FROM RESEARCH TO INDUSTRY

Lawrence Livermore National Laboratory

INSTITUT DE PHYSIQUE NUCLÉAIRE ORSAY

NUCLEAR STRUCTURE AND REACTIONS FROM CHIRAL INTERACTIONS

Collaborators:

- **A. Calci (TRIUMF)**
- J. Dohet-Eraly (TRIUMF)
- J. Langhammer (Private sector)
- **P. Navrátil (TRIUMF)**
- F. Raimondi (U. of Surrey)
- C. Romero-Redondo (LLNL)
- **R. Roth (TU Darmstadt)**
- **S. Quaglioni (LLNL)**

Guillaume Hupin

Progress in *Ab Initio* Techniques in Nuclear Physics, TRIUMF BC Canada, February 23th 2016.

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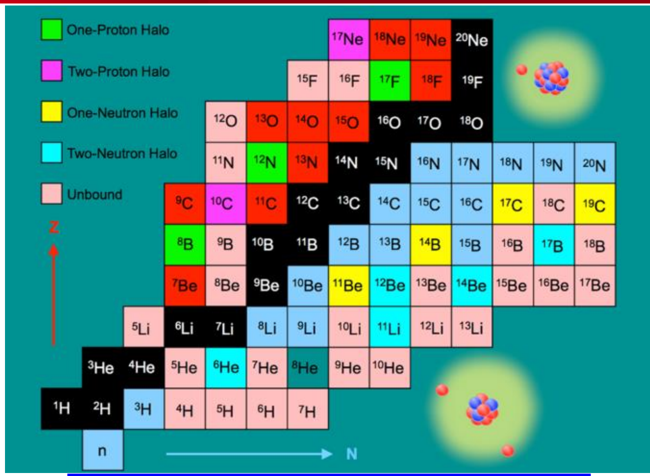
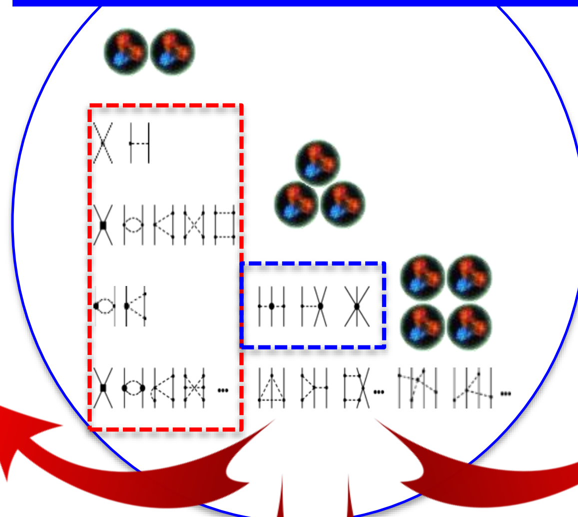
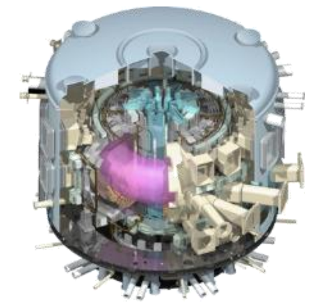
INTRODUCTION



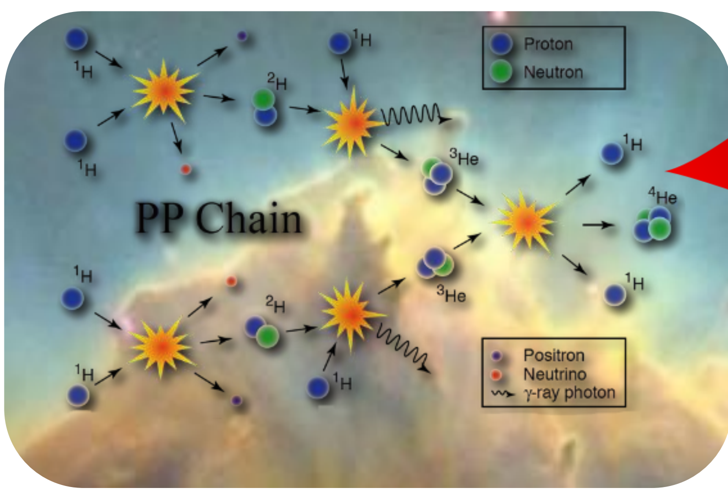
Structure of exotic nuclei

Ab initio structure and reaction





Fusion based energy generation



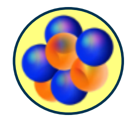
Nuclear astrophysics

Materials science

EQUAL TREATMENT OF BOUND AND RESONANT STATES: COUPLE NCSM AND NCSM/RGM (NCSMC)

- Methods develop in this presentation to solve the many body problem

$$\Psi^{(A)}_{NCSM} = |A\lambda J^{\pi} T\rangle = \sum_{\alpha} c_{\alpha} \, |A\alpha j_z{}^{\pi} t_z\rangle \Leftrightarrow |A\lambda J^{\pi} T\rangle_{SD} \phi_{00}(\vec{R}^{A}_{c.m.})$$

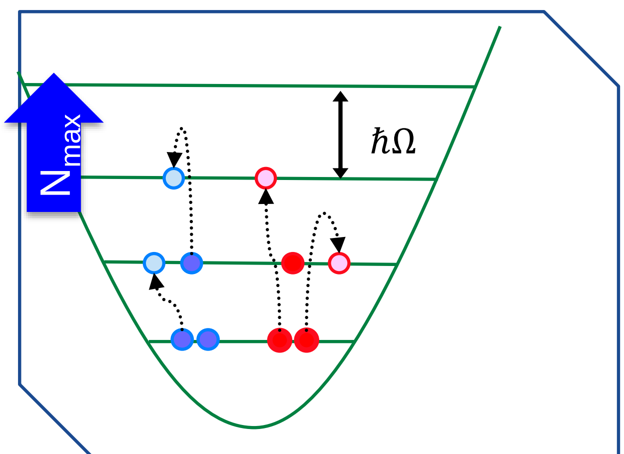


Mixing coefficients(unknown)

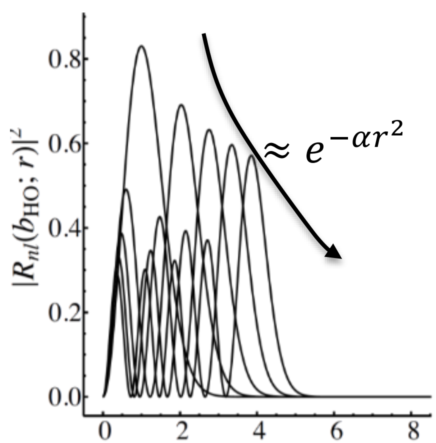
A-body harmonic oscillator states

Second quantization

Can address bound and low-lying resonances (short range correlations)



No-Core Shell Model



$$\Psi^{(A)}_{NCSMC} = \sum_{\lambda} c_{\lambda} |A\lambda J^{\pi} T\rangle$$

EQUAL TREATMENT OF BOUND AND RESONANT STATES: COUPLE NCSM AND NCSM/RGM (NCSMC)

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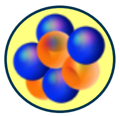


$$|A\lambda J^{\pi} T\rangle_{SD} \phi_{00}(\vec{R}^{A}_{c.m.})$$

Second quantization

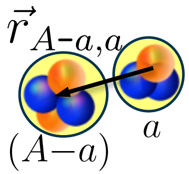
Can address bound and low-lying resonances (short range correlations)

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

Relative wave function (unknown)

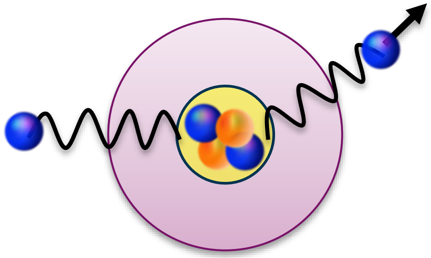
Antisymmetrizer

Channel basis



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

Cluster expansion technique



NCSM/RGM
Cluster formalism for elastic/inelastic

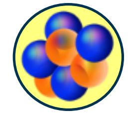
$$\Psi^{(A)}_{NCSMC} = \sum_{\lambda} c_{\lambda} |A\lambda J^{\pi} T\rangle + \sum_{\nu} \int d\vec{r} \, g_{\nu}(\vec{r}) \, \hat{A}_{\nu} \left| \Phi^{(A-a,a)}_{\nu\vec{r}} \right\rangle$$

EQUAL TREATMENT OF BOUND AND RESONANT STATES: COUPLE NCSM AND NCSM/RGM (NCSMC)

S. Baroni, P. Navrátil and S. Quaglioni PRL110 (2013); PRC93 (2013)

- Methods develop in this presentation to solve the many body problem

$$\Psi^{(A)}_{NCSM} = |A\lambda J^{\pi} T\rangle = \sum_{\alpha} c_{\alpha} \, |A\alpha j_z{}^{\pi} t_z\rangle \Leftrightarrow |A\lambda J^{\pi} T\rangle_{SD} \phi_{00}(\vec{R}^{A}_{c.m.})$$



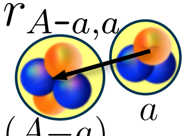
Mixing coefficients(unknown)

A-body harmonic oscillator states

Second quantization

Can address bound and low-lying resonances (short range correlations)

$$\Psi^{(A)}_{RGM} = \sum_{v} \int d\vec{r} \, g_v(\vec{r}) \, \hat{A}_v \left| \Phi^{(A-a,a)}_{v\vec{r}} \right\rangle \Leftrightarrow \psi^{(A-a)}_{\alpha_1} \psi^{(a)}_{\alpha_2} \, \delta(\vec{r} - \vec{r}_{A-a,a})$$



Relative wave function (unknown)

Antisymmetrizer

Channel basis

Cluster expansion technique

Design to account for scattering states (best for long range correlations)

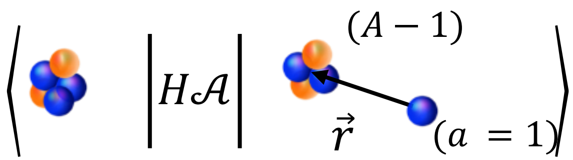
- The many body quantum problem is best described by the superposition of both type of wave functions

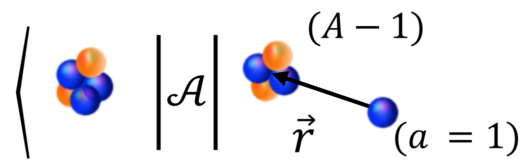
$$\Psi^{(A)}_{NCSMC} = \sum_{\lambda} c_{\lambda} |A\lambda J^{\pi} T\rangle + \sum_{v} \int d\vec{r} \, g_v(\vec{r}) \, \hat{A}_v \left| \Phi^{(A-a,a)}_{v\vec{r}} \right\rangle$$

NCSMC

COUPLED NCSMC EQUATIONS

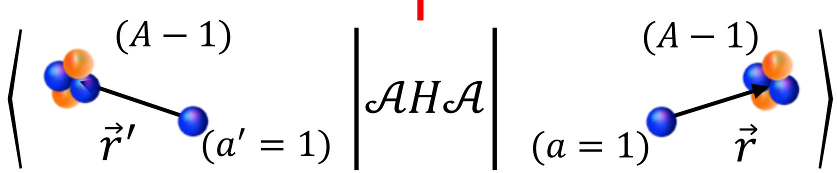
S. Baroni, P. Navrátil and S. Quaglioni PRL110 (2013); PRC93 (2013)





$E_\lambda\,\delta_{\lambda\lambda'}$

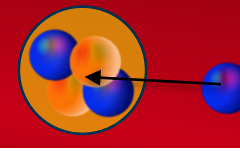
$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix}\begin{pmatrix} c \\ \gamma \end{pmatrix} = E\begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix}$$



Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic R-matrix on Lagrange mesh

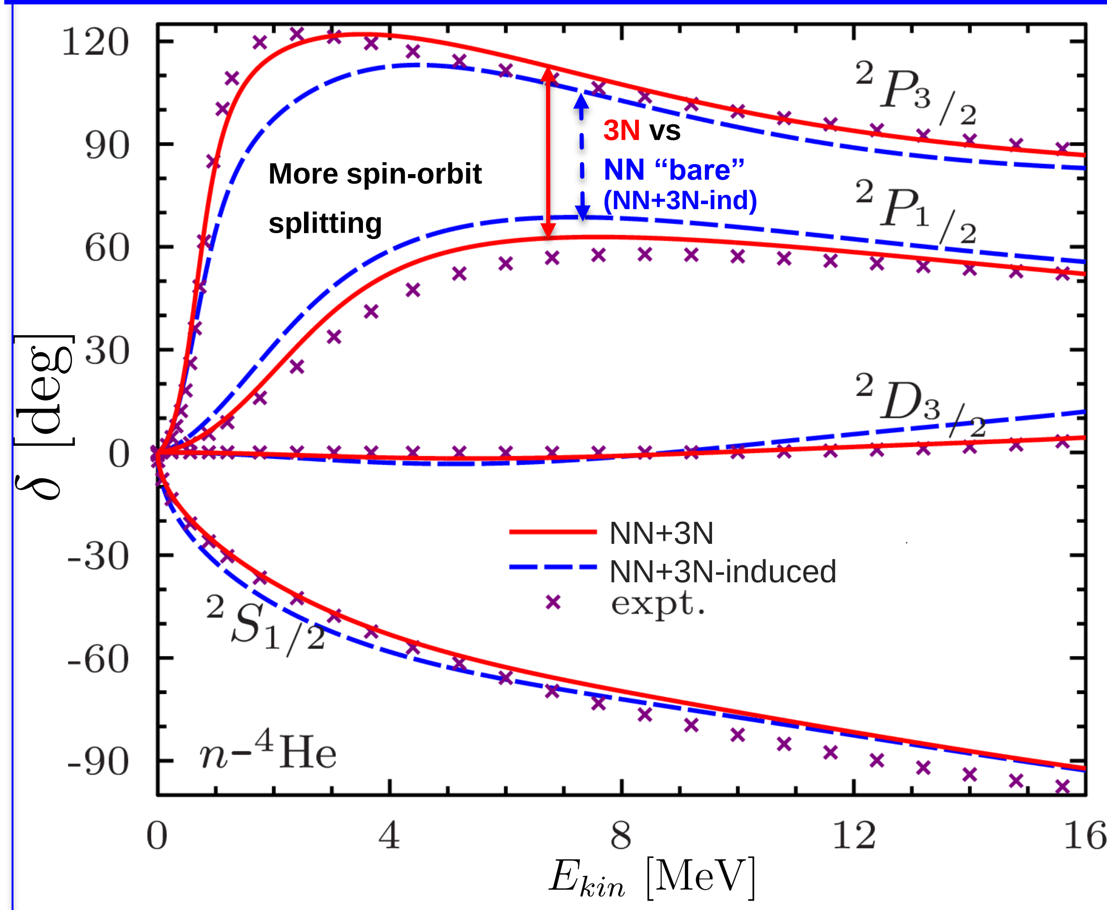
n-^{4}He SCATTERING: NN VERSUS 3N INTERACTIONS

G. Hupin, J. Langhammer *et al.* PRC88 (2013); G. Hupin, S. Quaglioni and P. Navrátil, to be published in Physica ScriptaSpecial Edition - Nobel Prize '75 anniversary



n-^{4}He scattering

Two scenarii of nuclear Hamiltonians

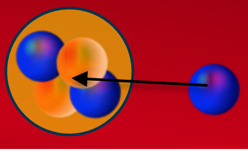


- The 3N interactions influence mostly the *P* waves.
- The largest splitting between *P* waves is obtained with NN+3N.

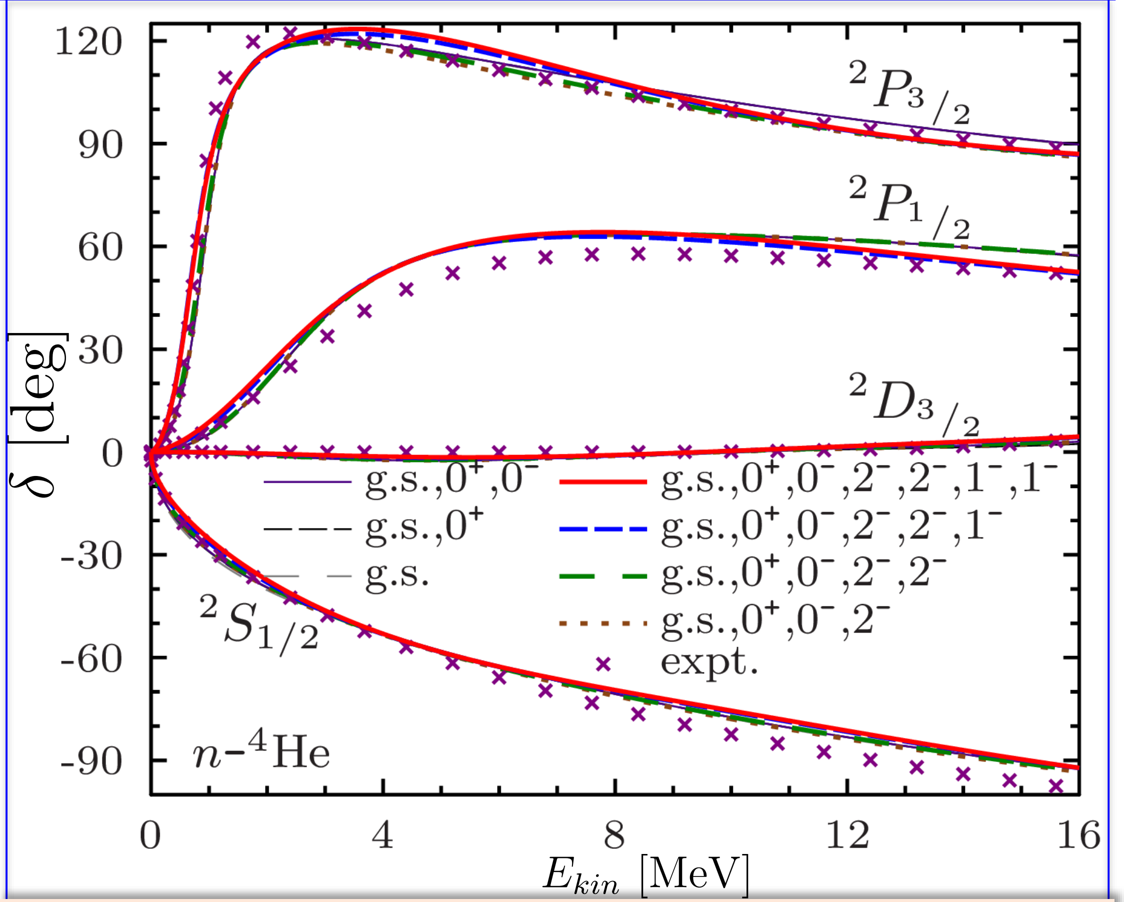
Comparison between NN+3N -ind and NN+3N at N_{max}=13 with six ^{4}He states and 14 ^{5}He states.

AB INITIO n-^{4}He SCATTERING

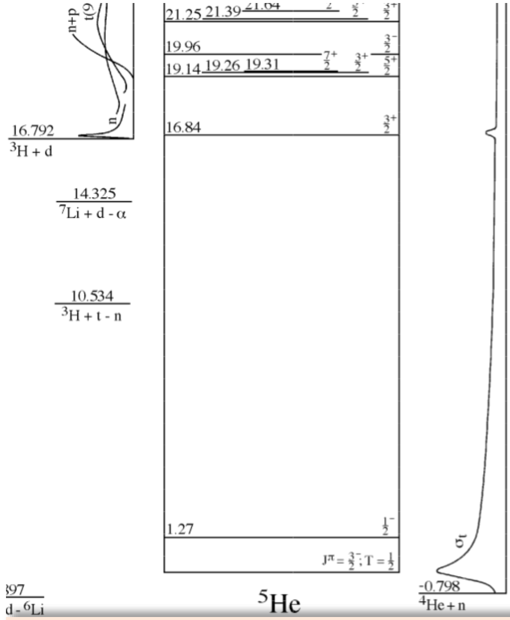
G. Hupin, J. Langhammer *et al.* PRC88 (2013); G. Hupin, S. Quaglioni and P. Navrátil, to be published in Physica ScriptaSpecial Edition - Nobel Prize '75 anniversary



Study of the convergence with respect to the # of ^{4}He low-lying states



n-^{4}He scattering phase-shifts for NN+3N potential with λ=2.0 fm^{-1} and first 14th low-lying state of ^{5}He.

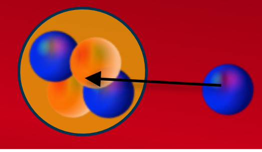


Experimental low-lying states of the A=5 nucleon systems.

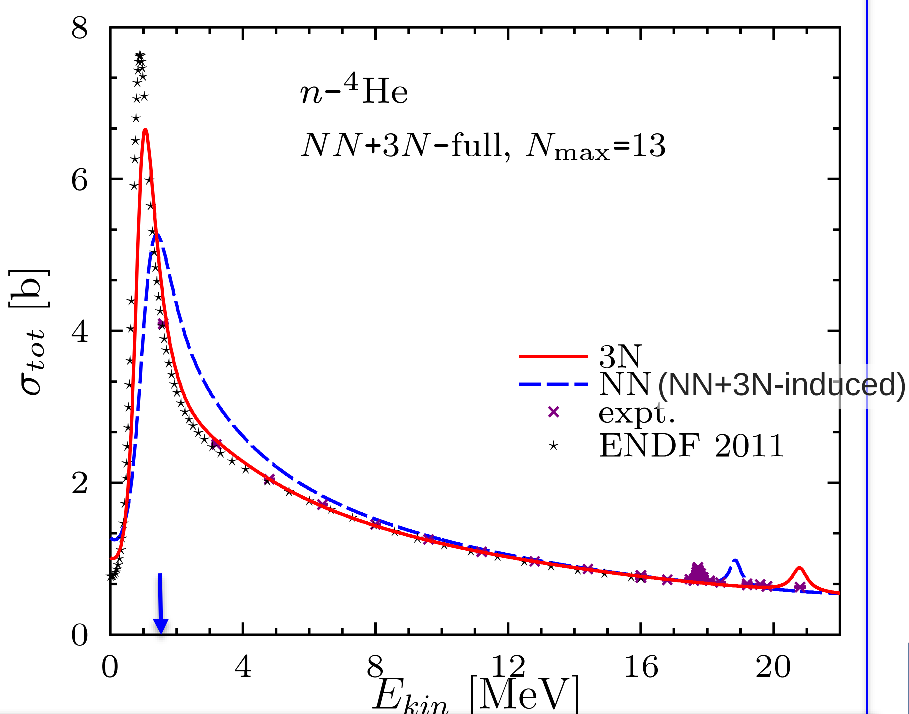
- The convergence pattern looks good.
- The experimental phase-shifts are well reproduced.

n-^{4}He ELASTIC CROSS-SECTIONS

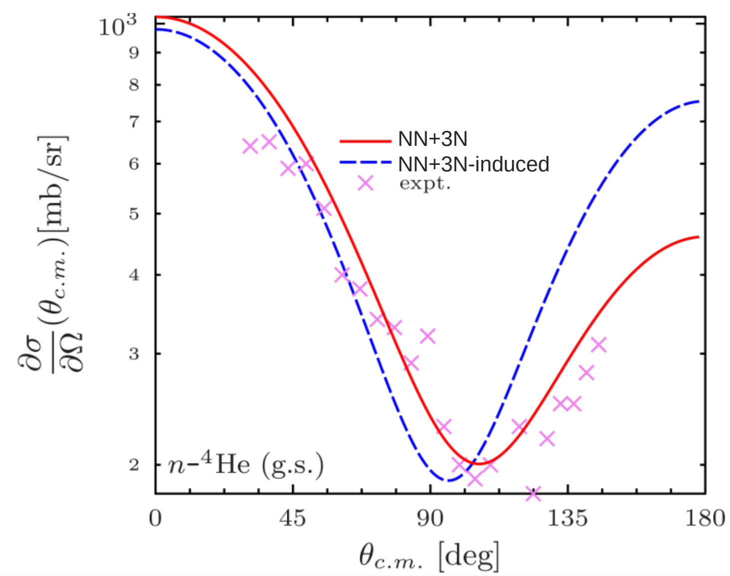
G. Hupin, S. Quaglioni and P. Navrátil, to be published as a contribution to the Special Physica Scripta Edition - 40 year anniversary - Nobel Prize '75



Comparison of the elastic cross-section between NN and NN+3N with ^{4}He (g.s.)



n-^{4}He elastic cross-section for NN+3N-induced, NN+3N potentials compared to expt. and ENDF evaluation.

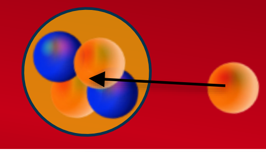


Differential cross-section at $E_{neutron}$ =1.79 MeV between NN+3N-ind and NN+3N.

- We obtained a better agreement with data when using NN+3N.
- The 3N force is constitutive to the reproduction of the $^3/_2{}^+$ resonance.

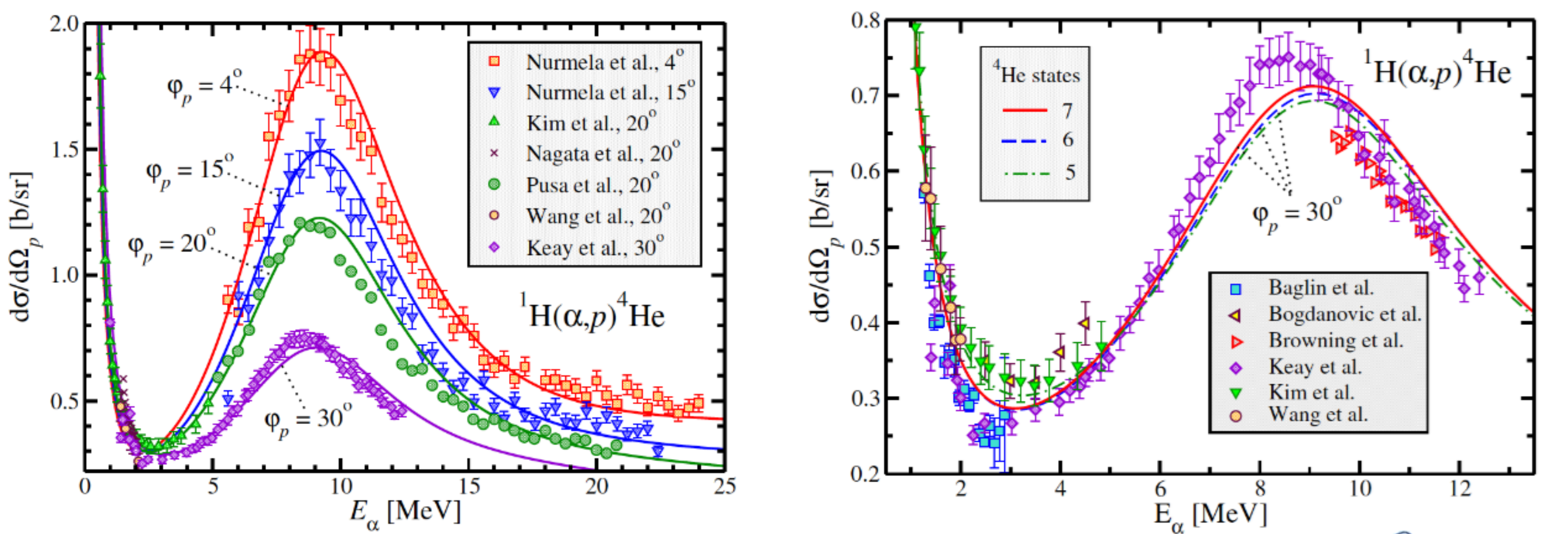
PREDICTION FOR ELASTIC RECOIL DETECTION (ERD)

G. Hupin, S. Quaglioni and P. Navrátil, PRC90 (2014)



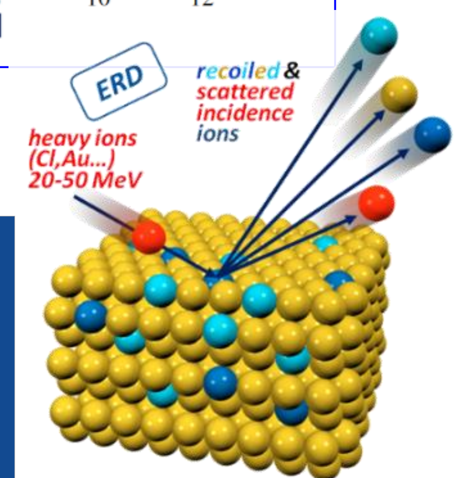
p-^{4}He scattering

Cross-section compared to experiments focused on proton recoil analysis



p-^{4}He differential cross-section for NN+3N at ^{4}He incident energies close to the Rutherford scattering.

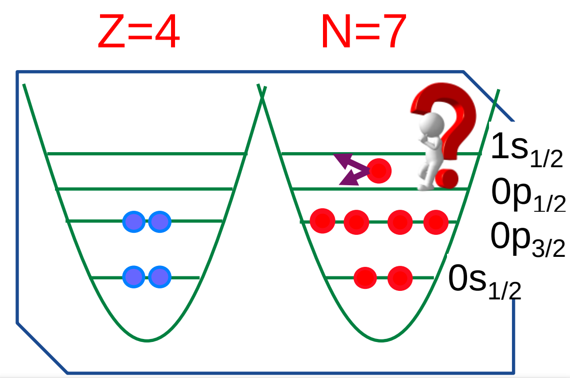
The widths predicted by our model (the only ingredient being the interaction) is too large compared to experiment. We can however discriminate between experimental data and provide accurate predictions for all angles at small and high energies.



NEUTRON-RICH HALO NUCLEUS ^{11}BE

- In the shell model picture g.s. expected to be $J^\pi=1/2^-$

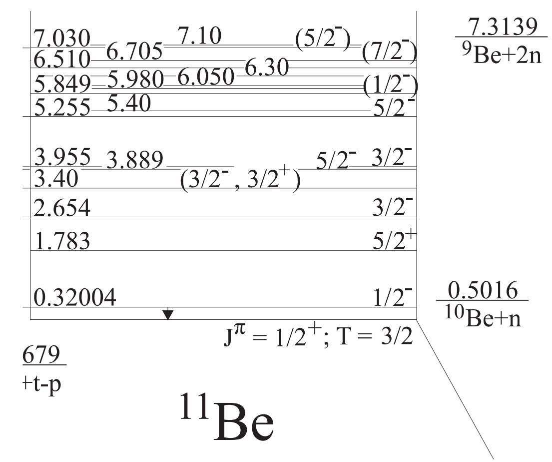
  (Z=6, N=7) ^{13}C and (Z=8, N=7) ^{15}O have $J^\pi=1/2^-$ g.s.
- In reality, ^{11}Be g.s. is **$J^\pi=1/2^+$** -- parity inversion
- Very weakly bound: E_{th}=-0.5 MeV **Halo state** -- dominated by ^{10}Be-n in the *S*-wave
- The 1/2$^-$ state also bound -- only by 180 keV



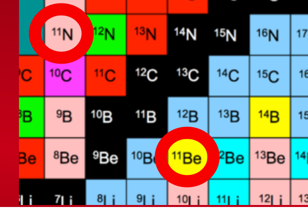
Single particle interpretation using nuclear shell model

Can we describe ^{11}Be in *ab initio* calculations?

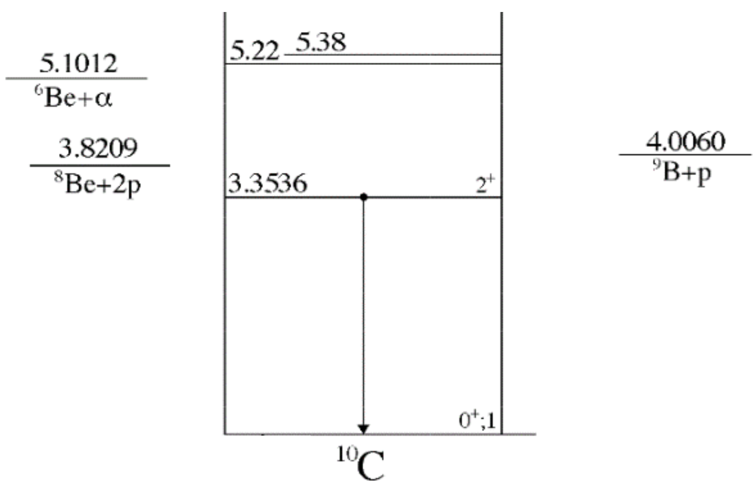
- Continuum must be included
- Does the 3N interaction play a role in the parity inversion?

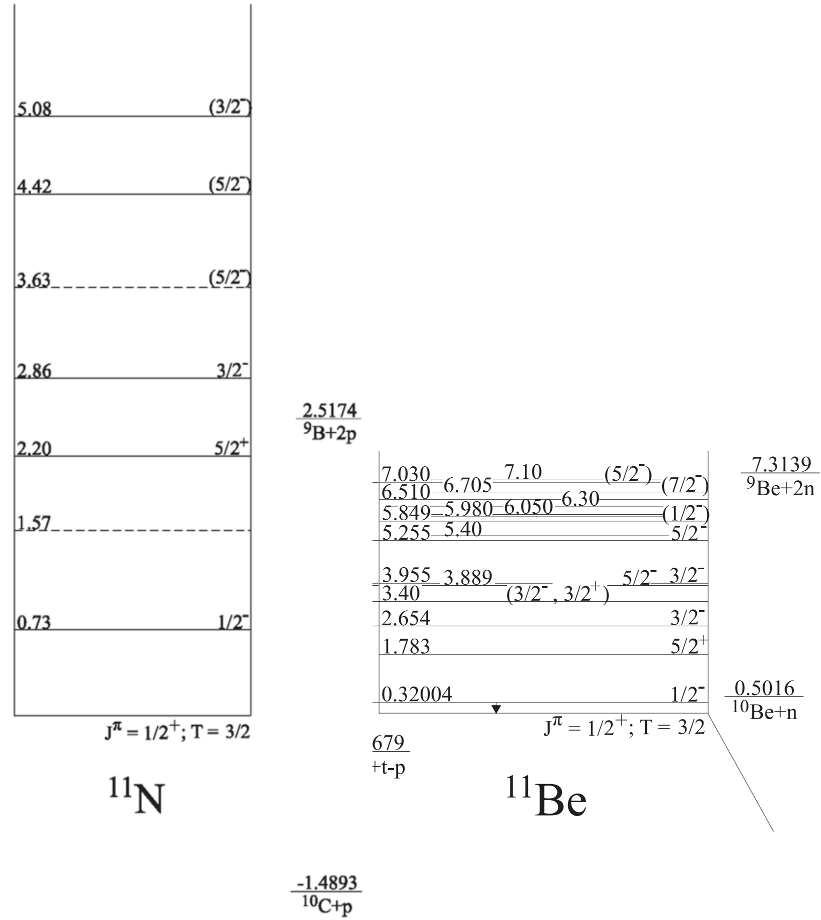


p-^{10}C SCATTERING: STRUCTURE OF ^{11}N RESONANCES



- Limited information about the structure of proton rich ^{11}N – mirror nucleus of ^{11}Be halo nucleus
- Incomplete knowledge of ^{10}C unbound excited states
- Importance of 3N force effects and continuum
- Can structure of exotic nuclei discriminate among different nuclear force models?

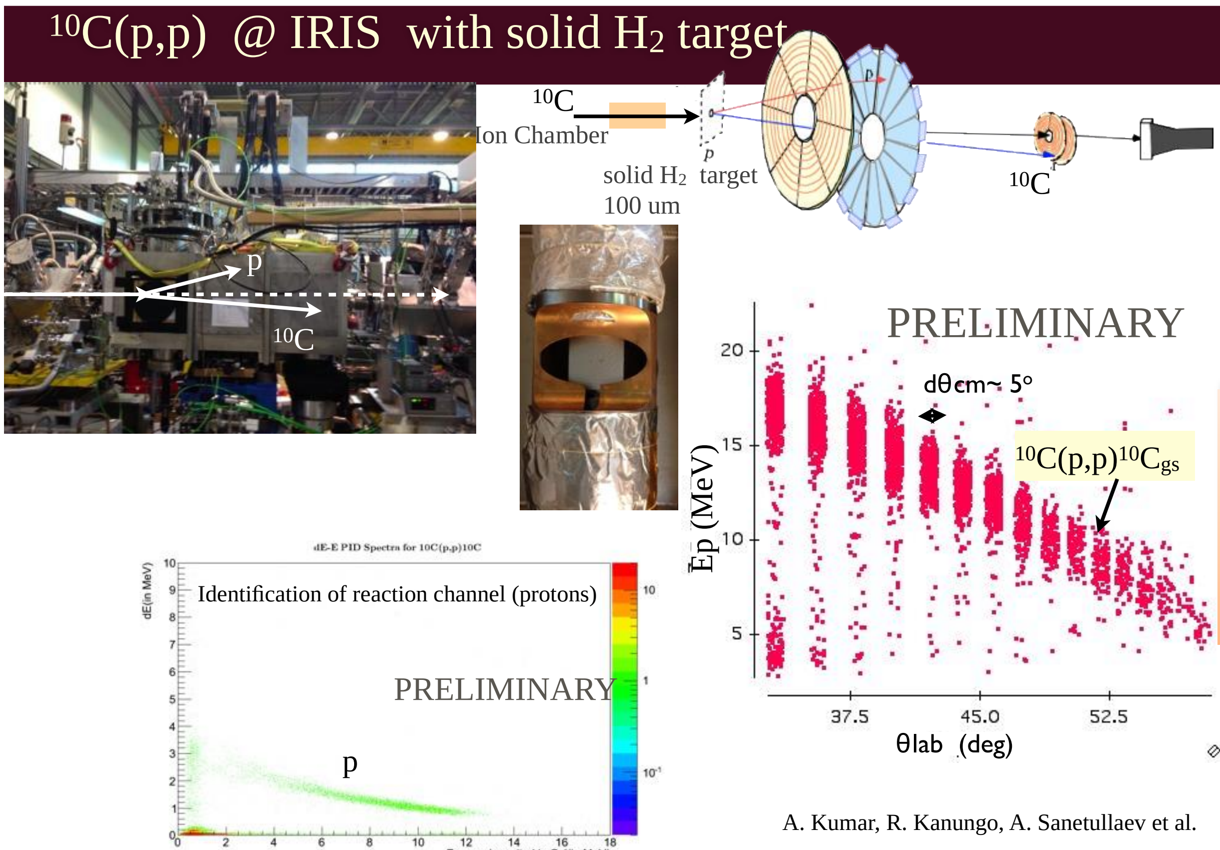




^{10}C(*p*,*p*) @ IRIS with solid H_2 target

New experiment at ISAC TRIUMF with reaccelerated ^{10}C

- The first ever ^{10}C beam at TRIUMF
- Angular distributions measured at E_{CM} ~ 4.16 MeV and 4.4 MeV



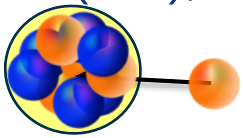
IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev *et al.*

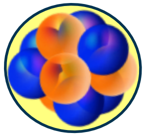
p-^{10}C SCATTERING: STRUCTURE OF ^{11}N RESONANCES

A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al.* with IRIS collaboration, in preparation

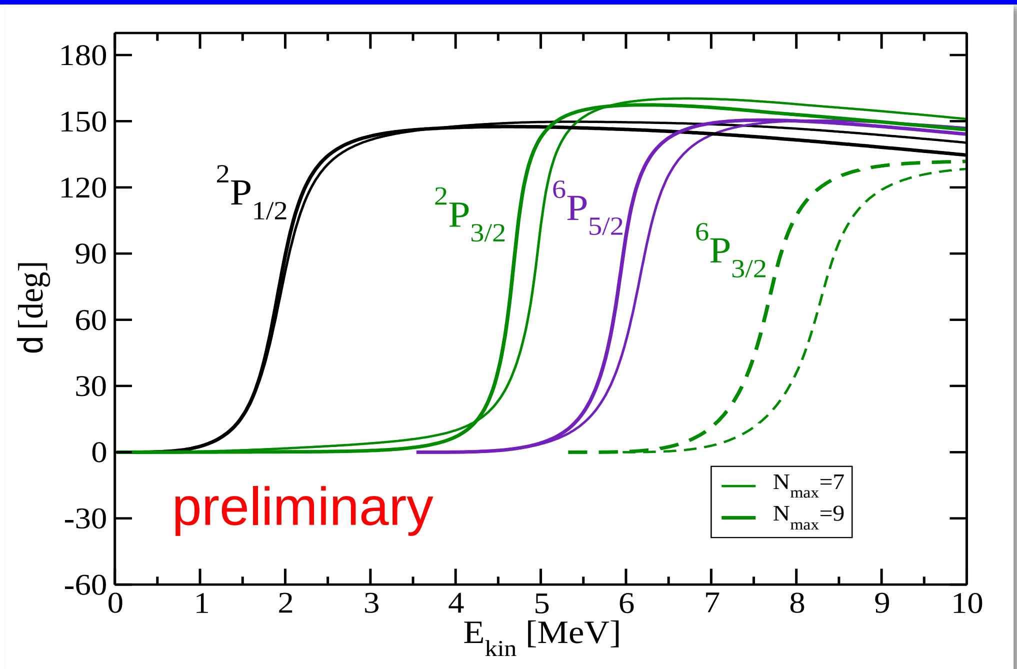
NCSMC calculations with **chiral NN+3N** [N^{3}LO NN+N^{2}LO 3NF(400), NNLOsat]

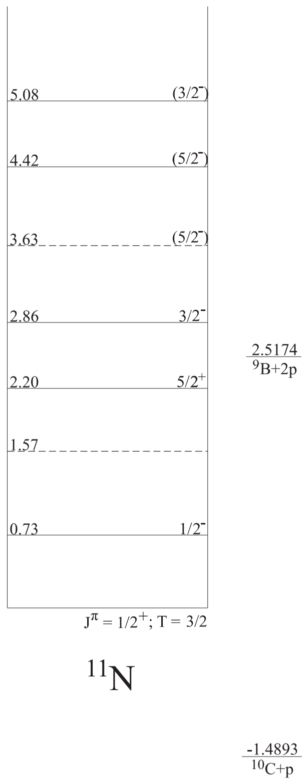
- ^{10}C: 0^+, 2^+, 2^+ NCSM eigenstates
- ^{11}N: ≥4 (π=-1= and ≥3 (π=+1) NCSM eigenstates





p-^{10}C phase shifts with NN+3N (Λ=400)





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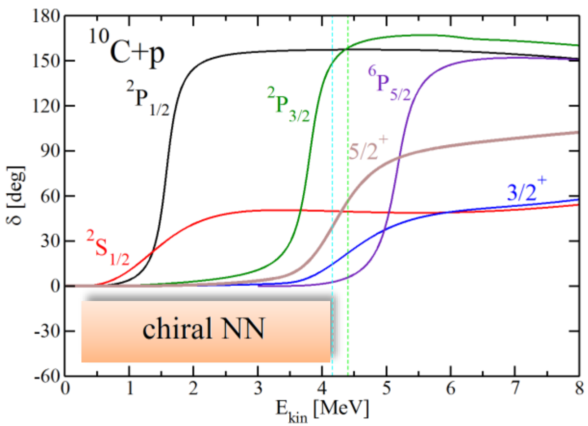

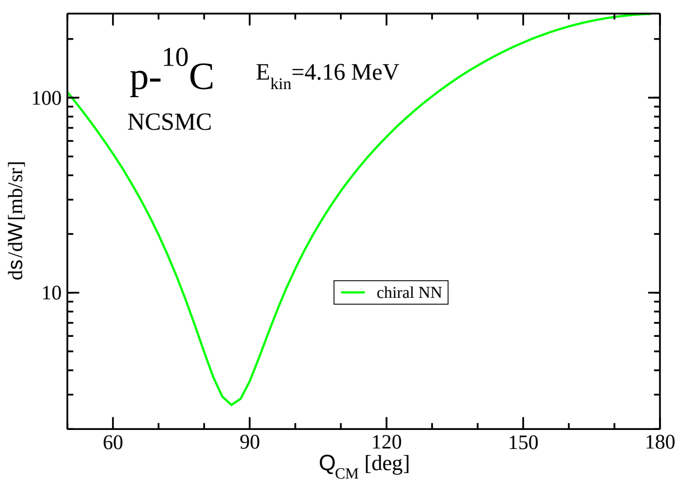

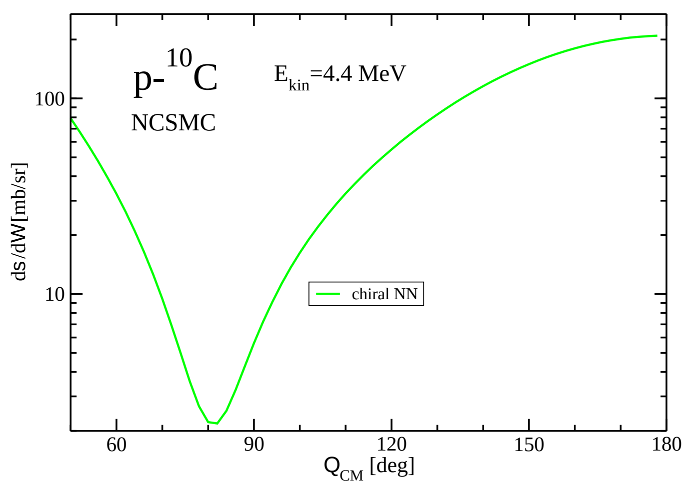

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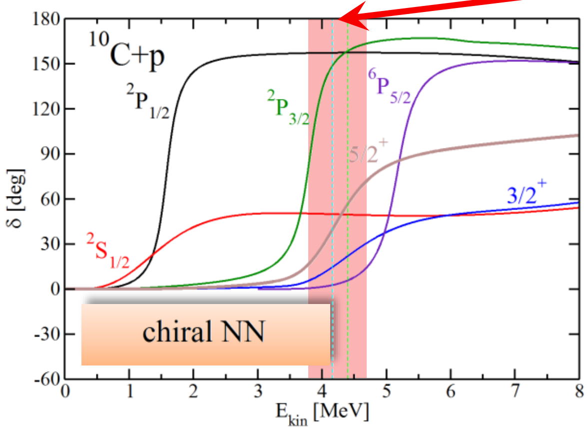
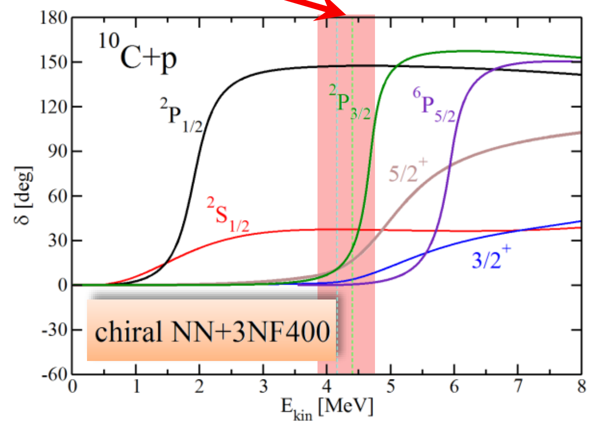
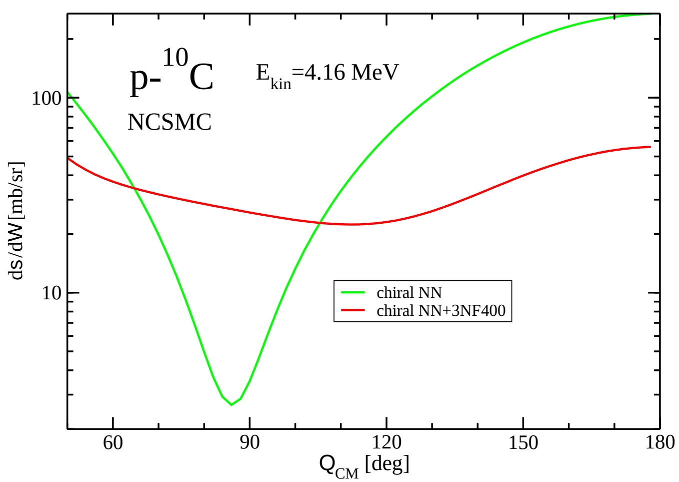
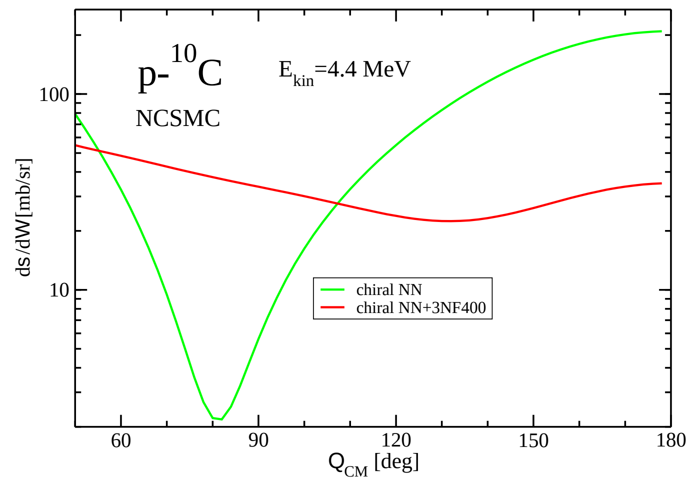
IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev *et al.*

Area where 3N force effect can be observed





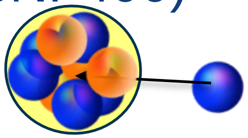




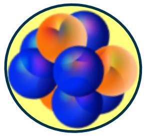
STRUCTURE OF ^{11}Be FROM CHIRAL NN+3N FORCES

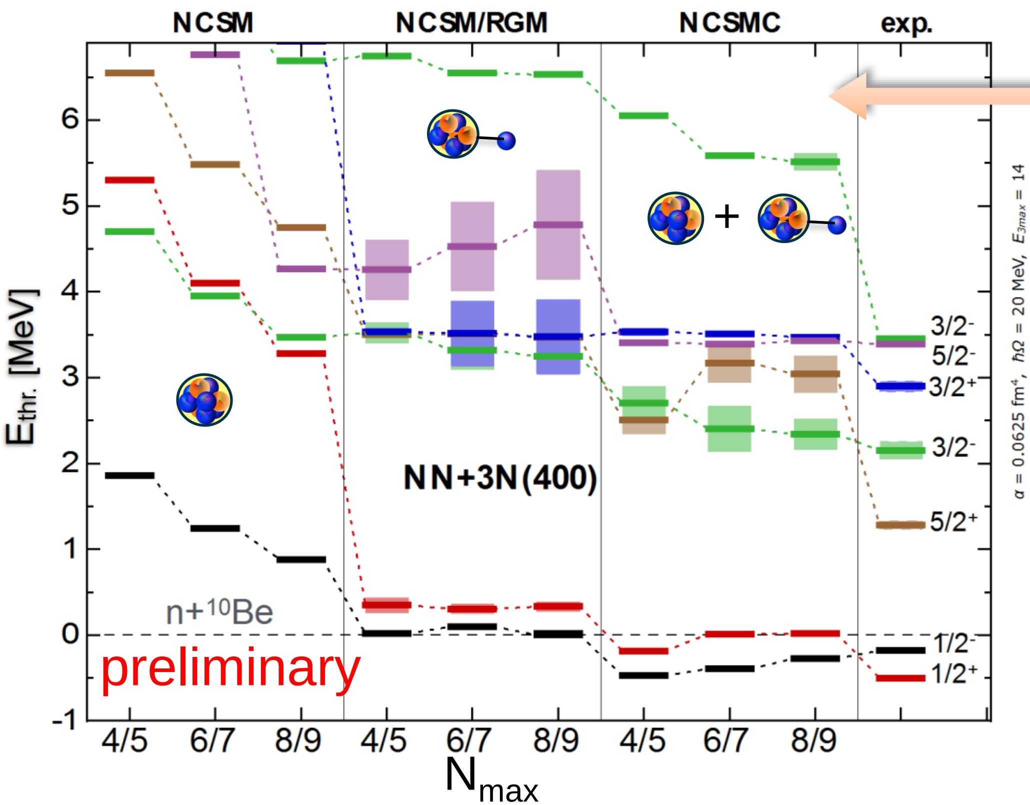
A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al.* with IRIS collaboration, in preparation

NCSMC calculations **including chiral 3N** (N^3LO NN+N^2LO 3NF400)

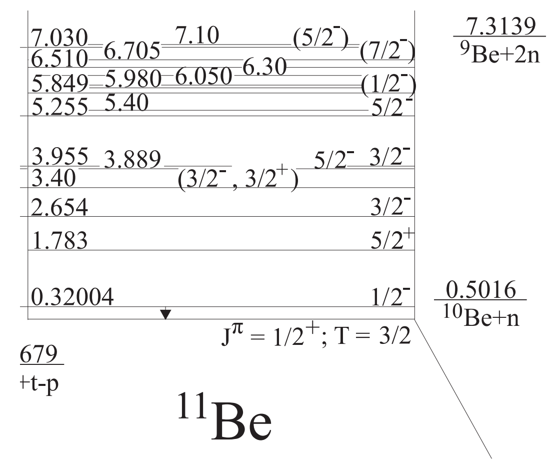


- ^{10}Be: 0^+, 2^+, 2^+ NCSM eigenstates
- ^{11}Be: ≥6 (π=-1) and ≥3 (π=+1) NCSM eigenstates



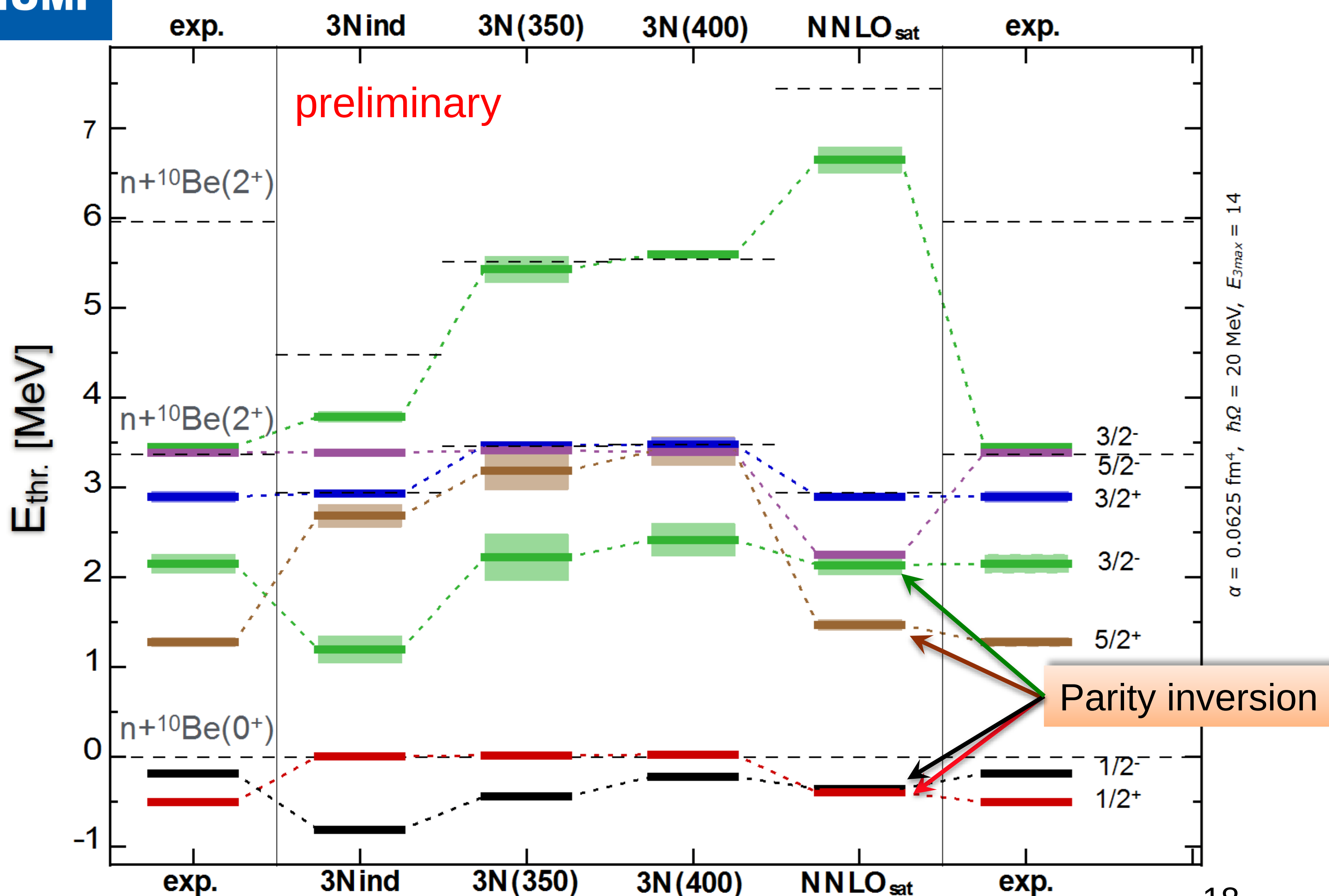


Continuum effects



^{11}Be WITHIN NCSMC: DISCRIMINATION AMONG CHIRAL NUCLEAR FORCES

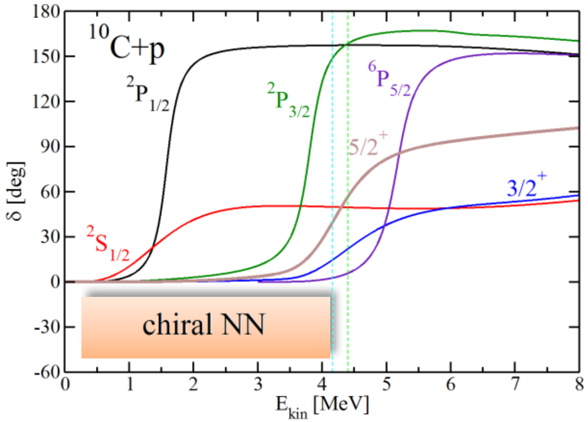
A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al.* with IRIS collaboration, in preparation

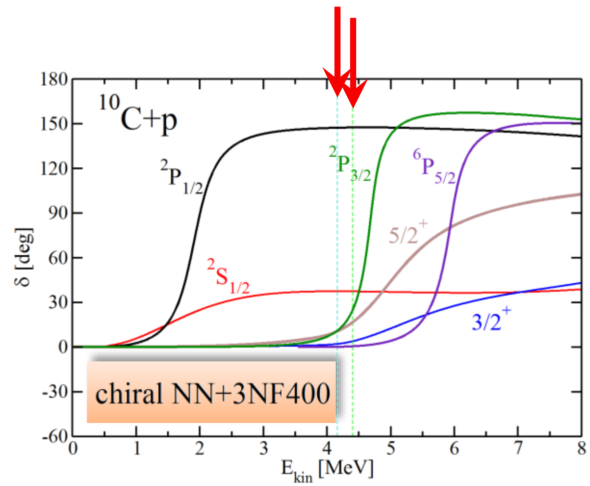


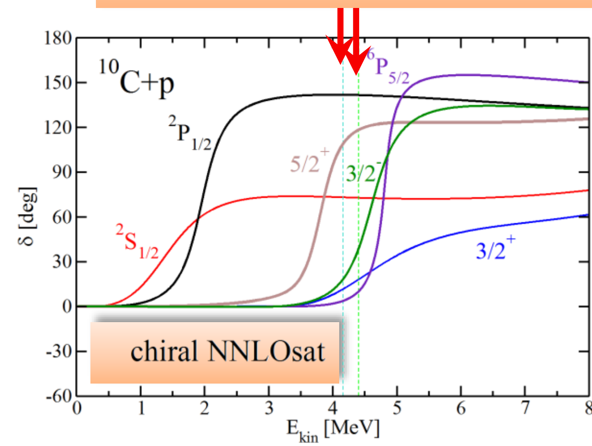
p-^{10}C SCATTERING: STRUCTURE OF ^{11}N RESONANCES

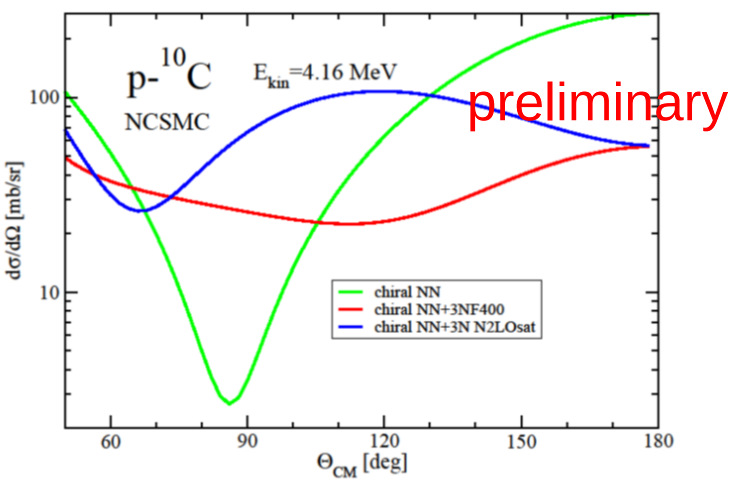
A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al.* with IRIS collaboration, in preparation

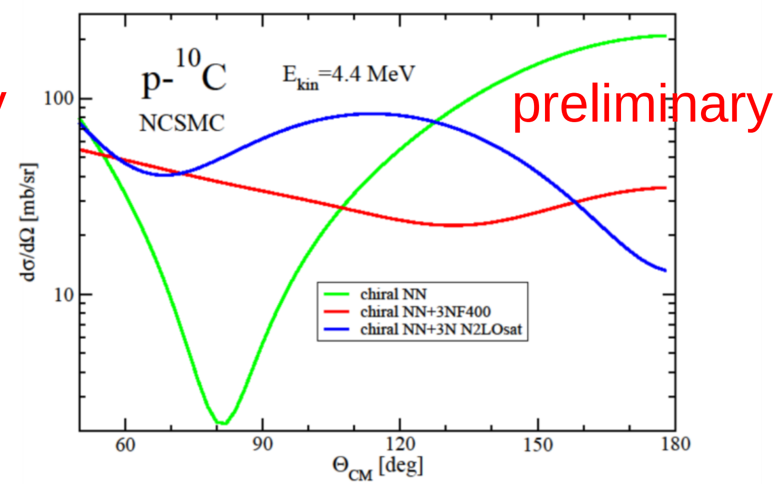
IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev *et al.*







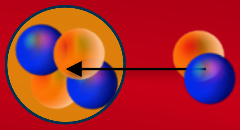




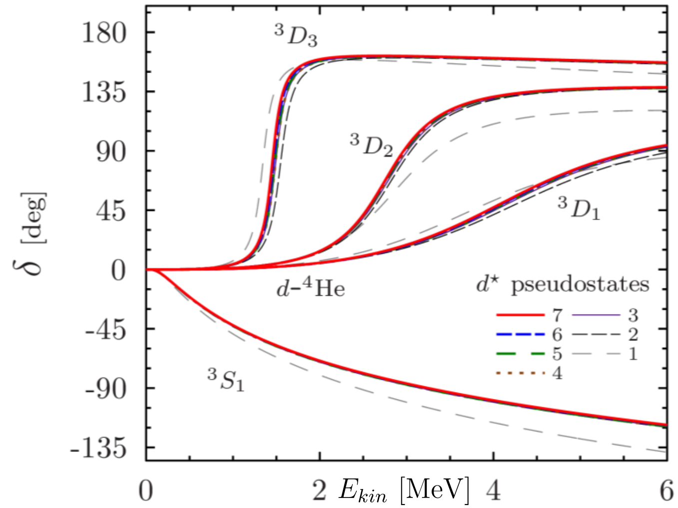
FROM RESEARCH TO INDUSTRY

^{4}He(d,d)^{4}He COMPARISON OF INTERACTION

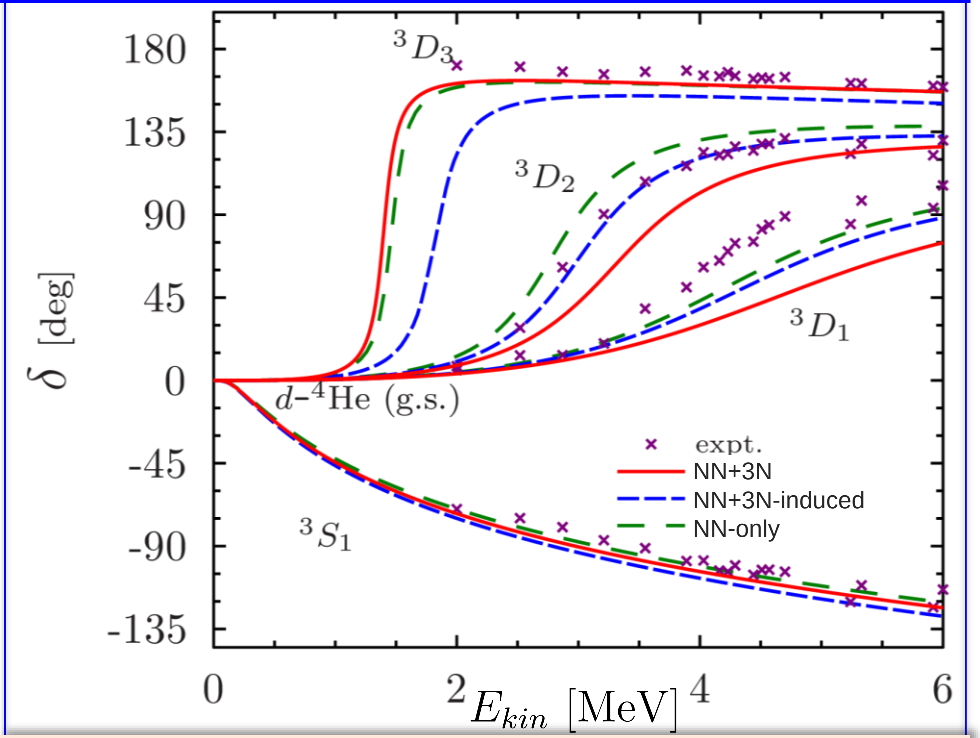
G. Hupin, S. Quaglioni and P. Navrátil, PRL114 (2015)



d-^{4}He scattering



Comparison of the d-α phase-shifts with different interactions (N_{max}=11)

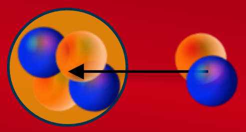


d-^{4}He(g.s.) scattering phase-shifts for NN-only, NN+3N-induced, NN+3N-full potential with λ=2.0 fm^{-1}.

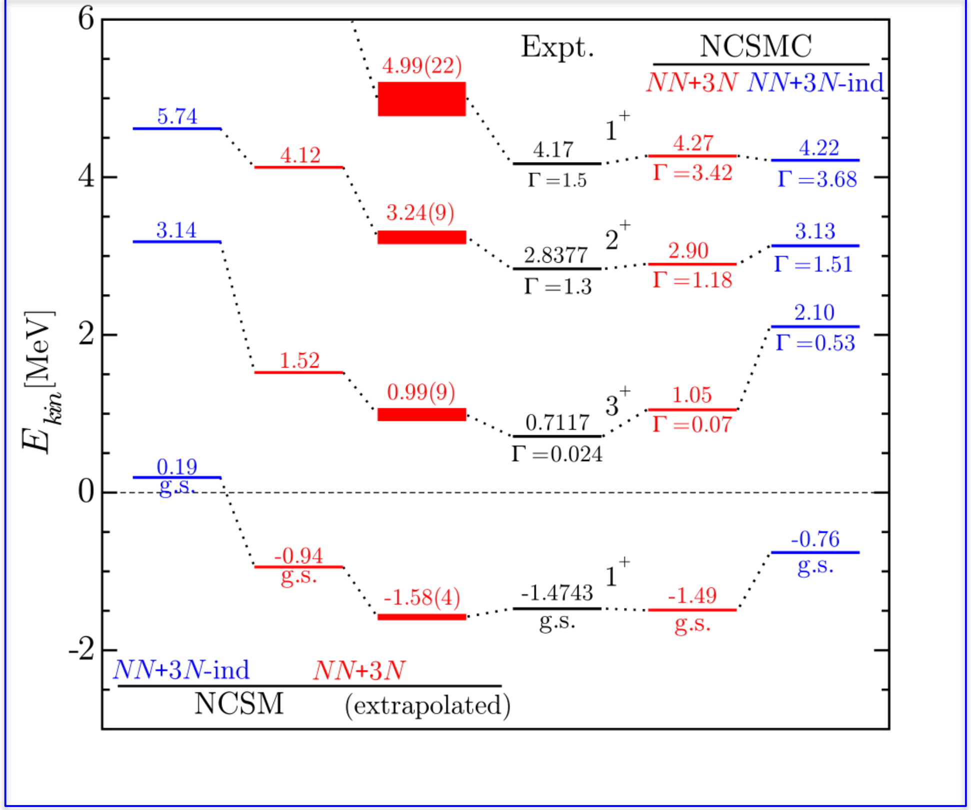
- Best results in a decent model space (N_{max}=11).
- The $^3D_3$ resonance is reproduced but the $^3D_2$ and $^3D_1$ resonance positions are underestimated.
- The 3N force corrects the D-wave resonance positions by increasing the spin-orbit splitting.
- There is room for improvements.

^{6}Li SPECTRUM, NCSMC VS NCSM/RGM

G. Hupin, S. Quaglioni and P. Navrátil, PRL114 (2015)



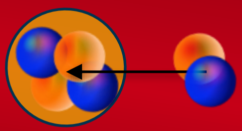
Comparison between NCSMC vs NCSM

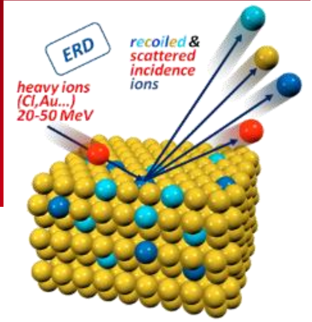


- The 3N force is essential to get the correct ^{6}Li g.s. energy and splitting between the 3^{+} and 2^{+} states.
- The ^{6}Li g.s. is well reproduced.
- There is room for improvements, in particular regarding the 3^{+} state.

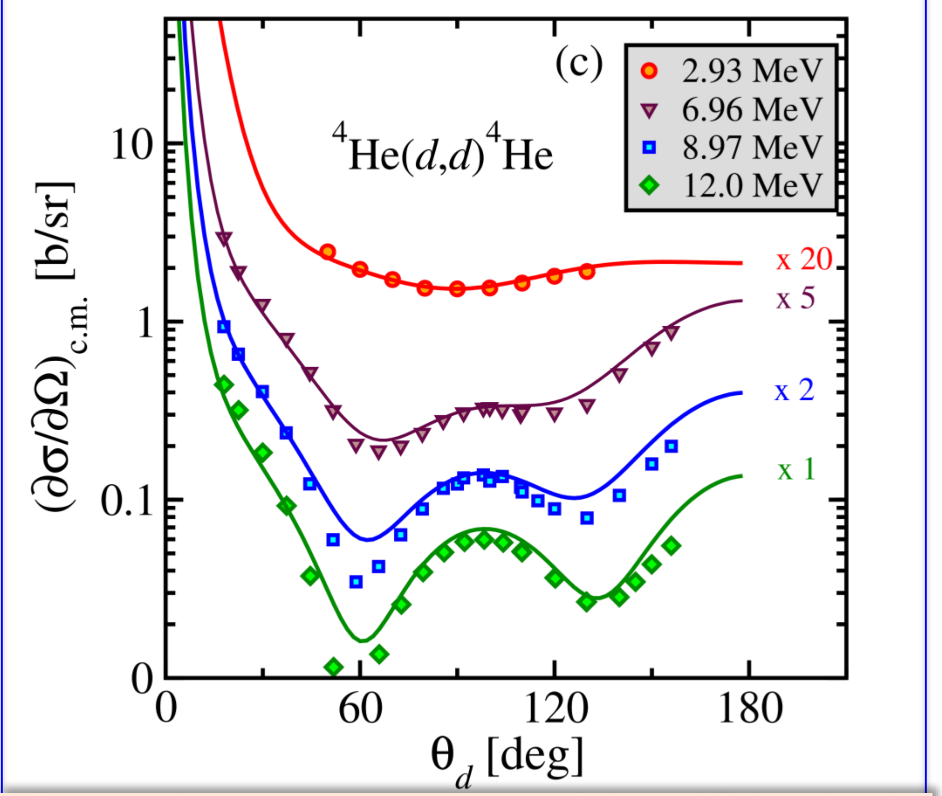
$^{4}He(d,d)^{4}He$ CROSS-SECTION

G. Hupin, S. Quaglioni and P. Navrátil, PRL114 (2015)





$^{4}He(d,d)\,^{4}He$ angular distribution for various E_d

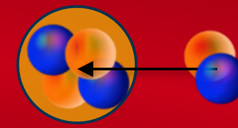


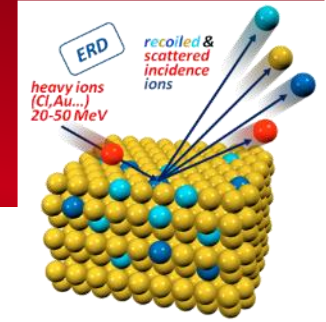
Comparison to experiment of the d-^{4}He elastic angular distribution of NCSMC with NN+3N potential at λ=2.0 fm^{-1}.

The bulk of the cross section is well reproduced for a large set of kinetic energy and scattering angle.

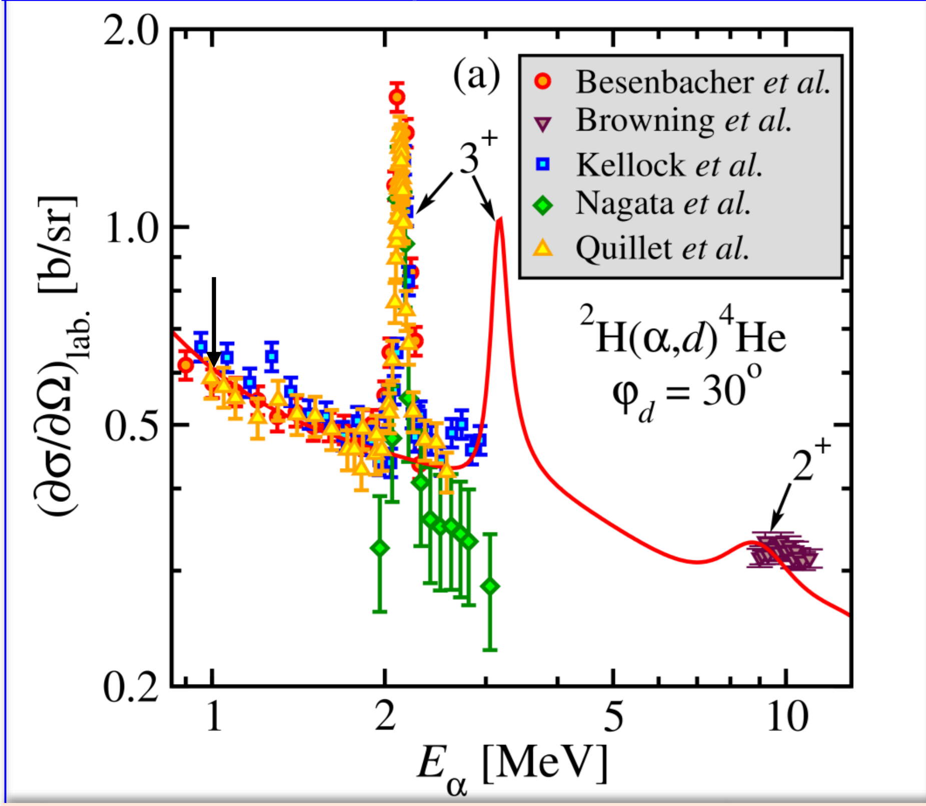
^{4}He(d,^{4}He)d CROSS-SECTION

G. Hupin, S. Quaglioni and P. Navrátil, PRL114 (2015)



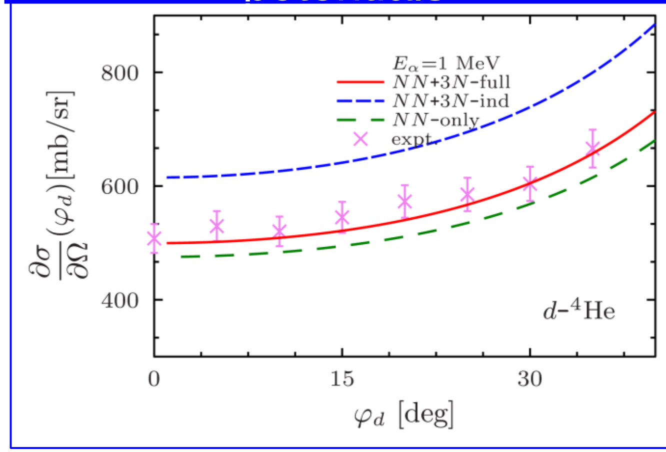


^{4}He(d,^{4}He)d differential cross section at $\varphi=30^0$



Comparison to experiment of the d-^{4}He elastic recoil differential cross section of NCSMC with NN+3N potential at λ=2.0 fm^{-1}.

Comparison between potentials

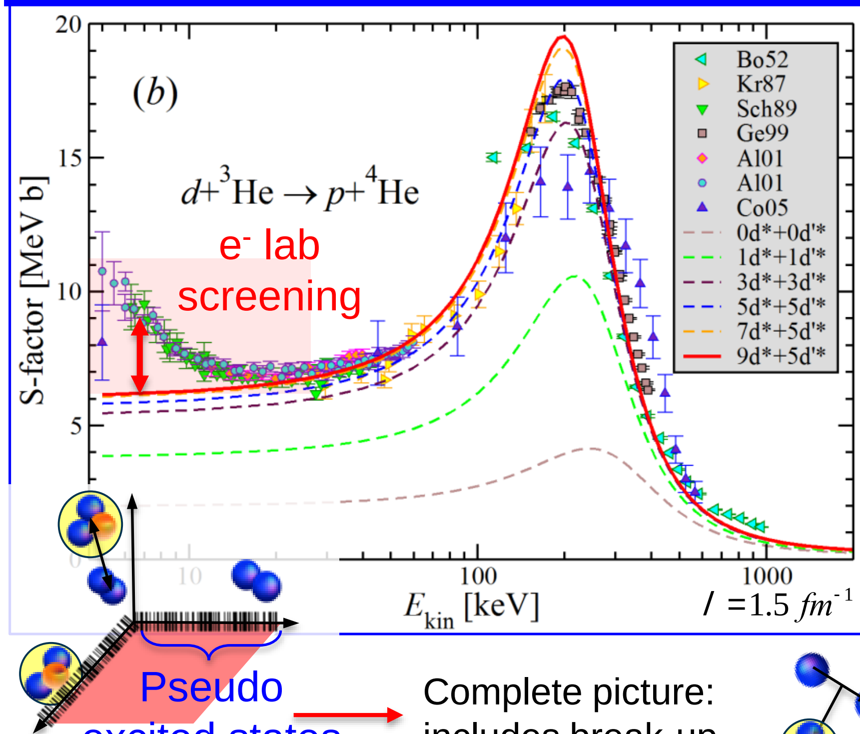


The 3$^+$ resonance is missed. As its width is very narrow, it has little impact and the bulk of the cross-section.

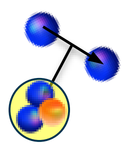
FIRST STEPS TOWARDS *AB INITIO* CALCULATIONS OF FUSION WITH NCSM/RGM

P. Navrátil, S. Quaglioni, PRL108 (2012)

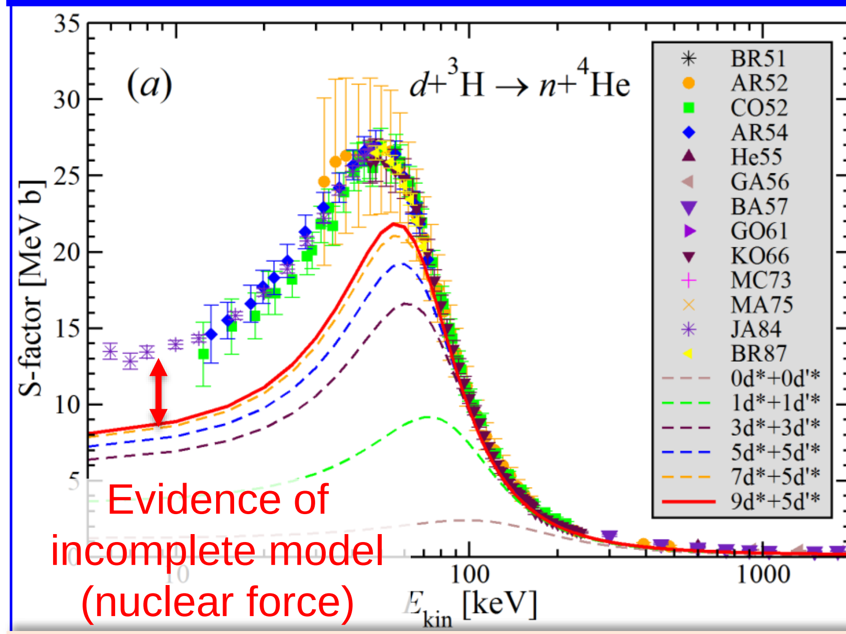
^{3}He(d,p)^{4}He astrophysical S-factor



Complete picture:
includes break-up



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



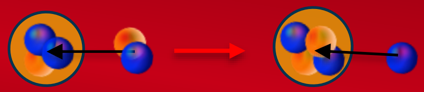
NCSM/RGM results for the ^{3}He(d,n)^{4}He astrophysical S-factor compared to beam-target measurements.

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 3N force (SRG-induced + “real”)

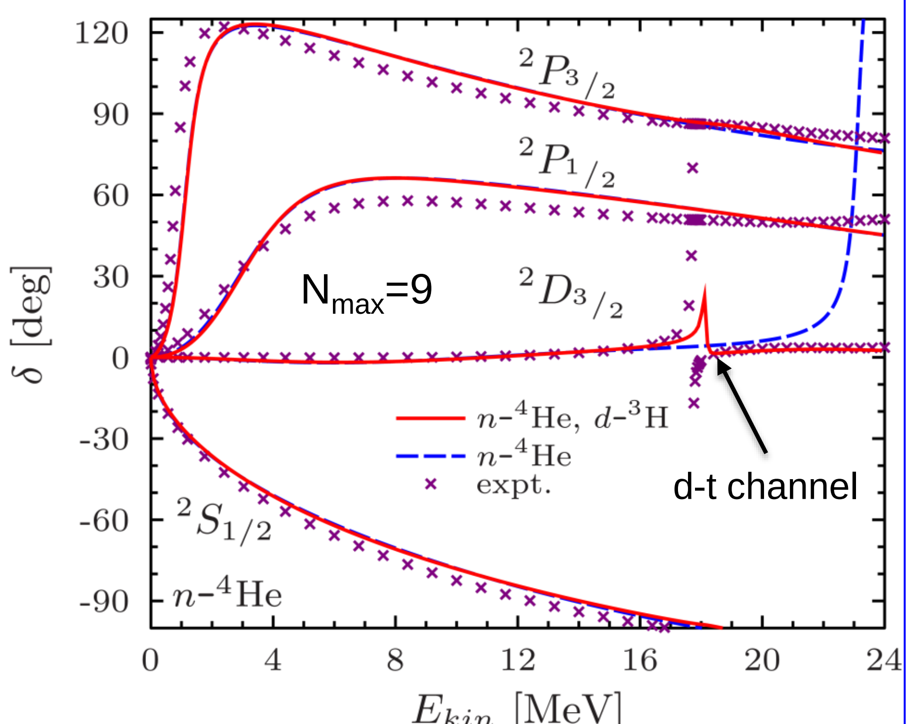
FIRST STEPS TOWARDS *AB INITIO* CALCULATIONS OF FUSION

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



d-t fusion

n-^{4}He phaseshifts with NCSMC and the chiral two- and three-nucleon force

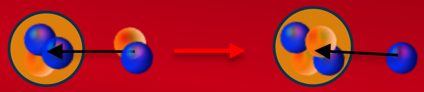


n+^{4}He(g.s.) phase shifts with NN+3N potential, λ=2.0 fm^{-1}, with eigenstates of ^{5}He at N_{max} =9.

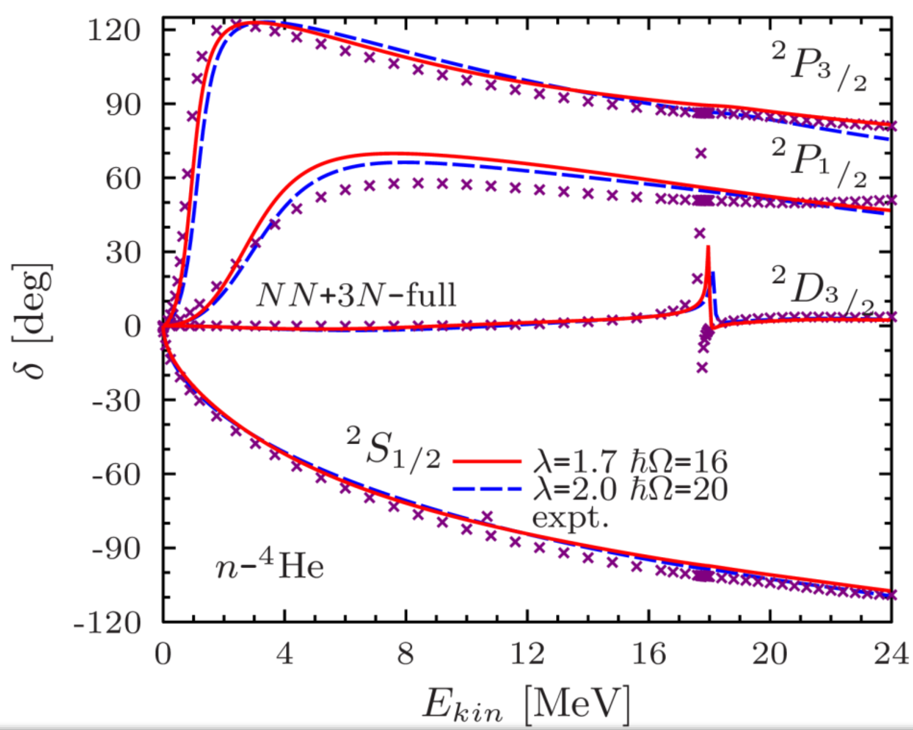
- Perspective to provide accurate t(*d*,*n*)^{4}He fusion cross-section for the effort toward earth-based fusion energy generation.
- The *d*-t fusion is known to be very sensitive to the spin-orbit and isospin part of the nuclear interaction.

FIRST STEPS TOWARDS *AB INITIO* CALCULATIONS OF FUSION

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



Towards d-t fusion with NCSMC: comparison between effective interactions



n+^{4}He(g.s.) phase shifts with NN+3N potential, with eigenstates of ^{5}He.

$\lambda = 1.7$ fm^{-1} and $\hbar\Omega = 16$ MeV

N_{max}	^{5}He ($\frac{3}{2}^+$)	^{4}He	^{3}H	d
6	-5.1574	-28.1739	-8.2909	-2.0404
8	-7.2529	-28.3677	-8.3893	-2.092
10	-8.1861	-28.4348	-8.4455	-2.1654
12			-8.4546	-2.1781
∞	-8.9373	-28.4693	-8.4565	-2.224

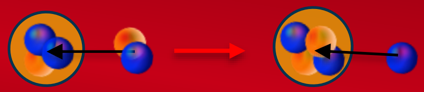
$\lambda = 2.0$ fm^{-1} and $\hbar\Omega = 20$ MeV

N_{max}	^{5}He ($\frac{3}{2}^+$)	^{4}He	^{3}H	d
6	-1.9037	-27.7923	-8.0971	-1.9199
8	-4.9122	-28.2341	-8.2721	-1.9633
10	-6.6422	-28.4078	-8.4099	-2.1172
12	-7.7062	-28.4438	-8.4387	-2.1351
∞	-9.1813	-28.4796	-8.4469	-2.224

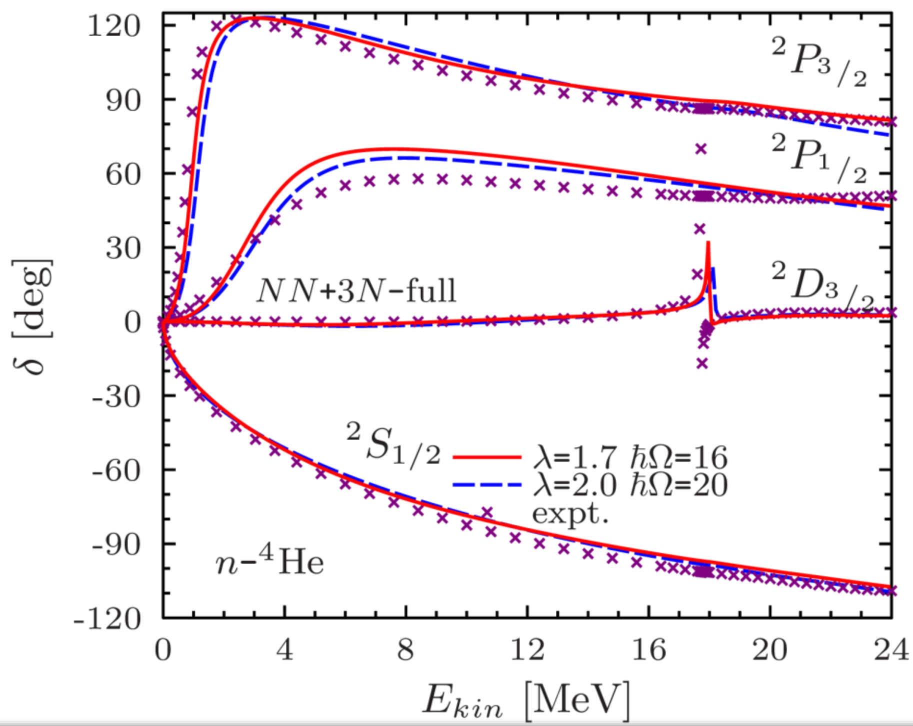
NCSM convergence of compound and cluster states.

FIRST STEPS TOWARDS *AB INITIO* CALCULATIONS OF FUSION

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



Towards d-t fusion with NCSMC: comparison between effective interactions



n+⁴He(g.s.) phase shifts with NN+3N potential, with eigenstates of ⁵He.

$\lambda = 1.7$ fm^{-1} and $\hbar\Omega = 16$ MeV

N_{max}	$^5He\ (\frac{3}{2}^+)$	^4He	^3H	d
6	42.29	1.04	1.96	8.26
8	18.85	0.36	0.80	5.94
10	8.41	0.12	0.13	2.63
12	-	-	0.02	2.06

$\lambda = 2.0$ fm^{-1} and $\hbar\Omega = 20$ MeV

N_{max}	$^5He\ (\frac{3}{2}^+)$	^4He	^3H	d
6	78.70	2.38	4.25	13.67
8	45.04	0.83	2.18	11.72
10	25.68	0.22	0.55	4.80
12	13.78	0.09	0.21	4.00

Relative error (%) with respect to converged value

A smaller frequency allows us to capture the dilute nature of the $^3/_2{}^+$ resonance.

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+3N interaction
- Deuterium-nucleus collisions with NN+3N interaction as the n-n
- NCSMC for single- and two-nucleon projectile

Work in progress:

- Fusion reactions with our best complete *ab initio* approach
- The present NNN force is "incomplete", need to go to N^3LO