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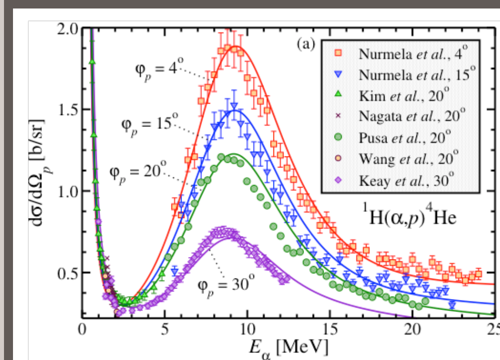
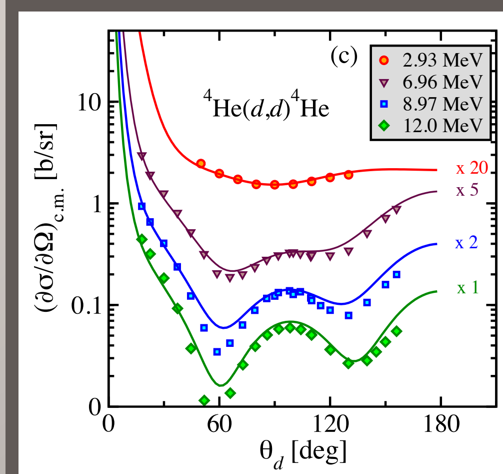
Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

Ab Initio Unified Approach to Nuclear Structure and Reactions





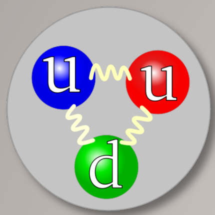
YIPQS Long-term workshop
Computational Advances in Nuclear and Hadron Physics (CANHP 2015)
Yukawa Institute for Theoretical Physics, Kyoto, Japan
October 13, 2015

Petr Navratil | TRIUMF

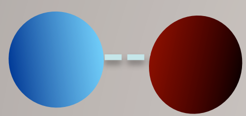
Outline

- NCSMC approach
- Nucleon-^{4}He scattering & ^{3}H(d,n)^{4}He
- Deuteron-^{4}He scattering and ^{6}Li structure
- ^{11}Be as a laboratory for testing of nuclear forces
- ^{3}He-^{4}He and ^{3}H-^{4}He radiative capture
- ^{6}He as ^{4}He-n-n system

From QCD to nuclei

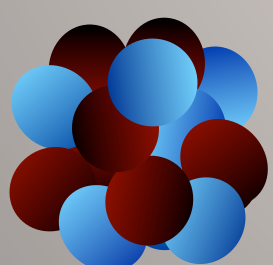


Low-energy QCD



NN+3N interactions from chiral EFT

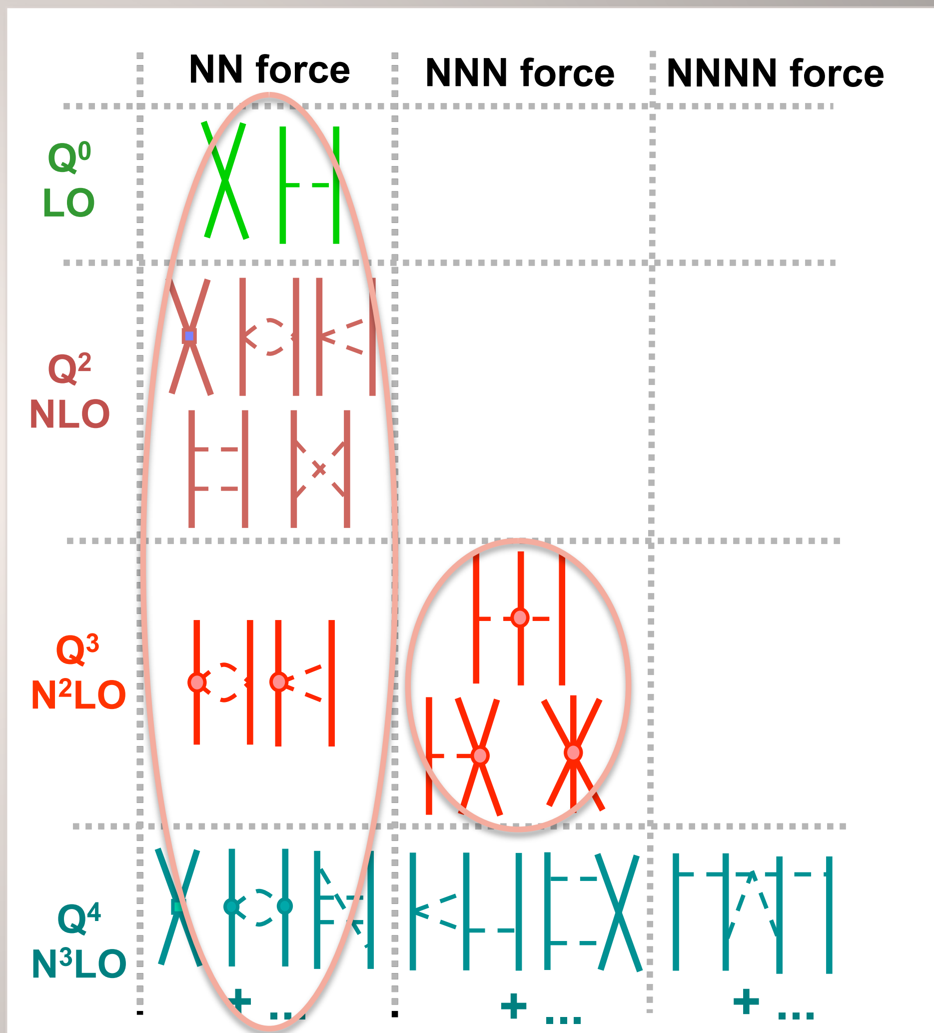
…or accurate meson-exchange potentials



Nuclear structure and reactions

Chiral Effective Field Theory

- 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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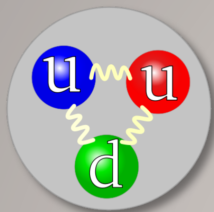
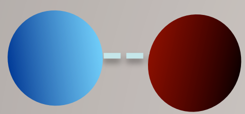
From QCD to nuclei





Low-energy QCD

↓

NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

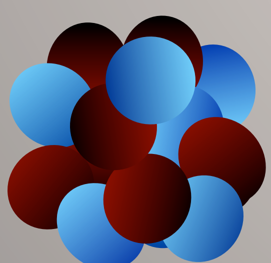
↓

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

Many-Body methods

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

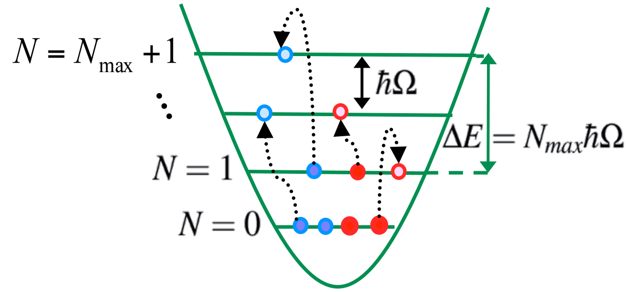
↓



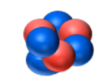
Nuclear structure and reactions

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

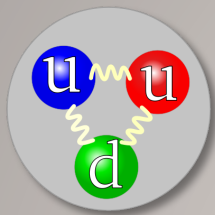


NCSM

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

Unknowns

From QCD to nuclei



Low-energy QCD

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NN+3N interactions from chiral EFT

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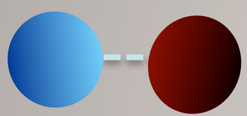

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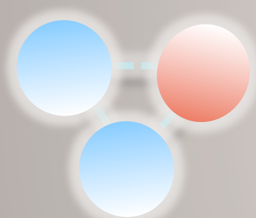
Unitary/similarity transformations

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



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Many-Body methods

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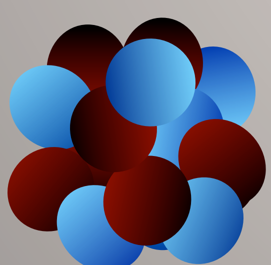
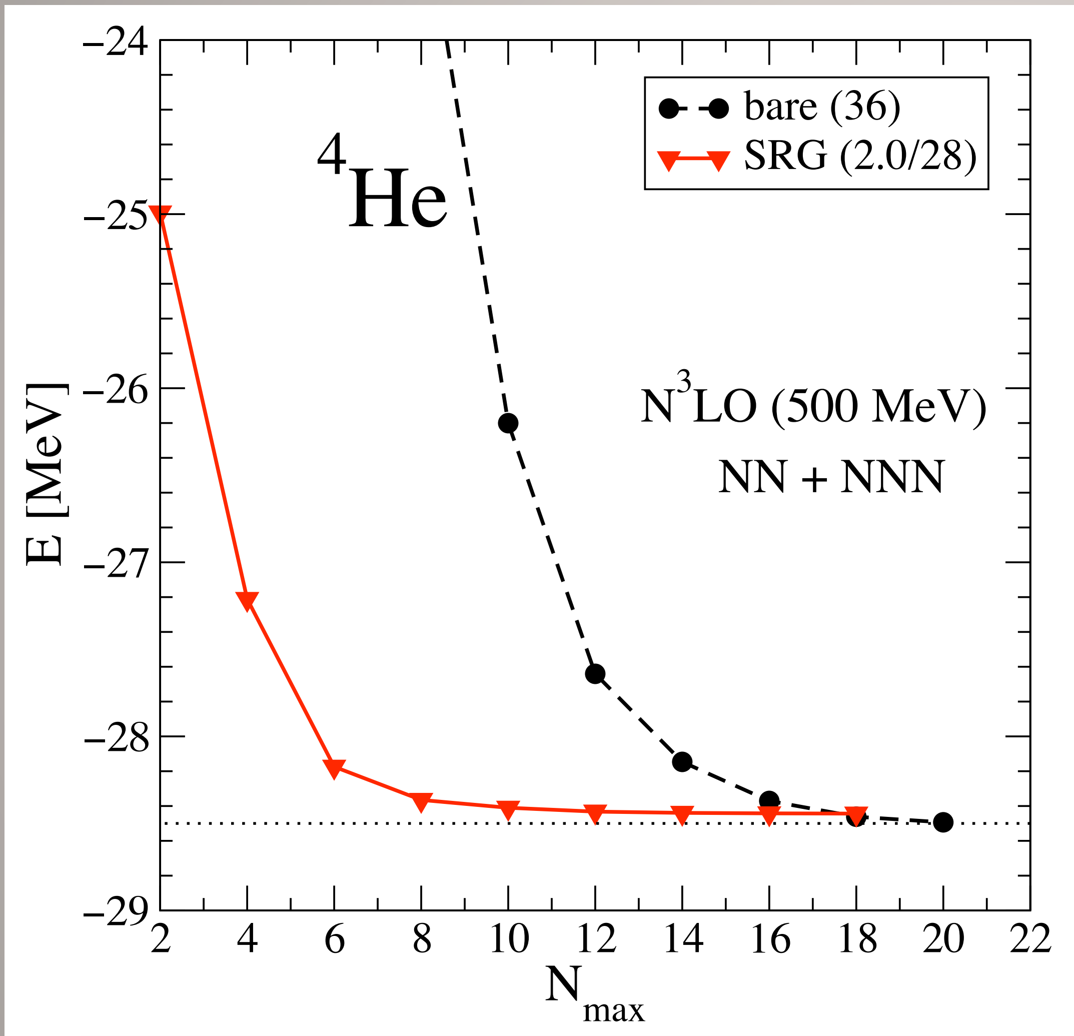
Nuclear structure and reactions



Calculations with chiral 3N: SRG softening needed




PRL **103**, 082501 (2009) PHYSICAL REVIEW LETTERS week ending 21 AUGUST 2009

Evolution of Nuclear Many-Body Forces with the Similarity Renormalization Group

E. D. Jurgenson,[1] P. Navrátil,[2] and R. J. Furnstahl[1]

A=3 binding energy and half life constraint
c_D=-0.2, c_E=-0.205, Λ=500 MeV

Chiral N^{3}LO NN plus N^{2}LO NNN potential

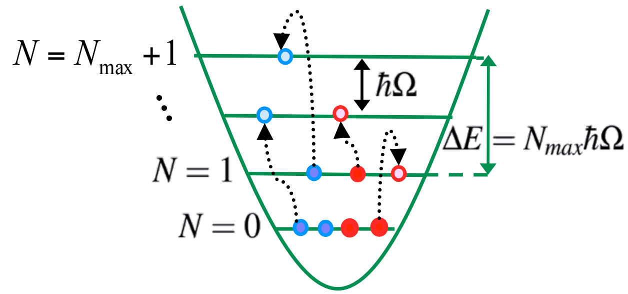
- Bare interaction (black line)
  - Strong short-range correlations
    - Large basis needed
- SRG evolved effective interaction (red line)
  - Unitary transformation

$$H_\alpha = U_\alpha H U_\alpha^+ \Rightarrow \frac{dH_\alpha}{d\alpha} = \left[\left[T, H_\alpha\right], H_\alpha\right] \quad \left(\alpha = 1/\lambda^4\right)$$

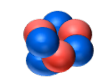
  - Two- plus *three*-body components, *four*-body omitted
  - Softens the interaction
    - Smaller basis sufficient

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



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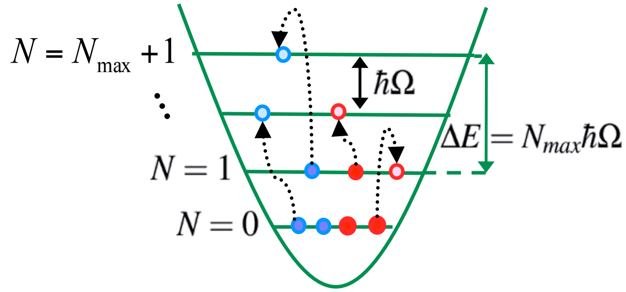

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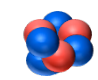
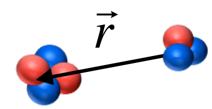


NCSM

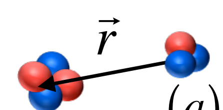
- …with resonating group method
  - Bound & scattering states, reactions
  - Cluster dynamics, long-range correlations



NCSM/RGM

NCSM/RGM channel states

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



Unknowns

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

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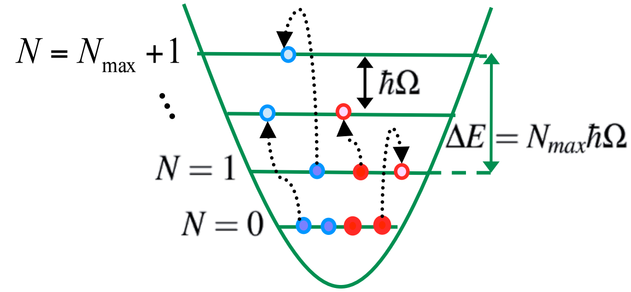
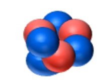


Harmonic oscillator basis



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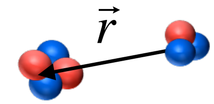


NCSM/RGM

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

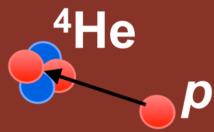
Coupled NCSMC equations

$$E_\lambda^{NCSM}\,\delta_{\lambda\lambda'} \qquad \left\langle (A) \middle| H\,\hat{A}_\nu \middle| (a) \overset{r}{\longrightarrow} (A-a) \right\rangle \qquad \delta_{\lambda\lambda'} \qquad \left\langle (A) \middle| \hat{A}_\nu \middle| (a) \overset{r}{\longrightarrow} (A-a) \right\rangle$$

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

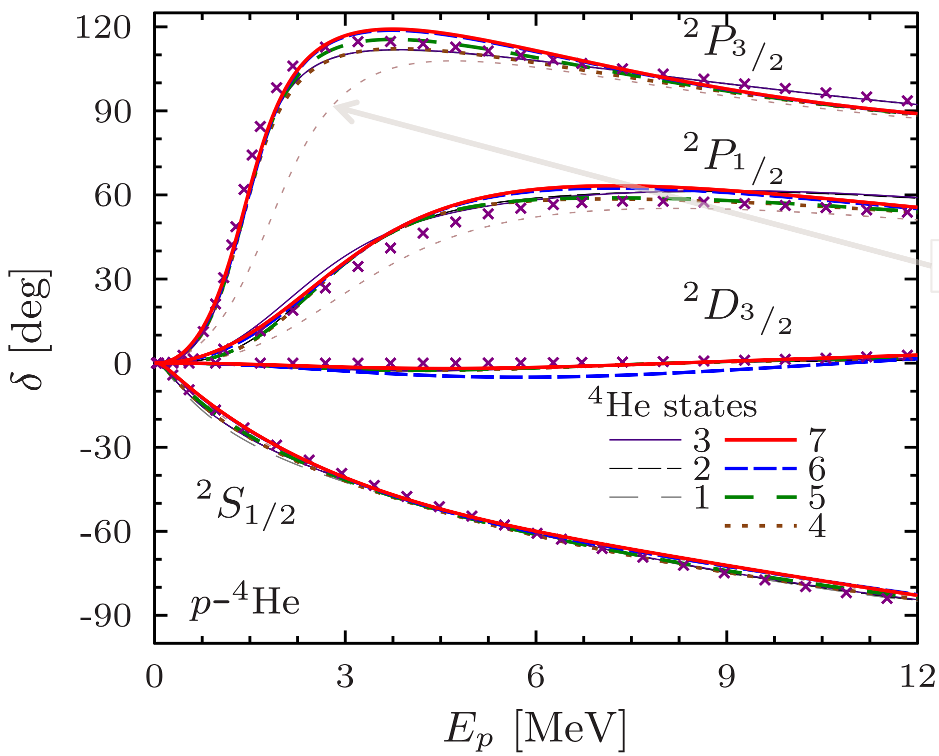
$$\left\langle (A-a) \overset{r'}{\longleftarrow} (a) \middle| \hat{A}_{\nu'}\,H\,\hat{A}_\nu \middle| (a) \overset{r}{\longrightarrow} (A-a) \right\rangle \qquad \left\langle (A-a) \overset{r'}{\longleftarrow} (a) \middle| \hat{A}_{\nu'}\,\hat{A}_\nu \middle| (a) \overset{r}{\longrightarrow} (A-a) \right\rangle$$

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

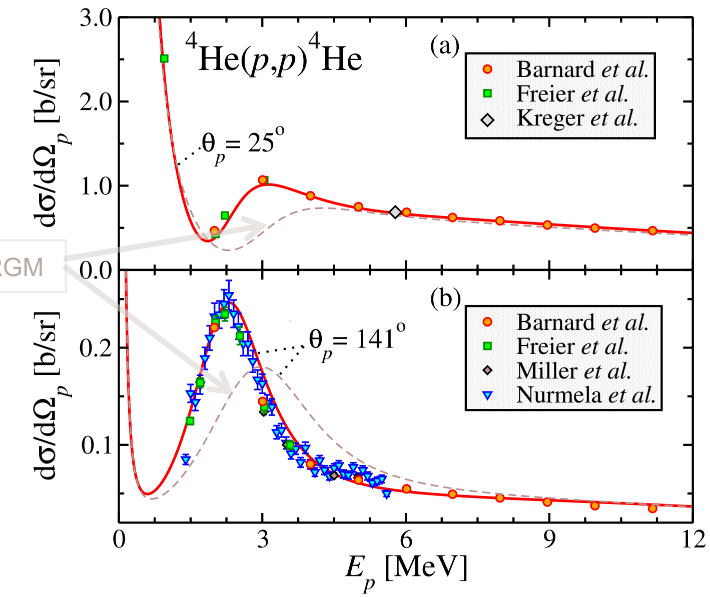


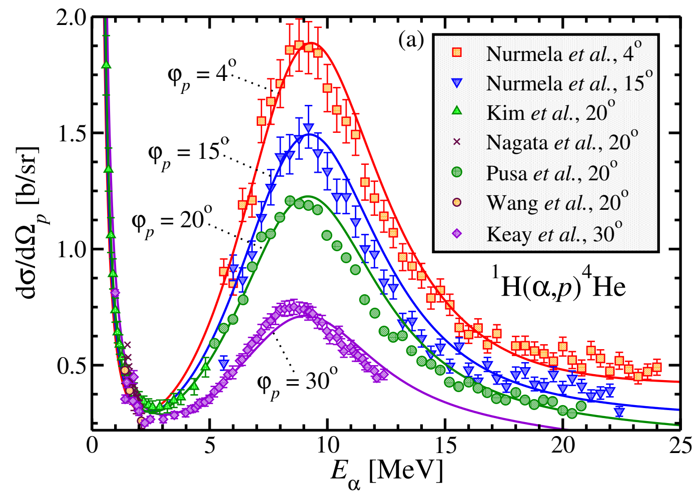
p-^{4}He scattering within NCSMC

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,‡]

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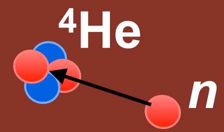
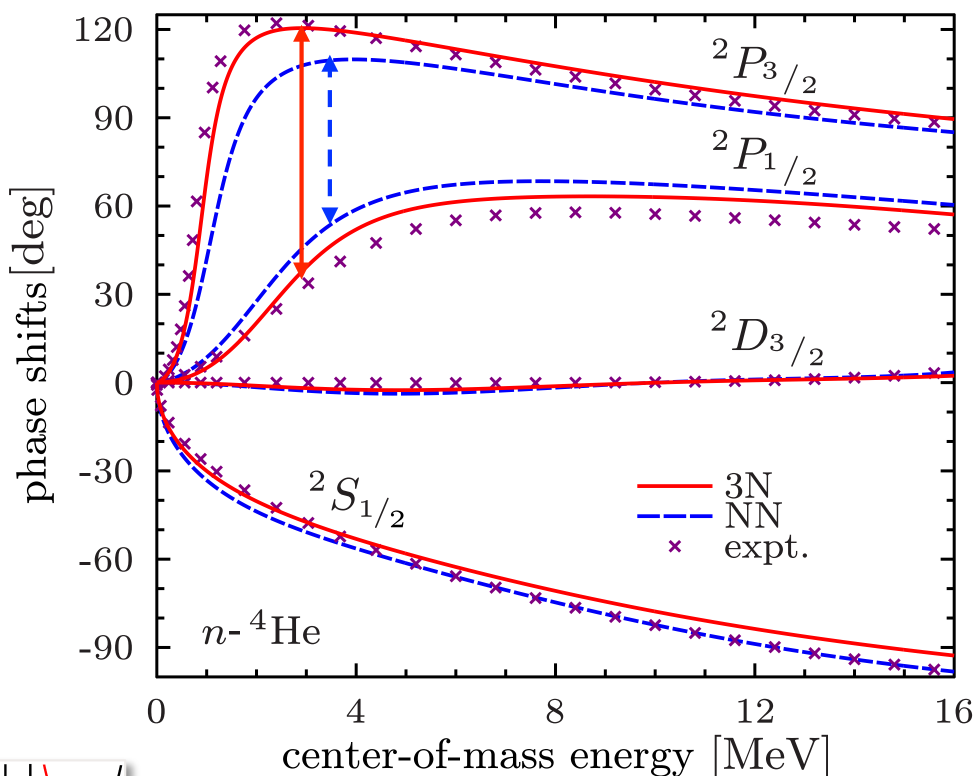
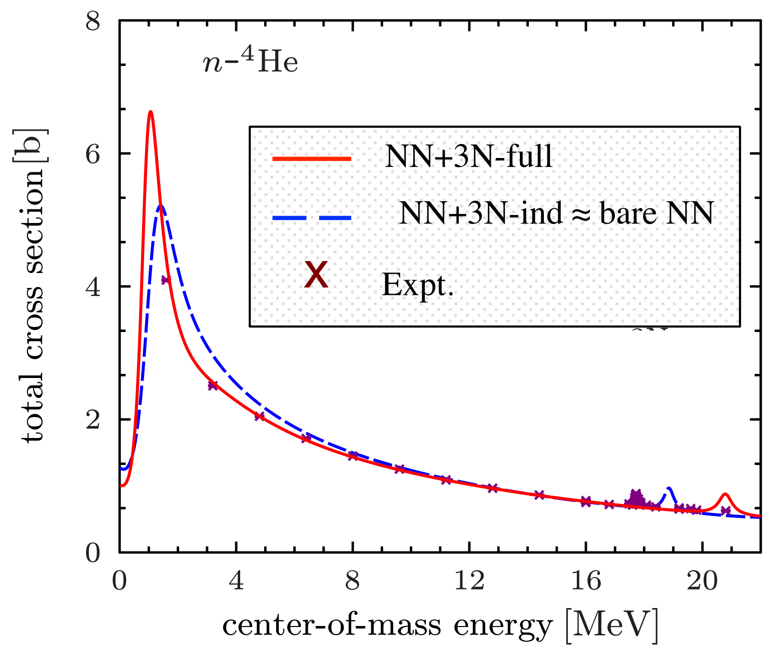


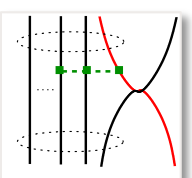
n-^{4}He scattering within NCSMC

n-^{4}He scattering phase-shifts for chiral NN and NN+3N potential

Total n-^{4}He cross section with NN and NN+3N potentials







3N force enhances 1/2$^-$ ←→ 3/2$^-$ splitting: Essential at low energies!

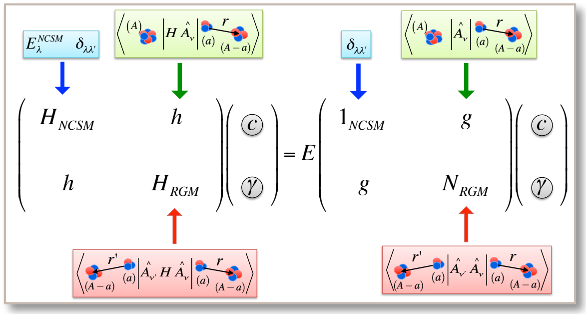
G. Hupin, S. Quaglioni and P. Navrátil

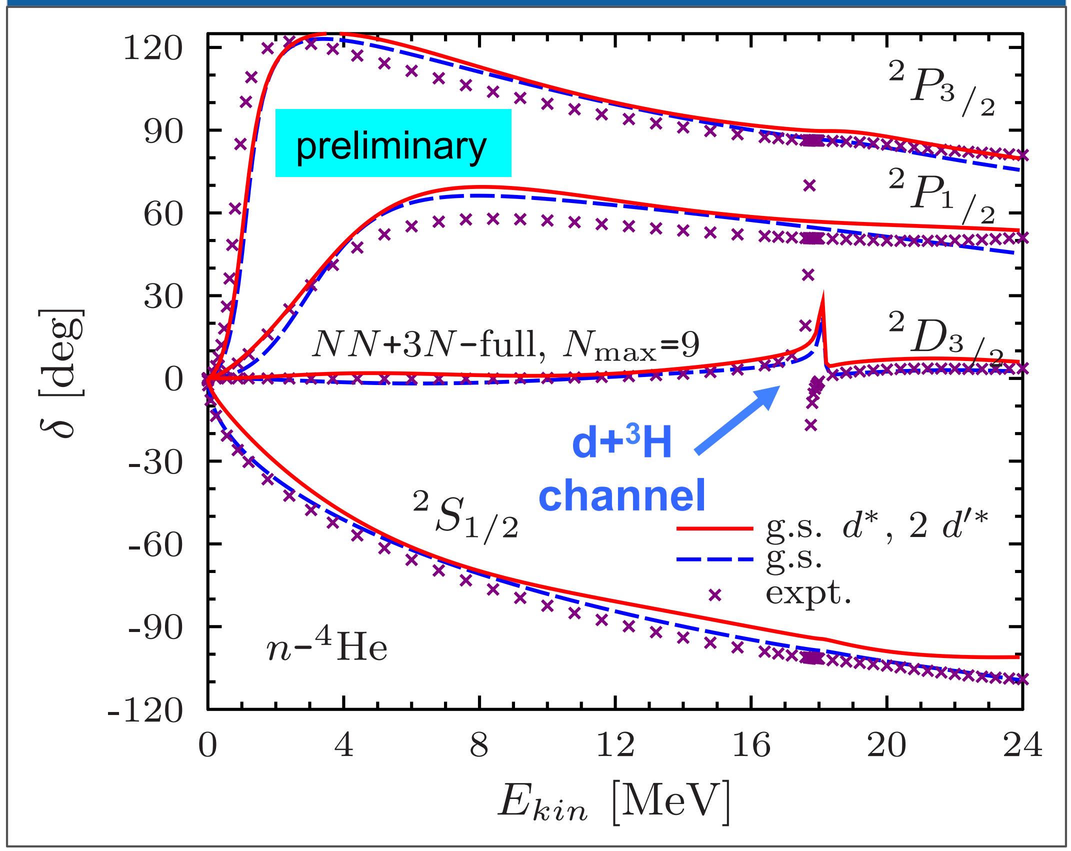
PHYSICAL REVIEW C **88**, 054622 (2013)

Ab initio **many-body calculations of nucleon-^{4}He scattering with three-nucleon forces**

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

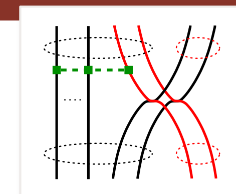
$^3H(d,n)^4He$ fusion with chiral NN+3N





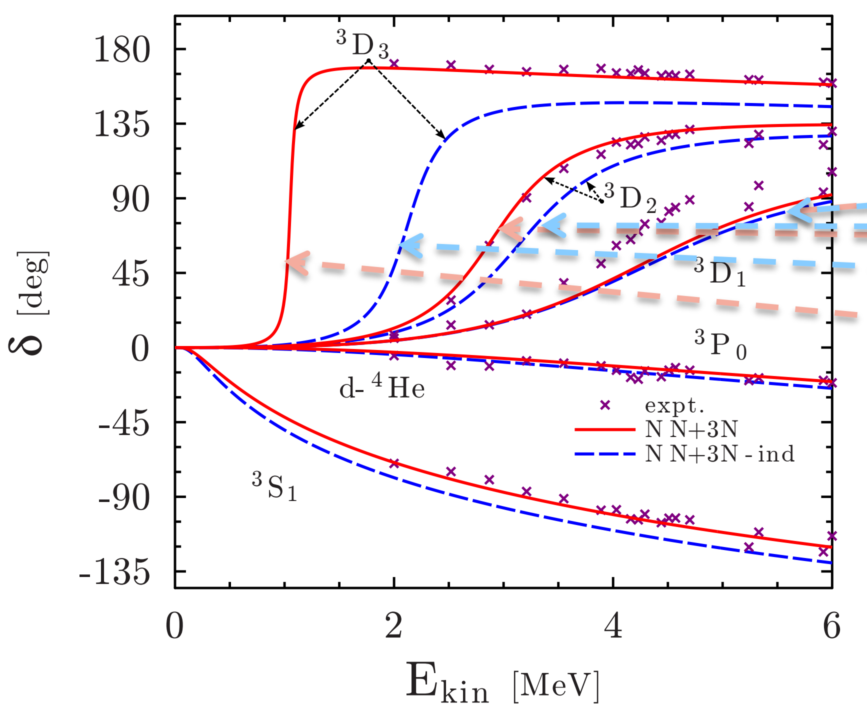
- Towards first ab initio calculation of $^3H(d,n)^4He$ fusion with 3N forces
  - N_{max} = 9 model space
  - n+^{4}He & d+^{3}H continuum channels
  - Up to 14 ^{5}He states
  - Only g.s. of ^{4}He and ^{3}H: effect of target excitation described by ^{5}He states
  - 3-body dynamics approximated above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

Unified description of ^{6}Li structure and d+^{4}He dynamics

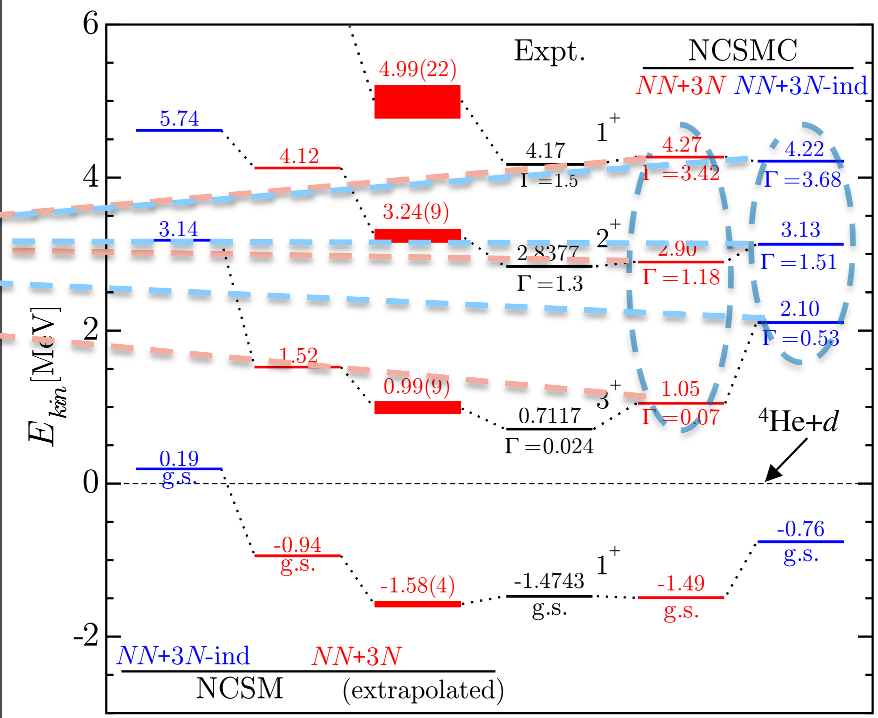


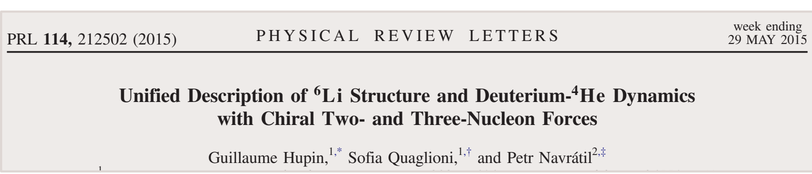
- Continuum and three-nucleon force effects on d+^{4}He and ^{6}Li

d+^{4}He Scattering Phase Shifts



^{6}Li vs. (^{4}He+d)+^{6}Li calculation



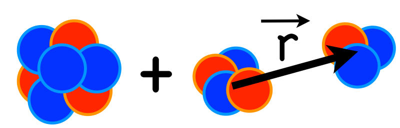


PRL 114, 212502 (2015) PHYSICAL REVIEW LETTERS week ending 29 MAY 2015

Unified Description of ^{6}Li Structure and Deuterium-^{4}He Dynamics with Chiral Two- and Three-Nucleon Forces

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

NCSMC



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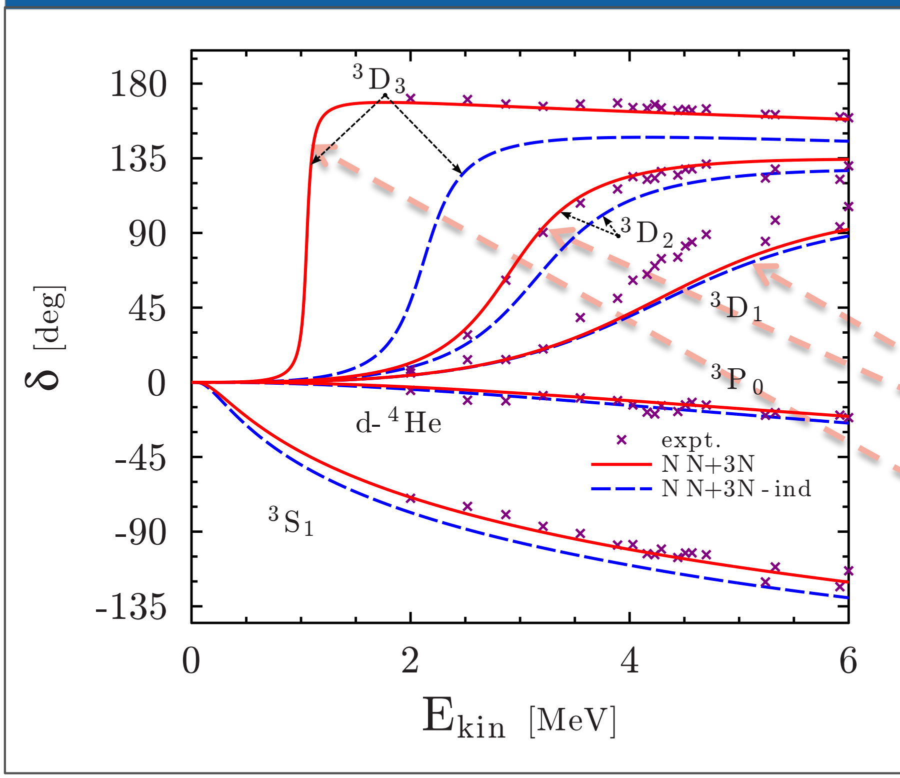

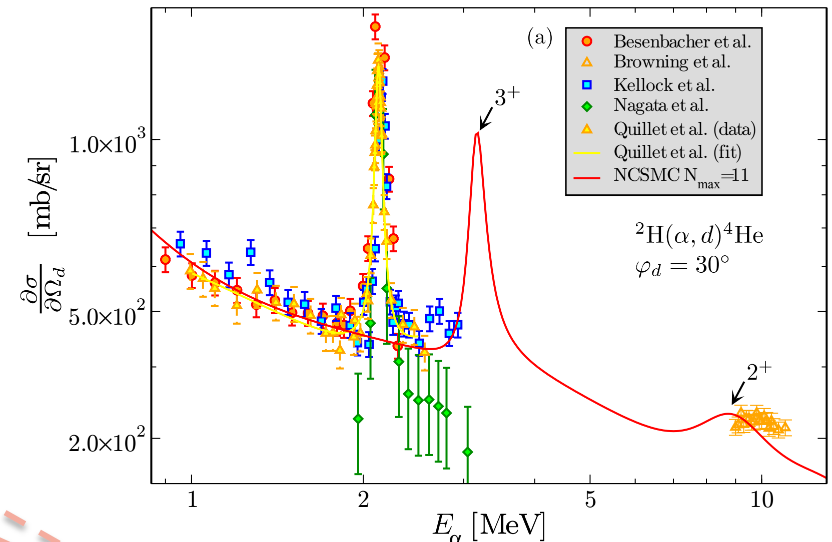

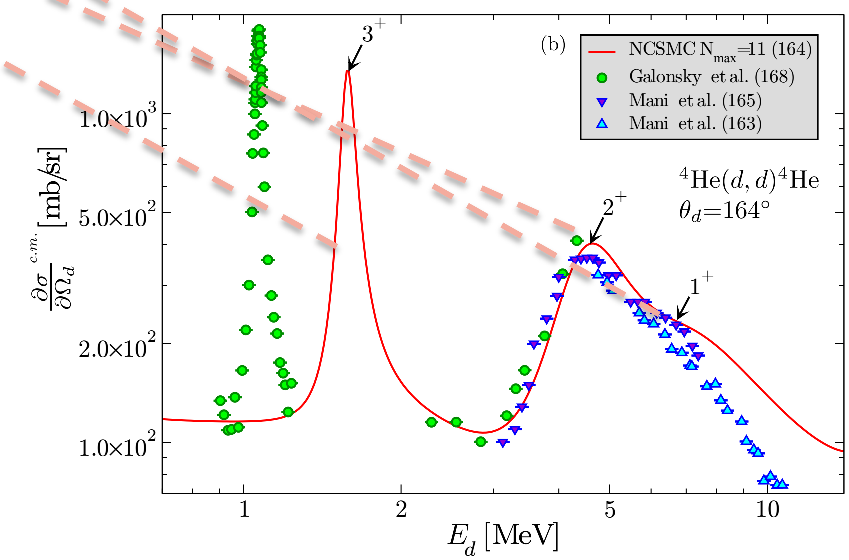

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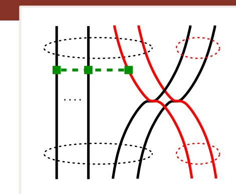

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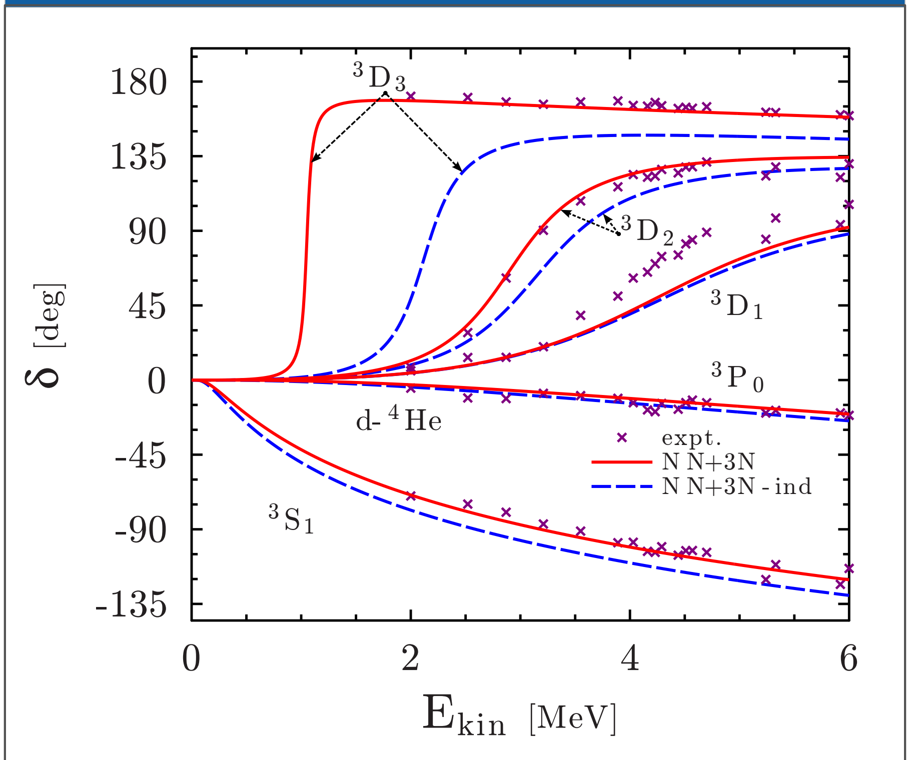

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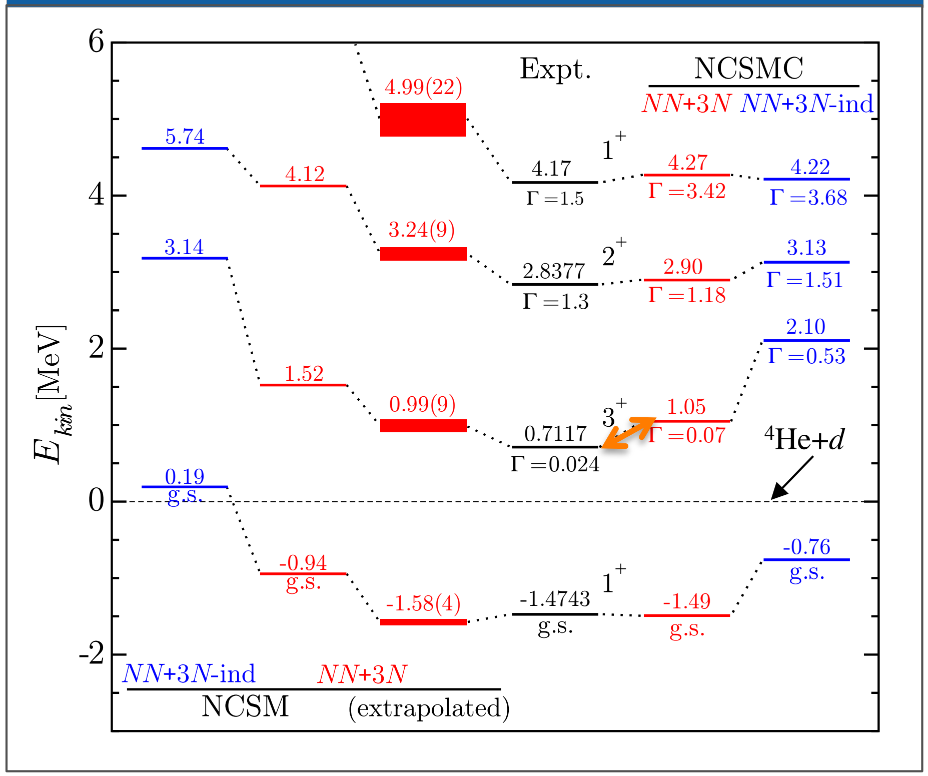

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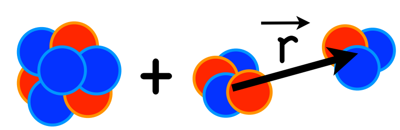
NCSMC



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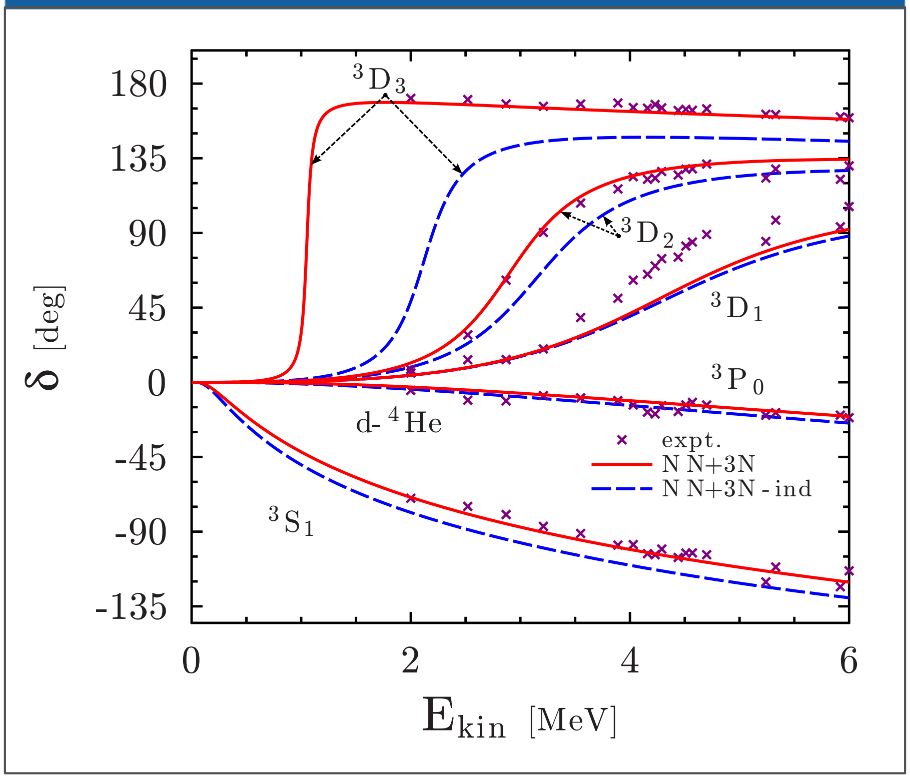

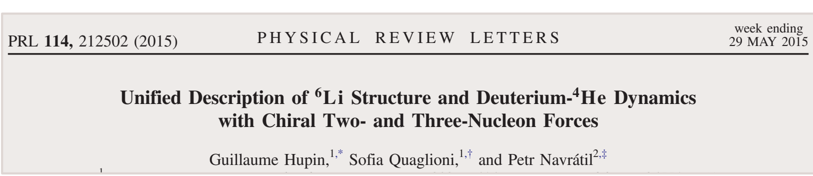
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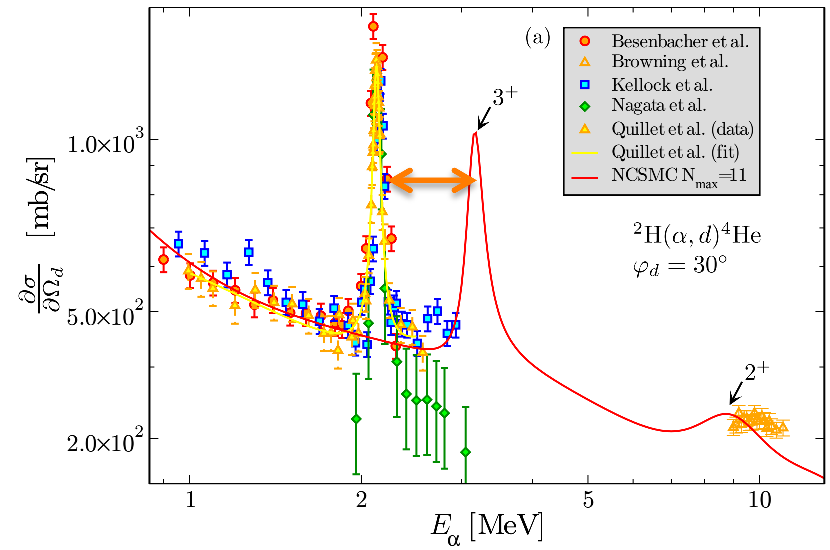
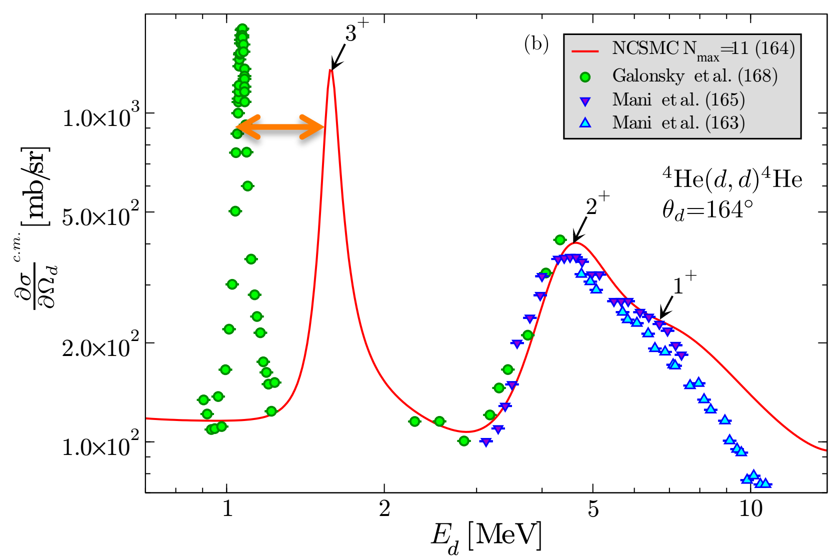
Unified Description of ^{6}Li Structure and Deuterium-^{4}He Dynamics with Chiral Two- and Three-Nucleon Forces

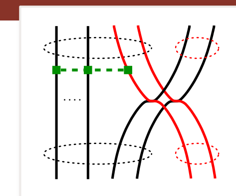
Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]



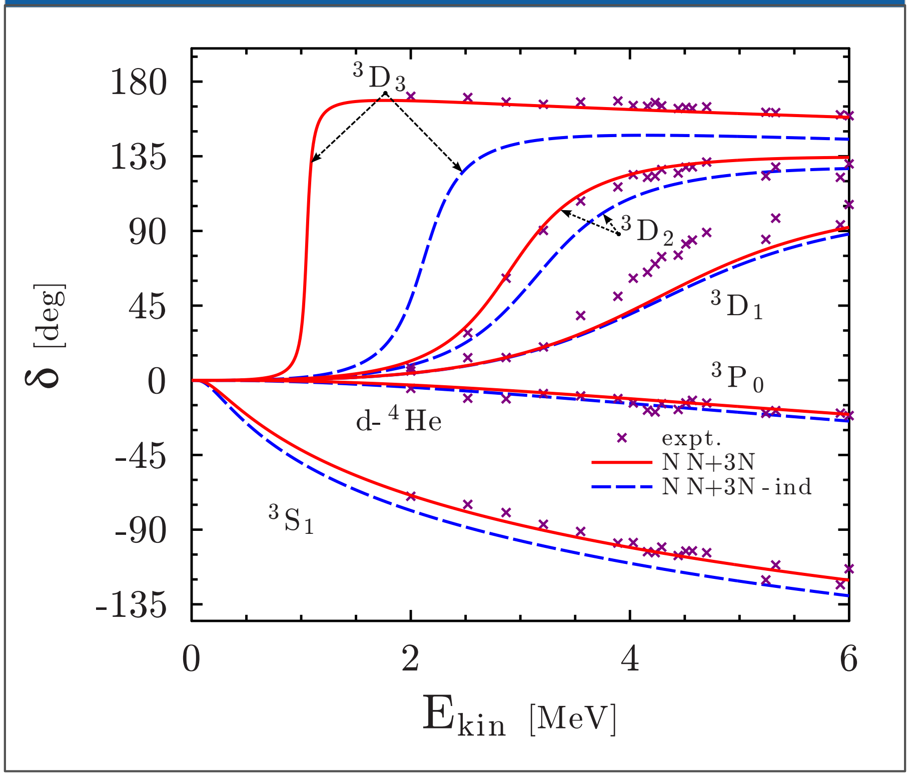


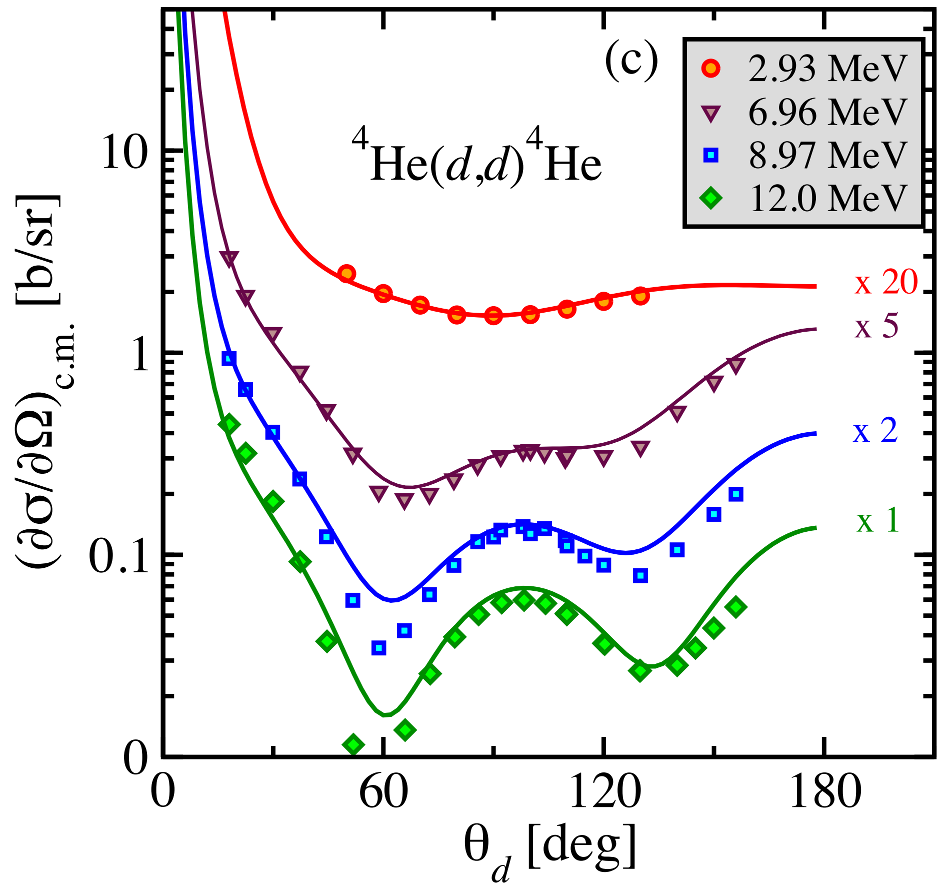
Unified description of ^{6}Li structure and d+^{4}He dynamics

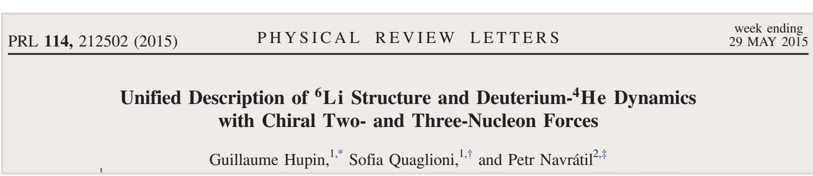
- Continuum and three-nucleon force effects on d+^{4}He and ^{6}Li



d+^{4}He Scattering Phase Shifts





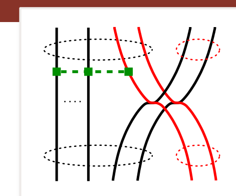

PRL 114, 212502 (2015) PHYSICAL REVIEW LETTERS week ending 29 MAY 2015

Unified Description of ^{6}Li Structure and Deuterium-^{4}He Dynamics with Chiral Two- and Three-Nucleon Forces

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

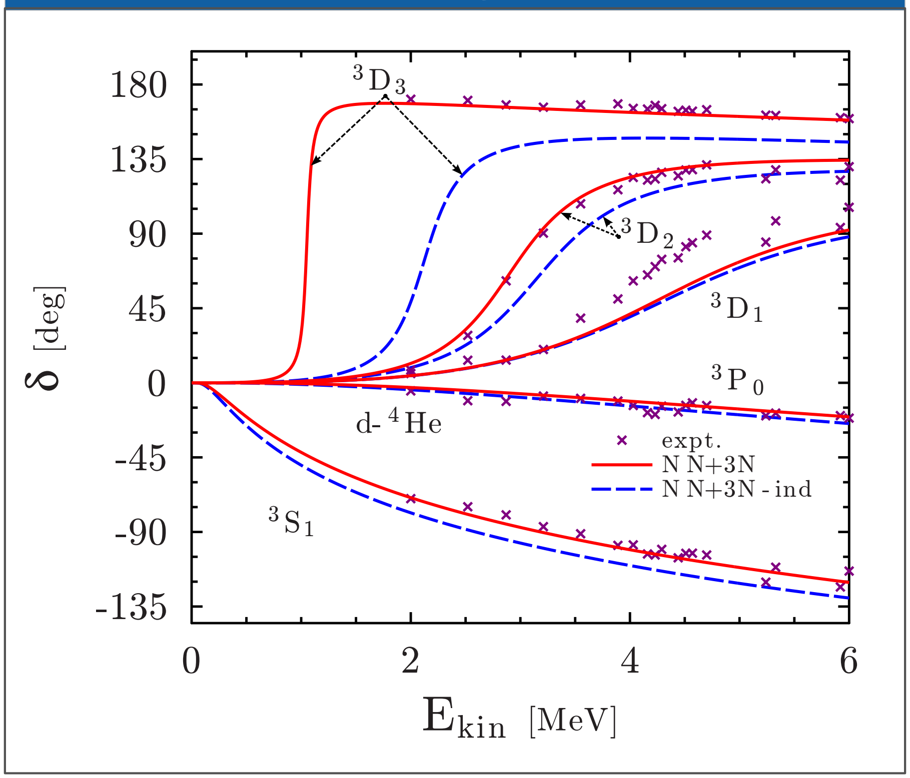
TRIUMF

Unified description of ^{6}Li structure and d+^{4}He dynamics



- *S*- and *D*-wave asymptotic normalization constants

d+^{4}He Scattering Phase Shifts

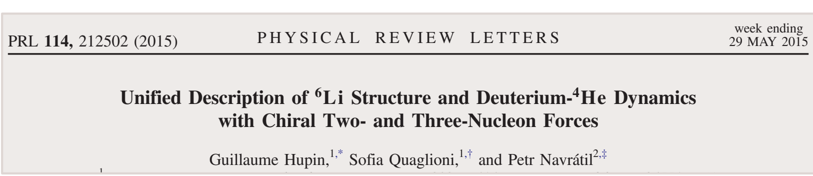


	NCSMC	Experiment			
C_0 [fm$^{-1/2}$]	2.695	2.91(9)	[39]	2.93(15)	[38]
C_2 [fm$^{-1/2}$]	−0.074	−0.077(18)	[39]		
C_2/C_0	−0.027	−0.025(6)(10)	[39]	0.0003(9)	[41]

[38] L. D. Blokhintsev, V. I. Kukulin, A. A. Sakharuk, D. A. Savin, and E. V. Kuznetsova, Phys. Rev. C **48**, 2390 (1993).

[39] E. A. George and L. D. Knutson, Phys. Rev. C **59**, 598 (1999).

[41] K. D. Veal, C. R. Brune, W. H. Geist, H. J. Karwowski, E. J. Ludwig, A. J. Mendez, E. E. Bartosz, P. D. Cathers, T. L. Drummer, K. W. Kemper, A. M. Eiró, F. D. Santos, B. Kozlowska, H. J. Maier, and I. J. Thompson, Phys. Rev. Lett. **81**, 1187 (1998).

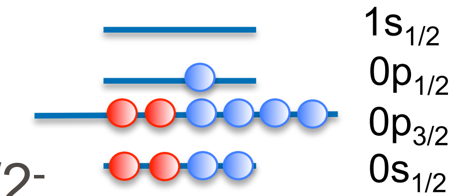


PRL **114,** 212502 (2015) PHYSICAL REVIEW LETTERS week ending 29 MAY 2015

Unified Description of ^{6}Li Structure and Deuterium-^{4}He Dynamics with Chiral Two- and Three-Nucleon Forces

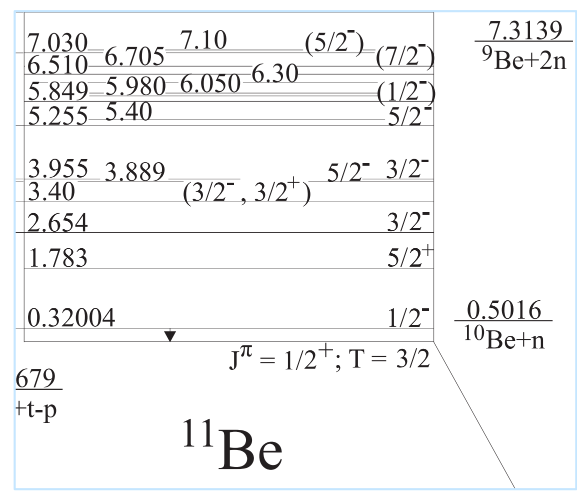
Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

Neutron-rich halo nucleus ^{11}Be



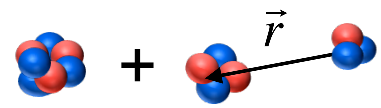
- Z=4, N=7
  - In the shell model picture g.s. expected to be $J^\pi=1/2^-$
    - Z=6, N=7 ^{13}C and Z=8, N=7 ^{15}O have $J^\pi=1/2^-$ g.s.
  - In reality, ^{11}Be g.s. is **$J^\pi=1/2^+$** - parity inversion
  - Very weakly bound: E_{th}=-0.5 MeV
    - Halo state – dominated by ^{10}Be-n in the *S*-wave
  - The $1/2^-$ state also bound – only by 180 keV

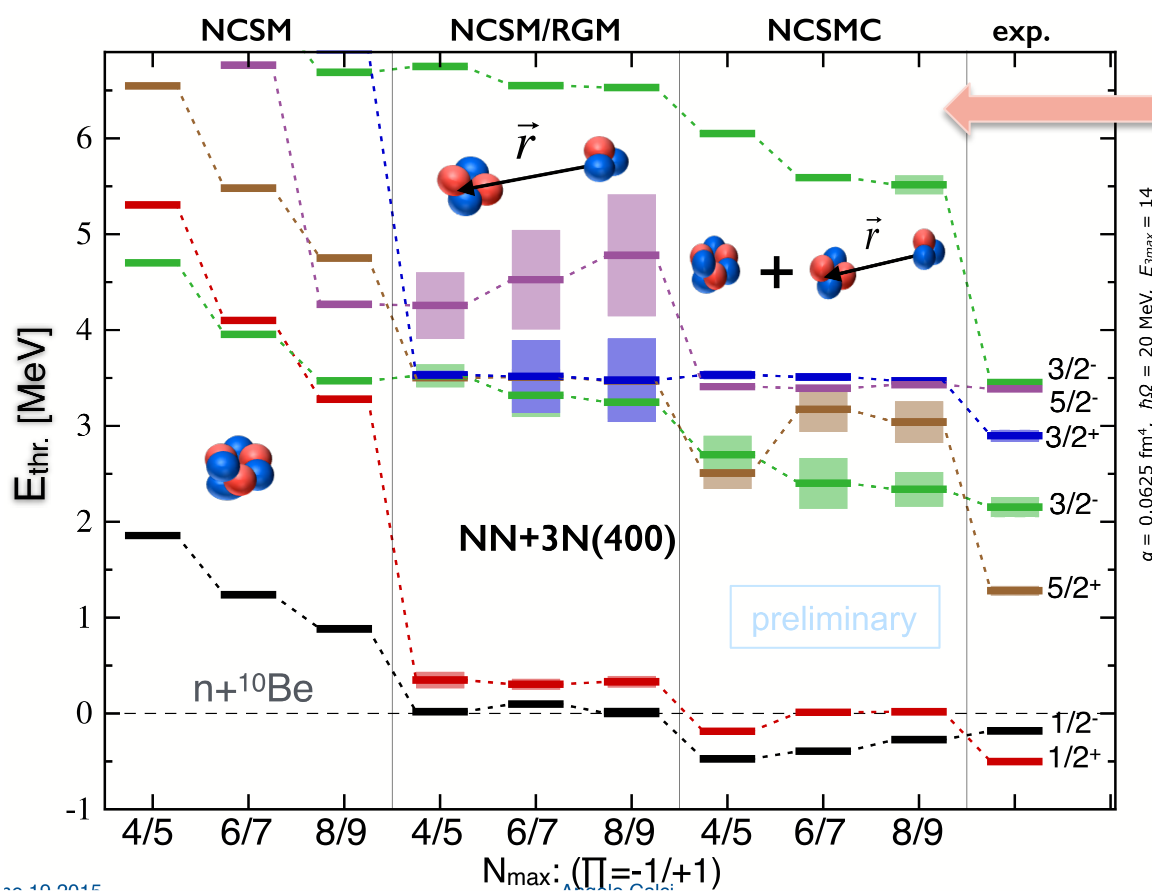
- Can we describe ^{11}Be in *ab initio* calculations?
  - Continuum must be included
  - Does the 3N interaction play a role in the parity inversion?



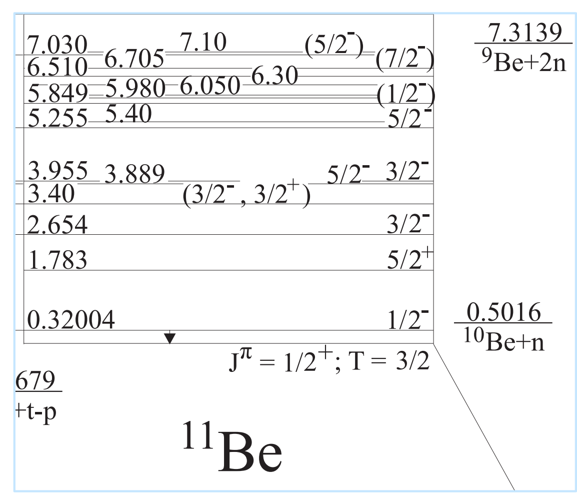
Structure of ^{11}Be from chiral NN+3N forces

- NCSMC calculations **including chiral 3N** (N^3LO NN+N^2LO 3NF400)
  - n-^{10}Be + ^{11}Be
    - ^{10}Be: 0^+, 2^+, 2^+ NCSM eigenstates
    - ^{11}Be: ≥6 π = -1 and ≥3 π = +1 NCSM eigenstates



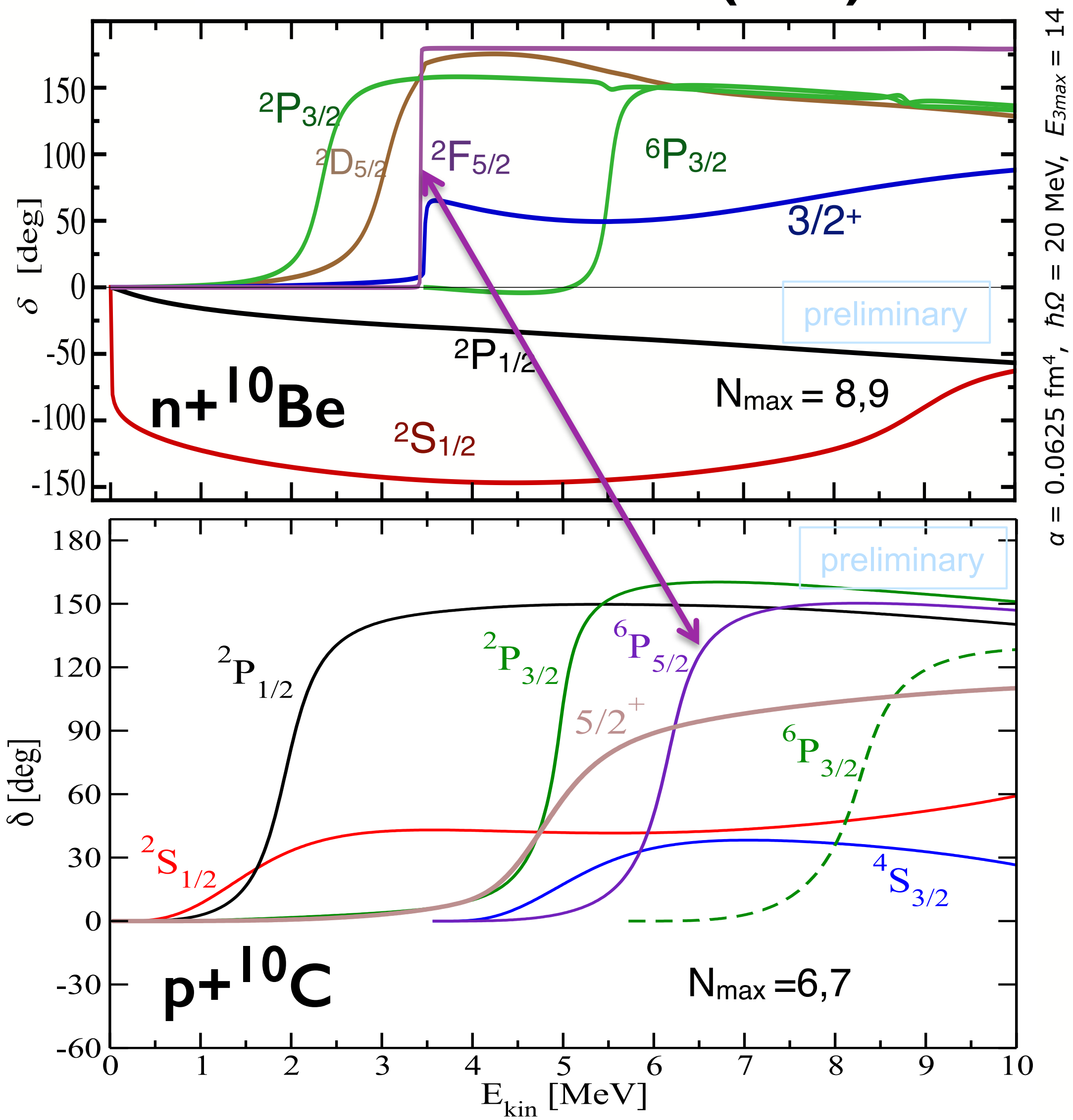


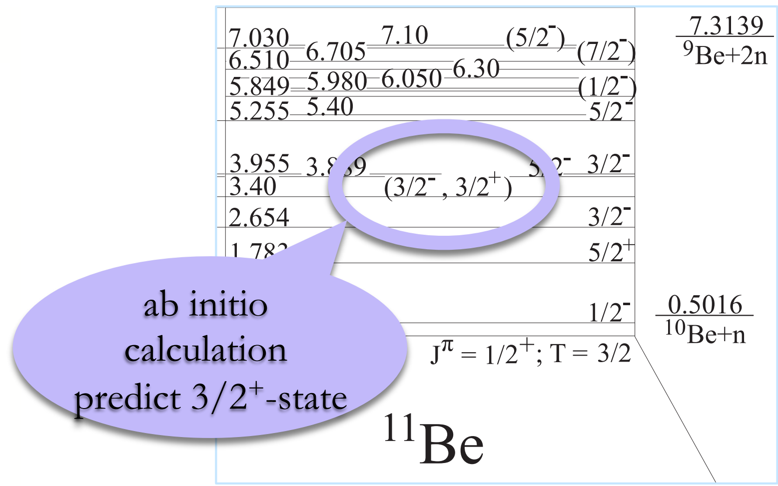
Continuum effects

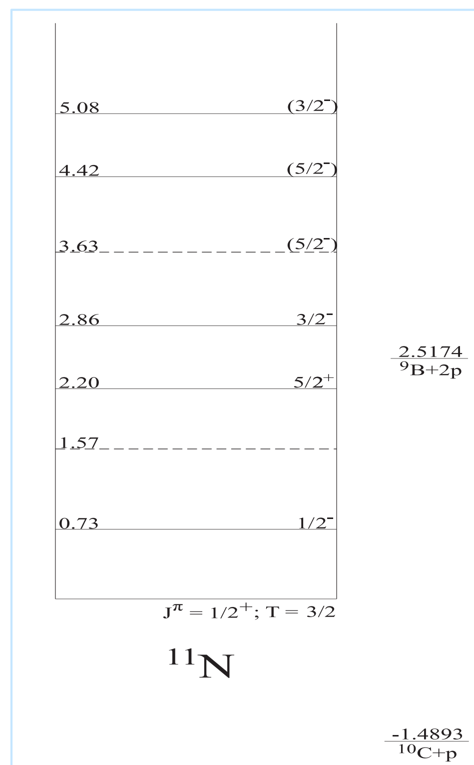


Mirror nuclei ^{11}Be and ^{11}N

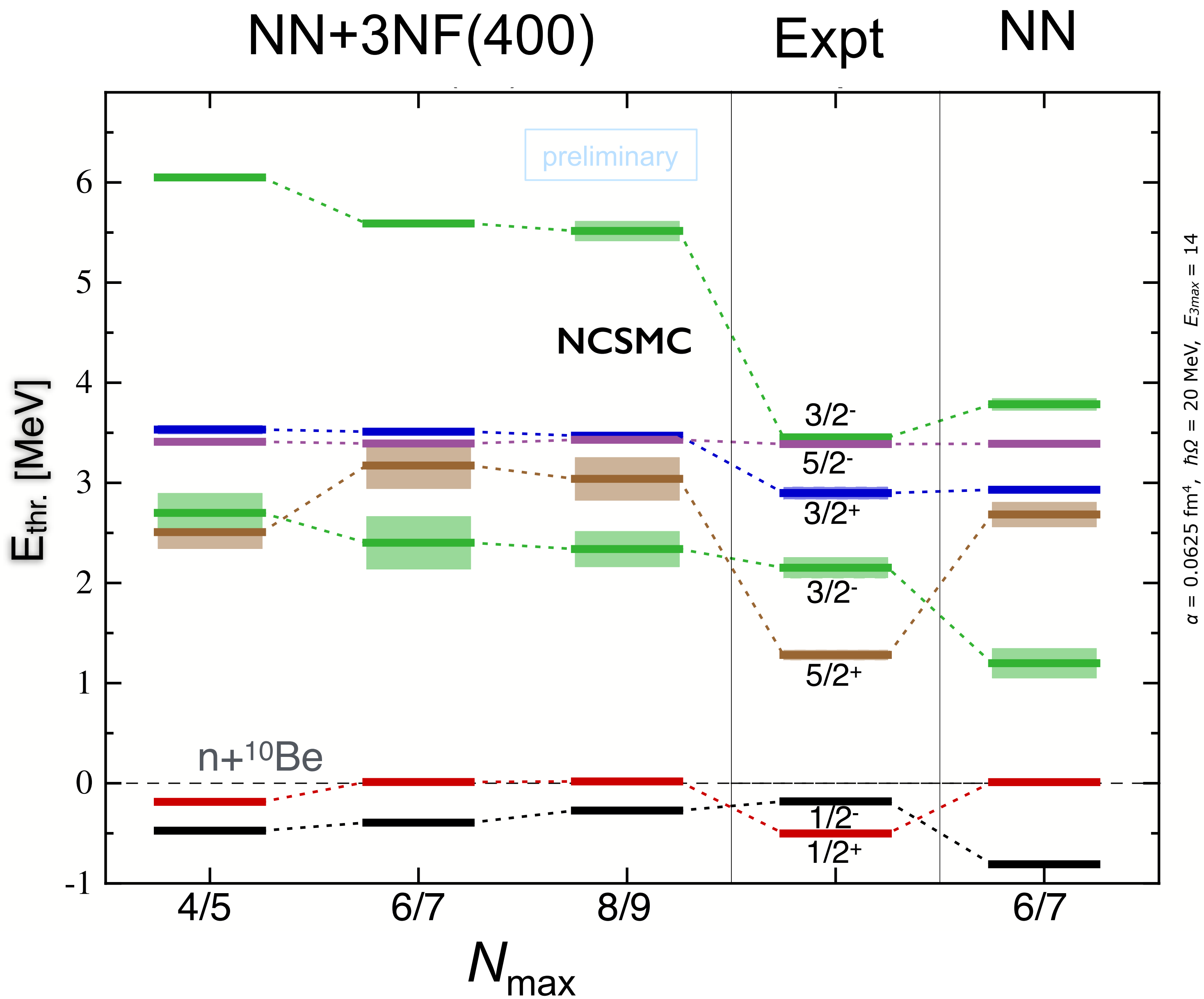
NN+3N(400)







Effects of 3N force in ^{11}Be



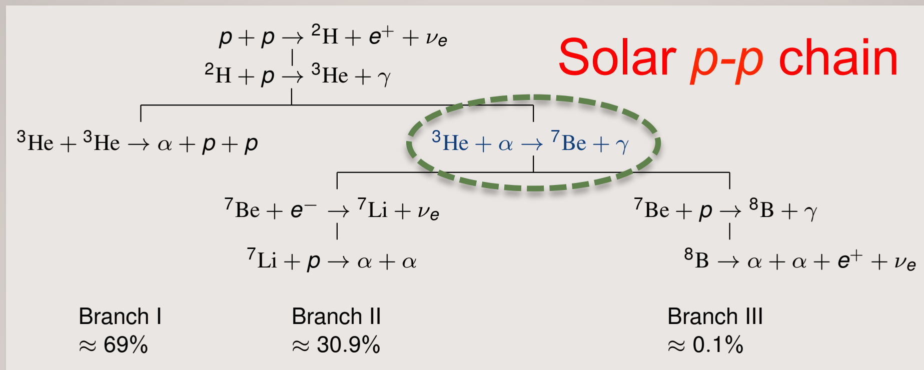
Much better agreement with experiment when 3N force included.

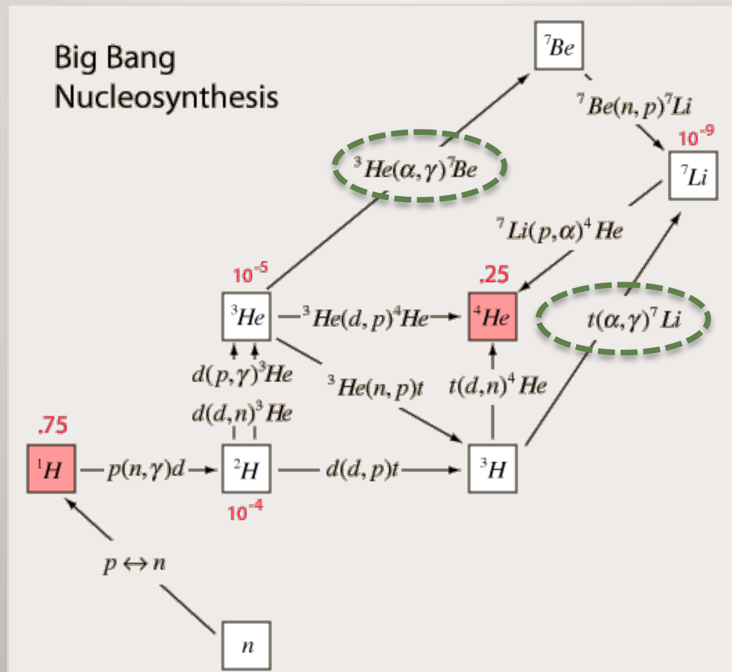
Parity inversion not reproduced.

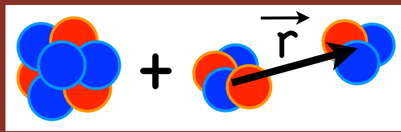
(More excited NCSM states?)

Other NN+3N?

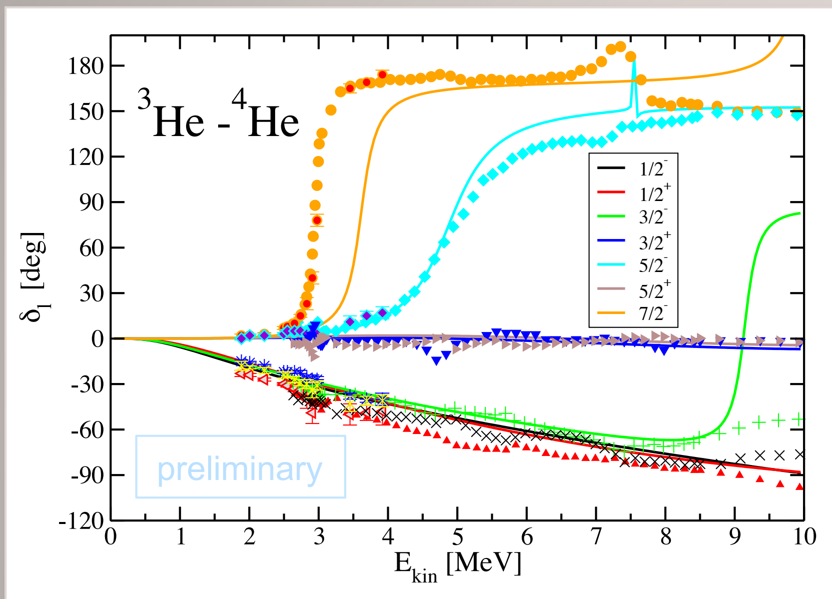
Capture reactions important for astrophysics







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



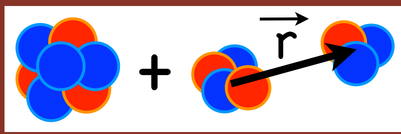
	^{7}Be		^{7}Li	
	NCSMC	Expt.	NCSMC	Expt.
$E_{3/2^-}$ [MeV]	-1.52	-1.586	-2.43	-2.467
$E_{1/2^-}$ [MeV]	-1.26	-1.157	-2.15	-1.989
r_{ch} [fm]	2.62	2.647(17)	2.42	2.390(30)
Q [e fm^2]	-6.14		-3.72	-4.00(3)
μ [μ_N]	-1.16	-1.3995(5)	+3.02	+3.256

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

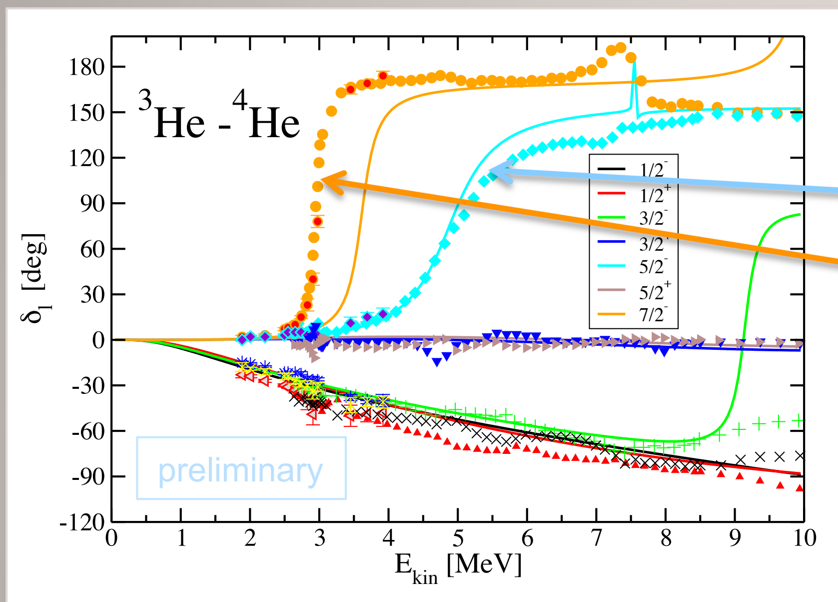
^{3}He, ^{3}H, ^{4}He ground state, 8(π-) + 6(π+) eigenstates of ^{7}Be and ^{7}Li

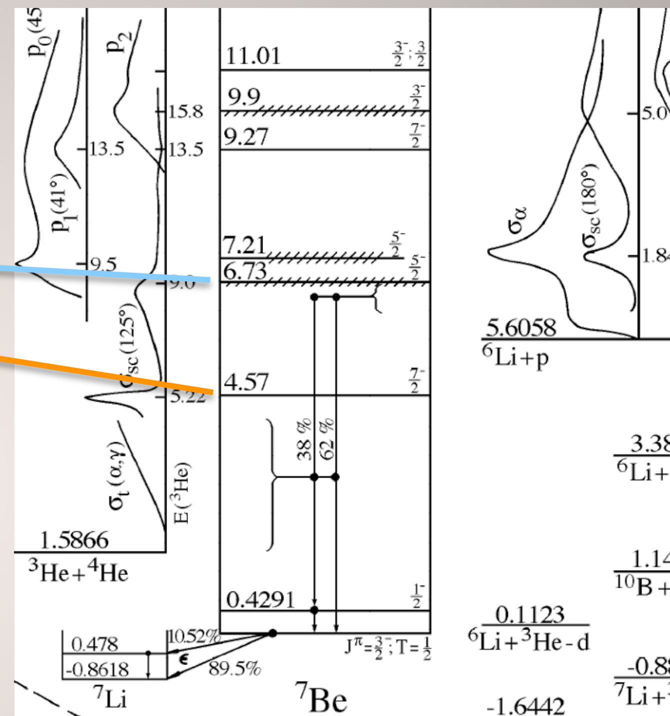
Preliminary: N_{max}=12, hΩ=20 MeV

TRIUMF



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





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

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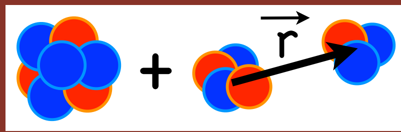
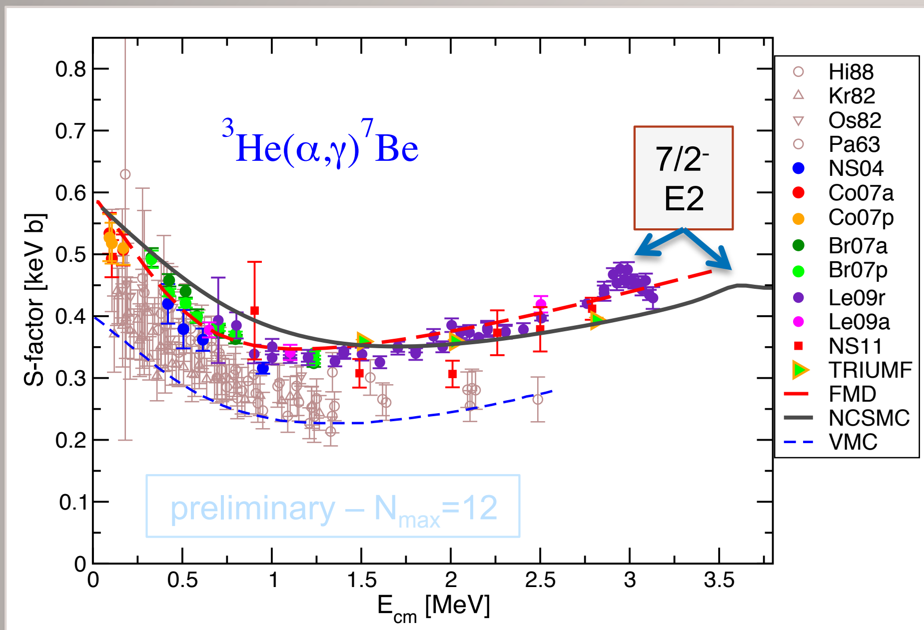
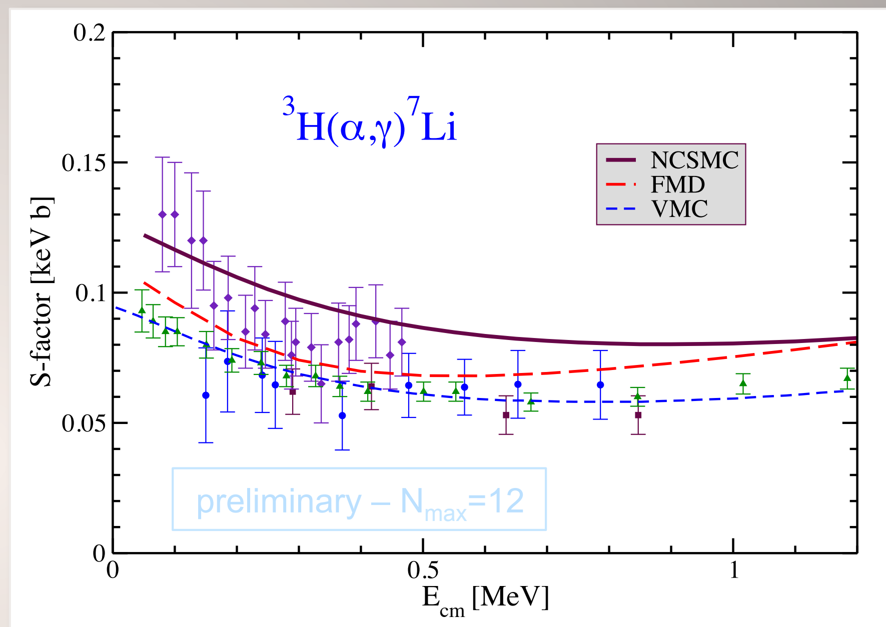
TRIUMF



^{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

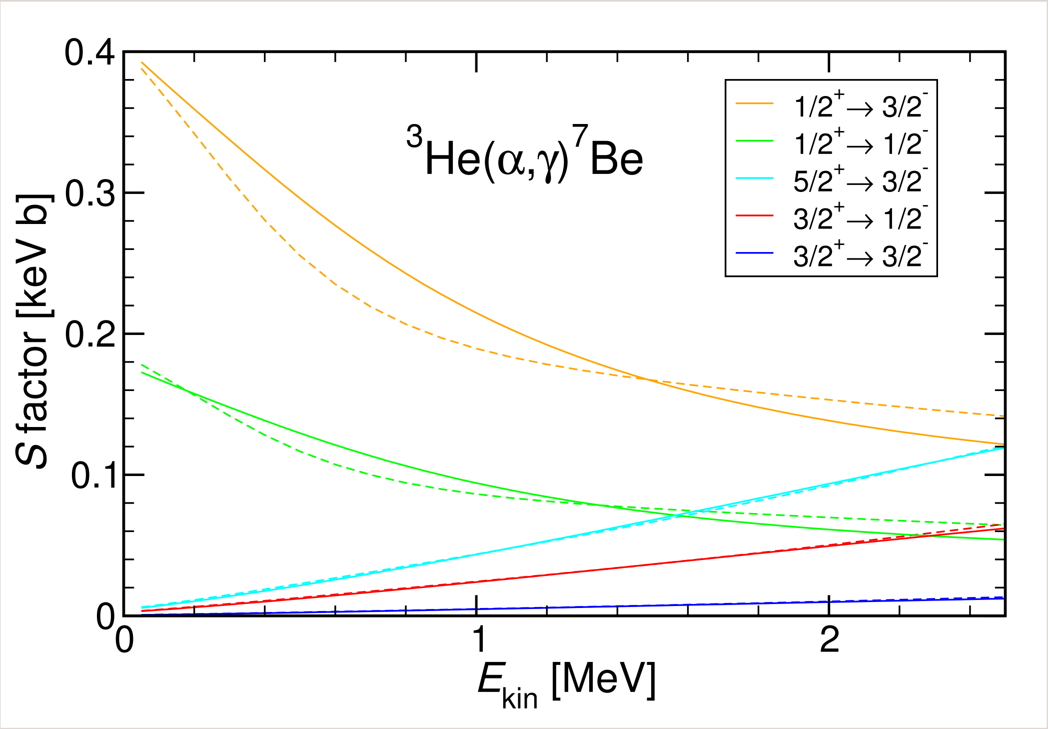
Preliminary: N_{max}=12, ħΩ=20 MeV

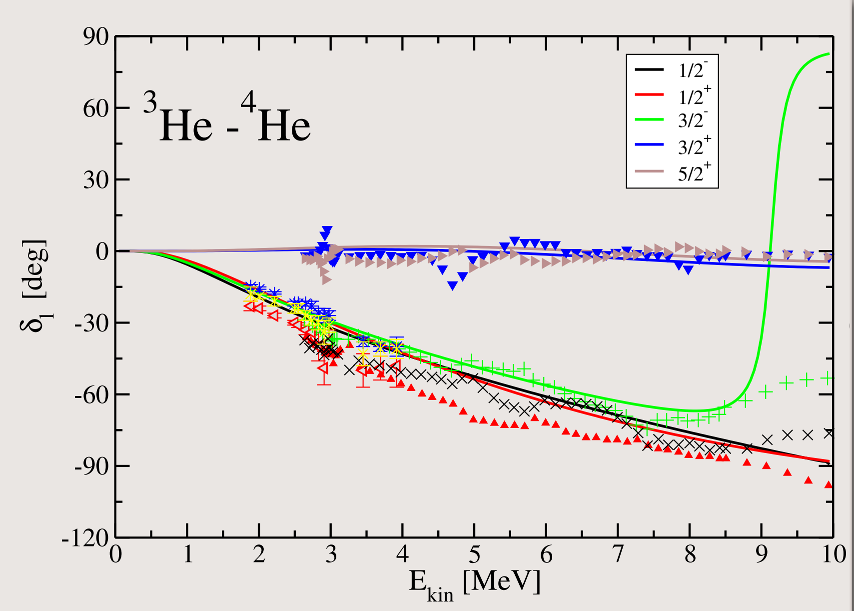
Theoretical calculations suggest that the most recent and precise ^{7}Be and ^{7}Li data are inconsistent

TRIUMF

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

- Comparison of the NCSMC and the FMD results





Differences in the S-wave contributions

NCSMC: 1/2$^+$ phase shift underestimated
Soft NN potential -> 3N needs to be included
Impact of N_{max} truncation

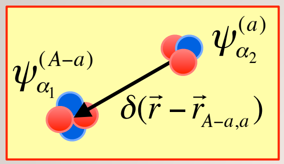
TRIUMF

Three-body clusters in *ab initio* NCSM/RGM

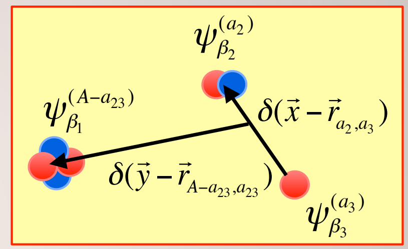
- Starts from:

$$\Psi^{(A)}_{RGM} = \sum_{\nu_2}\int g_{\nu_2}(\vec{r}\,)\hat{A}_{\nu_2}\left|\phi_{\nu_2\vec{r}}\right\rangle d\vec{r} + \sum_{\nu_3}\iint G_{\nu_3}(\vec{x},\vec{y})\;\hat{A}_{\nu_3}\left|\Phi_{\nu_3\vec{x}\vec{y}}\right\rangle d\vec{x}d\vec{y}$$

2-body channels

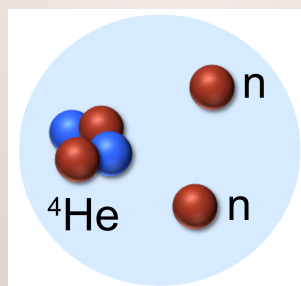


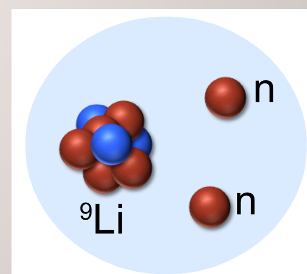
plus



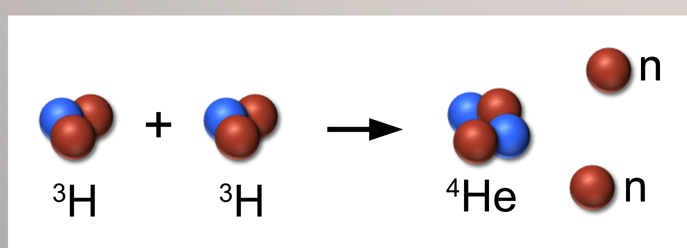
3-body channels

- Two-neutron halo nuclei





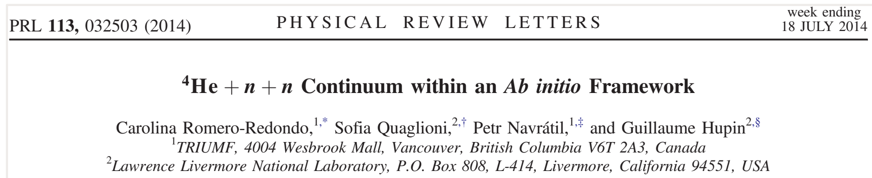
- Transfer reactions with three-body continuum final states



TRIUMF

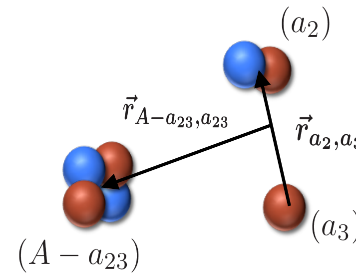
NCSM/RGM for three-body clusters: Structure of ^{6}He

^{4}He + n + n


PRL 113, 032503 (2014) PHYSICAL REVIEW LETTERS week ending 18 JULY 2014

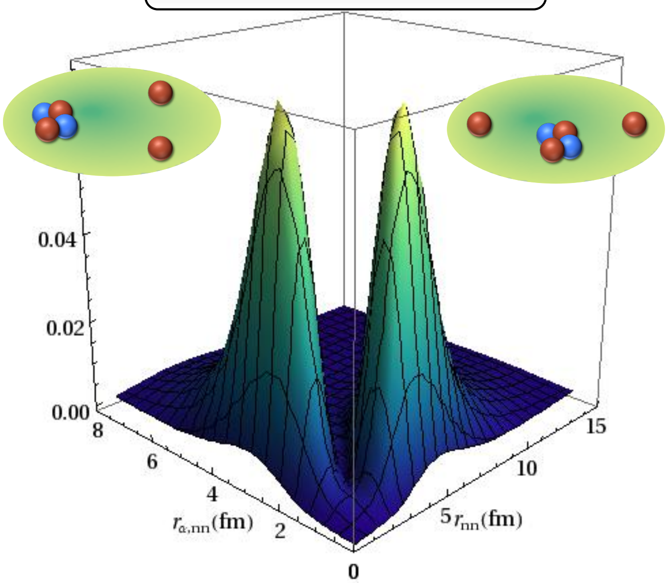
^{4}He + n + n Continuum within an *Ab initio* Framework

Carolina Romero-Redondo,[1,*] Sofia Quaglioni,[2,†] Petr Navrátil,[1,‡] and Guillaume Hupin[2,§]
[1]TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada
[2]Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA

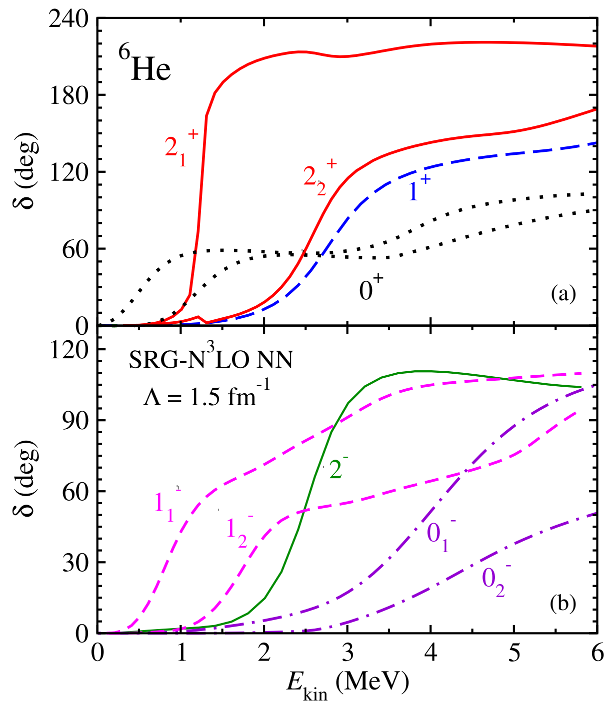


^{6}He bound 0$^+$ ground state

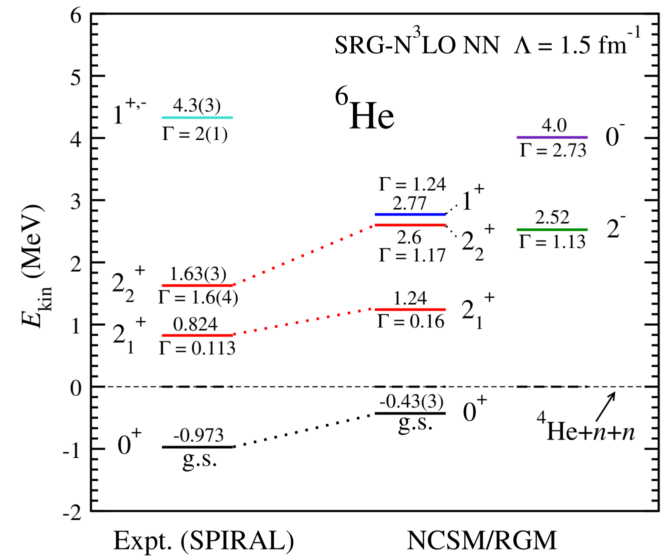
$\ell_x = \ell_y = L = S_{nn} = 0$



^{6}He resonances and continuum



Comparison to recent experiment

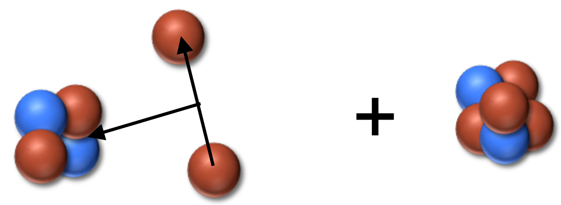


NCSMC implementation in progress…

^{5}H ≈ ^{4}He + n + n in progress

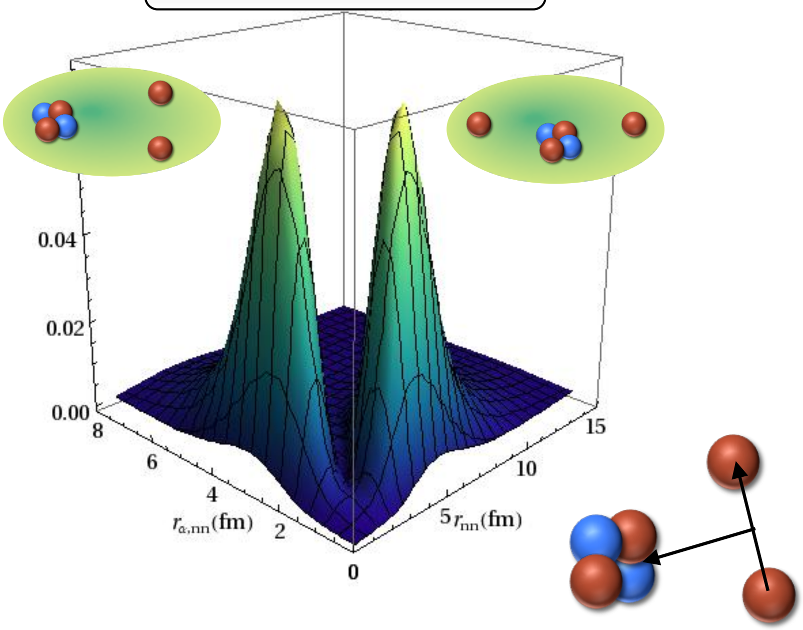
NCSM/RGM for three-body clusters: Structure of ^{6}He

^{4}He + n + n



^{6}He bound 0$^+$ ground state

$\ell_x = \ell_y = L = S_{nn} = 0$



N_{max}	NCSM/RGM	NCSM	NCSMC
8	−28.62	−28.95	−29.69
10	−28.72	−29.45	−29.86
12	−28.70	−29.66	−29.86
Extrapolation	—	−29.84(4)	—

C. Romero-Redondo, S. Quaglioni, P. Navratil, G.Hupin

arXiv: 1509.00878

NCSMC implementation in progress…

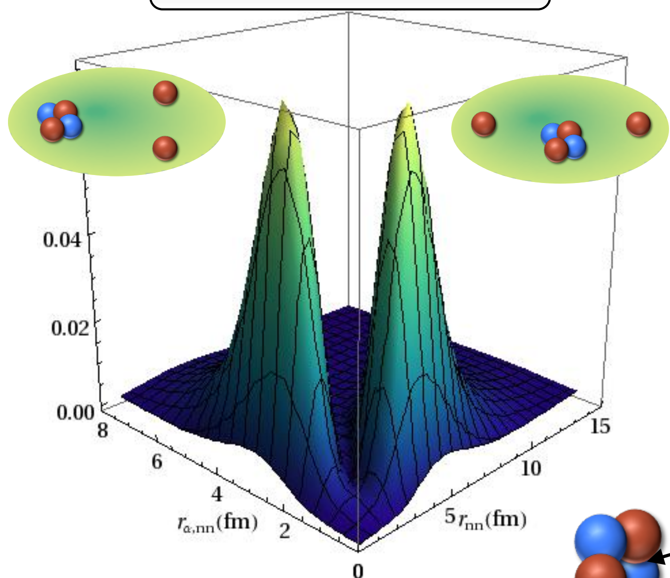
… excellent ground-state energy convergence

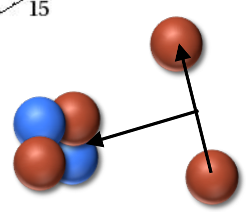
NCSM/RGM for three-body clusters: Structure of ^{6}He

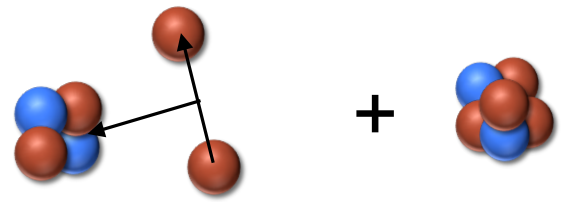
^{4}He + *n* + *n*

^{6}He bound 0^+ ground state

$$\ell_x = \ell_y = L = S_{nn} = 0$$







λ=1.5 fm^{-1}

	N_{max}=6	N_{max}=8	N_{max}=10	N_{max}=12	
Matter radius					
NCSM	2.14	2.18	2.22	2.25	
NCSMC	2.40	2.28	2.33	2.34	
Binding Energy					
NCSM	-28.95	-29.45	-29.66	-29.75	[-29.84(4)]
NCSMC	-30.02	-29.69	-29.86	-29.86	

PP radius	
NCSM	1.78
NCSMC	1.79

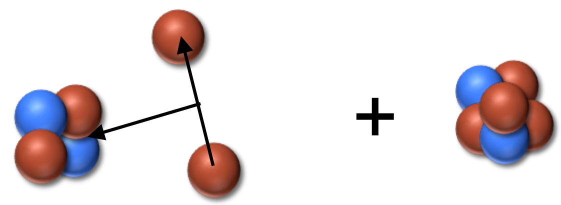
NCSMC implementation in progress…

… and improved matter radius convergence

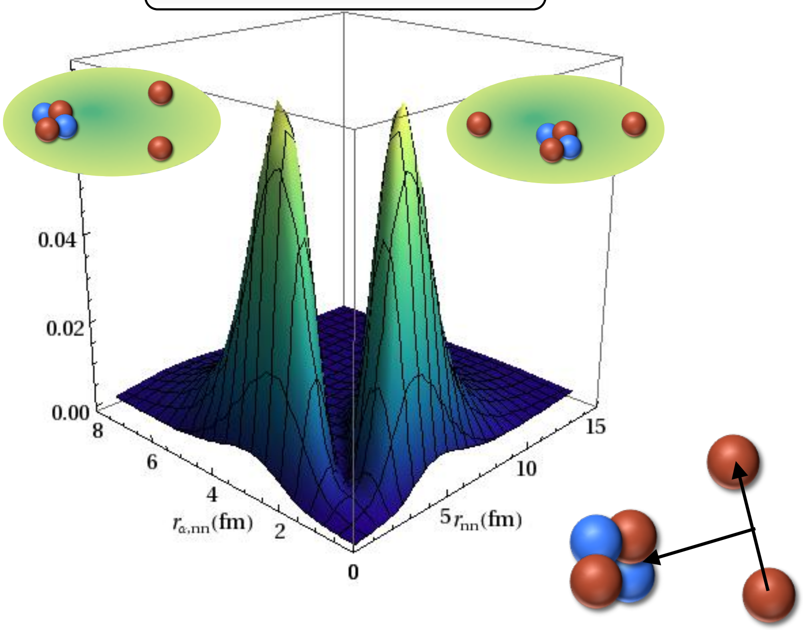
NCSM/RGM for three-body clusters: Structure of ^{6}He

^{4}He + *n* + *n*

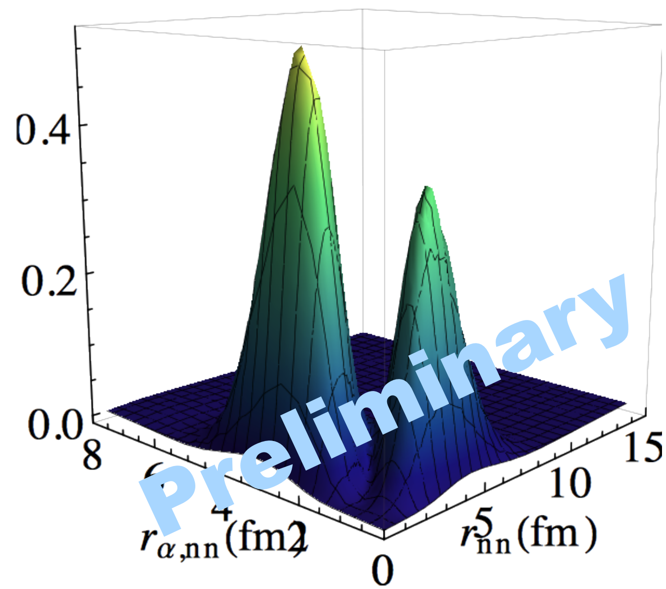
^{6}He bound 0^+ ground state



$\ell_x = \ell_y = L = S_{nn} = 0$



$\ell_x = \ell_y = L = S_{nn} = 0$



NCSMC implementation in progress…

…^{4}He core excitations enhance the di-neutron configuration

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

NCSMC and NCSM/RGM collaborators

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Guillaume Hupin (CNRS)

Wataru Horiuchi (Hokkaido)