

Bound and unbound states of nuclei from chiral interactions

FUSTIPEN Topical Meeting

«Future directions for nuclear structure and reaction theories:
Ab initio approaches for 2020»

March 14-18, 2016, GANIL, Caen, France

Petr Navratil | TRIUMF

Collaborators:

Sofia Quaglioni, Carolina Romero-Redondo (LLNL)

Guillaume Hupin (CEA/DAM)

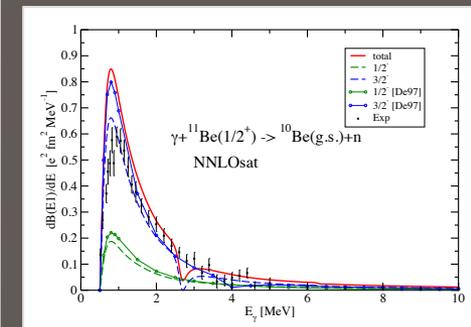
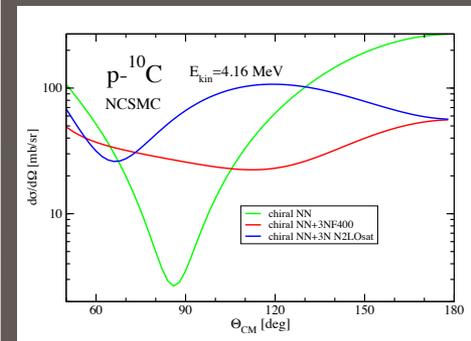
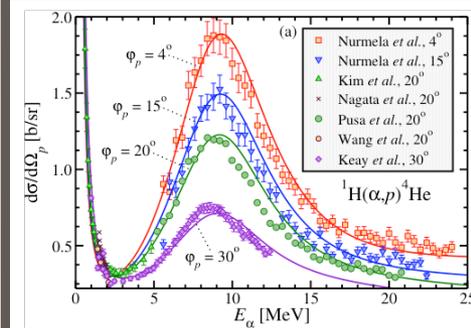
Jeremy Dohet-Eraly, Angelo Calci (TRIUMF)

Francesco Raimondi (Surrey), Wataru Horiuchi (Hokkaido)

Robert Roth (TU Darmstadt)

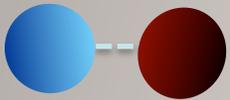
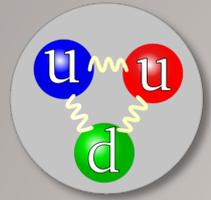
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- No-Core Shell Model with Continuum (NCSMC) approach
- N-⁴He scattering
- ⁶Li structure & d-⁴He scattering
- ¹¹Be as a laboratory for testing of nuclear forces
- ¹¹N and ¹⁰C-p scattering
- ³He-⁴He and ³H-⁴He radiative capture

From QCD to nuclei

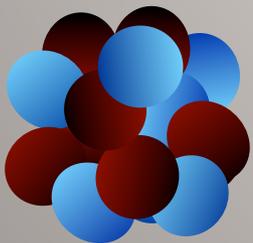


Low-energy QCD



NN+3N interactions
from chiral EFT

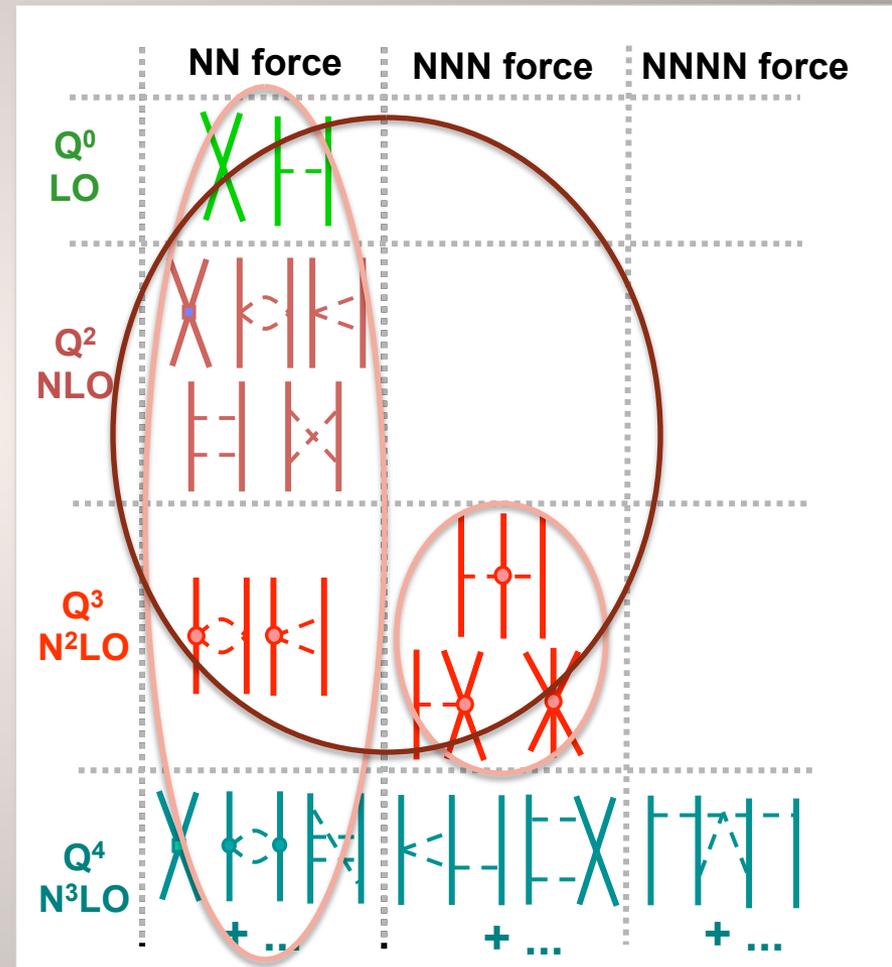
...or accurate
meson-exchange
potentials



Nuclear structure and reactions

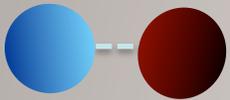
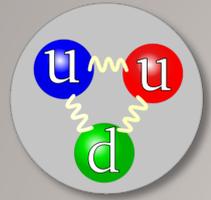
Chiral Effective Field Theory

- 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



$\Lambda_\chi \sim 1 \text{ GeV}$:
Chiral symmetry breaking scale

From QCD to nuclei

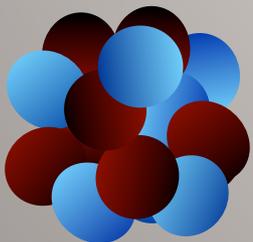


Low-energy QCD

NN+3N interactions
from chiral EFT

...or accurate
meson-exchange
potentials

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

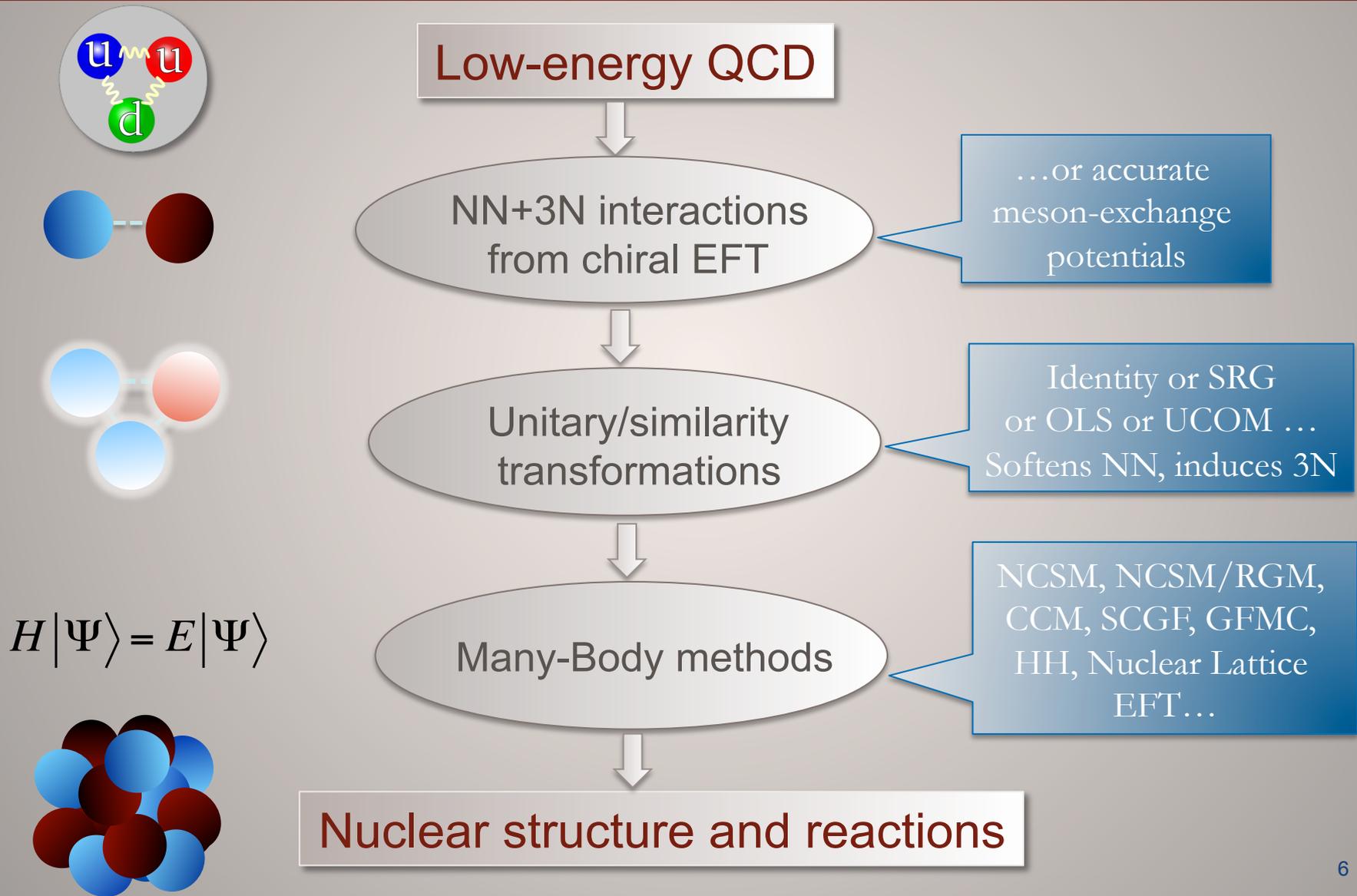


Many-Body methods

NCSM, NCSM/RGM,
NCSMC, CCM, SCGF,
GFMC, HH, Nuclear
Lattice EFT...

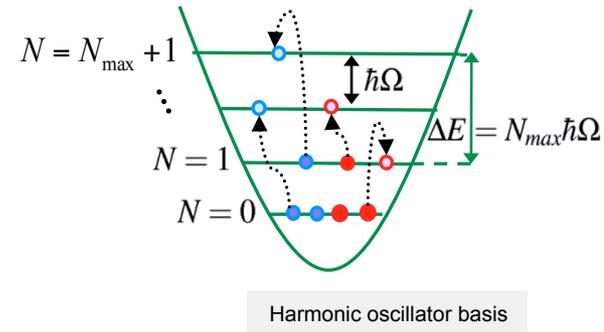
Nuclear structure and reactions

From QCD to nuclei



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



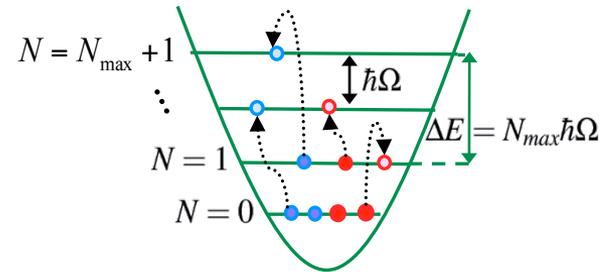
NCSM

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

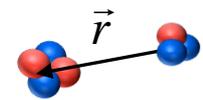
Unknowns

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



Harmonic oscillator basis



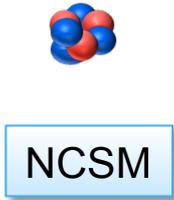
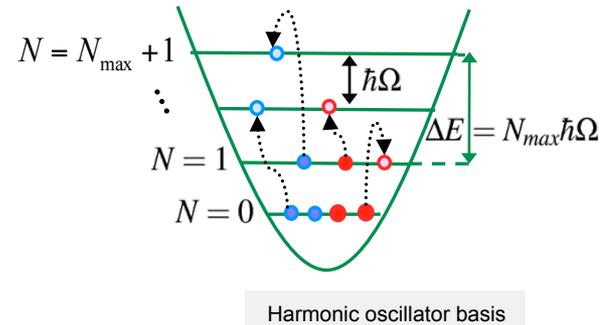
$$\Psi^{(A)} =$$

$$\sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left[\begin{array}{c} \text{NCSM/RGM} \\ \text{channel states} \\ \left(\begin{array}{c} \text{cluster } (A-a) \\ \text{cluster } (a) \end{array}, \nu \right) \end{array} \right]$$

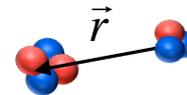
Unknowns 

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- ...with resonating group method
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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



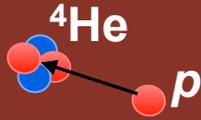
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left[\begin{array}{c} \text{NCSM eigenstates} \\ \left(\begin{array}{c} (A) \\ \text{Nucleon cluster} \end{array}, \lambda \right) \end{array} \right] + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left[\begin{array}{c} \text{NCSM/RGM} \\ \text{channel states} \\ \left(\begin{array}{c} \text{Nucleon cluster} \\ (A-a) \end{array}, \nu \right) \end{array} \right]$$

Unknowns

Coupled NCSMC equations

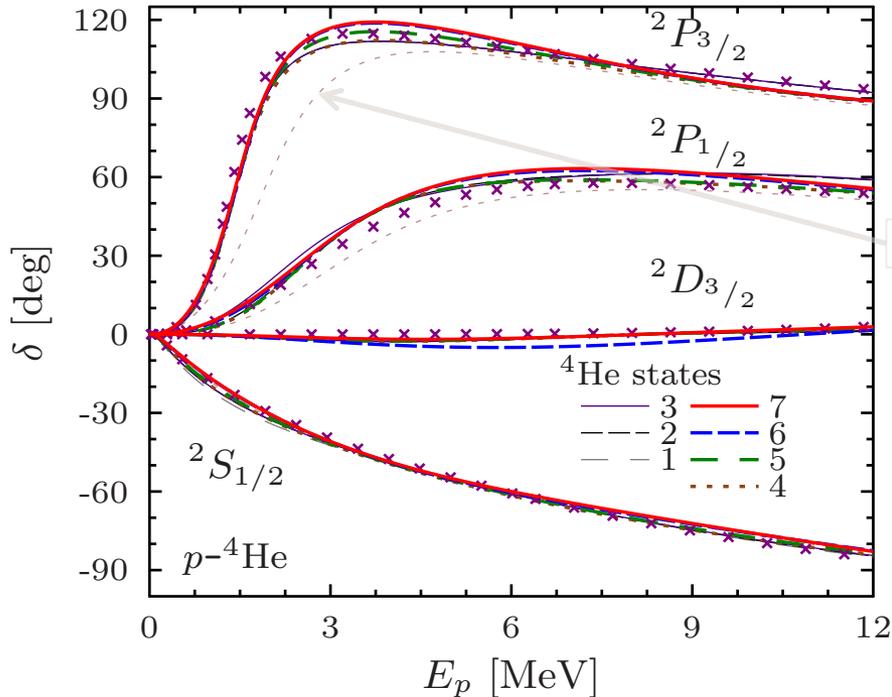
$$\begin{array}{c}
 \begin{array}{cc}
 \boxed{E_{\lambda}^{NCSM} \delta_{\lambda\lambda'}} & \boxed{\langle (A) \left| H \hat{A}_v \right| (a) (A-a) \rangle} \\
 \downarrow \text{blue} & \downarrow \text{green} \\
 \begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} & \begin{pmatrix} \textcircled{C} \\ \textcircled{\gamma} \end{pmatrix}
 \end{array} \\
 \uparrow \text{red} \\
 \boxed{\langle (A-a) (a) \left| \hat{A}_v H \hat{A}_v \right| (a) (A-a) \rangle}
 \end{array}
 = E
 \begin{array}{c}
 \begin{array}{cc}
 \boxed{\delta_{\lambda\lambda'}} & \boxed{\langle (A) \left| \hat{A}_v \right| (a) (A-a) \rangle} \\
 \downarrow \text{blue} & \downarrow \text{green} \\
 \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} & \begin{pmatrix} \textcircled{C} \\ \textcircled{\gamma} \end{pmatrix}
 \end{array} \\
 \uparrow \text{red} \\
 \boxed{\langle (A-a) (a) \left| \hat{A}_v \hat{A}_v \right| (a) (A-a) \rangle}
 \end{array}
 \end{array}$$

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



p - ^4He scattering within NCSMC

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



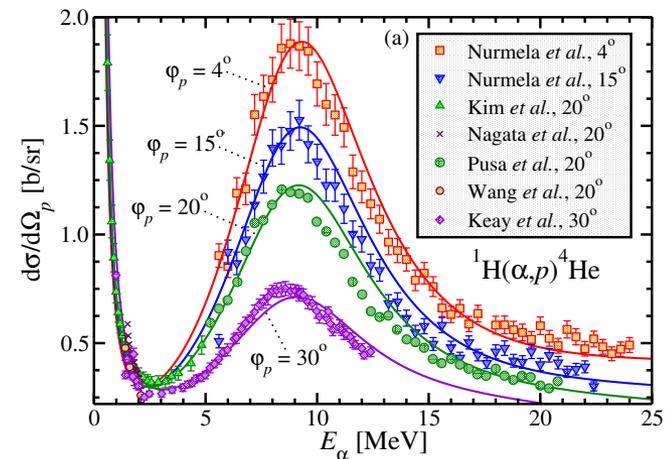
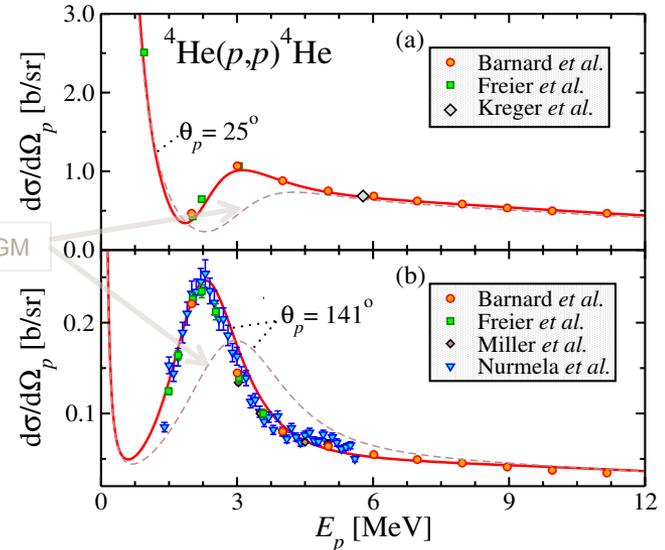
Predictive power in the 3/2- resonance region:
Applications to material science

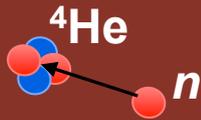
PHYSICAL REVIEW C **90**, 061601(R) (2014)

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

Guillaume Hupin,^{1,*} Sofia Quaglioni,^{1,†} and Petr Navrátil^{2,‡}

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

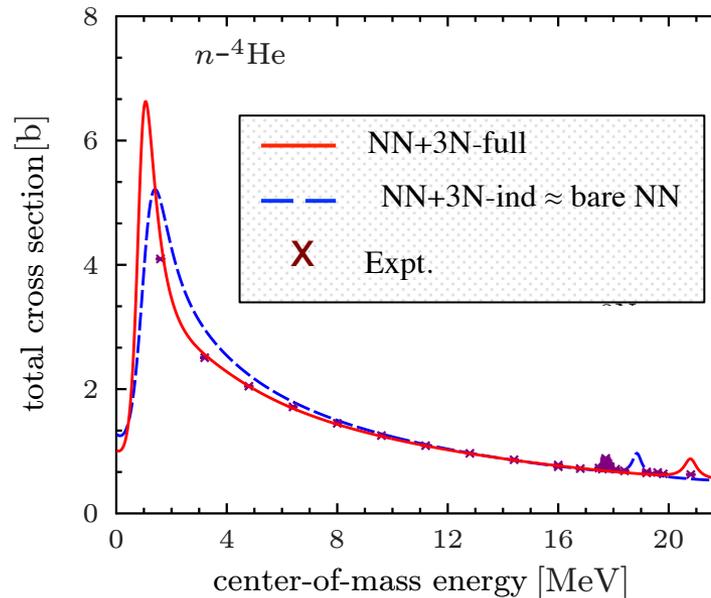
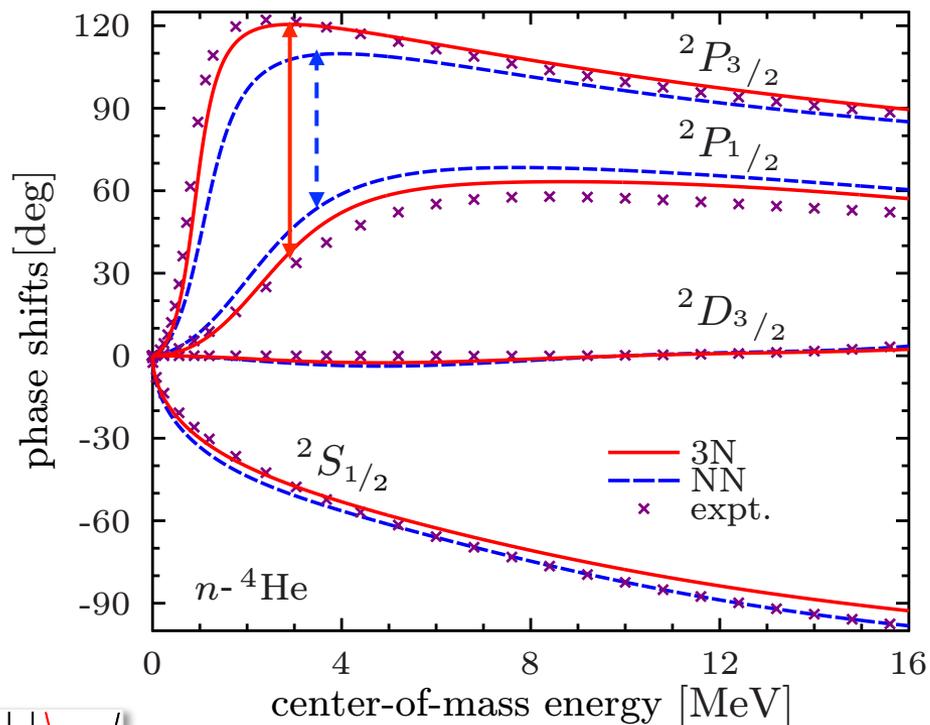




n - ^4He scattering within NCSMC

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

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



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

IOP Publishing | Royal Swedish Academy of Sciences
Phys. Scr. 99 (2016) 020000 (7pp)

Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

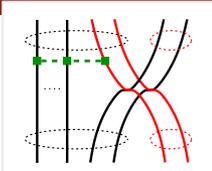
Petr Navrátil^{1,*}, Sofia Quaglioni^{2,†}, Guillaume Hupin^{3,‡}, Carolina Romero-Redondo⁴ and Angelo Calci⁵

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

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

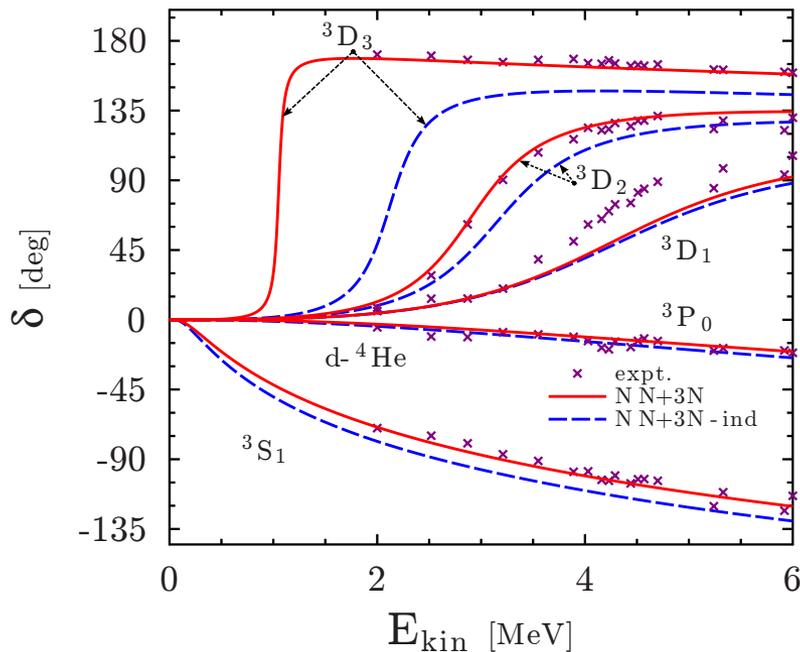
Guillaume Hupin,^{1,*} Joachim Langhammer,^{2,†} Petr Navrátil,^{3,‡} Sofia Quaglioni,^{1,§} Angelo Calci,^{2,||} and Robert Roth^{2,¶}

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

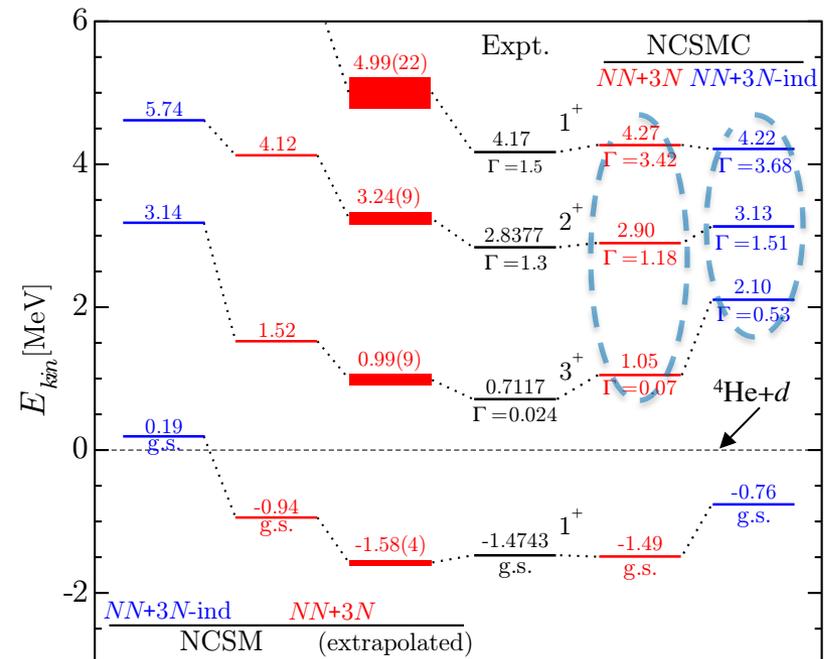


- Continuum and three-nucleon force effects on $d+{}^4\text{He}$ and ${}^6\text{Li}$

$d+{}^4\text{He}$ Scattering Phase Shifts

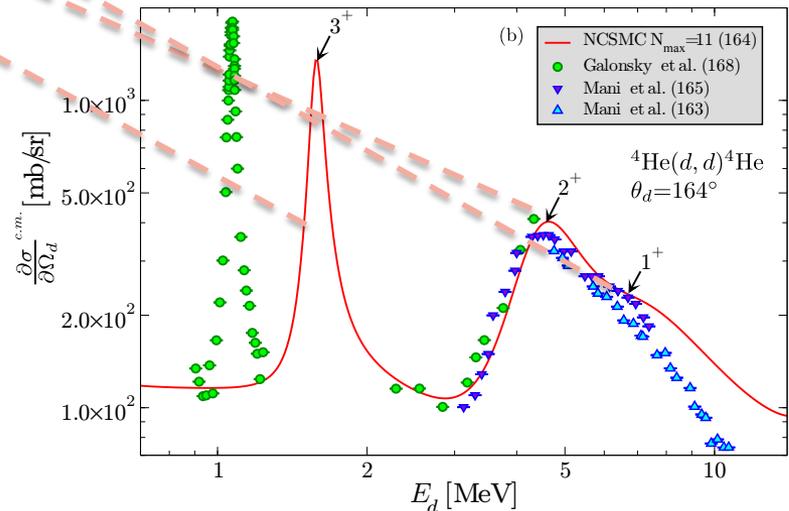
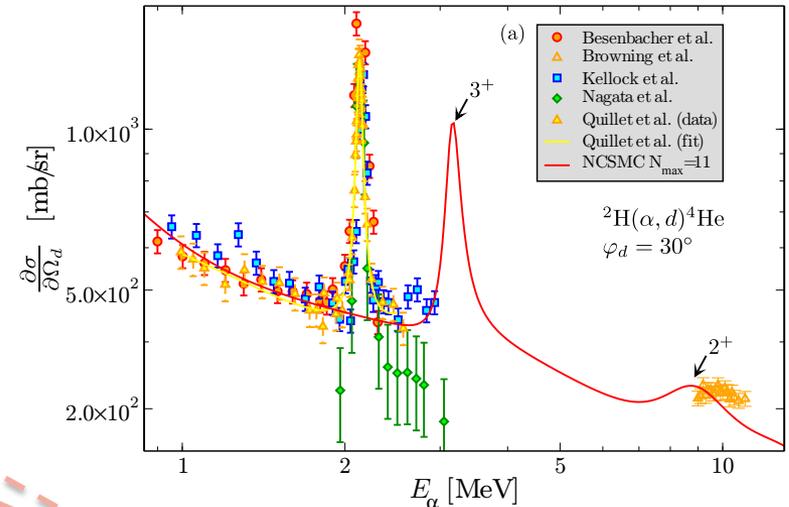
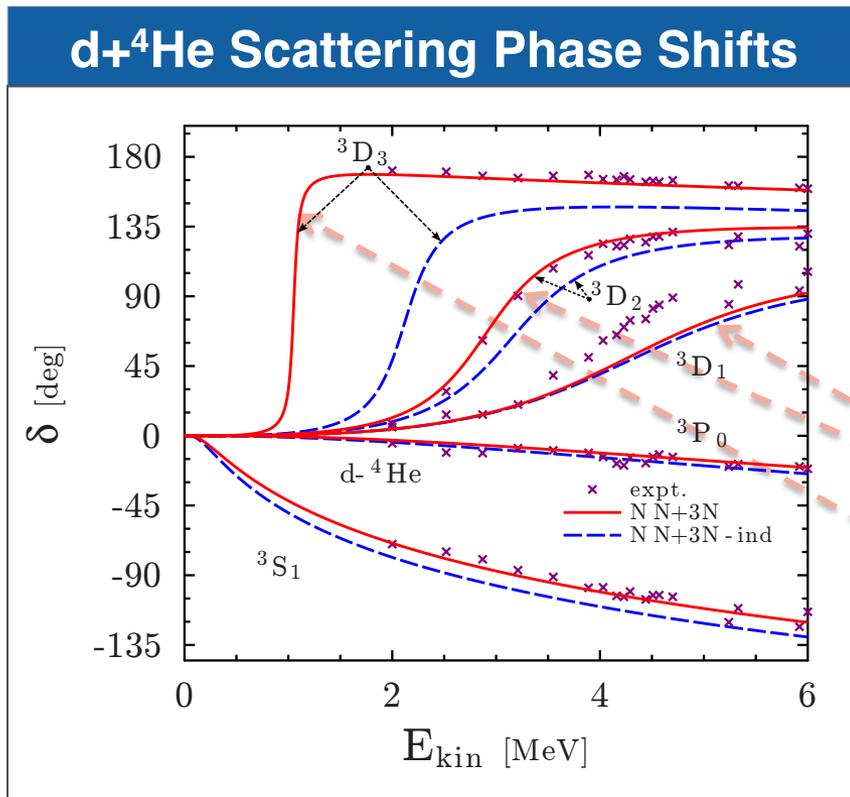


${}^6\text{Li}$ vs. $({}^4\text{He}+d)+{}^6\text{Li}$ calculation

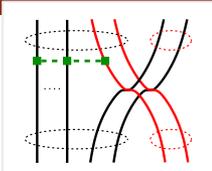


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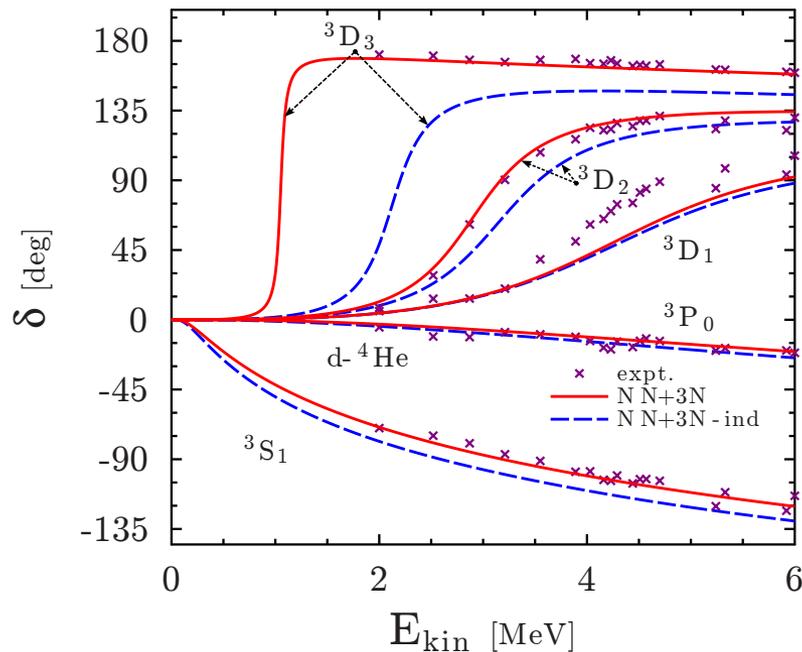


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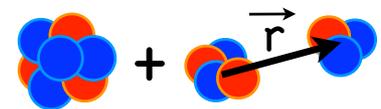
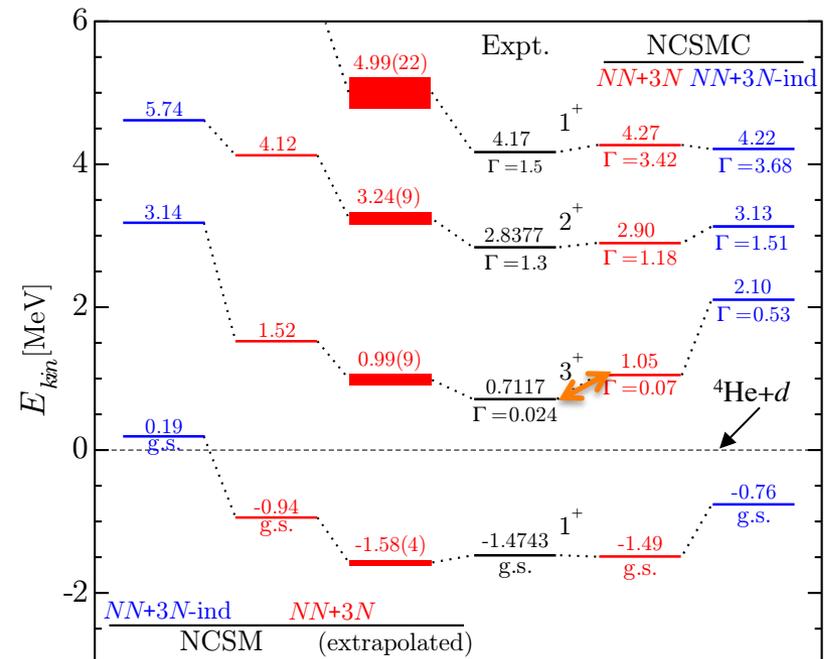


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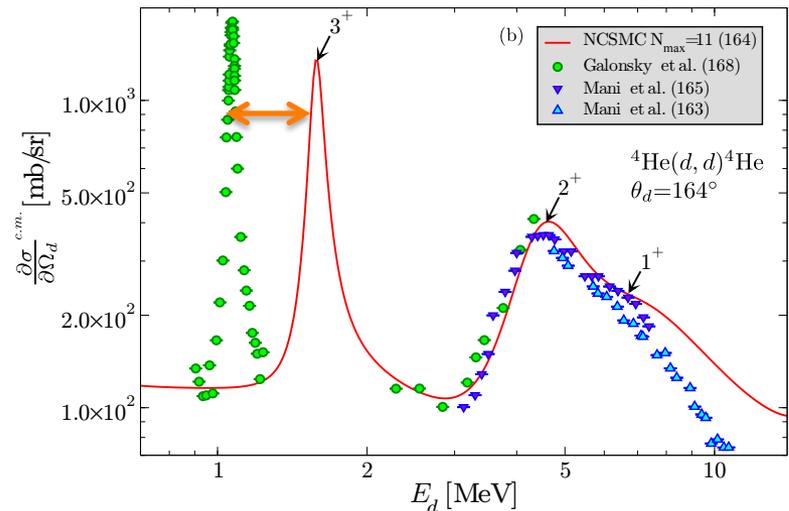
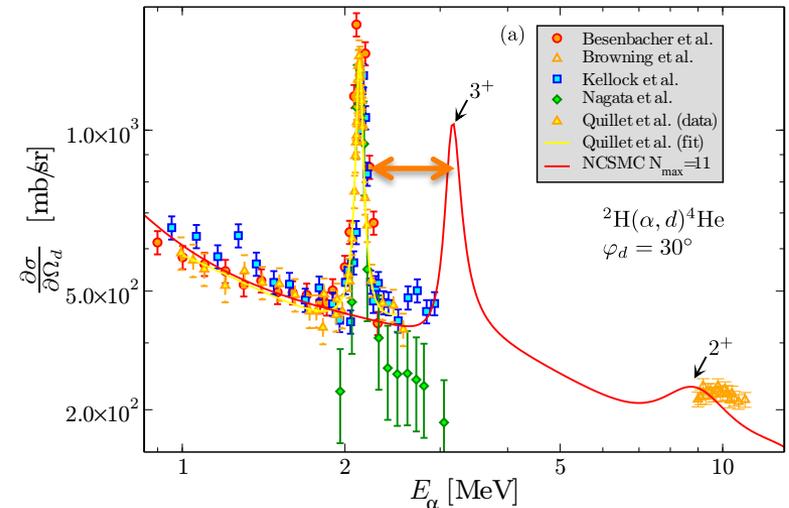
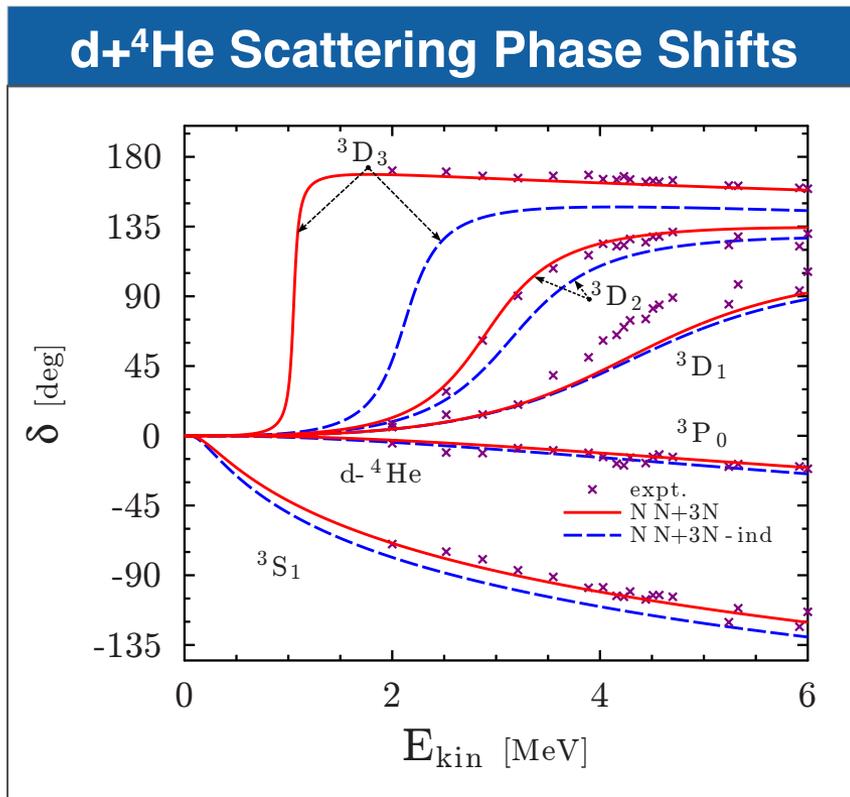


${}^6\text{Li}$ vs. $({}^4\text{He}+d)+{}^6\text{Li}$ calculation

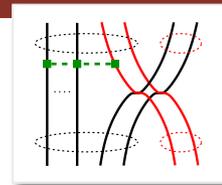


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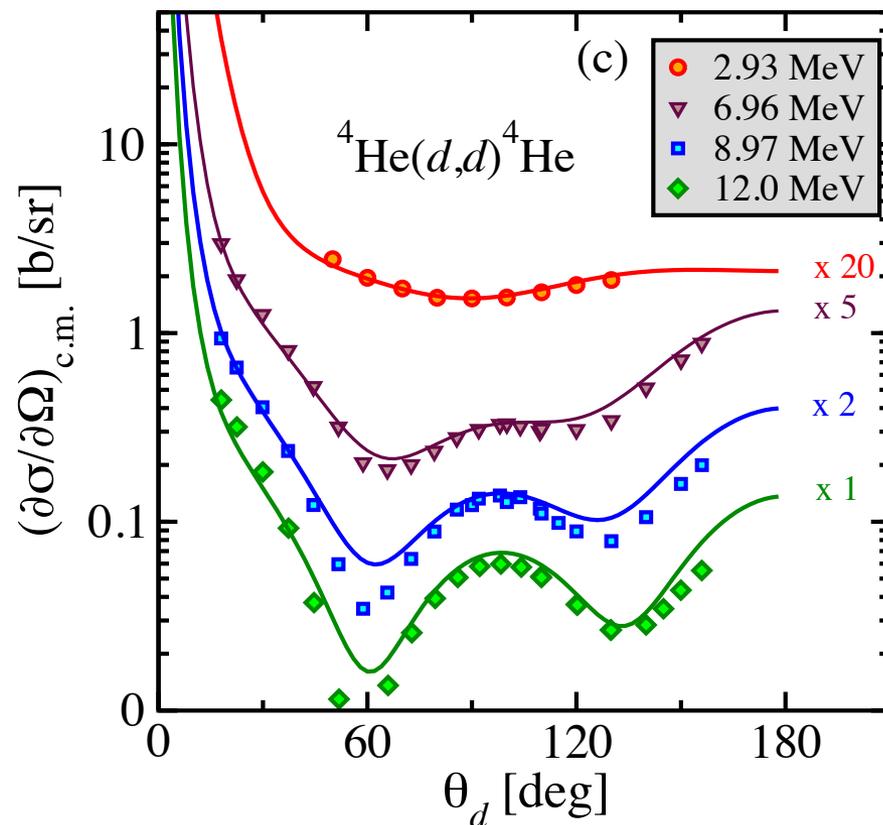
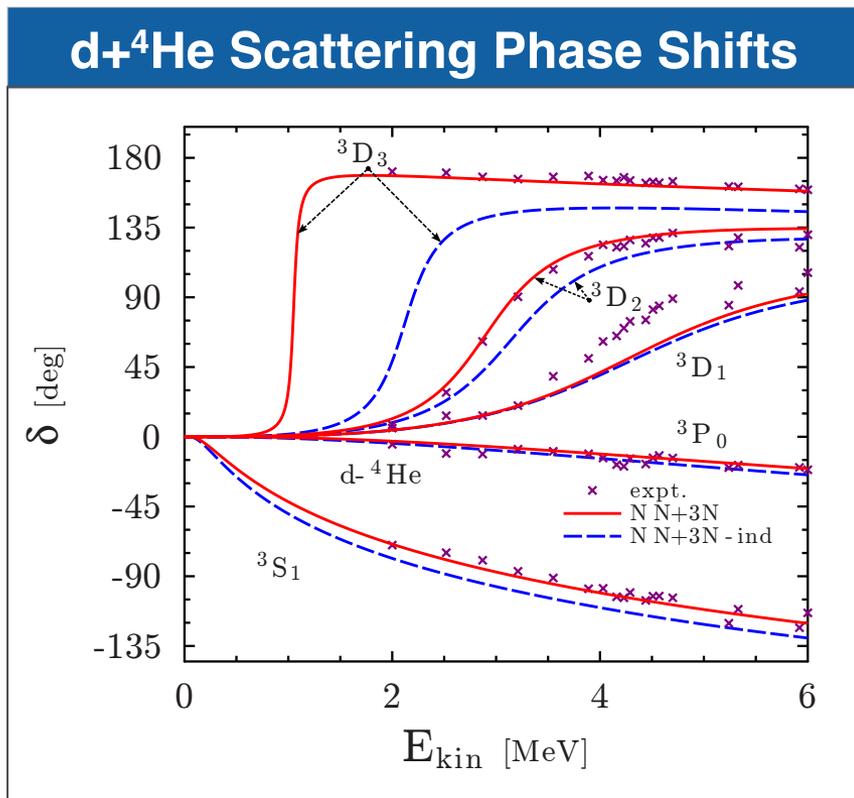
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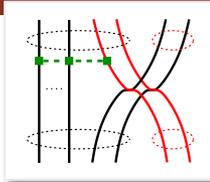
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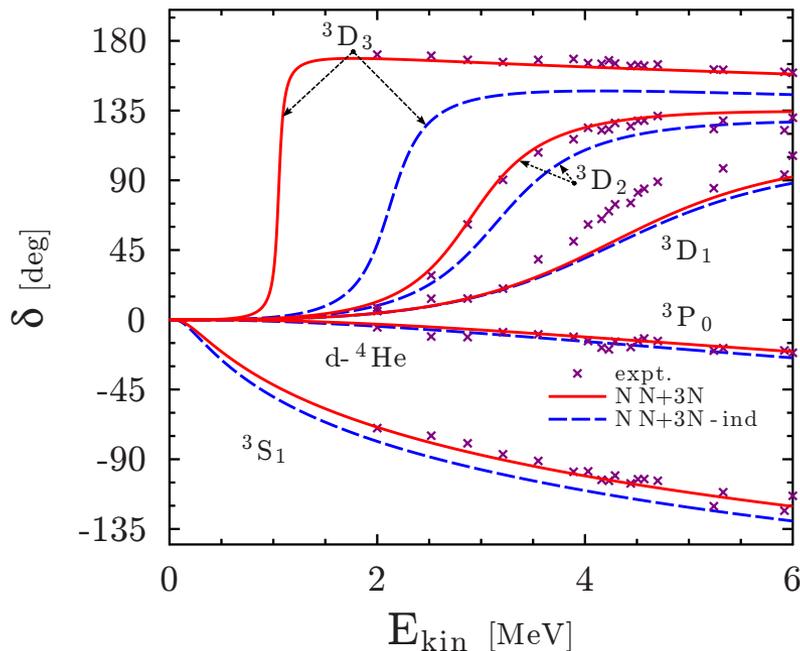


Unified description of ${}^6\text{Li}$ structure and $d+{}^4\text{He}$ dynamics



- S- and D-wave asymptotic normalization constants

$d+{}^4\text{He}$ Scattering Phase Shifts



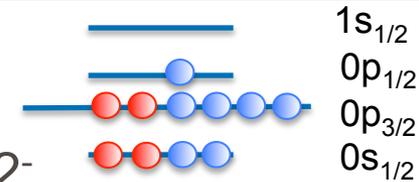
	NCSMC		Experiment	
C_0 [$\text{fm}^{-1/2}$]	2.695	2.91(9) [39]	2.93(15) [38]	
C_2 [$\text{fm}^{-1/2}$]	-0.074	-0.077(18) [39]		
C_2/C_0	-0.027	-0.025(6)(10) [39]	0.0003(9) [41]	

- [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. Kozłowska, H. J. Maier, and I. J. Thompson, *Phys. Rev. Lett.* **81**, 1187 (1998).

Neutron-rich halo nucleus ^{11}Be

- $Z=4, N=7$

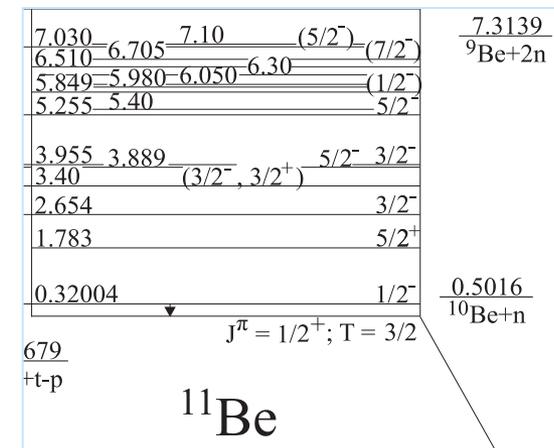
- In the shell model picture g.s. expected to be $J^\pi=1/2^-$
 - $Z=6, N=7$ ^{13}C and $Z=8, N=7$ ^{15}O have $J^\pi=1/2^-$ g.s.
- In reality, ^{11}Be g.s. is $J^\pi=1/2^+$ - parity inversion
- Very weakly bound: $E_{\text{th}}=-0.5$ MeV
 - Halo state – dominated by $^{10}\text{Be-n}$ in the S -wave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



- Can we describe ^{11}Be

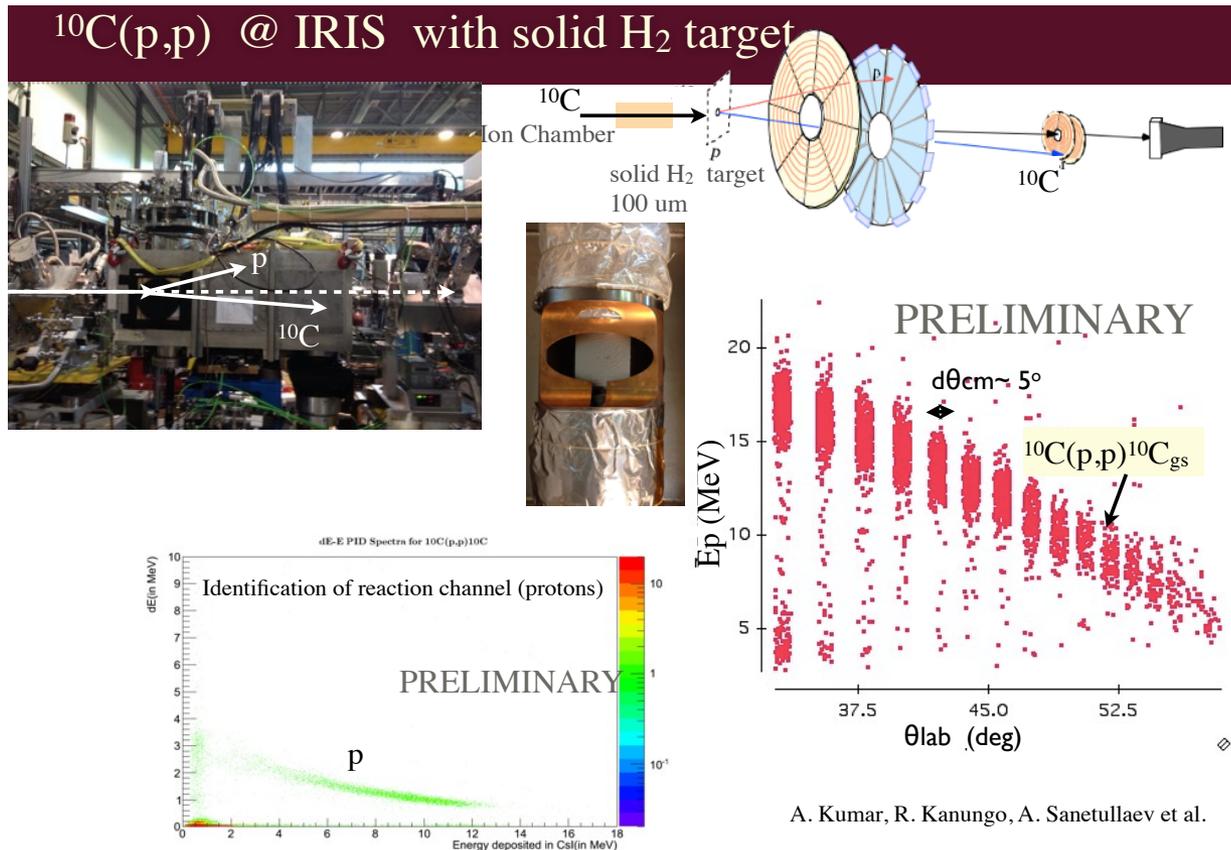
in *ab initio* calculations?

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



$^{10}\text{C}(p,p) @ \text{IRIS}$ 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 $E_{\text{CM}} \sim 4.16 \text{ MeV}$ and 4.4 MeV



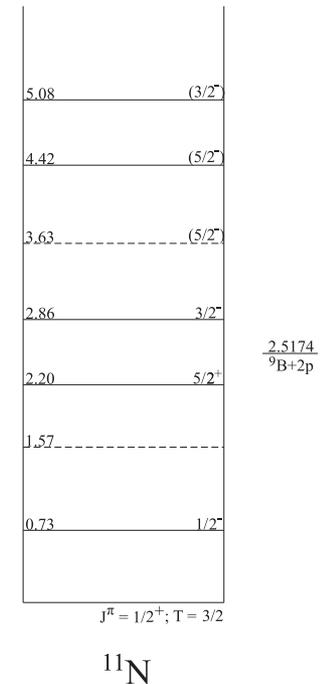
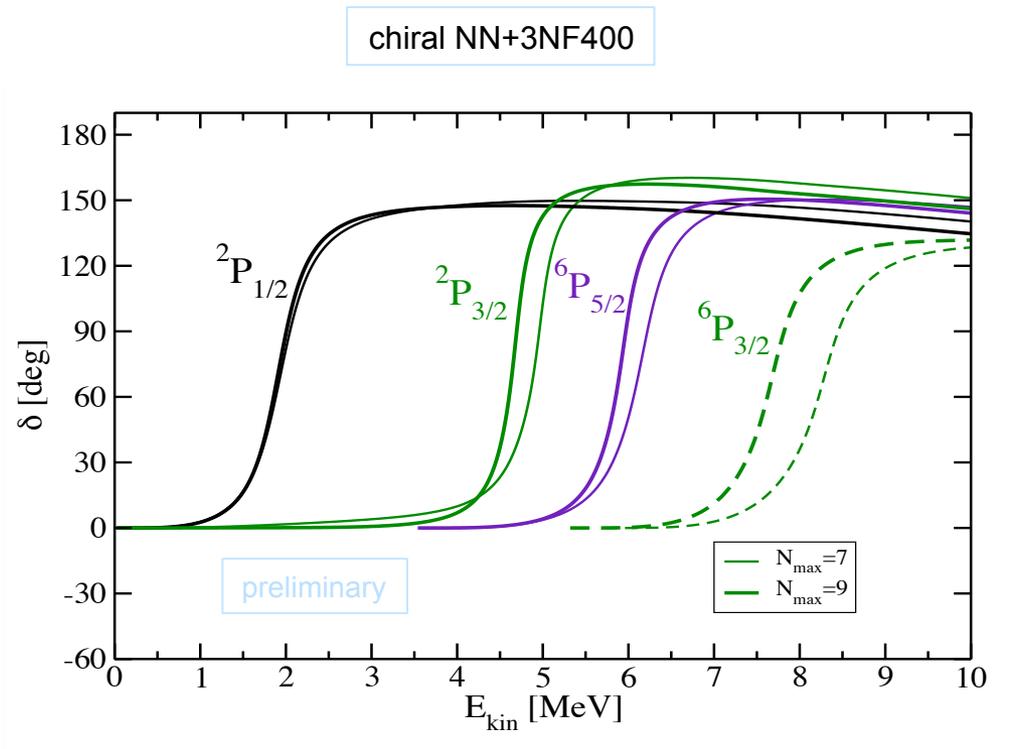
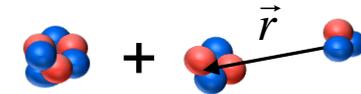
IRIS collaboration:
A. Kumar, R. Kanungo,
A. Sanetullaev *et al.*

p+¹⁰C scattering: structure of ¹¹N resonances

- NCSMC calculations with **chiral NN+3N** (N³LO NN+N²LO 3NF400, NNLOsat)

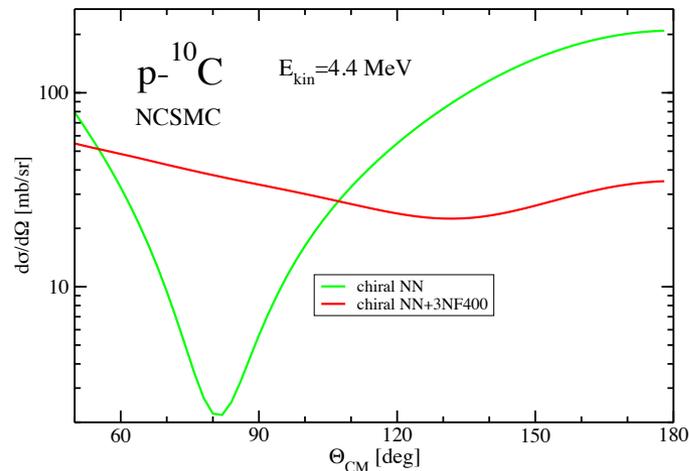
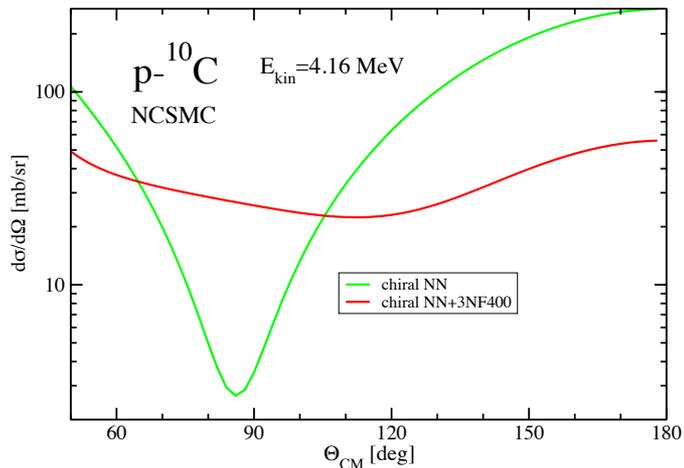
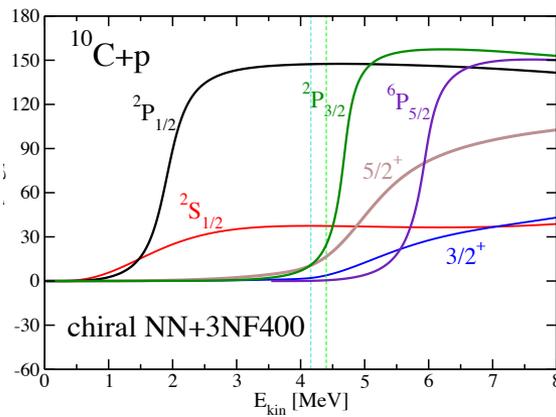
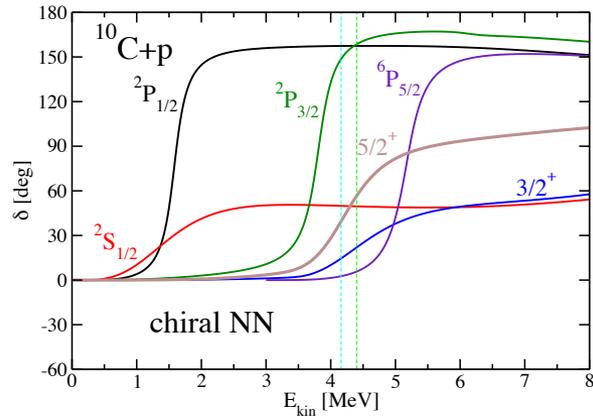
– p-¹⁰C + ¹¹N

- ¹⁰C: 0⁺, 2⁺, 2⁺ NCSM eigenstates
- ¹¹N: ≥4 π = -1 and ≥3 π = +1 NCSM eigenstates

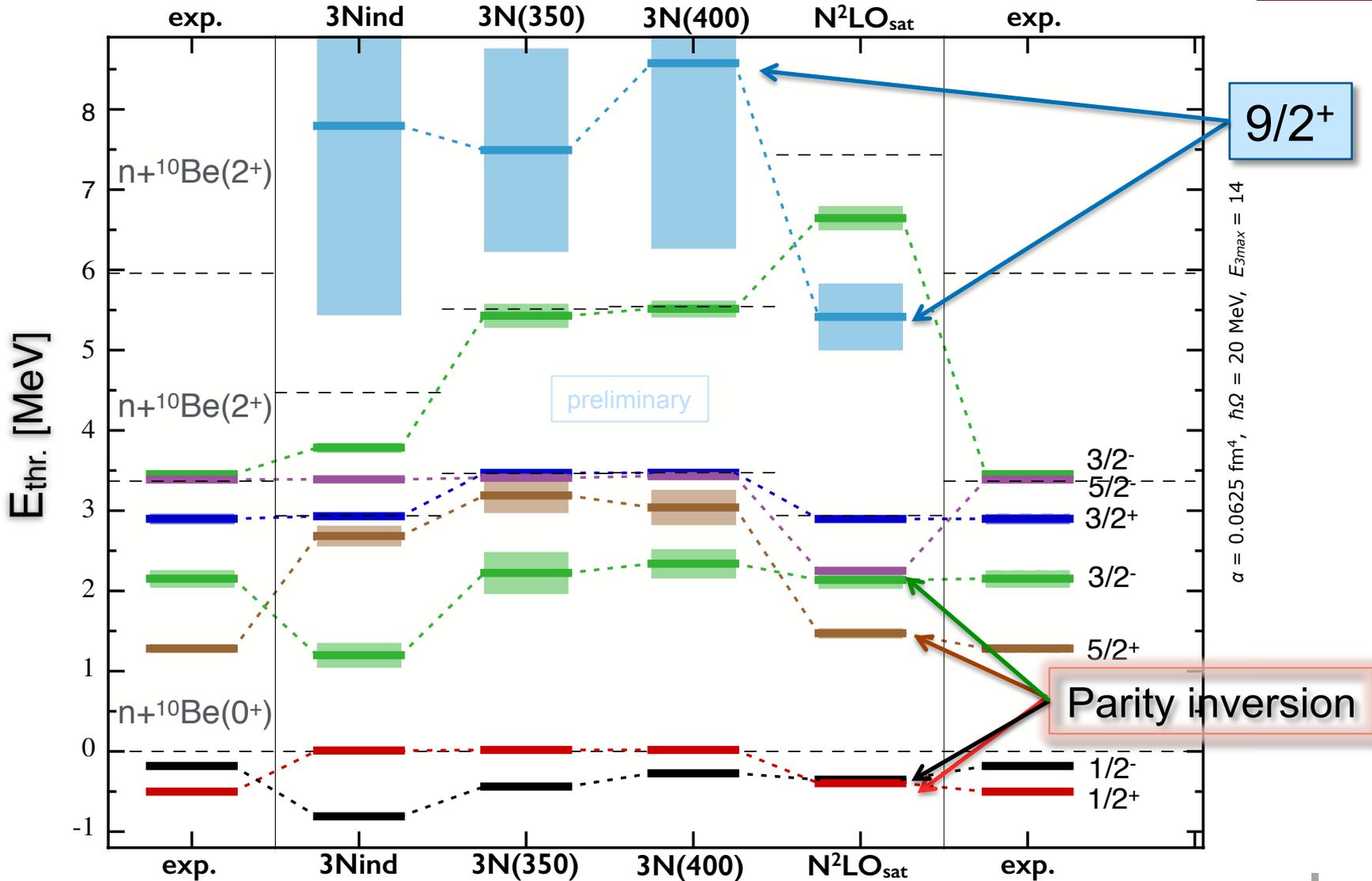


$\frac{-1.4893}{10C+p}$

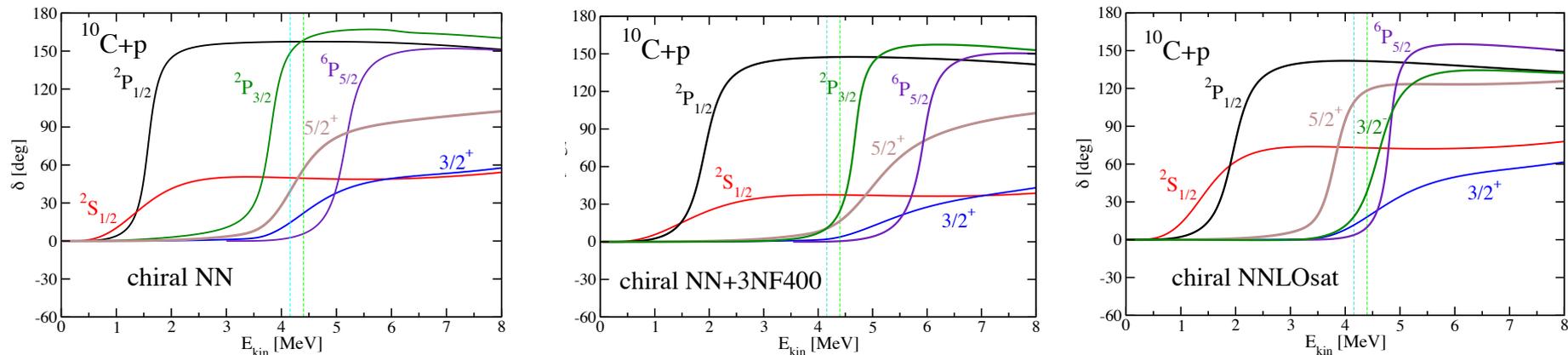
p+¹⁰C scattering: structure of ¹¹N resonances



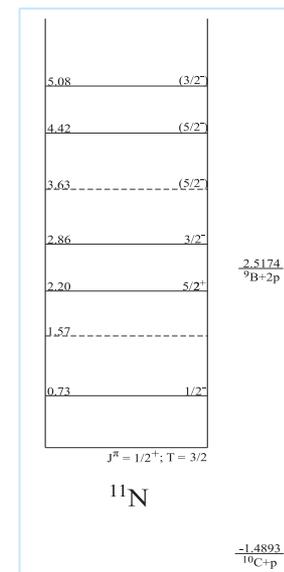
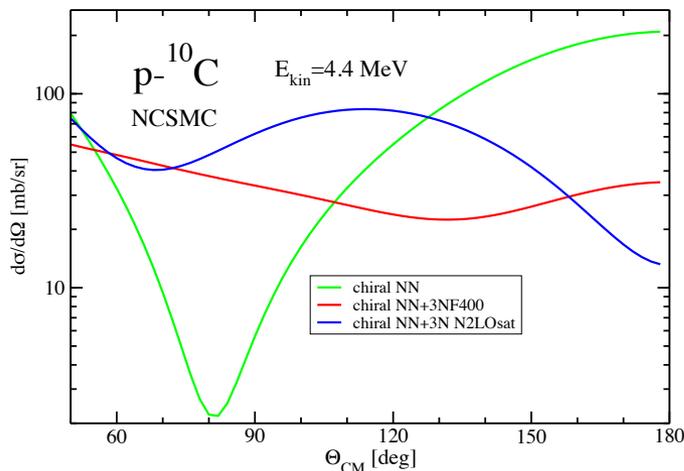
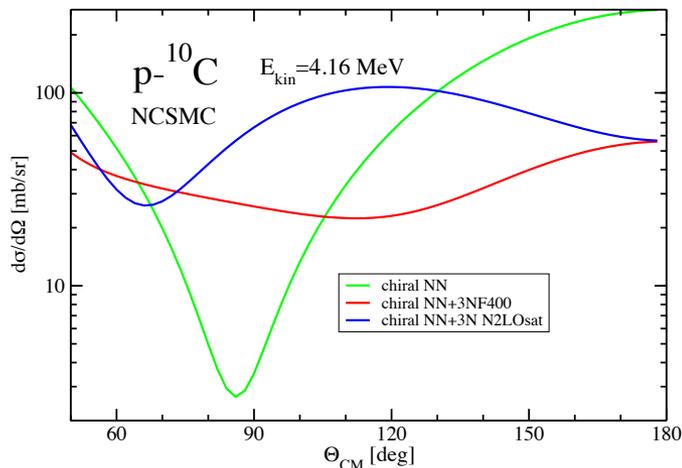
^{11}Be within NCSMC: Discrimination among chiral nuclear forces



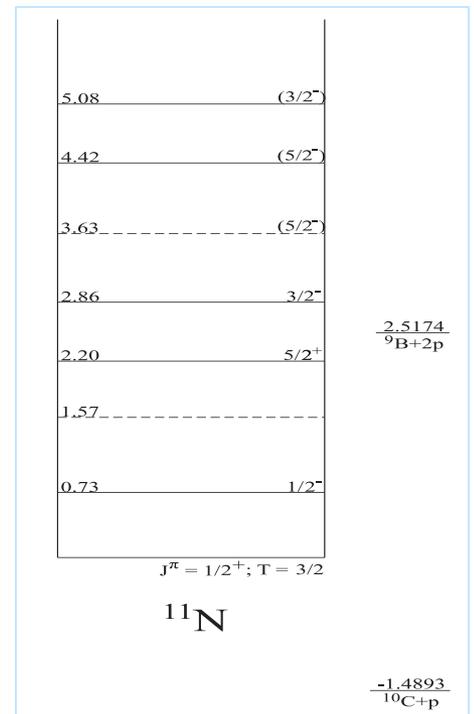
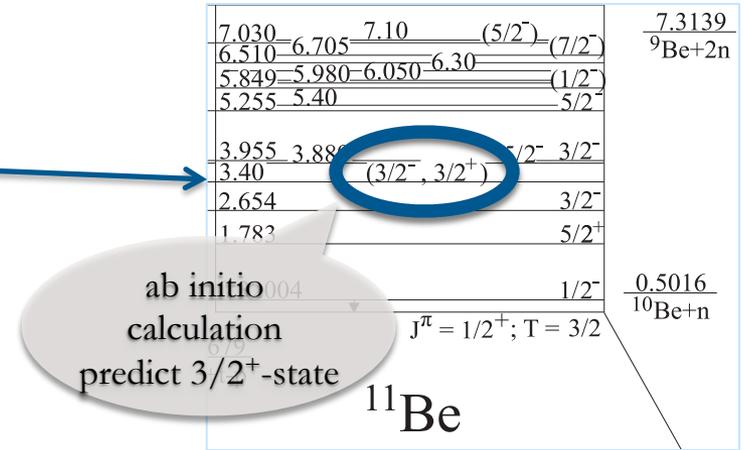
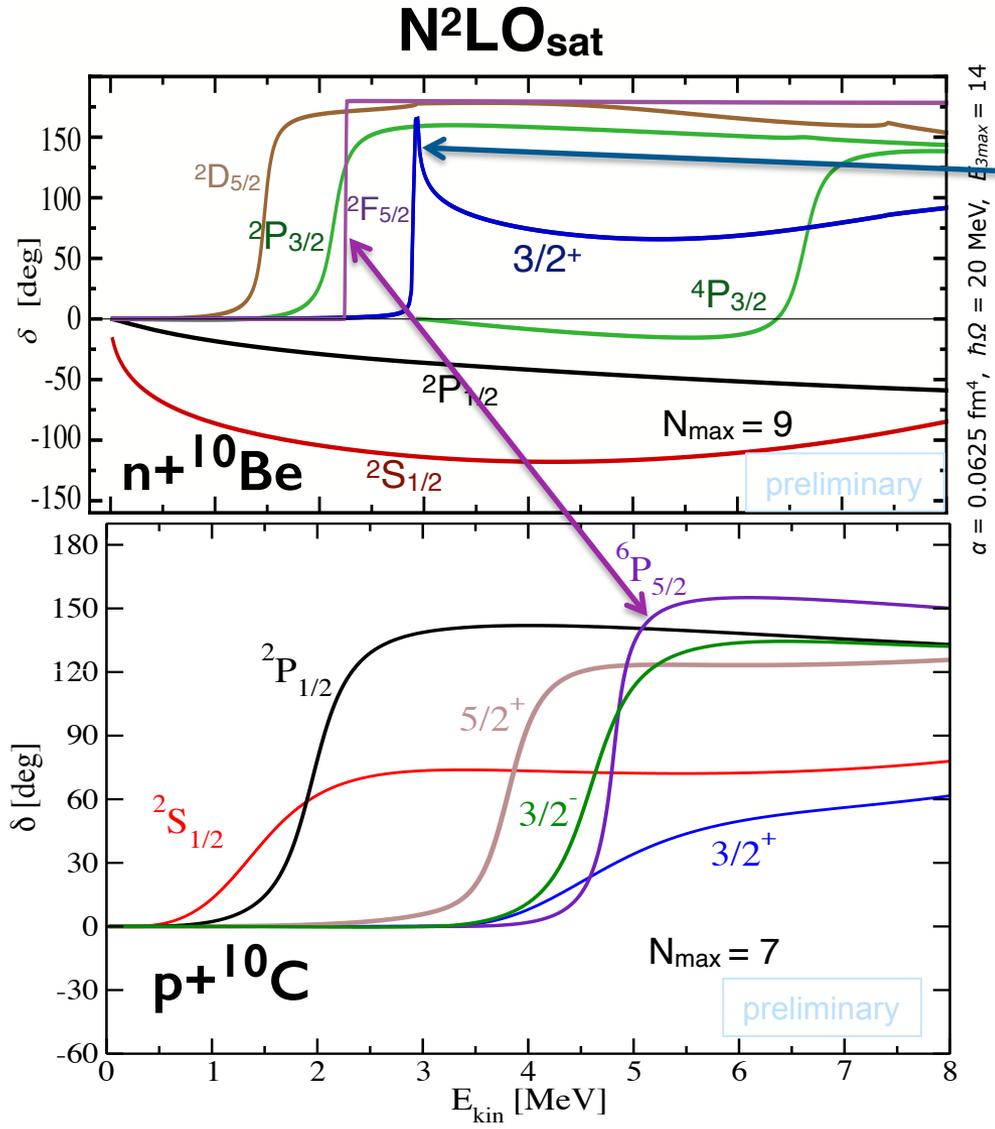
p+¹⁰C scattering: structure of ¹¹N resonances



Discrimination among chiral nuclear forces



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



NCSMC wave function

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

$$\begin{aligned} |\Psi_A^{J^{\pi T}}\rangle &= \sum_{\lambda} |A\lambda J^{\pi T}\rangle \left[\sum_{\lambda'} (N^{-\frac{1}{2}})^{\lambda\lambda'} \bar{c}_{\lambda'} + \sum_{\nu'} \int dr' r'^2 (N^{-\frac{1}{2}})_{\nu'r'}^{\lambda} \frac{\bar{\chi}_{\nu'}(r')}{r'} \right] \\ &+ \sum_{\nu\nu'} \int dr r^2 \int dr' r'^2 \hat{A}_{\nu} |\Phi_{\nu r}^{J^{\pi T}}\rangle \mathcal{N}_{\nu\nu'}^{-\frac{1}{2}}(r, r') \left[\sum_{\lambda'} (N^{-\frac{1}{2}})_{\nu'r'}^{\lambda'} \bar{c}_{\lambda'} + \sum_{\nu''} \int dr'' r''^2 (N^{-\frac{1}{2}})_{\nu'r'\nu''r''} \frac{\bar{\chi}_{\nu''}(r'')}{r''} \right]. \end{aligned}$$

Asymptotic behavior $r \rightarrow \infty$:

$$\bar{\chi}_{\nu}(r) \sim C_{\nu} W(k_{\nu} r) \qquad \bar{\chi}_{\nu}(r) \sim v_{\nu}^{-\frac{1}{2}} \left[\delta_{\nu i} I_{\nu}(k_{\nu} r) - U_{\nu i} O_{\nu}(k_{\nu} r) \right]$$

Bound state

Scattering state

 Scattering matrix

E1 transitions in NCSMC

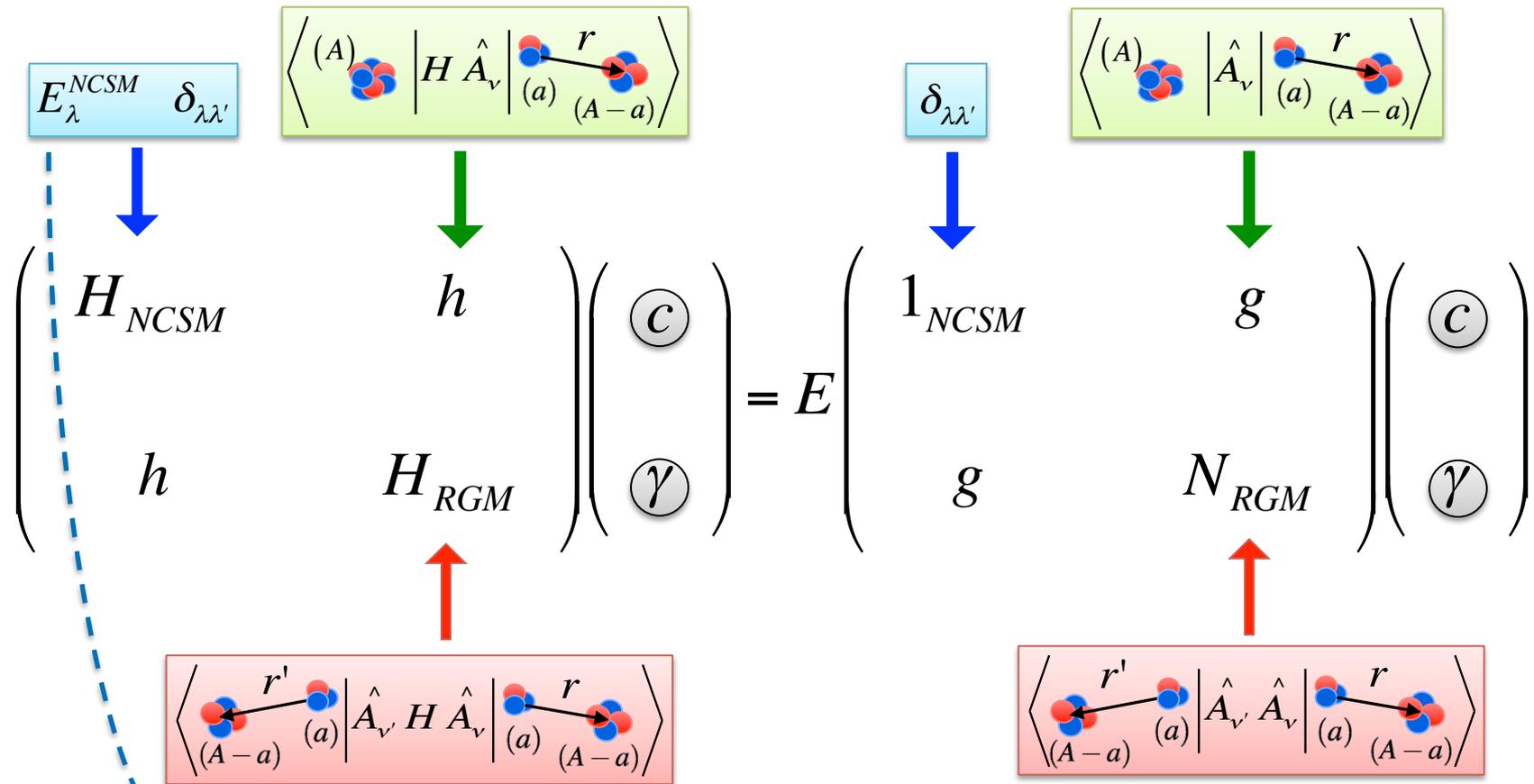
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{cluster} \end{array}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} (A-a) \\ \text{cluster} \end{array}, \nu \right\rangle$$

$$\begin{aligned} \vec{E}1 &= e \sum_{i=1}^{A-a} \frac{1 + \tau_i^{(3)}}{2} (\vec{r}_i - \vec{R}_{\text{c.m.}}^{(A-a)}) \\ &+ e \sum_{j=A-a+1}^A \frac{1 + \tau_j^{(3)}}{2} (\vec{r}_j - \vec{R}_{\text{c.m.}}^{(a)}) \\ &+ e \frac{Z_{(A-a)}a - Z_{(a)}(A-a)}{A} \vec{r}_{A-a,a}. \end{aligned}$$

$$\mathcal{M}_{1\mu}^E = e \sum_{j=1}^A \frac{1 + \tau_j^{(3)}}{2} |\vec{r}_j - \vec{R}_{\text{c.m.}}^{(A)}| Y_{1\mu}(r_j - \widehat{R}_{\text{c.m.}}^{(A)})$$

$$\begin{aligned} \mathcal{B}_{fi}^{E1} &= \sum_{\lambda\lambda'} c_{\lambda'}^{*f} \langle A\lambda' J_f^{\pi f} T_f || \mathcal{M}_1^E || A\lambda J_i^{\pi i} T_i \rangle c_{\lambda}^i \\ &+ \sum_{\lambda'\nu} \int dr r^2 c_{\lambda'}^{*f} \langle A\lambda' J_f^{\pi f} T_f || \mathcal{M}_1^E \hat{A}_{\nu} || \Phi_{\nu r}^i \rangle \frac{\gamma_{\nu}^i(r)}{r} \\ &+ \sum_{\lambda\nu'} \int dr' r'^2 \frac{\gamma_{\nu'}^{*f}(r')}{r'} \langle \Phi_{\nu' r'}^f || \hat{A}_{\nu'} \mathcal{M}_1^E || A\lambda J_i^{\pi i} T_i \rangle c_{\lambda}^i \\ &+ \sum_{\nu\nu'} \int dr' r'^2 \int dr r^2 \frac{\gamma_{\nu'}^{*f}(r')}{r'} \langle \Phi_{\nu' r'}^f || \hat{A}_{\nu'} \mathcal{M}_1^E \hat{A}_{\nu} || \Phi_{\nu r}^i \rangle \frac{\gamma_{\nu}^i(r)}{r}. \end{aligned}$$

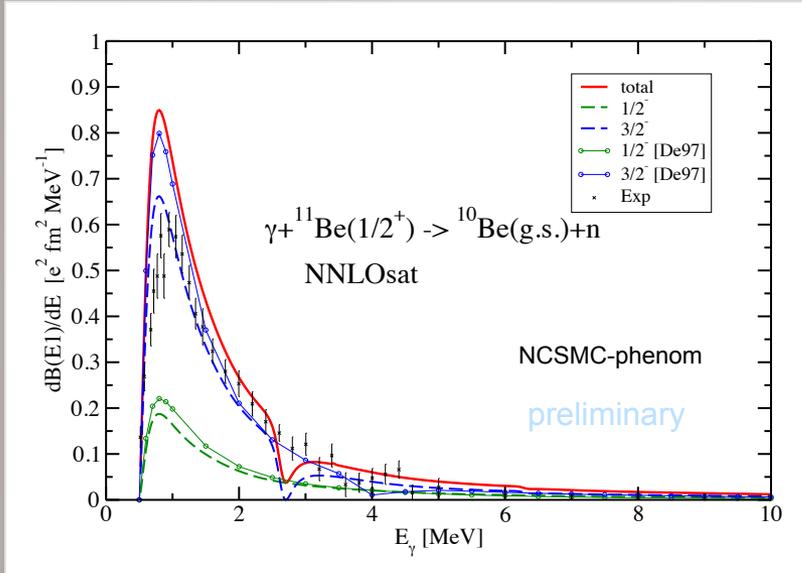
NCSMC phenomenology



E_λ^{NCSM} energies treated as adjustable parameters
 Cluster excitation energies set to experimental values

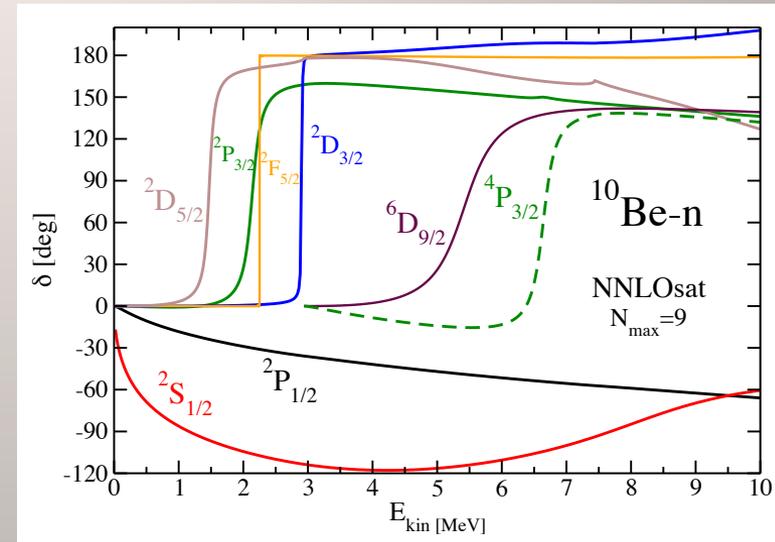
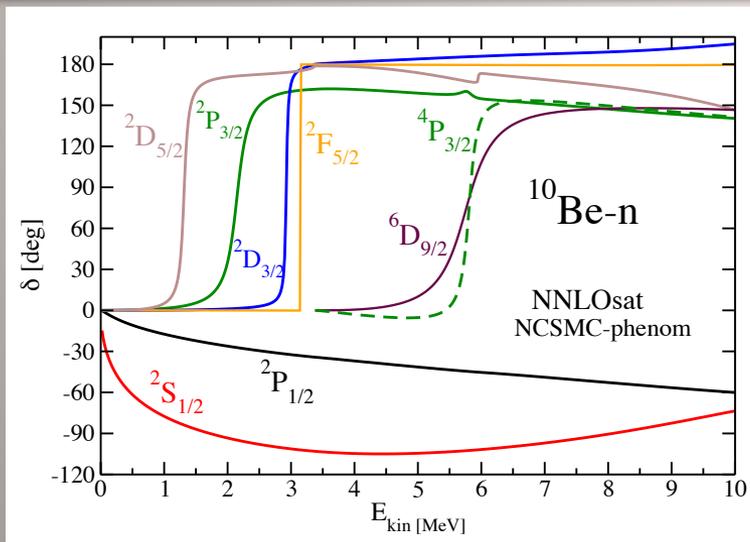
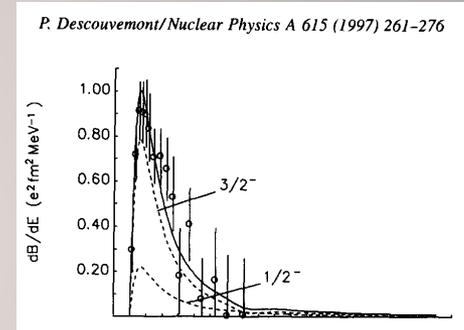
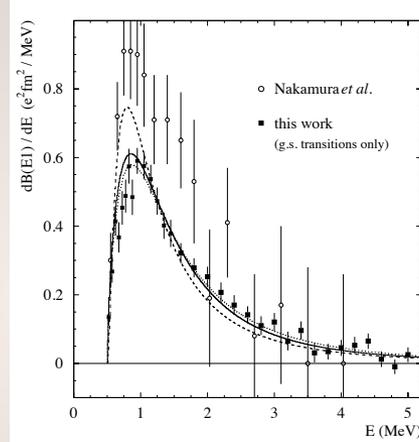
Photo-disassociation of ^{11}Be

Bound to continuum

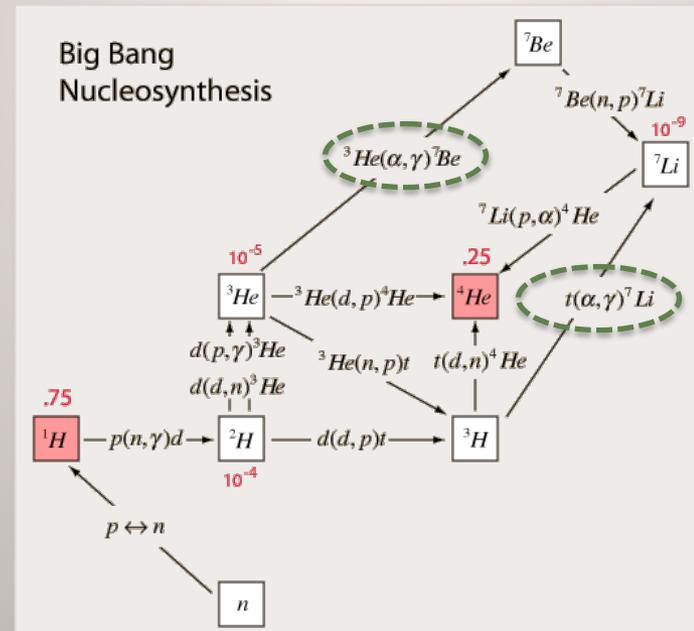
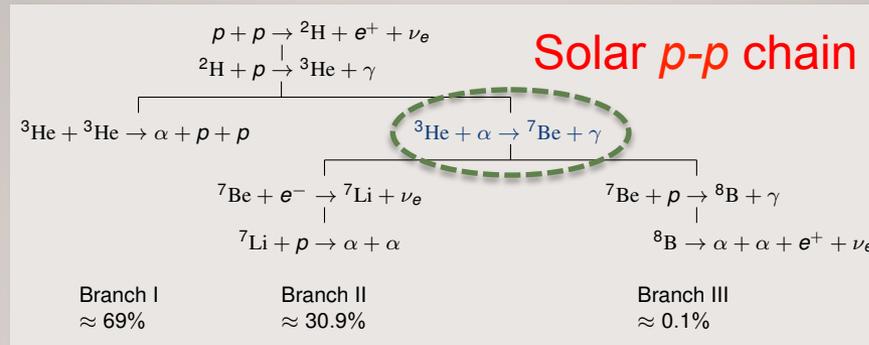


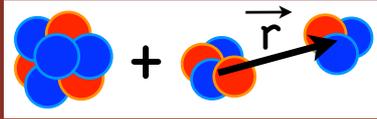
Bound to bound	NCSM	NCSMC-phenom	Expt.
$B(E1; 1/2^+ \rightarrow 1/2^-)$ [$e^2 \text{fm}^2$]	5×10^{-6}	0.118	0.102(2)

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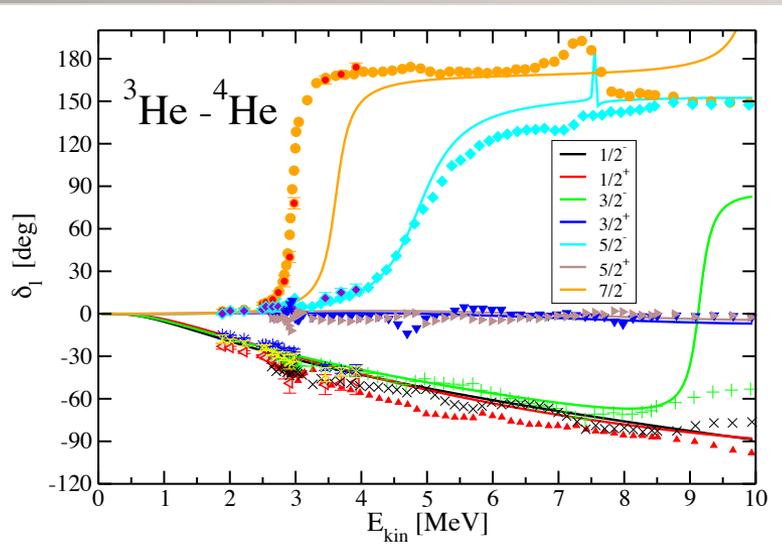


Capture reactions important for astrophysics





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



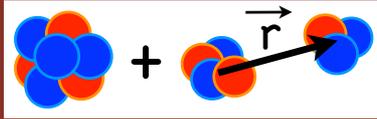
	^7Be		^7Li	
	NCSMC	Expt.	NCSMC	Expt.
$E_{3/2^-}$ [MeV]	-1.52	-1.586	-2.43	-2.467
$E_{1/2^-}$ [MeV]	-1.26	-1.157	-2.15	-1.989
r_{ch} [fm]	2.62	2.647(17)	2.42	2.390(30)
Q [$e \text{ fm}^2$]	-6.14		-3.72	-4.00(3)
μ [μ_N]	-1.16	-1.3995(5)	+3.02	+3.256

J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, arXiv:1510.07717 [nucl-th]

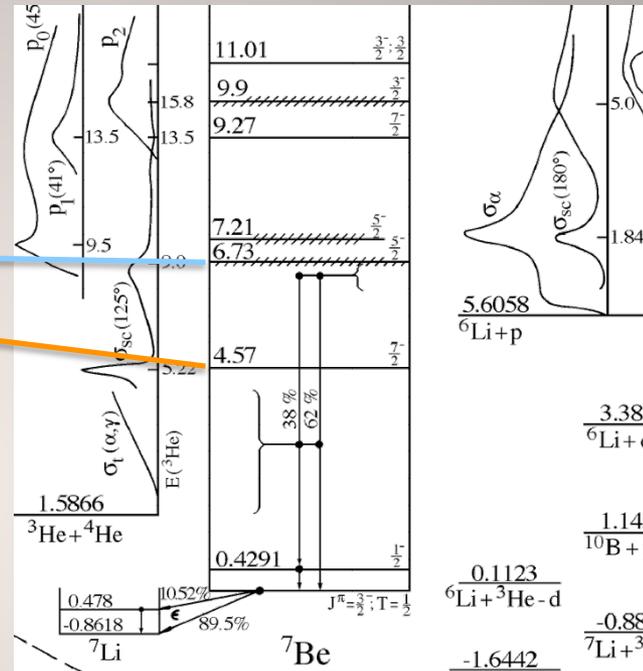
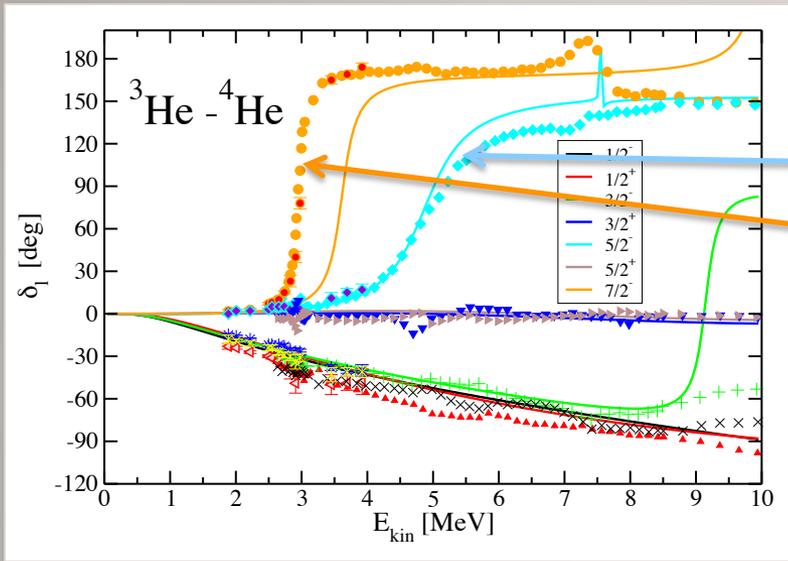
NCSMC calculations with chiral SRG- $N^3\text{LO}$ NN potential ($\lambda=2.15 \text{ fm}^{-1}$)

^3He , ^3H , ^4He ground state, $8(\pi^-) + 6(\pi^+)$ eigenstates of ^7Be and ^7Li

Preliminary: $N_{\text{max}}=12$, $h\Omega=20 \text{ MeV}$



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

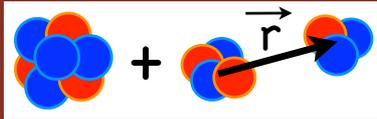


J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, arXiv:1510.07717 [nucl-th]

NCSMC calculations with chiral SRG- $N^3\text{LO}$ NN potential ($\lambda=2.15 \text{ fm}^{-1}$)

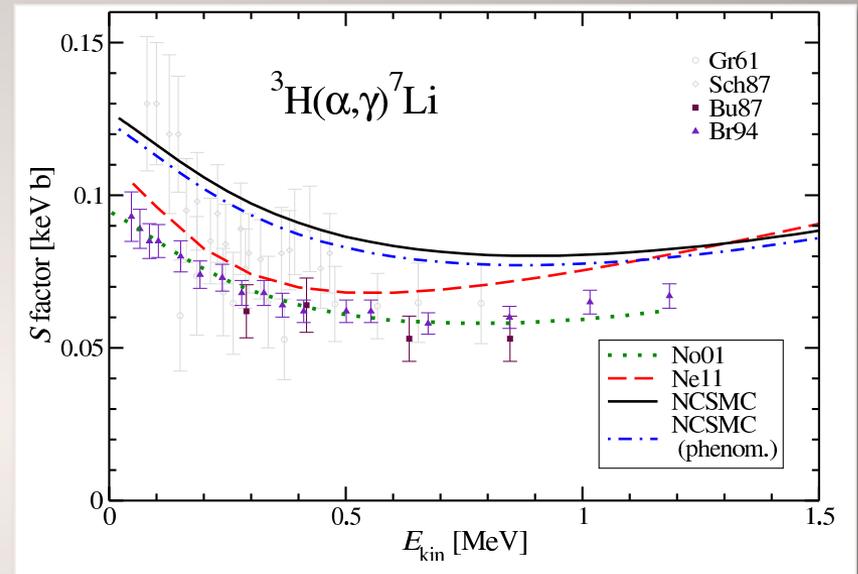
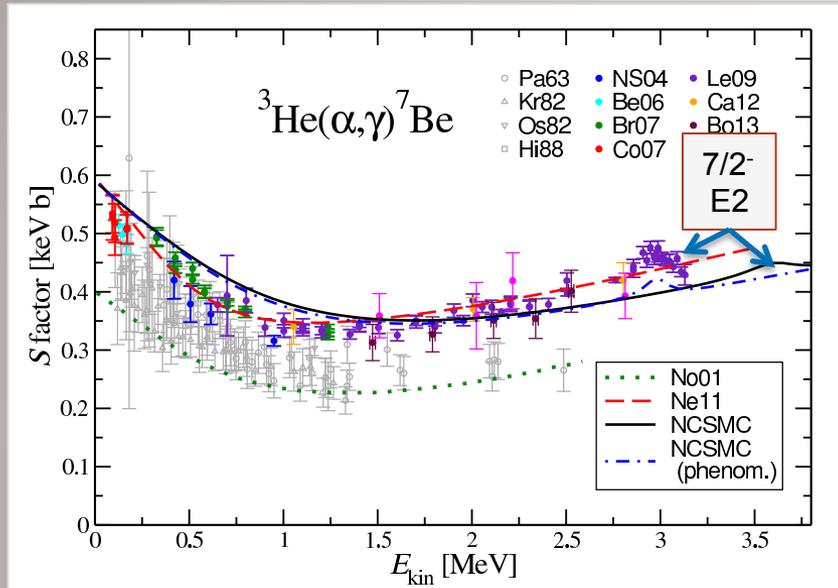
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^3He - ^4He and ^3H - ^4He capture

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



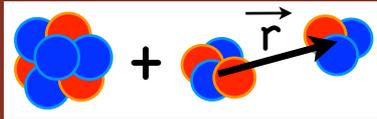
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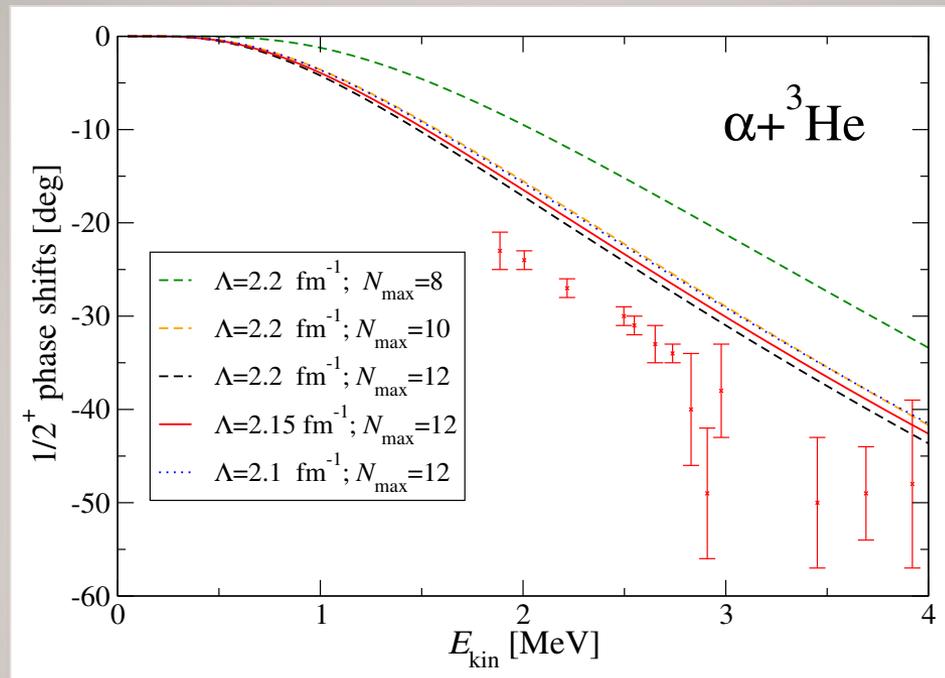
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Theoretical calculations suggest that the most recent and precise ^7Be and ^7Li data are inconsistent



^3He - ^4He S-wave phase shifts



J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, arXiv:1510.07717 [nucl-th]

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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
 - Structure of halo ^{11}Be and exotic ^{11}N discriminates among chiral interaction models
 - Extension to three-body clusters ($^6\text{He} \sim ^4\text{He} + n + n$): NCSMC in progress
- Ongoing projects:
 - Transfer reactions
 - Applications to capture reactions important for astrophysics
 - Bremsstrahlung
- Outlook
 - Alpha-clustering (^4He projectile)
 - ^{12}C and Hoyle state: $^8\text{Be} + ^4\text{He}$
 - ^{16}O : $^{12}\text{C} + ^4\text{He}$