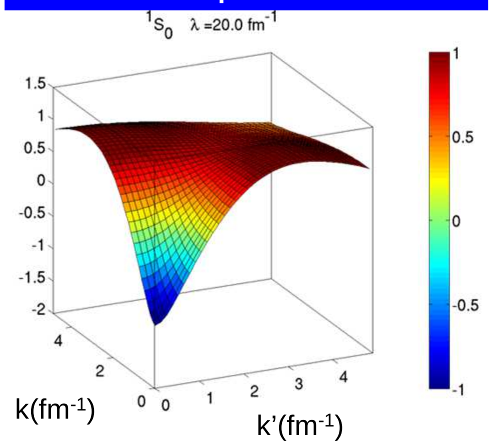
$$H_\lambda = U_\lambda H U_\lambda^{+}$$

Unitary transformations

$$\begin{cases} \dfrac{dH_\lambda}{d\lambda} = \left[\eta(\lambda), H_\lambda\right] \\[2ex] \eta(\lambda) = \dfrac{dU_\lambda}{d\lambda} U_\lambda^{+} \end{cases}$$

Flow parameter

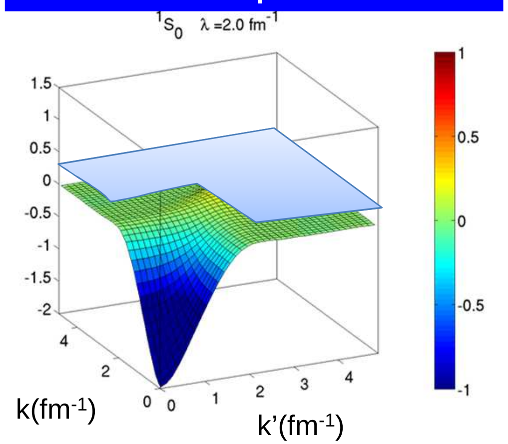
Bare potential



Evolution with flow parameter λ

- Preserves the physics
- Decouples high and low momentum
- Induces many-body forces

Evolved potential



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

☑ Nucleon-nucleus collisions

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

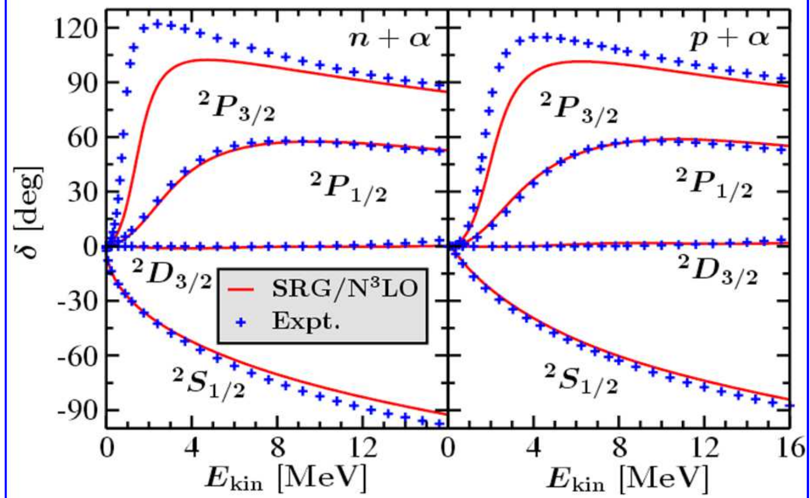
☑Deuterium-nucleus collisions

- ✓ d-^{4}He scattering and ^{6}Li structure with SRG-N^{3}LO

☑(d,N) transfer reactions

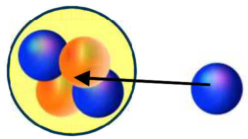
- ✓ ^{3}H(d,n)^{4}He and ^{3}He(d,p)^{4}He reactions with SRG-N^{3}LO

n-He^4 phase-shift NN only



λ dependent

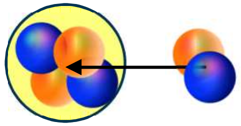
Good reproduction, but still incomplete



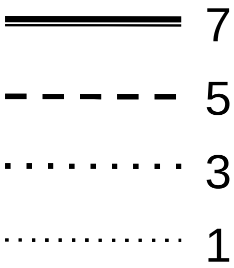
n on ^{4}He scattering

^{4}He(d,d)^{4}He with NN-only

S. Quaglioni and P. Navratil

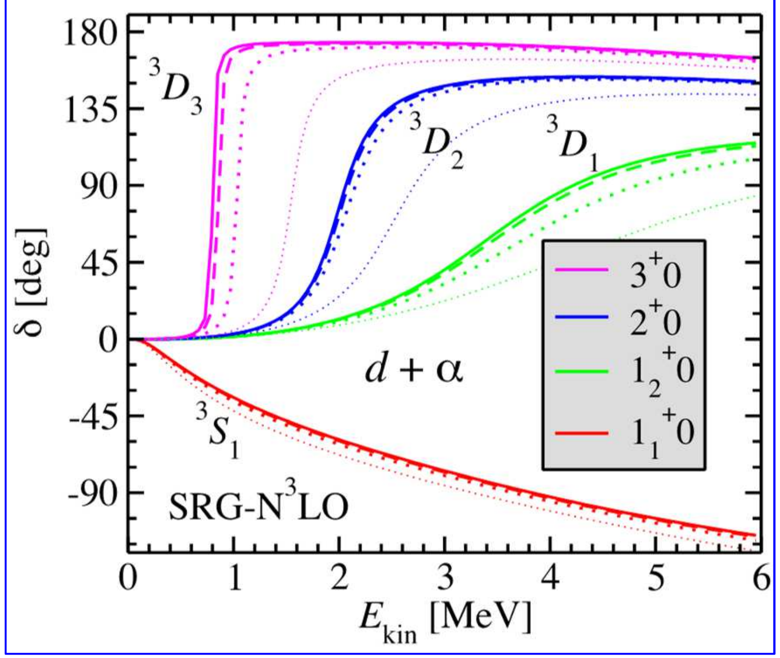


d-^{4}He scattering

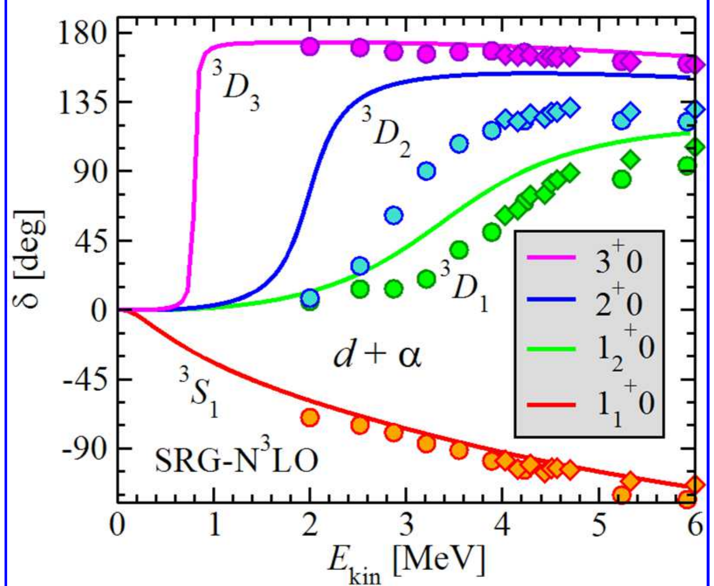


Deuteron Pseudo-states in each channel

^{4}He(d,d)^{4}He phase shifts



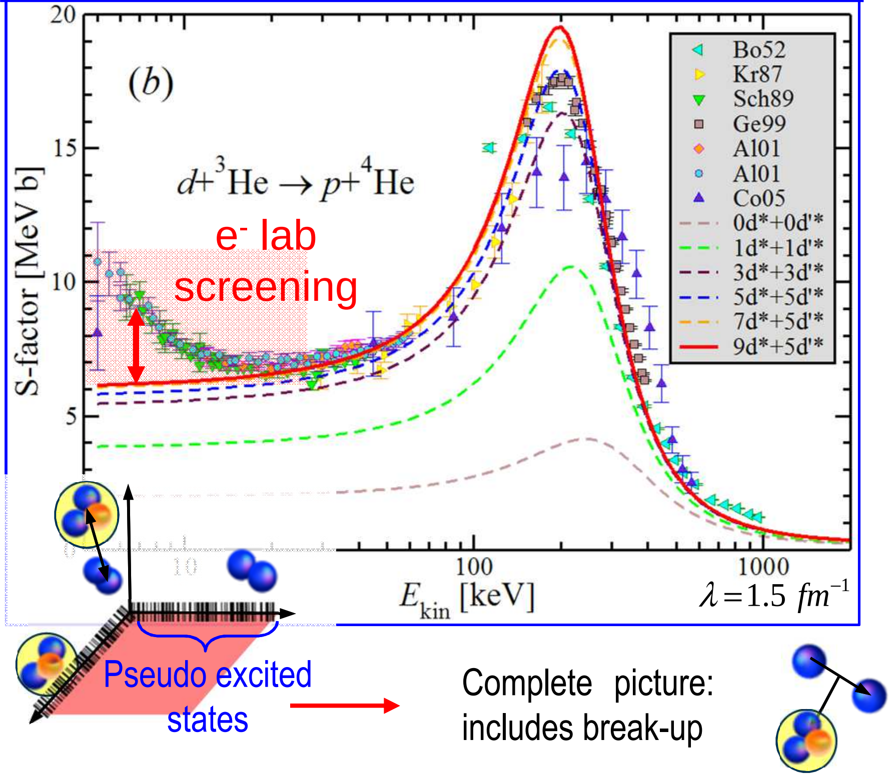
Phase shifts with λ= 1.5 fm^{-1}



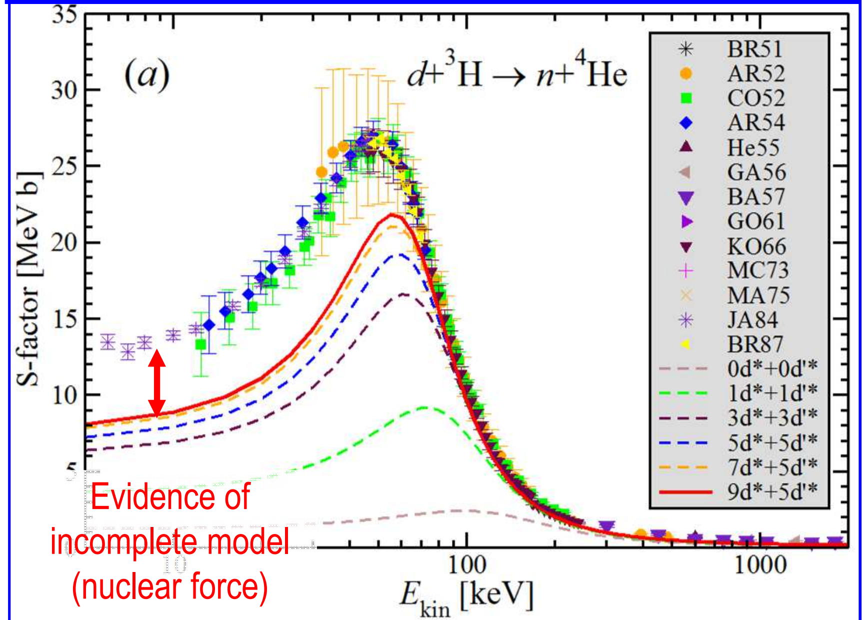
N_{max}= 12 d(g.s.,$^3S_1$-$^3D_1$, $^3D_2$, $^3D_3$-$^3G_3$) + ^{4}He(g.s.) SRG-N^{3}LO NN potential with λ=1.5 fm^{-1}.

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)

^{3}He(d,p)^{4}He astrophysical S-factor



^{3}H(d,n)^{4}He astrophysical S-factor



NCSM/RGM results for the ^{3}He(d,n)^{4}He astrophysical S-factor compared to beam-target measurements.

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.

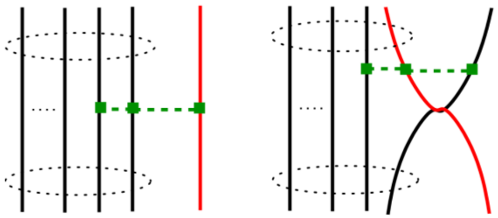
Incomplete nuclear interaction: requires NNN force (SRG-induced + “real”)

Including the NNN force into the NCSM/RGM approach

nucleon-nucleus formalism

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} V^{NNN} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle \; (A-1) \; r' \; (a'=1) \middle| V^{NNN}\left(1-\sum_{i=1}^{A-1}\hat{P}_{iA}\right) \middle| (a=1) \; r \; (A-1) \right\rangle$$

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

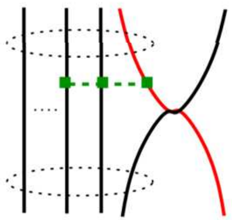


(a) (b)

Direct potential:

$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha'_1} \middle| a^+_i a^+_j a_l a_k \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

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



(c)

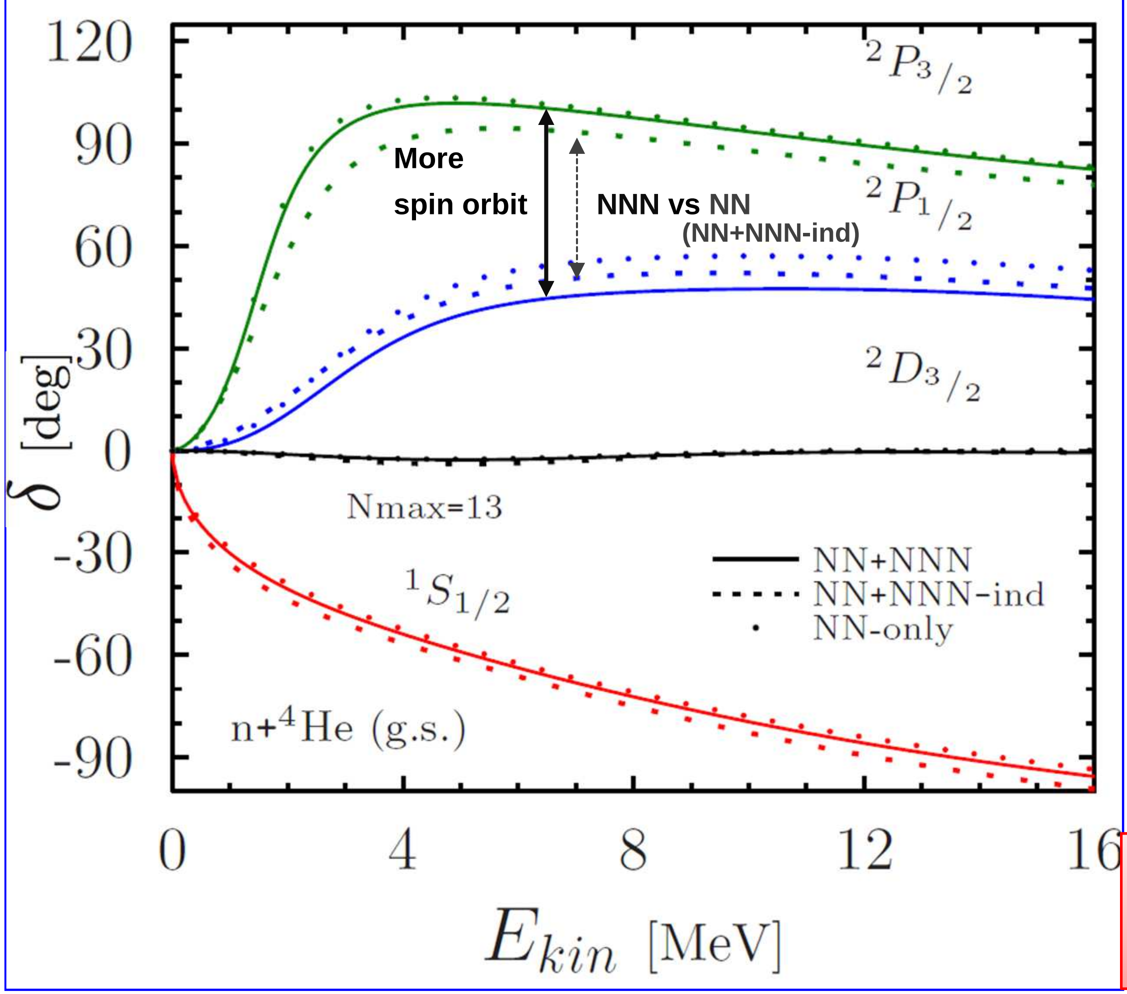
Exchange potential:

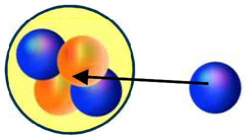
$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha'_1} \middle| a^+_h a^+_i a^+_j a_m a_l a_k \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

n-^{4}He scattering: NN versus NNN interactions, first results

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

From NN-only (NN+NNN-ind) to NN+NNN





n-^{4}He scattering

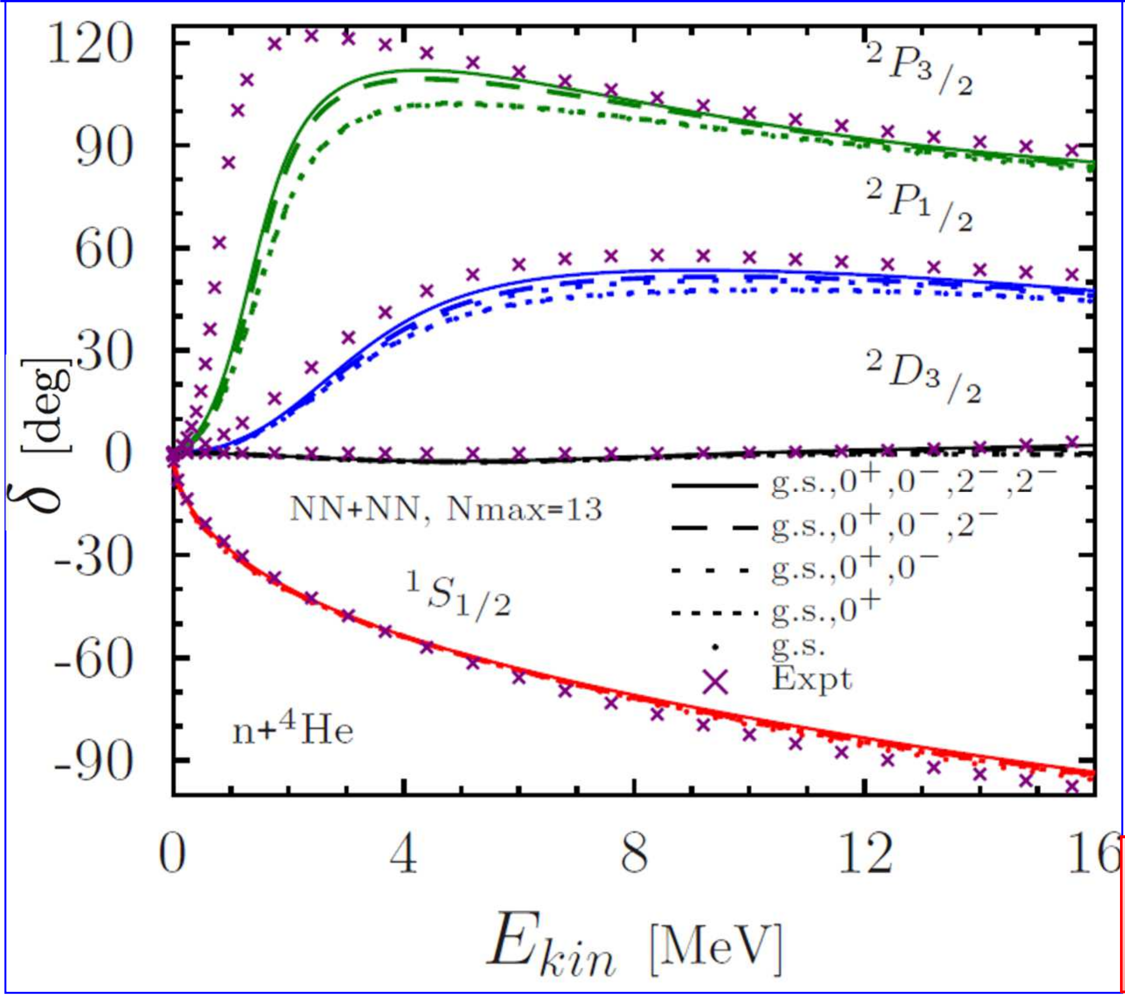
- The largest splitting between *P* waves is obtained with NN+NNN.

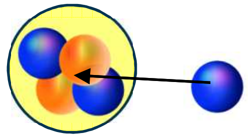
Comparison between NN, NN+NNN-ind and NN+NNN at Nmax=13

n-^{4}He scattering: NN+NNN with the first three excited states

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

^{4}He(n,n)^{4}He phase-shifts with four excited states





n-^{4}He scattering

- The largest splitting between *P* waves is obtained with NN+NNN.
- A better reproduction of data is expected when all the first six excited state of ^{4}He included (following).
- The present NNN force is incomplete (N^{2}LO only).

Comparison between NN+NNN and experiment at Nmax=13 and λ=2.0

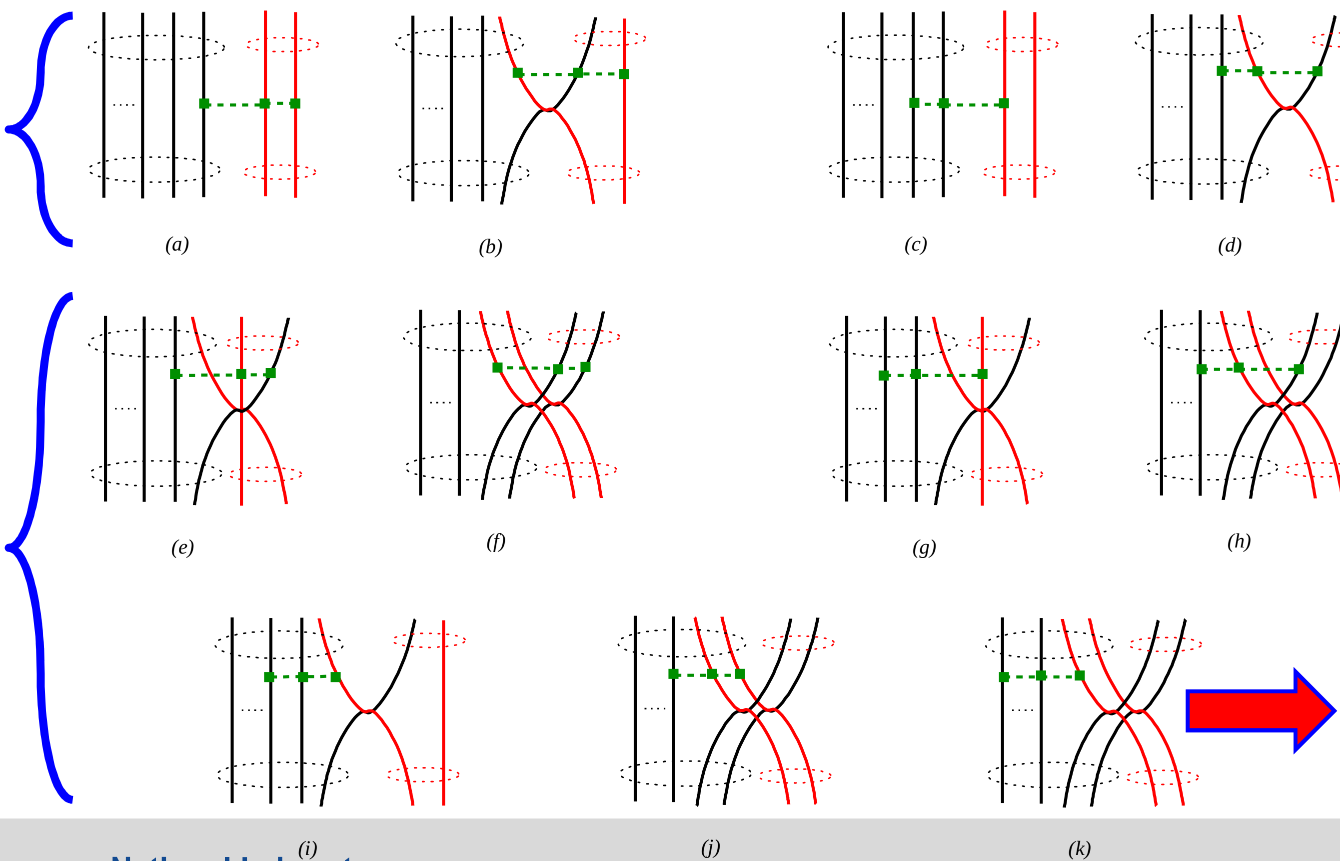
Including the NNN force into the NCSM/RGM approach

deuteron-nucleus formalism

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} V^{NNN} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle \underset{(a'=2)}{\overset{(A-2)}{r'}} \middle| V^{NNN} \left(1 - \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{i,k} + \sum_{i<j=1}^{A-2} \hat{P}_{i,A-1} \hat{P}_{j,A} \right) \middle| \underset{(a=2)}{\overset{(A-2)}{r}} \right\rangle$$

Direct

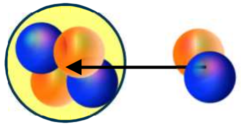
Exchange

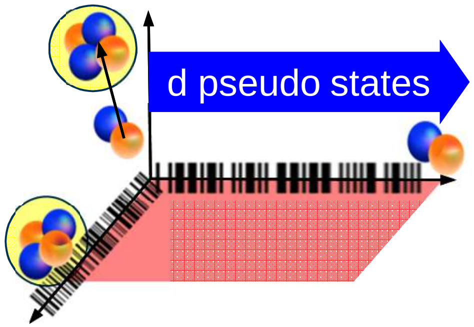


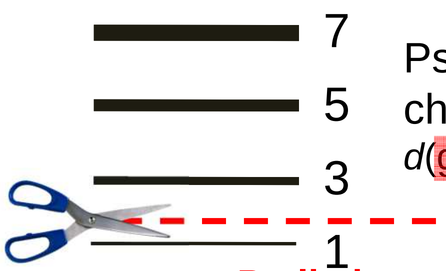
four body density

^{4}He(d,d)^{4}He with NN+NNN interaction

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



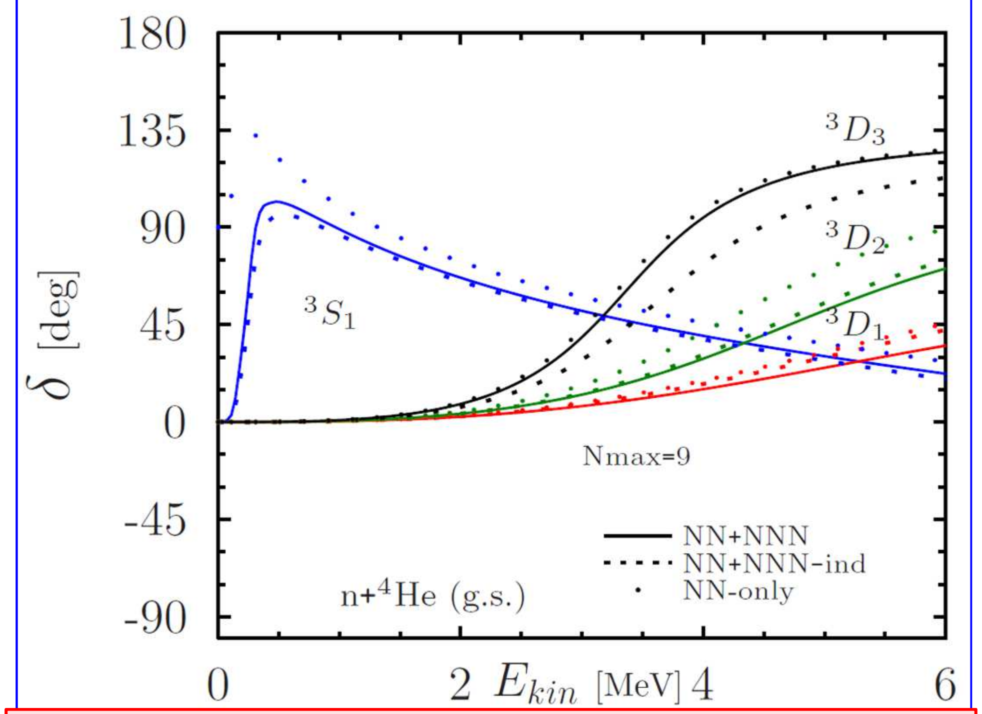




Pseudo-states in each channel
d(g.s.,$^3S_1$-$^3D_1$, $^3D_2$, $^3D_3$-$^3G_3$)

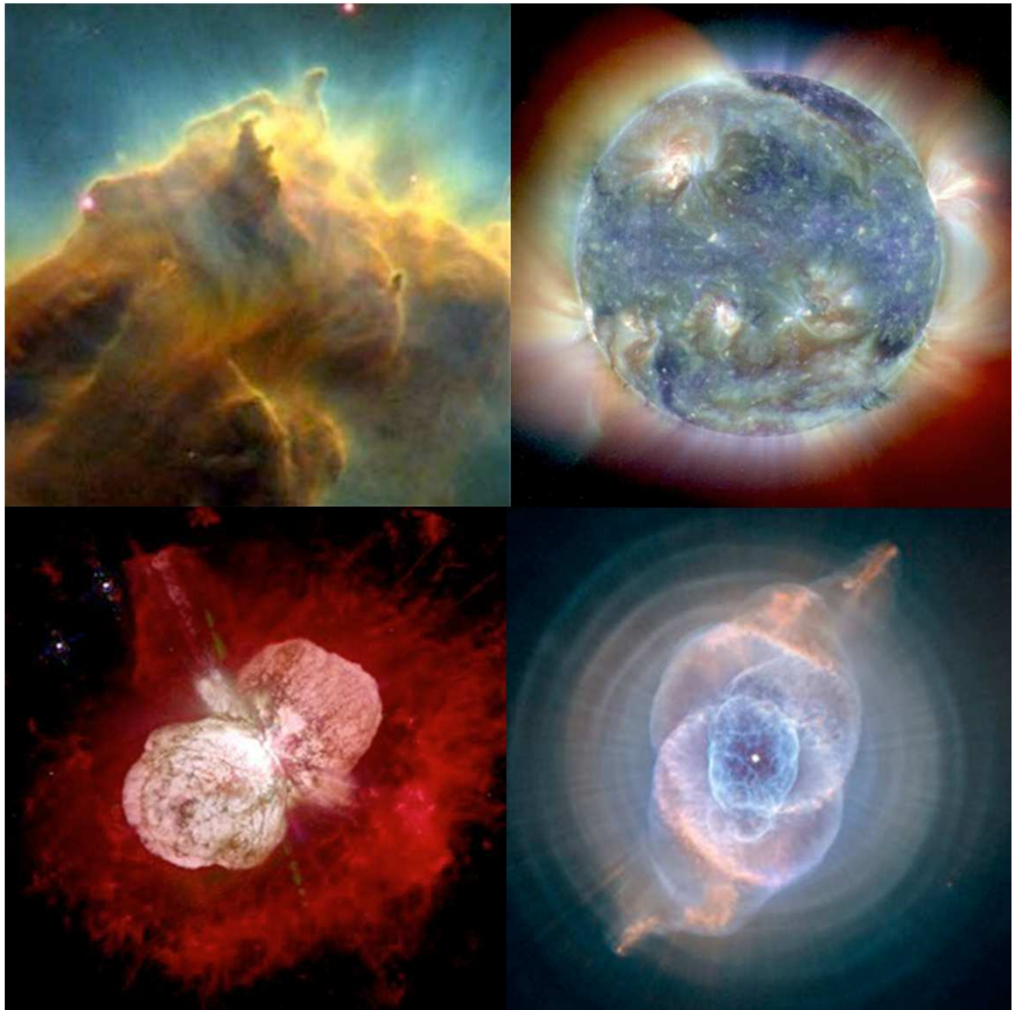
Preliminary results in a small model space and with only d and ^{4}He g.s., look promising

Comparison between NN-only, NN+NNN-ind and NN+NNN ^{4}He(d,d)^{4}He phase-shifts



d(g.s.) + ^{4}He(g.s.) scattering phase-shifts for NN, NN+NNN-induced and NN+NNN potential with hω=20, λ=2 fm^{-1} and Nmax=9.

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^3LO
  - Before definite conclusion
    - Study of λ dependence
    - Study of $\hbar\omega$ dependence
  - Scattering of heavier target