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Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

Ab Initio calculations of Nuclear Structure and Reactions

2015 CAP Congress
Edmonton, Alberta
June 13–19, 2015

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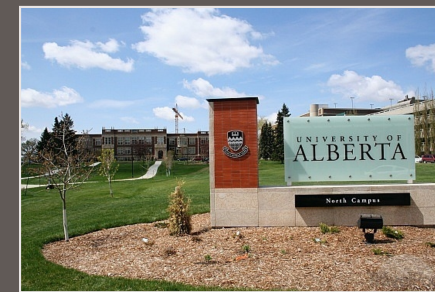
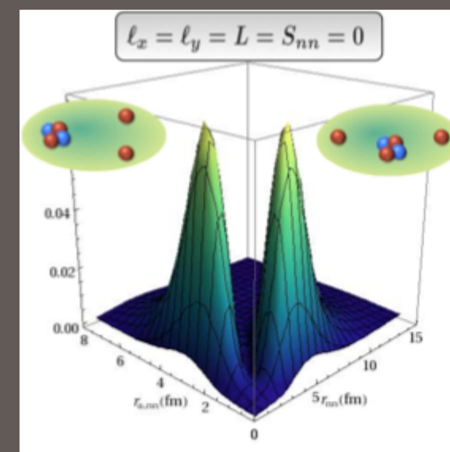
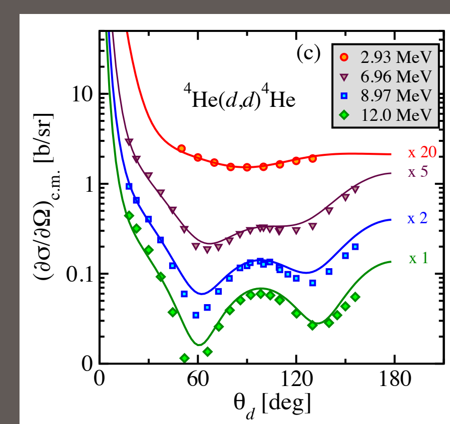
Guillaume Hupin | CNRS

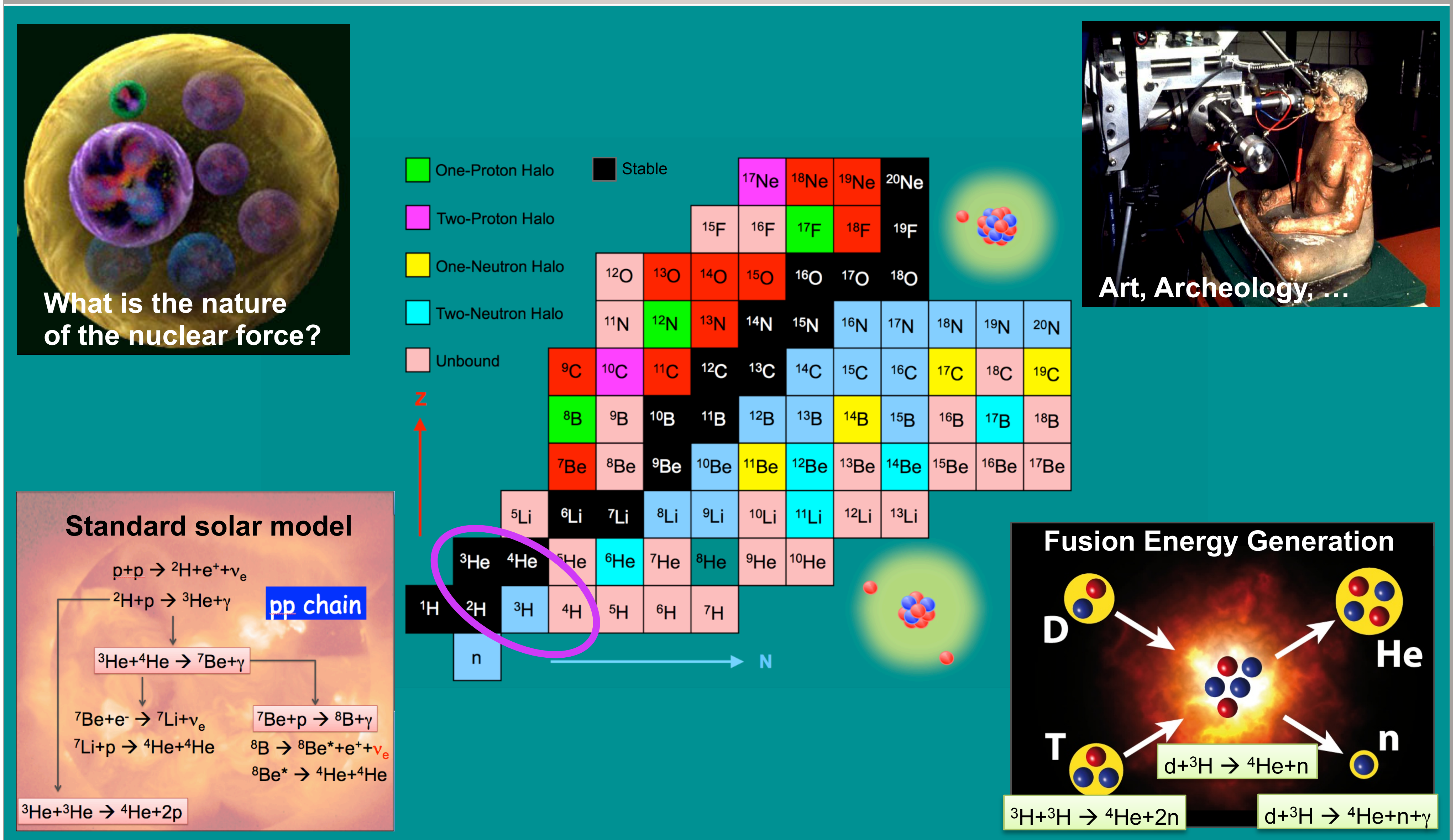




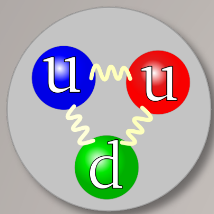


Accelerating Science for Canada
Un accélérateur de la démarche scientifique canadienne

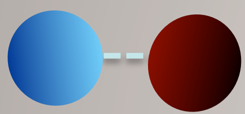
Our goal is to develop a fundamental theory for the description of structure and dynamics of light nuclei



From QCD to nuclei

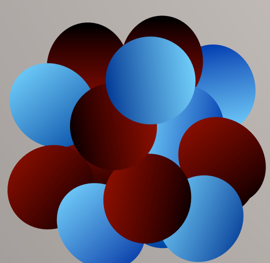


Low-energy QCD



NN+3N interactions from chiral EFT

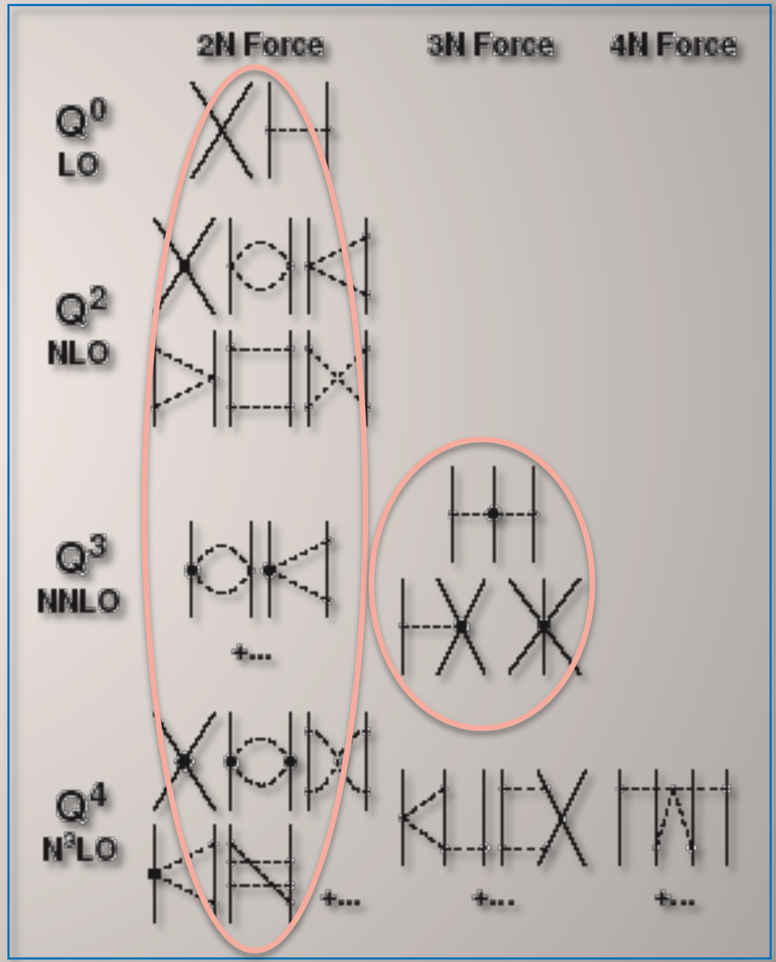
…or accurate meson-exchange potentials



Nuclear structure and reactions

Chiral Effective Field Theory

- **First principles for Nuclear Physics:**
  QCD
  - Non-perturbative at low energies
  - Lattice QCD in the future
- ***For now a good place to start:***
- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order (Q/Λ_χ)
  - Hierarchy
  - Consistency
  - Low energy constants (LEC)
    - Fitted to data
    - Can be calculated by lattice QCD



Λ_χ~1 GeV :
Chiral symmetry breaking scale

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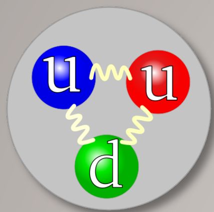
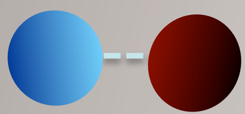
From QCD to nuclei



Low-energy QCD



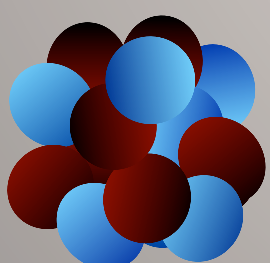
NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

$$H|\Psi\rangle = E|\Psi\rangle$$

Many-Body methods

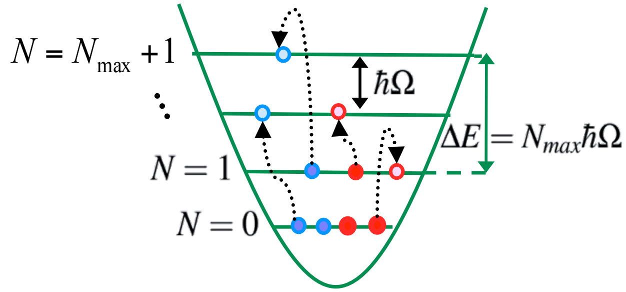
NCSM, NCSM/RGM, NCSMC, CCM, GFMC, HH, Nuclear Lattice EFT…



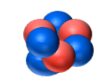
Nuclear structure and reactions

Unified approach to bound & continuum states; to nuclear structure & reactions

- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances



Harmonic oscillator basis

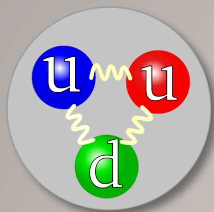


NCSM

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

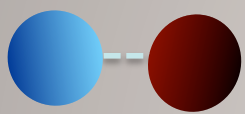
Unknowns

From QCD to nuclei



Low-energy QCD

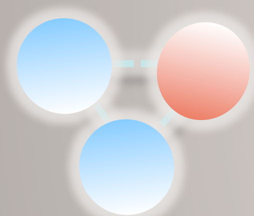
↓



NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

↓



Unitary/similarity transformations

Identity or SRG or OLS or UCOM …
Softens NN, induces 3N

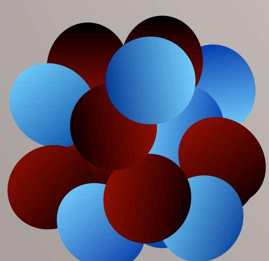
↓

$$H|\Psi\rangle = E|\Psi\rangle$$

Many-Body methods

NCSM, NCSM/RGM, CCM, GFMC, HH, Nuclear Lattice EFT…

↓



Nuclear structure and reactions

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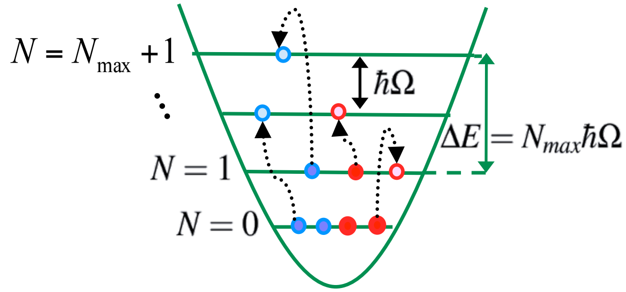

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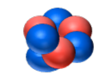
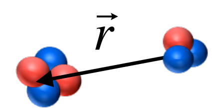


NCSM

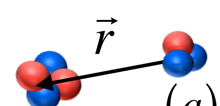
- …with resonating group method
  - Bound & scattering states, reactions
  - Cluster dynamics, long-range correlations



NCSM/RGM

NCSM/RGM channel states

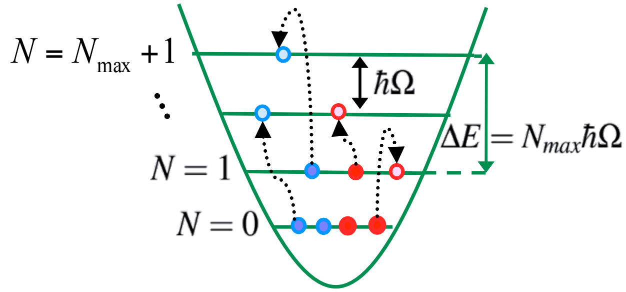
$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\, \gamma_{\nu}(\vec{r})\, \hat{A}_{\nu} \left| \;^{(A-a)} \quad ^{(a)}, \nu \right\rangle$$



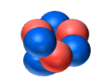
Unknowns

Unified approach to bound & continuum states; to nuclear structure & reactions

- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances



Harmonic oscillator basis



NCSM

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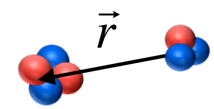


NCSM/RGM

S. Baroni, P. Navratil, and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

- Most efficient: *ab initio* no-core shell model with continuum

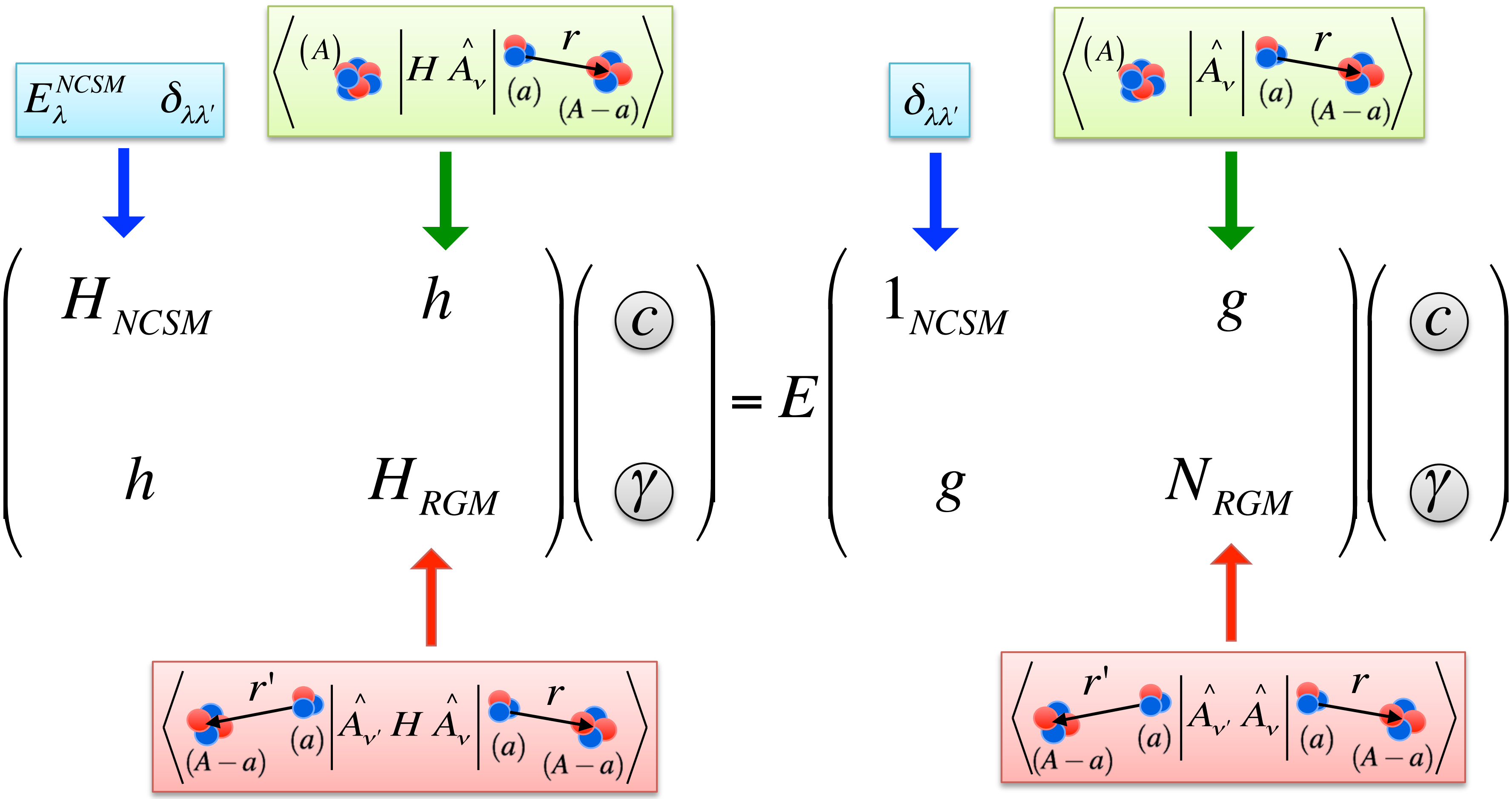
NCSMC

NCSM eigenstates — NCSM/RGM channel states

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

Unknowns

Coupled NCSMC equations



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

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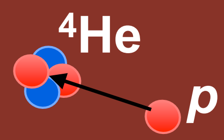
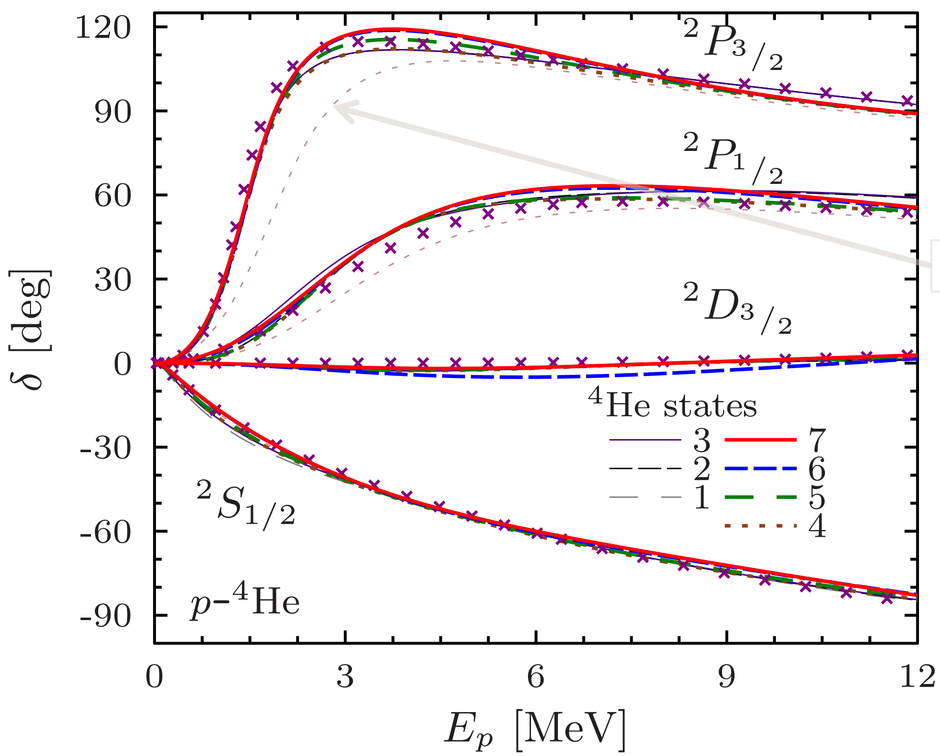
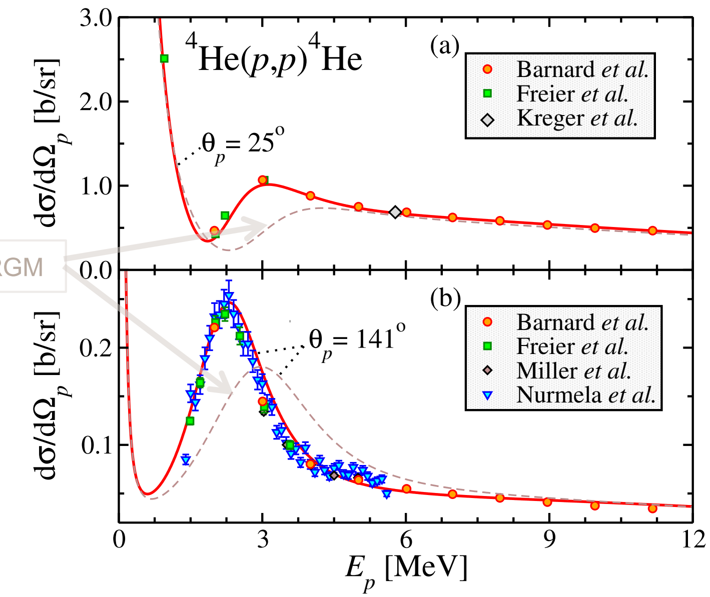


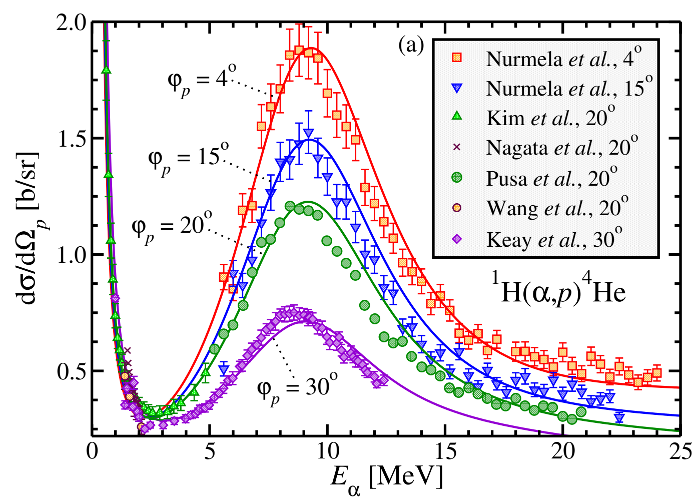
p-^{4}He scattering within NCSMC

p-^{4}He scattering phase-shifts for NN+3N potential: Convergence



Differential p-^{4}He cross section with NN+3N potentials





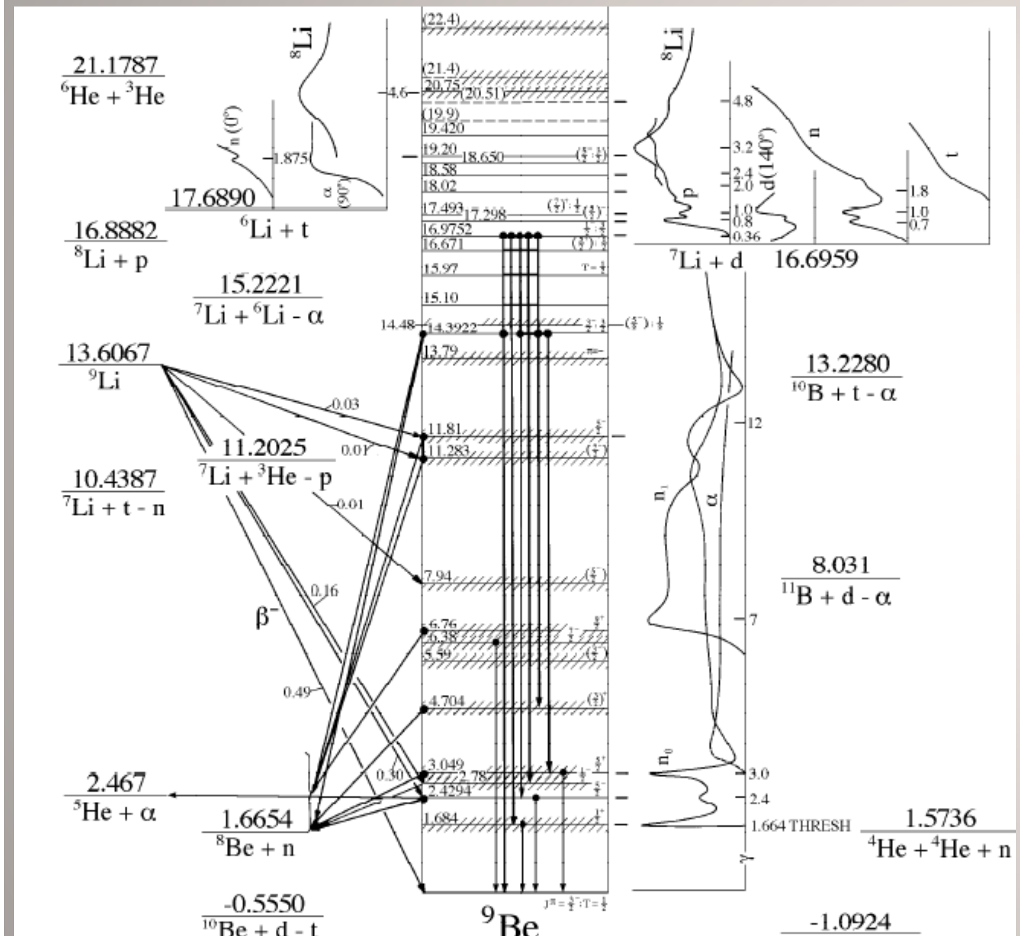
Predictive power in the 3/2$^-$ resonance region: Applications to material science

PHYSICAL REVIEW C **90**, 061601(R) (2014)

Predictive theory for elastic scattering and recoil of protons from ^{4}He

Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

Structure of ^9Be



^9Be is a stable nucleus

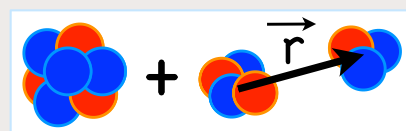
… but all its excited states unbound

A proper description requires to include effects of continuum

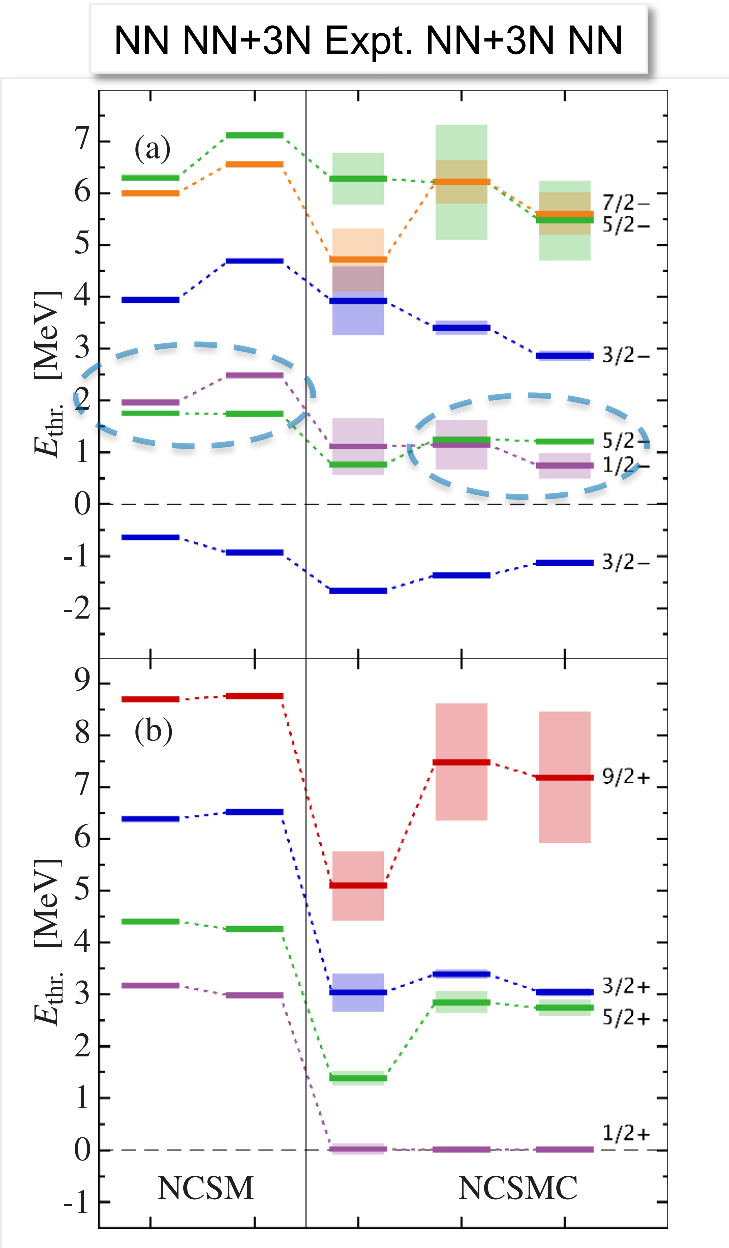
The lowest threshold: n-^8Be (n-α-α)

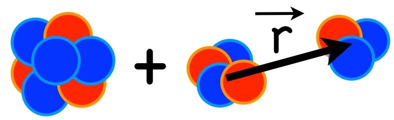
Optimal description:

Square-integrable ^9Be basis + n-^8Be clusters



NCSMC with chiral NN+3N: Structure of ^{9}Be

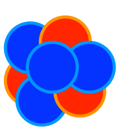




^{9}Be is a stable nucleus
… but all its excited states unbound
A proper description requires to include effects of continuum

Three-nucleon interaction *and* continuum improve agreement with experiment for negative parity states

Continuum crucial for the description of positive-parity states

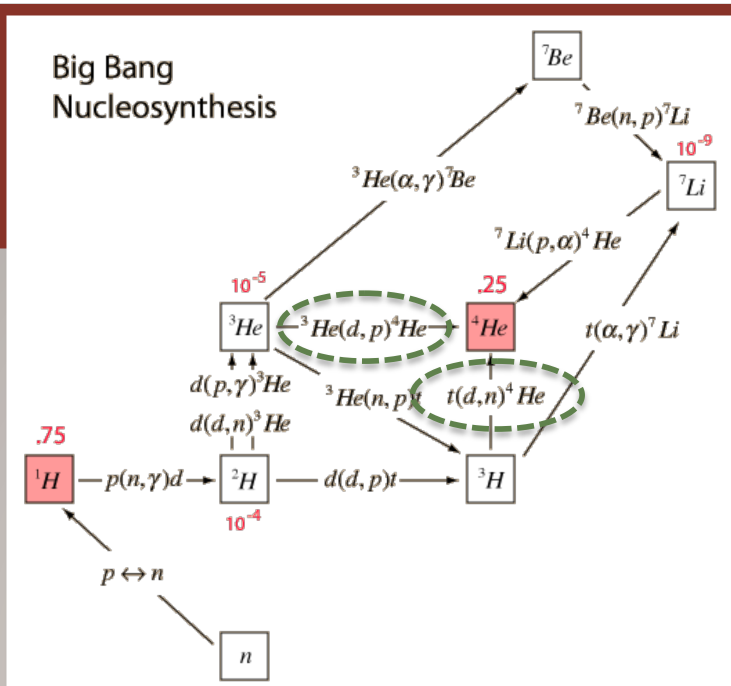


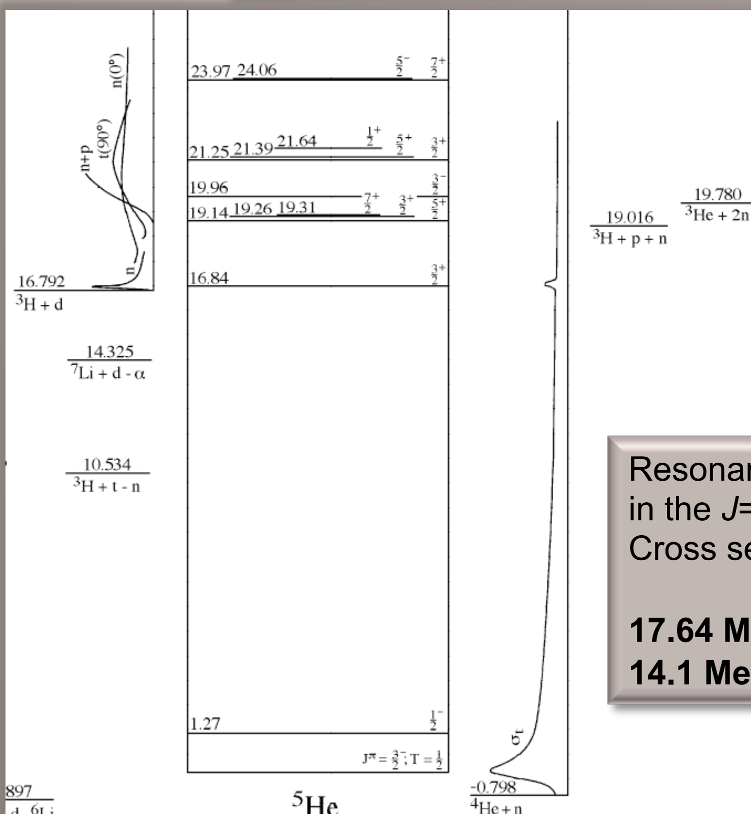
PHYSICAL REVIEW C **91**, 021301(R) (2015)

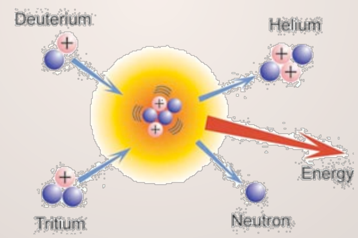
Continuum and three-nucleon force effects on ^{9}Be energy levels

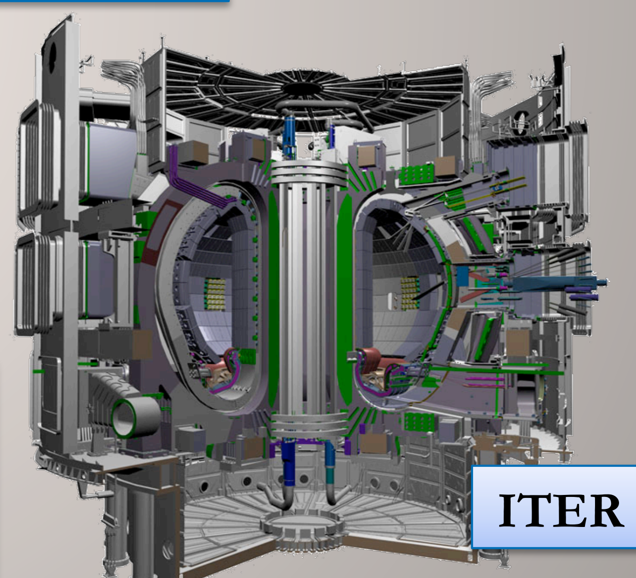
Joachim Langhammer,[1,*] Petr Navrátil,[2,†] Sofia Quaglioni,[3] Guillaume Hupin,[3,‡] Angelo Calci,[1,2] and Robert Roth[1,§]

Deuterium-Tritium fusion









Resonance at E_{cm} =48 keV (E_d=105 keV) in the J=3/2$^+$ channel
Cross section at the peak: 4.88 b

17.64 MeV energy released:
14.1 MeV neutron and 3.5 MeV alpha

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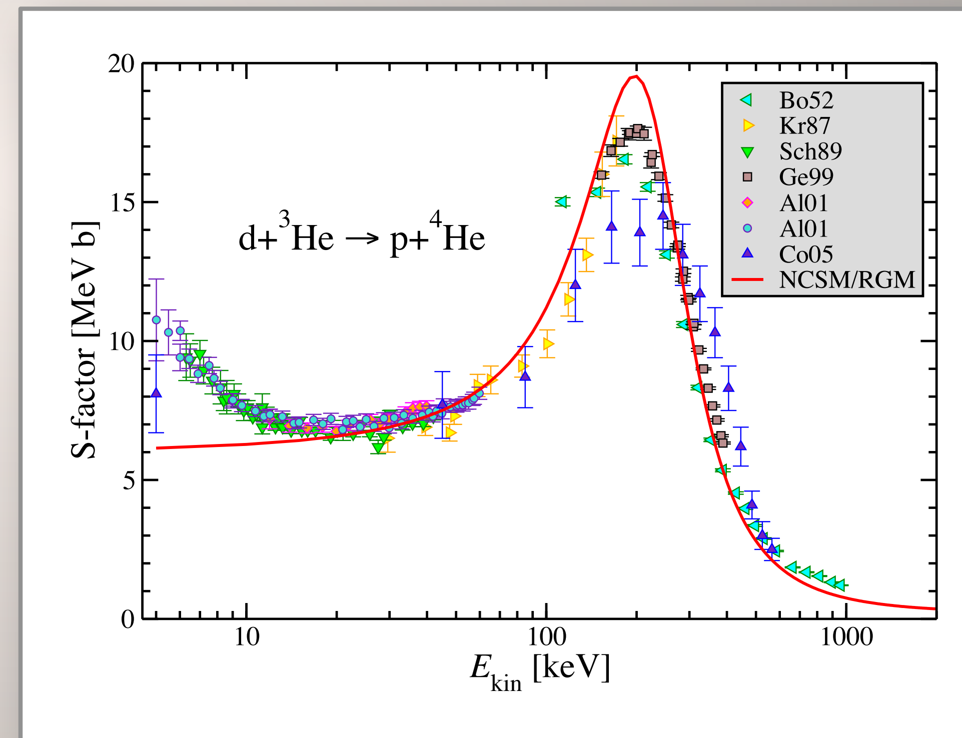
NCSM/RGM calculations of transfer reactions

$$\int dr\, r^2 \begin{pmatrix} \langle \vec r'\, n\,\alpha | \hat A_1 (H-E) \hat A_1 | \alpha\, n\, \vec r \rangle & \langle \vec r'\, n\,\alpha | \hat A_1 (H-E) \hat A_2 | {}^3\mathrm{H}\, d\, \vec r \rangle \\ \langle \vec r'\, d\, {}^3\mathrm{H} | \hat A_2 (H-E) \hat A_1 | \alpha\, n\, \vec r \rangle & \langle \vec r'\, d\, {}^3\mathrm{H} | \hat A_2 (H-E) \hat A_2 | {}^3\mathrm{H}\, d\, \vec r \rangle \end{pmatrix} \begin{pmatrix} \frac{g_1(r)}{r} \\ \frac{g_2(r)}{r} \end{pmatrix} = 0$$

Straightforward to couple different mass partitions in the NCSM/RGM formalism

Applications to (d,p) and (d,n) reactions
Example: **^{3}He(d,p)^{4}He**



$$S(E) = E\sigma(E)\exp[2\pi\eta(E)]$$

$$\eta(E) = Z_{A-a} Z_a e^2 / \hbar v_{A-a,a}$$

PRL 108, 042503 (2012) PHYSICAL REVIEW LETTERS week ending 27 JANUARY 2012

***Ab Initio* Many-Body Calculations of the ^{3}H(d,n)^{4}He and ^{3}He(d,p)^{4}He Fusion Reactions**

Petr Navrátil[1,2] and Sofia Quaglioni[2]

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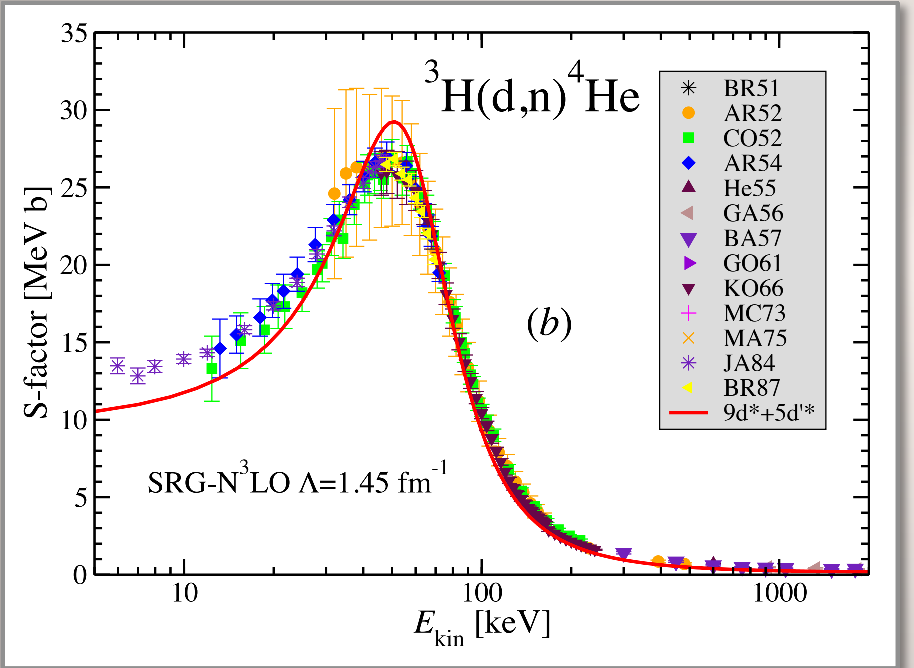
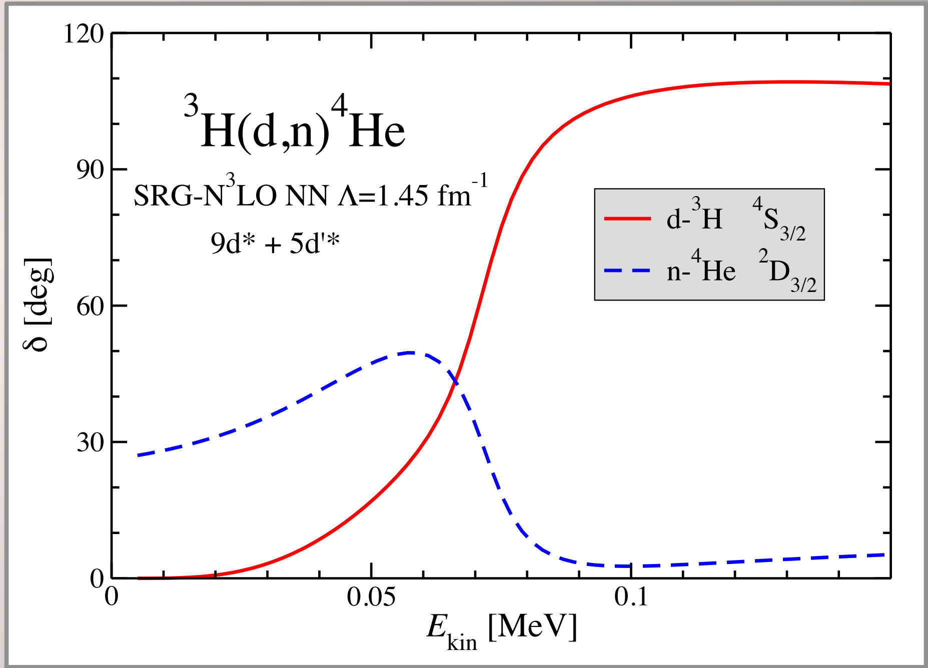
^{3}H(d,n)^{4}He cross section

- SRG-N^{3}LO (Λ=1.45 fm^{-1}) NN potential
  - Position of the resonance matches experiment

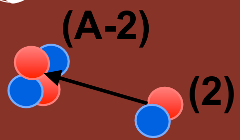




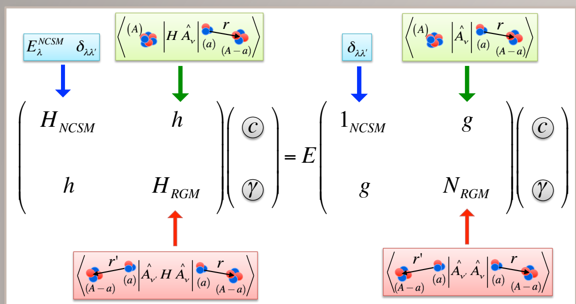
S-factor narrower than the data

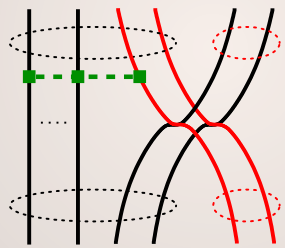
Resonance in the d-^{3}H $^4S_{1/2}$ partial wave

n-^{4}He $^2D_{3/2}$ decreasing, does not cross 90 degrees



The deuteron-projectile formalism: Three-nucleon interaction and/or A_1>4 target

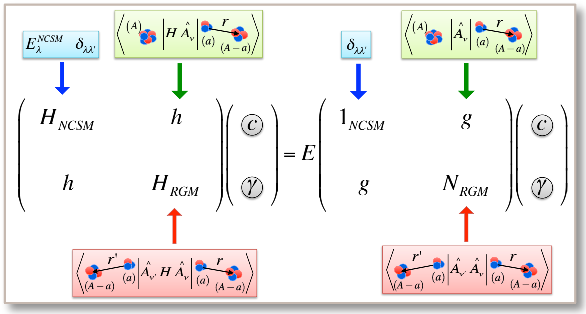




$$ {}_{\mathrm{SD}}\left\langle \psi_{\mu_1}^{(A-2)} \right| a^+ a^+ a^+ a^+ a\, a\, a\, a \left| \psi_{\nu_1}^{(A-2)} \right\rangle_{\mathrm{SD}} $$

For A=6 use completeness
For A>6 a sophisticated algorithm required

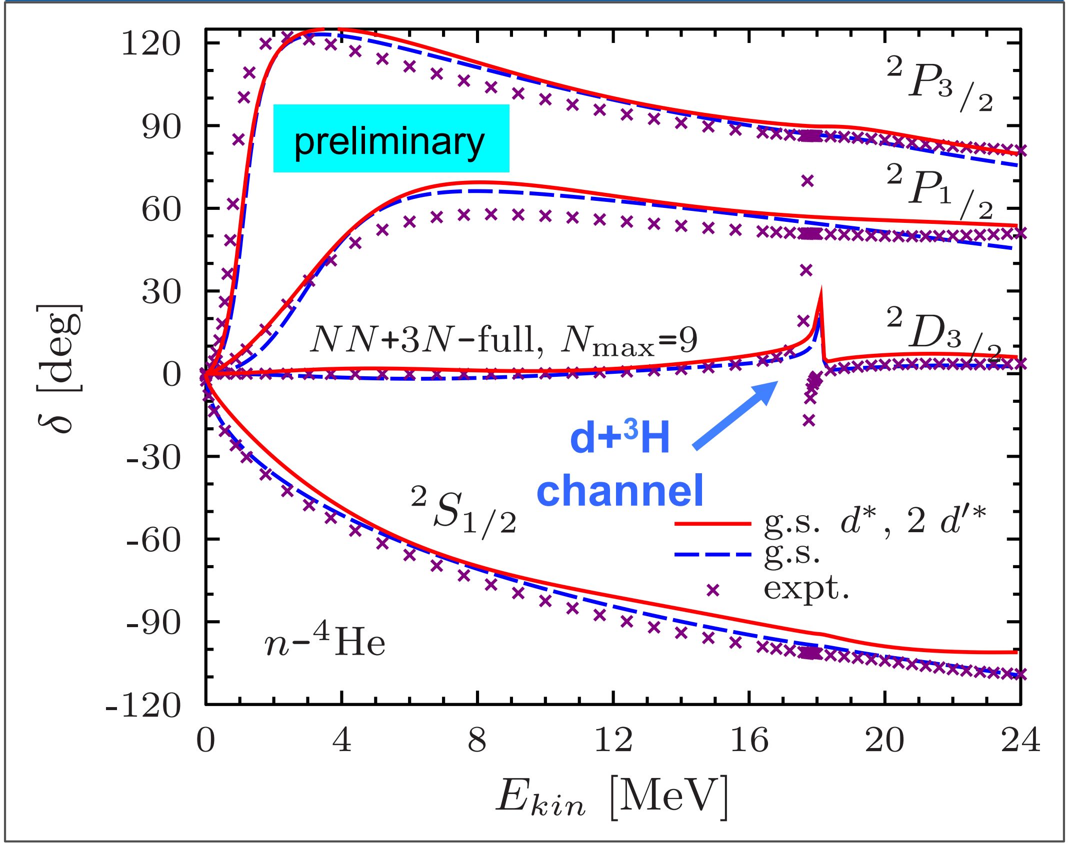
^{3}H(d,n)^{4}He fusion with chiral NN+3N



NCSMC

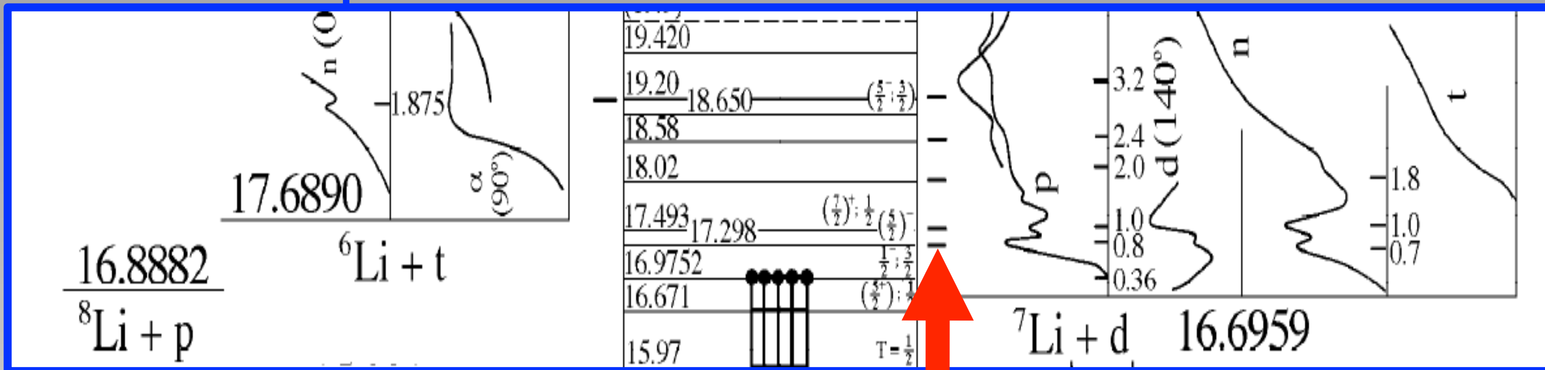
- Towards first ab initio calculation of ^{3}H(d,n)^{4}He fusion with 3N forces
  - N_{max} = 9 model space
  - n+^{4}He & d+^{3}H continuum channels
  - Up to 14 ^{5}He states
  - Only g.s. of ^{4}He and ^{3}H: effect of target excitation described by ^{5}He states
  - 3-body dynamics approximated above deuteron breakup

n-^{4}He scattering phase shifts



Spin-parity assignment of 0.78 MeV resonance of ^{9}Be

^{9}Be spectrum above *d*-^{7}Li threshold



Low peak in the experimental total cross section:
E(5/2^{-})~0.78 MeV above the threshold
(Uncertain spin-parity assignment)

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

- Possible mechanism of destruction of ^{7}Li in the context of baryon-inhomogeneus models of the primordial nucleosynthesis (Primordial Lithium abundance problem)

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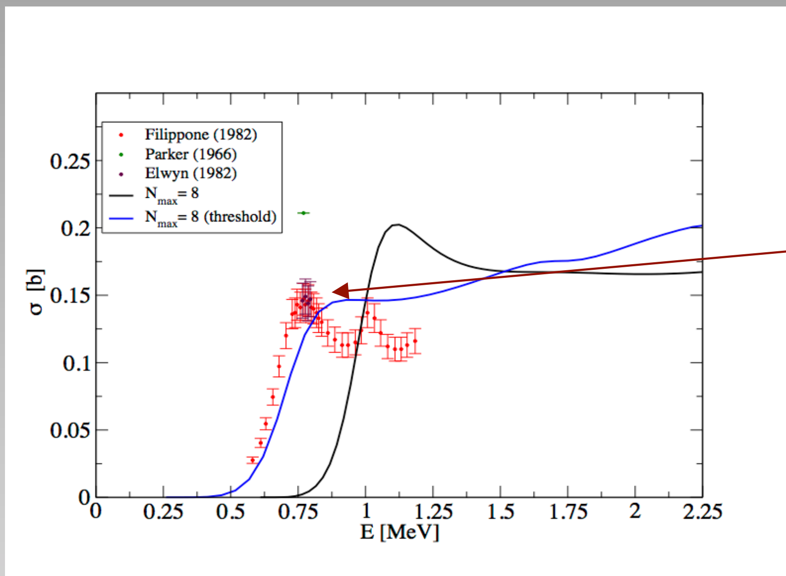
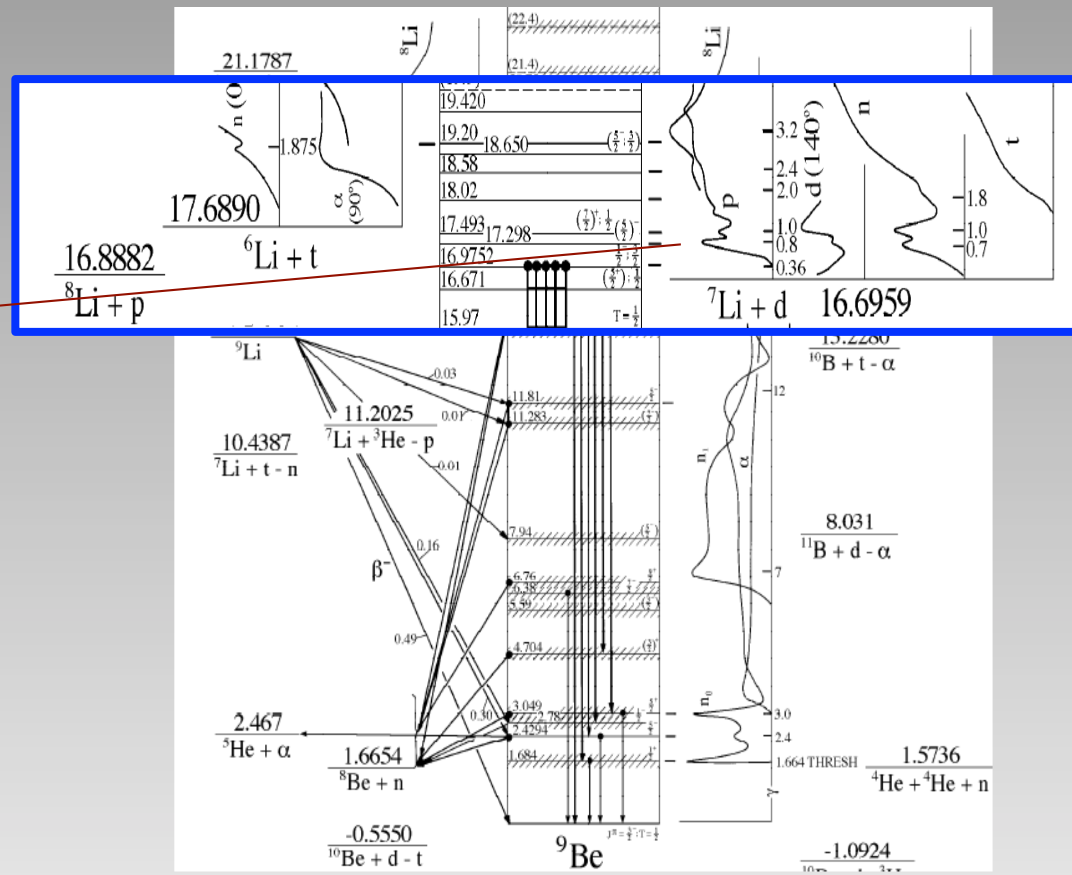
$^{7}Li(d,p)^{8}Li$ scattering results (NCSM-RGM)





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 SRG-evolved (λ=2.02 fm^{-1}) chiral N^{3}LO NN potentials
4 eigenstates of ^{8}Li, 2 eigenstates of ^{7}Li and 5 pseudostates of deuteron
N_{max}=8, $h\Omega$=20 MeV

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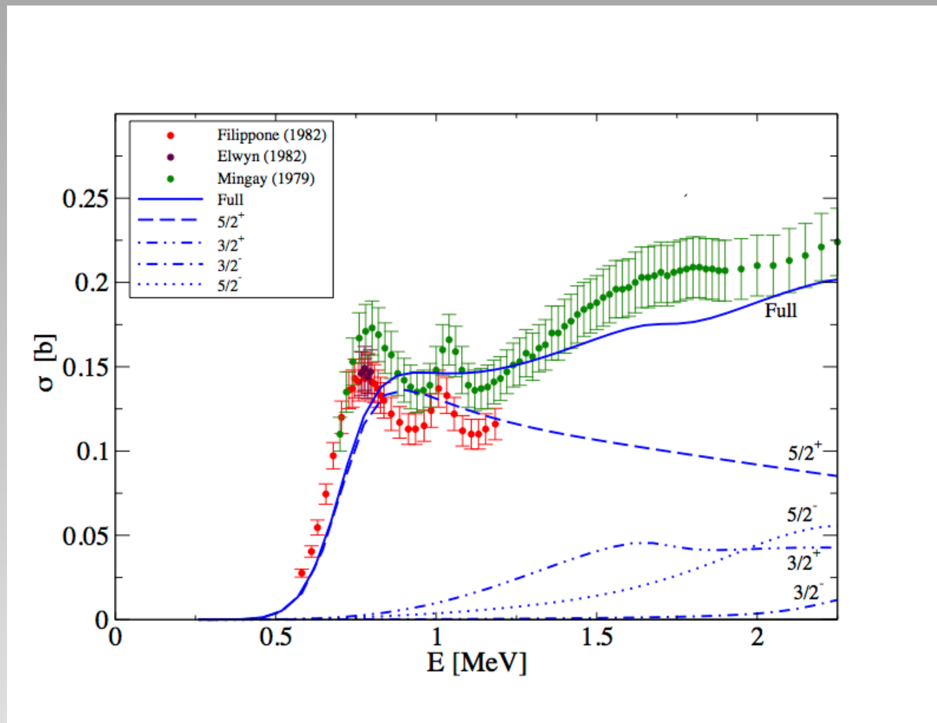
Impact of different partial waves (NCSM-RGM)

$^{7}Li(d,p)^{8}Li$ cross section



- Position of the first resonant peak slightly overestimated
- Increasing trend up to deuteron break-up fairly well reproduced (contribution from $3/2^{+}$ partial wave)
- Double-peak structure at low energy not resolved

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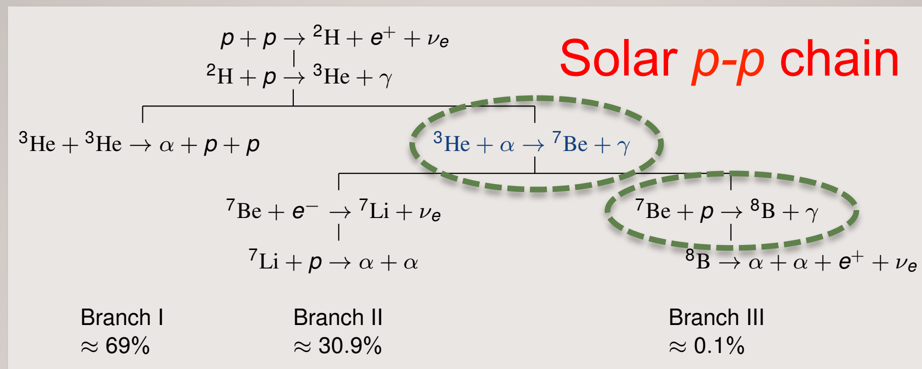
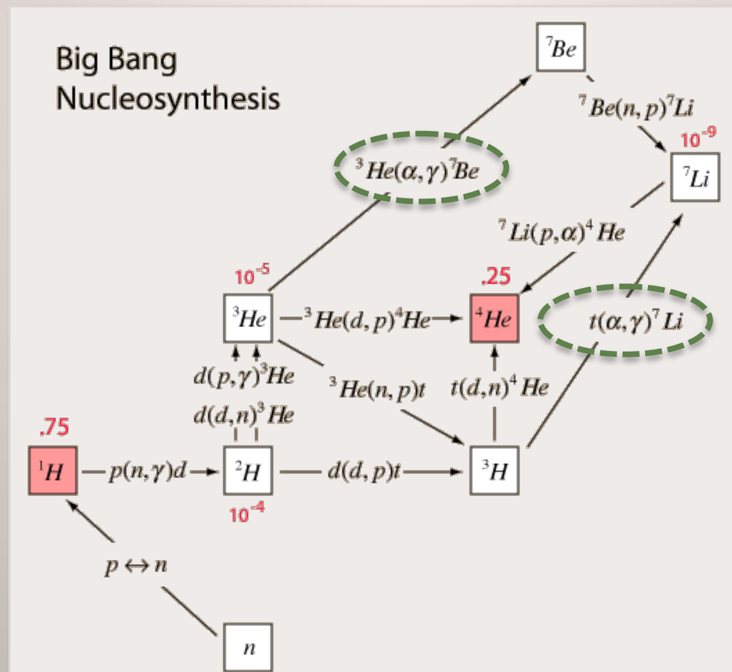
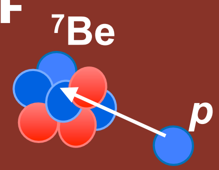
Capture reactions important for astrophysics

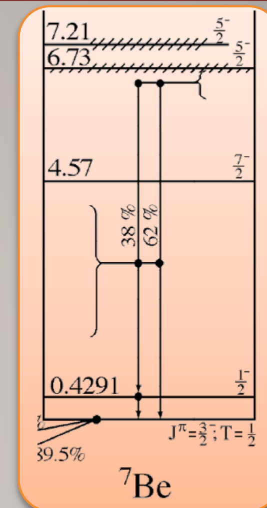






^{7}Be(p,γ)^{8}B radiative capture

- NCSM/RGM calculation of ^{7}Be(p,γ)^{8}B radiative capture
  - ^{7}Be states 3/2$^-$,1/2$^-$, 7/2$^-$, 5/2$^-_1$, 5/2$^-_2$
  - Soft NN potential (SRG-N^{3}LO with Λ = 1.86 fm^{-1})



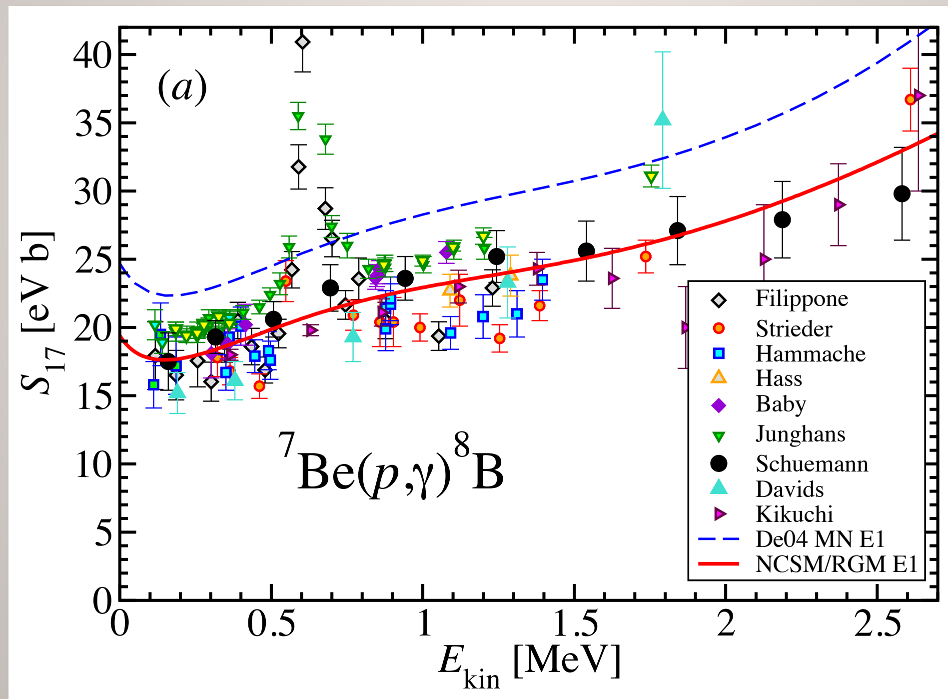
^{8}B 2$^+$ g.s. **bound** by 136 keV

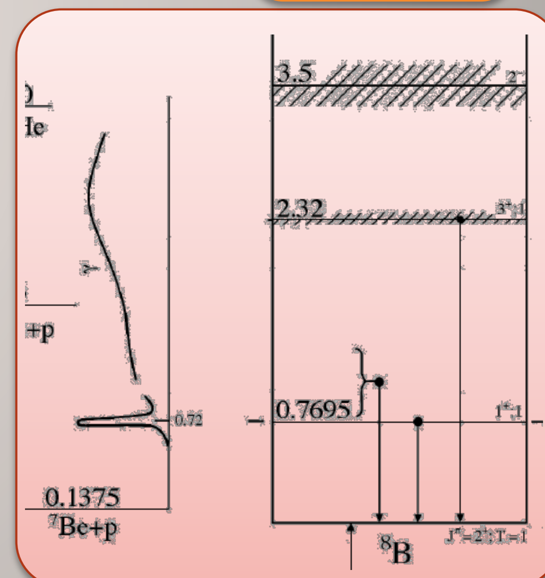
(expt. 137 keV)

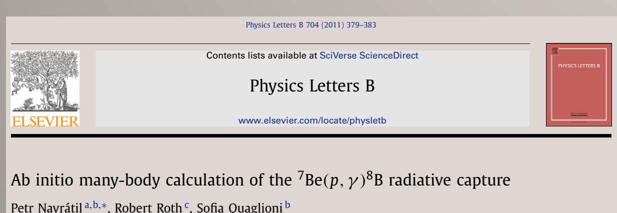
S(0) ~ 19.4(0.7) eV b

Data evaluation:

S(0)=20.8(2.1) eV b



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

Petr Navrátil[a,b,*], Robert Roth[c], Sofia Quaglioni[b]

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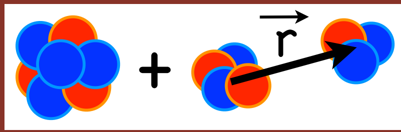
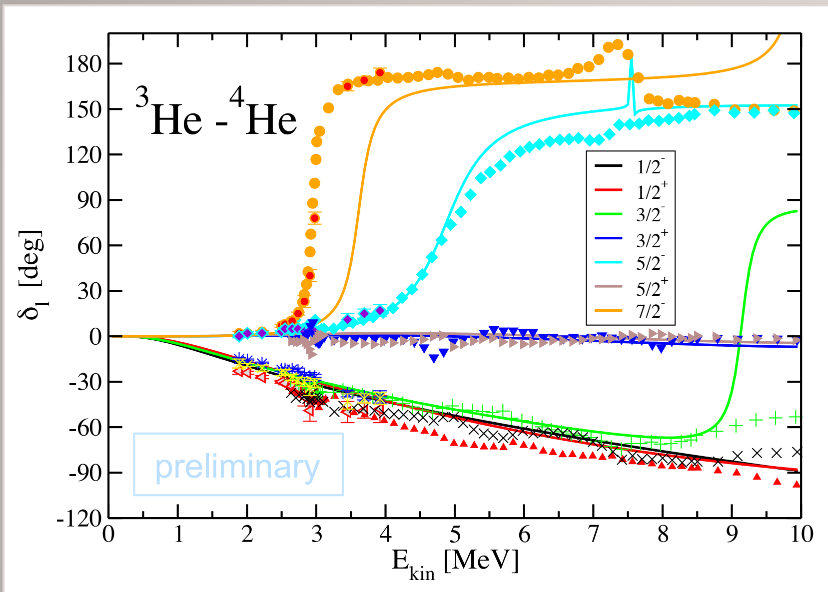


^{3}He-^{4}He and ^{3}H-^{4}He scattering



	^{7}Be		^{7}Li	
	NCSMC	Expt.	NCSMC	Expt.
$E_{3/2^-}$ [MeV]	-1.52	-1.586	-2.43	-2.467
$E_{1/2^-}$ [MeV]	-1.26	-1.157	-2.15	-1.989
r_{ch} [fm]	2.62	2.647(17)	2.42	2.390(30)
Q [e fm^2]	-6.14		-3.72	-4.00(3)
μ [μ_N]	-1.20	-1.3995(5)	+3.08	+3.256

NCSMC calculations with chiral SRG-N^{3}LO *NN* potential (λ=2.15 fm^{-1})

^{3}He, ^{3}H, ^{4}He ground state, 8(π-) + 6(π+) eigenstates of ^{7}Be and ^{7}Li

Preliminary: N_{max}=12, hΩ=20 MeV

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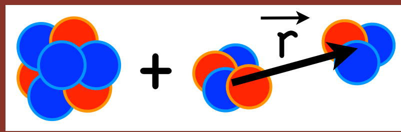

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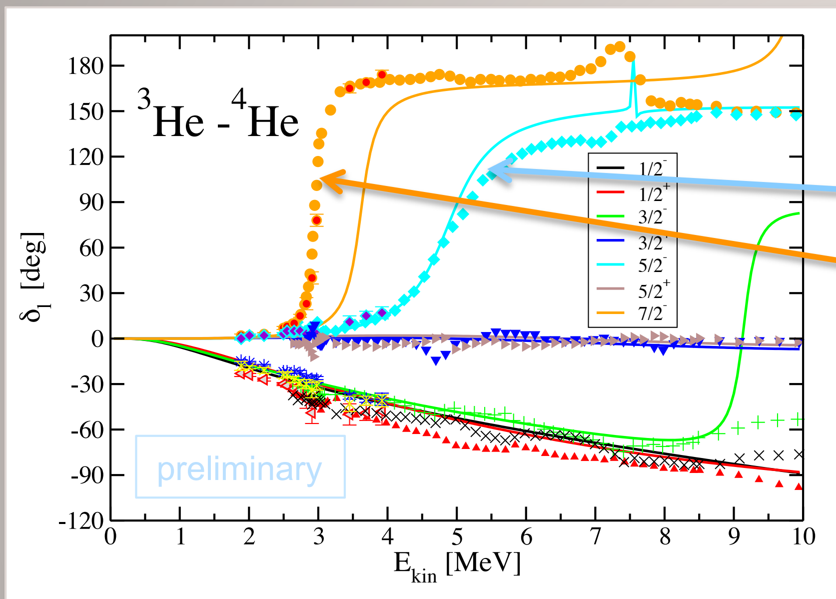

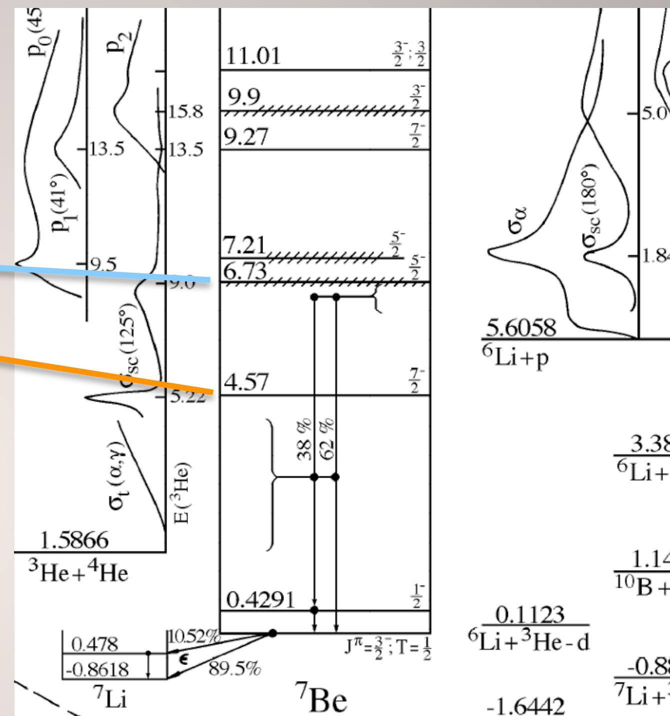

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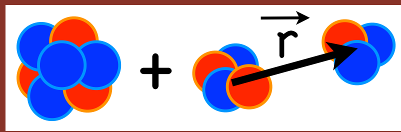
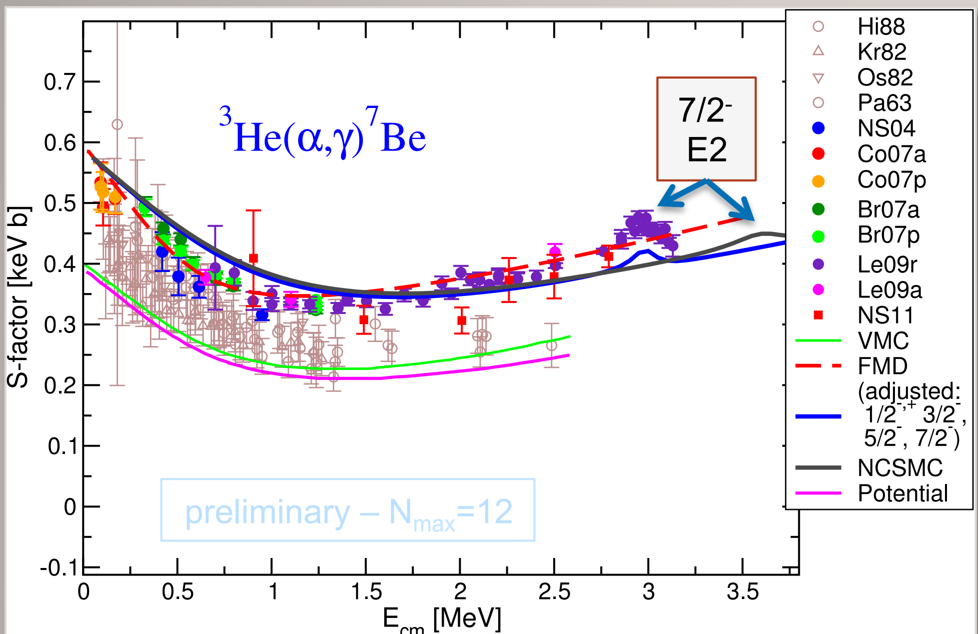
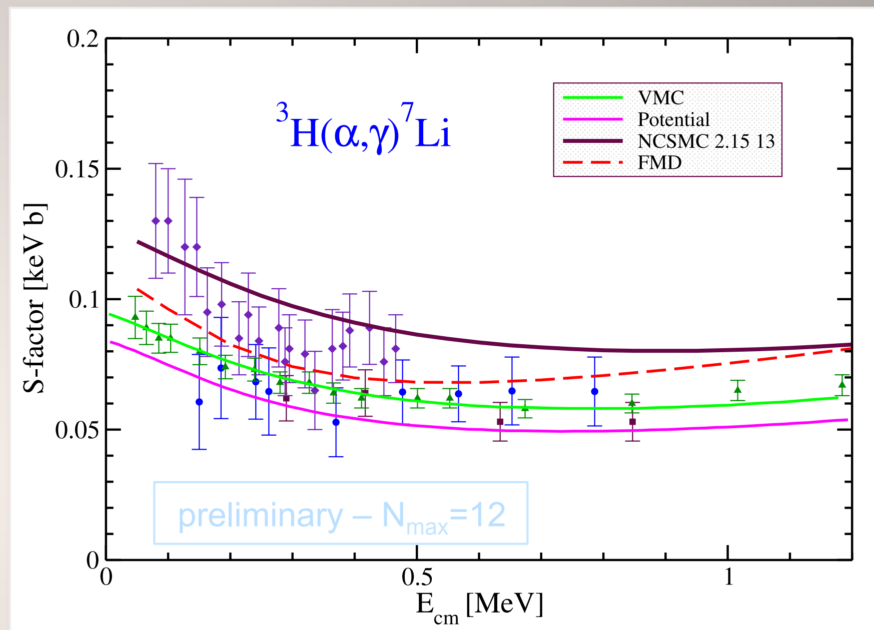


^{3}He-^{4}He and ^{3}H-^{4}He capture

E1 radiative capture with small E2 contribution at $7/2^-$ resonance





In progress

J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi

NCSMC calculations with chiral SRG-N^{3}LO *NN* potential (λ=2.15 fm^{-1})

^{3}He, ^{3}H, ^{4}He ground state, 8(π-) + 6(π+) eigenstates of ^{7}Be and ^{7}Li

Preliminary: N_{max}=12, hΩ=20 MeV

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Conclusions and Outlook

- *Ab initio* calculations of nuclear structure and reactions is a dynamic field with significant advances

- We developed a new unified approach to nuclear bound and unbound states
  - Merging of the NCSM and the NCSM/RGM = **NCSMC**
  - Inclusion of three-nucleon interactions in reaction calculations for *A*>5 systems
  - Extension to three-body clusters (^{6}He ~ ^{4}He+n+n): NCSMC in progress

- Ongoing projects:
  - Transfer reactions
  - Applications to capture reactions important for astrophysics
  - Bremsstrahlung

- Outlook
  - Alpha-clustering (^{4}He projectile)
    - ^{12}C and Hoyle state: ^{8}Be+^{4}He
    - ^{16}O: ^{12}C+^{4}He