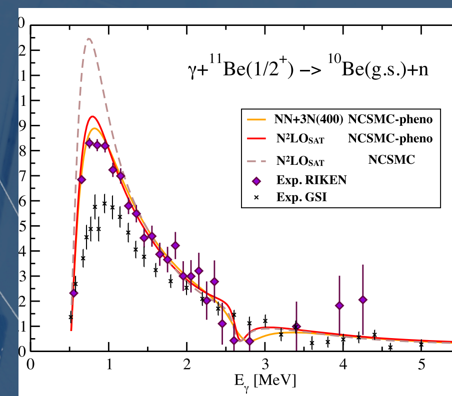
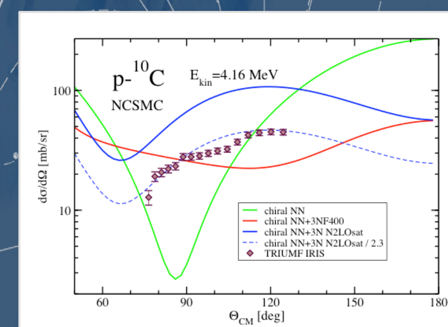
Canada's national laboratory for particle and nuclear physics and accelerator-based science

Bound and Unbound Light Nuclei from *Ab Initio* Theory

Shapes and Symmetries in Nuclei: from Experiment to Theory SSNET 2017
Centre de Sciences Nucléaires et Sciences de la Matière,
CNRS, Gif sur Yvette, France, 6-10 November, 2017

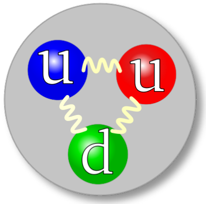
Petr Navratil | TRIUMF



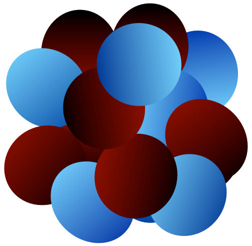


Collabrorators:
Sofia Quaglioni, Carolina Romero-Redondo (LLNL)
Guillaume Hupin (CNRS)
Angelo Calci, Matteo Vorabbi (TRIUMF)
Jeremy Dohet-Eraly (INFN), Robert Roth (TU Darmstadt)

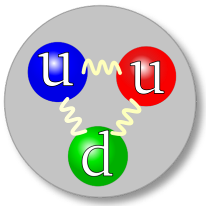
- Nuclear structure and reactions from first principles
- No-Core Shell Model with Continuum (NCSMC) approach
- n-^{4}He scattering benchmark
- ^{11}Be parity inversion in low-lying states, photo-dissociation
- Structure of unbound ^{9}He
- Synergy between *ab initio* theory and TRIUMF experiments
  - ^{11}N and ^{10}C(p,p) scattering - IRIS
  - ^{12}N, ^{11}C(p,p) scattering and ^{11}C(p,γ)^{12}N capture - TUDA
  - Quadrupole moment of ^{12}C 2^{+} state - TIGRESS



Low-energy QCD



Nuclear structure and reactions



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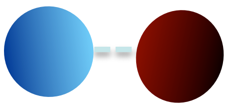
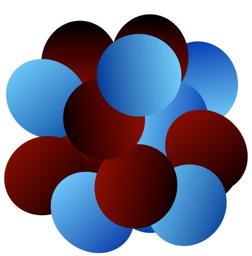


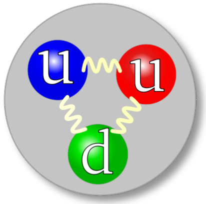
NN+3N interactions from chiral EFT

...or accurate meson-exchange potentials



Nuclear structure and reactions

From QCD to nuclei



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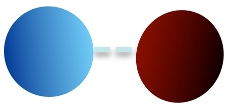


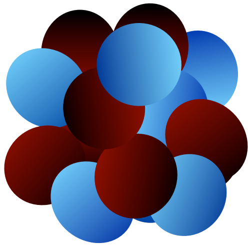
NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

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

Many-Body methods

NCSM, NCSMC, CCM, IM-SRG, SCGF, GFMC, HH, Nuclear Lattice EFT…



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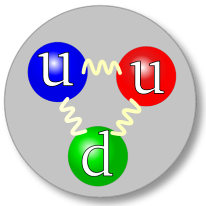

Low-energy QCD

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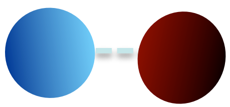
NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials



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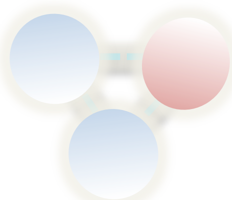
Unitary/similarity transformations

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



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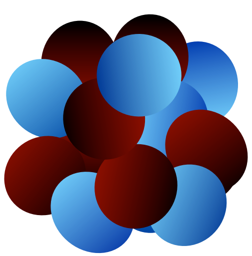
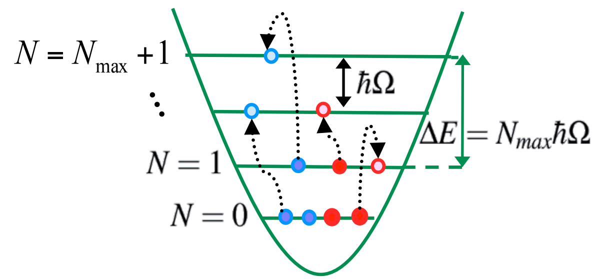
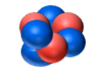
Nuclear structure and reactions



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



Harmonic oscillator basis

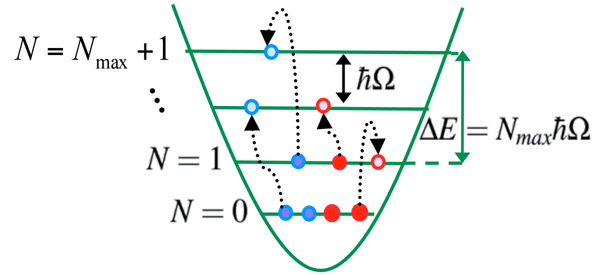


NCSM

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

Unknowns

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



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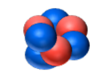
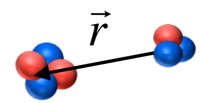


NCSM

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



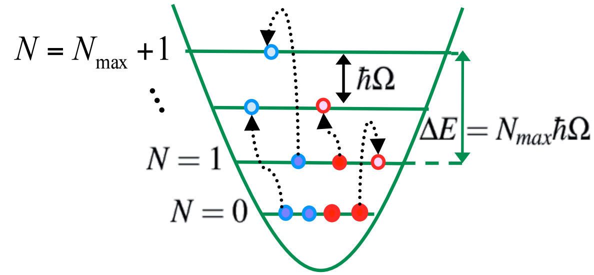
NCSM/RGM

NCSM/RGM channel states

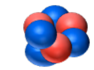
$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r}\,)\; \hat{A}_{\nu} \left| \underbrace{\vec{r}\;(A-a)\;(a)}\;, \nu \right\rangle$$

Unknowns

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



Harmonic oscillator basis



NCSM

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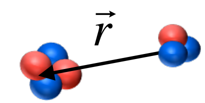


NCSM/RGM

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

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

NCSMC

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \overbrace{\left| {}^{(A)} \, , \lambda \right\rangle}^{\text{NCSM eigenstates}} + \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r}\,)\; \hat{A}_{\nu} \overbrace{\left| {}_{(A-a)} \quad \vec{r} \quad {}_{(a)} \, , \nu \right\rangle}^{\text{NCSM/RGM channel states}}$$

Unknowns

Coupled NCSMC equations

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

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

$$E_{\lambda}^{NCSM}\;\delta_{\lambda\lambda'}$$

$$\left\langle {}^{(A)} \middle| H\,\hat{A}_{\nu} \middle| {}^{(a)} \; r \; {}_{(A-a)} \right\rangle$$

$$\delta_{\lambda\lambda'}$$

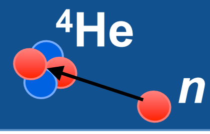
$$\left\langle {}^{(A)} \middle| \hat{A}_{\nu} \middle| {}^{(a)} \; r \; {}_{(A-a)} \right\rangle$$

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

$$\left\langle {}_{(A-a)} \; r' \; {}^{(a)} \middle| \hat{A}_{\nu'}\, H\, \hat{A}_{\nu} \middle| {}^{(a)} \; r \; {}_{(A-a)} \right\rangle$$

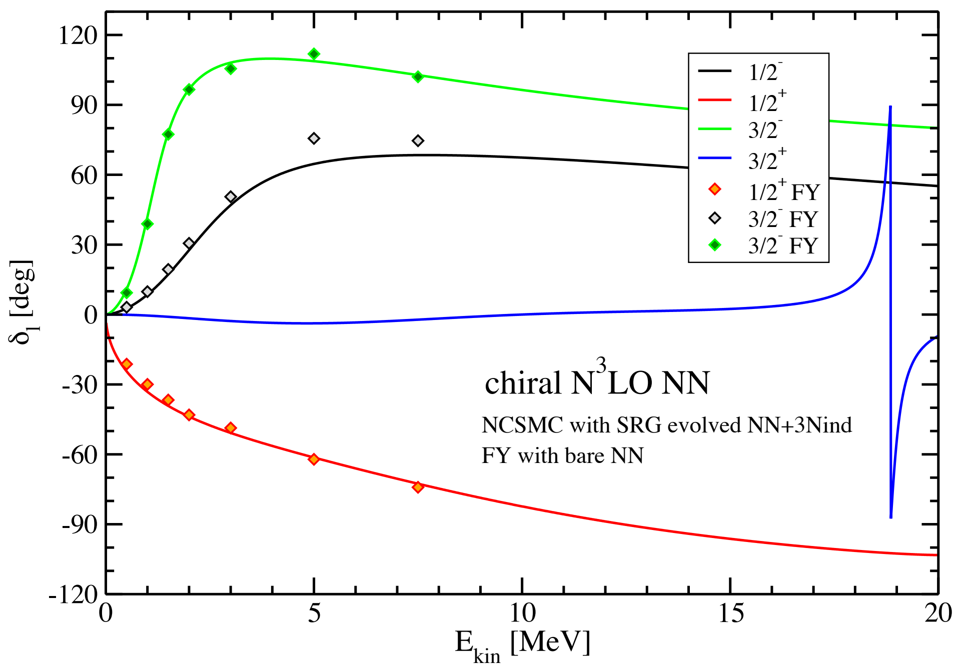
$$\left\langle {}_{(A-a)} \; r' \; {}^{(a)} \middle| \hat{A}_{\nu'}\, \hat{A}_{\nu} \middle| {}^{(a)} \; r \; {}_{(A-a)} \right\rangle$$

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



n-^{4}He scattering within NCSMC

n-^{4}He scattering phase-shifts for chiral NN



FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta

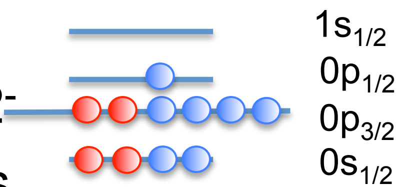
Phys. Scr. 00 (2016) 000000 (37pp)

Invited Comment

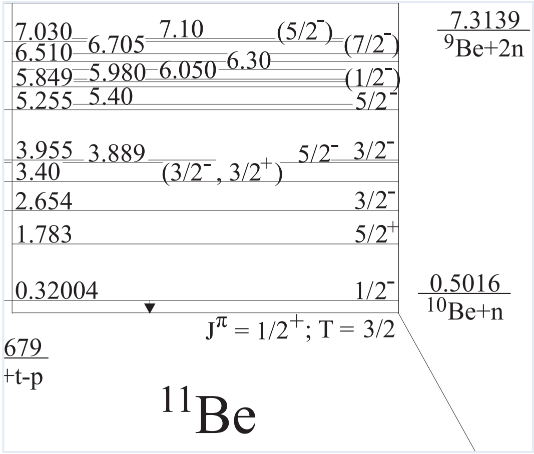
Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]

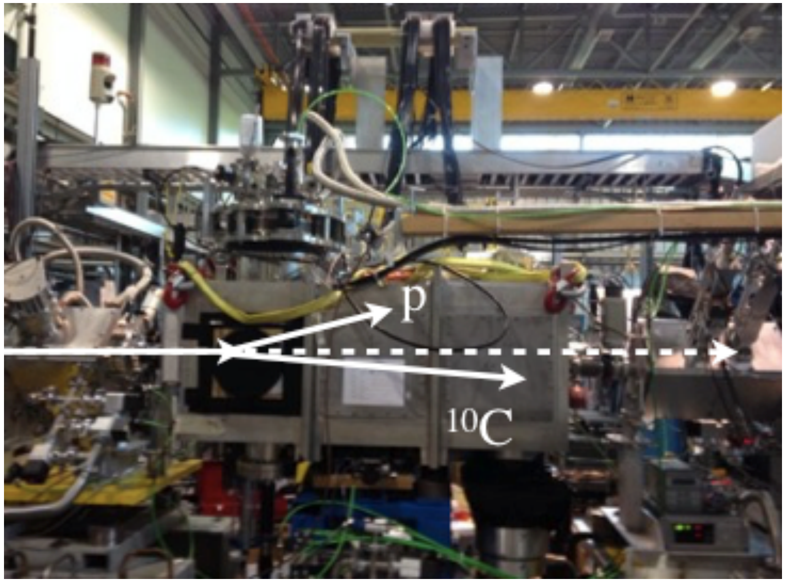
- Z=4, N=7
  - In the shell model picture g.s. expected to be $J^\pi=1/2^-$
    - Z=6, N=7 ^{13}C and Z=8, N=7 ^{15}O have $J^\pi=1/2^-$ g.s.
  - In reality, ^{11}Be g.s. is $\mathbf{J^\pi=1/2^+}$ - parity inversion
  - Very weakly bound: E_{th}=-0.5 MeV
    - Halo state – dominated by ^{10}Be-n in the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

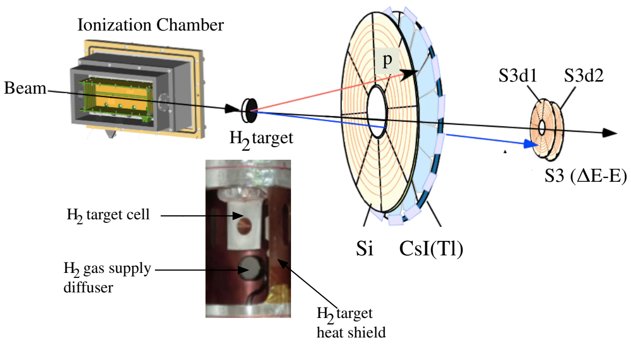


- Can we describe ^{11}Be in *ab initio* calculations?
  - Continuum must be included
  - Does the 3N interaction play a role in the parity inversion?



- Experiment at TRIUMF with the novel IRIS solid H_2 target
  - First re-accelerated ^{10}C beam at TRIUMF
  - $^{10}C(p,p)$ angular distributions measured at E_{CM} ~ 4.15 MeV and 4.4 MeV



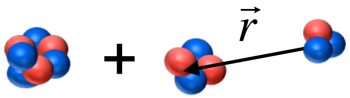


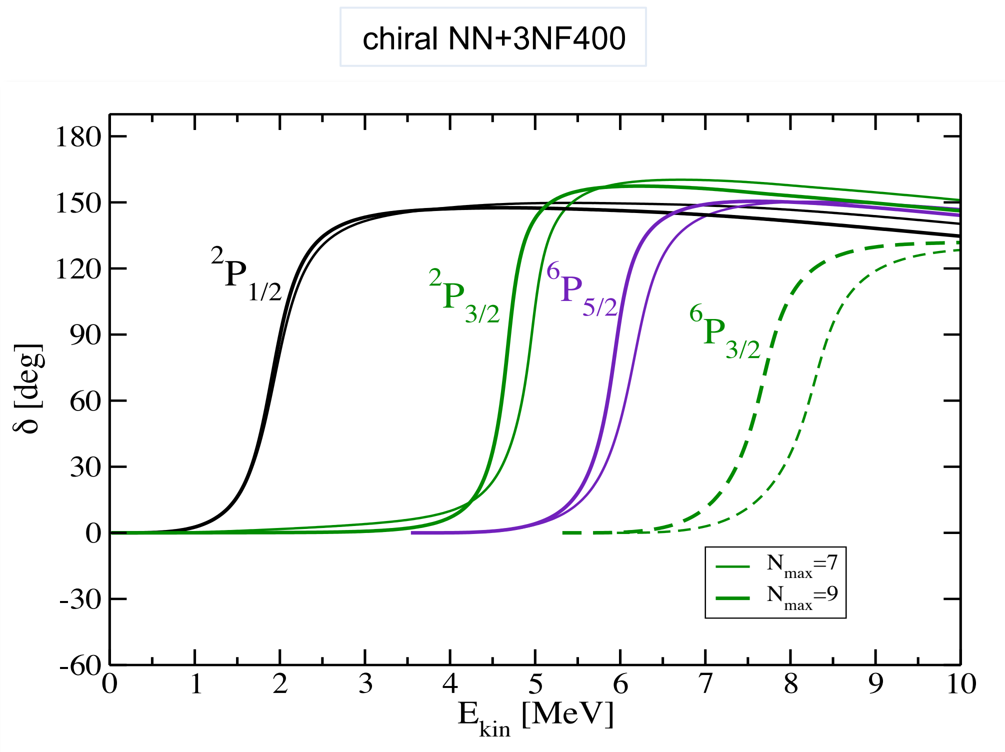
^{11}N ~ ^{10}C+p unbound mirror system of ^{11}Be ~ ^{10}Be+n

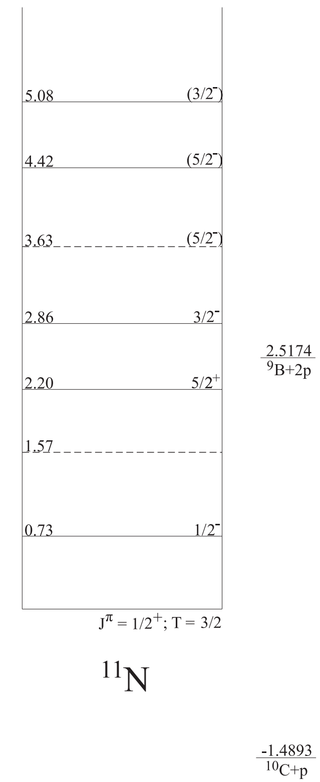
IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev *et al.*

p+^{10}C scattering: structure of ^{11}N resonances

- NCSMC calculations with **chiral NN+3N** (N^{3}LO NN+N^{2}LO 3NF400, NNLOsat)
  - (^{11}N)$_{NCSM}$ + (p-^{10}C)$_{NCSM/RGM}$
    - ^{10}C: 0$^+$, 2$^+$, 2$^+$ NCSM eigenstates
    - ^{11}N: ≥4 π = -1 and ≥3 π = +1 NCSM eigenstates





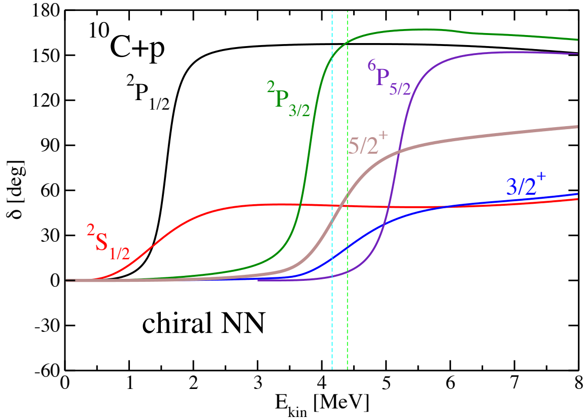


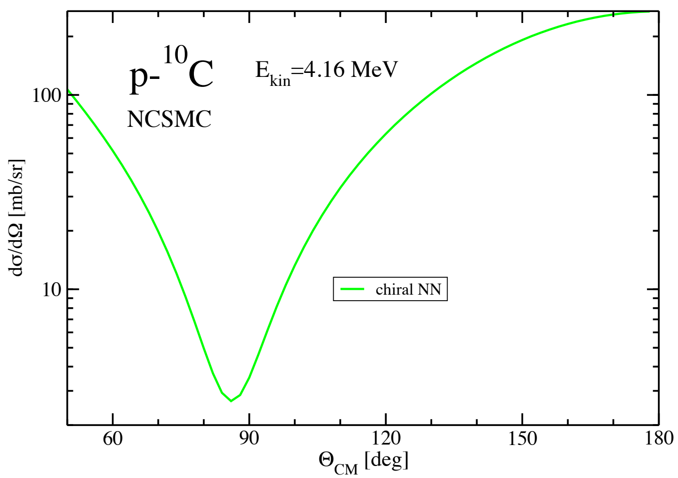
p+^{10}C scattering: structure of ^{11}N resonances

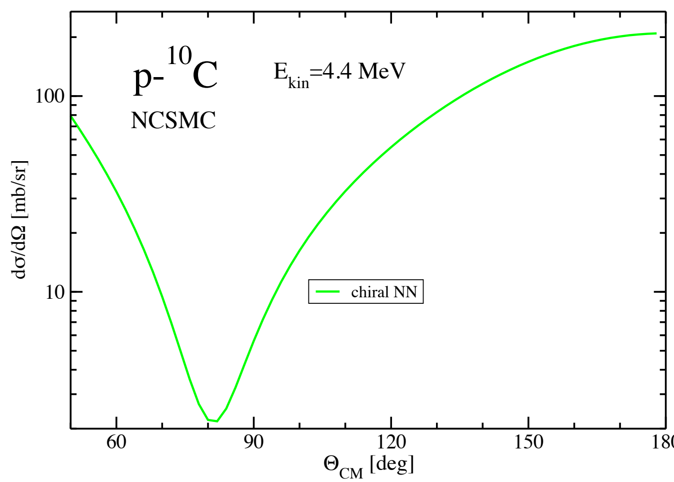
Selected for a Viewpoint in *Physics*
PRL **118,** 262502 (2017) PHYSICAL REVIEW LETTERS week ending 30 JUNE 2017

Nuclear Force Imprints Revealed on the Elastic Scattering of Protons with ^{10}C

A. Kumar,[1] R. Kanungo,[1*] A. Calci,[2] P. Navrátil,[2†] A. Sanetullaev,[1,2] M. Alcorta,[2] V. Bildstein,[3] G. Christian,[2] B. Davids,[2] J. Dohet-Eraly,[2,4] J. Fallis,[2] A. T. Gallant,[2] G. Hackman,[2] B. Hadinia,[3] G. Hupin,[5,6] S. Ishimoto,[7] R. Krücken,[2,8] A. T. Laffoley,[3] J. Lighthall,[2] D. Miller,[2] S. Quaglioni,[9] J. S. Randhawa,[1] E. T. Rand,[3] A. Rojas,[2] R. Roth,[10] A. Shotter,[11] J. Tanaka,[12] I. Tanihata,[12,13] and C. Unsworth[2]







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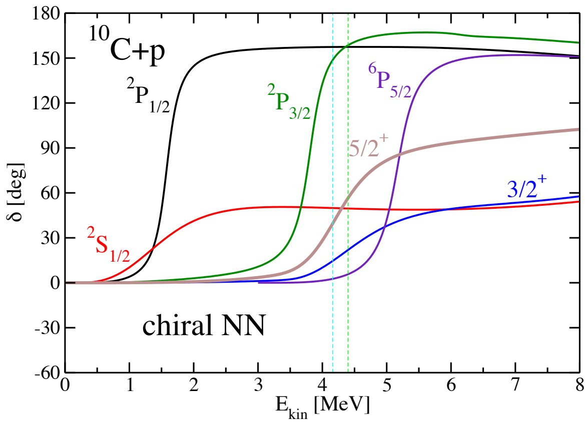

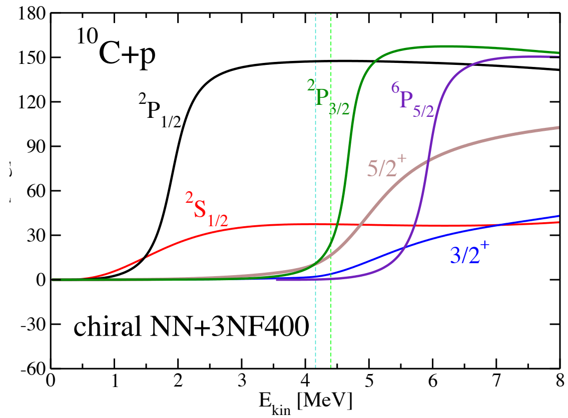

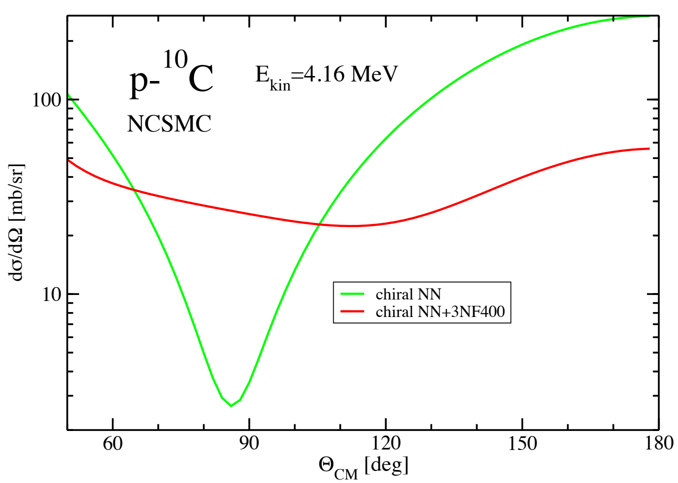

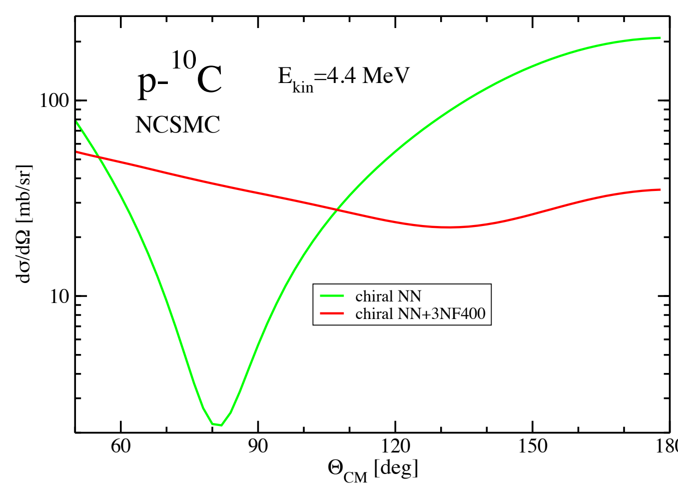

p+^{10}C scattering: structure of ^{11}N resonances

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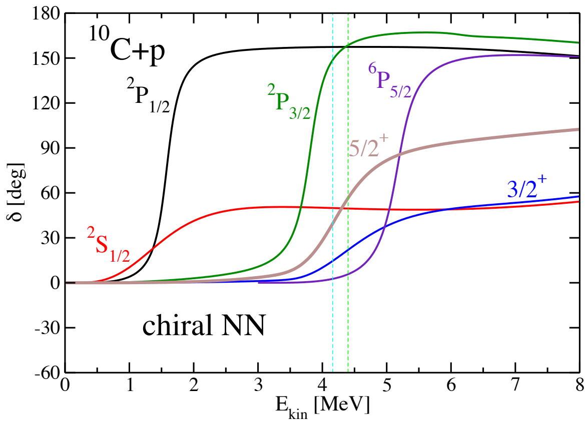
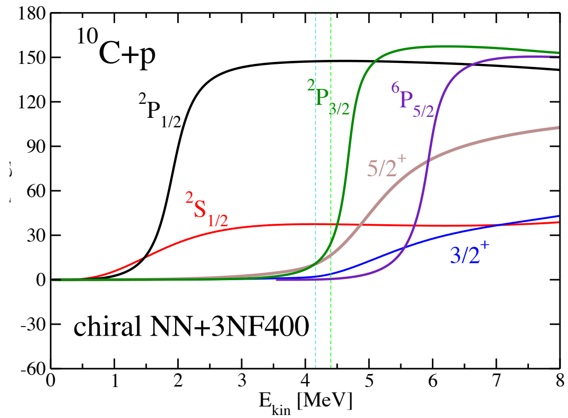
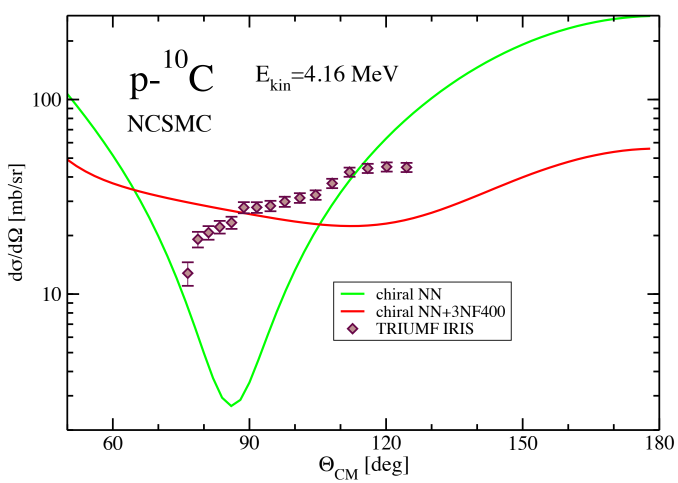
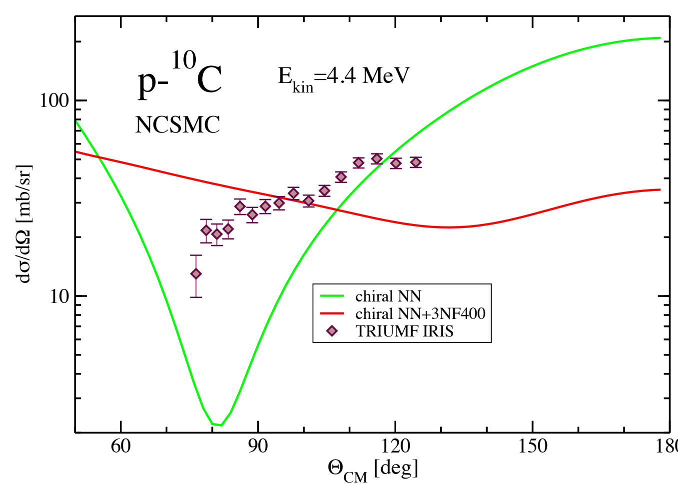
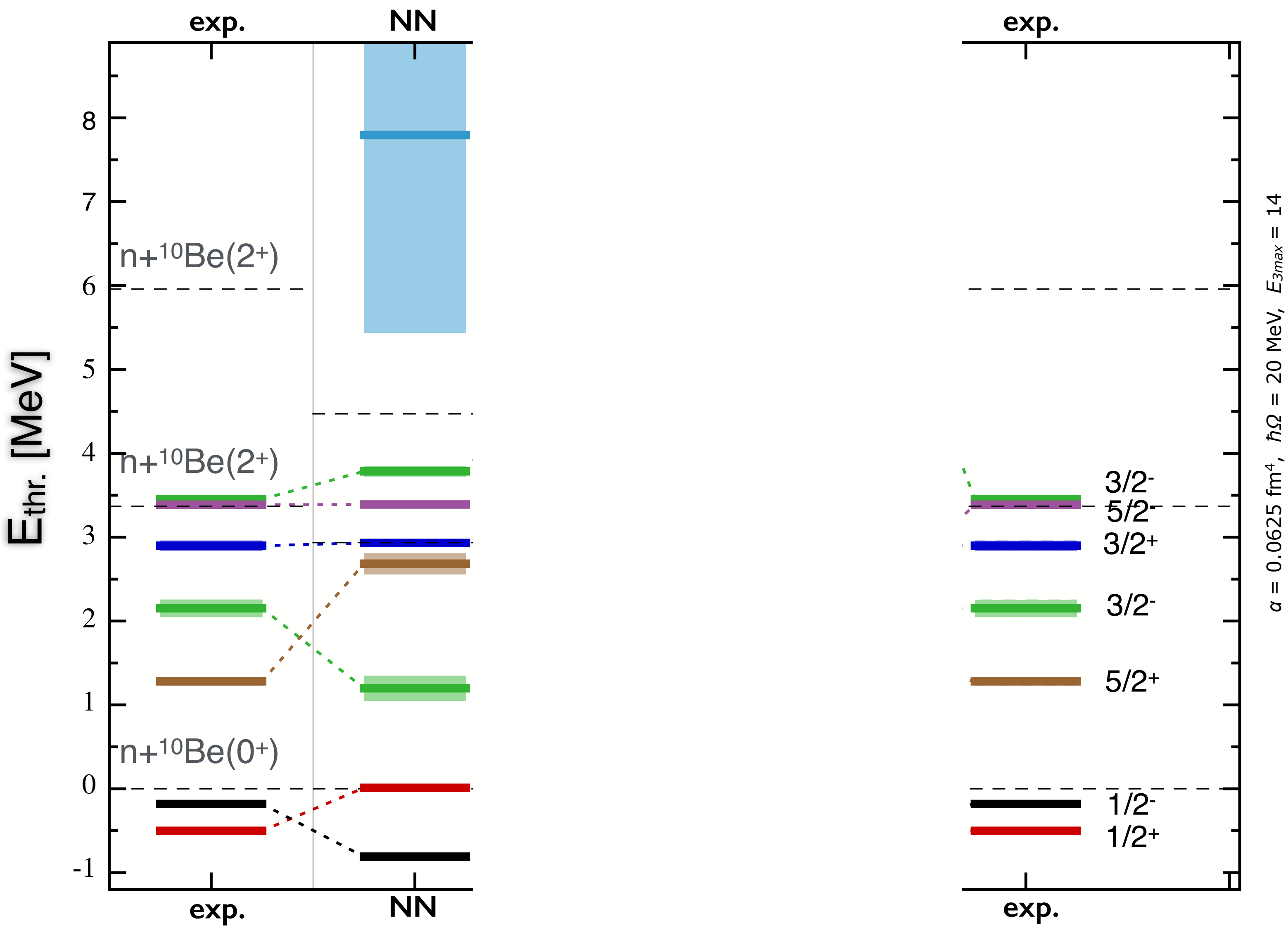








^{11}Be within NCSMC: Discrimination among chiral nuclear forces



A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, PRL 117, 242501 (2016)

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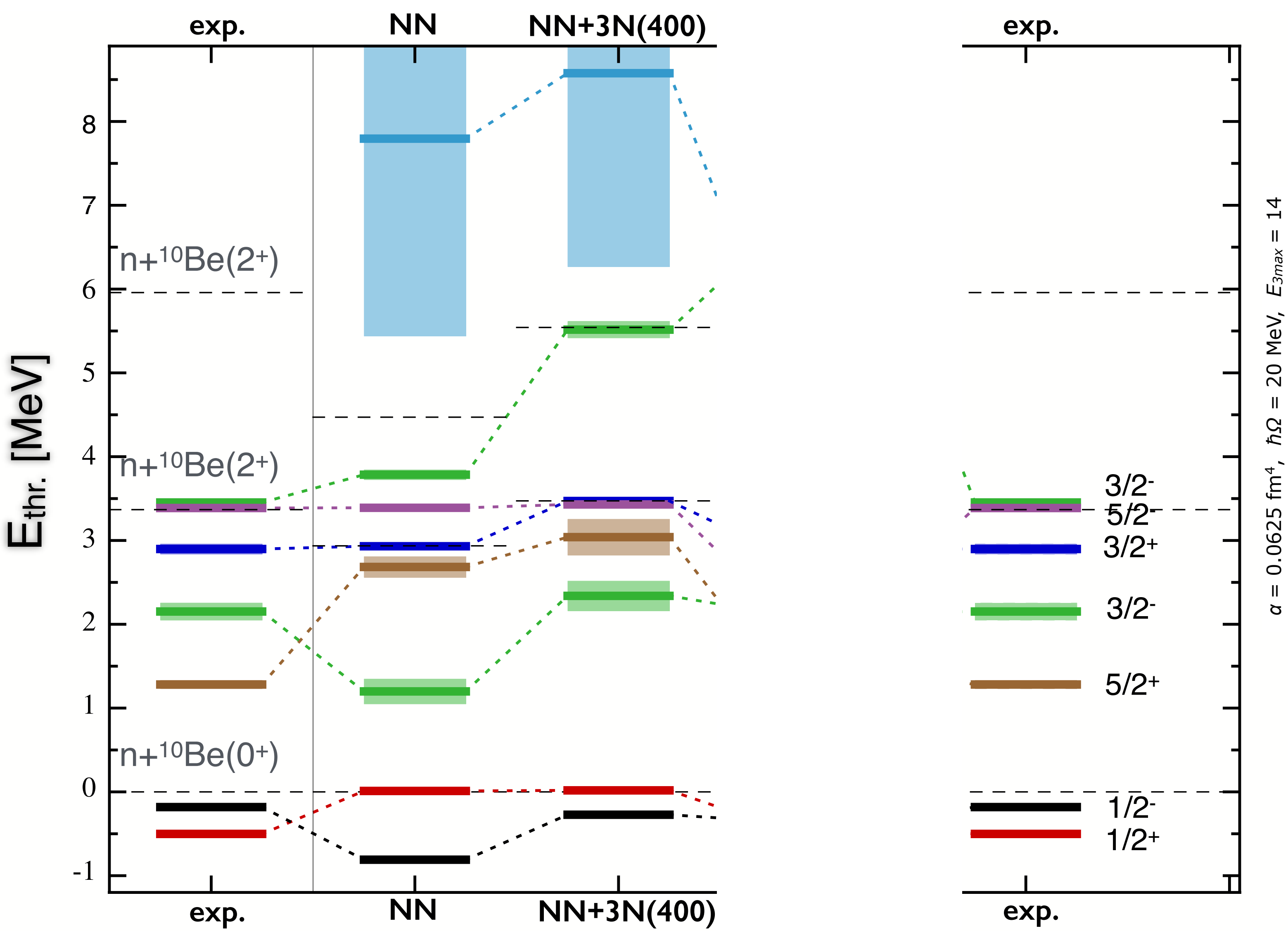

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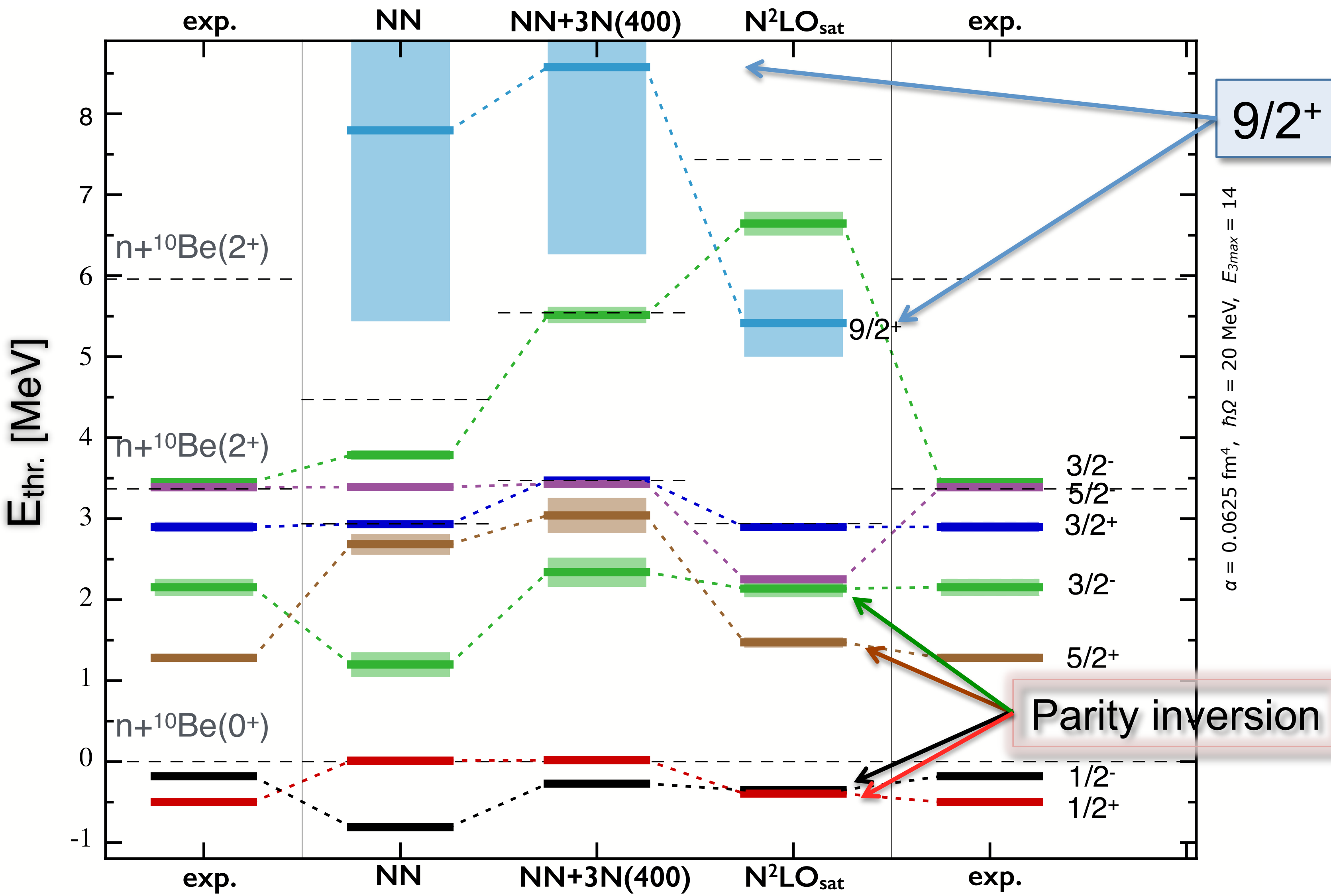

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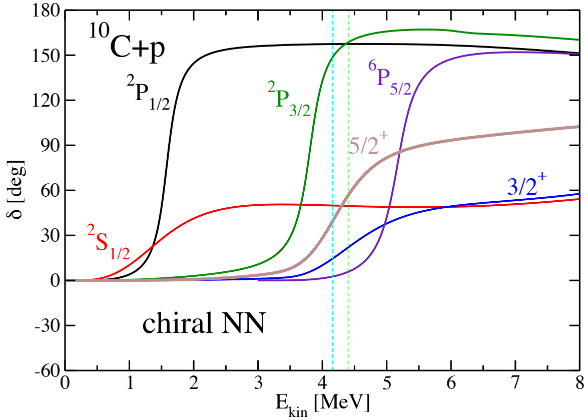

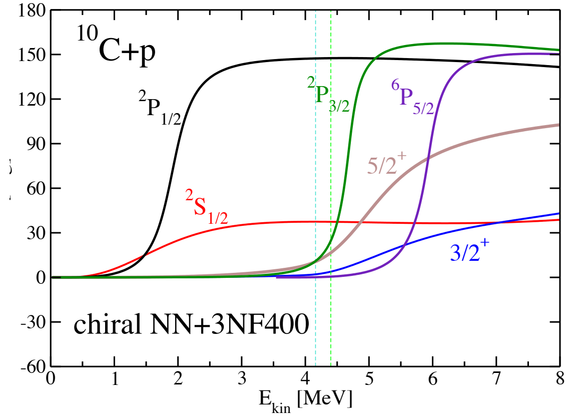

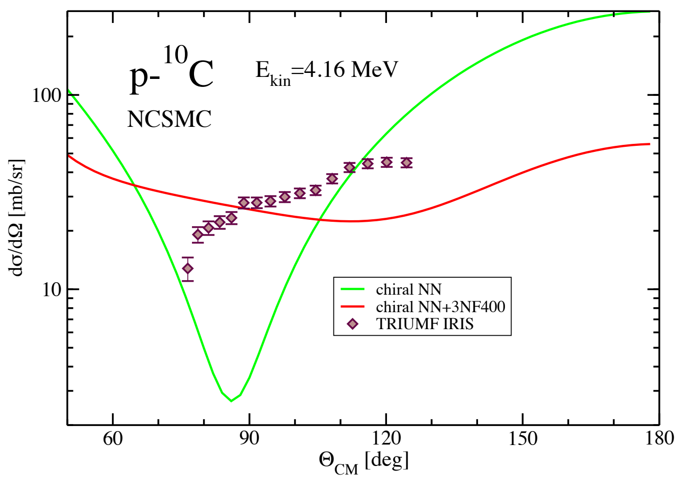

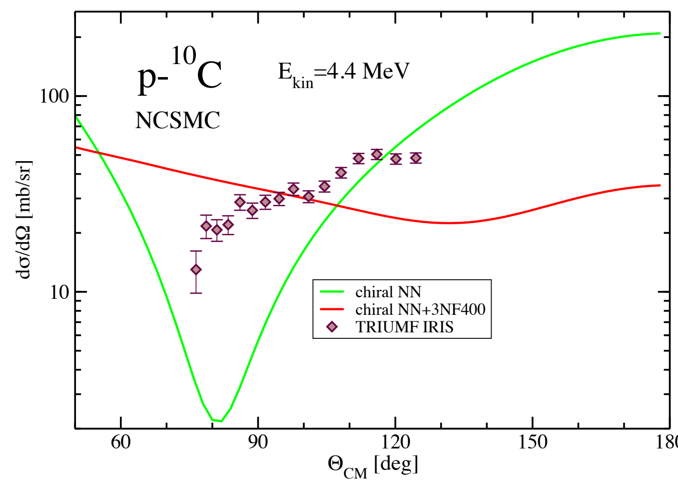

p+^{10}C scattering: structure of ^{11}N resonances

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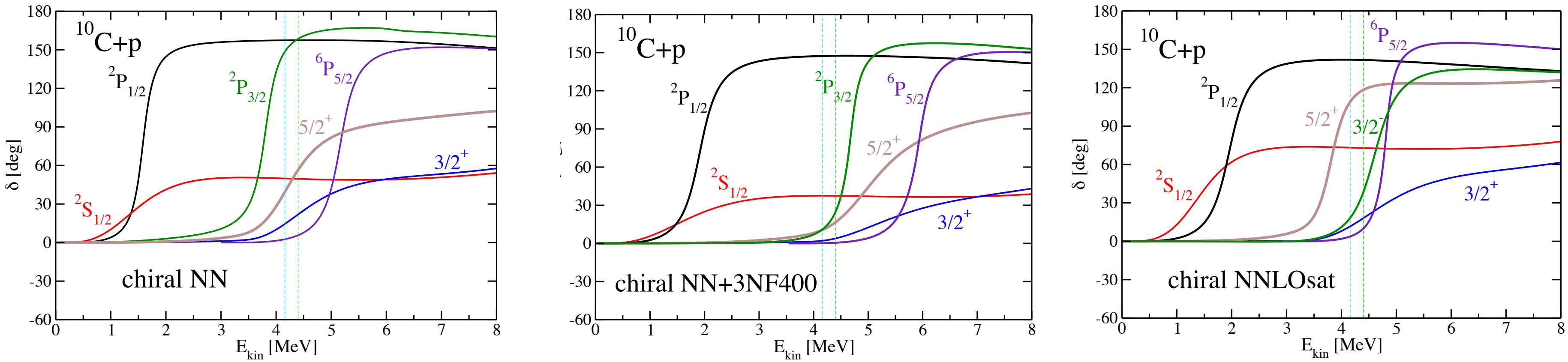

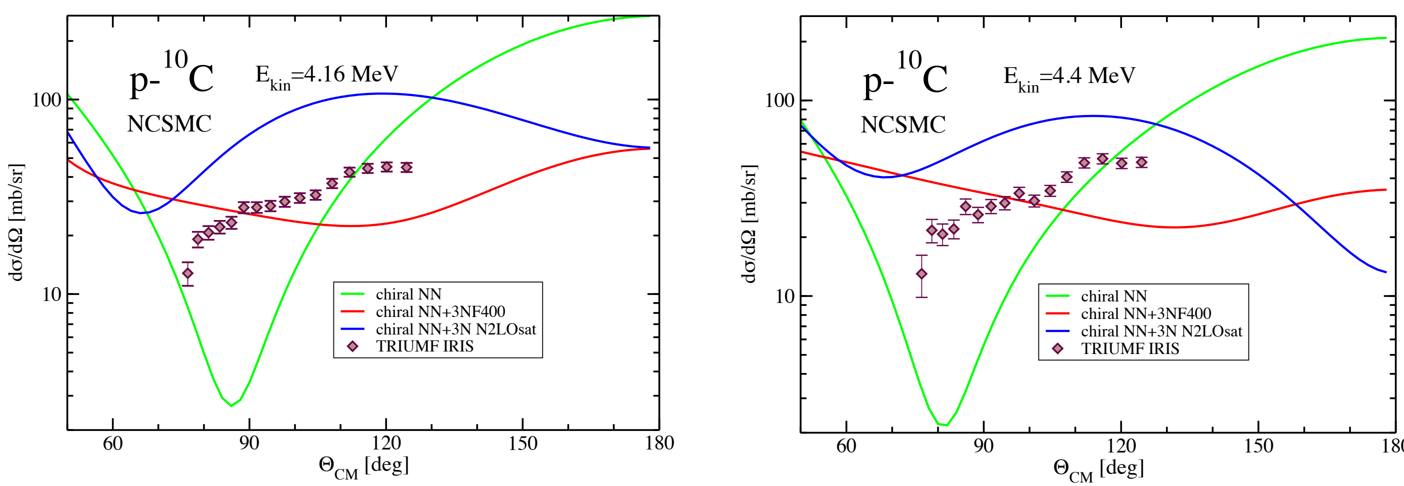

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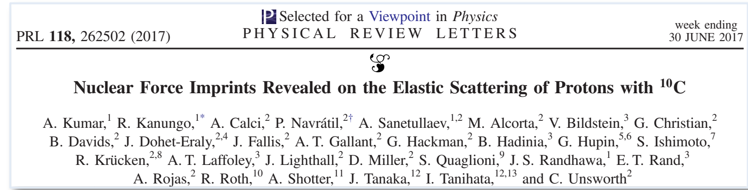

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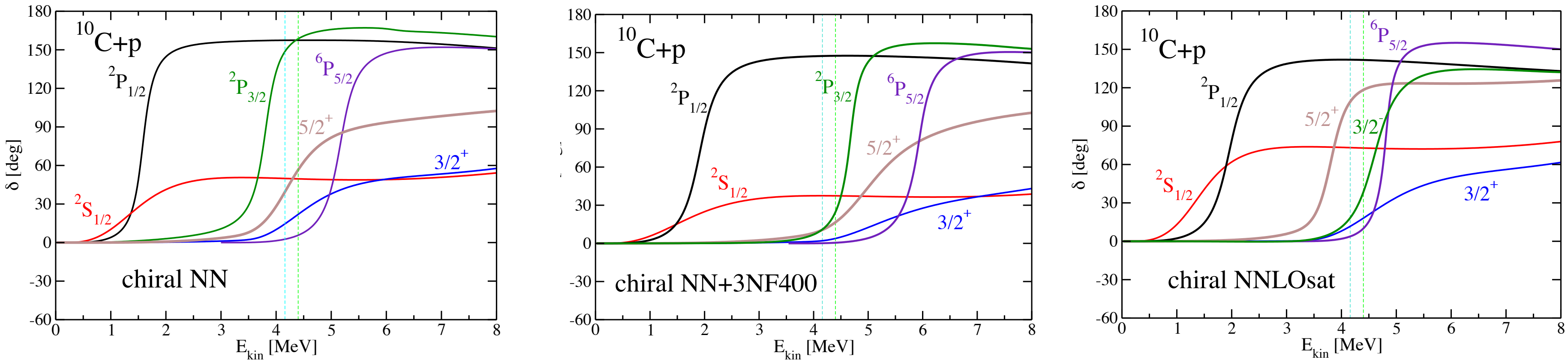
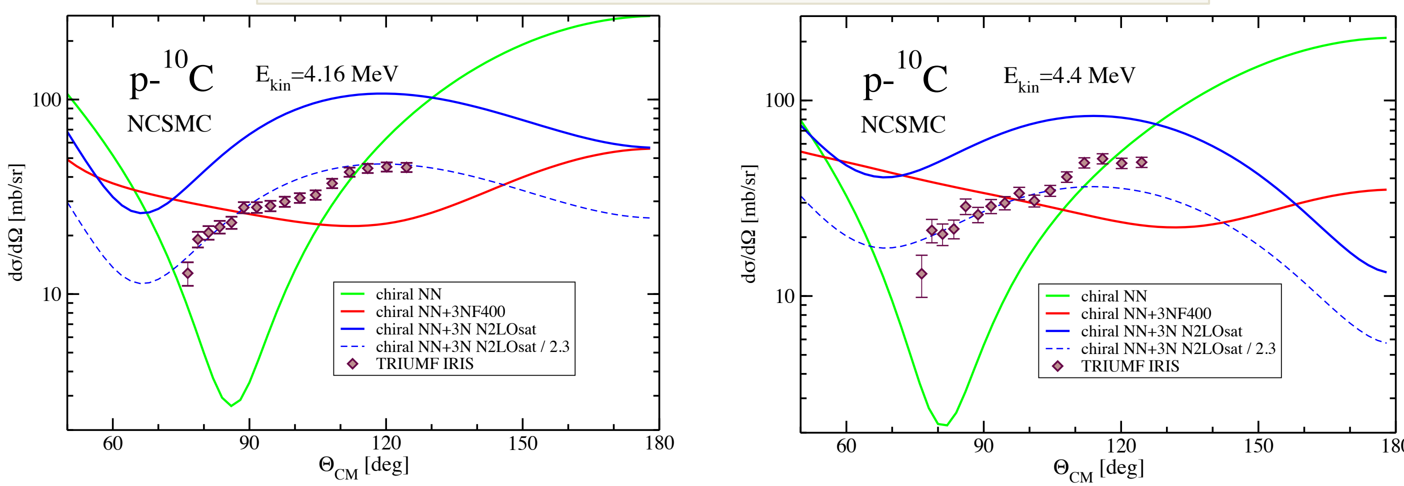


Discrimination among chiral nuclear forces



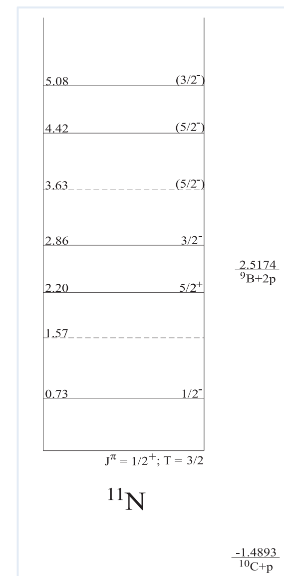
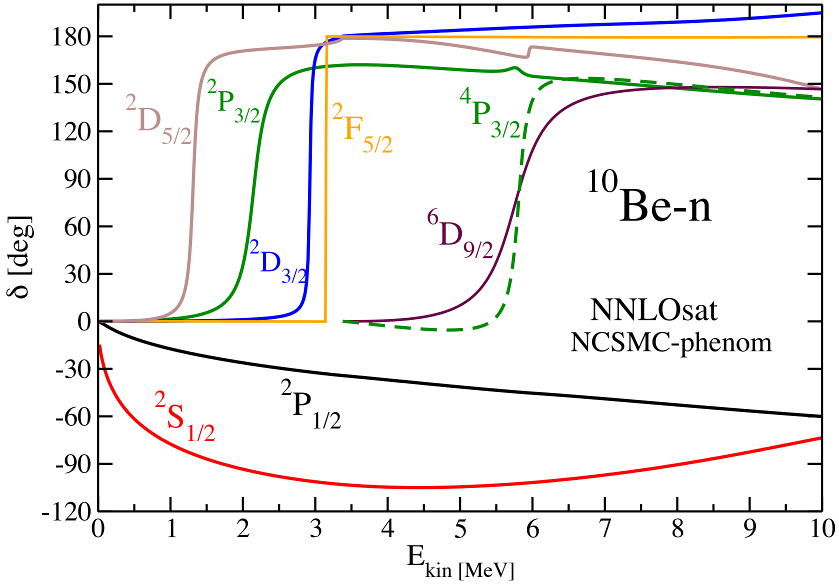


Photo-disassociation of ^{11}Be

Bound to bound	NCSM	NCSMC-phenom	Expt.
B(E1; $1/2^+ \rightarrow 1/2^-$) [e^2 fm^2]	0.0005	0.117	0.102(2)



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Bound to bound	NCSM	NCSMC-phenom	Expt.
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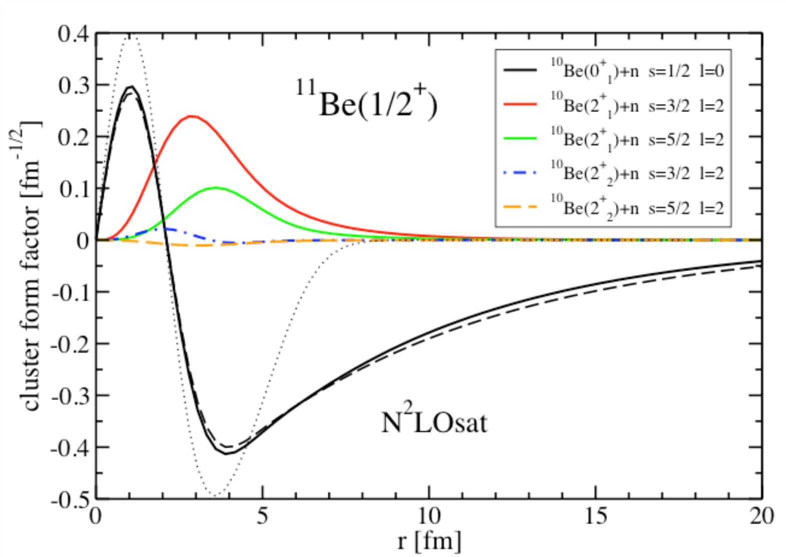
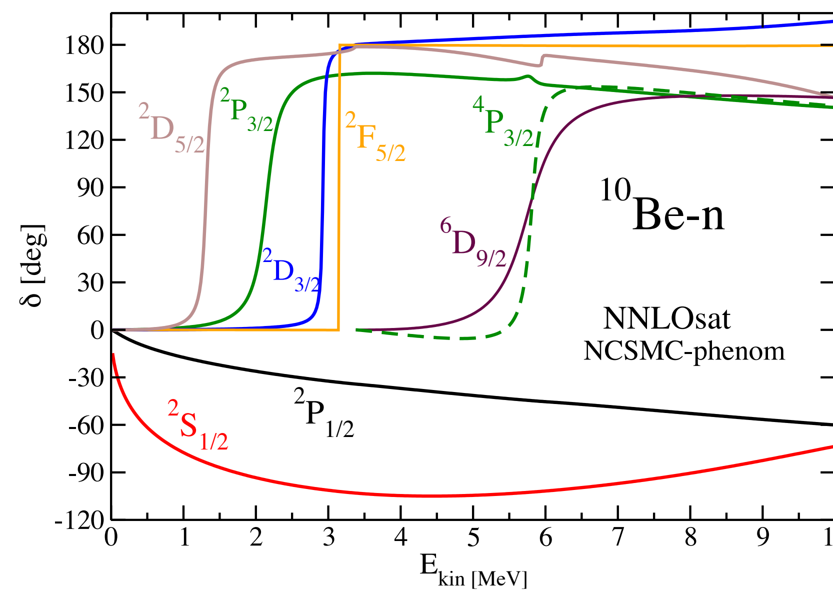
Halo structure





cluster form factor

$$= r \left\langle \Phi_{\nu r}^{J^\pi T} \middle| \hat{A}_\nu \middle| \psi^{J^\pi T} \right\rangle$$

$$\left|\Phi_{\nu r}^{J^\pi T}\right\rangle = \left[\left(\left|{}^{10}\mathrm{Be}\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|n\ \tfrac{1}{2}^+\ \tfrac{1}{2}\right\rangle\right)^{(sT)} Y_\ell(\hat{r}_{10,1})\right]^{(J^\pi T)} \frac{\delta(r - r_{10,1})}{r r_{10,1}}$$

PRL 117, 242501 (2016) PHYSICAL REVIEW LETTERS week ending 9 DECEMBER 2016

Can *Ab Initio* Theory Explain the Phenomenon of Parity Inversion in ^{11}Be?

Angelo Calci,[1,*] Petr Navrátil,[1,†] Robert Roth,[2] Jérémy Dohet-Eraly,[1,‡] Sofia Quaglioni,[3] and Guillaume Hupin[4,5]

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Bound to bound	NCSM	NCSMC-phenom	Expt.
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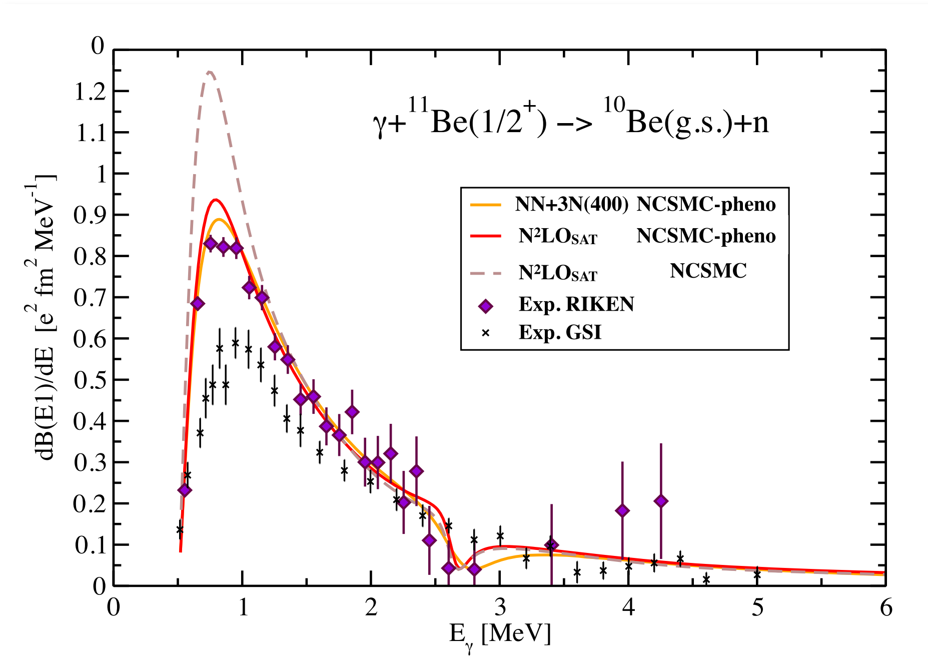
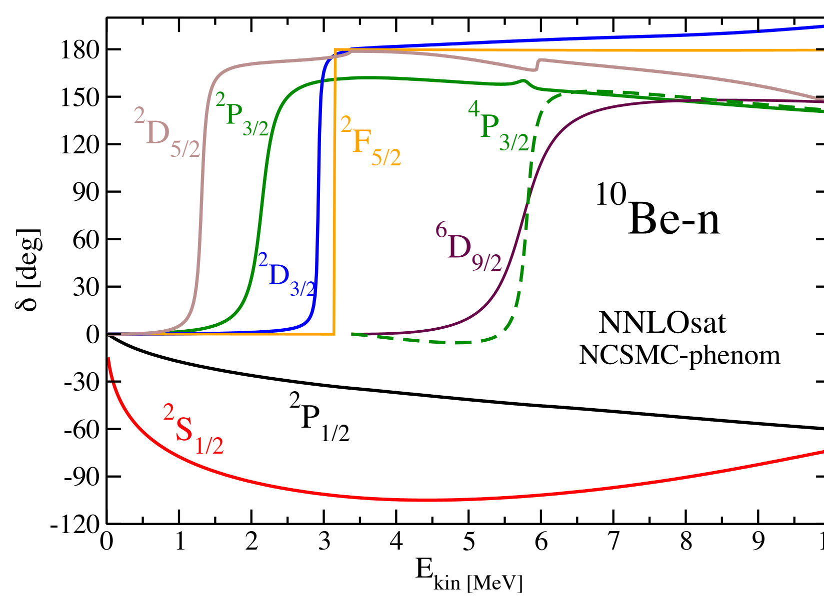
Bound to continuum





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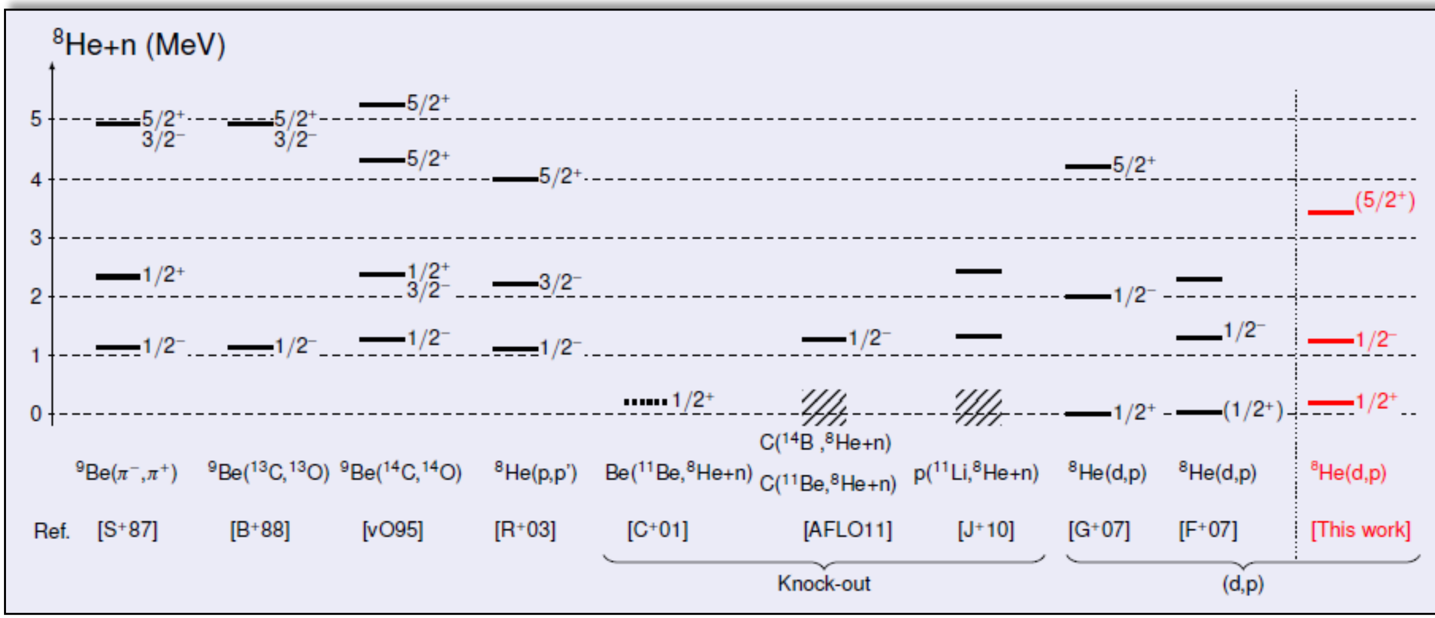
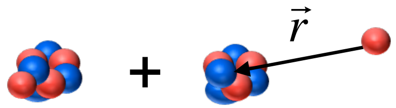
A still lighter N=7 isotone: ^{9}He

- Controversial experimental situation
  - From talk by Nigel Orr at ECT* in 2013



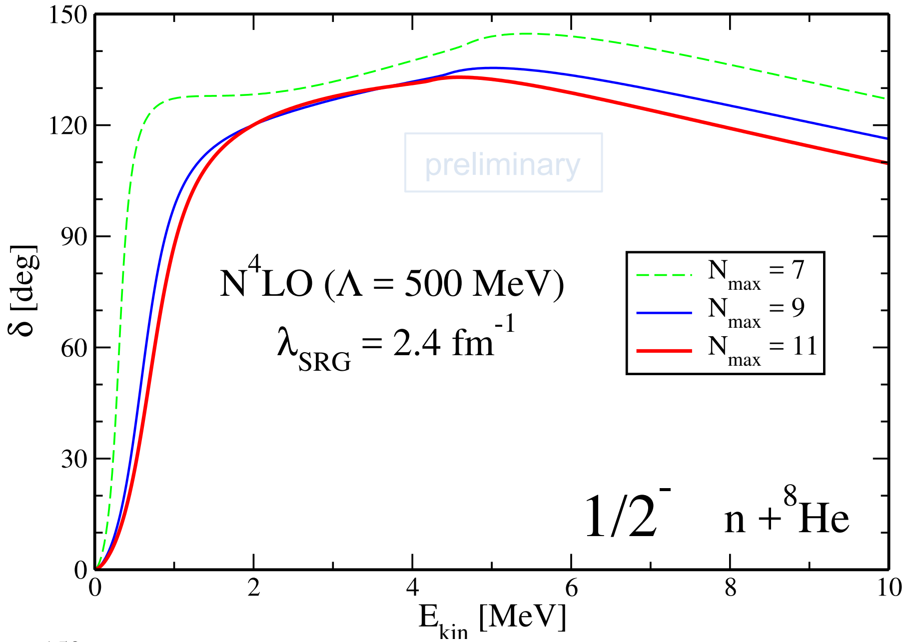
  - No bound state
  - Most experiments see 1/2$^-$ resonance ~ 1 MeV
  - Is there a 1/2$^+$ resonance? Is the ground state 1/2$^+$ or 1/2$^-$?
    - a_0~ -10 fm (Chen et al.)
    - a_0~ -3 fm (Al Falou, et al.)
  - Any higher-lying resonances?
  - Recent ^{8}He(p,p) measurement at TRIUMF by Rogachev found no T=5/2 resonances (PLB 754 (2016) 323)

- NCSMC calculations with several interactions
  - ^{9}He ~ $(^{9}\text{He})_{\text{NCSM}}$ + $(\text{n-}^{8}\text{He})_{\text{NCSM/RGM}}$
    - ^{8}He: 0^{+} and 2^{+} NCSM eigenstates
    - ^{9}He: ≥4 π = -1 and ≥4 π = +1 NCSM eigenstates

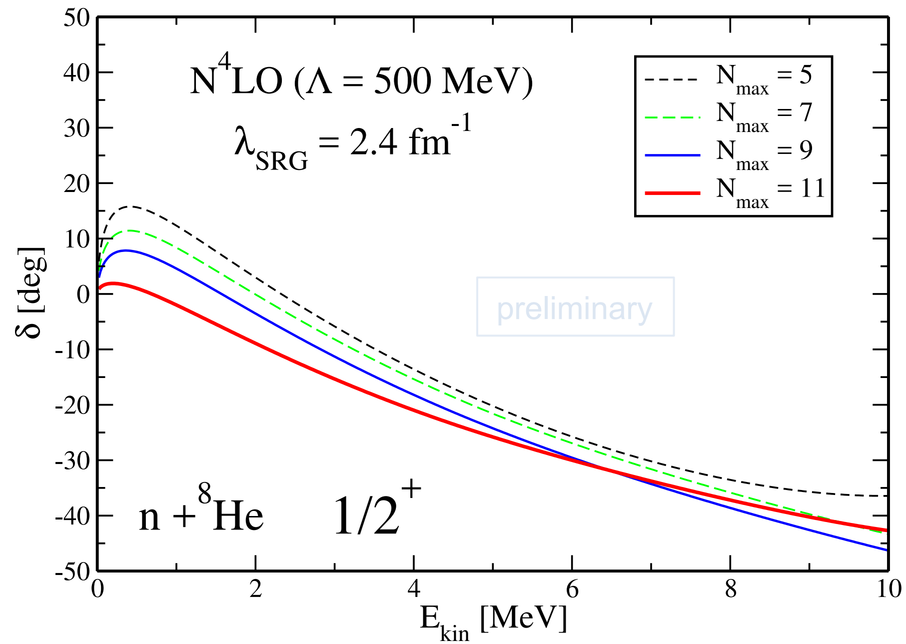


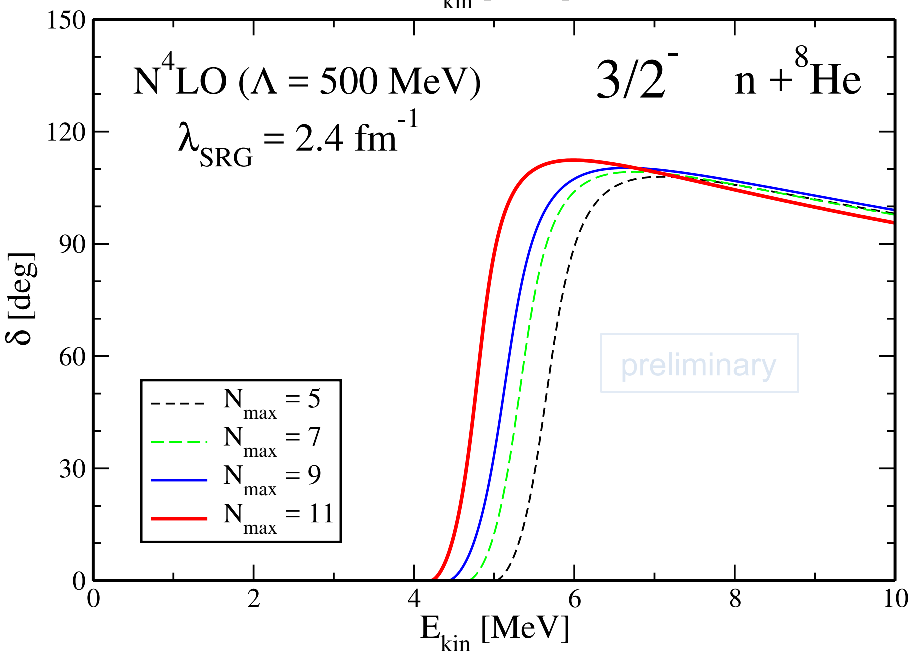
  - Importance of large N_{max} basis:
    - SRG-N^{4}LO500 NN with λ=2.4 fm^{-1}
      - up to N_{max}=11 with ^{9}He NCSM m-scheme basis of 350 million

G.s. energy [MeV]	^{4}He	^{6}He	^{8}He
SRG-N^{4}LO500 λ=2.4	-28.36	-28.9(2)	-30.1(2)
Expt	-28.30	-29.27	-31.41



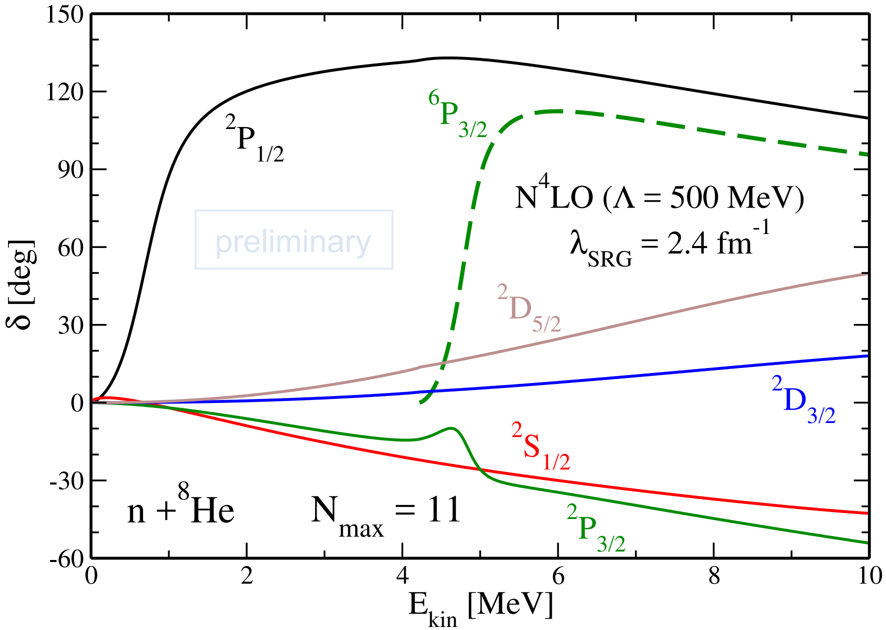
Phase shift convergence with SRG-N^{4}LO500 NN λ=2.4 fm^{-1}

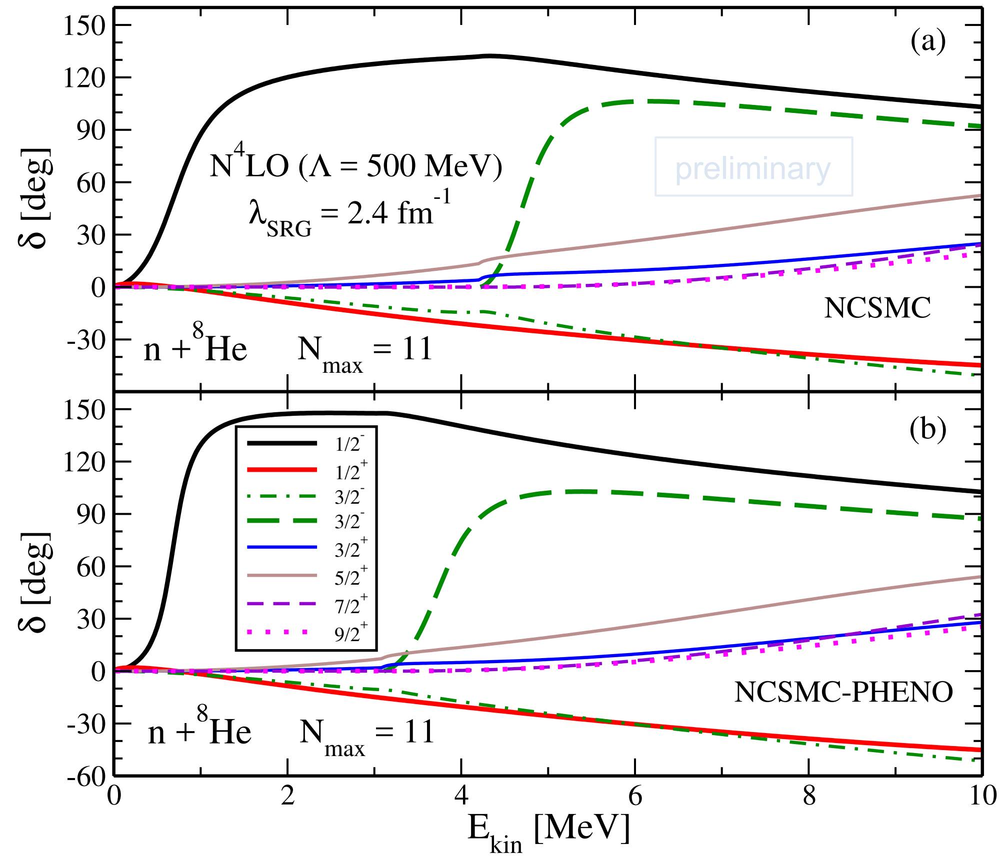




No bound state

Phase shift and eigenphase shifts with SRG-N^{4}LO500 NN λ=2.4 fm^{-1}





J^π	NCSMC		PHENO-NCSMC	
$1/2^-$	$E_R = 0.69$	$\Gamma = 0.83$	$E_R = 0.68$	$\Gamma = 0.37$
$3/2^-$	$E_R = 4.70$	$\Gamma = 0.74$	$E_R = 3.72$	$\Gamma = 0.95$

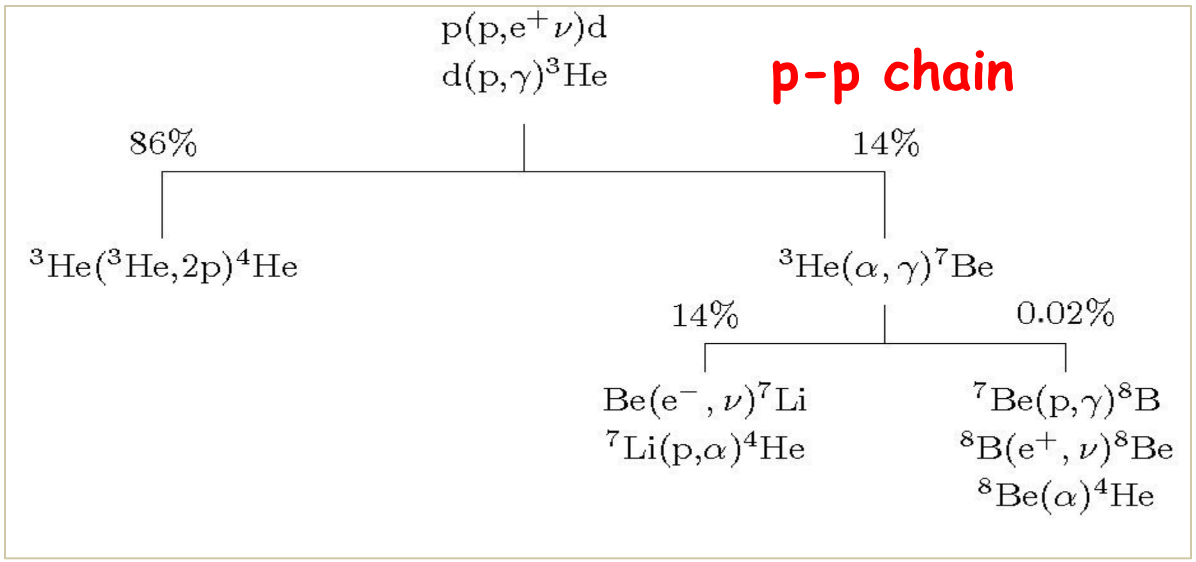
Robust results for **1/2$^-$** (~ 1MeV) and **3/2$^-$** (~4 MeV) **P-wave** resonances
(3/2$^-$ resonance in n-^{8}He(2$^+$) channel)
1/2$^+$ S-wave with vanishing scattering length: a_s= 0 ~ -1 fm
No evidence for other higher lying resonances

p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

- Measurement of ^{11}C(p,p) resonance scattering planned at TRIUMF
  - TUDA facility
  - ^{11}C beam of sufficient intensity produced
- NCSMC calculations of ^{11}C(p,p) with chiral NN+3N under way
- Obtained wave functions will be used to calculate ^{11}C(p,γ)^{12}N capture relevant for astrophysics

p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

- ^{11}C(p,γ)^{12}N capture relevant in hot *p-p* chain: Link between pp chain and the CNO cycle - bypass of slow triple alpha capture ^{4}He(αα,γ)^{12}C



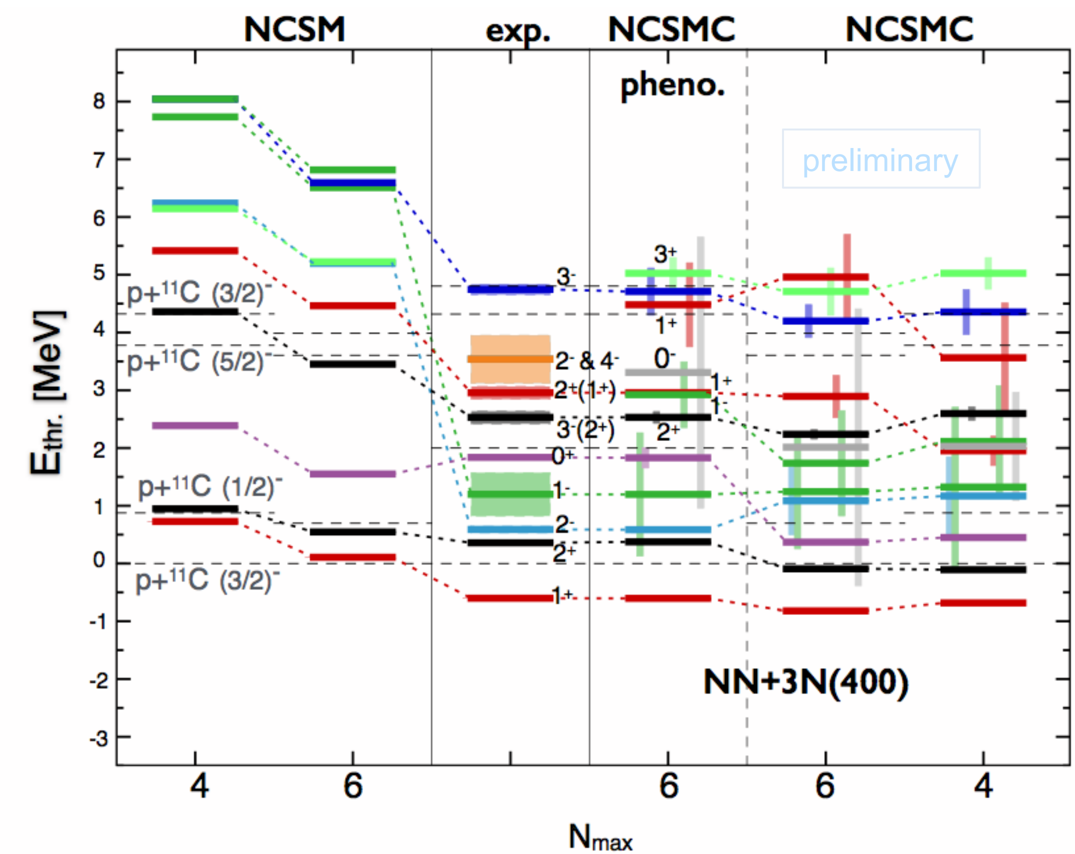
$$^{3}He(\alpha,\gamma)^{7}Be(\alpha,\gamma)^{11}C(p,\gamma)^{12}N(p,\gamma)^{13}O(\beta^{+},\nu)^{13}N(p,\gamma)^{14}O$$

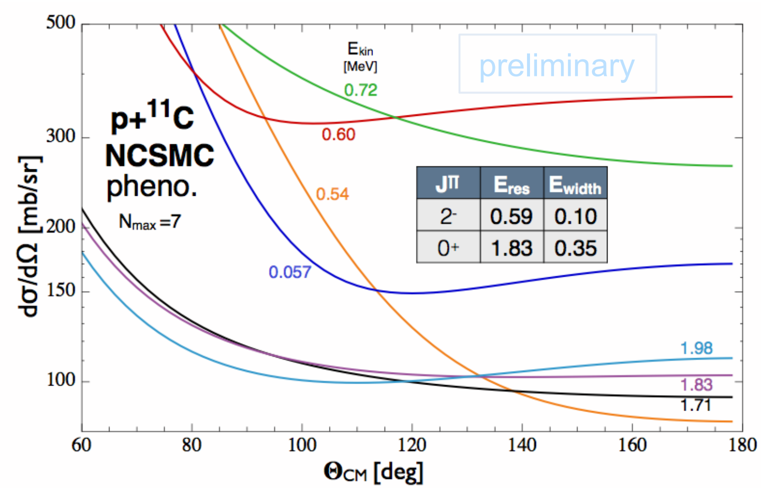
$$^{3}He(\alpha,\gamma)^{7}Be(\alpha,\gamma)^{11}C(p,\gamma)^{12}N(\beta^{+},\nu)^{12}C(p,\gamma)^{13}N(p,\gamma)^{14}O$$

$$^{11}\mathrm{C}(\beta^{+}\ \nu)^{11}\mathrm{B}(p,\alpha)^{8}\mathrm{Be}(^{4}\mathrm{He},^{4}\mathrm{He})$$

Next: p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

- NCSMC calculations of ^{11}C(p,p) with chiral NN+3N under way
  - ^{11}C: $3/2^-$, $1/2^-$, $5/2^-$, $3/2^-$ NCSM eigenstates
  - ^{12}N: ≥6 π = +1 and ≥4 π = -1 NCSM eigenstates





NCSMC calculations to be validated by measured cross sections and applied to calculate the ^{11}C(p,γ)^{12}N capture

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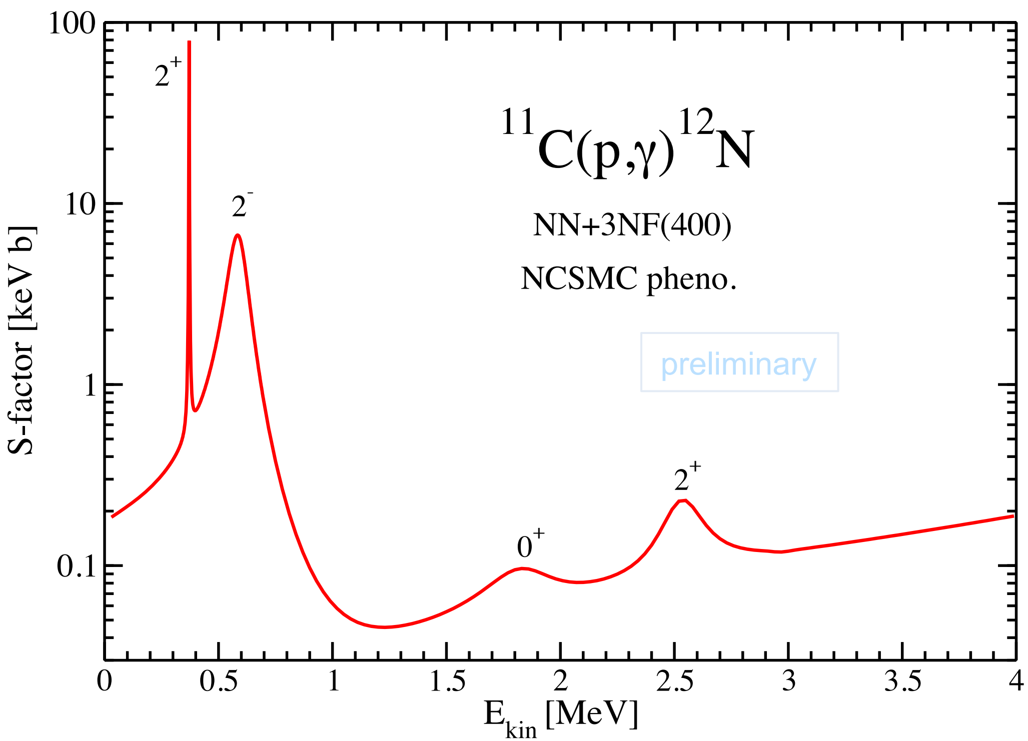
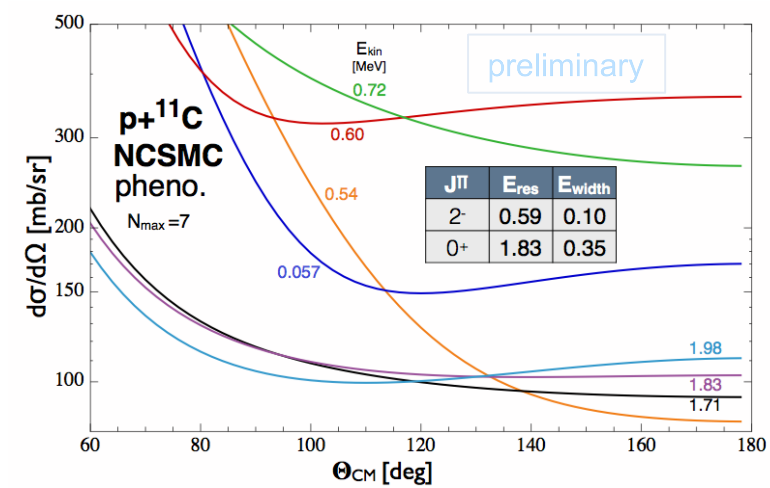




NCSMC calculations to be validated by measured cross sections and applied to calculate the ^{11}C(p,γ)^{12}N capture

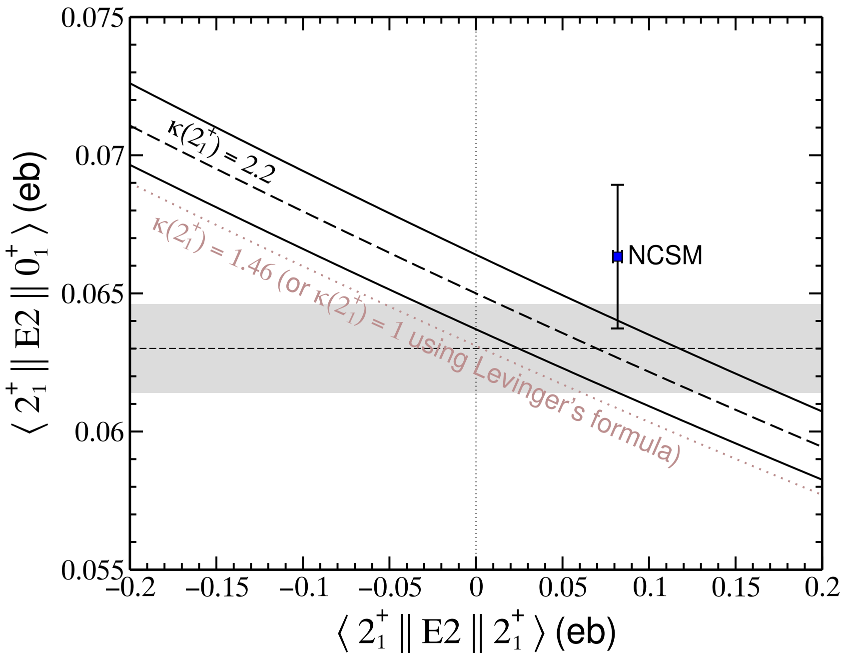
- New Coulomb excitation reorientation-effect measurement at TRIUMF
  - TIGRESS array, particle-gamma coincidence
  - Analysis by the semi-classical coupled-channel Coulomb-excitation least-squares code GOSIA
  - Extraction of $\langle 2^+_1 \,||\, E2 \,||\, 2^+_1 \rangle$ matrix element
- Nuclear polarizability for the ground and the 2^+_1 states needed
  - Calculated by the no-core shell model (NCSM) using chiral NN and NN+3N interaction

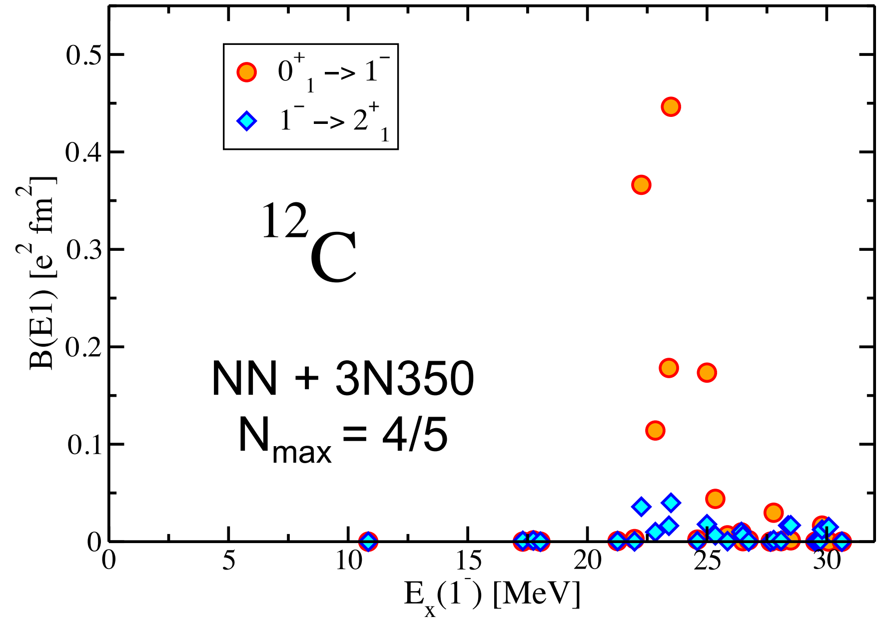
$$\frac{\sum_n W(11J_iJ_f,2J_n)\,\frac{\langle i||\hat{E}1||n\rangle\langle n||\hat{E}1||f\rangle}{E_n-E_i}}{\langle i\,||\,\hat{E}2\,||\,f\rangle}$$

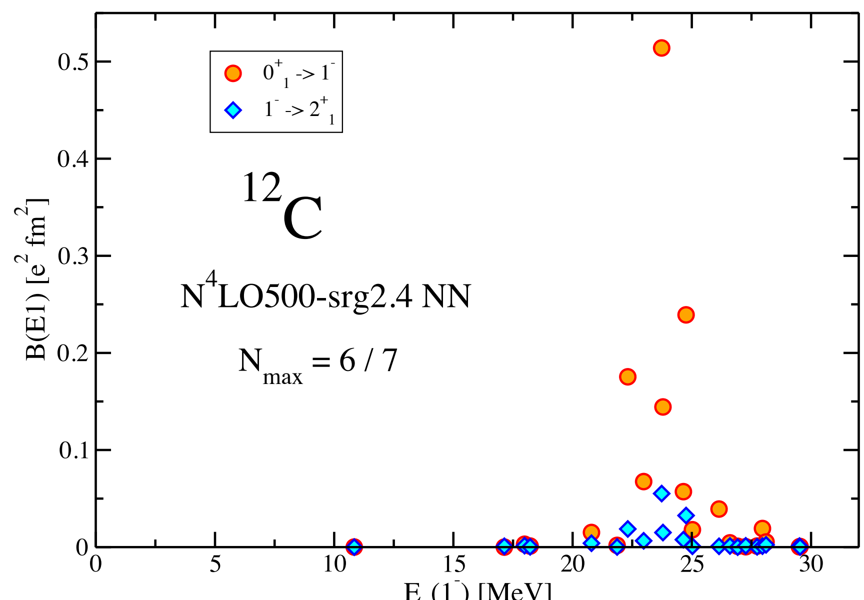
Quadrupole moment of ^{12}C 2^+ state

M. Kumar Raju *et al.*, arXiv 1709.07501

$$\frac{\sum_n W(11J_iJ_f,2J_n)\,\frac{\langle i||\hat{E}1||n\rangle\langle n||\hat{E}1||f\rangle}{E_n-E_i}}{\langle i\,||\,\hat{E}2\,||\,f\rangle}$$







New determination:
Oblate shape

$$Q_S(2_1^+) = +0.071(25)\ \mathrm{eb}$$

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)

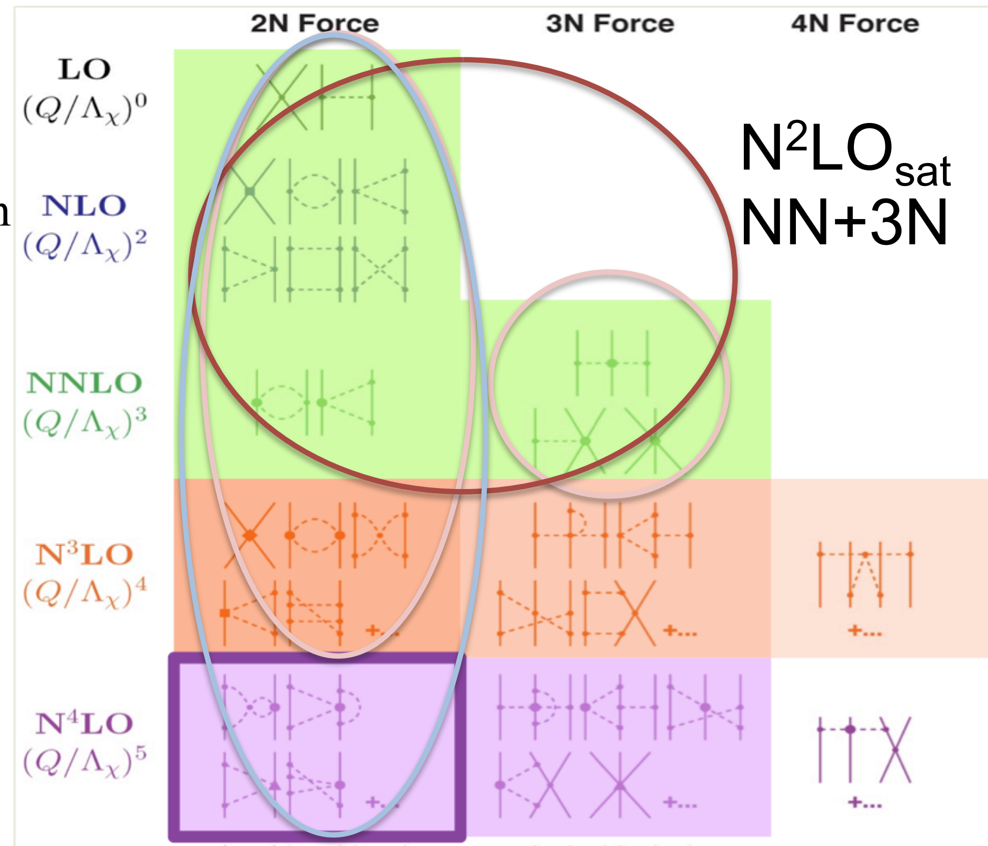
- Synergy between theory and experiment:
  - Calculations of ^{10}C(p,p) compared to TRIUMF/IRIS measurement
    - Test of chiral forces
  - Calculations of ^{11}C(p,p) to be compared to approved TRIUMF/TUDA experiment
    - Determination of ^{11}C(p,γ)^{12}N
  - Nuclear polarizability for the determination of ^{12}C 2^+ quadrupole moment
    - TRIUMF/TIGRESS experiment

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

TRIUMF

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

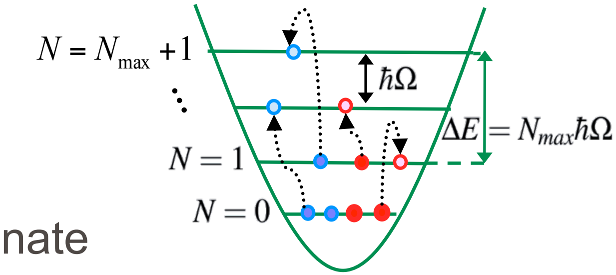


N^{4}LO500 NN

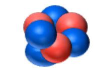
N^{3}LO NN+N^{2}LO 3N
(NN+3N400, NN+3N500)

Λ_χ~1 GeV :
Chiral symmetry breaking scale

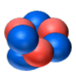
- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances
  - Equivalent description in relative-coordinate and Slater determinant basis



Harmonic oscillator basis

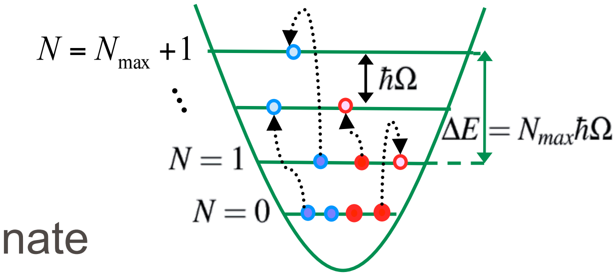


NCSM

(A) 

$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^{HO}(\vec{\eta}_1, \vec{\eta}_2, \ldots, \vec{\eta}_{A-1})$$

- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances
  - Equivalent description in relative-coordinate and Slater determinant basis



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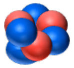


NCSM

(A) 

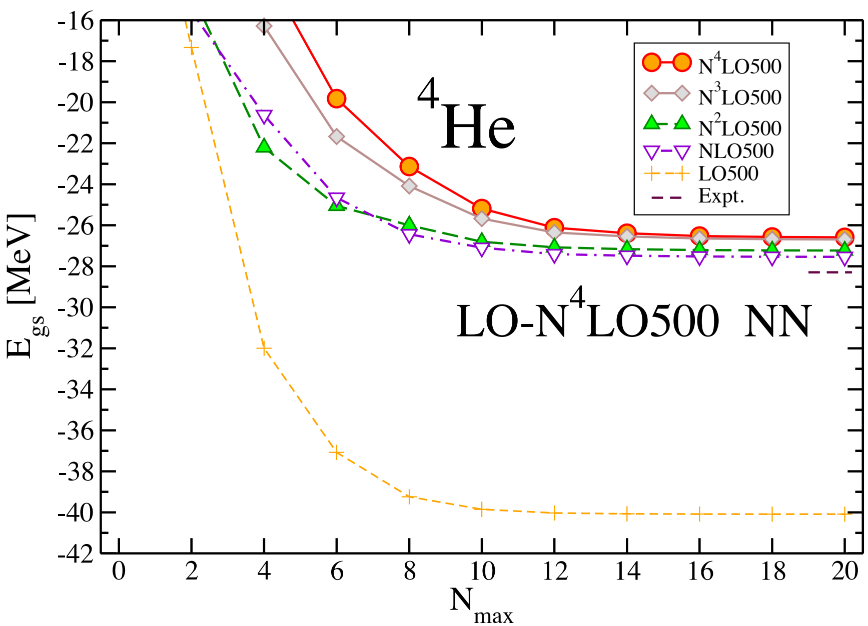
$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni}\, \Phi_{Ni}^{HO}(\vec{\eta}_1, \vec{\eta}_2, \ldots, \vec{\eta}_{A-1})$$

(A) 

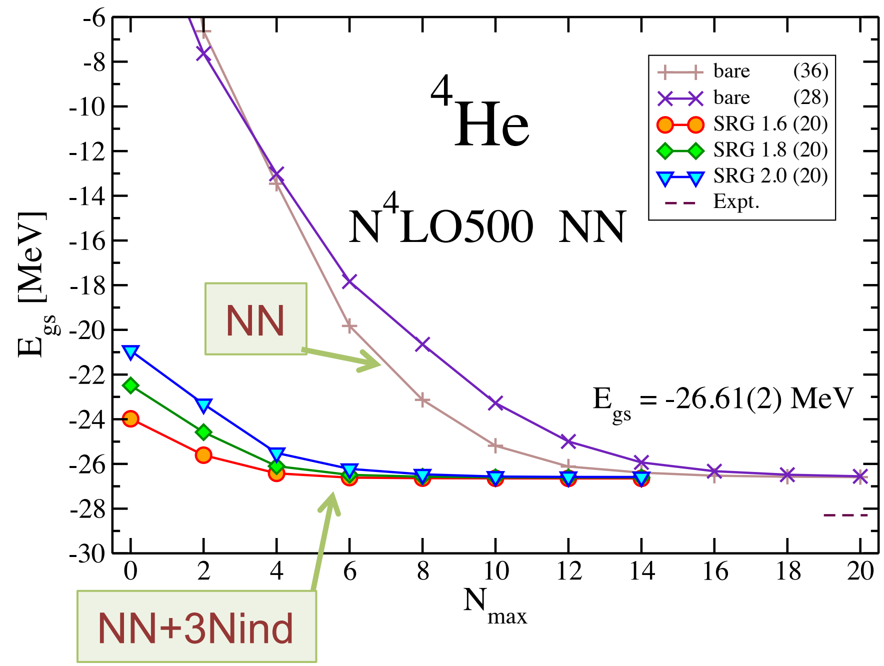
$$\Psi_{\mathrm{SD}}^A = \sum_{N=0}^{N_{\max}} \sum_j c_{Nj}^{\mathrm{SD}}\, \Phi_{\mathrm{SD}\,Nj}^{HO}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = \Psi^A\, \varphi_{000}(\vec{R}_{CM})$$

Chiral EFT interactions up to N^{4}LO

- Systematic from LO to N^{4}LO
- High precision – χ^2/datum = 1.15
  - D. R. Entem, N. Kaiser, R. Machleidt, and Y. Nosyk, Phys. Rev. C 91, 014002 (2015).
  - D. R. Entem, R. Machleidt, and Y. Nosyk, Phys. Rev. C 96, 024004 (2017).



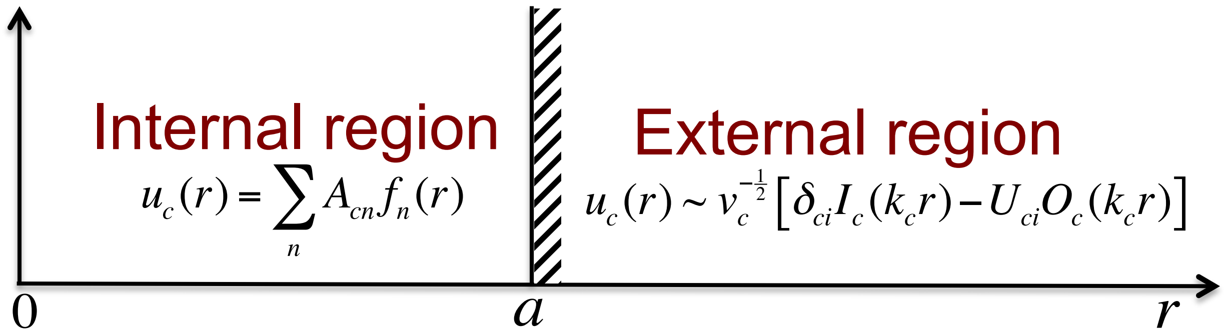
Original EM 2003 N^{3}LO NN E_{gs}=-25.39 MeV

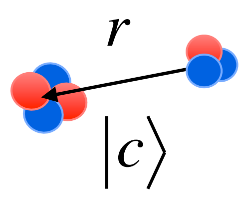


TRIUMF

Microscopic *R*-matrix theory on Lagrange mesh

- Separation into “internal” and “external” regions at the channel radius a





  - This is achieved through the Bloch operator: $L_c = \frac{\hbar^2}{2\mu_c} \delta(r-a) \left(\frac{d}{dr} - \frac{B_c}{r} \right)$
  - System of Bloch-Schrödinger equations:

$$\left[\hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r) - (E - E_c) \right] u_c(r) + \sum_{c'} \int dr' r' W_{cc'}(r,r') u_{c'}(r') = L_c u_c(r)$$

  - Internal region: expansion on Lagrange square-integrable basis $u_c(r) = \sum_n A_{cn} f_n(r)$
  - External region: asymptotic form for large r

$u_c(r) \sim C_c W(k_c r)$ or $u_c(r) \sim v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r) \right]$

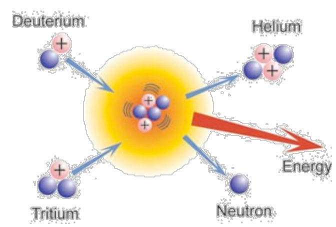
Scattering matrix

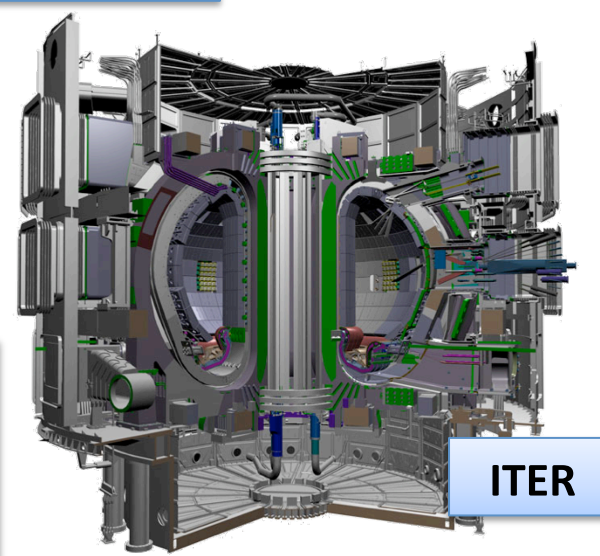
Bound state

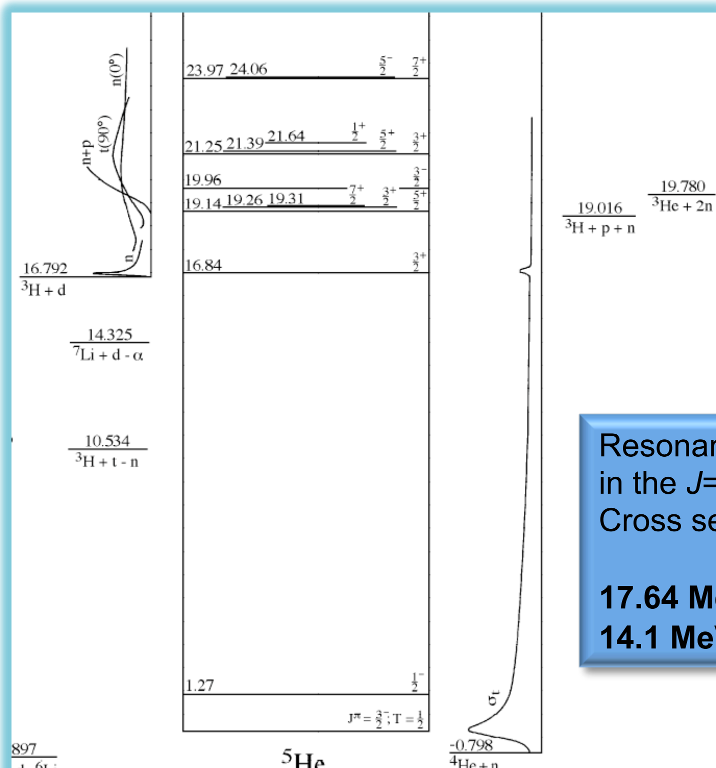
Scattering state

Deuterium-Tritium fusion

- The d+^{3}H→n+^{4}He reaction
  - The most promising for the production of fusion energy in the near future
  - Used to achieve inertial-confinement (laser-induced) fusion at NIF, and magnetic-confinement fusion at ITER
  - With its mirror reaction, ^{3}He(d,p)^{4}He, important for Big Bang nucleosynthesis

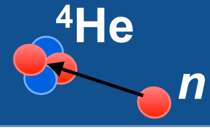






Resonance at E_{cm} =48 keV (E_d=105 keV) in the J=3/2$^+$ channel
Cross section at the peak: 4.88 b

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

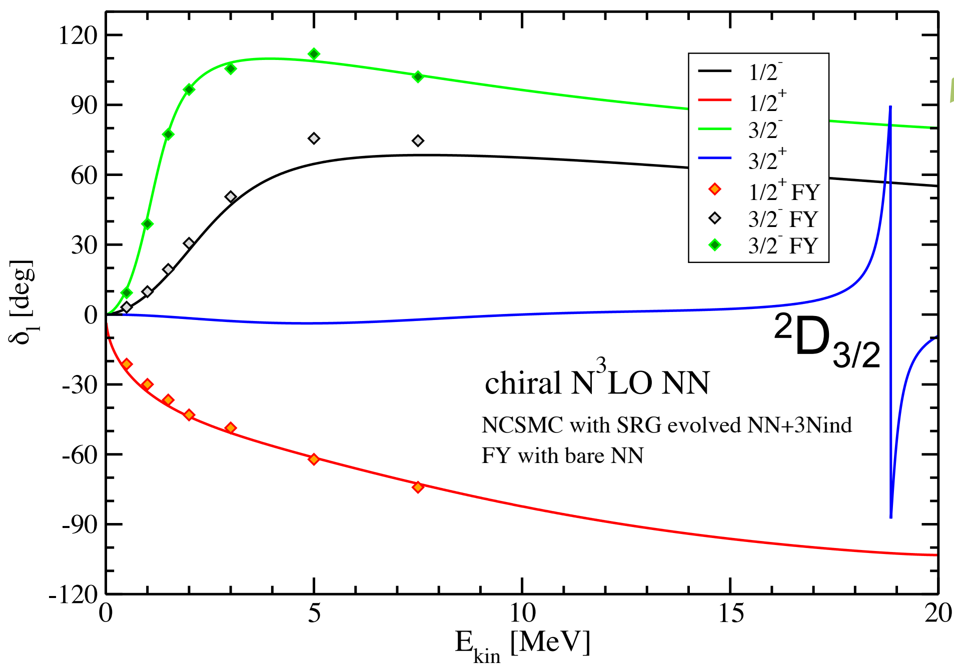


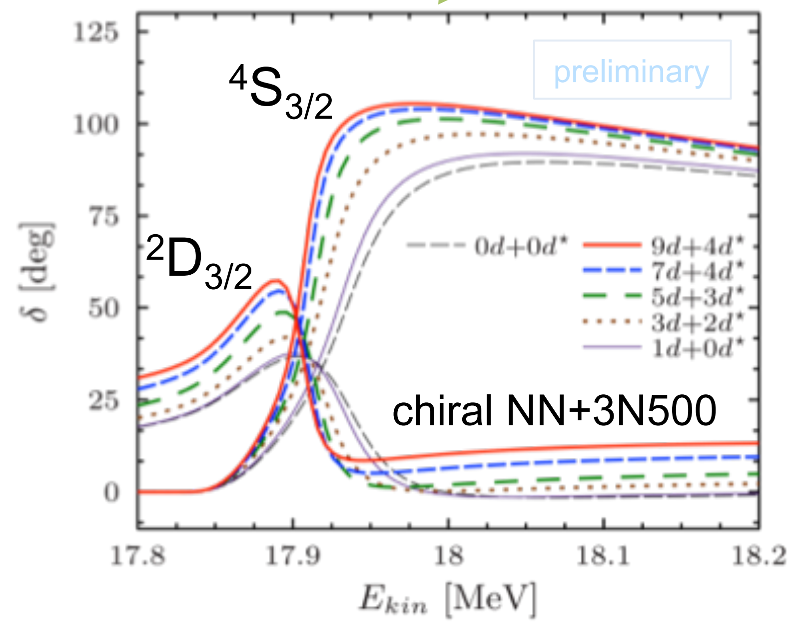
n-^{4}He scattering within NCSMC

n-^{4}He scattering phase-shifts for chiral NN

^{4}He+n

^{4}He+n -> ^{3}H+d





FY: Faddeev-Yakubovsky method - Rimantas Lazauskas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Phys. Scr. 00 (2016) 000000 (37pp)

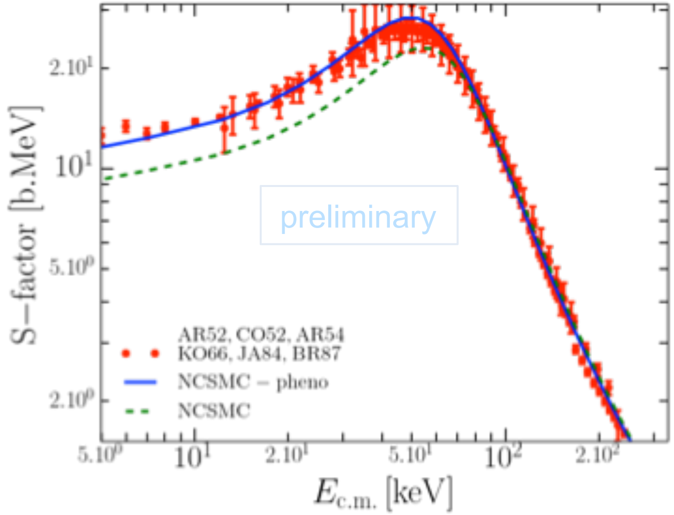
Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]

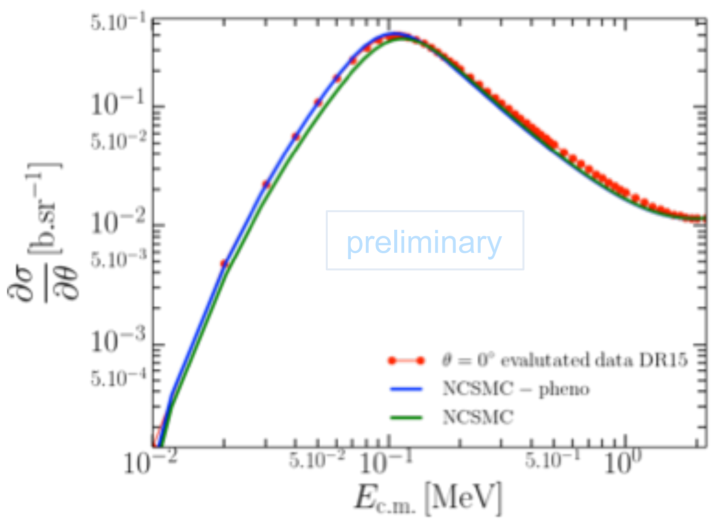
The d-^{3}H fusion takes place through a transition of d+^{3}H is S-wave to n+^{4}He in D-wave: Importance of the **tensor and 3N force**

$^3H(d,n)^4He$ with chiral NN+3N500 interaction

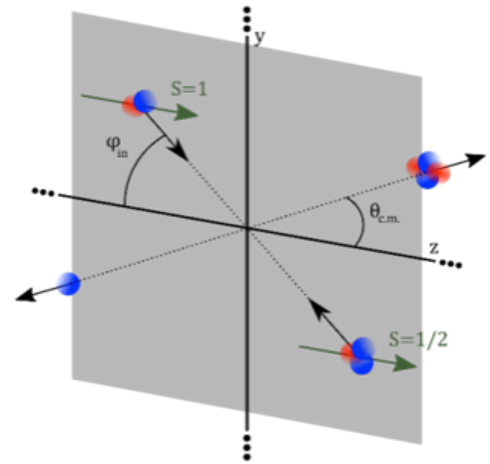


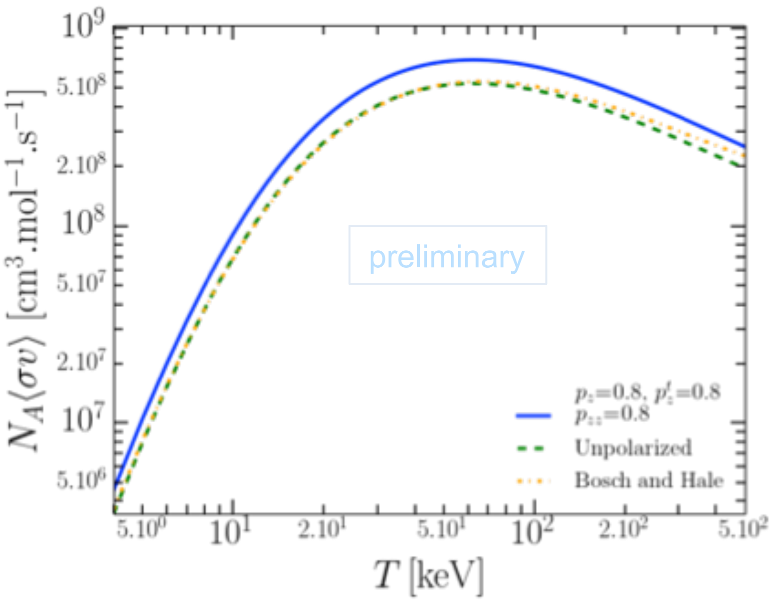
$$S(E) = E\sigma(E)\exp[2\pi\eta(E)]$$

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



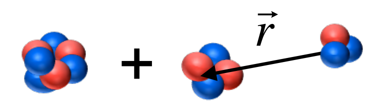
Polarized fusion

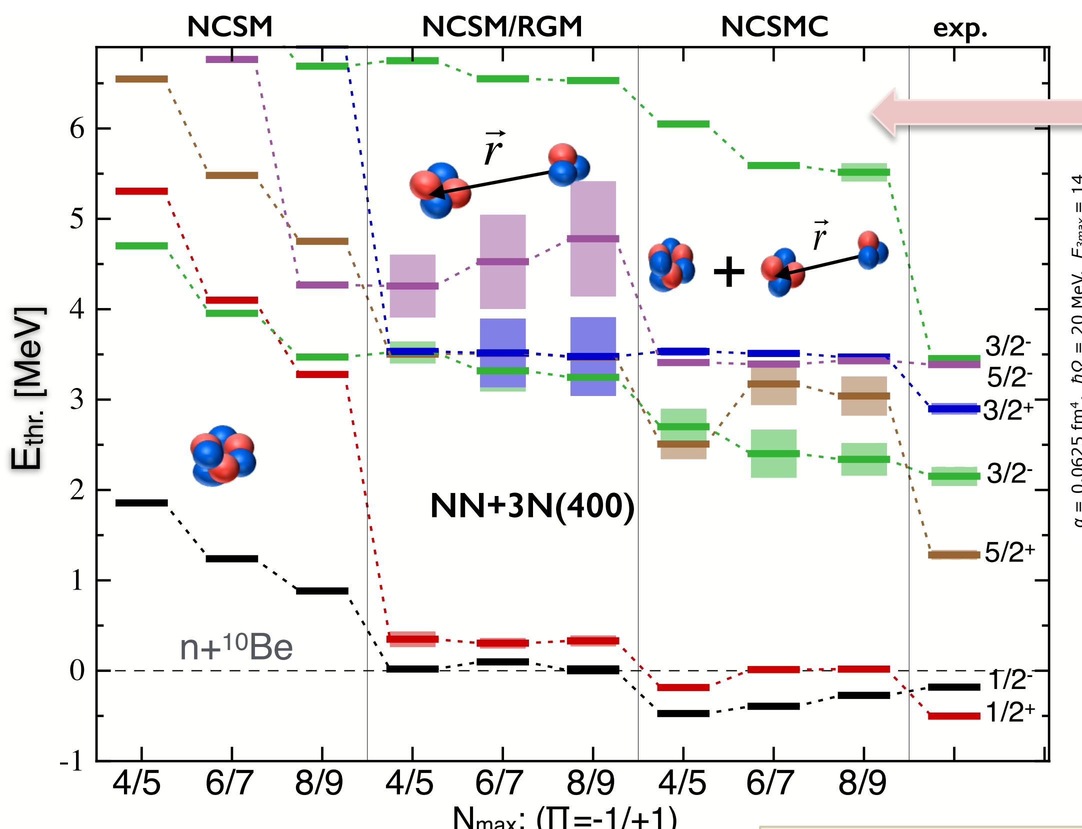




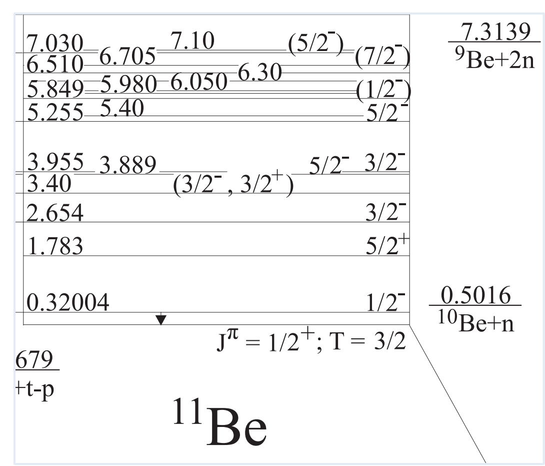
Structure of ^{11}Be from chiral NN+3N forces

- 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





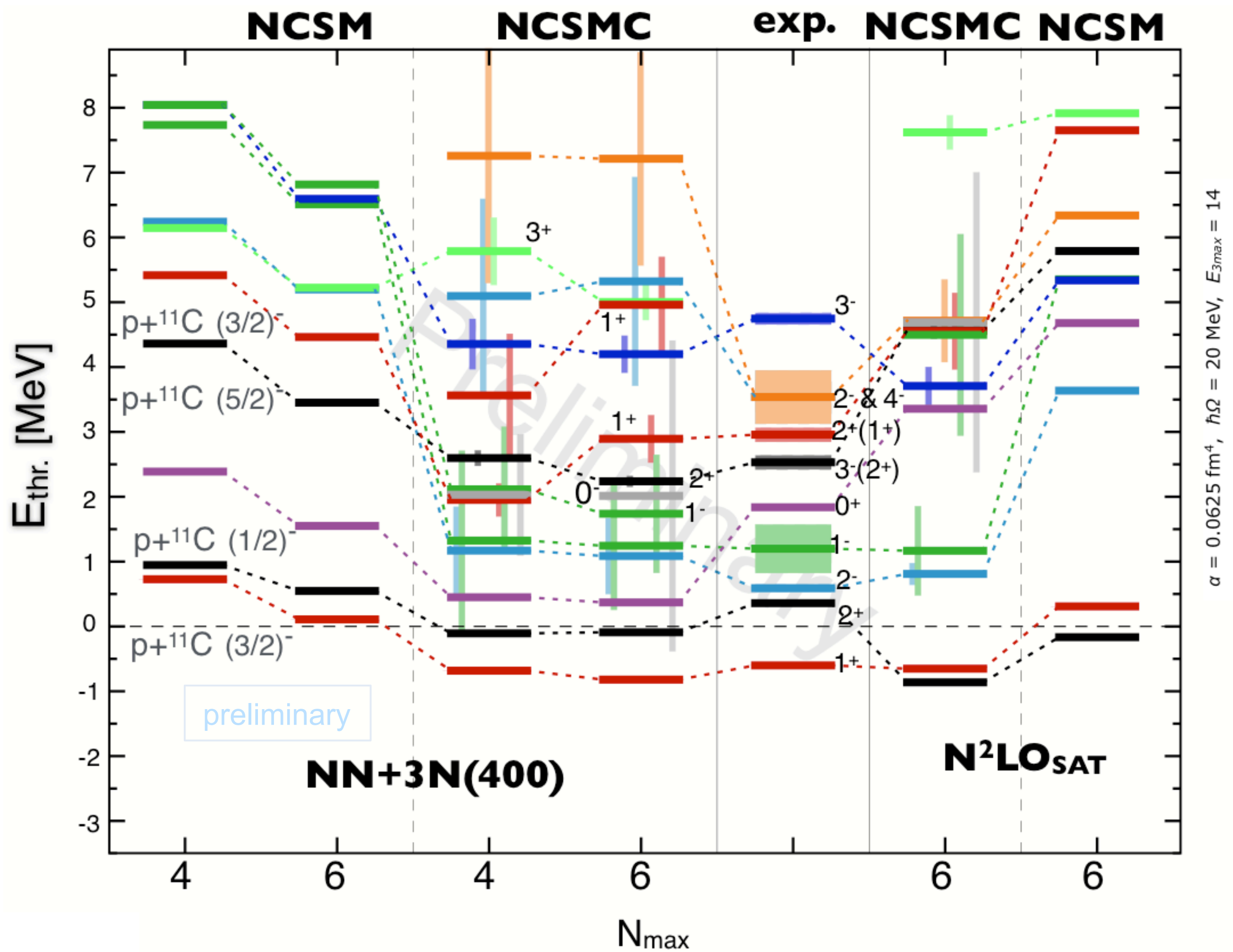
Continuum effects



A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, PRL 117, 242501 (2016)

p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

- NCSMC calculations of ^{11}C(p,p) with chiral NN+3N under way



Similarity Renormalization Group (SRG) evolution

- Continuous transformation driving Hamiltonian to band-diagonal form with respect to a chosen basis
- Unitary transformation $H_\alpha = U_\alpha H U_\alpha^+$ $\qquad U_\alpha U_\alpha^+ = U_\alpha^+ U_\alpha = 1$

$$\frac{dH_\alpha}{d\alpha} = \frac{dU_\alpha}{d\alpha} U_\alpha^+ H_\alpha + H_\alpha U_\alpha \frac{dU_\alpha^+}{d\alpha} = [\eta_\alpha, H_\alpha]$$

$$\eta_\alpha \equiv \frac{dU_\alpha}{d\alpha} U_\alpha^+ = -\eta_\alpha^+$$

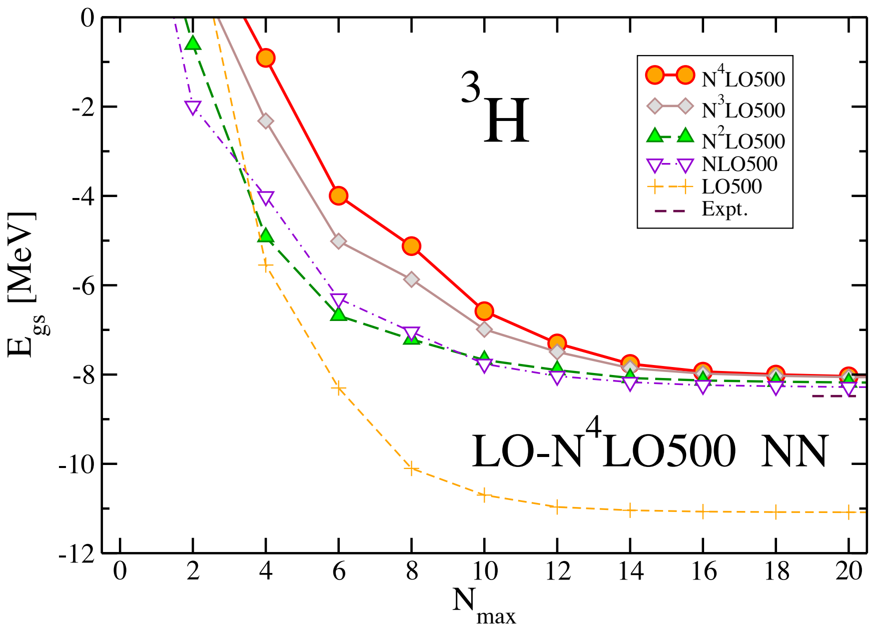
anti-Hermitian generator

- Setting $\eta_\alpha = [G_\alpha, H_\alpha]$ with Hermitian G_α

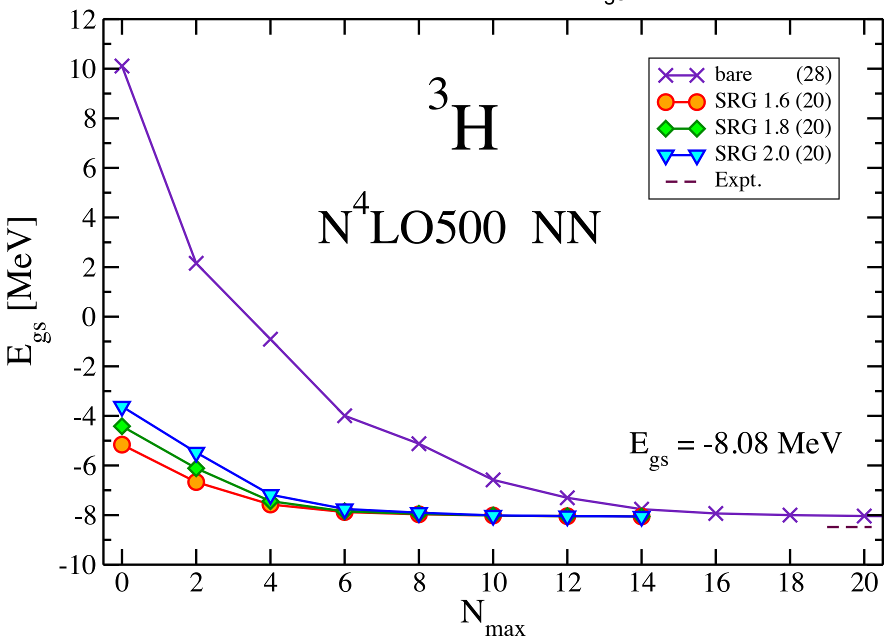
$$\frac{dH_\alpha}{d\alpha} = [[G_\alpha, H_\alpha], H_\alpha]$$

- Customary choice in nuclear physics $G_\alpha = T$ …kinetic energy operator
  - band-diagonal in momentum space plane-wave basis
- Initial condition $H_{\alpha=0} = H_{\lambda=\infty} = H$ $\qquad \lambda^2 = 1/\sqrt{\alpha}$
- **Induces many-body forces**
  - **In applications to chiral interactions three-body induced terms large, four-body small**

- Systematic from LO to N^4LO
- High precision – χ^2/datum = 1.15
  - D. R. Entem, N. Kaiser, R. Machleidt, and Y. Nosyk, Phys. Rev. C 91, 014002 (2015).
  - D. R. Entem, R. Machleidt, and Y. Nosyk, arXiv:1703.05454.



Original EM 2003 N^3LO NN E_{gs}=-7.85 MeV



Chiral EFT interactions up to N^4LO

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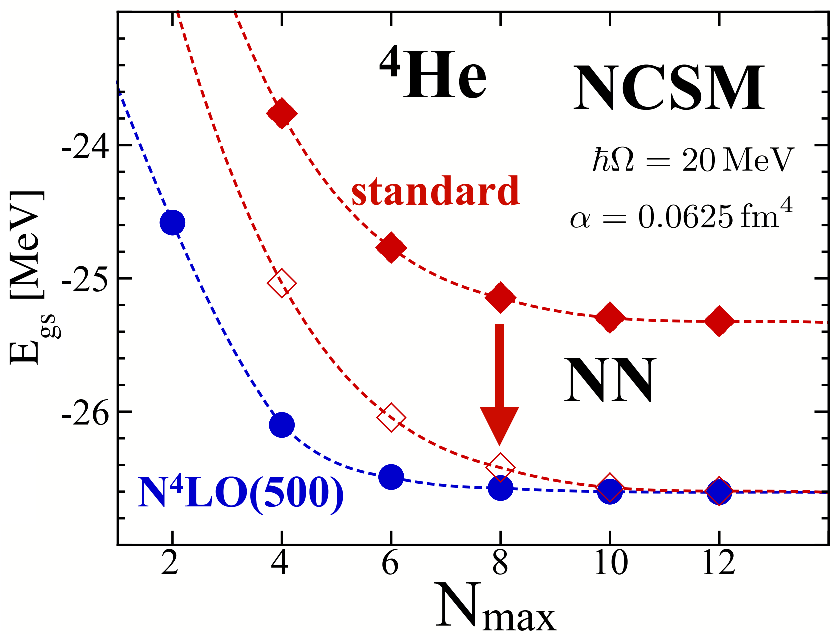
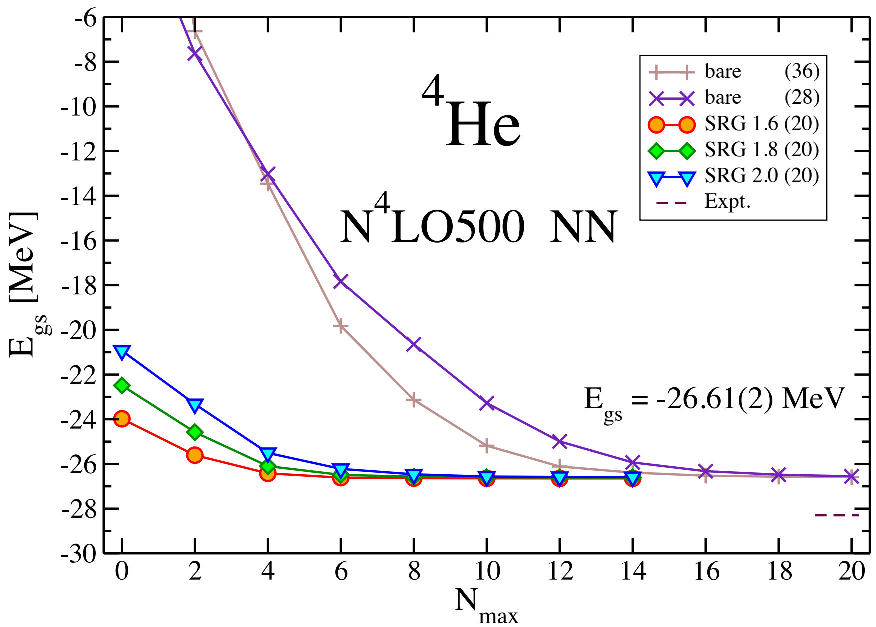


Original EM 2003 N^3LO NN E_{gs}=-25.39 MeV



Chiral EFT interactions up to N^4LO

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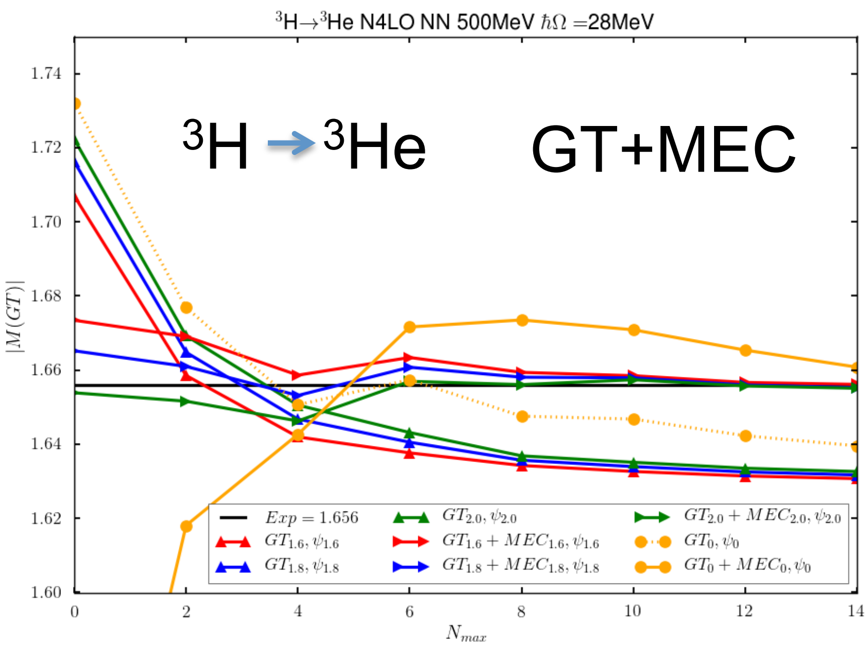
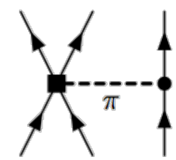


Determination of the c_D parameter relevant to chiral 3N force c_D=0.45 (3N repulsive)

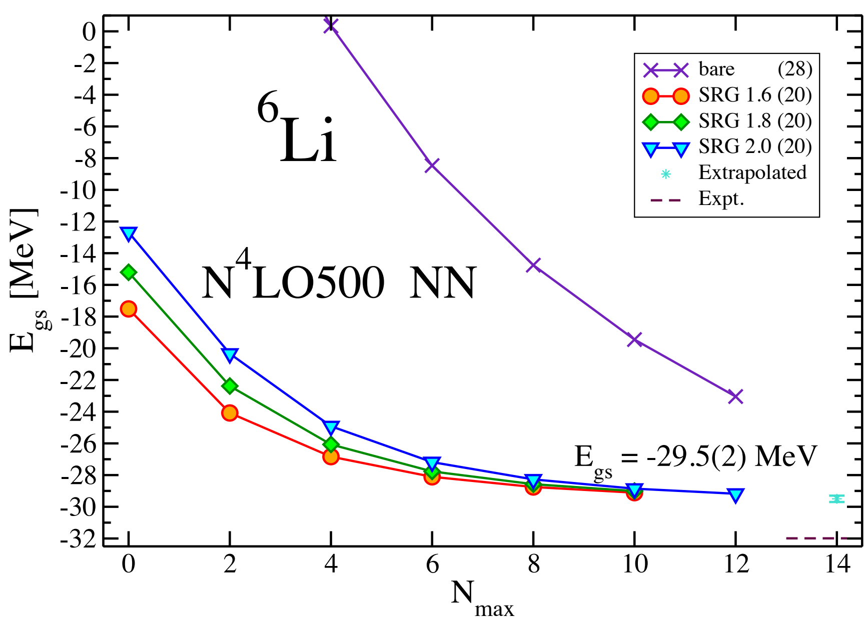


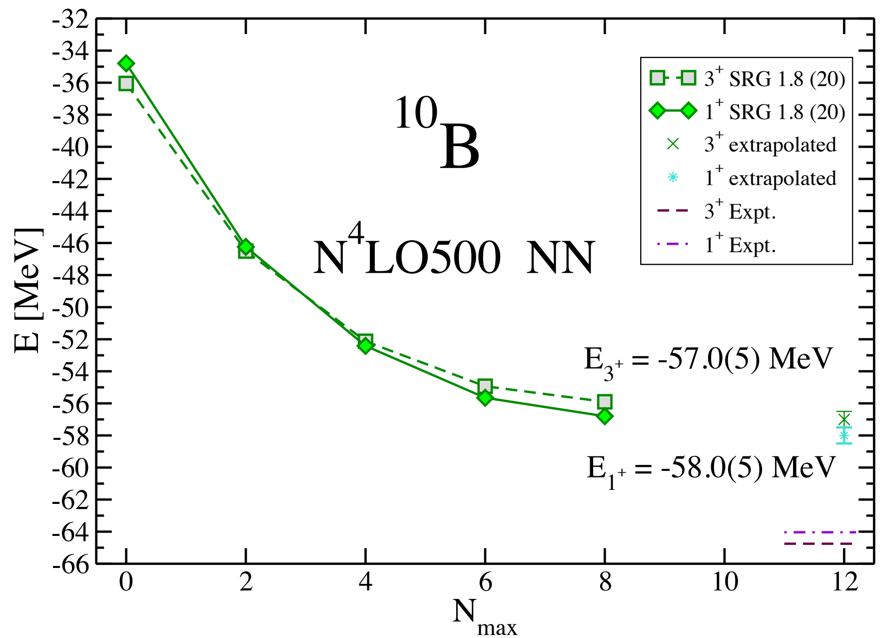
Original EM 2003 N^3LO NN c_D=-0.2 (3N attractive)

Chiral EFT interactions up to N^4LO

- Systematic from LO to N^4LO
- High precision – χ^2/datum = 1.15
  - D. R. Entem, N. Kaiser, R. Machleidt, and Y. Nosyk, Phys. Rev. C 91, 014002 (2015).
  - D. R. Entem, R. Machleidt, and Y. Nosyk, arXiv:1703.05454.

Original EM 2003 N^3LO NN E_{gs}=-28.0(5) MeV

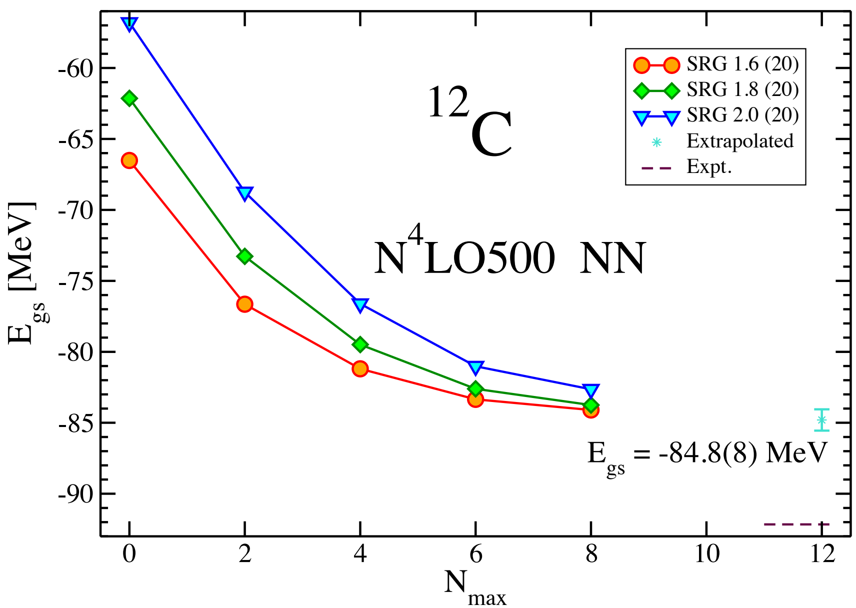




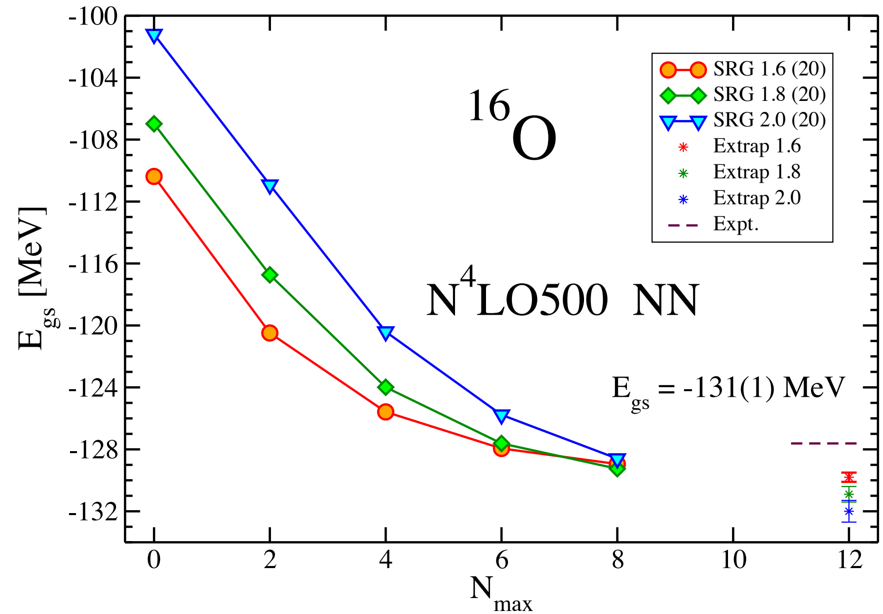
Chiral EFT interactions up to N^{4}LO

- Systematic from LO to N^{4}LO
- High precision – χ^2/datum = 1.15
  - D. R. Entem, N. Kaiser, R. Machleidt, and Y. Nosyk, Phys. Rev. C 91, 014002 (2015).
  - D. R. Entem, R. Machleidt, and Y. Nosyk, arXiv:1703.05454.

Original EM 2003 N^{3}LO NN E_{gs}=-77.2(3) MeV



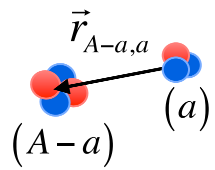
Original EM 2003 N^{3}LO NN E_{gs}=-119.5(5) MeV



Binary cluster Resonating Group Method

- Working in partial waves ($\nu \equiv \left\{A-a\ \alpha_1 I_1^{\pi_1} T_1; a\ \alpha_2 I_2^{\pi_2} T_2; s\ell\right\}$)

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \hat{A}_\nu \left[\left(\underbrace{\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle}_{\text{Target}}\underbrace{\left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle}_{\text{Projectile}}\right)^{(sT)} Y_\ell(\hat{r}_{A-a,a})\right]^{(J^\pi T)} \frac{\gamma_\nu^{J^\pi T}(r_{A-a,a})}{r_{A-a,a}}$$

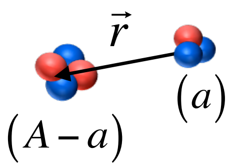


- Introduce a dummy variable $\vec{r}$ with the help of the delta function

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{\gamma_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle\left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell(\hat{r})\right]^{(J^\pi T)} \delta(\vec{r}-\vec{r}_{A-a,a})\ r^2 dr\, d\hat{r}$$

  - Allows to bring the wave function of the relative motion in front of the antisymmetrizer

$$\sum_\nu \int d\vec{r}\ \gamma_\nu(\vec{r})\ \hat{A}_\nu \Big| \quad , \nu \Big\rangle$$



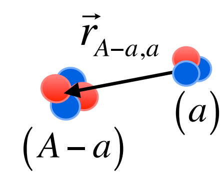
TRIUMF

Binary cluster Resonating Group Method

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{\gamma_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle \right)^{(sT)} Y_\ell(\hat{r}) \right]^{(J^\pi T)} \delta(\vec{r} - \vec{r}_{A-a,a})\ r^2 dr\, d\hat{r}$$

- Now introduce partial wave expansion of delta function

$$\delta(\vec{r} - \vec{r}_{A-a,a}) = \sum_{\lambda\mu} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}} Y^*_{\lambda\mu}(\hat{r}) Y_{\lambda\mu}(\hat{r}_{A-a,a})$$



- After integration in the solid angle one obtains:

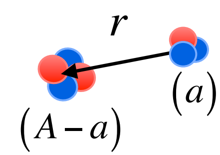
$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{\gamma_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \underbrace{\left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi T)} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}}}_{\left|\Phi_{\nu r}^{J^\pi T}\right\rangle} r^2 dr$$

(Jacobi) channel basis

TRIUMF

Binary cluster Resonating Group Method

- Trial wave function: $\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{\gamma_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \left|\Phi_{\nu r}^{J^\pi T}\right\rangle r^2 dr$



- Projecting the Schrödinger equation on the channel basis yields:

$$\sum_\nu \int \Big[\underbrace{H_{\nu'\nu}^{J^\pi T}(r',r)}_{\left\langle \Phi_{\nu' r'}^{J^\pi T} \right| \hat{A}_{\nu'} H \hat{A}_\nu \left| \Phi_{\nu r}^{J^\pi T} \right\rangle} - E \; \underbrace{N_{\nu'\nu}^{J^\pi T}(r',r)}_{\left\langle \Phi_{\nu' r'}^{J^\pi T} \right| \hat{A}_{\nu'} \hat{A}_\nu \left| \Phi_{\nu r}^{J^\pi T} \right\rangle} \Big] \frac{\gamma_\nu^{J^\pi T}(r)}{r} \; r^2 \, d\,r = 0$$

Hamiltonian kernel

Overlap (or norm) kernel

- Breakdown of approach:
  1. Build channel basis states from input target and projectile wave functions
  2. Calculate Hamiltonian and norm kernels
  3. Solve RGM equations: find unknown relative motion wave functions
     - Bound-state / scattering boundary conditions

How to calculate the RGM kernels?

- Since we are using NCSM wave functions, it is convenient to introduce Jacobi channel states in the HO space

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle = \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell(\hat{r}_{A-a,a})\right]^{(J^\pi T)} R_{n\ell}(r_{A-a,a})$$

- Note :
  - The coordinate space channel states are given by

$$\left|\Phi^{J^\pi T}_{\nu r}\right\rangle = \sum_n R_{n\ell}(r)\left|\Phi^{J^\pi T}_{\nu n}\right\rangle$$

    - We used the closure properties of HO radial wave functions

Trick #1

$$\frac{\delta(r - r_{A-a,a})}{r\, r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

Note that this is OK,
in particular when the sum
is truncated,
ONLY for localized
parts of the kernels

  - We call them Jacobi channel states because they describe only the internal motion
    - Target and projectile wave functions are both translational invariant NCSM eigenstates calculated in the Jacobi coordinate basis

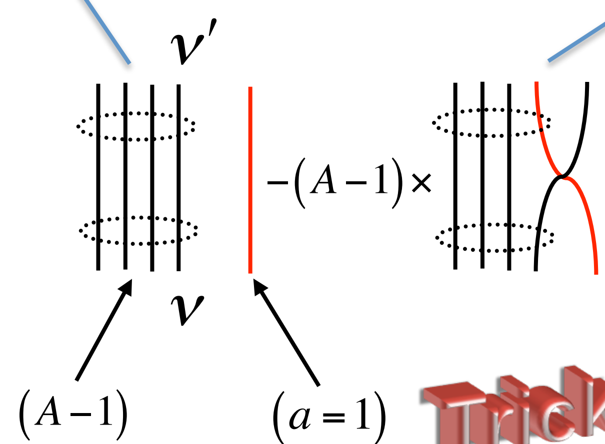
Norm kernel (Pauli principle): Single-nucleon projectile

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \right| \hat{A}_{\nu'} \hat{A}_{\nu} \left| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle \;(A-1)\quad r' \quad (a'=1) \;\right| 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \left|\; (a=1) \quad r \quad (A-1) \;\right\rangle$$

$$N^{J^\pi T}_{\nu'\nu}(r',r) = \underbrace{\delta_{\nu'\nu} \frac{\delta(r'-r)}{r' r}} - \underbrace{(A-1) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \right| \hat{P}_{A-1,A} \left| \Phi^{J^\pi T}_{\nu n} \right\rangle}$$

$$\boxed{{}_{SD}\left\langle \psi^{(A-1)}_{\mu_1} \right| a^{+} a \left| \psi^{(A-1)}_{\nu_1} \right\rangle_{SD}}$$

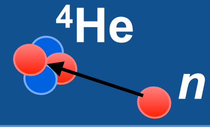
Direct term:
Treated exactly!
(in the full space)



Exchange term:
Obtained in the model space!
(Many-body correction due to the exchange part of the inter-cluster antisymmetrizer)

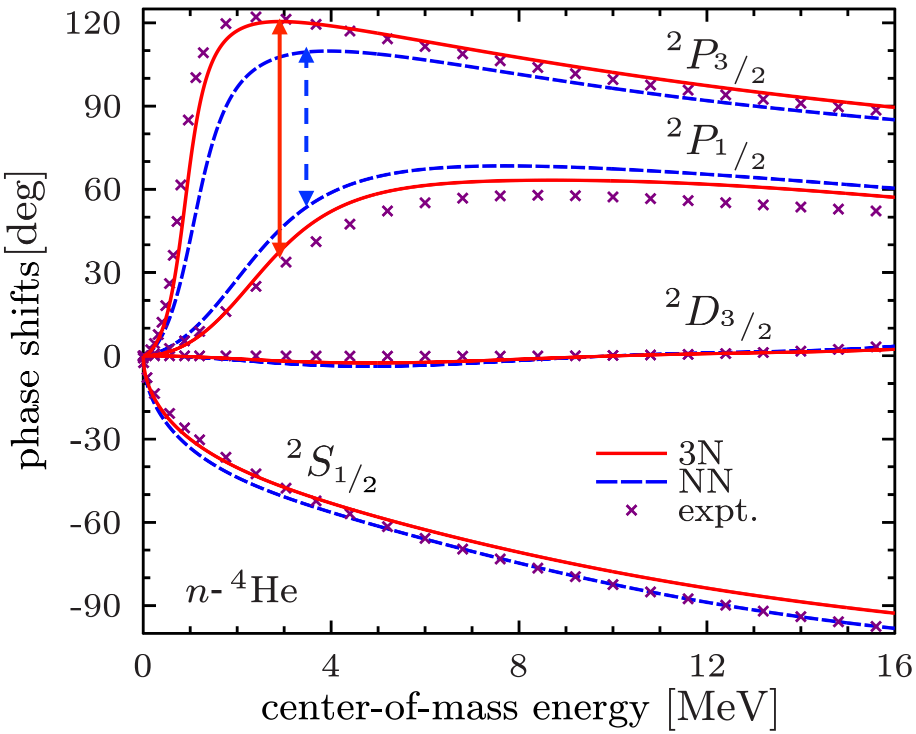
Trick #1
$$\frac{\delta(r - r_{A-a,a})}{r\, r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

Trick #2 Target wave functions expanded in the SD basis, the CM motion exactly removed

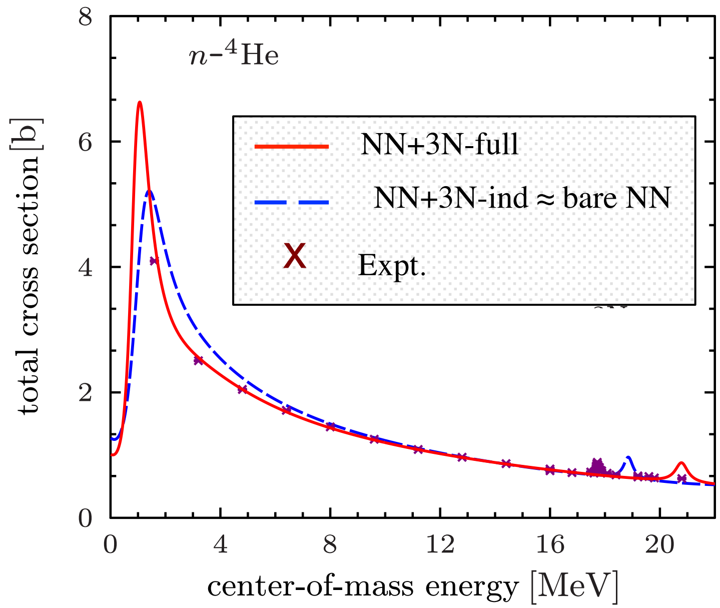


n-^{4}He scattering within NCSMC

n-^{4}He scattering phase-shifts for chiral NN and NN+3N500 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!

IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta
Phys. Scr. 00 (2016) 000000 (37pp)

Invited Comment

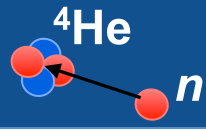
Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]

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

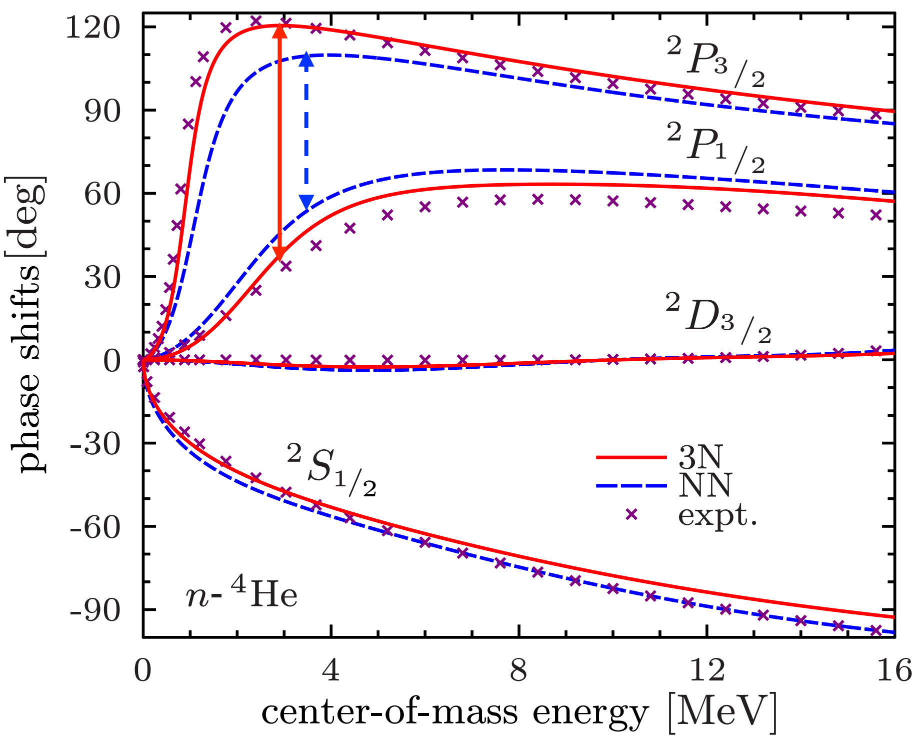
***Ab initio* many-body calculations of nucleon-^{4}He scattering with three-nucleon forces**

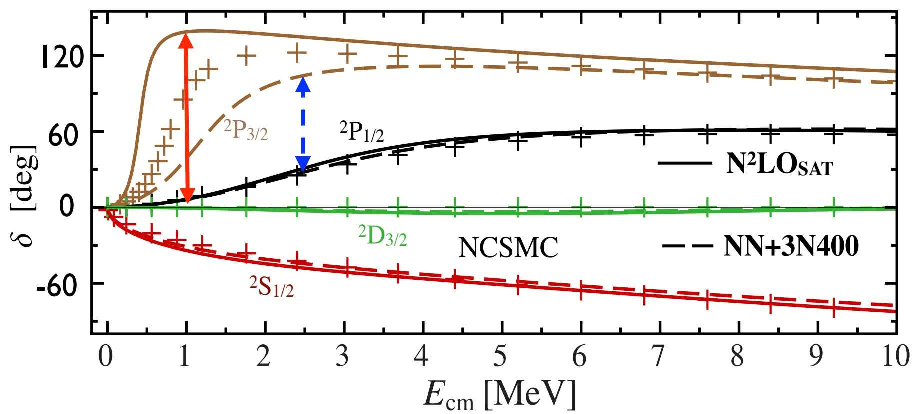
Guillaume Hupin,[1,*] Joachim Langhammer,[2,†] Petr Navrátil,[3,‡] Sofia Quaglioni,[1,§] Angelo Calci,[2,‖] and Robert Roth[2,¶]



n-^{4}He scattering within NCSMC

n-^{4}He scattering phase-shifts for chiral NN and NN+3N500 potential	n-^{4}He scattering phase-shifts for chiral N^2LO_{sat} and NN+3N400 potentials





3N force enhances 1/2⁻ ←→ 3/2⁻ splitting: Essential at low energies!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Phys. Scr. 00 (2016) 000000 (37pp)

Invited Comment

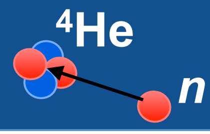
Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]

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

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

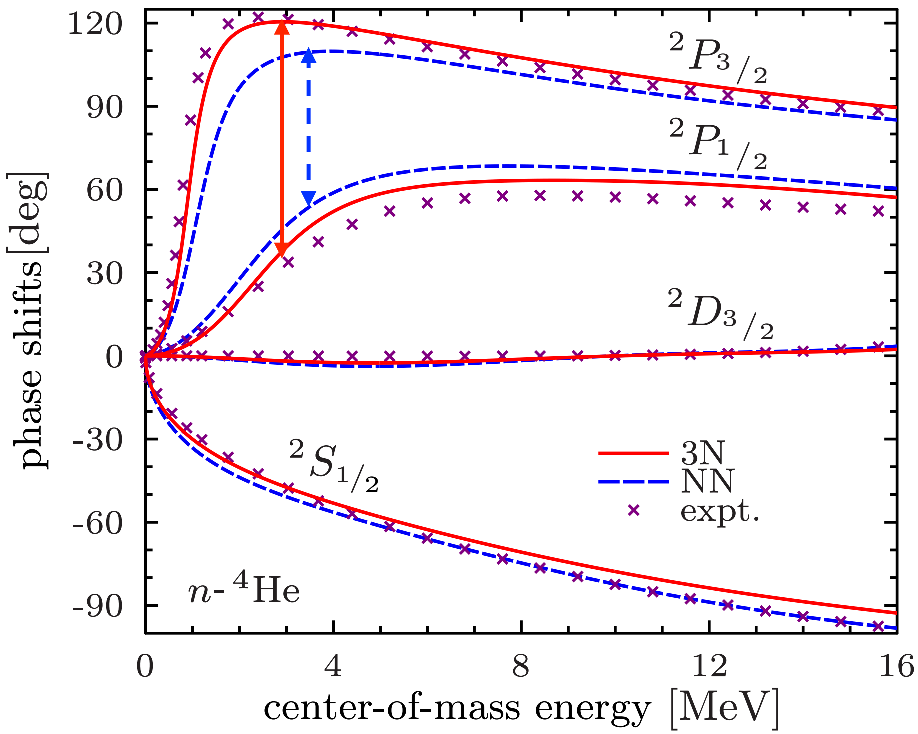
Guillaume Hupin,[1,*] Joachim Langhammer,[2,†] Petr Navrátil,[3,‡] Sofia Quaglioni,[1,§] Angelo Calci,[2,‖] and Robert Roth[2,¶]

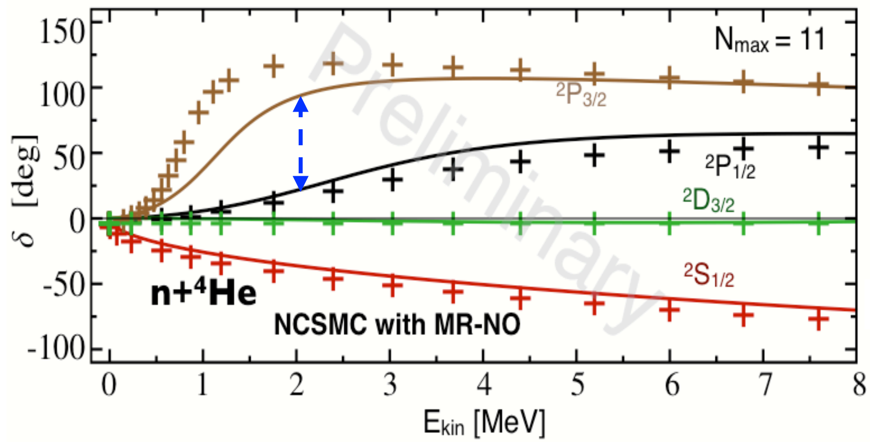


n-^{4}He scattering within NCSMC

n-^{4}He scattering phase-shifts for chiral NN and NN+3N500 potential

n-^{4}He scattering phase-shifts for chiral N^{4}LO500 NN potential





3N force enhances $1/2^-$ ←→ $3/2^-$ splitting: Essential at low energies!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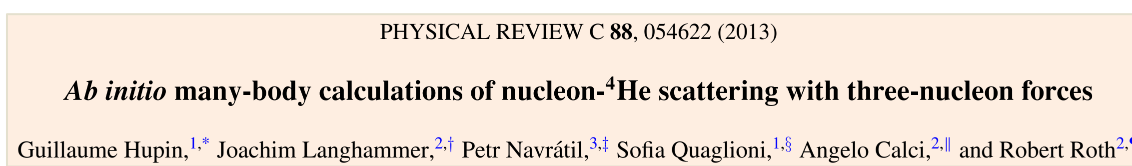
PHYSICAL REVIEW C **88**, 054622 (2013)

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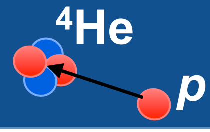
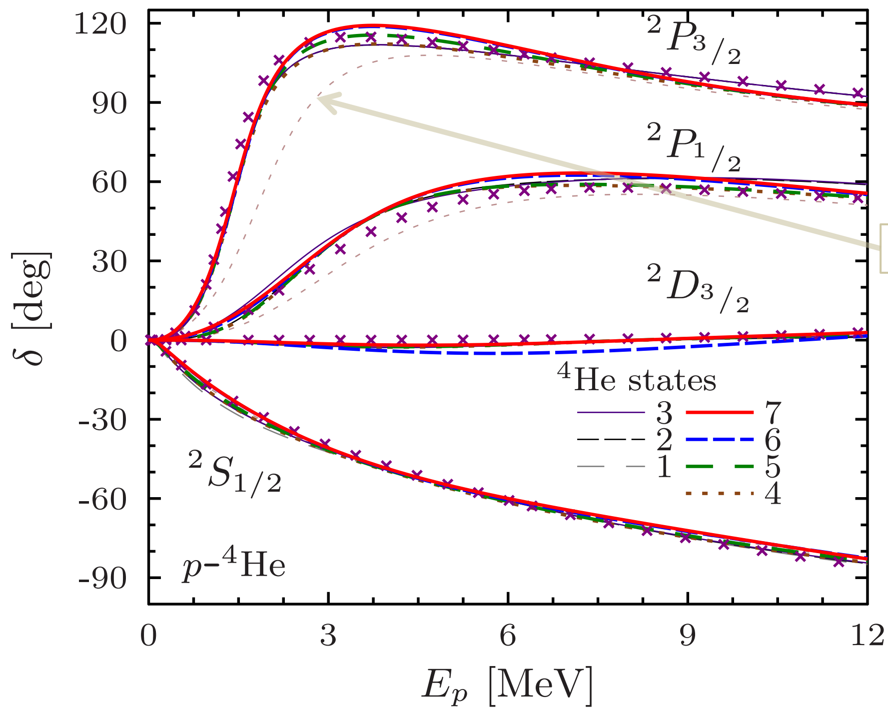
Guillaume Hupin,[1,*] Joachim Langhammer,[2,†] Petr Navrátil,[3,‡] Sofia Quaglioni,[1,§] Angelo Calci,[2,‖] and Robert Roth[2,¶]

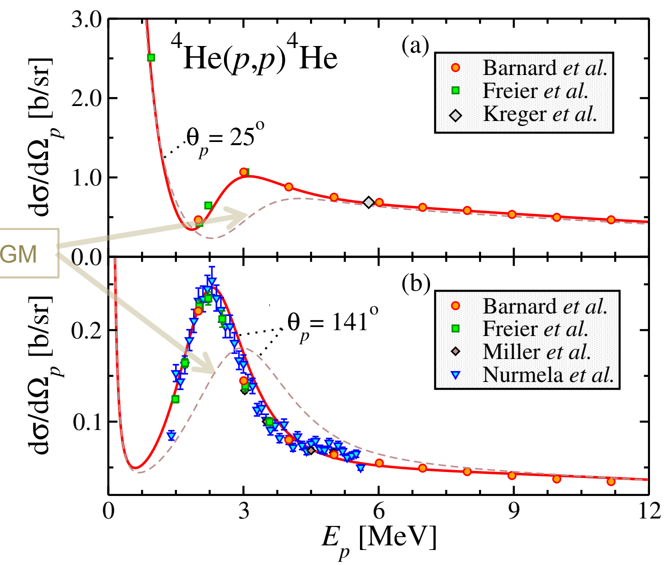


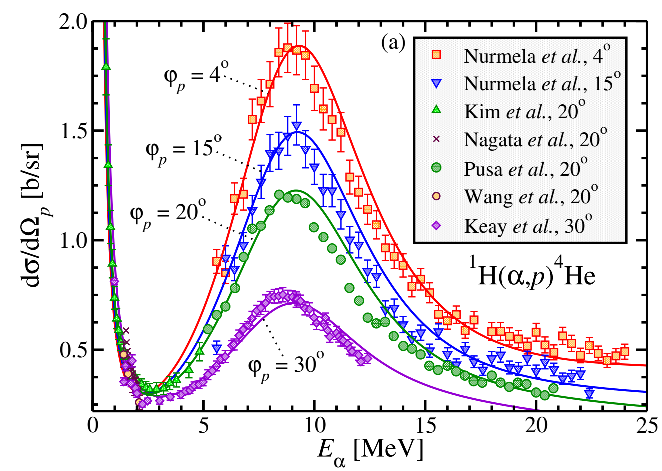
p-^{4}He scattering within NCSMC

p-^{4}He scattering phase-shifts for NN+3N500 potential: Convergence



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





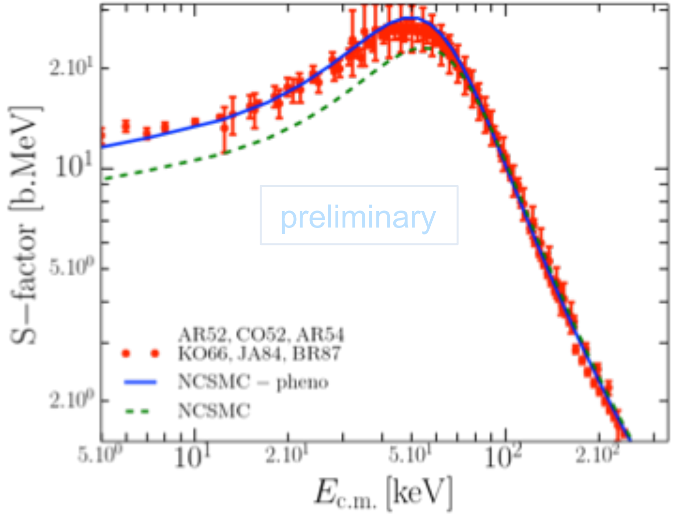
Predictive power in the 3/2$^-$ resonance region: Applications to material science

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

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

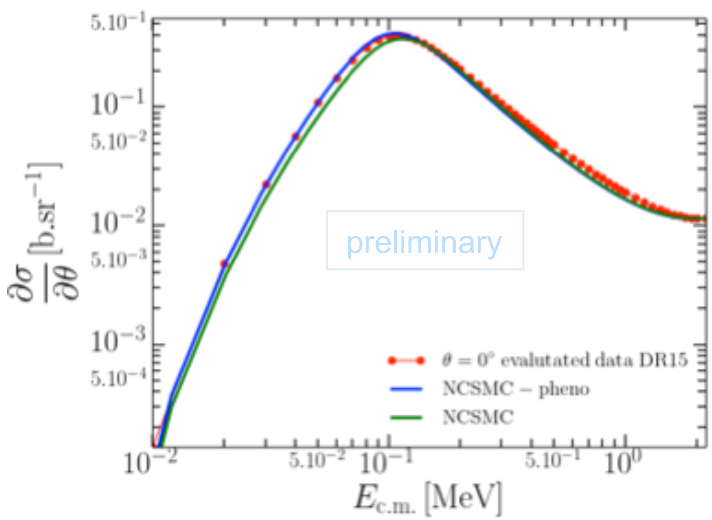
Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

$^3H(d,n)^4He$ with chiral NN+3N500 interaction

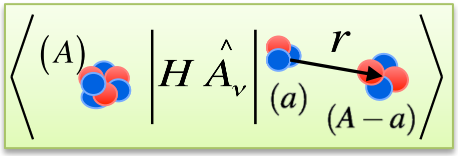


$$S(E) = E\sigma(E)\exp[2\pi\eta(E)]$$

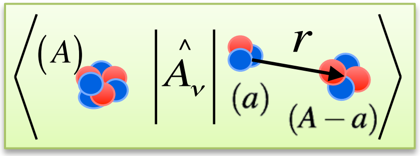
$$\eta(E) = Z_{A-a}Z_a e^2 / \hbar v_{A-a,a}$$



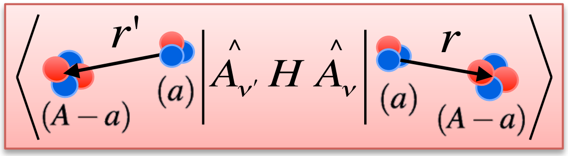
$E_\lambda^{NCSM}\,\delta_{\lambda\lambda'}$

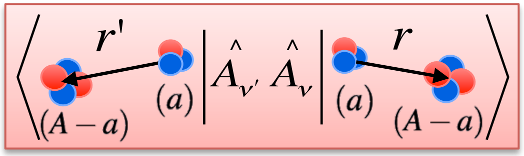


$\delta_{\lambda\lambda'}$



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

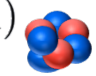
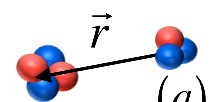




E_λ^{NCSM} energies treated as adjustable parameters

Cluster excitation energies set to experimental values

NCSMC wave function

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

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

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

Asymptotic behavior $r \to \infty$:

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

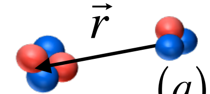
Bound state

Scattering state

Scattering matrix

E1 transitions in NCSMC

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



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

$$\begin{aligned} M^{E1}_{fi} = & \sum_{\lambda\lambda'} c^{*f}_{\lambda'} \langle A\lambda' J_f^{\pi_f} T_f || \vec{E}1 || A\lambda J_i^{\pi_i} T_i \rangle \, c^i_\lambda \\ & + \sum_{\lambda'\nu} \int drr^2 \, c^{*f}_{\lambda'} \langle A\lambda' J_f^{\pi_f} T_f || \vec{E}1 \hat{\mathcal{A}}_\nu || \Phi^i_{\nu r} \rangle \, \frac{\gamma^i_\nu(r)}{r} \\ & + \sum_{\lambda\nu'} \int dr' r'^2 \frac{\gamma^{*f}_{\nu'}(r')}{r'} \langle \Phi^f_{\nu' r'} || \hat{\mathcal{A}}_{\nu'} \vec{E}1 || A\lambda J_i^{\pi_i} T_i \rangle \, c^i_\lambda \\ & + \sum_{\nu\nu'} \int dr' r'^2 \int drr^2 \frac{\gamma^{*f}_{\nu'}(r')}{r'} \langle \Phi^f_{\nu' r'} || \hat{\mathcal{A}}_{\nu'} \vec{E}1 \hat{\mathcal{A}}_\nu || \Phi^i_{\nu r} \rangle \, \frac{\gamma^i_\nu(r)}{r} \end{aligned}$$