TRIUMF

Canada's national laboratory for particle and nuclear physics

Laboratoire national canadien pour la recherche en physique nucléaire

et en physique des particules

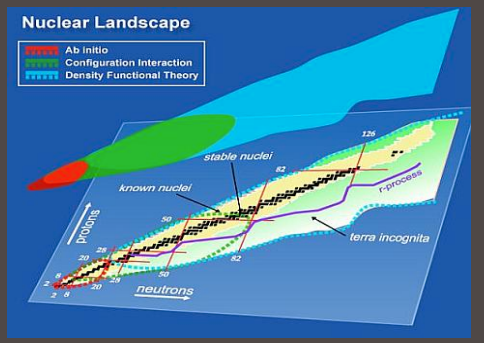
Deuteron scattering and transfer reactions within NCSM-RGM and NCSMC

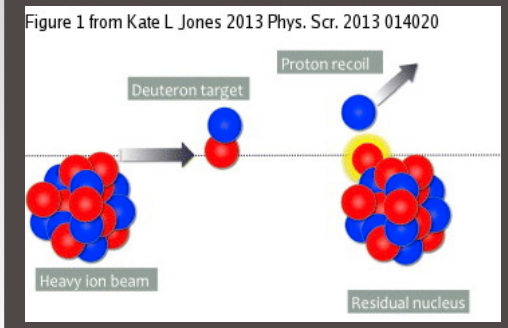
TRIUMF Workshop
19 February 2015
Vancouver, Canada

Francesco Raimondi, TRIUMF

In collaboration with:

G. Hupin, P. Navrátil, S. Quaglioni





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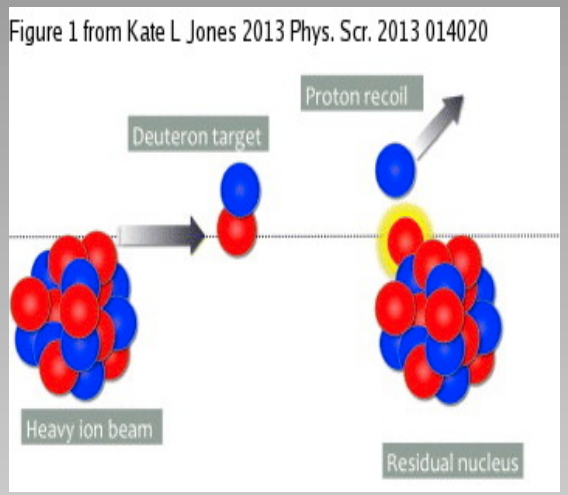
Outline

- ✔ Motivations for *ab initio* study of transfer reactions
- ✔ Interest of ^{7}Li(*d*,p)^{8}Li reaction
- ✔ Results on the first resonance of ^{9}Be above *d*-^{7}Li threshold
- ✔ Recent progress on inclusion of 3N forces in transfer reaction (s-shell nuclei)

  (on behalf of: G. Hupin, P. Navrátil, S. Quaglioni)
- ✔ Conclusions

Deuteron-nucleus reaction: experimental motivations



(*d*,p) reaction in inverse kinematics

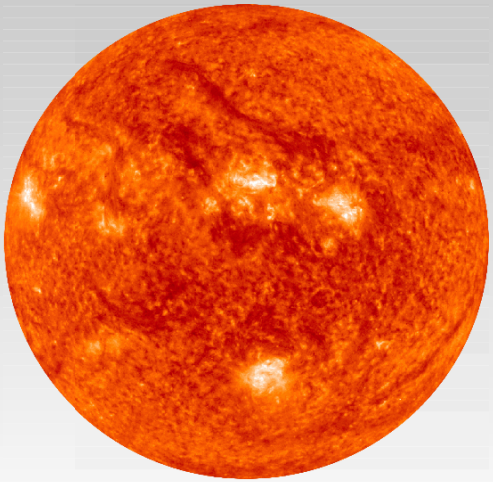
Intense experimental activity (now with exotic nuclei beams in RIB facilities):

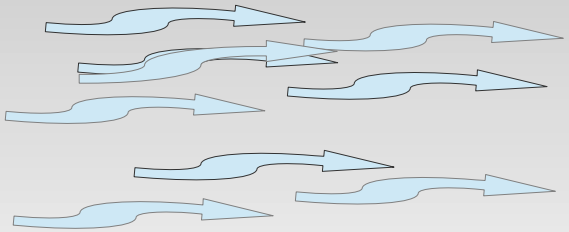
- Structure and spectroscopy of nuclei (^{11}Be(*d*,p)^{12}Be at ISAC - TRIUMF)
- Nucleosynthesis and nuclear fusion applications (^{3}H(*d*,n)^{4}He reaction)
- Surrogate for (p/n) capture reactions (^{14}C(*d*,p)^{15}C as surrogate of ^{14}C(n, γ)^{15}C)

^{7}Li(*d*,p)^{8}Li transfer reaction

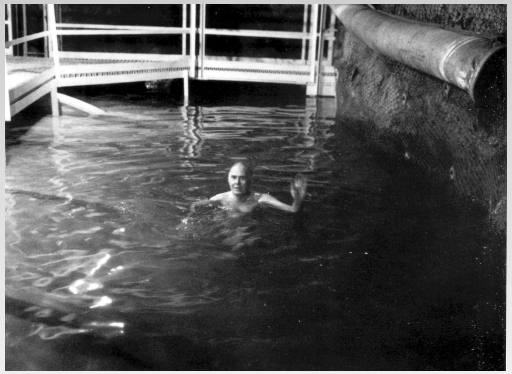
- Calibration reaction for astrophysical process: ^{7}Li(*d*,p)^{8}Li as target calibration for ^{7}Be(p,γ)^{8}B

Solar neutrino problem:





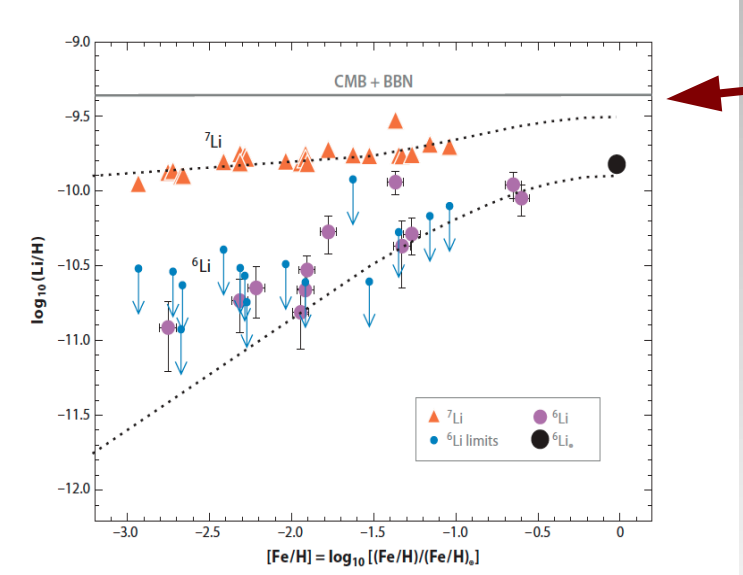
$\nu_e + {}^{37}Cl \rightarrow {}^{37}Ar + e^-$



R. Davis Jr takes a dip
At Homestake Mine (1971)

^{7}Li(*d*,p)^{8}Li transfer reaction

- Calibration reaction for astrophysical process: ^{7}Li(*d*,p)^{8}Li as target calibration for ^{7}Be(p,γ)^{8}B
- Possible mechanism of destruction of ^{7}Li in the context of baryon-inhomogeneus models of the primordial nucleosynthesis

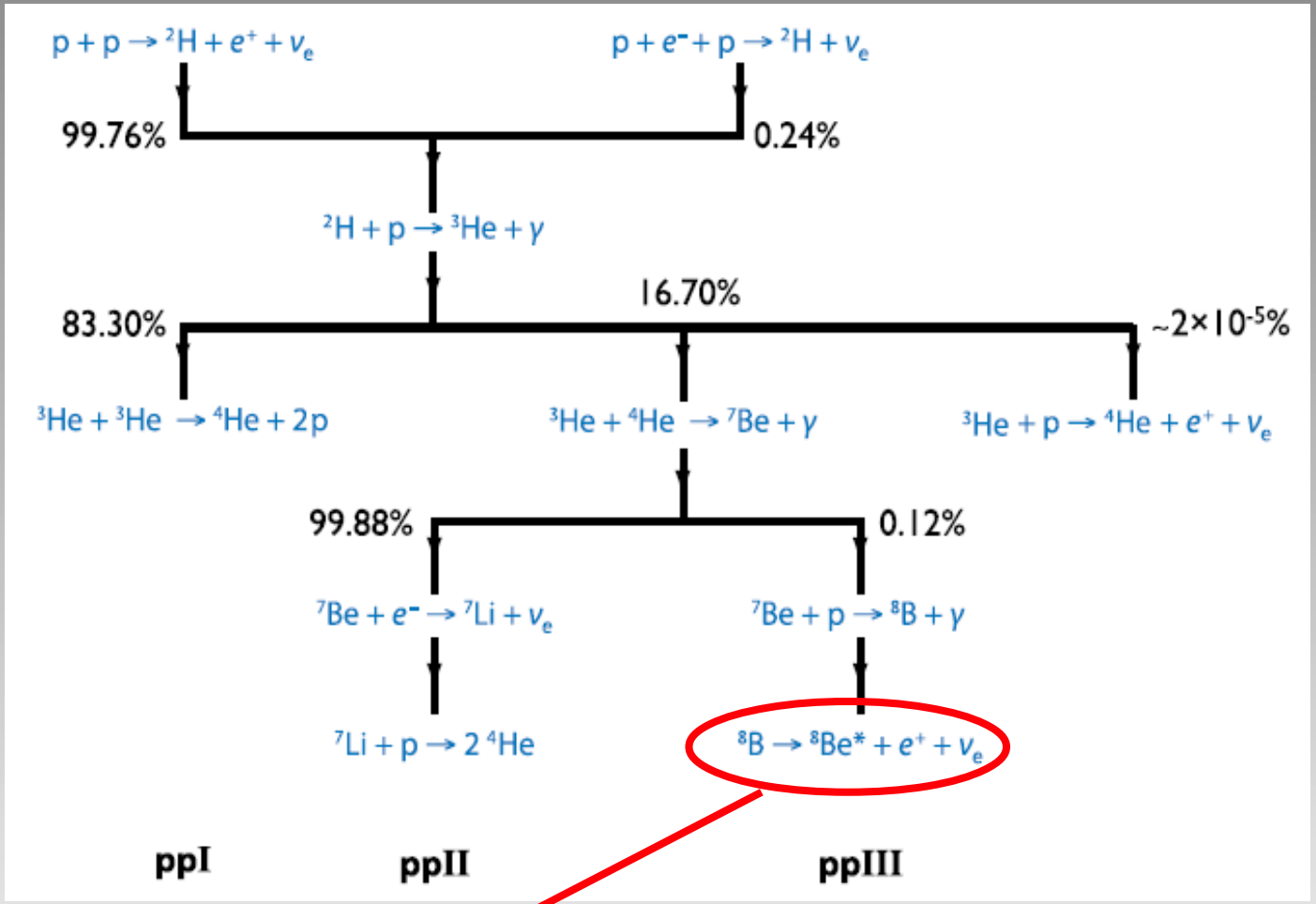


Primordial Lithium problem:

- 4-5σ discrepancy between observed and calculated (CMB+BBN) abundance of ^{7}Li
- Nuclear solution to the problem: *d*-^{7}Li destruction mechanism is ruled out (but only in a standard BBN scenario PRC 47, 2369 1993)

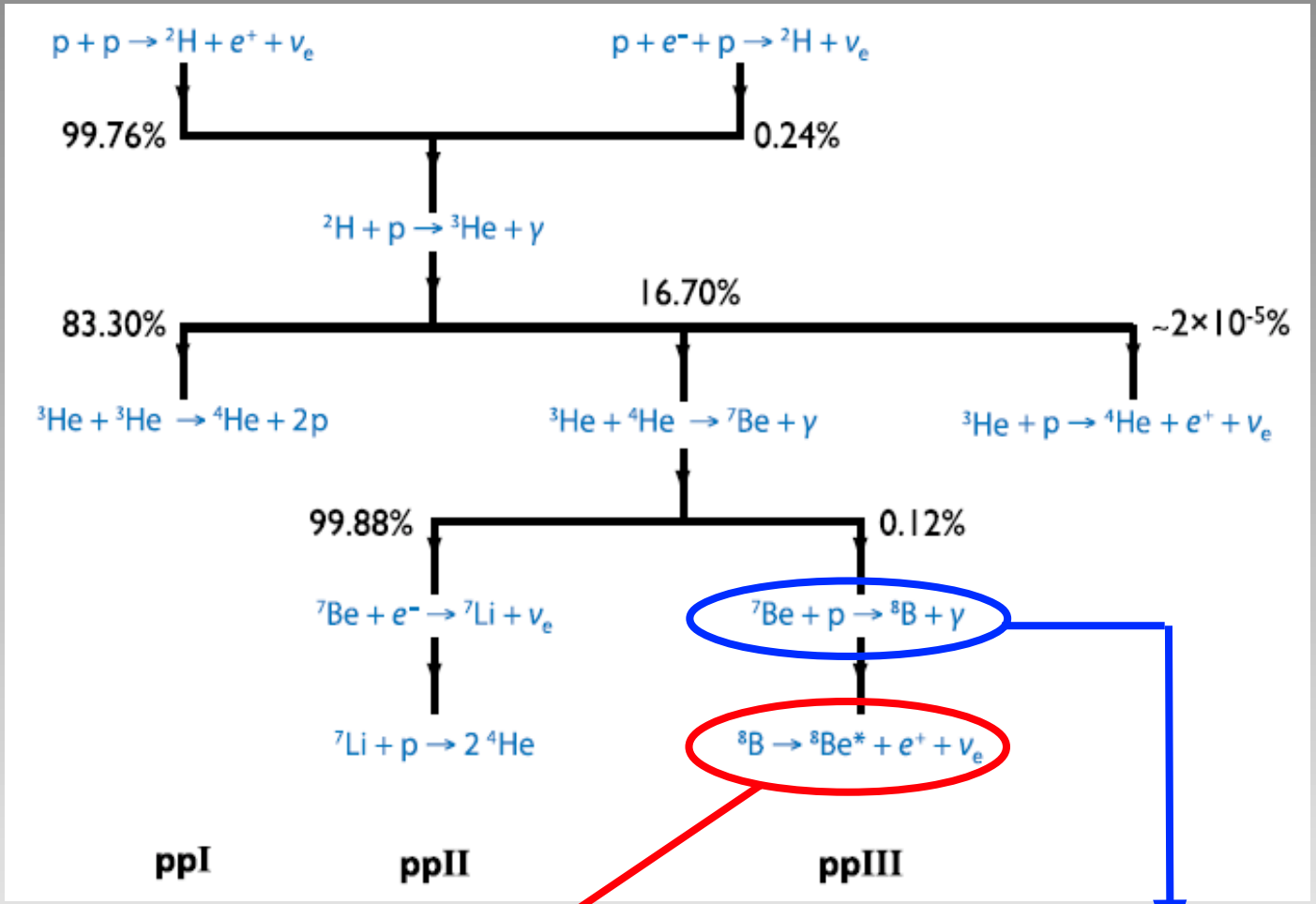
Annu Rev. Nucl. Part. Sci. 2011 61:47-68

Solar p-p chain



High-energy solar neutrinos
(E_ν up to 15 MeV)

Solar p-p chain



$S_{17}(0)$ crucial input to estimate solar neutrino flux

"Prudent conservative range" $S_{17}(0)=20.8(2.1)$ eV b

(Rev Mod Phys 83, 1 (2011))

High-energy solar neutrinos (E_ν up to 15 MeV)

$^{7}Be(p,\gamma)^{8}B$ direct measurements

Solar fusion cross sections (Rev Mod Phys 70, 4, 1265 (1998))

- At low energy, it is an external, direct-capture process (Q=137.5 ± 1.2 KeV)

- Experimental uncertainties:
  - Need to be extrapolated to astrophysical relevant regime (E_p < 134 KeV)
  - ^{7}Be target is radioactive: Areal density of ^{7}Be difficult to estimate (required for normalization of the cross section)

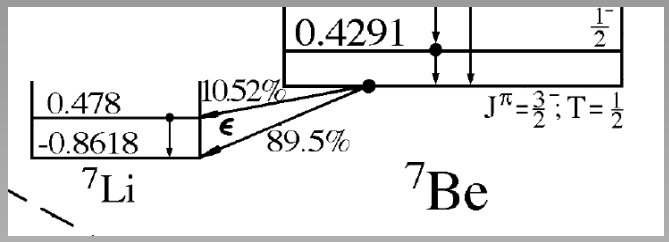
- Two possible strategies:
  - Direct: counting 429 KeV photons of ^{7}Be decay (Filippone 1983)
  - Indirect: measuring the $^{7}Li(d,p)^{8}Li$ yield on the resonance ($\Gamma \approx 0.2$ MeV) at $E_d = 0.78$ MeV) (Kavanagh 1960, Parker 1966, Filippone 1982, Weissman 1998)

^{7}Li(*d*,p)^{8}Li calibration reaction (Normalization procedure)

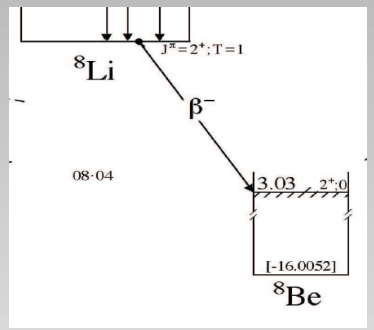
1) Buildup of ^{7}Li in ^{7}Be

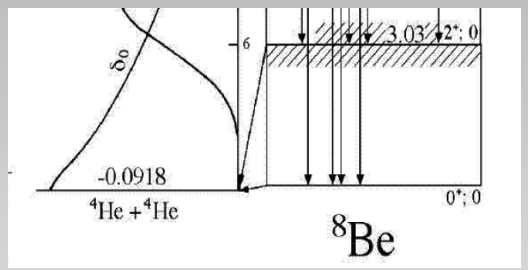
$$N_{^7Li}(t) = N_{^7Be}(0)(1 - e^{\lambda t}) + N_{^7Li}(0)$$

N_i areal density at time t



2) Counting ^{7}Li through the yield of (*d*,p) reaction





Beta-delayed alphas detected

3) Areal density of Li from total σ

$$\sigma(E_d) \sim \frac{Y_\alpha(E)\beta(^8Li)}{N_d N_{^7Li}(t)}$$

$Y_\alpha(E)$ α-particle yield

$\beta(^8Li)$ depends on decay constant of ^{8}Li

^{7}Li(*d*,p)^{8}Li calibration reaction (Normalization procedure)

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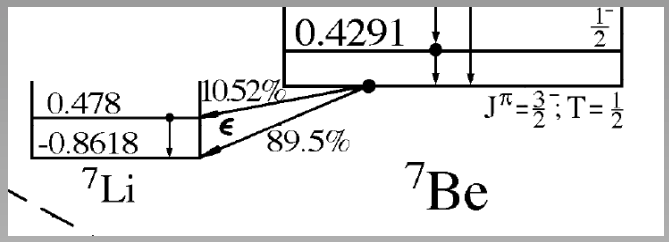

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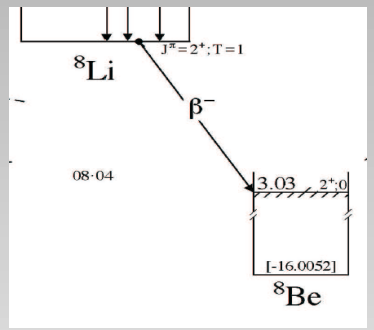

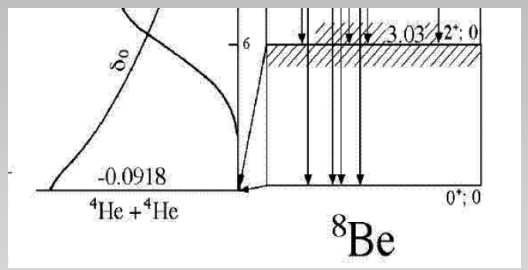

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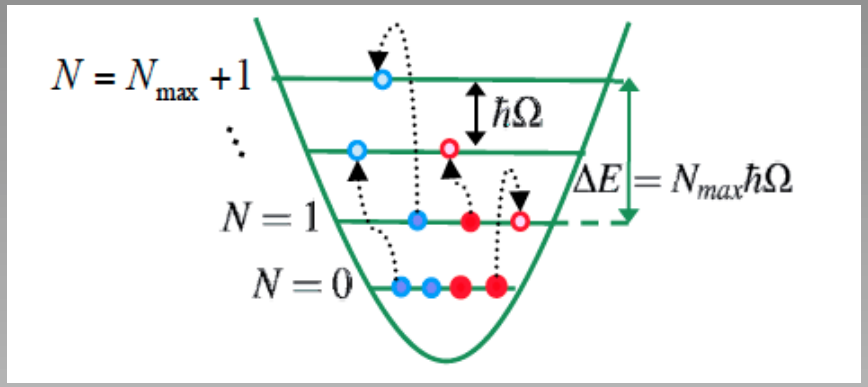
No-core shell model with continuum

- No-core shell model (NCSM):
  - A-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - Short- and medium-range correlations
  - Bound states and narrow resonances



$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| (A) \right., \lambda \rangle$$

Unknowns

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No-core shell model with continuum

- NCSM with Resonating Group Method (NCSM/RGM):

  - Cluster expansion
  - Proper asymptotic behaviour
  - Long-range correlations

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

Unknowns

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No-core shell model with continuum

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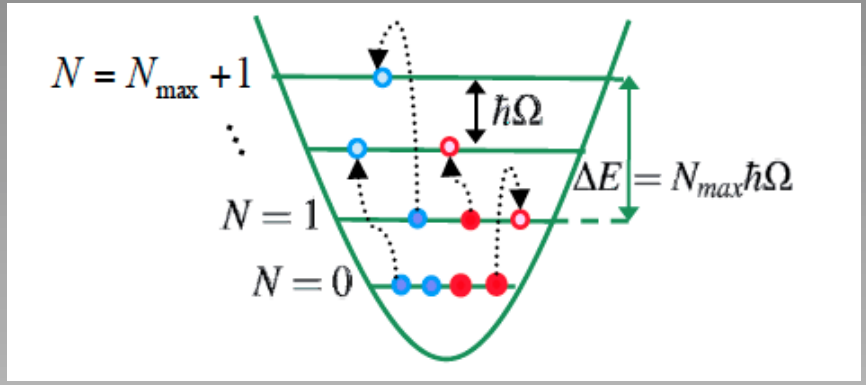
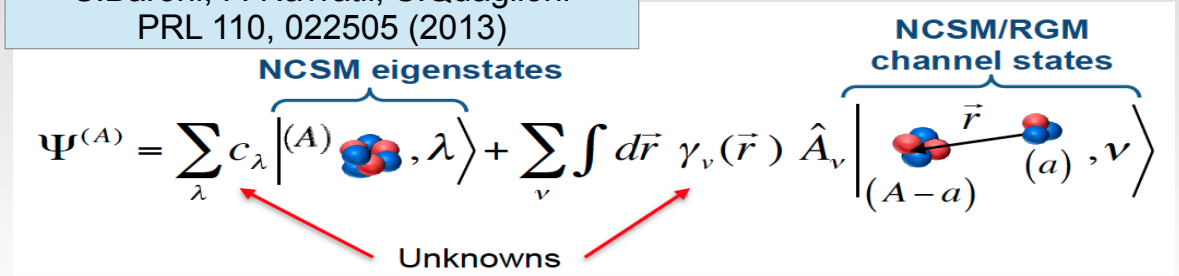


- NCSM with Resonating Group Method (NCSM/RGM):
  - Cluster expansion
  - Proper asymptotic behavior
  - Long-range correlations

The most efficient:
No-Core Shell Model with Continuum (NCSMC)

S.Baroni, P. Návratil, S.Quaglioni
PRL 110, 022505 (2013)



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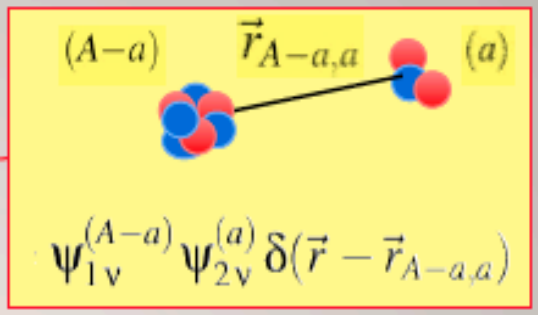
The *ab initio* NCSM-RGM equation

- Ansatz: $\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\, \varphi_{\nu}(\vec{r})\, \hat{\mathcal{A}}\, \Phi^{(A-a,a)}_{\nu\vec{r}}$



eigenstates of $H_{(A-a)}$ and $H_{(a)}$ in the *ab initio* NCSM basis

- Many-body Schrödinger equation:

$$H\Psi^{(A)} = E\Psi^{(A)}$$

$$T_{\rm rel}(r) + \mathcal{V}_{\rm rel} + \bar{V}_{\rm Coul}(r) + H_{(A-a)} + H_{(a)}$$

realistic nuclear Hamiltonian

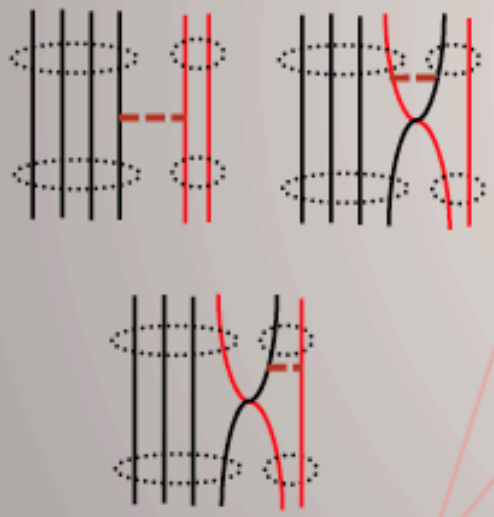
$$\sum_{\nu} \int d\vec{r} \left[\mathcal{H}^{(A-a,a)}_{\mu\nu}(\vec{r}',\vec{r}) - E\mathcal{N}^{(A-a,a)}_{\mu\nu}(\vec{r}',\vec{r}) \right] \varphi_{\nu}(\vec{r}) = 0$$

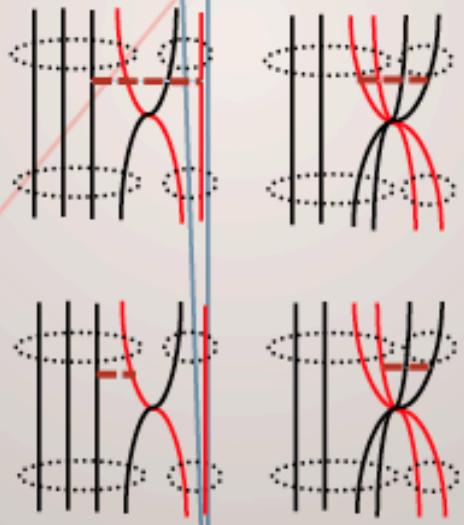
$\langle \Phi^{(A-a,a)}_{\mu\vec{r}'} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$ — Hamiltonian kernel

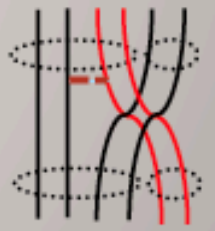
$\langle \Phi^{(A-a,a)}_{\mu\vec{r}'} | \hat{\mathcal{A}}^2 | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$ — Norm kernel

The deuteron projectile: Hamiltonian kernel

$$\left\langle (1,\ldots,A\text{-}2)\ r' \ (A\text{-}1,A) \right| \begin{aligned} & 2(A-2)V_{A-1,A-2}(1-P_{A-1,A-2}) - 2(A-2)V_{A,A-2}\hat{P}_{A-2,A-1} \\ & -2(A-2)(A-3)V_{A,A-3}(1-\hat{P}_{A,A-3})\hat{P}_{A-2,A-1} \\ & -2(A-2)(A-3)V_{A-1,A-3}\hat{P}_{A-2,A-1} \\ & +(A-2)(A-3)(A-4)V_{A-1,A-4}\hat{P}_{A-2,A}\hat{P}_{A-3,A-1} \end{aligned} \left| (1,\ldots,A\text{-}2)\ (A\text{-}1,A)\ r \right\rangle$$







$${}_{SD}\left\langle \psi^{(A-2)}_{\mu_1} \middle| a^+ a \middle| \psi^{(A-2)}_{\nu_1} \right\rangle_{SD}$$

$${}_{SD}\left\langle \psi^{(A-2)}_{\mu_1} \middle| a^+ a^+ a\, a \middle| \psi^{(A-2)}_{\nu_1} \right\rangle_{SD}$$

$${}_{SD}\left\langle \psi^{(A-2)}_{\mu_1} \middle| a^+ a^+ a^+ a\, a\, a \middle| \psi^{(A-2)}_{\nu_1} \right\rangle_{SD}$$

... and 'offdiagonal' coupling kernels $< \ |V\hat{P}| \ >$

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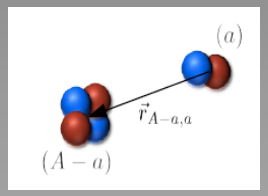
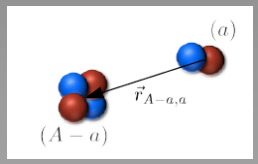
Three-body density Hamiltonian kernel



$$\left\langle \Phi^{J^\pi T}_{k'_{ab}} \middle| \left(V_{A,A-4} \hat{P}_{A-2,A-1} \hat{P}_{A-3,A} \right) \middle| \Phi^{J^\pi T}_{k_{ab}} \right\rangle$$



$$\underbrace{{}_{\mathrm{SD}}\langle A{-}2\alpha' | \hat{a}^\dagger_{\beta_{A-4}} \hat{a}^\dagger_a \hat{a}^\dagger_b \hat{a}_{b'} \hat{a}_{\beta'_{A-3}} \hat{a}_{\beta'_{A-4}} | A{-}2\alpha \rangle_{\mathrm{SD}}}_{\text{Three-body density matrix}} \underbrace{{}_a\langle \beta_{A-4}, a' | V_{A,A-4} | \beta'_{A-4} \beta'_{A-3} \rangle_a}_{\text{Two-body potential}}$$

- Number of three-body matrix elements increases fast with basis size
- Optimized numerical algorithm: On-the-fly calculation of the needed three-body matrix elements for a given target nucleus in the m-scheme

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Memory size issue in kernels computation

Dimension of the RGM kernels affects the calculation:

- Memory of a node could be insufficient to handle kernels files
- R-matrix solver is slowed down by the reading-in of huge kernel files

Three different 'representations' of the three-body kernels:

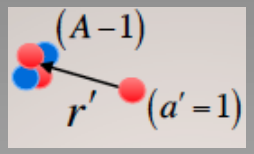
1) $${}_{\rm SD}\langle A\!-\!2\,\alpha_1' I_1' M_1' T_1' M_{T_1}' | \hat{a}^\dagger_{\beta_{A-4}} \hat{a}^\dagger_{n_a \ell_a j_a m_{j_a} \frac{1}{2} m_{t_a}} \hat{a}^\dagger_{n_b \ell_b j_b m_{j_b} \frac{1}{2} m_{t_b}} \hat{a}_{n_b' \ell_b' j_b' m_{j_b'}' \frac{1}{2} m_{t_b'}'} \hat{a}_{\beta'_{A-3}} \hat{a}_{\beta'_{A-4}} | A\!-\!2\,\alpha_1 I_1 M_1 T_1 M_{T_1} a \rangle_{\rm SD}$$

2) $$\left\langle \Phi^{J^\pi T}_{k'_{ab}} \middle| \left(V_{A,A-4} \hat{P}_{A-2,A-1} \hat{P}_{A-3,A} \right) \middle| \Phi^{J^\pi T}_{k_{ab}} \right\rangle$$

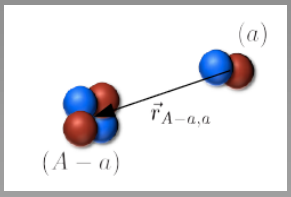
3) $$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \left(V_{A,A-4} \hat{P}_{A-2,A-1} \hat{P}_{A-3,A} \right) \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle$$

Nmax (single-channel d-^{4}He)	1) # 3-body density matrix	2) # Kernels in SD-basis	3) # Kernels in physical basis
2	~10^5	~10^2	20
4	~10^7	~10^3	70
6	~10^9	~10^4	167
8	~10^{10}	~10^5	325

Coupling Hamiltonian kernel



$$\left\langle \Phi^{J^\pi T}_{k'_a} \middle| \left(V_{A-3,A-2} \hat{P}_{A-2,A} \right) \middle| \Phi^{J^\pi T}_{k_{ab}} \right\rangle$$



$$_{\mathrm{SD}}\langle A-1\alpha' | \hat{a}^\dagger_{\beta_{A-3}} \hat{a}^\dagger_b \hat{a}^\dagger_a \hat{a}_{\beta'_{A-2}} \hat{a}_{\beta'_{A-3}} | A-2\alpha \rangle_{\mathrm{SD}} \; {}_a\langle \beta_{A-3}, a' | V_{A-3,A-2} | \beta'_{A-3} \beta'_{A-2} \rangle_a$$

"Not-diagonal" density matrix

Two-body potential

(A-2,2) mass partition in the entrance channel
(A-1,1) mass partition in the exit channel

- Inclusion of coupling kernel describing the dominant channel in a (*d*,p/n) transfer reaction

< d,^{7}Li | ^{9}Be > & < p,^{8}Li | ^{9}Be > cluster overlaps

$N_{max} = 6$

- Understand cluster structure of ^{9}Be

Cluster overlaps from NCSM eigenstates

$$g(r) = < \Psi^{(A)} | \mathcal{A} \Psi^{(A-a)} \Psi^{(a)} \delta_{r, r_{A,A-a}} >$$

Large overlap of mass partitions considered with compound nucleus in the $5/2^{+}$ partial wave

< ^{9}Be | p + ^{8}Li > E_{thr} = -37.60 MeV

$J^{\pi}T$	E (^{9}Be) [Mev]	(2s,l)	S
$(3/2^{+}1/2)_{5}$	4.49	$(3,0)^{*}$	0.356
$(5/2^{-}1/2)_{6}$	3.87	$(5,1)^{*}$	0.052
$(5/2^{+}1/2)_{4}$	3.46	(5,0)	0.593

< ^{9}Be | d + ^{7}Li > E_{thr} = -38.16 MeV

$J^{\pi}T$	E (^{9}Be) [MeV]	(2s,l)	S
$(1/2^{-}1/2)_{4}$	2.98	$(1,0)^{*}$	0.140
$(5/2^{-}1/2)_{6}$	4.43	$(5,0)^{*}$	0.153
$(5/2^{+}1/2)_{4}$	3.46	(5,1)	0.371

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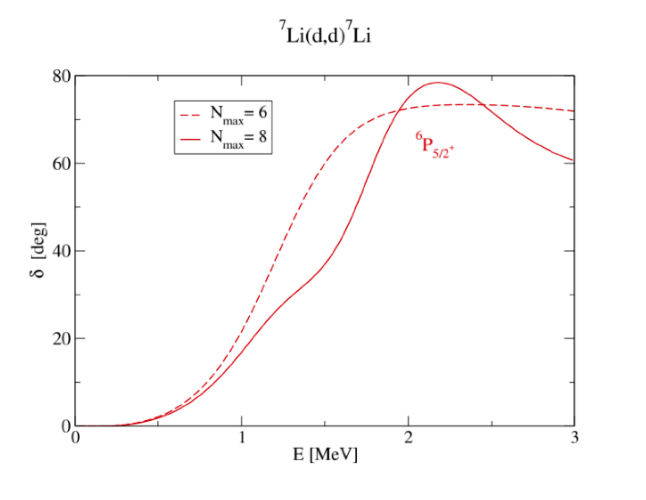
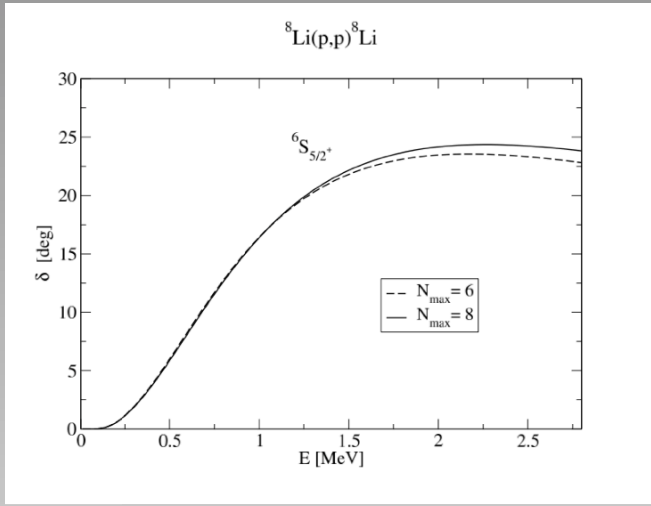
Phase shifts analysis (NCSM-RGM)

Analysis of the partial wave phase shifts: spin and parity (J^π) of the resonance

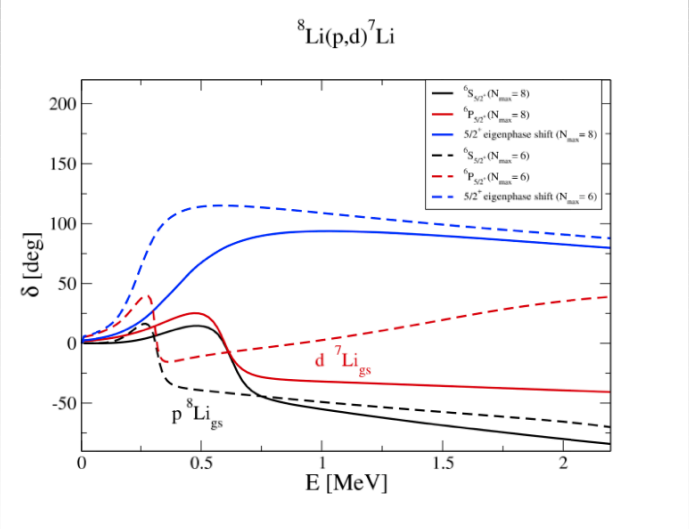


$J^\pi = 5/2^+$

dominant resonance at low energy

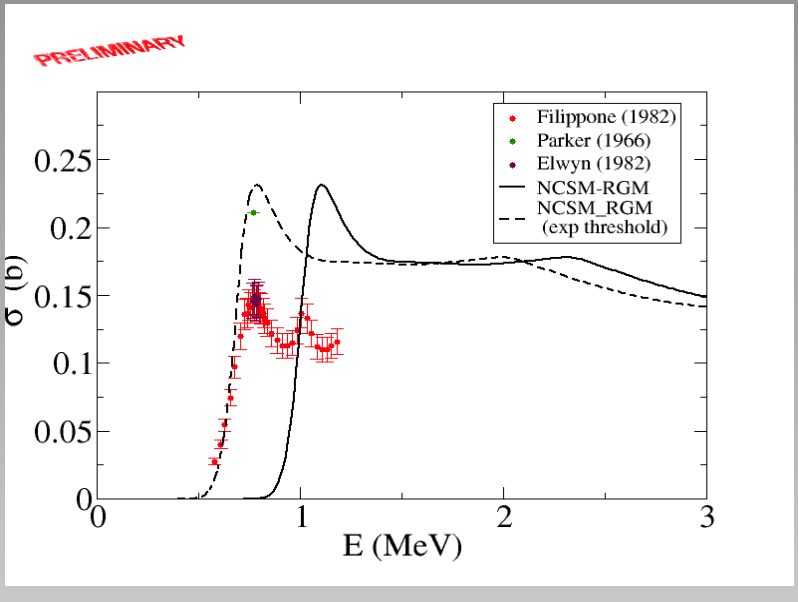


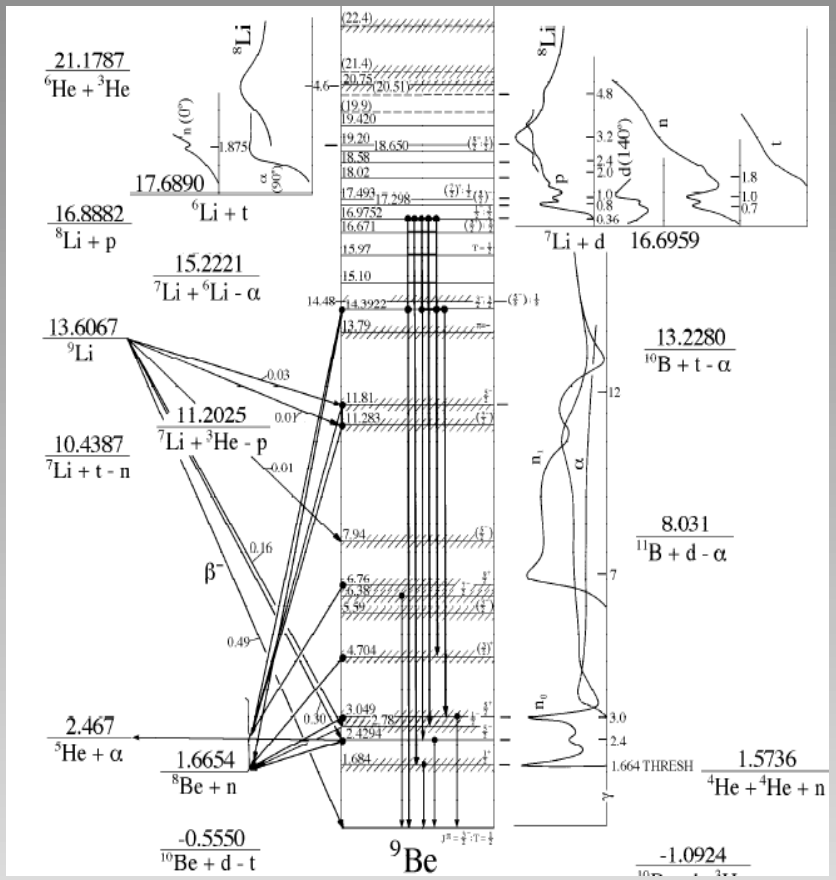
Effect of the coupling: contribution from 'offdiagonal' elements of the collision matrix



Eigenphase shifts convey informations on all the matrix elements of the collision matrix

^{7}Li(*d*,p)^{8}Li scattering results (NCSM-RGM)



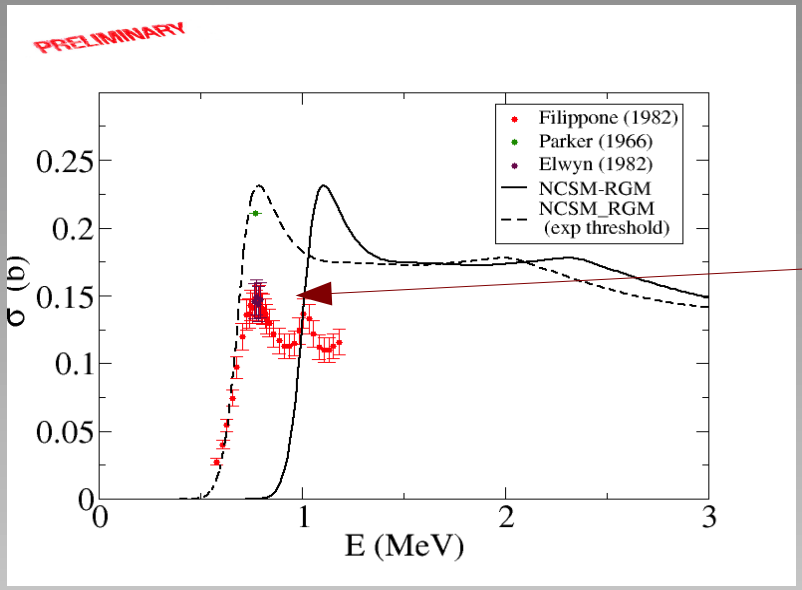


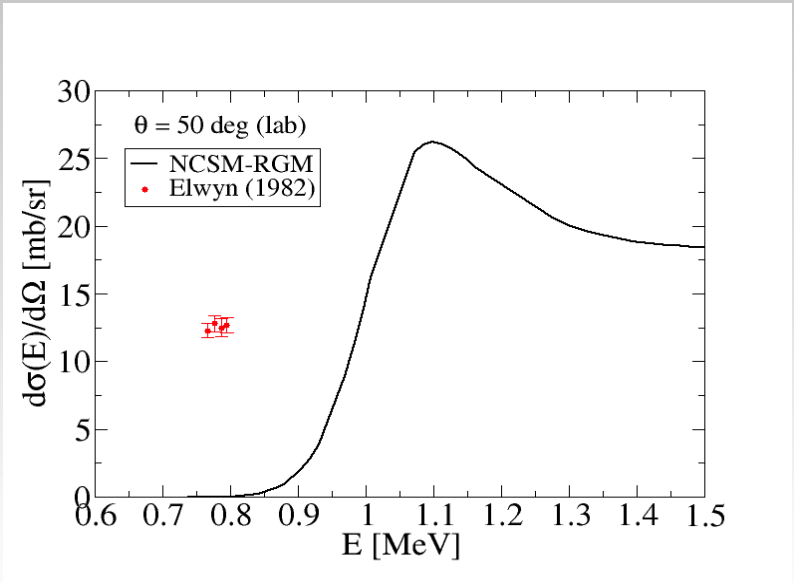
Included channels:
(1) p, ^{8}Li (2) *d*, ^{7}Li (3) coupling (*d*,p)
(4) virtual breakup of *d*

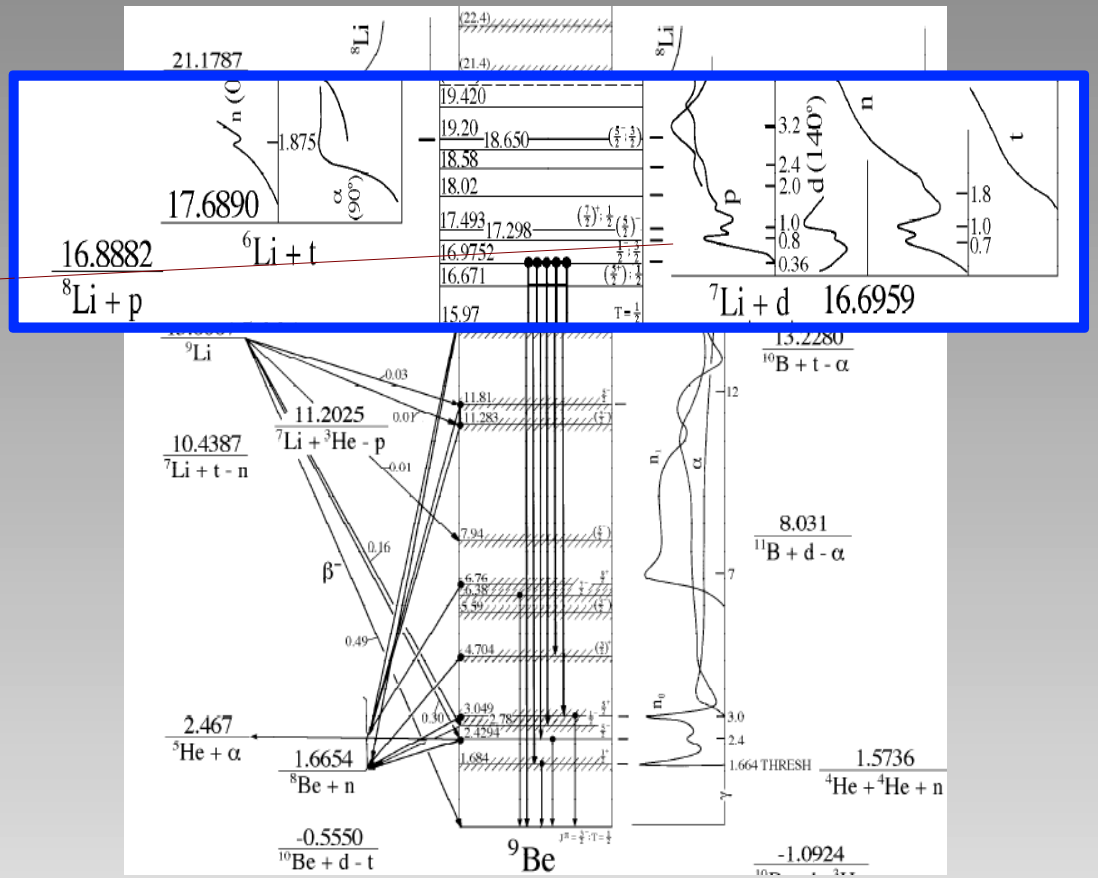
Not-included channels: (1)^{8}Be, n (2) ^{6}Li, t

NCSM-RGM calculations with chiral N^{3}LO NN potentials (SRG λ=2.02 fm^{-1})
4 eigenstates of ^{8}Li, 2 eigenstates of ^{7}Li and 5 pseudostates of deuteron
Preliminary: Nmax=6, hΩ=20 MeV

^{7}Li(*d*,p)^{8}Li scattering results (NCSM-RGM)





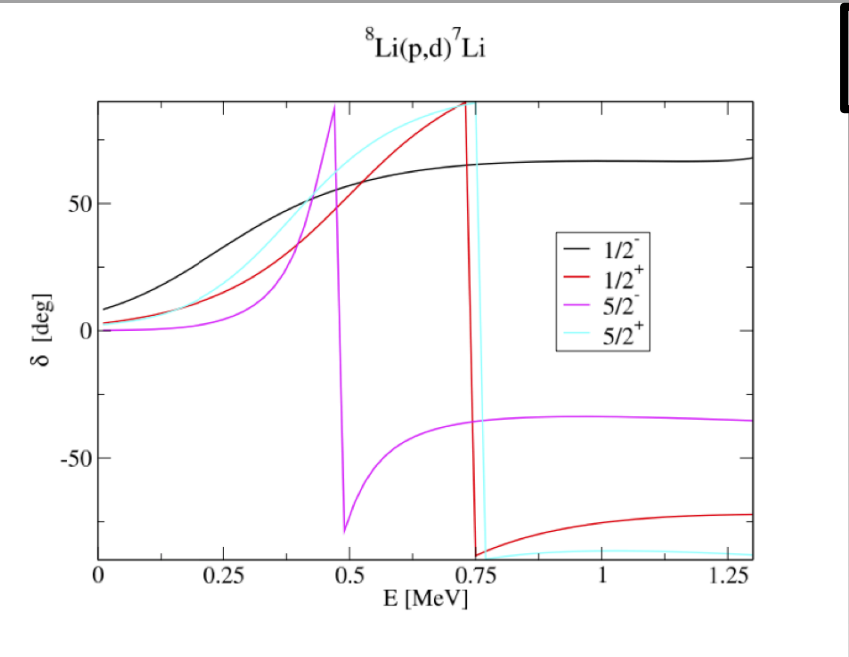


Lowest peak in the experimental total cross section:
(E(5/2^{-})~0.8 MeV above the threshold)

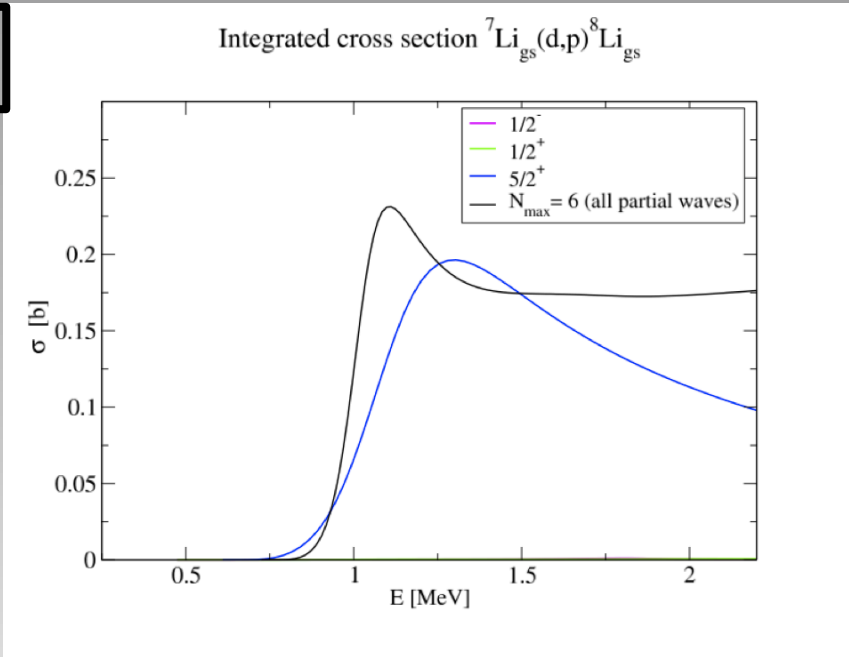
(Uncertain spin-parity assignment)

Impact of $5/2^+$ resonance on cross section

Cross section calculated from selected partial waves:



$N_{max} = 8$



Main eigenphase shifts at low energy of deuteron: $5/2^+$ stable when increasing the model space dimension

$5/2^+$ partial wave accounts for most of the strength of the first resonance above the *d*-^{7}Li thresholds.

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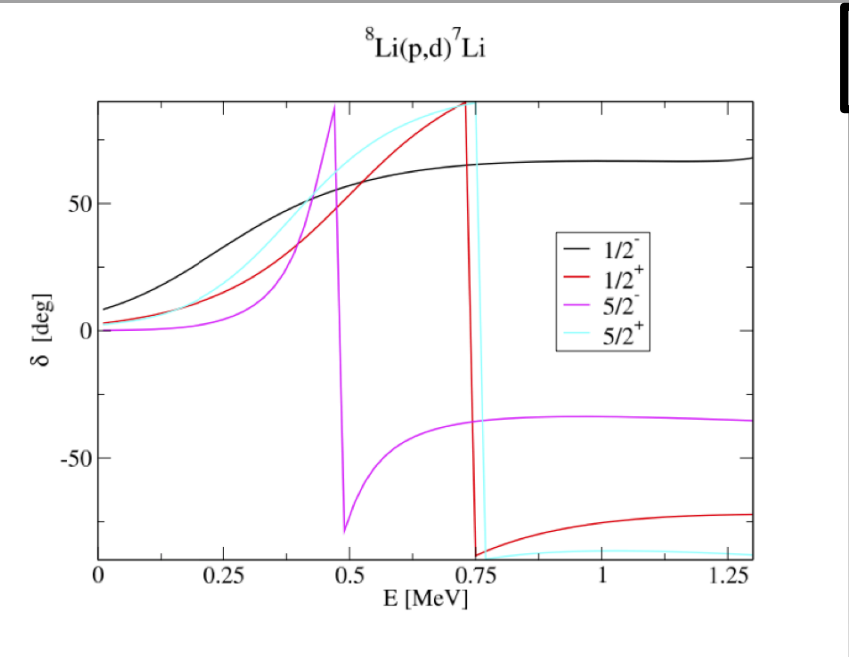
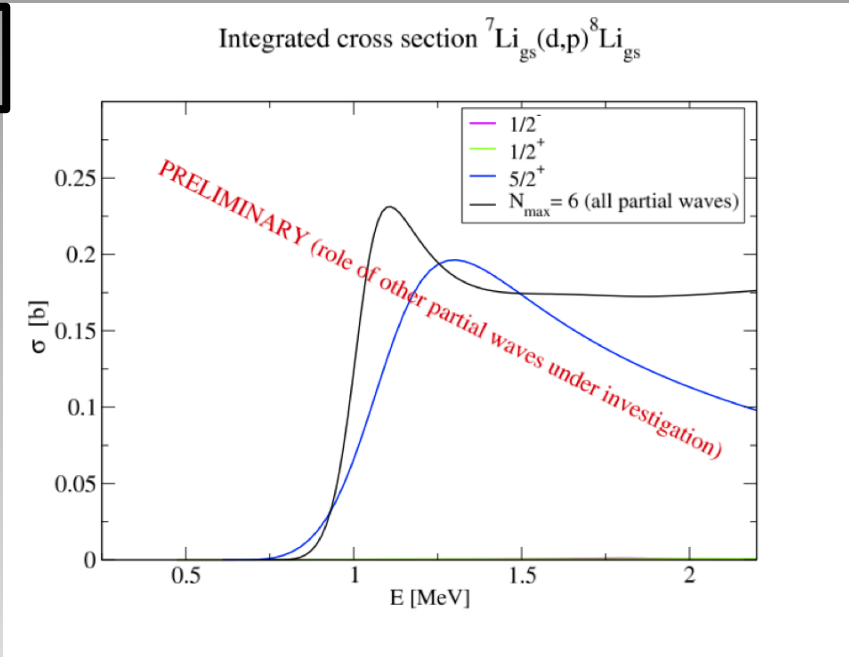
Impact of $5/2^+$ resonance on cross section

Cross section calculated from selected partial waves:



$N_{max} = 8$

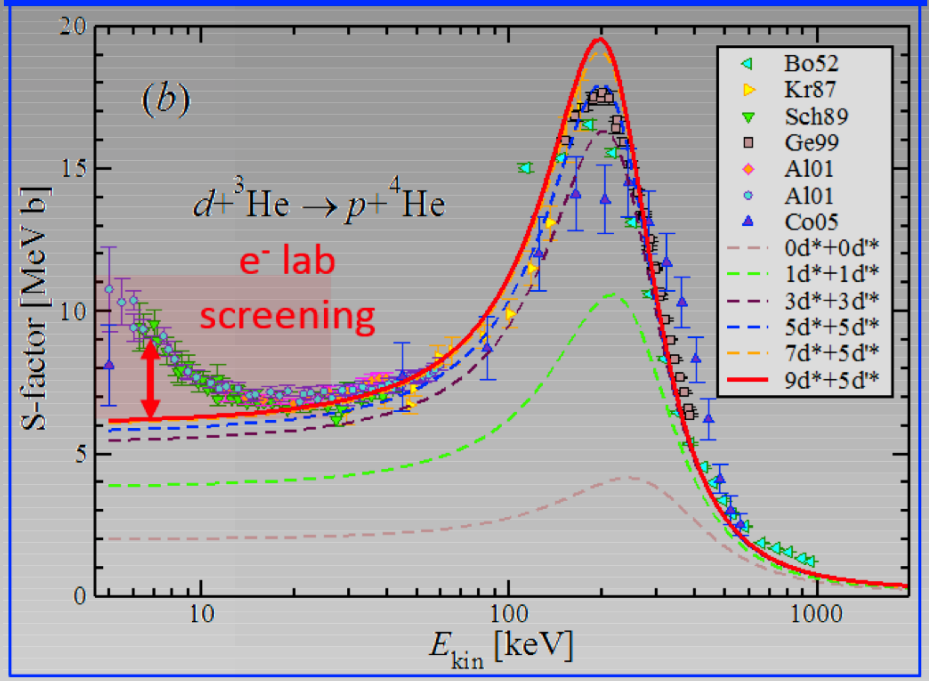


Main eigenphase shifts at low energy of deuteron: $5/2^+$ stable when increasing the model space dimension

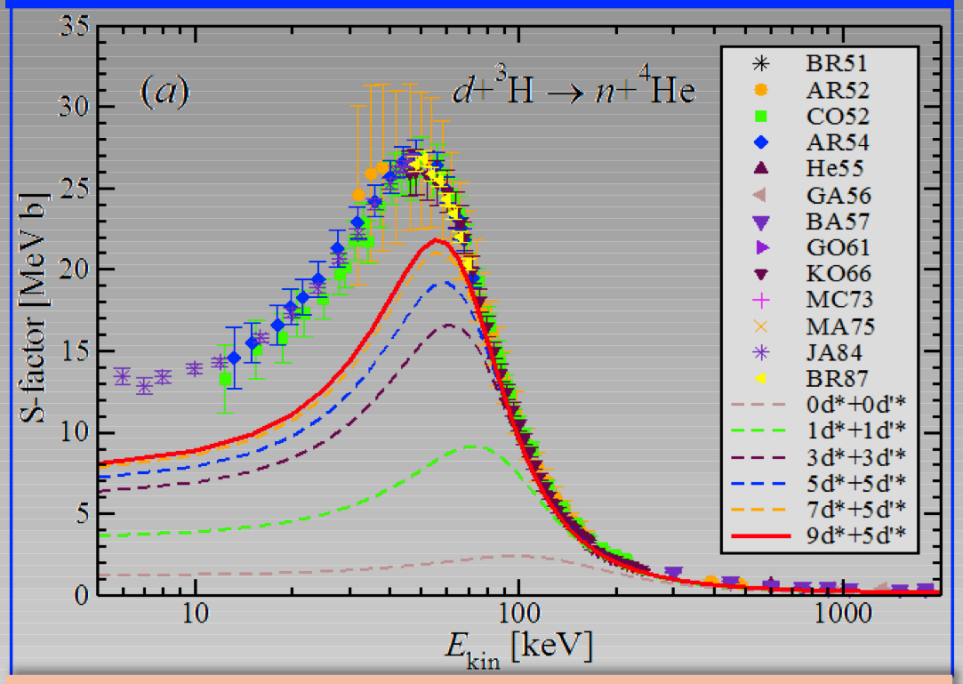
$5/2^+$ partial wave accounts for most of the strength of the first resonance above the *d*-^{7}Li thresholds.

First step towards *ab initio* calculation transfer reactions (Navrátil, Quaglioni PRL108, 2012)

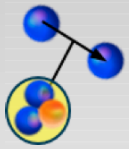
^{3}He(d,p)^{4}He astrophysical S-factor



^{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.



Deuterium breakup:

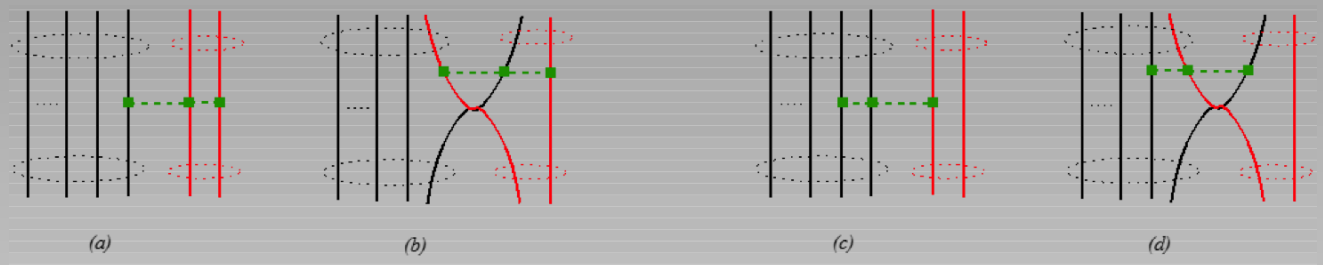
Calculated S-factors converge with the inclusion of virtual breakup of the Deuterium, obtained by means of excited $^3S_1$-$^3D_1$(d^*) and $^3D_2$(d^*) pseudostates

Incomplete nuclear ineraction: Requires 3N forces (SRG-induced + “real”)

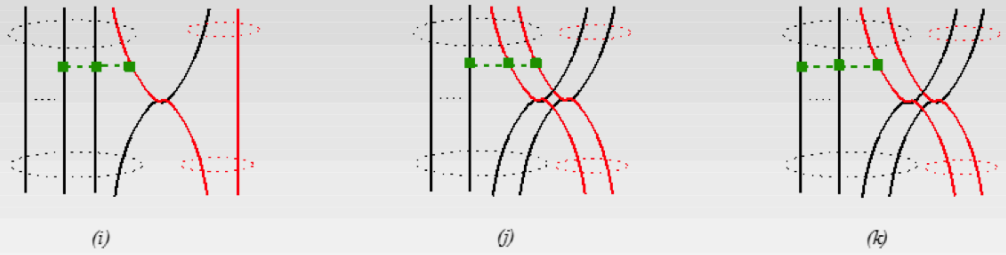
Including 3N force into the description of deuteron-nucleus scattering

$$\left\langle \Phi^{J^\pi T}_{v'r'} \middle| \hat{A}_{v'} V^{NNN} \hat{A}_v \middle| \Phi^{J^\pi T}_{v\,r} \right\rangle = \left\langle \begin{matrix} (A-2) \\ \vec{r}\,' \\ (a'=2) \end{matrix} \middle| V^{NNN}\left(1 - \sum_{i=1}^{A-2}\sum_{k=A-1}^{A} \hat{P}_{ik} + \sum_{i<j=1}^{A-2} \hat{P}_{iA-1}\hat{P}_{jA}\right) \middle| \begin{matrix} (A-2) \\ \vec{r} \\ (a=2) \end{matrix} \right\rangle$$

Direct



Exchange



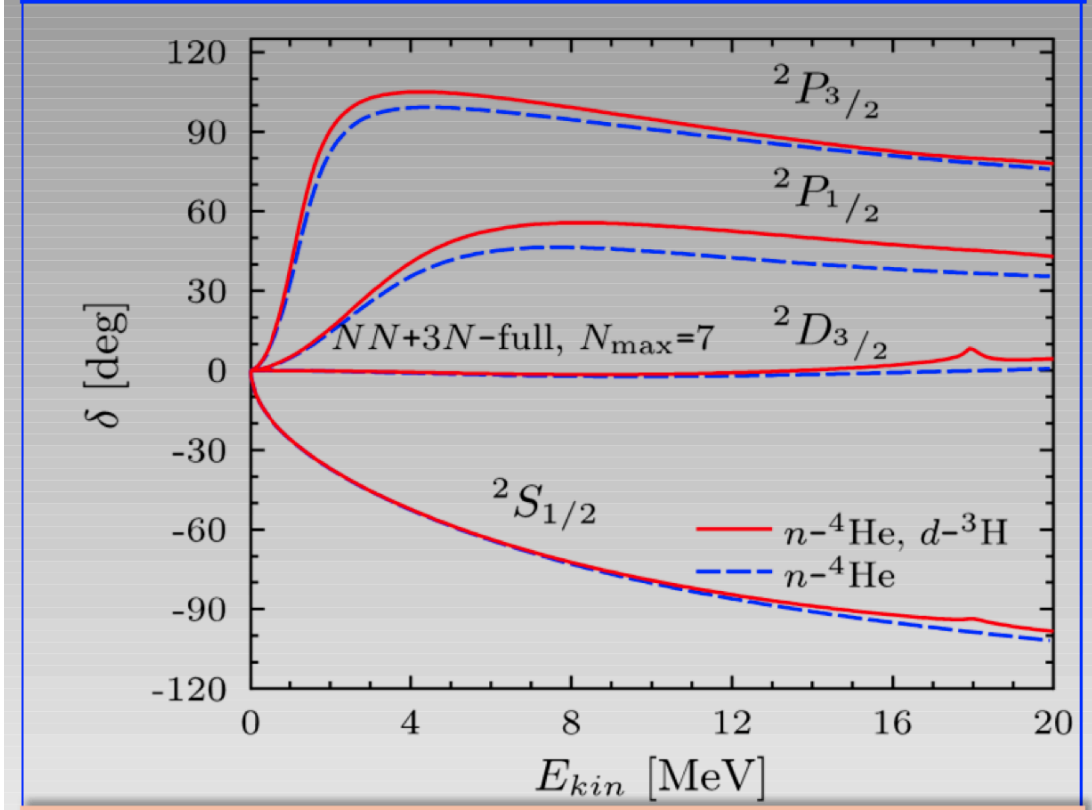
→ Four body density

NCSM-RGM calculation of transfer reaction ^{3}H(d,n)^{4}He with 3N forces

^{4}He fusion

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

n-^{4}He with the d-^{3}H channel with the chiral two- and three-nucleon force (preliminary)

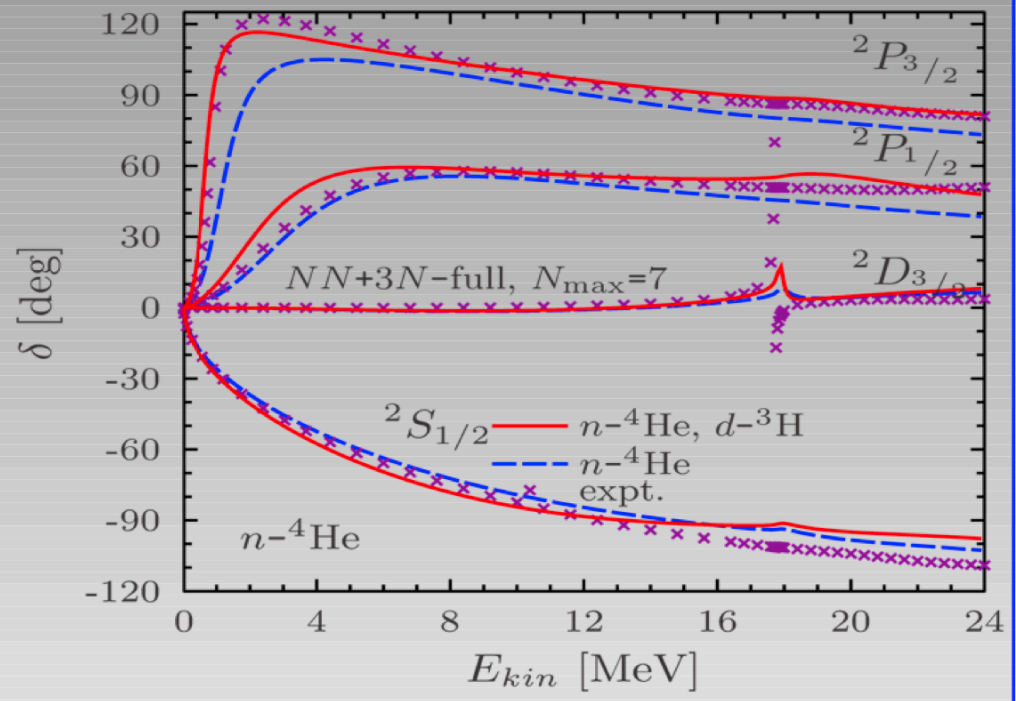


n+^{4}He(g.s.) phase shifts with NN+3N potential, λ=2.0 fm^{-1}, no ^{5}He eigenstates, with/o coupling to d-t.

- 7 diagrams (+ exchange) arising from the coupling of n-α with d-t through the three-nucleon force.
- Next step: Coupling to the compound ^{5}He eigenstates

NCSMC calculation of transfer reaction ^{3}H(d,n)^{4}He with 3N forces

^{4}He fusion with NCSMC and the chiral two- and three-nucleon force (preliminary)



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

^{4}He fusion

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

- Preliminary, small N_{MAX} = 7

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Conclusions & Perspectives

First application of the NCSM-RGM for deuteron-projectile and p-shell nucleus as target:

- Inclusion of the “elastic” and coupling channel in the description of transfer reactions

Analysis of the ^{9}Be resonances above *d*-^{7}Li threshold:

- Discussion of the spin-parity assignment of 0.78 MeV resonance

RGM and NCSMC results on *d*-t and *d*-^{3}He transfer reaction with 3N force

To be done:

- Complete the calculation (Nmax=8) of the ^{7}Li(*d*,p)^{8}Li transfer reaction in NCSM-RGM and NCSMC
- Include 3N force also for p-shell nuclei