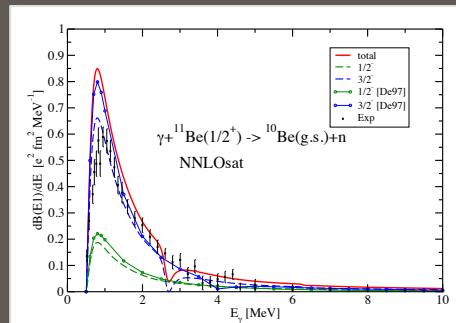
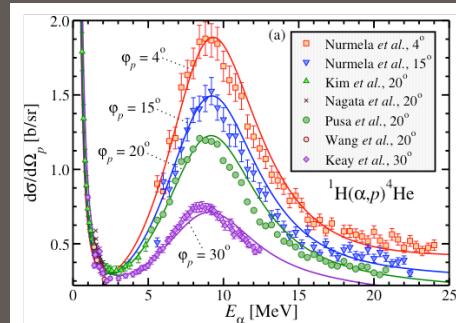


Ab Initio Unified Approach to Nuclear Structure and Reactions

INT Program INT 16-1
 Nuclear Physics from Lattice QCD
 April 5, 2016

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)

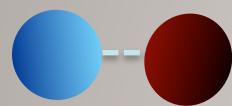
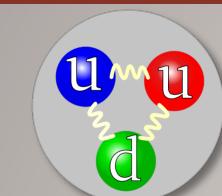
Accelerating Science for Canada
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Owned and operated as a joint venture by a consortium of Canadian universities via a contribution through the National Research Council Canada
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Outline

- No-Core Shell Model with Continuum (NCSMC) approach
- Connection to nuclear lattice EFT
- N- ${}^4\text{He}$ scattering
- ${}^6\text{Li}$ structure & d- ${}^4\text{He}$ scattering
- ${}^{11}\text{Be}$ as a laboratory for testing of nuclear forces
- ${}^{11}\text{N}$ and ${}^{10}\text{C}$ -p scattering
- ${}^3\text{He}$ - ${}^4\text{He}$ and ${}^3\text{H}$ - ${}^4\text{He}$ radiative capture

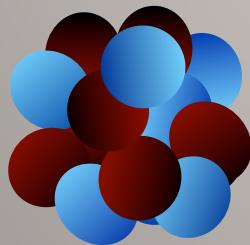
From QCD to nuclei



Low-energy QCD

NN+3N interactions
from chiral EFT

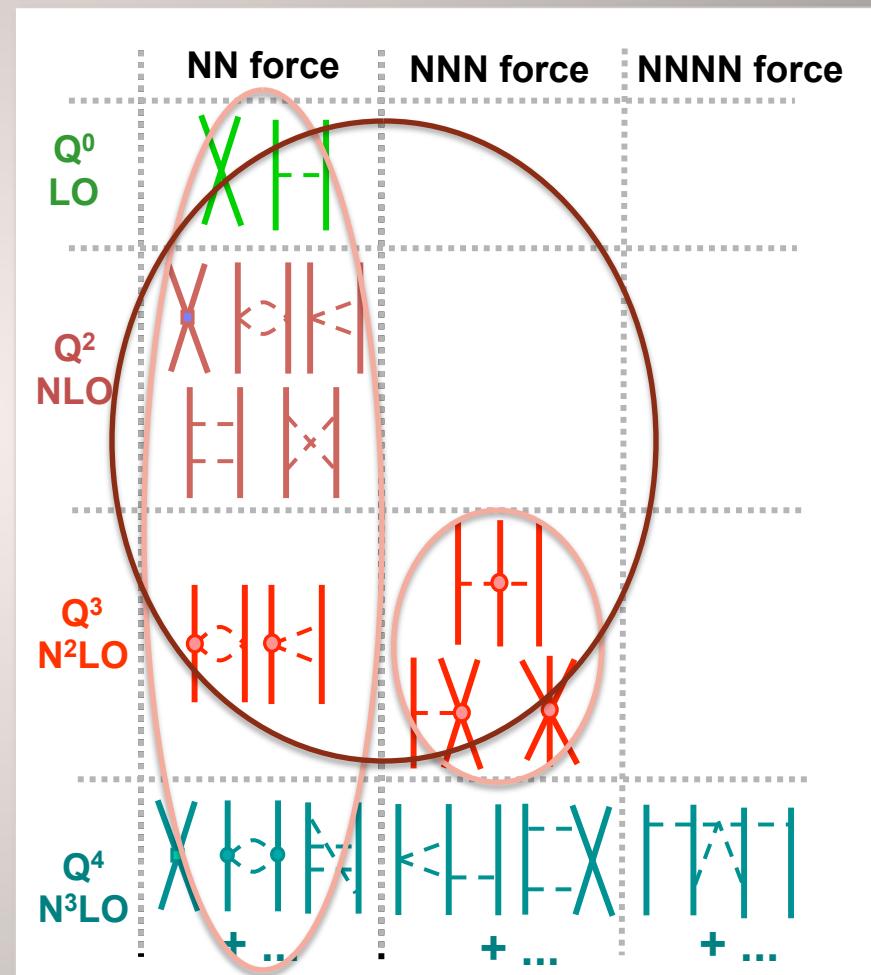
...or accurate
meson-exchange
potentials



Nuclear structure and reactions

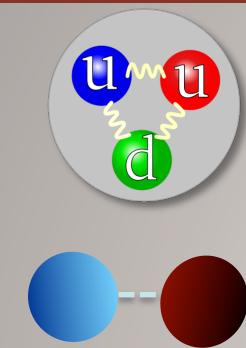
Chiral Effective Field Theory

- 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_x)
 - Hierarchy
 - Consistency
 - Low energy constants (LEC)
 - Fitted to data
 - Can be calculated by lattice QCD

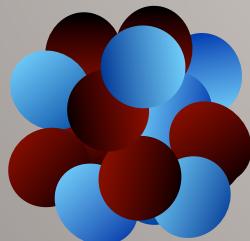


$\Lambda_x \sim 1 \text{ GeV}$:
Chiral symmetry breaking scale

From QCD to nuclei



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



Low-energy QCD

NN+3N interactions
from chiral EFT

...or accurate
meson-exchange
potentials

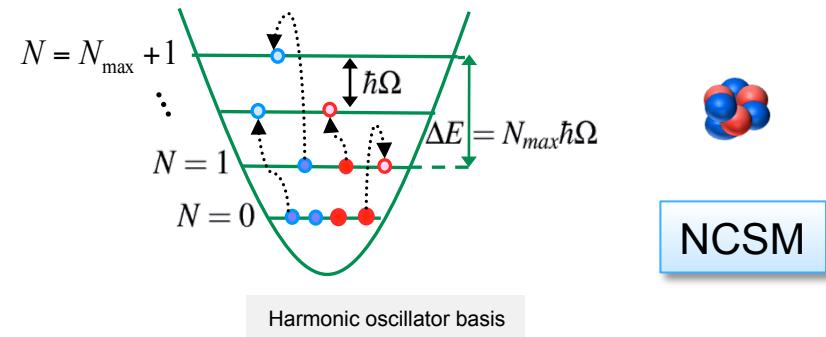
Many-Body methods

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

Nuclear structure and reactions

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

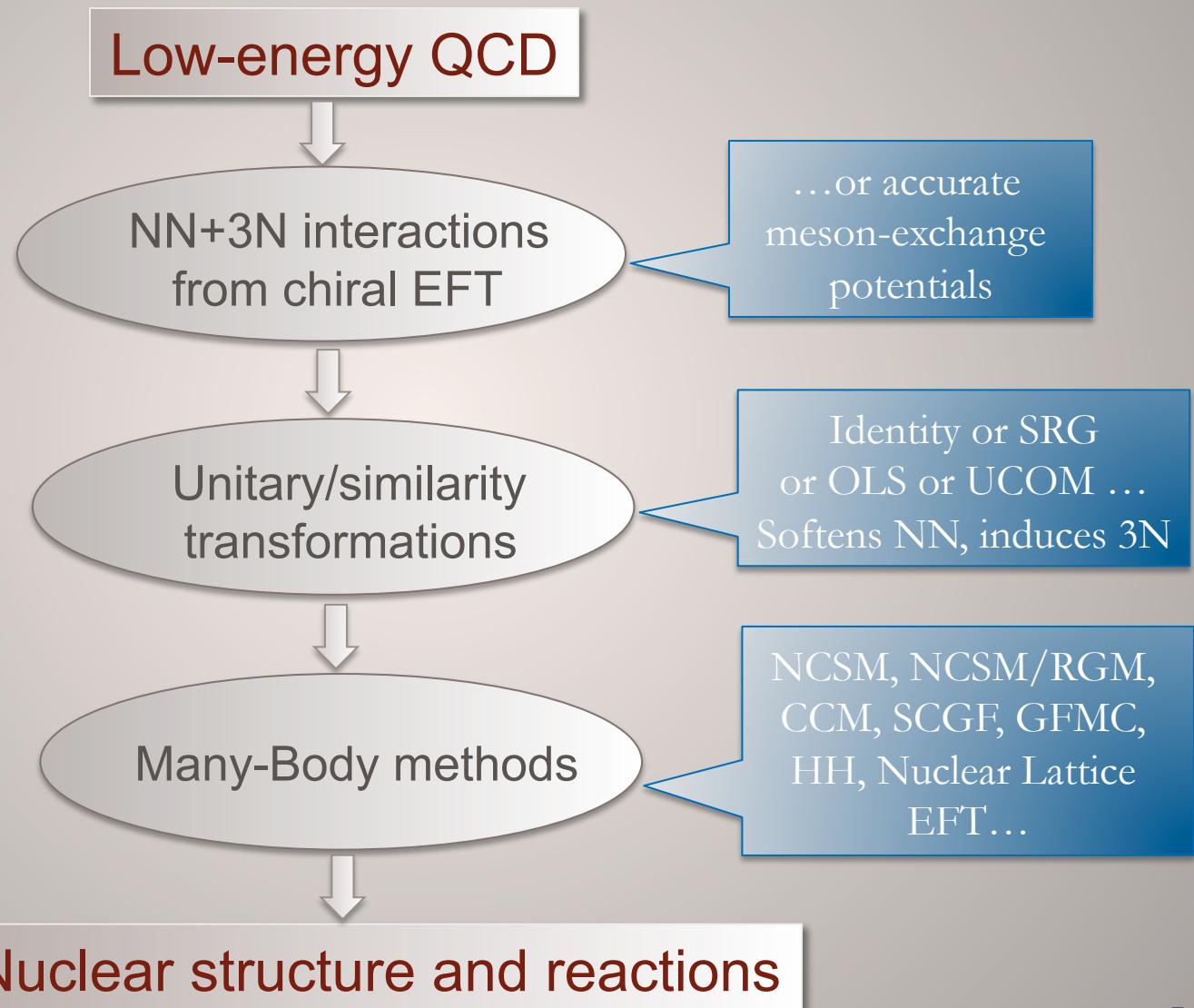
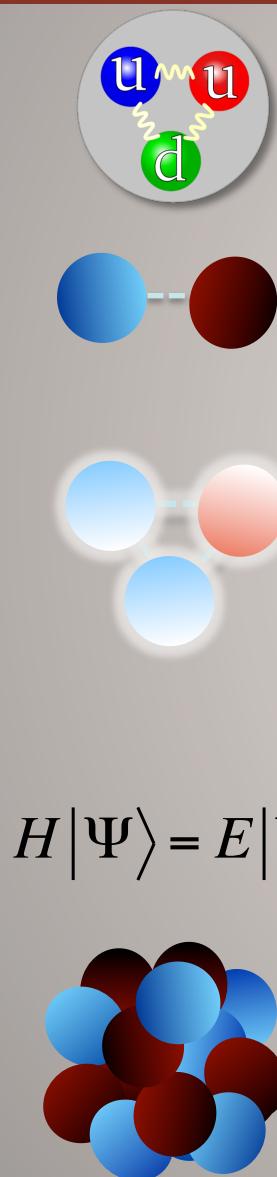
- *Ab initio* no-core shell model
 - Short- and medium range correlations
 - Bound-states, narrow resonances



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

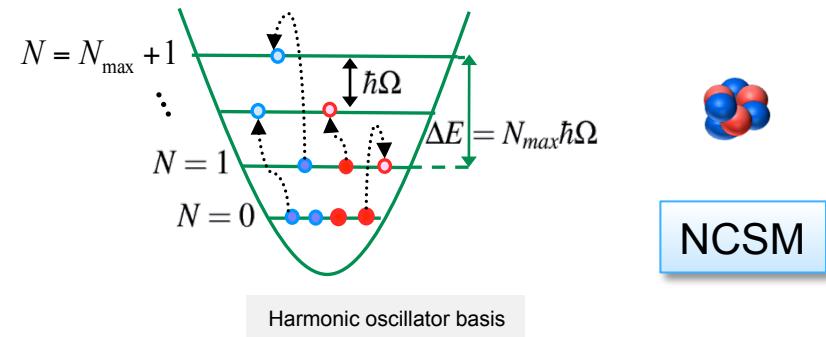
Unknowns

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

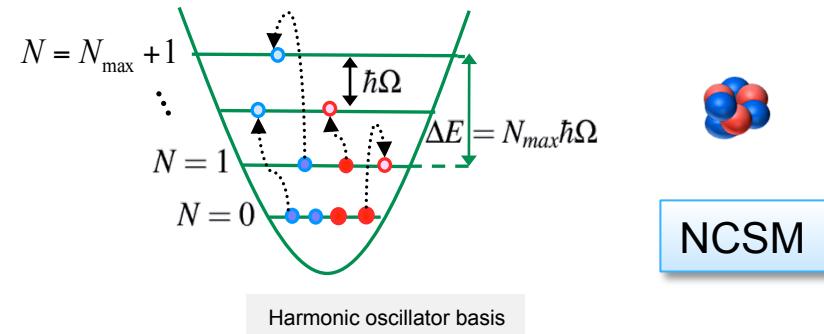


$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} |(A) \text{ (nucleus)}, \lambda \rangle$$

Unknowns

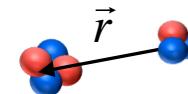
Unified approach to bound & continuum states; to nuclear structure & reactions

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



NCSM

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



NCSM/RGM

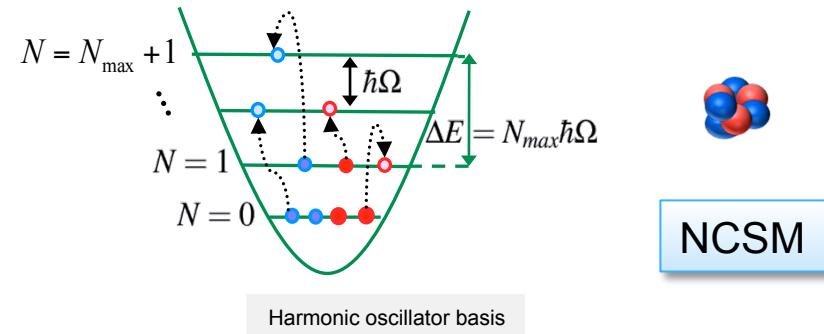
$$\Psi^{(A)} = \sum_v \int d\vec{r} \gamma_v(\vec{r}) \hat{A}_v \left| \begin{array}{c} \text{NCSM/RGM} \\ \text{channel states} \end{array} \right\rangle_{(A-a), v}$$

Unknowns

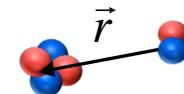
A red arrow points from the text "Unknowns" to the integration variable $d\vec{r}$ in the equation.

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



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

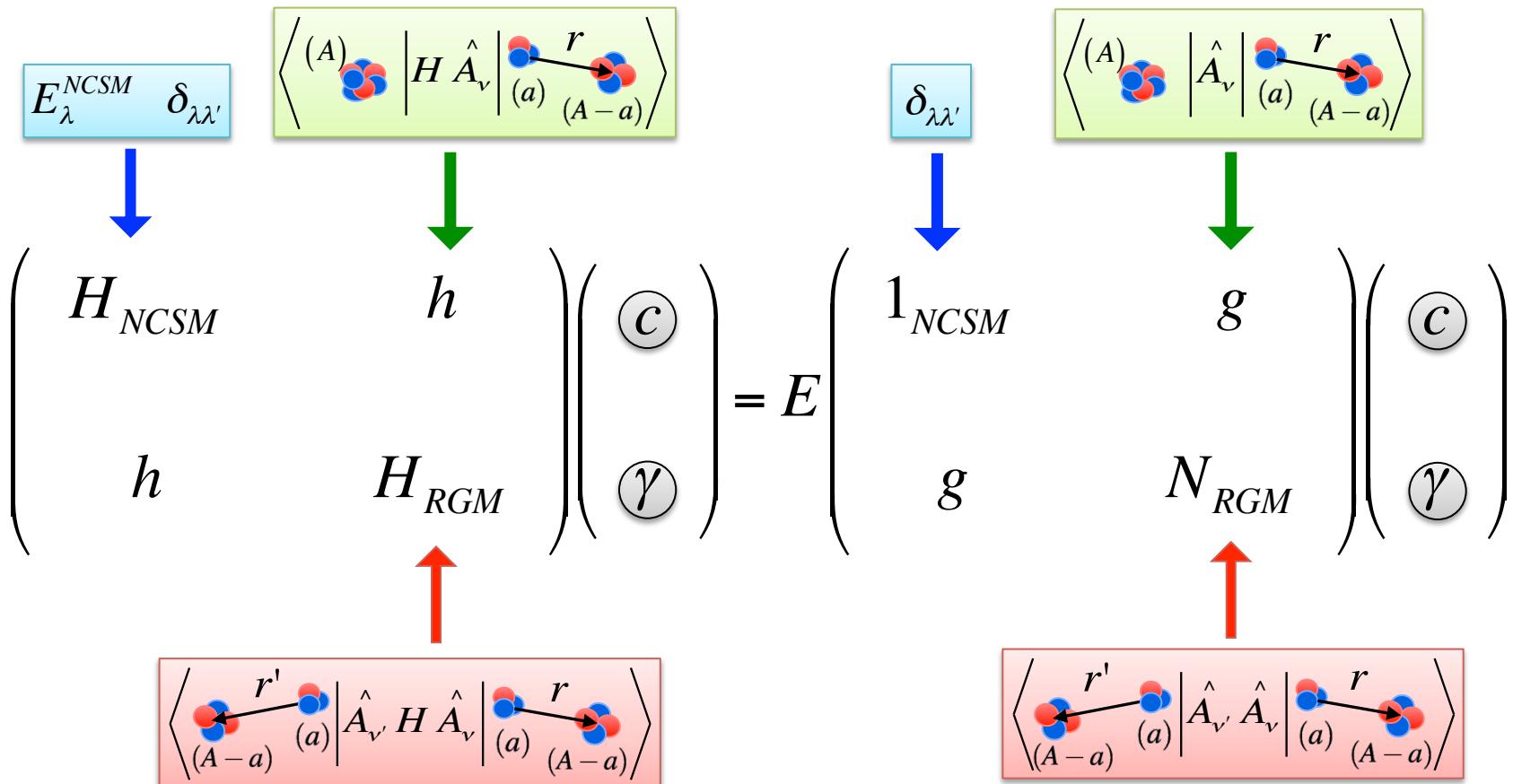
- Most efficient: *ab initio* no-core shell model with continuum

NCSMC

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

The equation shows the *ab initio* no-core shell model with continuum (NCSMC) wavefunction. It is a sum of two terms. The first term, labeled "NCSM eigenstates", contains a molecule icon and a parameter λ . The second term, labeled "NCSM/RGM channel states", contains a cluster icon and a parameter ν . Red arrows point from the labels "NCSM eigenstates" and "NCSM/RGM channel states" to their respective parts of the equation. A label "Unknowns" is positioned below the integration term.

Coupled NCSMC equations



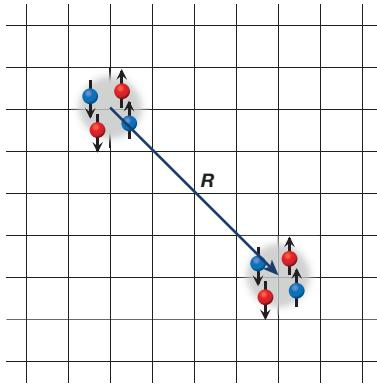
Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic R -matrix on Lagrange mesh

Connection to nuclear lattice EFT

doi:10.1038/nature16067

Ab initio alpha–alpha scattering

Serdar Elhatisari¹, Dean Lee², Gautam Rupak³, Evgeny Epelbaum⁴, Hermann Krebs⁴, Timo A. Lähde⁵, Thomas Luu^{1,5} & Ulf-G. Meißner^{1,5,6}



Lattice EFT
Adiabatic projection method

$$|\mathbf{R}\rangle = \sum_{\mathbf{r}} |\mathbf{r} + \mathbf{R}\rangle_1 \otimes |\mathbf{r}\rangle_2$$

$$|R\rangle^{\ell,\ell_z} = \sum_{R'} Y_{\ell,\ell_z}(R') \delta_{R,R'} |\mathbf{R}'\rangle$$

$$|R\rangle_{\tau}^{\ell,\ell_z} = \exp(-H\tau) |R\rangle^{\ell,\ell_z}$$

NCSM/RGM

$$\hat{A}_v \left|_{(A-a)}^{(a)}, v \right\rangle$$

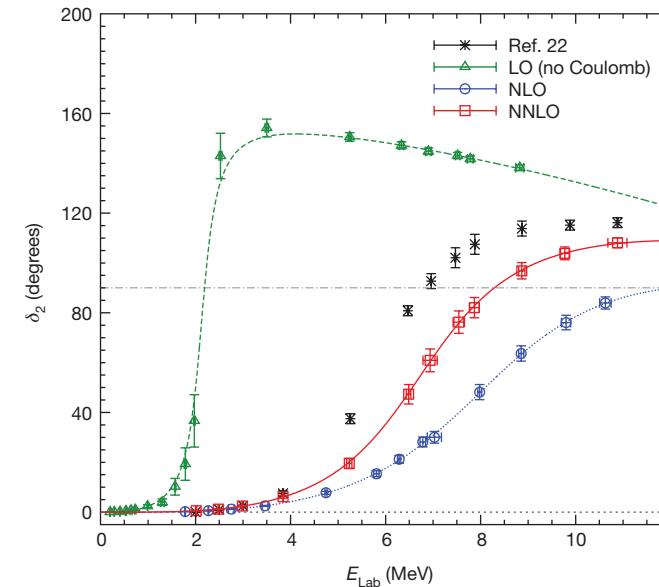
NCSM/RGM

Lattice EFT
Auxiliary field MC

$$[H_{\tau}]_{R,R'}^{\ell,\ell_z} = {}^{\ell,\ell_z}_{\tau} \langle R | H | R' \rangle_{\tau}^{\ell,\ell_z}$$

$$[N_{\tau}]_{R,R'}^{\ell,\ell_z} = {}^{\ell,\ell_z}_{\tau} \langle R | R' \rangle_{\tau}^{\ell,\ell_z}$$

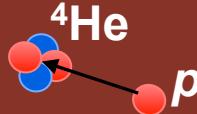
$$[H_{\tau}^a]_{R,R'}^{\ell,\ell_z} = [N_{\tau}^{-1/2} H_{\tau} N_{\tau}^{-1/2}]_{R,R'}^{\ell,\ell_z}$$



Scattering states

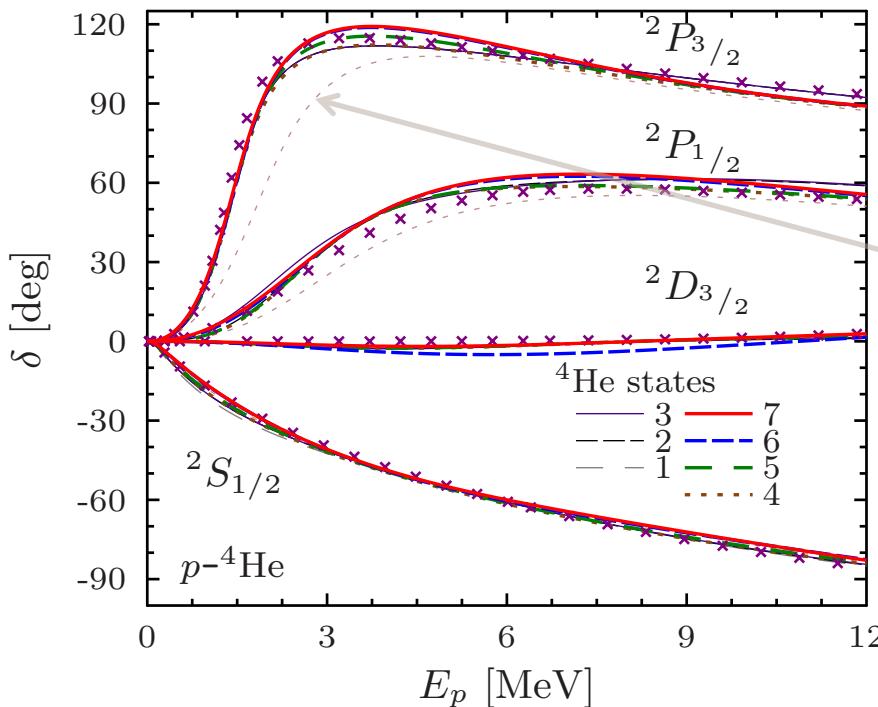
Lattice EFT –
hard spherical wall

NCSM/RGM –
Microscopic R-matrix



$p\text{-}{}^4\text{He}$ scattering within NCSMC

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



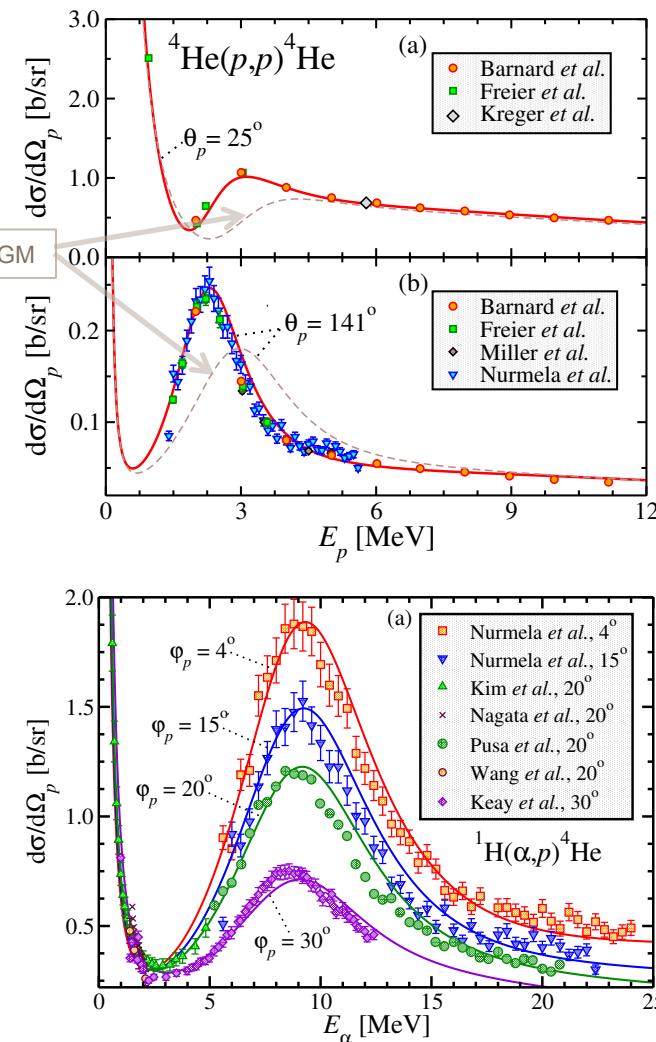
Predictive power in the $3/2^-$ resonance region:
Applications to material science

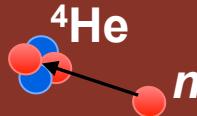
PHYSICAL REVIEW C 90, 061601(R) (2014)

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

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

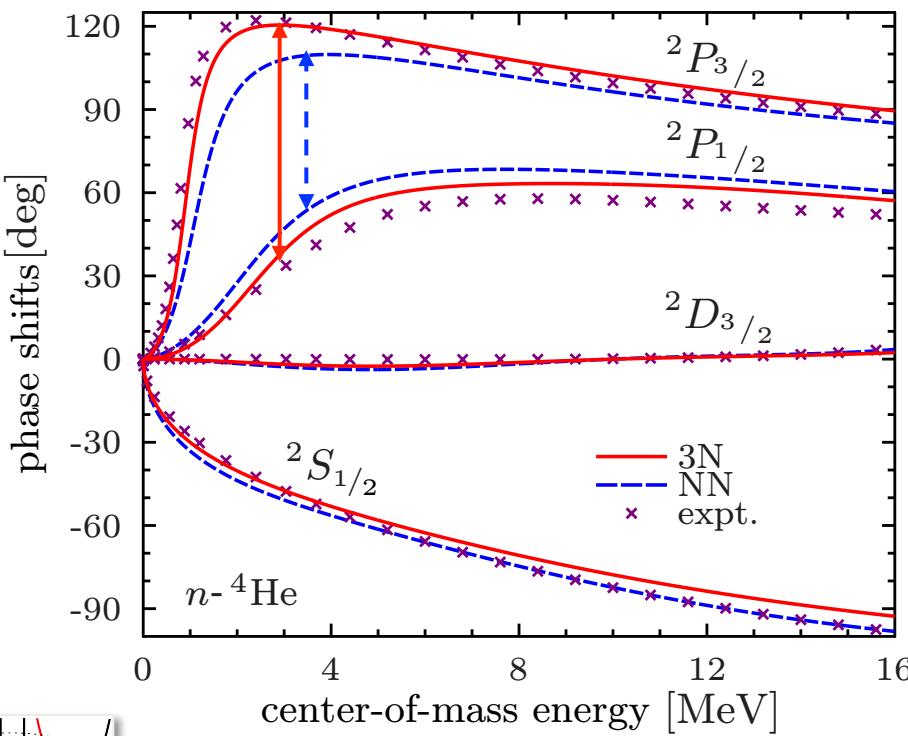
Differential $p\text{-}{}^4\text{He}$ cross section with NN+3N potentials



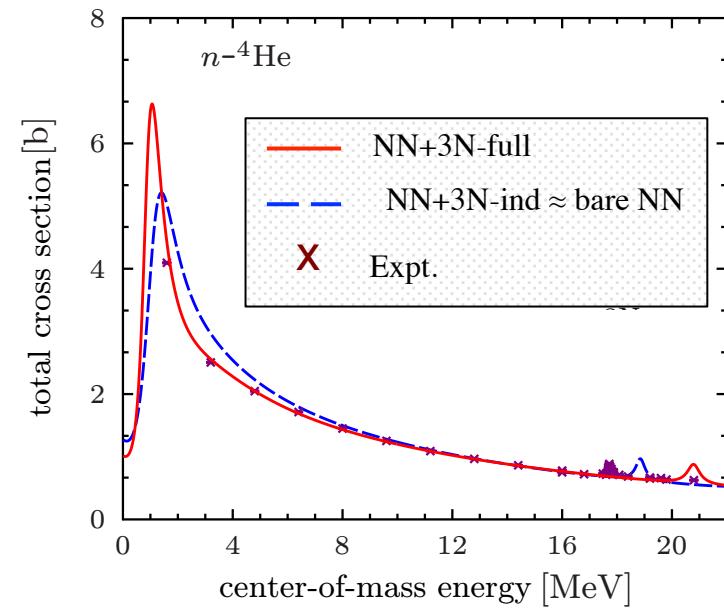


$n\text{-}{}^4\text{He}$ scattering within NCSMC

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



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



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



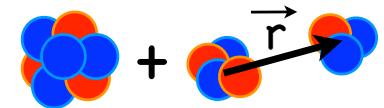
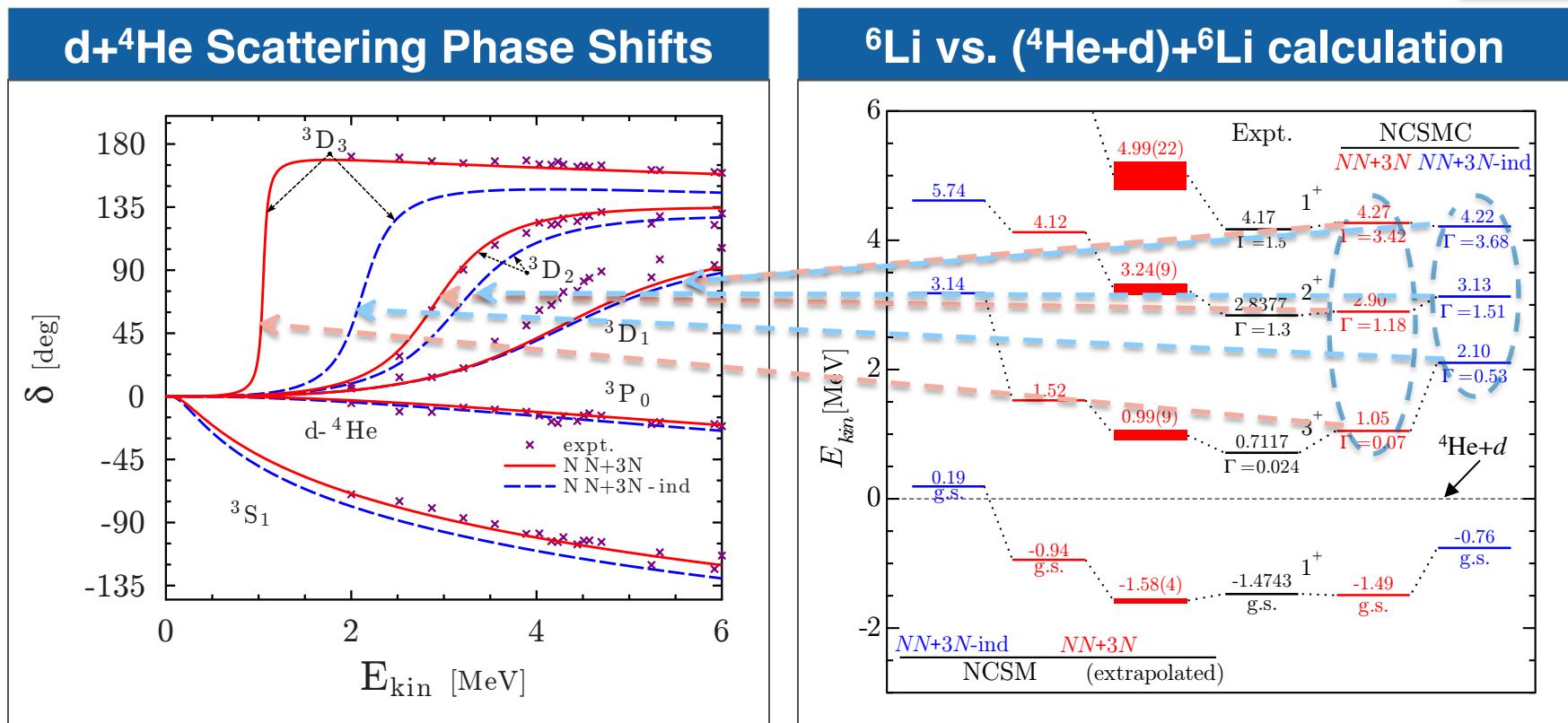
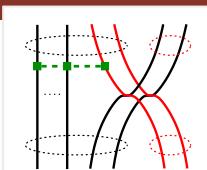
PHYSICAL REVIEW C 88, 054622 (2013)

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

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

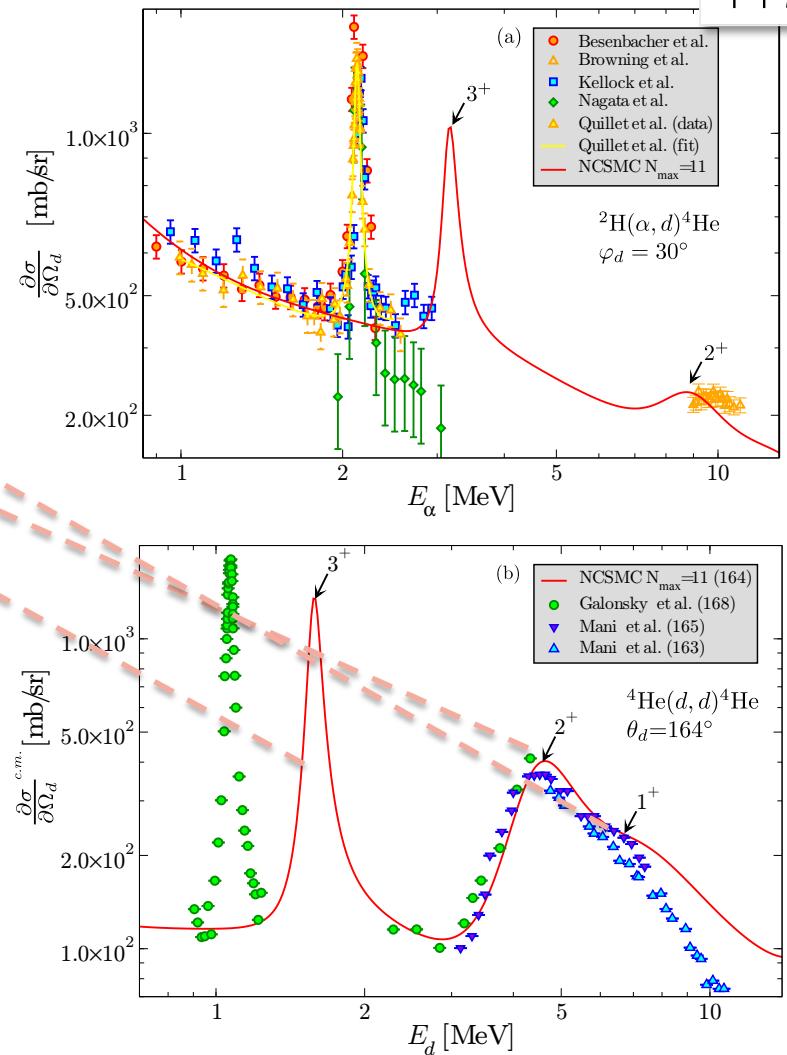
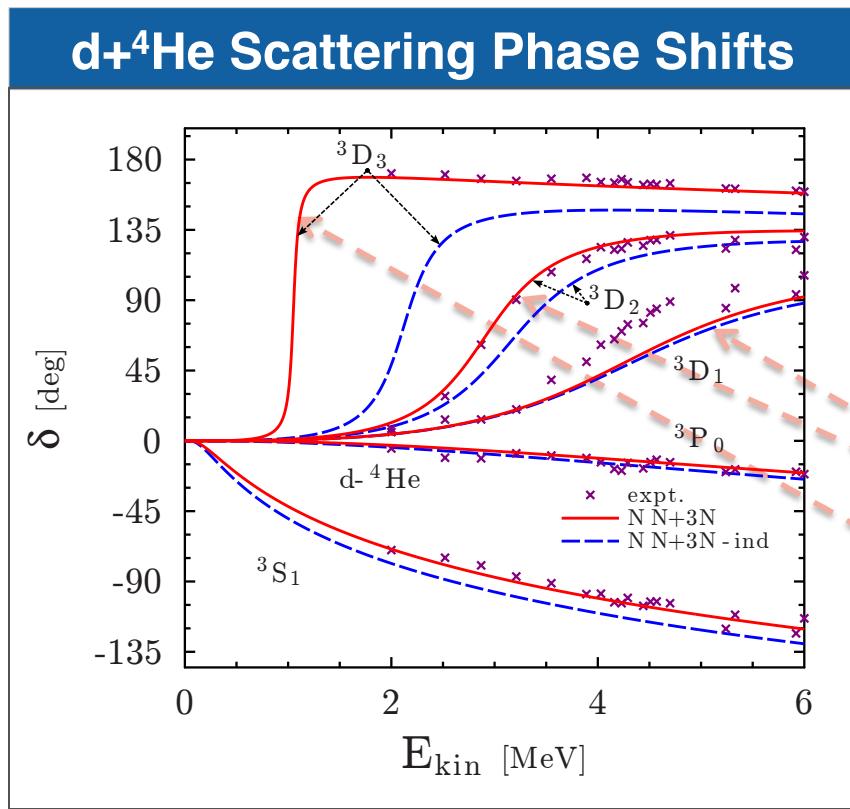
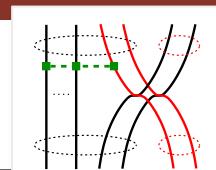
Unified description of ${}^6\text{Li}$ structure and $\text{d}+{}^4\text{He}$ dynamics

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



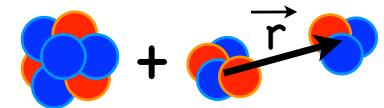
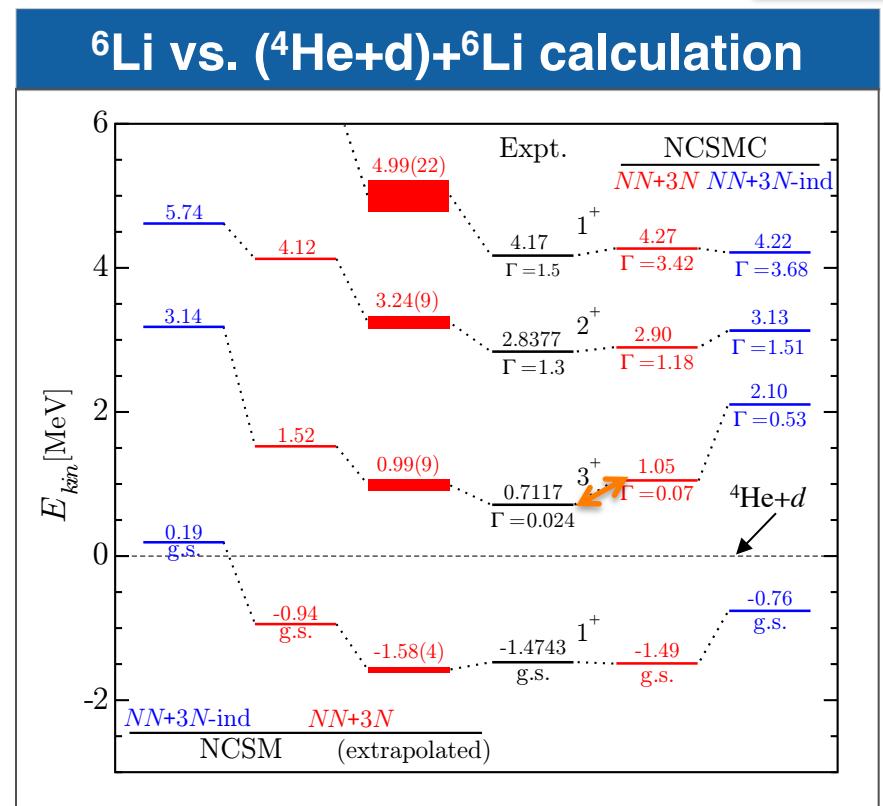
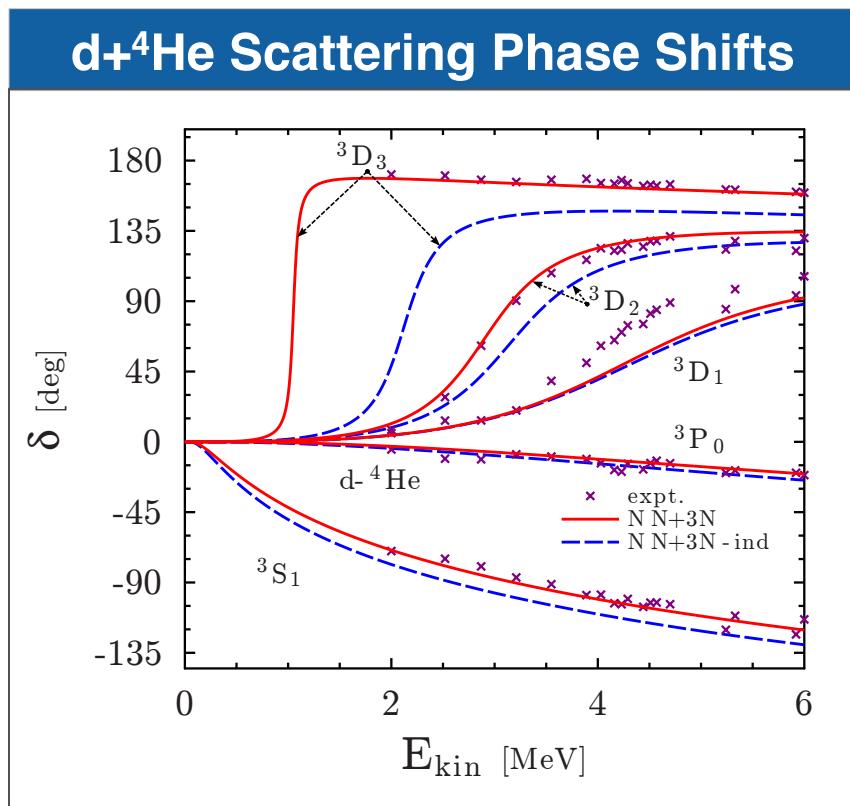
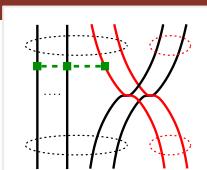
Unified description of ${}^6\text{Li}$ structure and $\text{d}+{}^4\text{He}$ dynamics

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



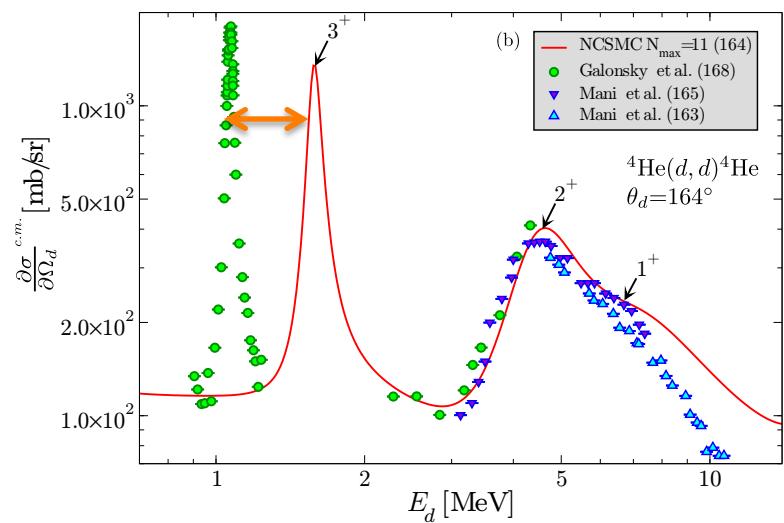
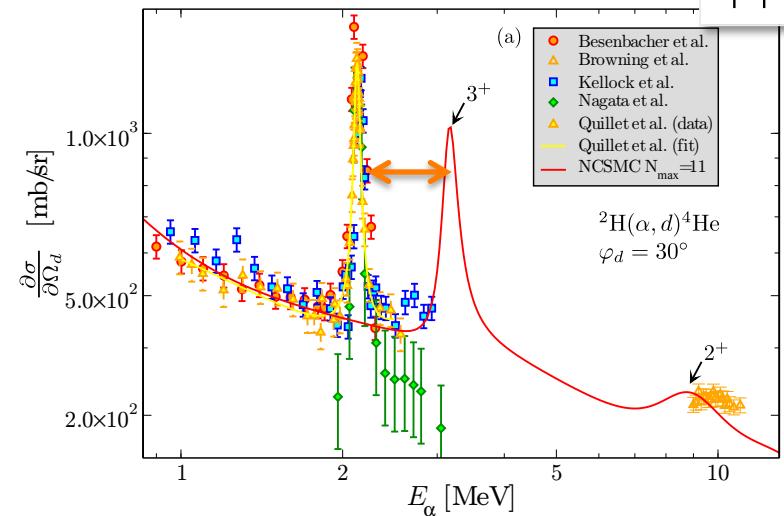
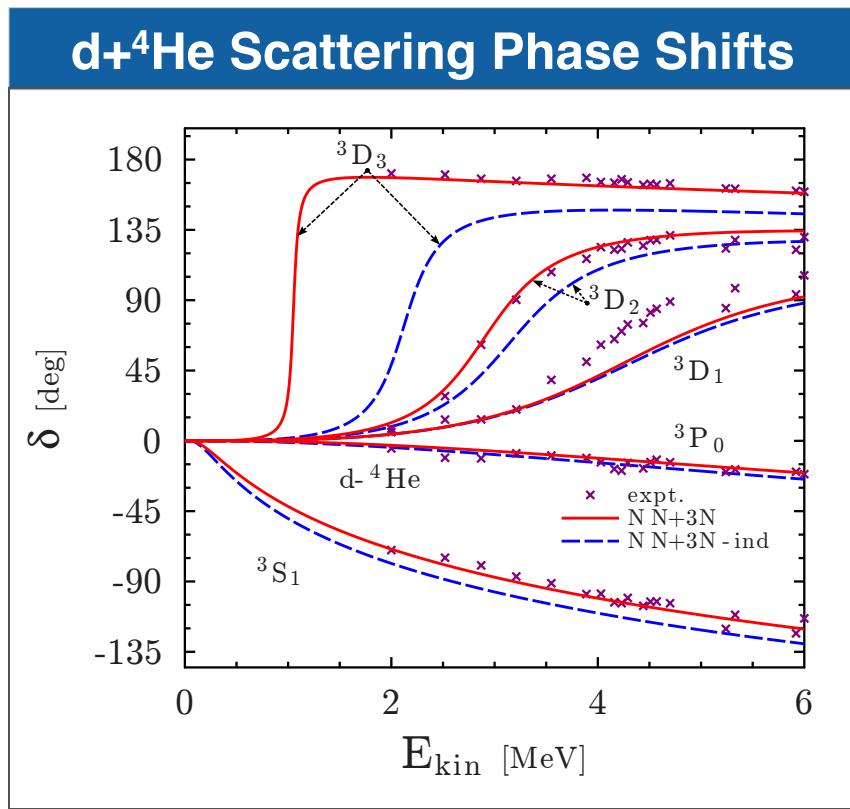
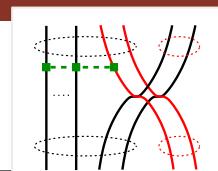
Unified description of ${}^6\text{Li}$ structure and $\text{d}+{}^4\text{He}$ dynamics

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



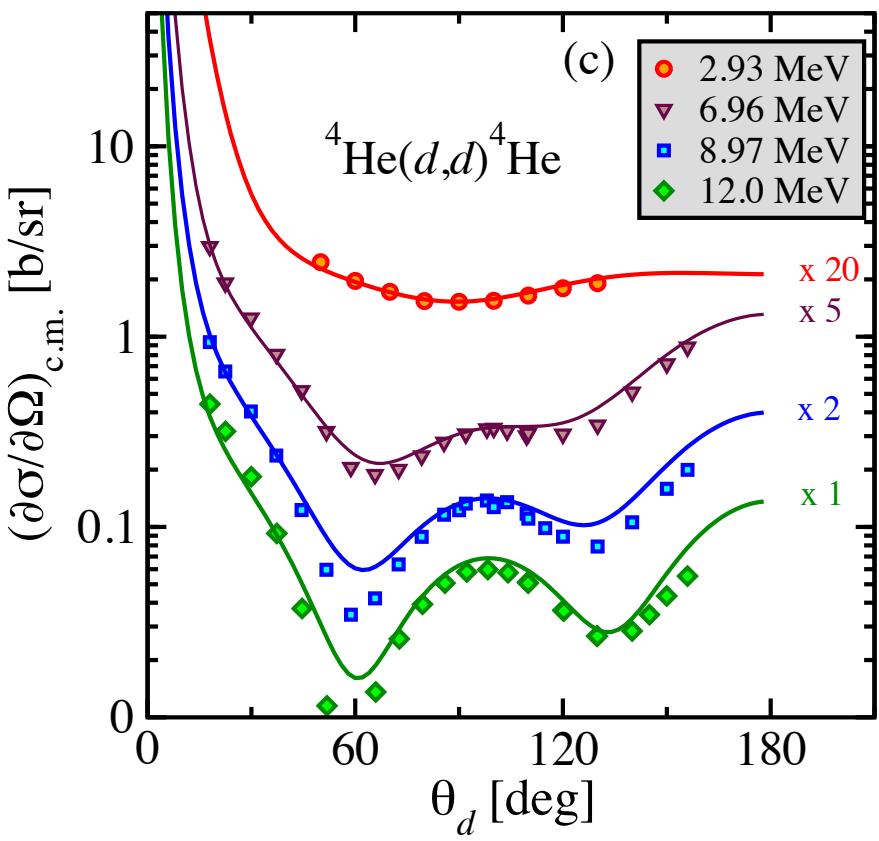
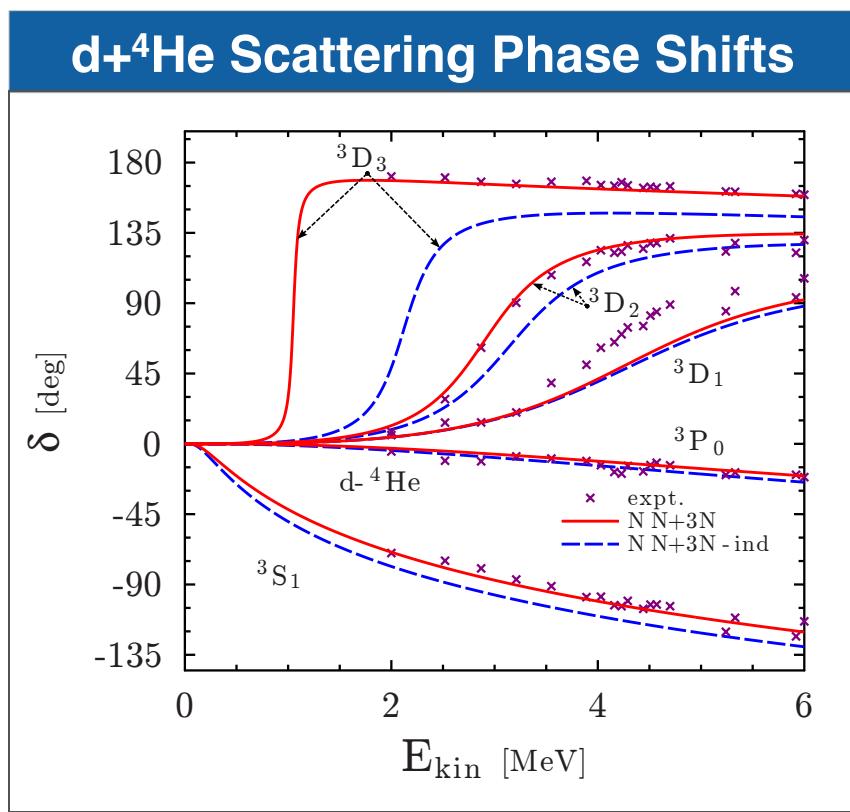
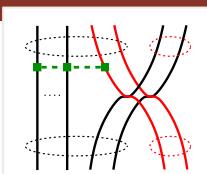
Unified description of ${}^6\text{Li}$ structure and $\text{d}+{}^4\text{He}$ dynamics

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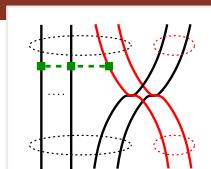


Unified description of ${}^6\text{Li}$ structure and $\text{d}+{}^4\text{He}$ dynamics

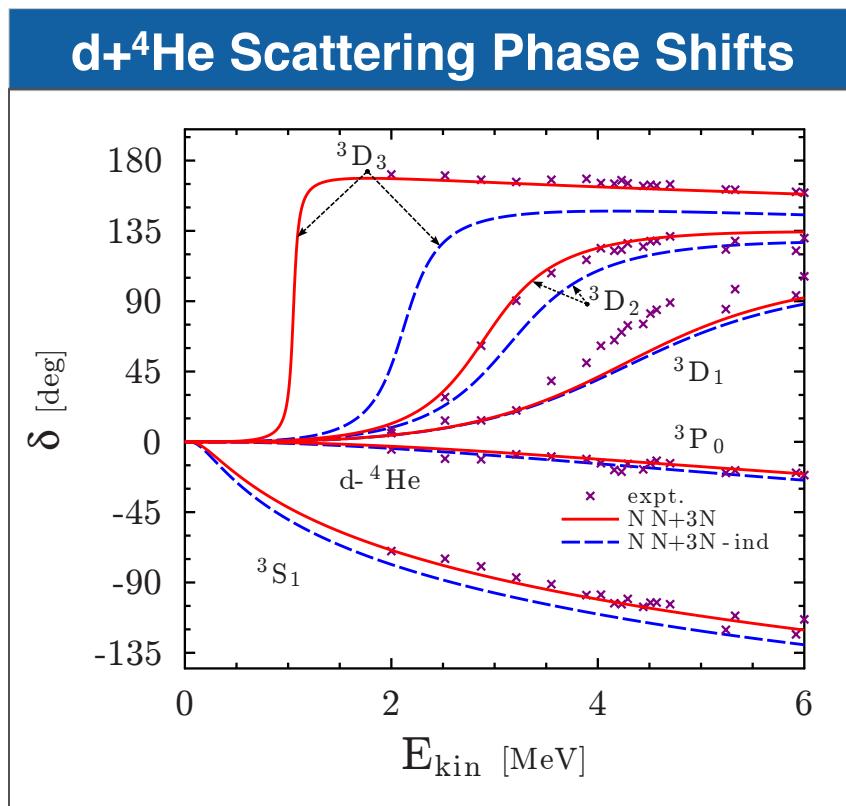
- Continuum and three-nucleon force effects on $\text{d}+{}^4\text{He}$ and ${}^6\text{Li}$



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



- S- and D-wave asymptotic normalization constants



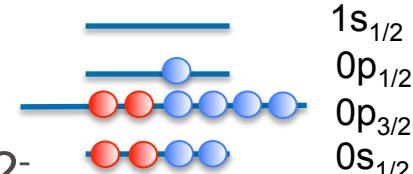
	NCSMC	Experiment
C_0 [fm $^{-1/2}$]	2.695	2.91(9) [39]
C_2 [fm $^{-1/2}$]	-0.074	-0.077(18) [39]
C_2/C_0	-0.027	-0.025(6)(10) [39]
		0.0003(9) [41]

- [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).

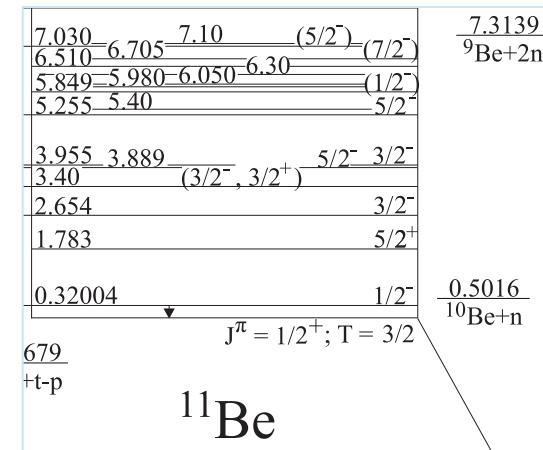
Neutron-rich halo nucleus ^{11}Be

- $Z=4, N=7$

- 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

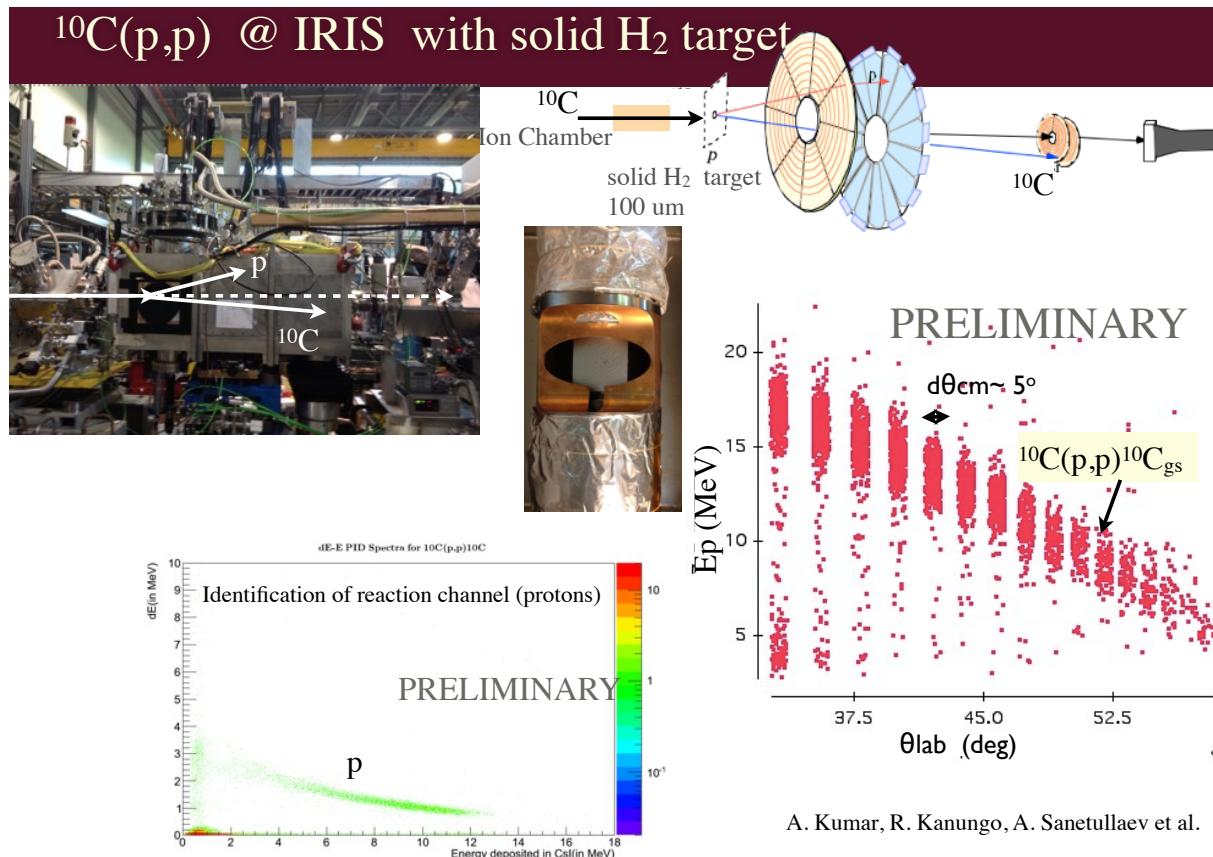


- Can we describe ^{11}Be in *ab initio* calculations?
 - Continuum must be included
 - Does the 3N interaction play a role in the parity inversion?



$^{10}\text{C}(\text{p},\text{p})$ @ IRIS with solid H_2 target

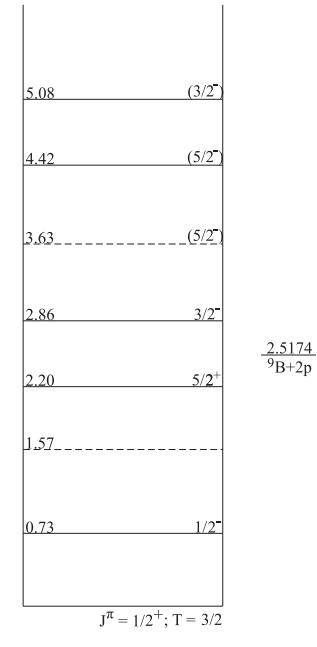
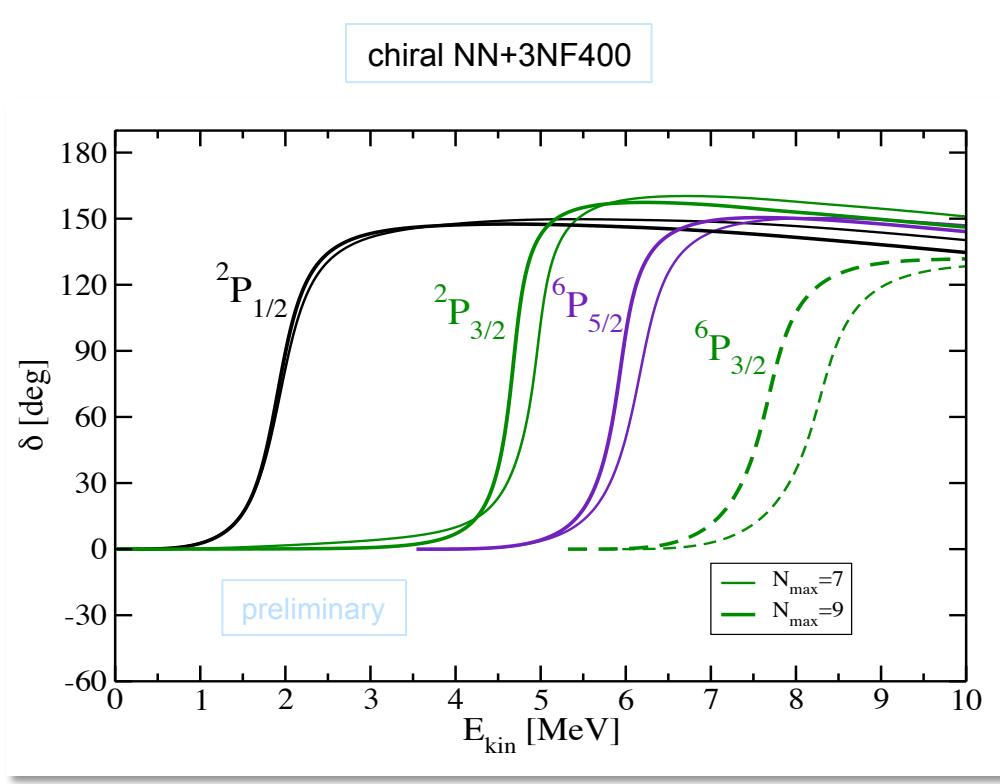
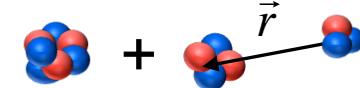
- New experiment at ISAC TRIUMF with reaccelerated ^{10}C
 - The first ever ^{10}C beam at TRIUMF
 - Angular distributions measured at $E_{\text{CM}} \sim 4.16 \text{ MeV}$ and 4.4 MeV



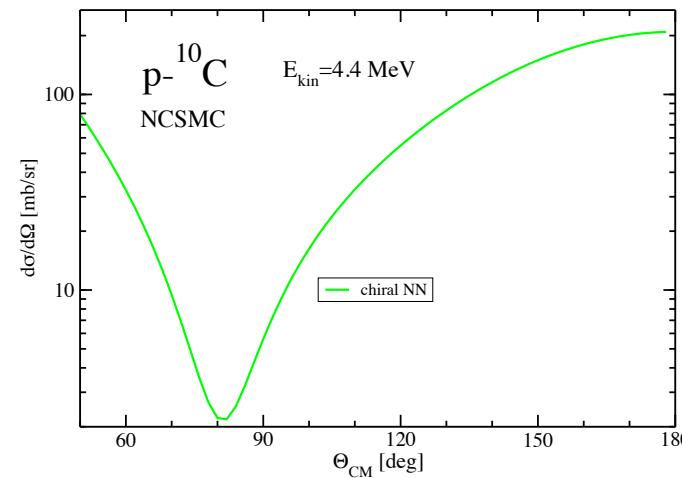
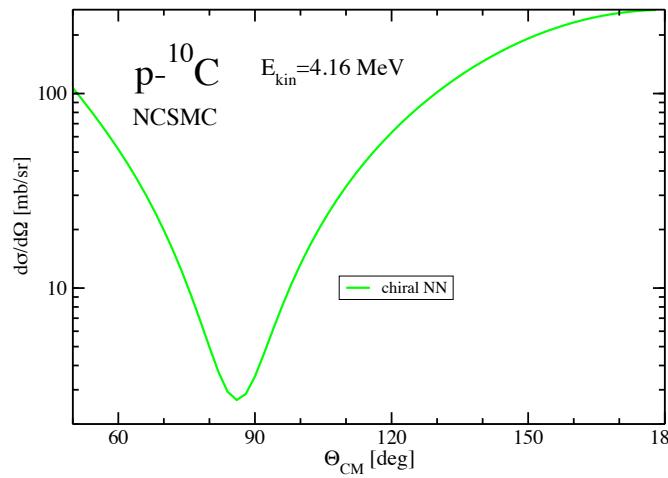
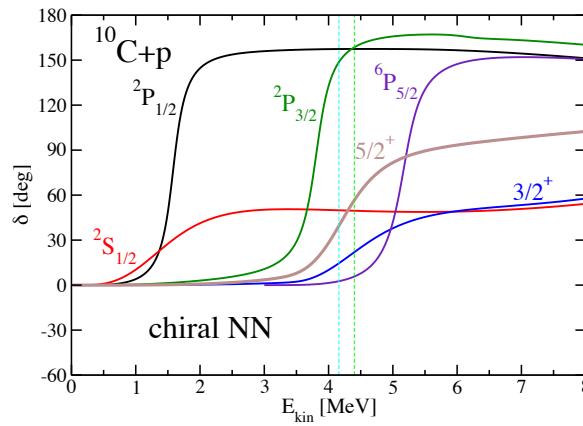
IRIS collaboration:
A. Kumar, R. Kanungo,
A. Sanetullaev *et al.*

p+¹⁰C scattering: structure of ¹¹N resonances

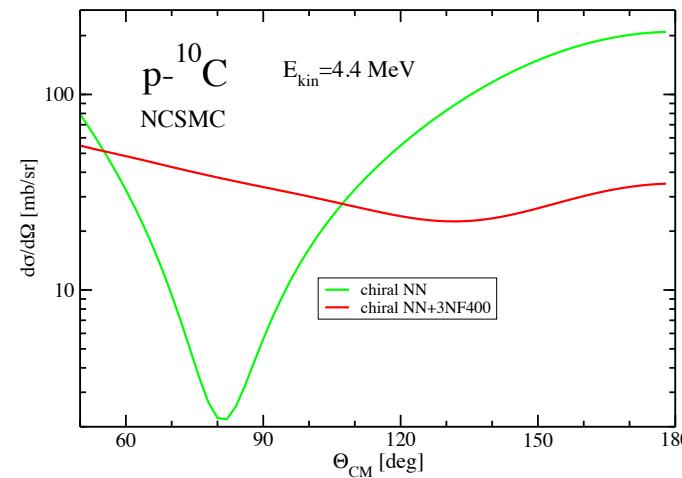
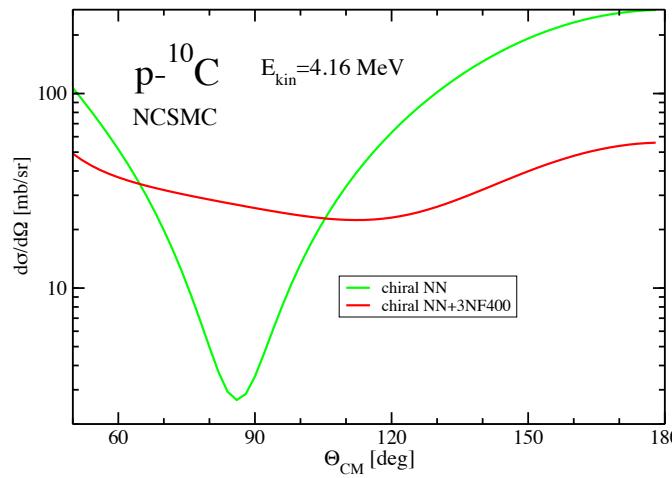
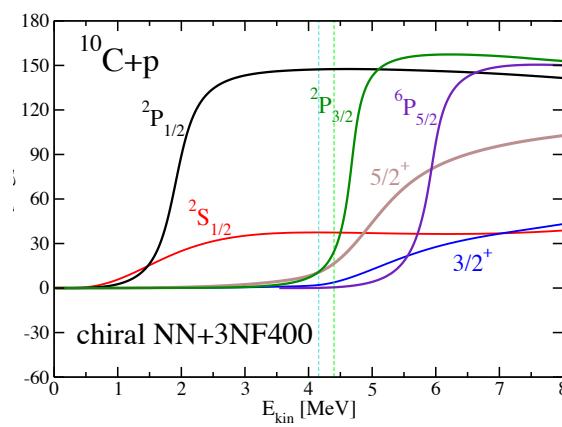
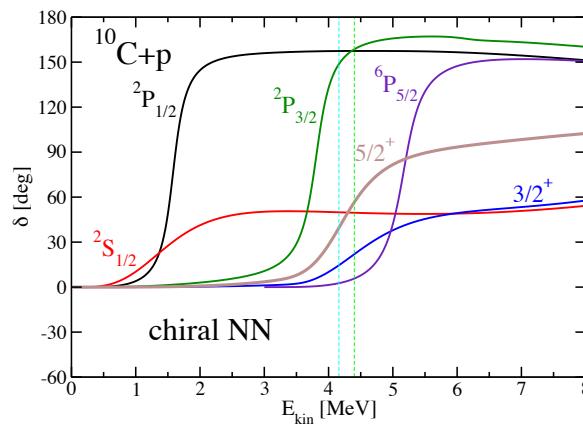
- NCSMC calculations with **chiral NN+3N** (N^3LO NN+N 2LO 3NF400, NNLOsat)
 - p-¹⁰C + ¹¹N
 - ¹⁰C: 0^+ , 2^+ , 2^+ NCSM eigenstates
 - ¹¹N: $\geq 4 \pi = -1$ and $\geq 3 \pi = +1$ NCSM eigenstates

¹¹N^{-1.4893}
¹⁰C+p

p+¹⁰C scattering: structure of ¹¹N resonances

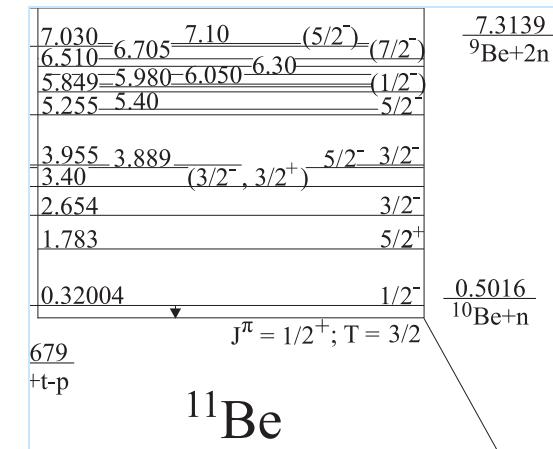
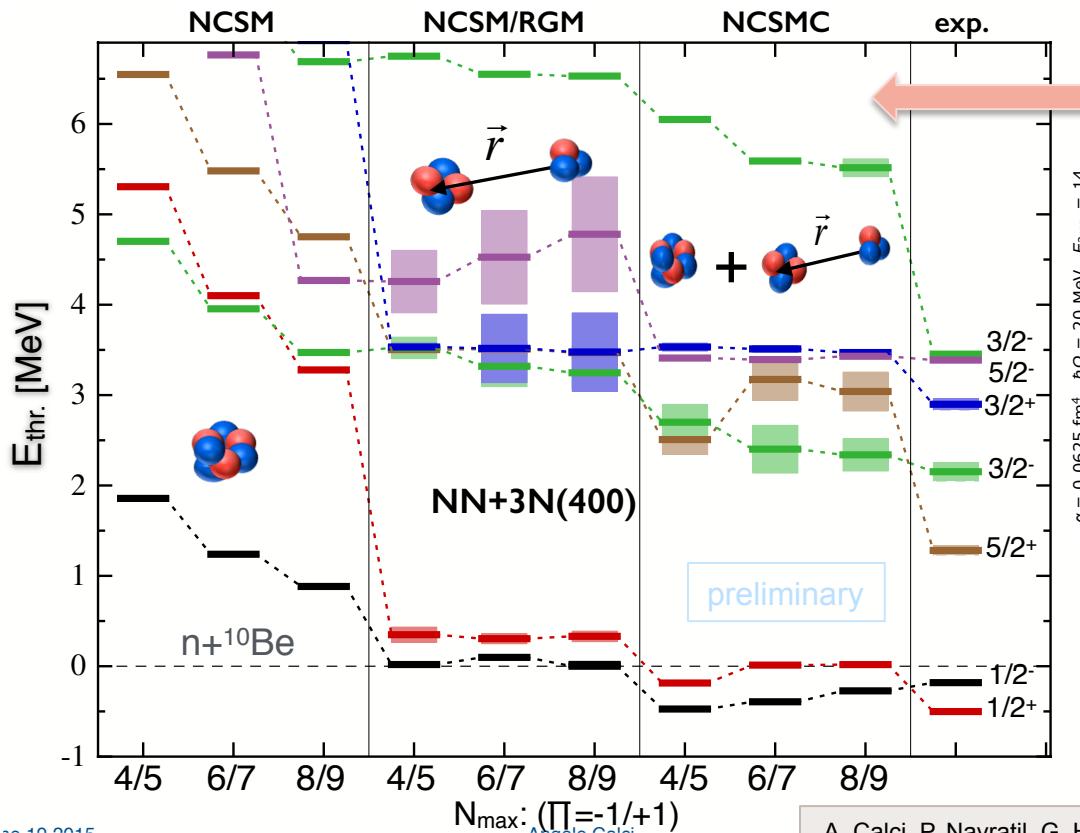


p+¹⁰C scattering: structure of ¹¹N resonances

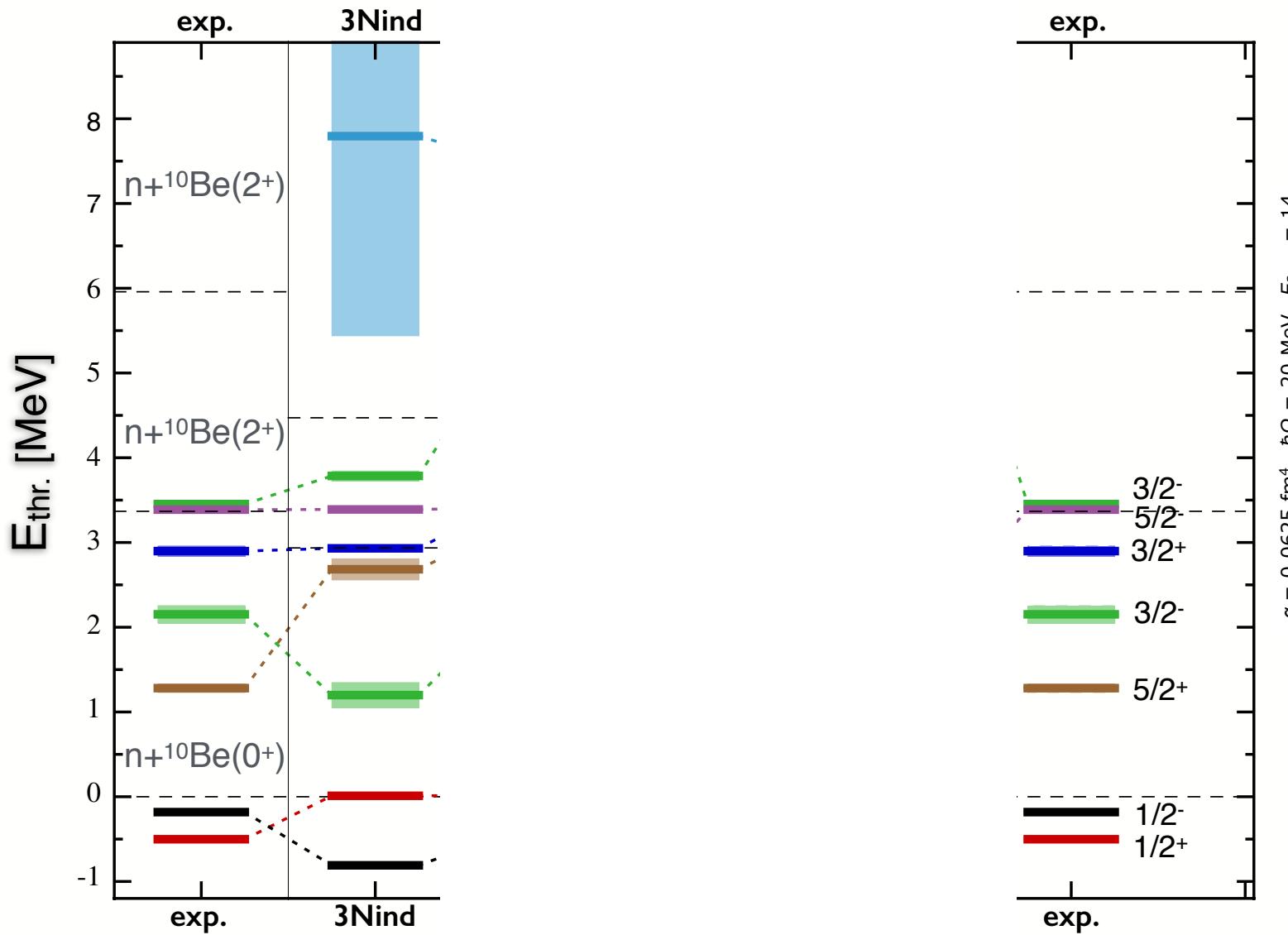


Structure of ^{11}Be from chiral NN+3N forces

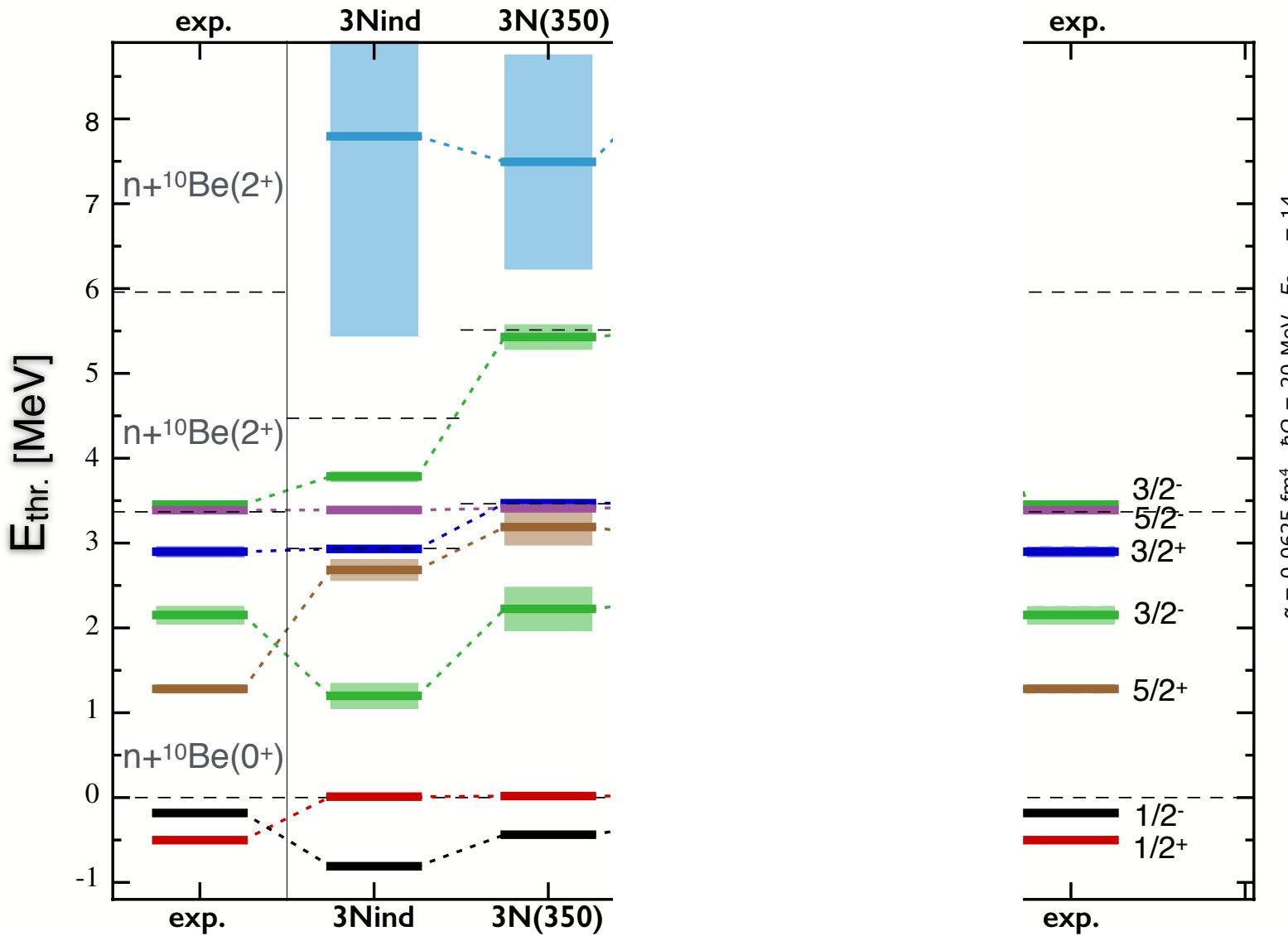
- NCSMC calculations including chiral 3N (N³LO NN+N²LO 3NF400)
 - $n-^{10}\text{Be} + ^{11}\text{Be}$
 - ^{10}Be : 0⁺, 2⁺, 2⁺ NCSM eigenstates
 - ^{11}Be : $\geq 6 \pi = -1$ and $\geq 3 \pi = +1$ NCSM eigenstates



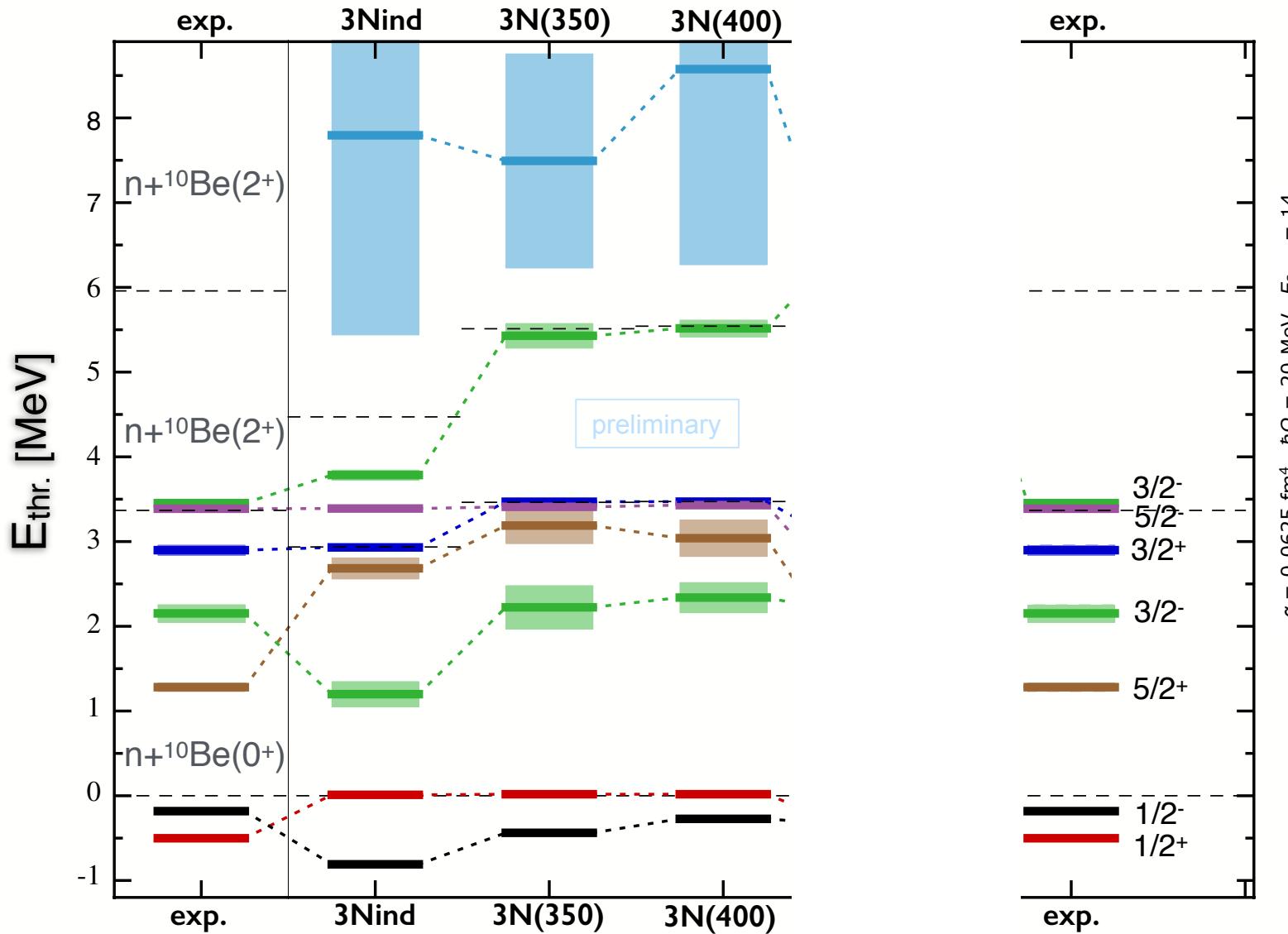
^{11}Be within NCSMC: Discrimination among chiral nuclear forces



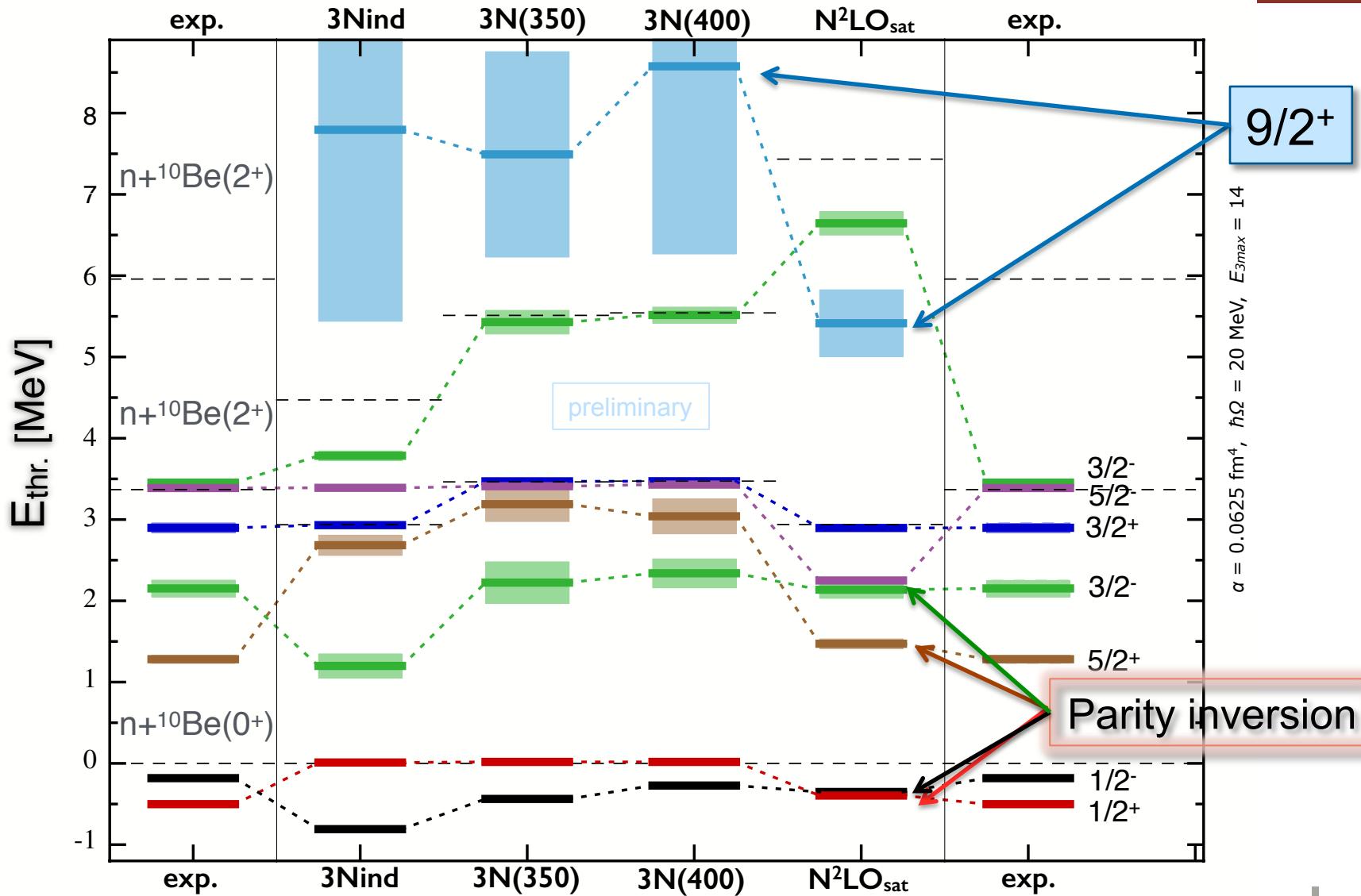
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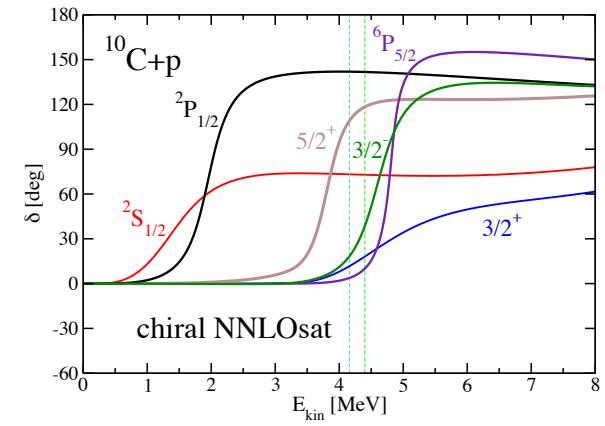
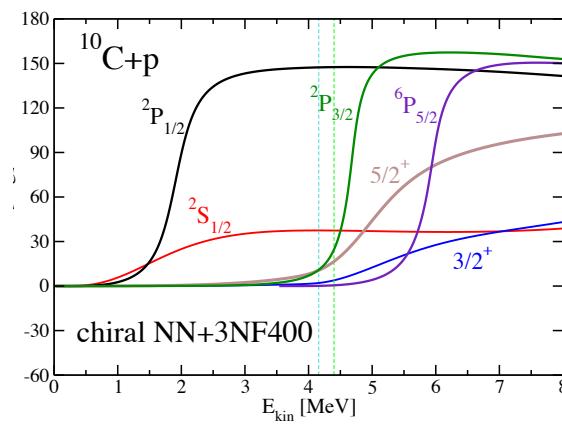
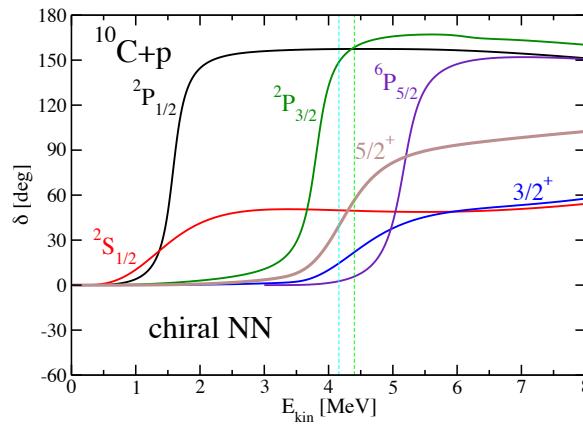
^{11}Be within NCSMC: Discrimination among chiral nuclear forces



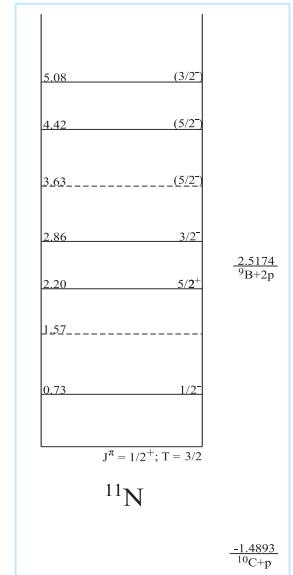
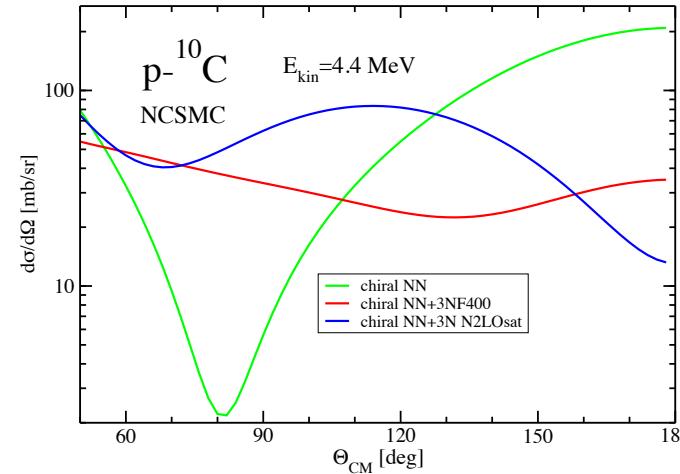
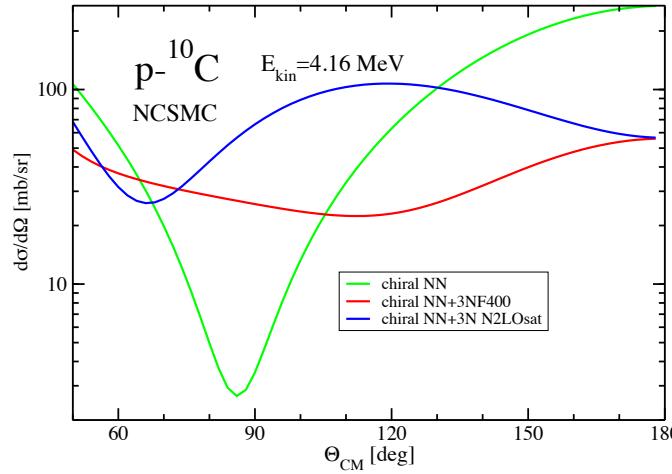
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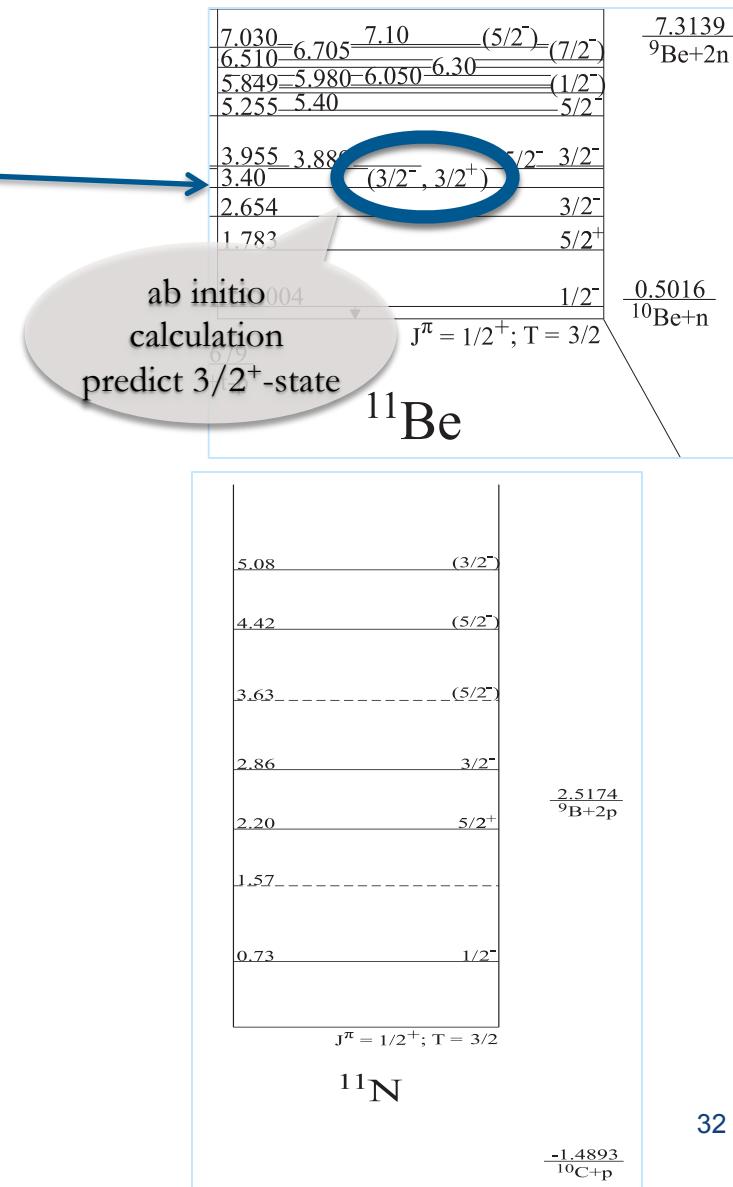
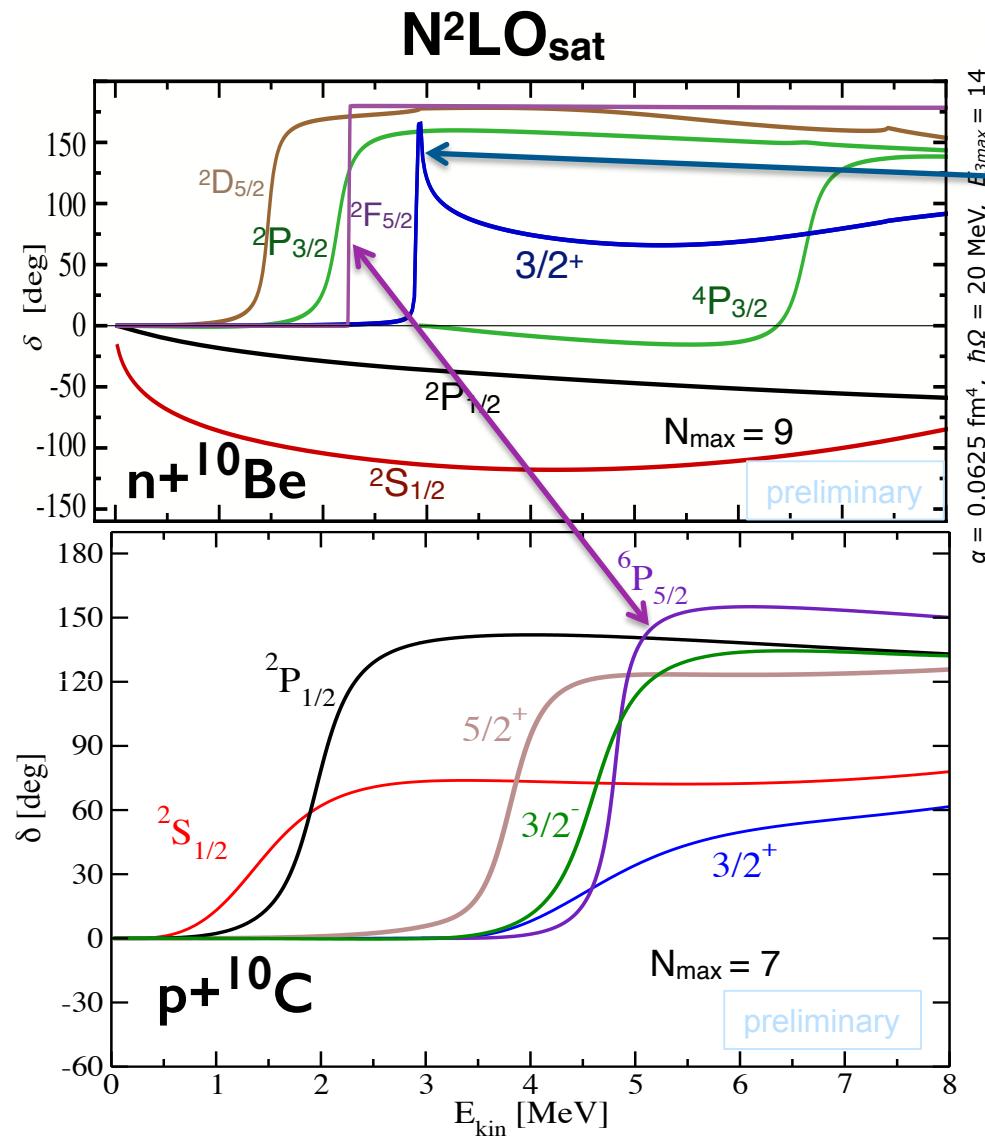
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Discrimination among chiral nuclear forces



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



NCSMC wave function

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

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

Asymptotic behavior $r \rightarrow \infty$:

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

Bound state

Scattering state

Scattering matrix

E1 transitions in NCSMC

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

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

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

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

Photo-disassocation of ^{11}Be

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

NCSMC phenomenology

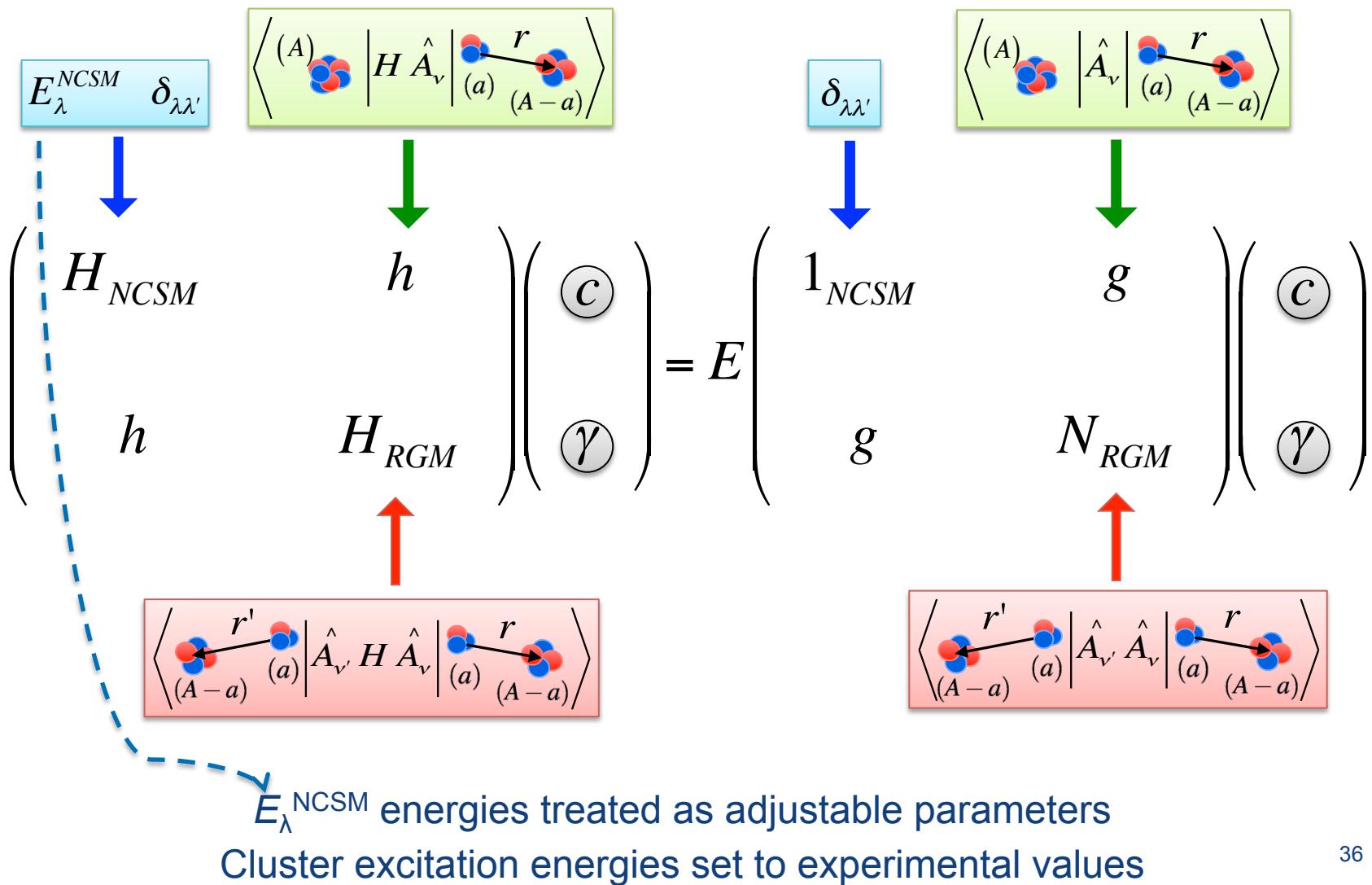
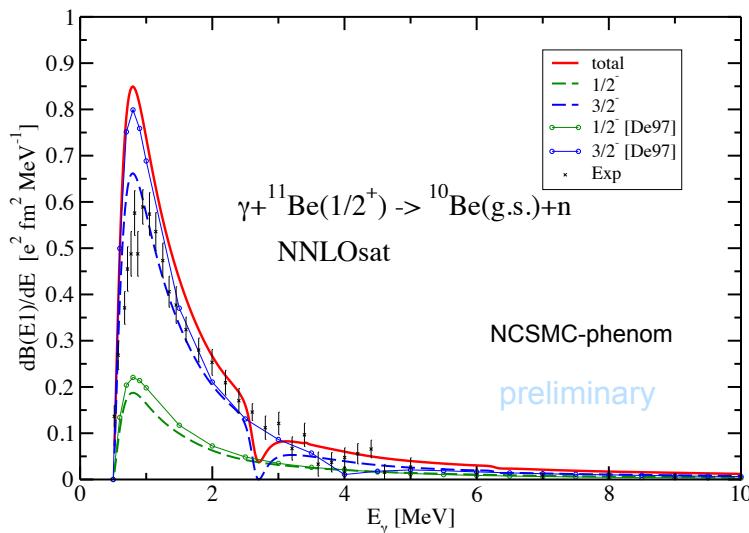


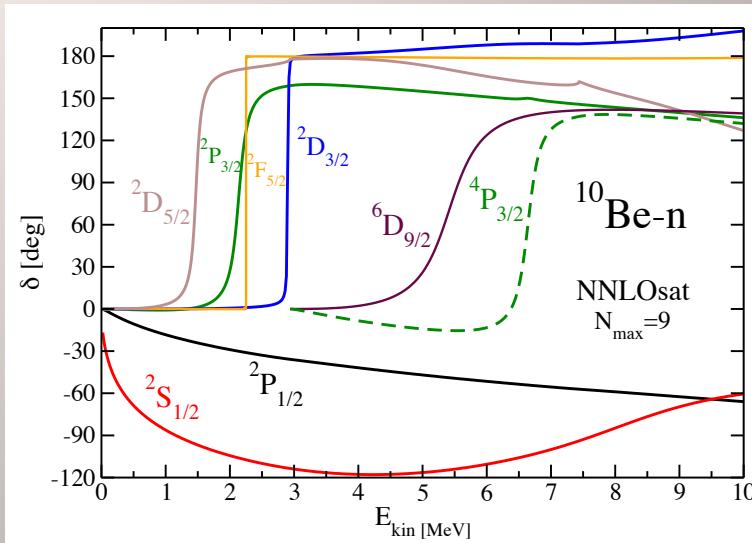
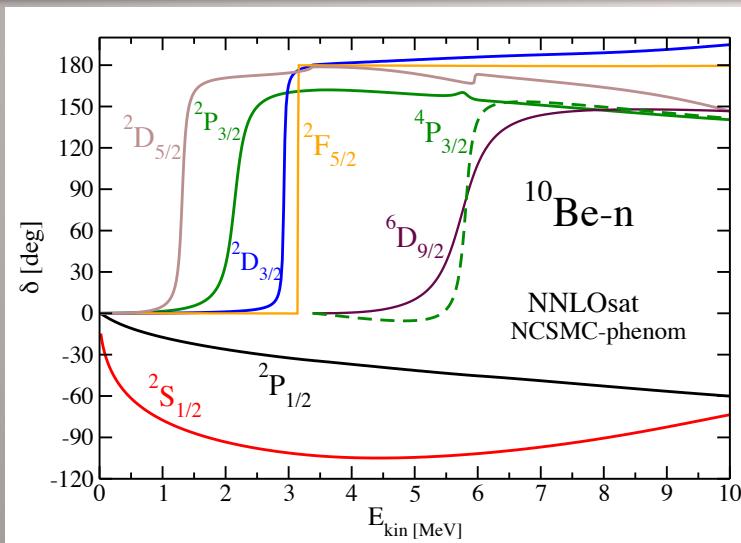
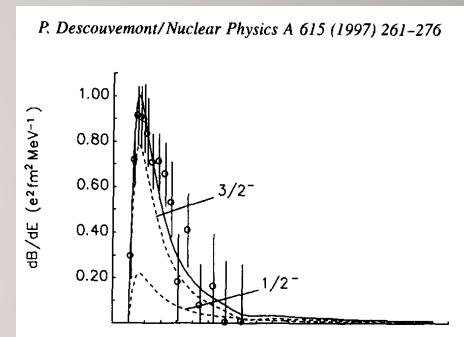
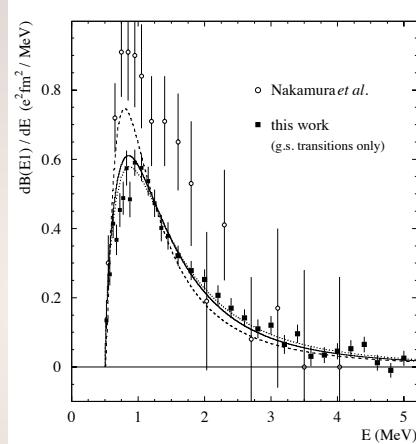
Photo-disassocation of ^{11}Be

Bound to continuum

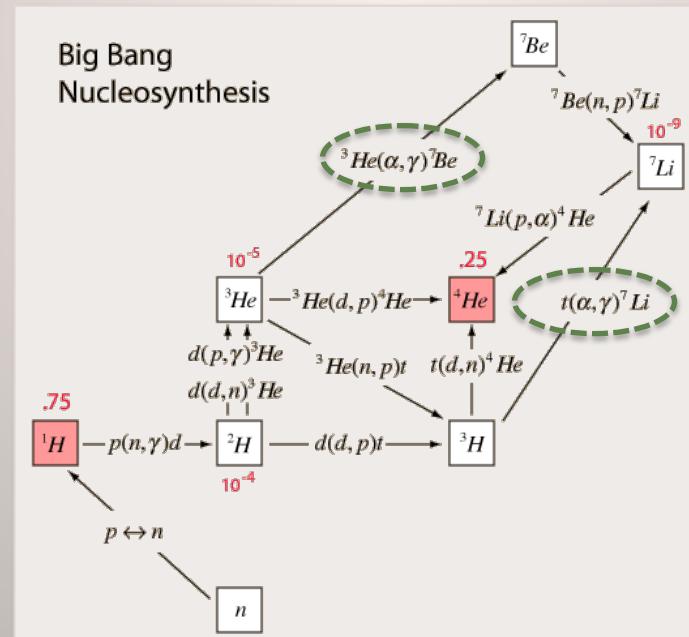
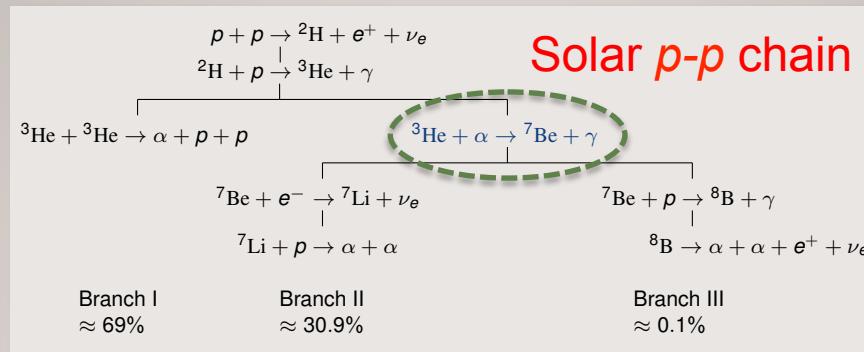


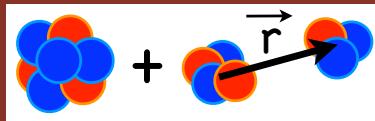
Bound to bound	NCSM	NCSMC-phenom	Expt.
$B(E1; 1/2^+ \rightarrow 1/2^-) [\text{e}^2 \text{ fm}^2]$	5×10^{-6}	0.118	0.102(2)

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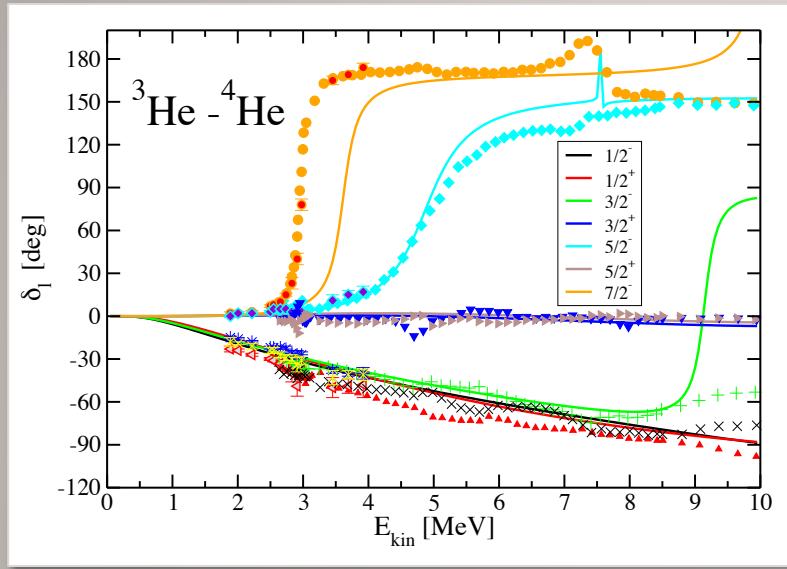


Capture reactions important for astrophysics





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



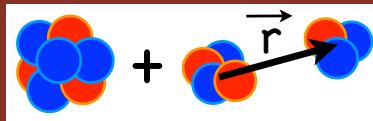
	^7Be		^7Li	
	NCSMC	Expt.	NCSMC	Expt.
$E_{3/2}^-$ [MeV]	-1.52	-1.586	-2.43	-2.467
$E_{1/2}^-$ [MeV]	-1.26	-1.157	-2.15	-1.989
r_{ch} [fm]	2.62	2.647(17)	2.42	2.390(30)
Q [e fm ²]	-6.14		-3.72	-4.00(3)
μ [μ_{N}]	-1.16	-1.3995(5)	+3.02	+3.256

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

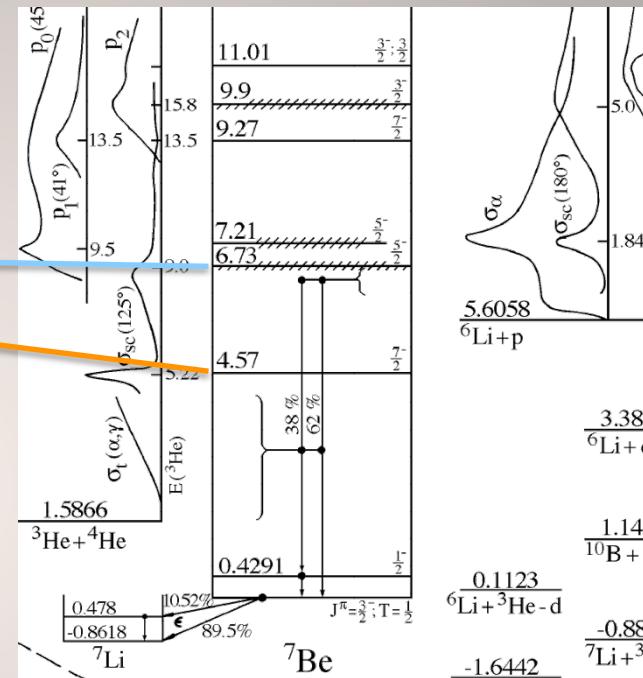
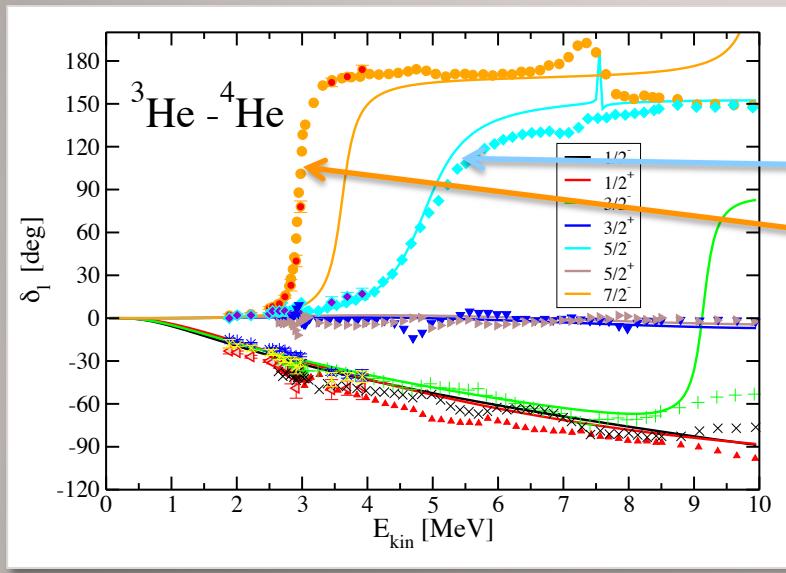
NCSMC calculations with chiral SRG-N³LO NN potential ($\lambda=2.15$ fm⁻¹)

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

Preliminary: $N_{\text{max}}=12$, $\hbar\Omega=20$ 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-N³LO NN potential ($\lambda=2.15 \text{ fm}^{-1}$)

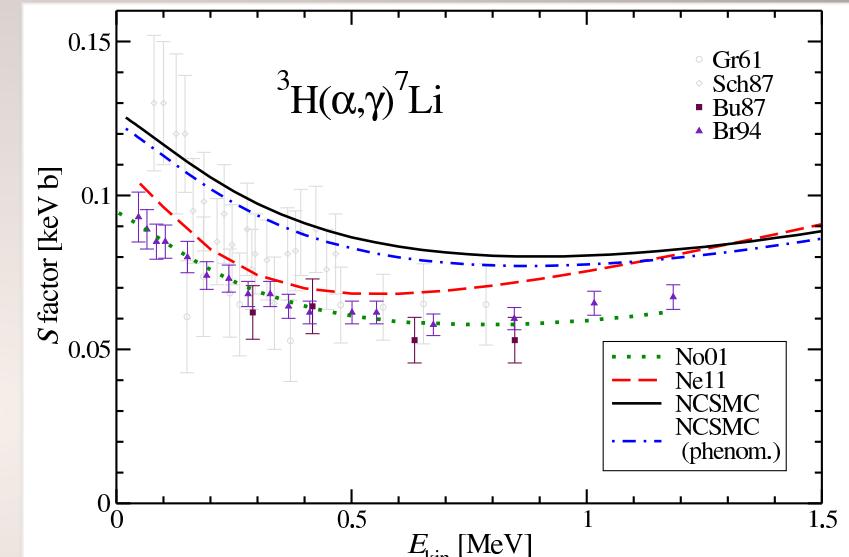
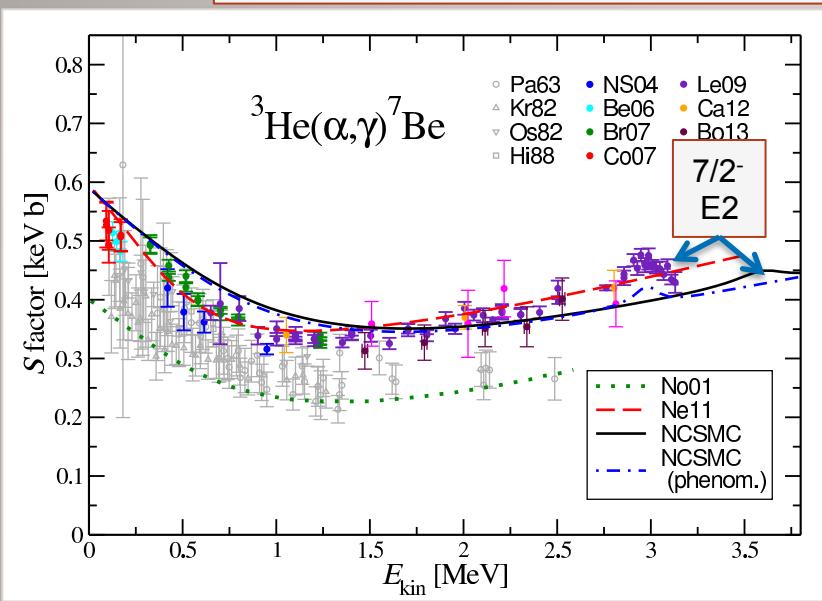
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^3He - ^4He and ^3H - ^4He capture

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



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

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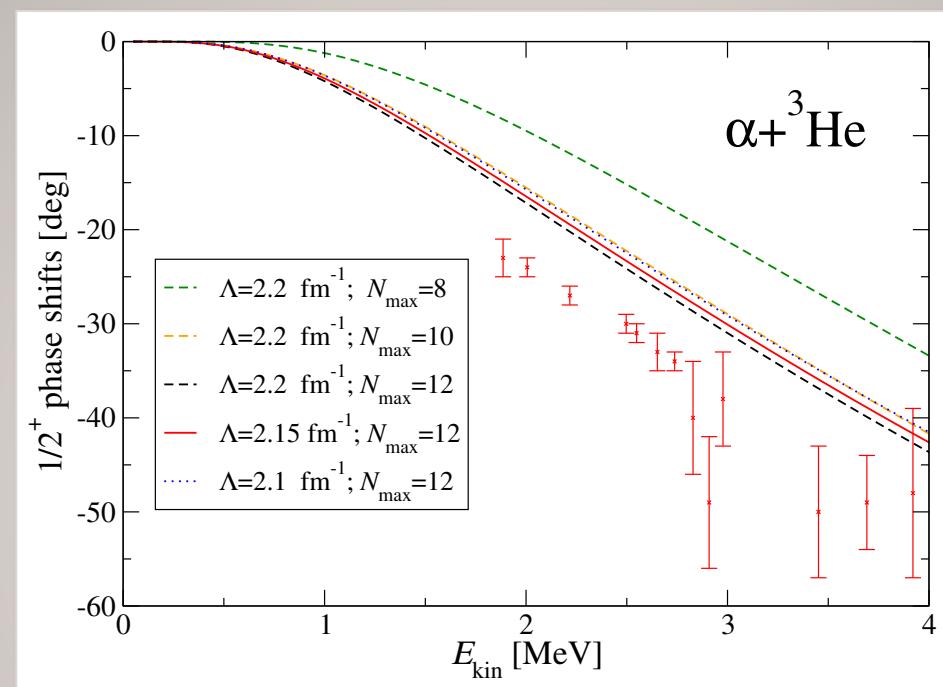
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Theoretical calculations suggest that the most recent and precise
 ^7Be and ^7Li data are inconsistent



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



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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 (${}^6\text{He} \sim {}^4\text{He}+n+n$): NCSMC in progress
- Ongoing projects:
 - Transfer reactions
 - Sensitivity analysis of nuclear interactions for halo ${}^{11}\text{Be}$ and exotic ${}^{11}\text{N}$
 - Applications to capture reactions important for astrophysics
 - Bremsstrahlung
- Outlook
 - Alpha-clustering (${}^4\text{He}$ projectile)
 - ${}^{12}\text{C}$ and Hoyle state: ${}^8\text{Be}+{}^4\text{He}$
 - ${}^{16}\text{O}$: ${}^{12}\text{C}+{}^4\text{He}$