TRIUMF

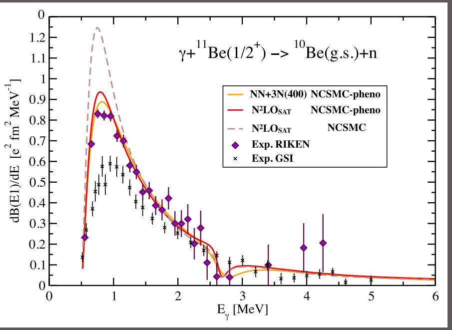
Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire
et en physique des particules

Weakly bound and unbound light nuclei from *ab initio* theory

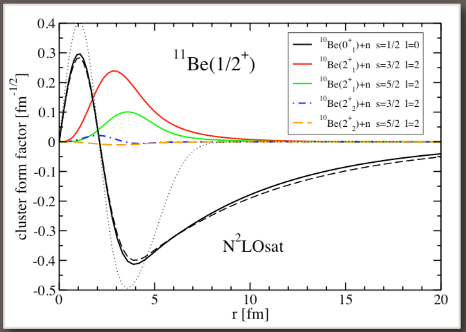
INT Program INT 17-1a

Toward Predictive Theories of Nuclear Reactions Across the Isotopic Chart

March 16, 2017



Petr Navratil | TRIUMF



Collabrorators:

Sofia Quaglioni, Carolina Romero-Redondo (LLNL)

Guillaume Hupin (CEA/DAM)

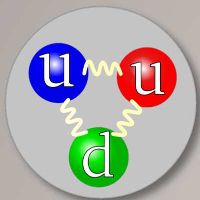
Jeremy Dohet-Eraly, **Angelo Calci, Peter Gysbers** (TRIUMF)

Robert Roth (TU Darmstadt)

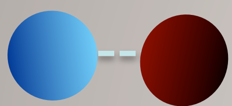
Outline

- New high precision chiral interactions
- No-Core Shell Model with Continuum (NCSMC) approach
- N-^{4}He scattering
- ^{11}Be parity inversion in low-lying states, photo-dissociation
- ^{11}N and ^{10}C(p,p) scattering
- ^{12}N and ^{11}C(p,p) scattering and ^{11}C(p,γ)^{12}N

From QCD to nuclei

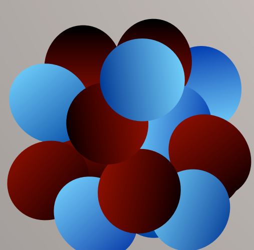


Low-energy QCD



NN+3N interactions
from chiral EFT

…or accurate
meson-exchange
potentials



Nuclear structure and reactions

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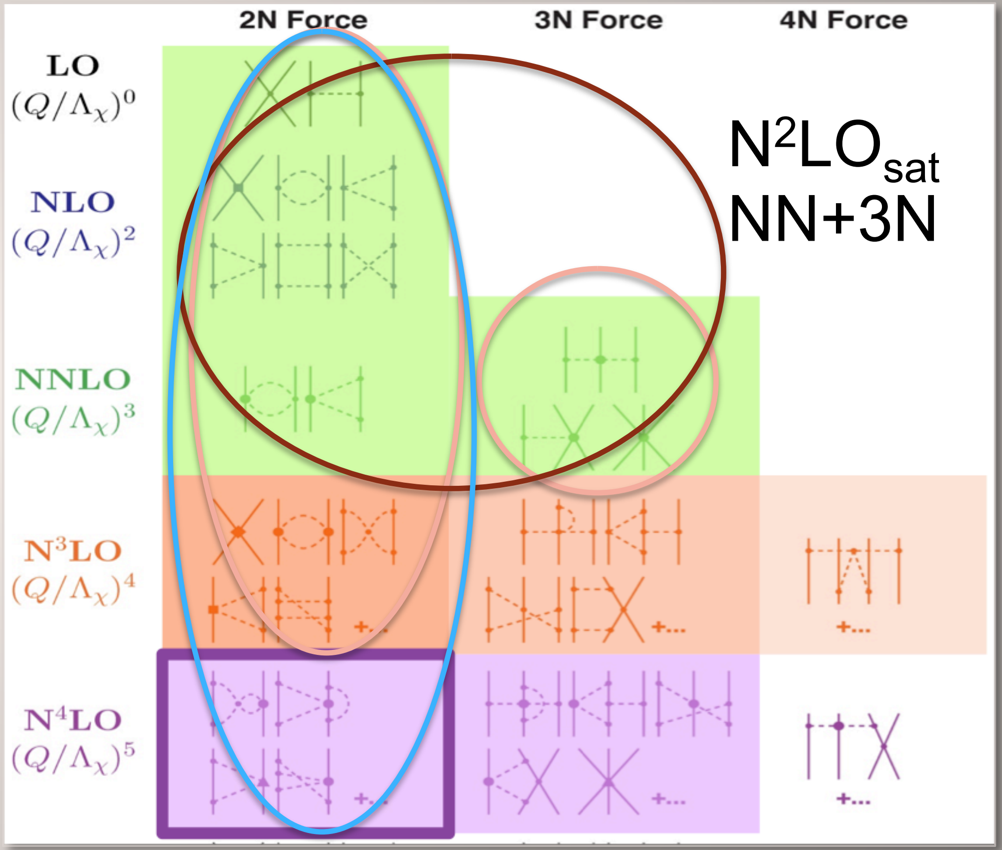
Chiral Effective Field Theory

- 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

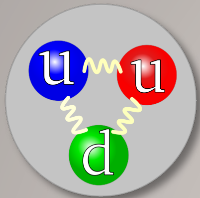


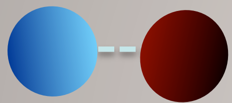
N^4LO500 NN

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

Λ_χ~1 GeV : Chiral symmetry breaking scale

From QCD to nuclei





Low-energy QCD

↓

NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

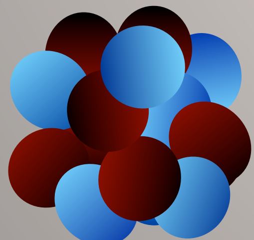
↓

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

Many-Body methods

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

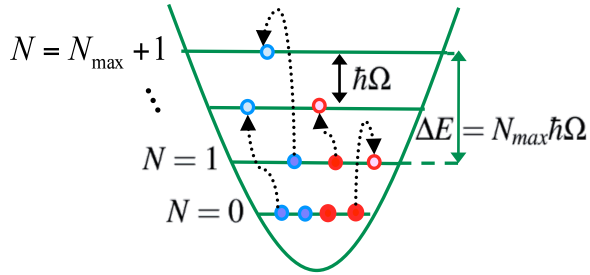
↓



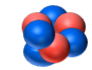
Nuclear structure and reactions

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

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



Harmonic oscillator basis

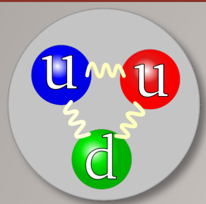


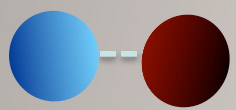
NCSM

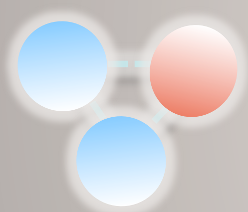
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)}, \lambda \right\rangle$$

Unknowns

From QCD to nuclei







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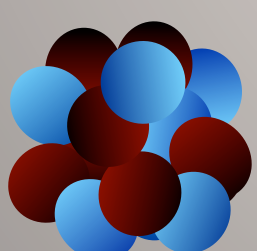


Low-energy QCD

↓

NN+3N interactions from chiral EFT — …or accurate meson-exchange potentials

↓

Unitary/similarity transformations — Identity or SRG or OLS or UCOM … Softens NN, induces 3N

↓

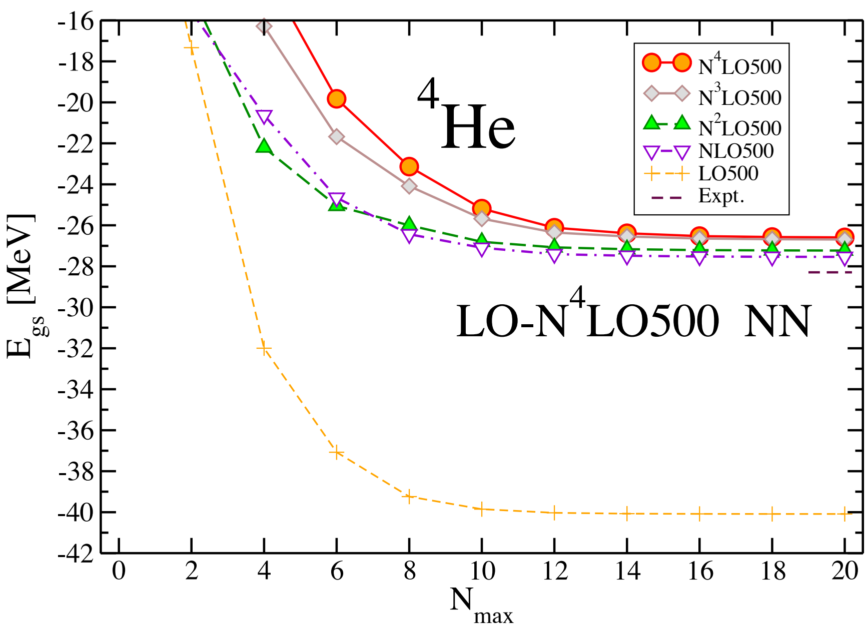
Many-Body methods — NCSM, NCSM/RGM, CCM, SCGF, GFMC, HH, Nuclear Lattice EFT…

↓

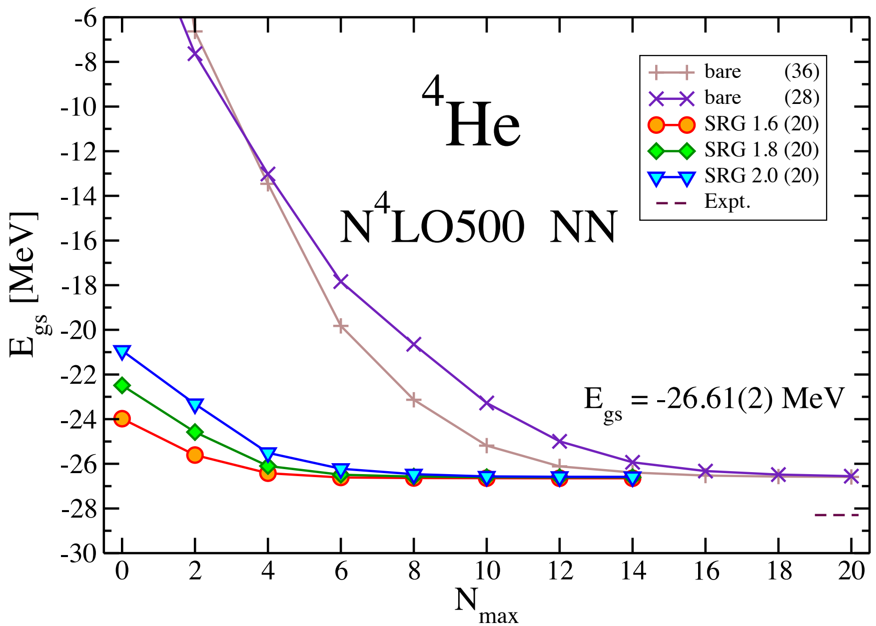
Nuclear structure and reactions

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, to be published.



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



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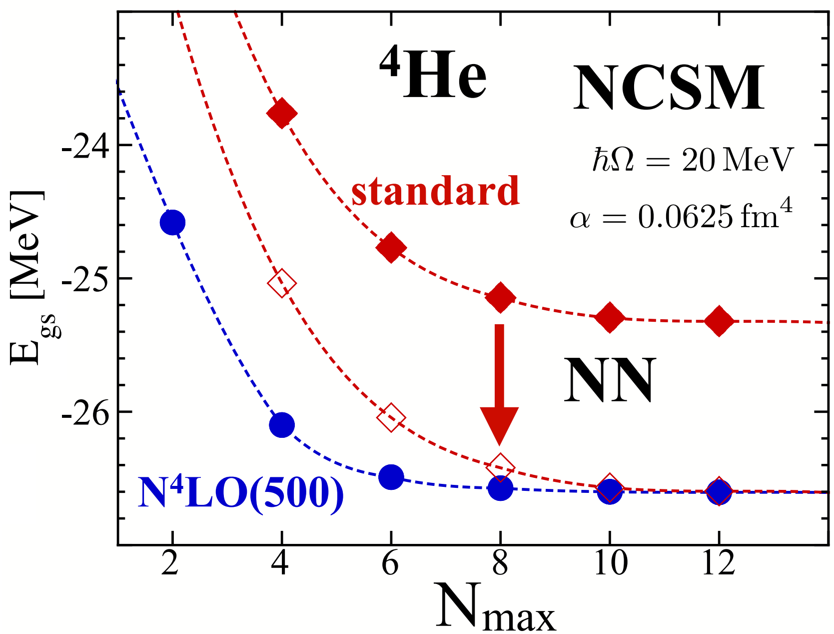

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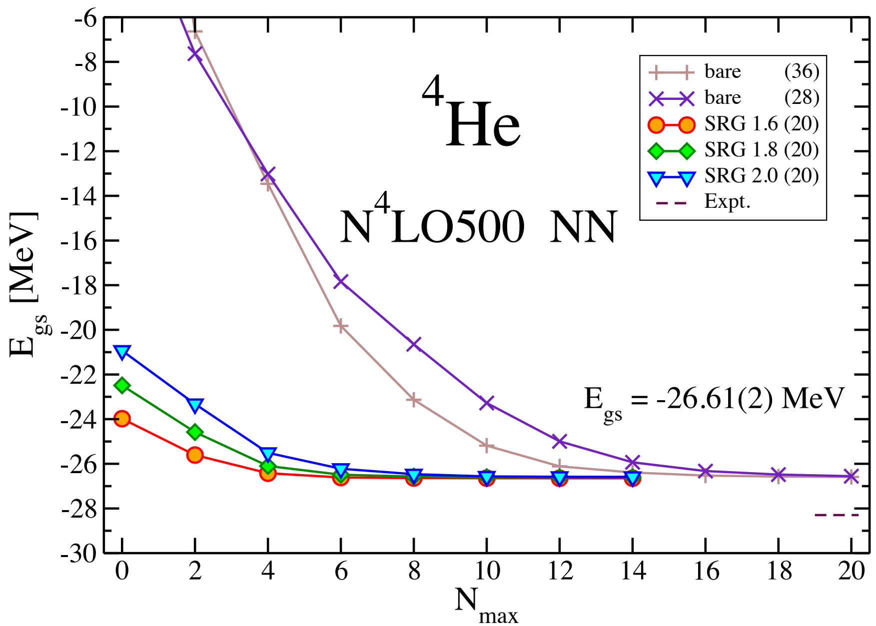

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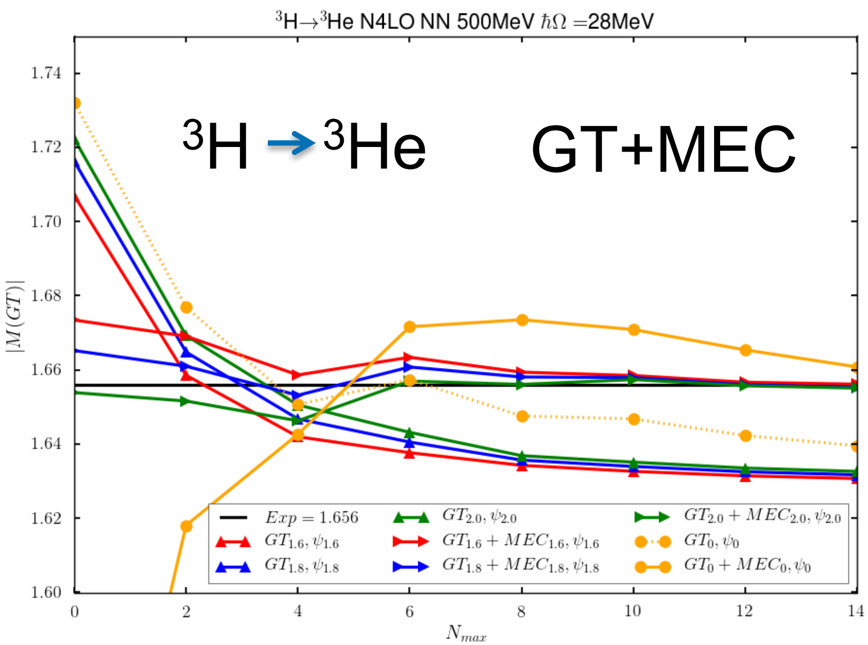
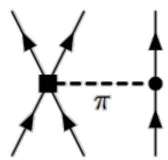


Determination of the c_D parameter relevant to chiral 3N force

c_D=0.45 (3N repulsive)



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

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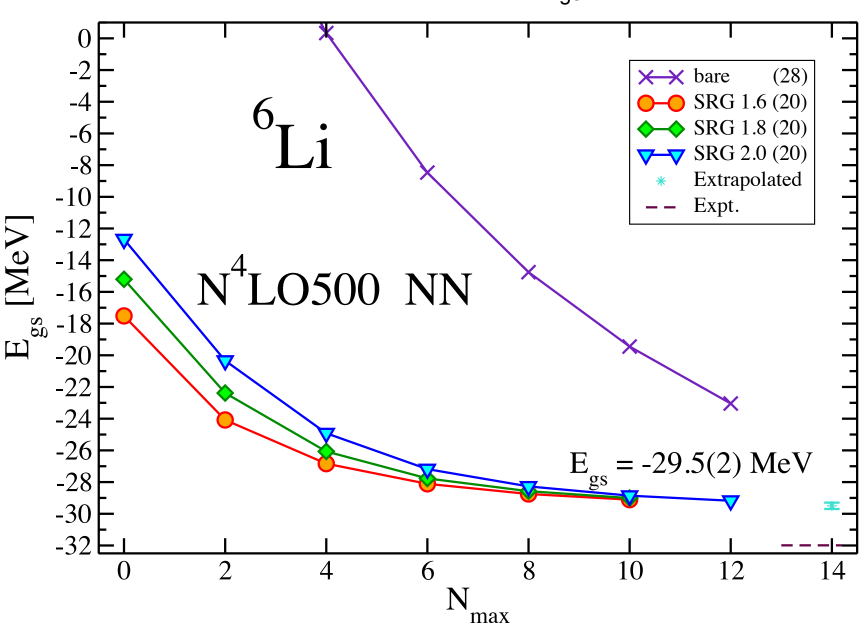
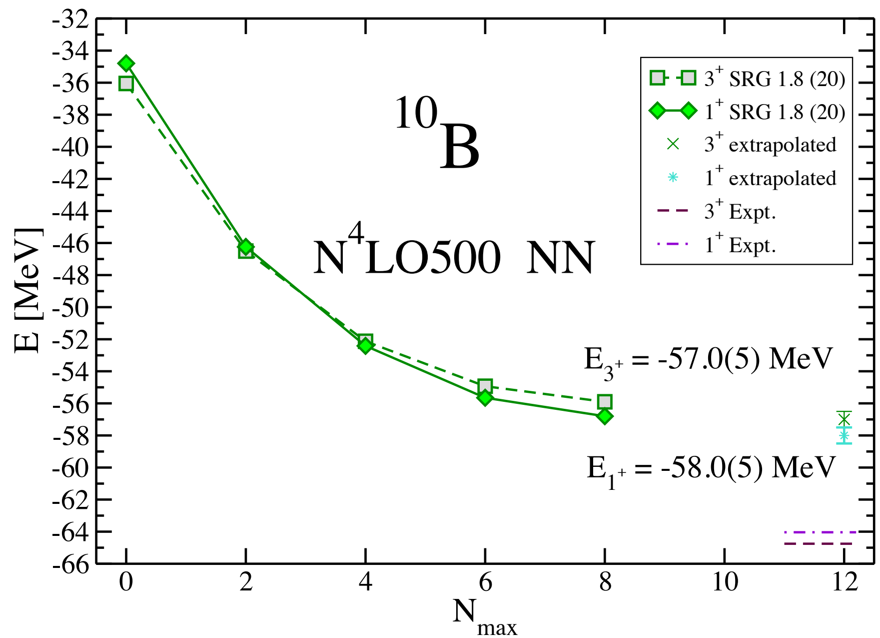
Original EM 2003 N^3LO NN E_{gs}=-28.0(5) MeV





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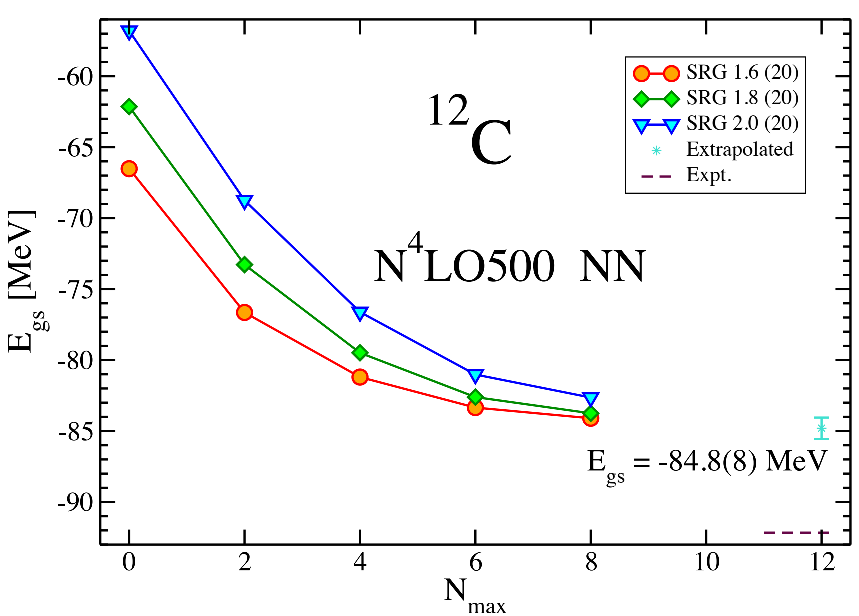
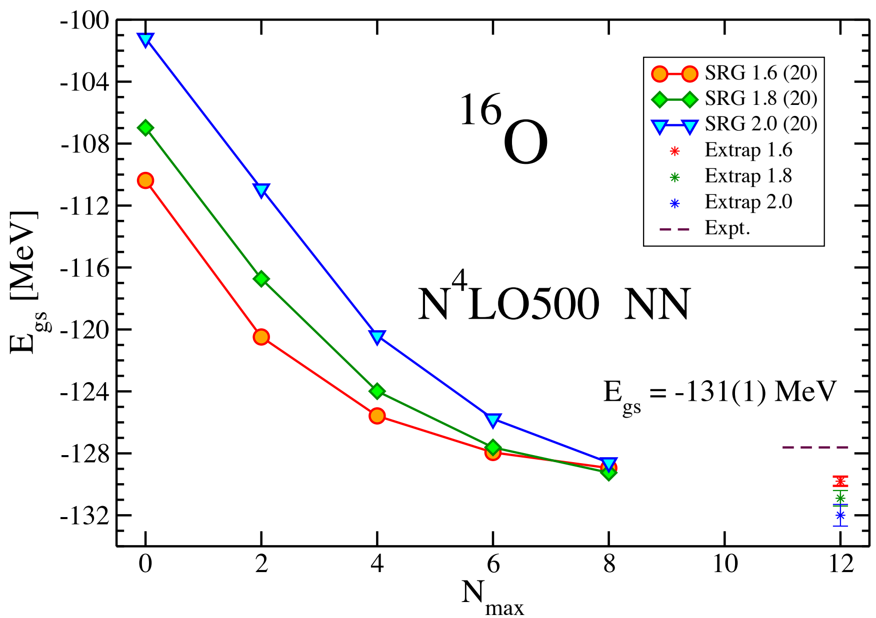
  - D. R. Entem, R. Machleidt, and Y. Nosyk, to be published.

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

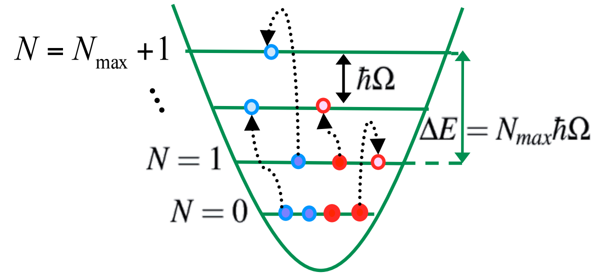


Original EM 2003 N^3LO NN E_{gs}=-119.5(5) MeV

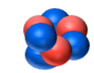


Unified approach to bound & continuum states; to nuclear structure & reactions

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



Harmonic oscillator basis



NCSM

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

Unknowns

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

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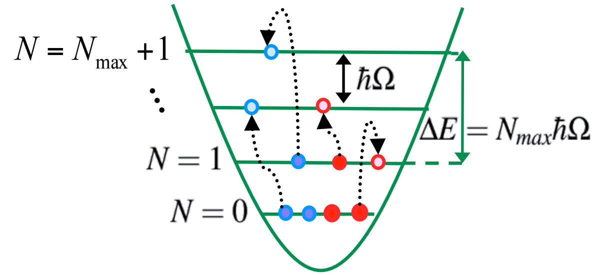

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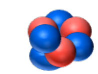
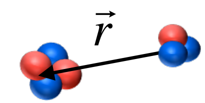


NCSM

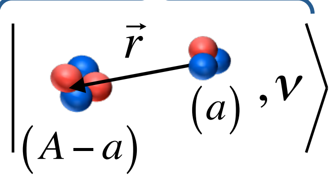
- …with resonating group method
  - Bound & scattering states, reactions
  - Cluster dynamics, long-range correlations



NCSM/RGM

NCSM/RGM channel states

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



Unknowns

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

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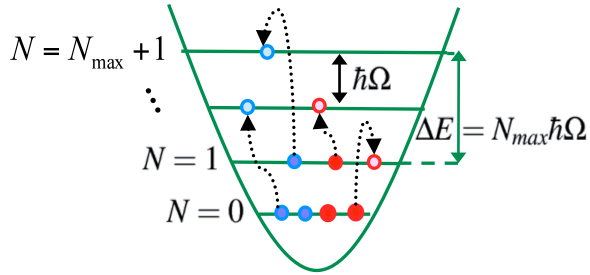

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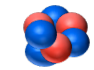

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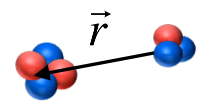


NCSM/RGM

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

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

NCSMC

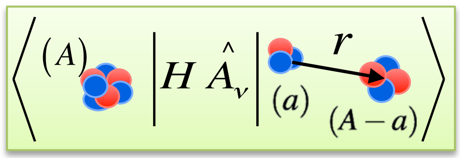
NCSM eigenstates; NCSM/RGM channel states

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

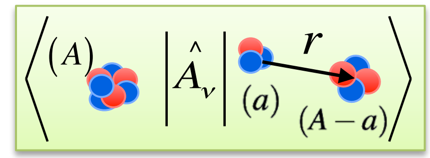
Unknowns

Coupled NCSMC equations

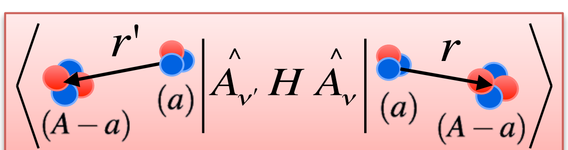
$E_{\lambda}^{NCSM}\,\delta_{\lambda\lambda'}$

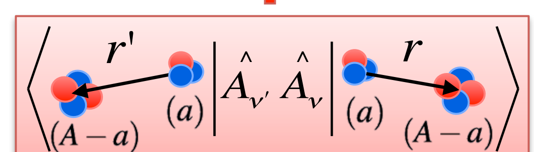


$\delta_{\lambda\lambda'}$



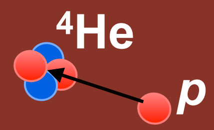
$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix}\begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix}\begin{pmatrix} c \\ \gamma \end{pmatrix}$$



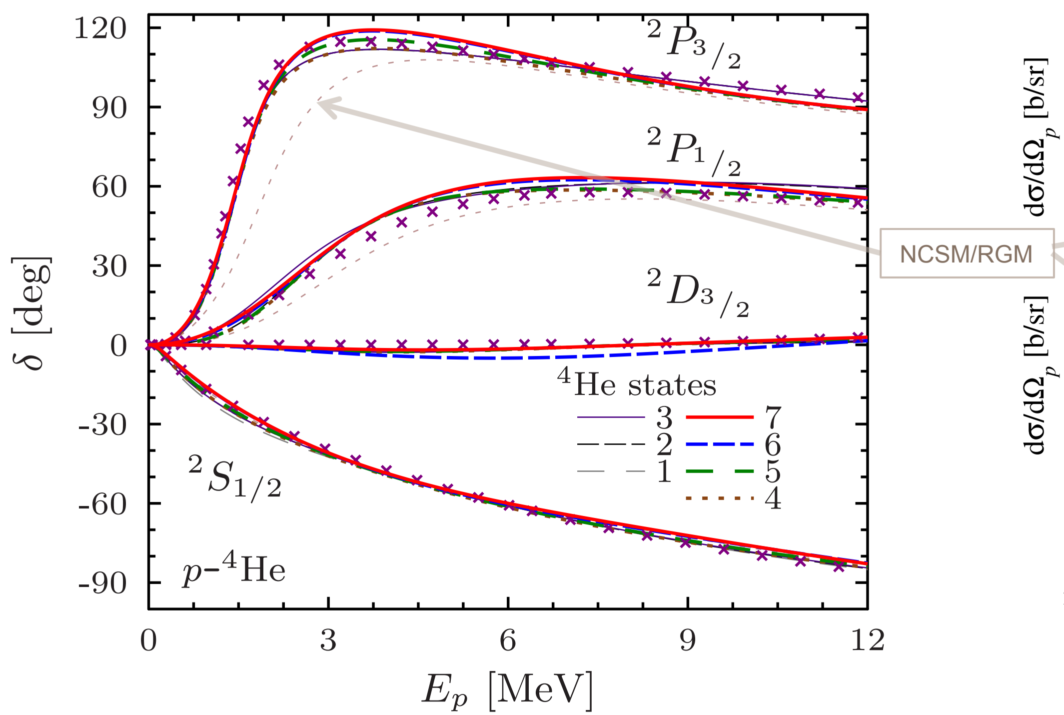


Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic *R*-matrix on Lagrange mesh

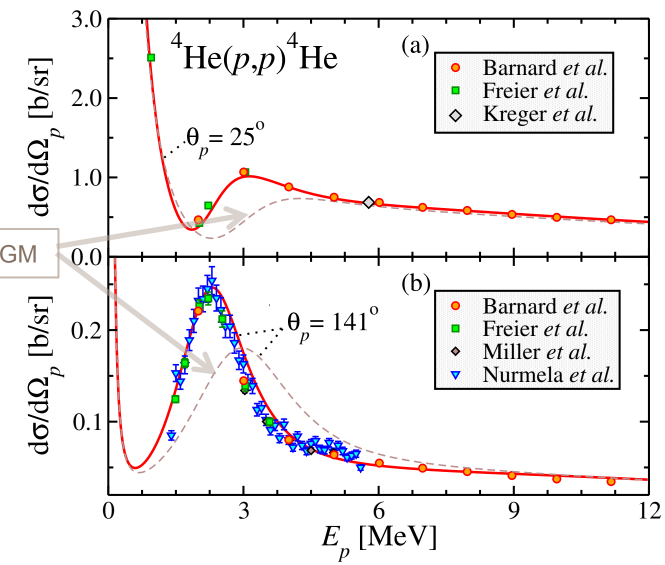
p-^{4}He scattering within NCSMC

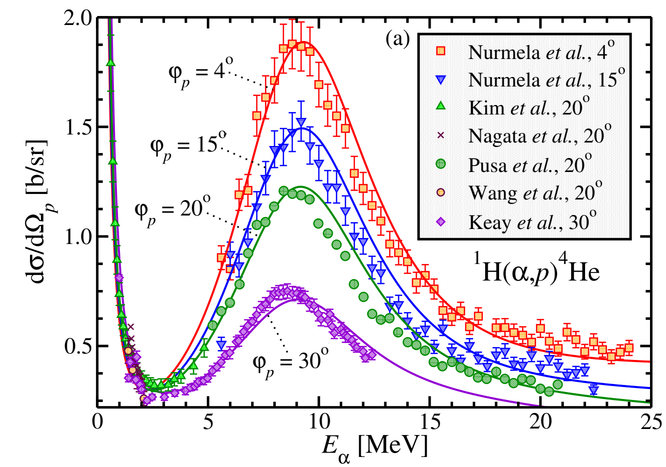


p-^{4}He scattering phase-shifts for NN+3N500 potential: Convergence



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,‡]

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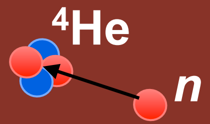
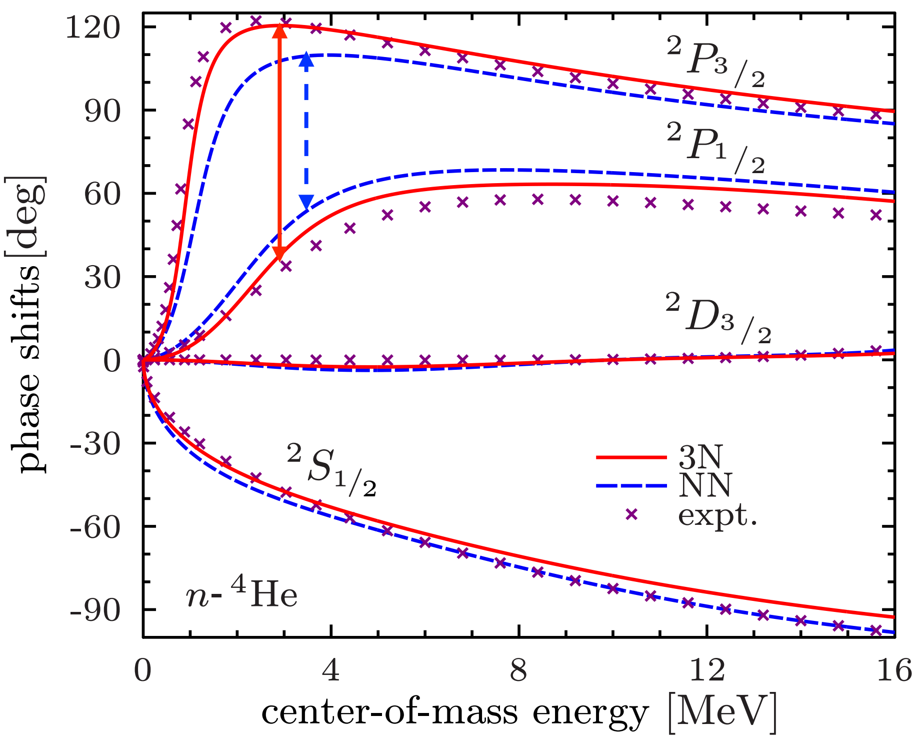
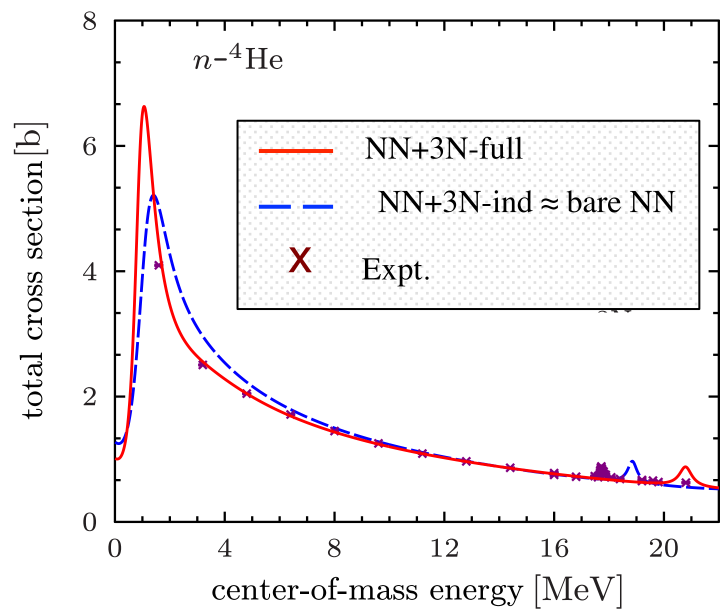


n-^{4}He scattering within NCSMC

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!

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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,¶]

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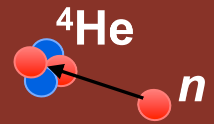
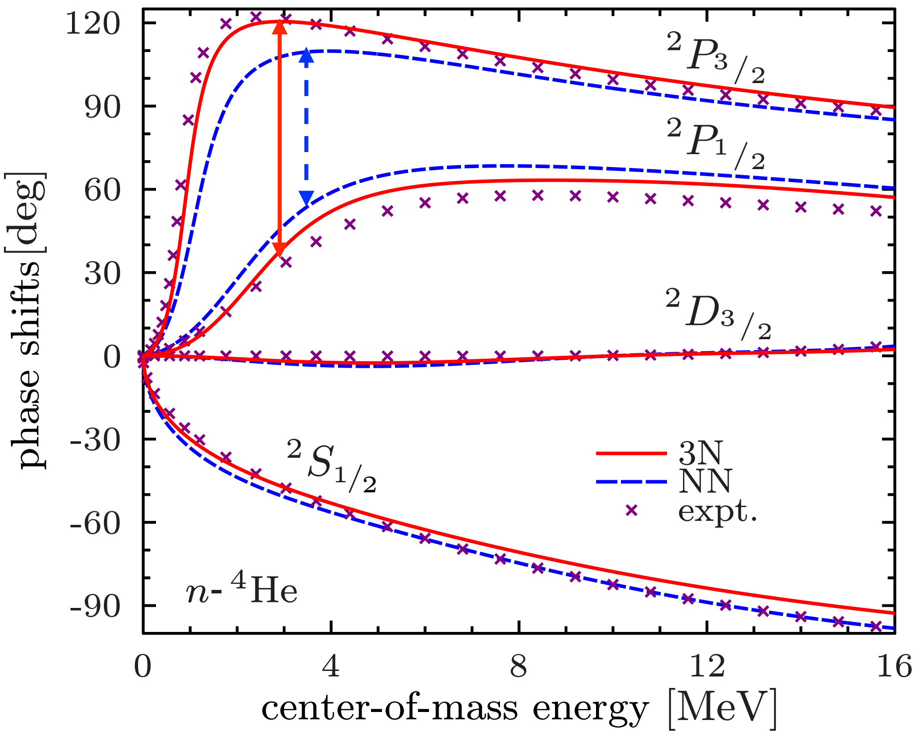
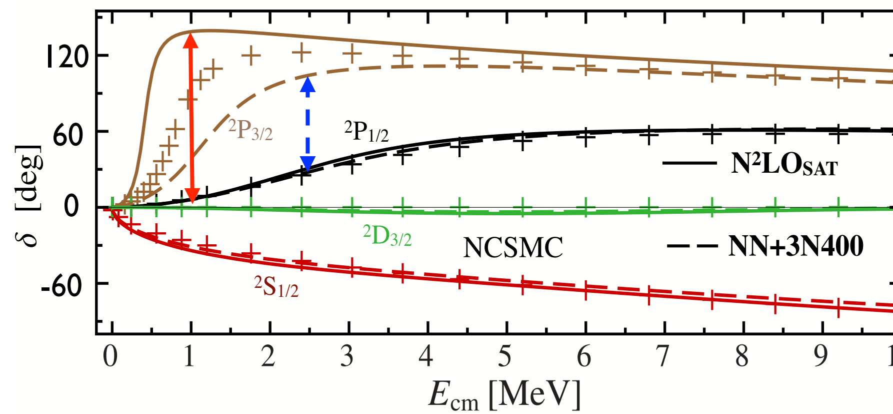


n-^{4}He scattering within NCSMC

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





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IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta

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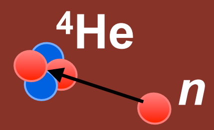
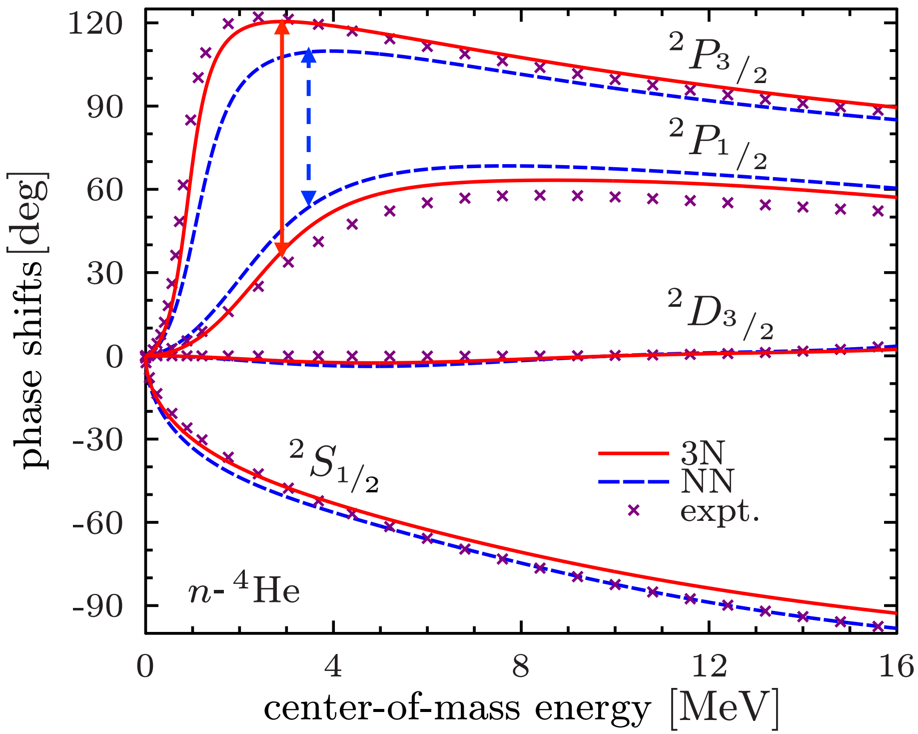
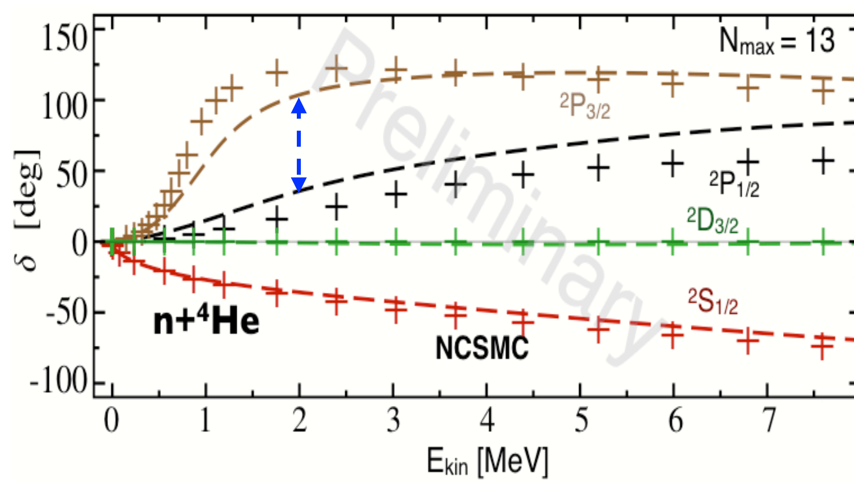


n-^{4}He scattering phase-shifts for chiral NN and NN+3N500 potential

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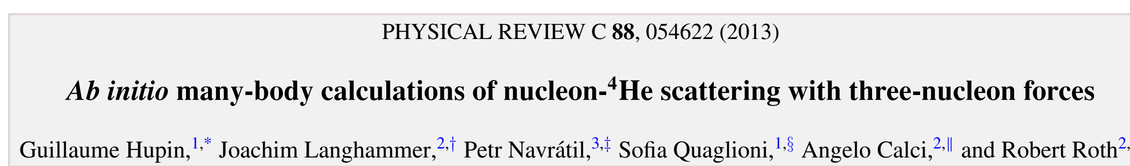
Phys. Scr. 00 (2016) 000000 (37pp)

Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

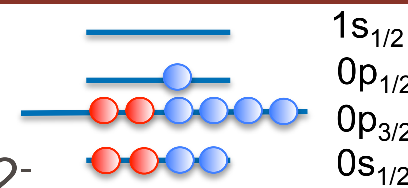
Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]


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

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

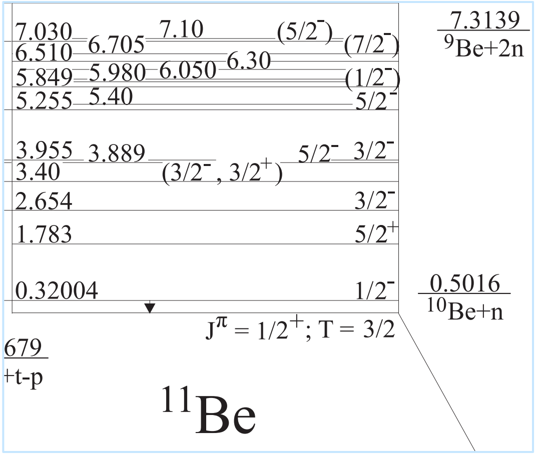
Guillaume Hupin,[1,*] Joachim Langhammer,[2,†] Petr Navrátil,[3,‡] Sofia Quaglioni,[1,§] Angelo Calci,[2,‖] and Robert Roth[2,¶]

Neutron-rich halo nucleus ^{11}Be



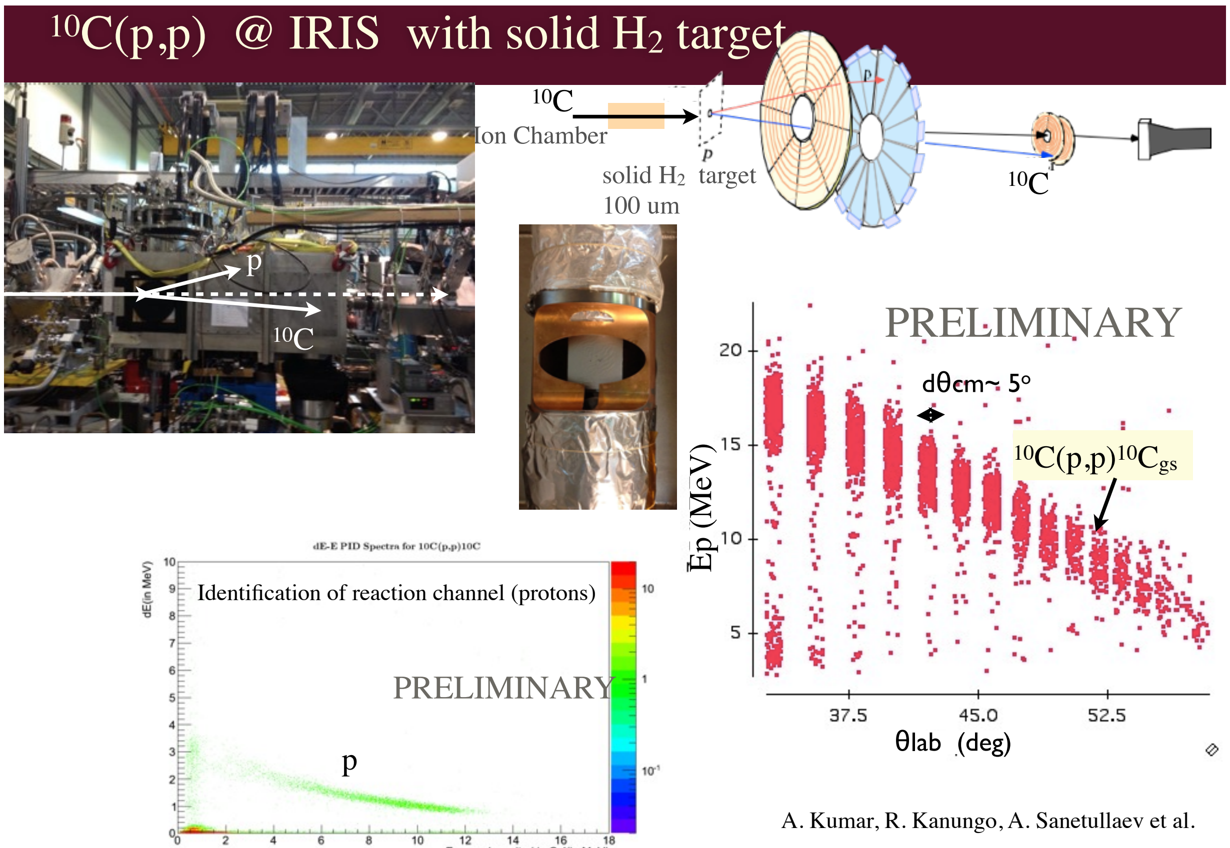
- Z=4, N=7
  - In the shell model picture g.s. expected to be $J^\pi=1/2^-$
    - Z=6, N=7 ^{13}C and Z=8, N=7 ^{15}O have $J^\pi=1/2^-$ g.s.
  - In reality, ^{11}Be g.s. is $\mathbf{J^\pi=1/2^+}$ - parity inversion
  - Very weakly bound: E_{th}=-0.5 MeV
    - Halo state – dominated by ^{10}Be-n in the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



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

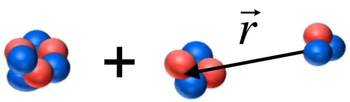
- New experiment at TRIUMF with the novel IRIS solid H_2 target
  - First re-accelerated ^{10}C beam at TRIUMF
  - $^{10}C(p,p)$ angular distributions measured at E_{CM} ~ 4.16 MeV and 4.4 MeV



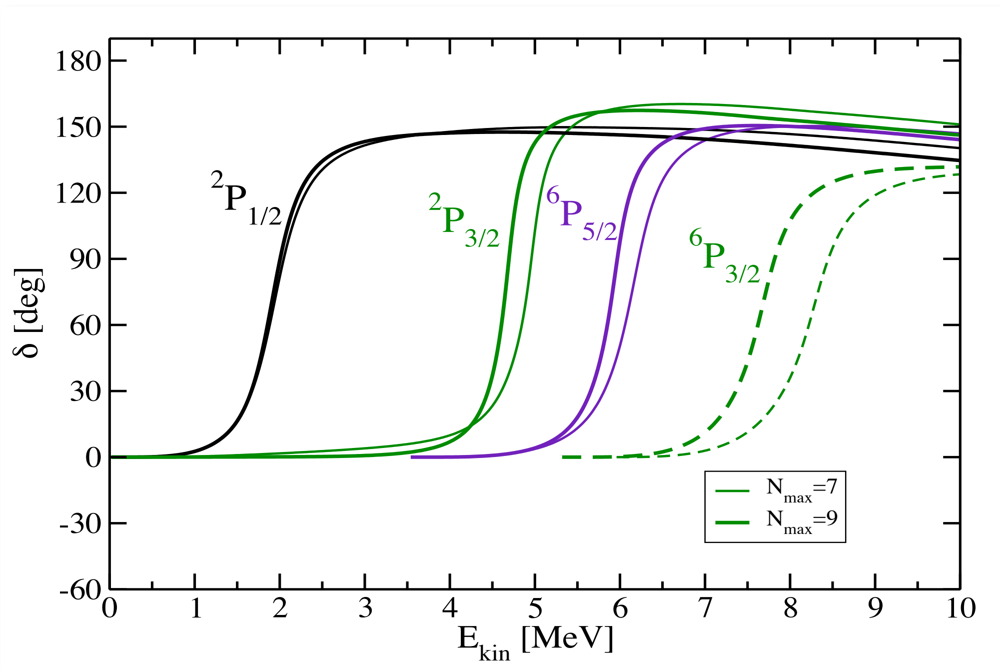
IRIS collaboration:
A. Kumar, R. Kanungo,
A. Sanetullaev *et al.*

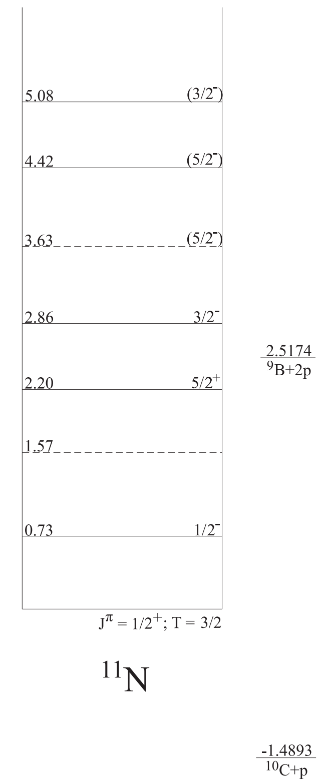
p+^{10}C scattering: structure of ^{11}N resonances

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



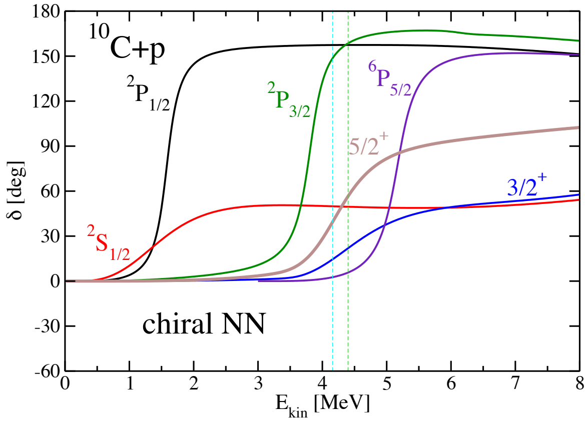
chiral NN+3NF400

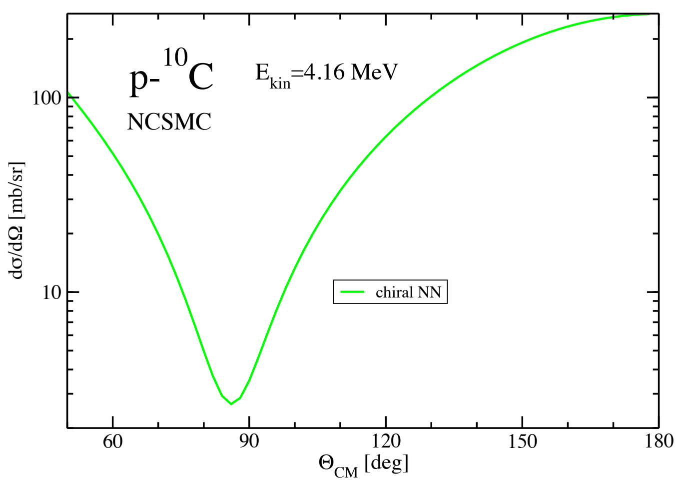


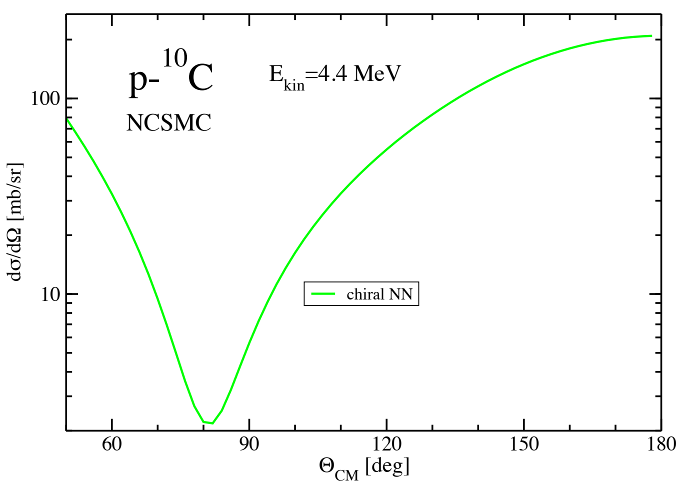


A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al* with IRIS collaboration, submitted

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







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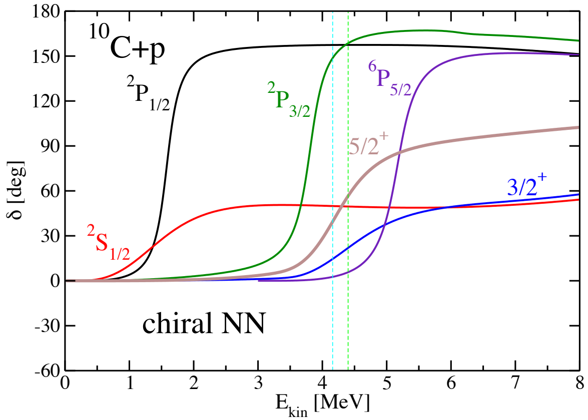

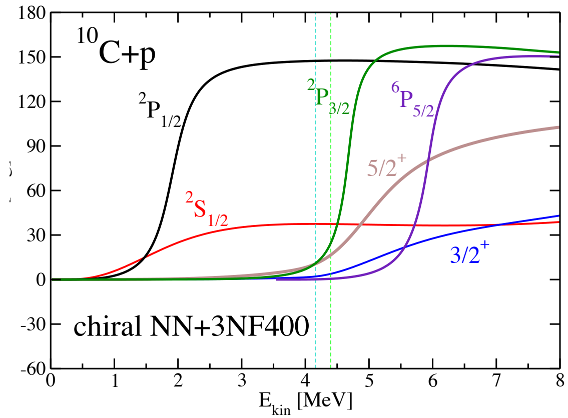

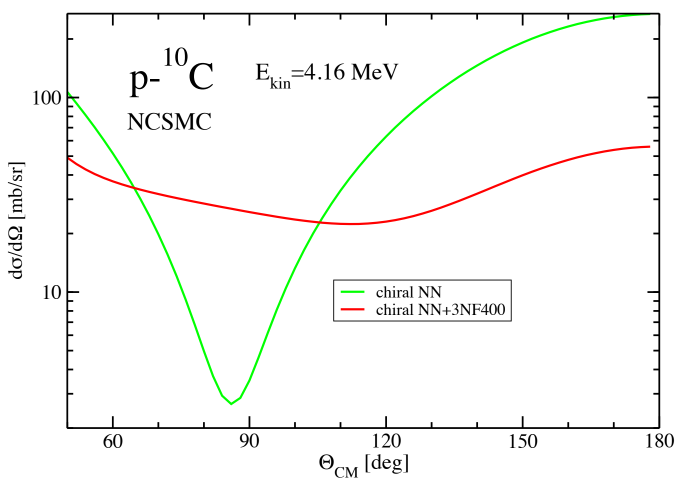

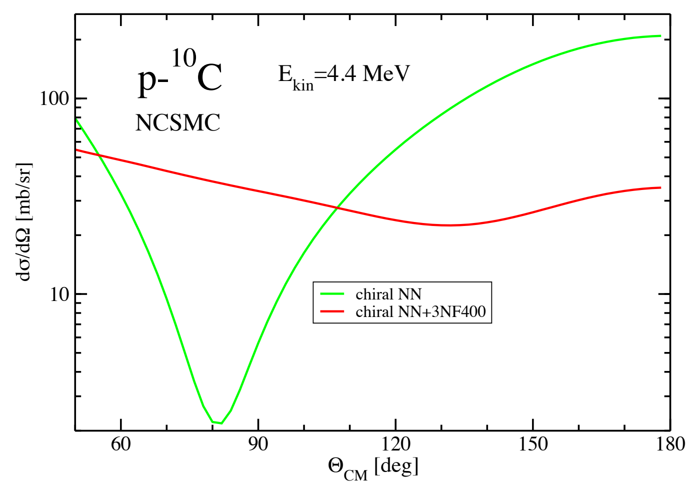

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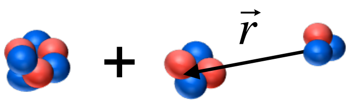
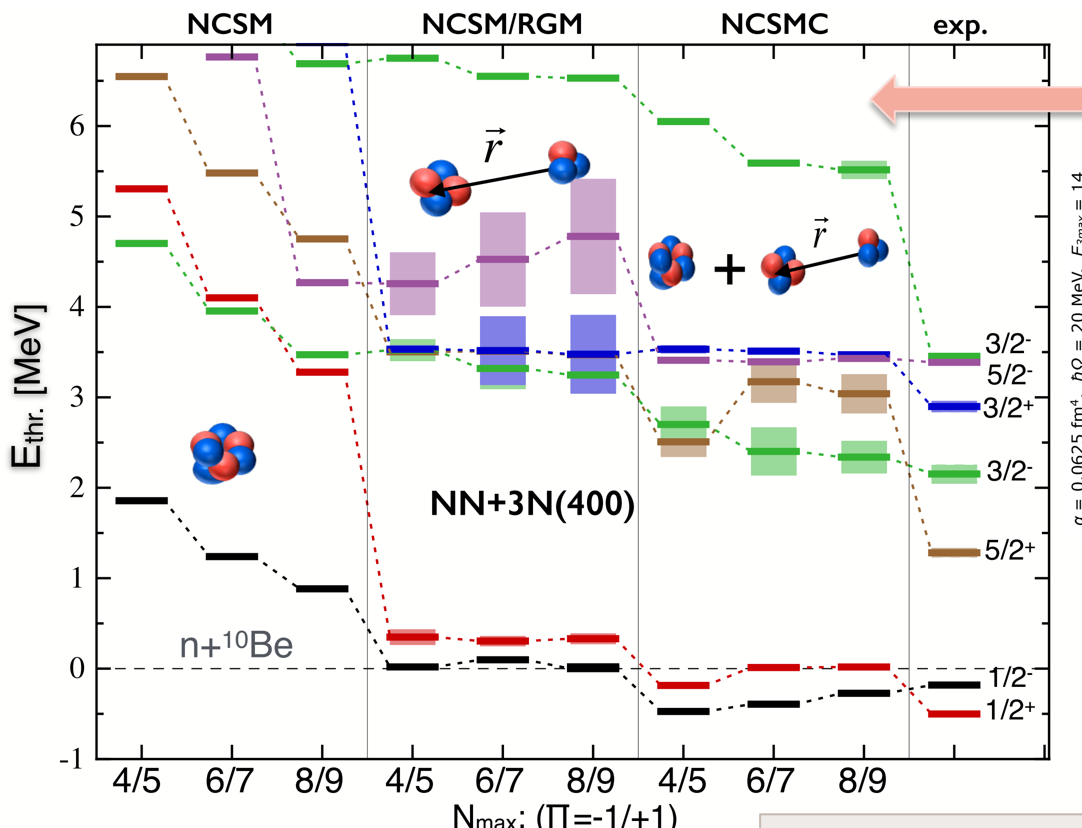
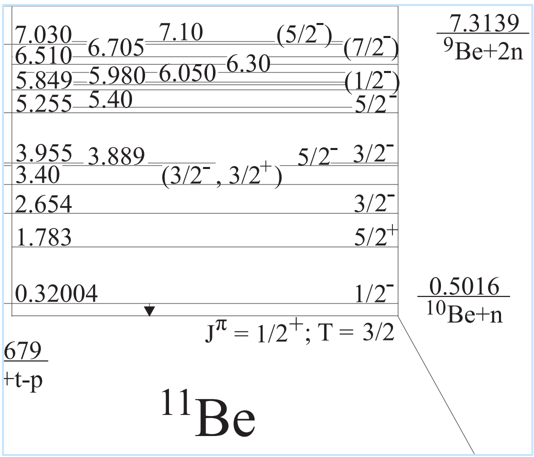
Structure of ^{11}Be from chiral NN+3N forces

- 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





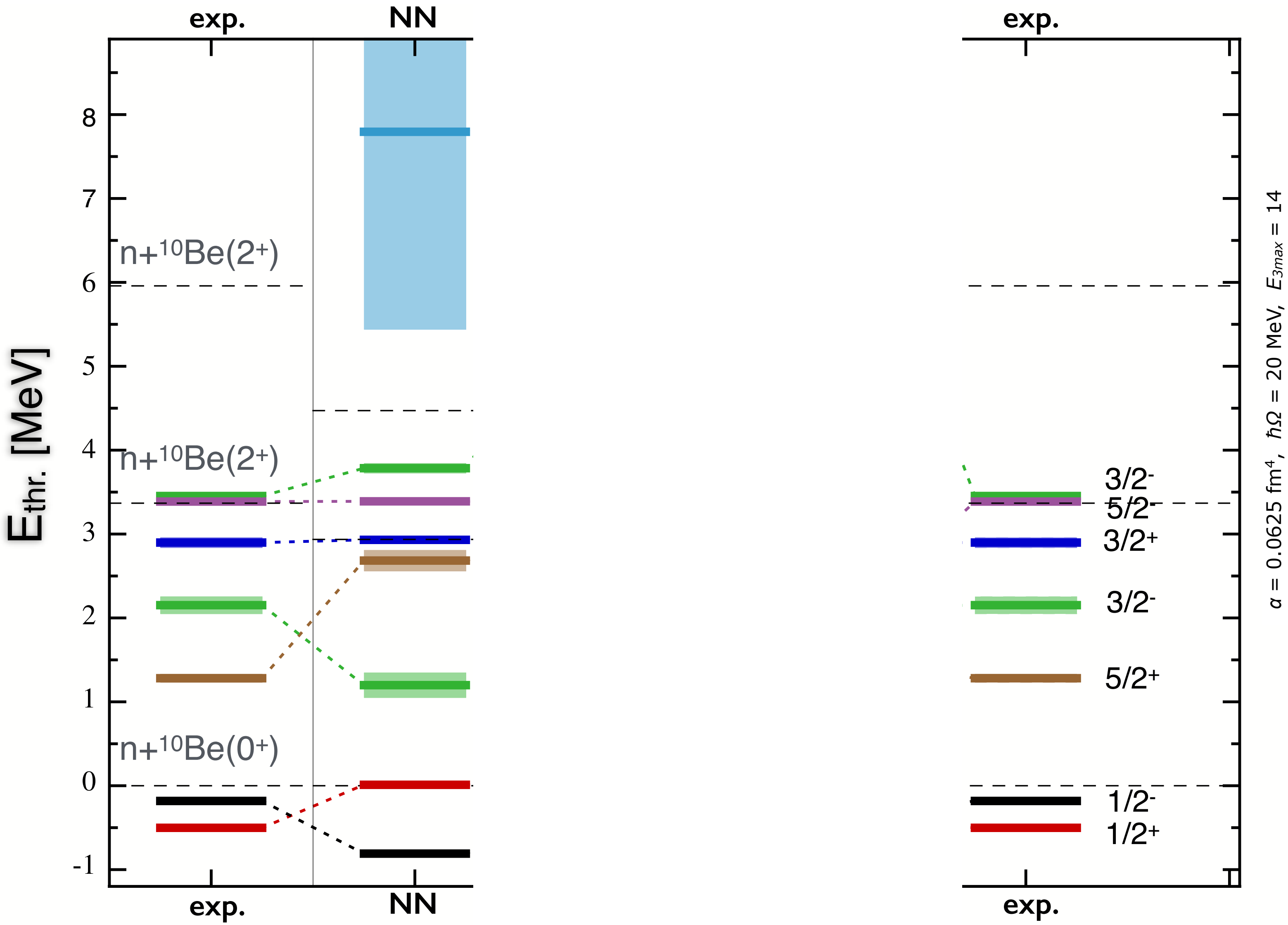
Continuum effects



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

TRIUMF

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



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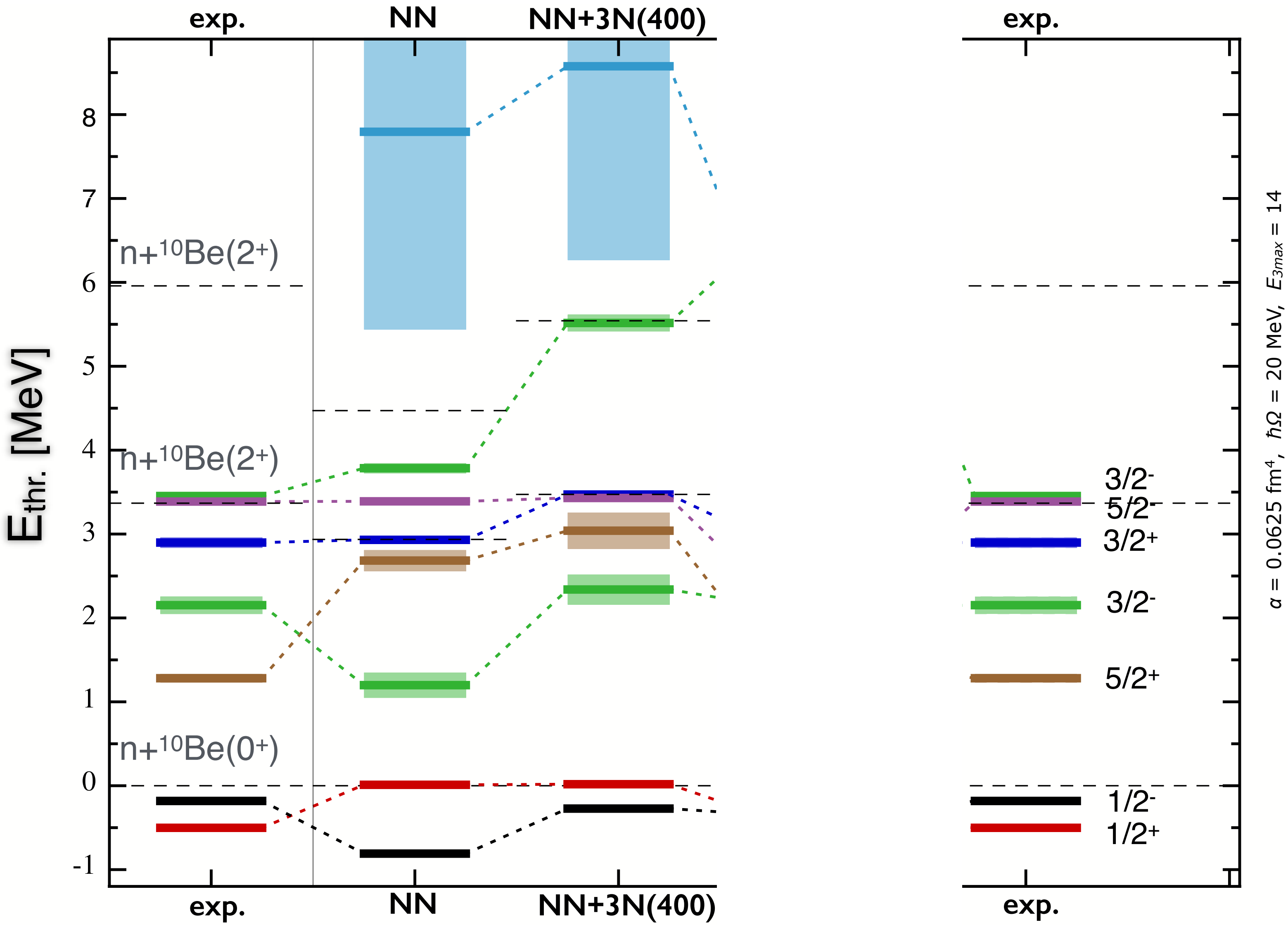

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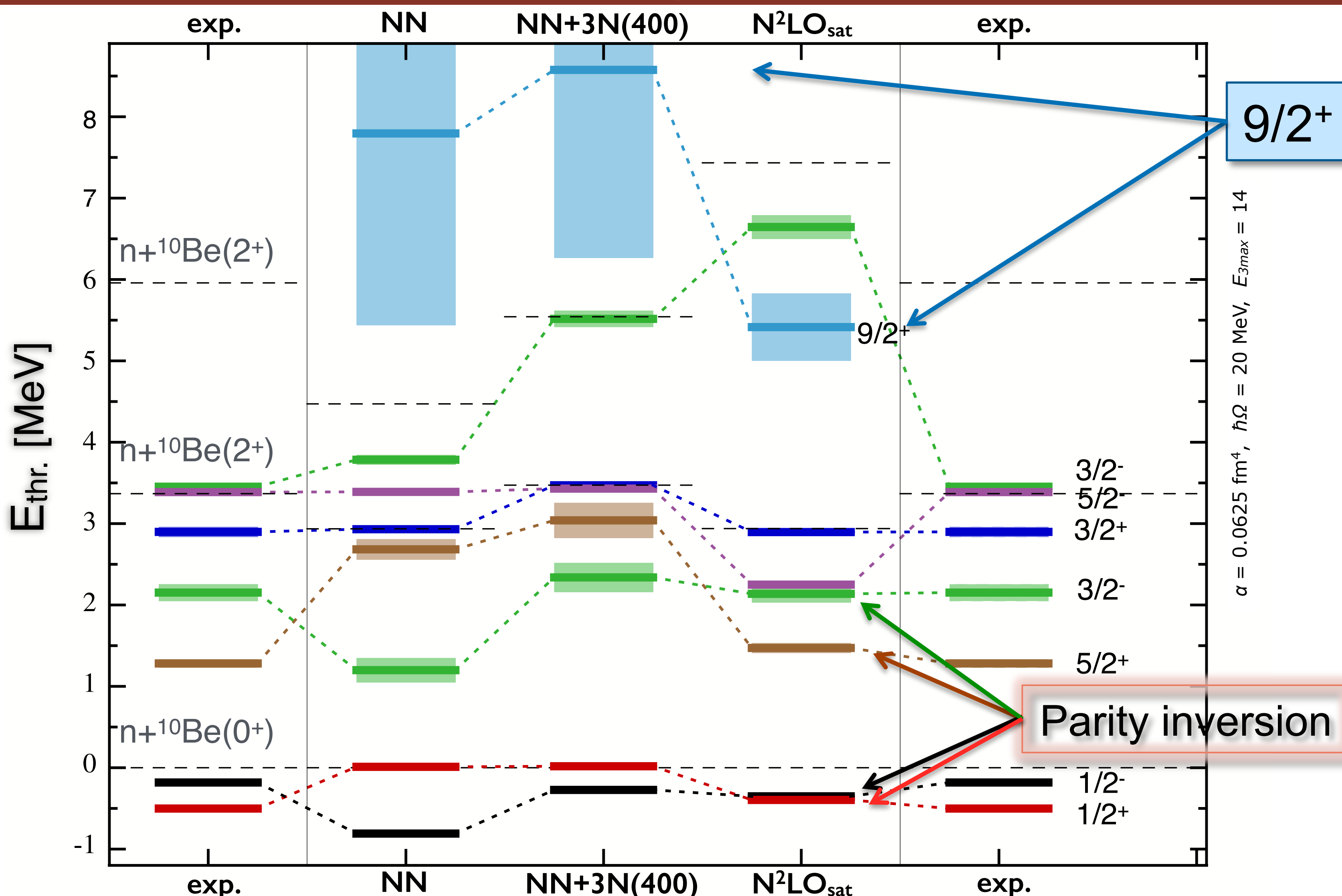

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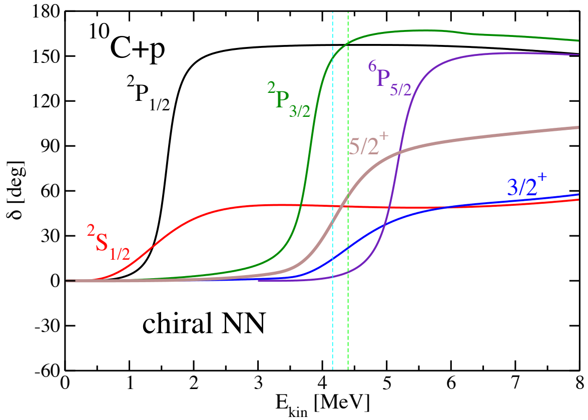
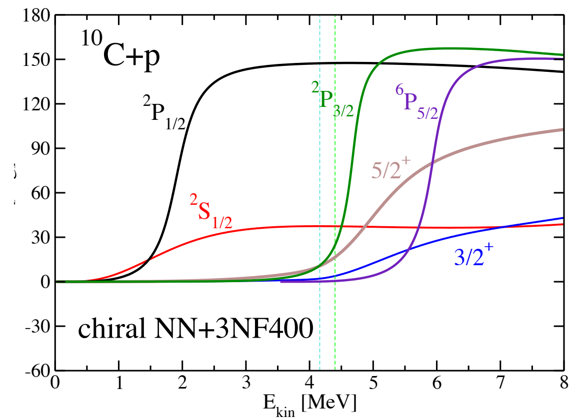
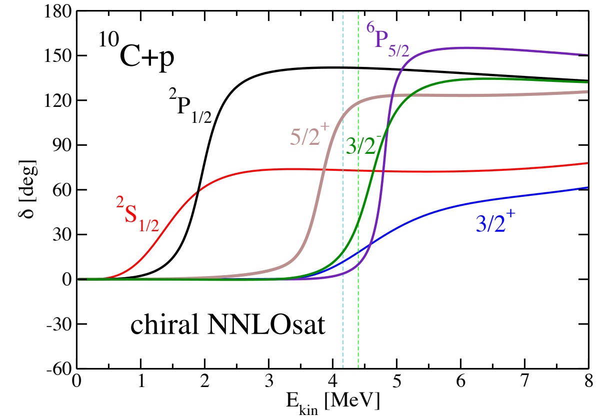
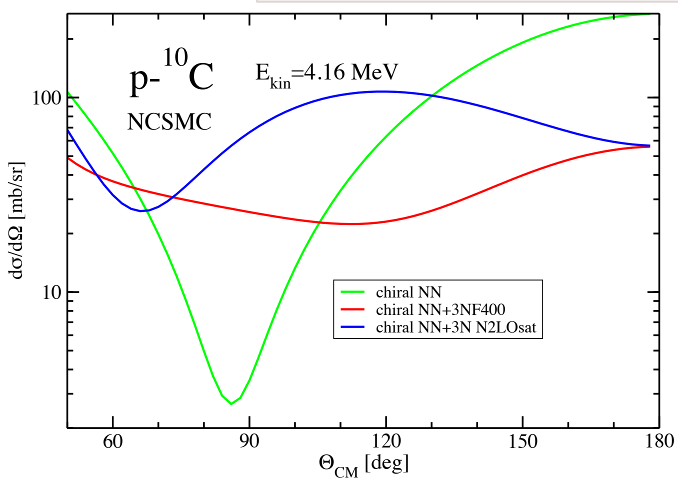
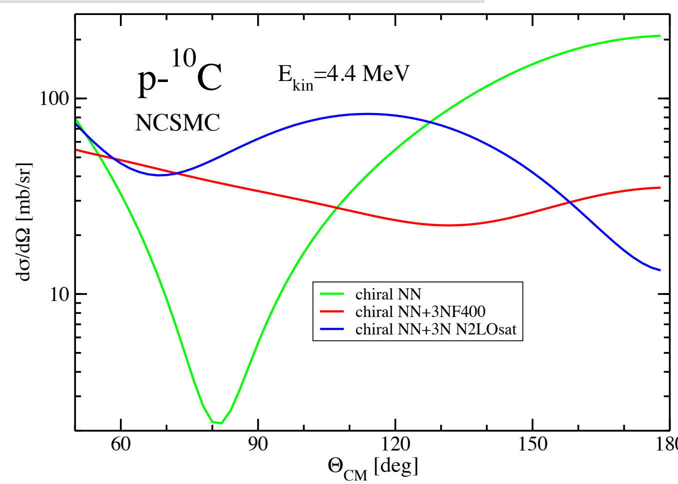


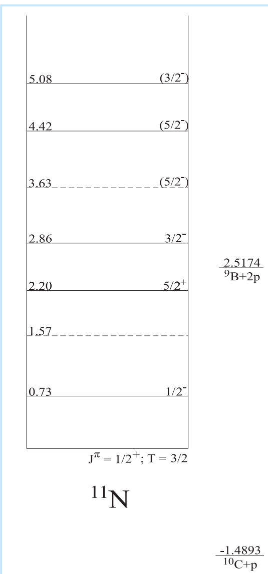




Discrimination among chiral nuclear forces







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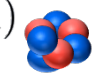
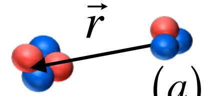
A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al* with IRIS collaboration, submitted

NCSMC wave function

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

$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_\lambda |A\lambda J^\pi T\rangle \left[\sum_{\lambda'} (N^{-\frac12})^{\lambda\lambda'} \bar c_{\lambda'} + \sum_{\nu'} \int dr'\, r'^2 (N^{-\frac12})^{\lambda}_{\nu' r'} \frac{\bar\chi_{\nu'}(r')}{r'}\right]$$

$$+ \sum_{\nu\nu'} \int dr\, r^2 \int dr'\, r'^2 \hat{\mathcal A}_\nu \left|\Phi^{J^\pi T}_{\nu r}\right\rangle \mathcal N^{-\frac12}_{\nu\nu'}(r,r') \left[\sum_{\lambda'} (N^{-\frac12})^{\lambda'}_{\nu' r'} \bar c_{\lambda'} + \sum_{\nu''}\int dr''\, r''^2 (N^{-\frac12})_{\nu' r' \nu'' r''} \frac{\bar\chi_{\nu''}(r'')}{r''}\right].$$

Asymptotic behavior $r \rightarrow \infty$:

$$\bar\chi_\nu(r) \sim C_\nu W(k_\nu r) \qquad \bar\chi_\nu(r) \sim \mathrm{v}_\nu^{-\frac12}\left[\delta_{\nu i} I_\nu(k_\nu r) - U_{\nu i} O_\nu(k_\nu r)\right]$$

Bound state

Scattering state

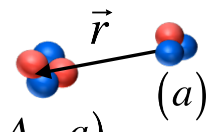
Scattering matrix

TRIUMF

E1 transitions in NCSMC

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

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



$$\left. , \nu \right\rangle$$

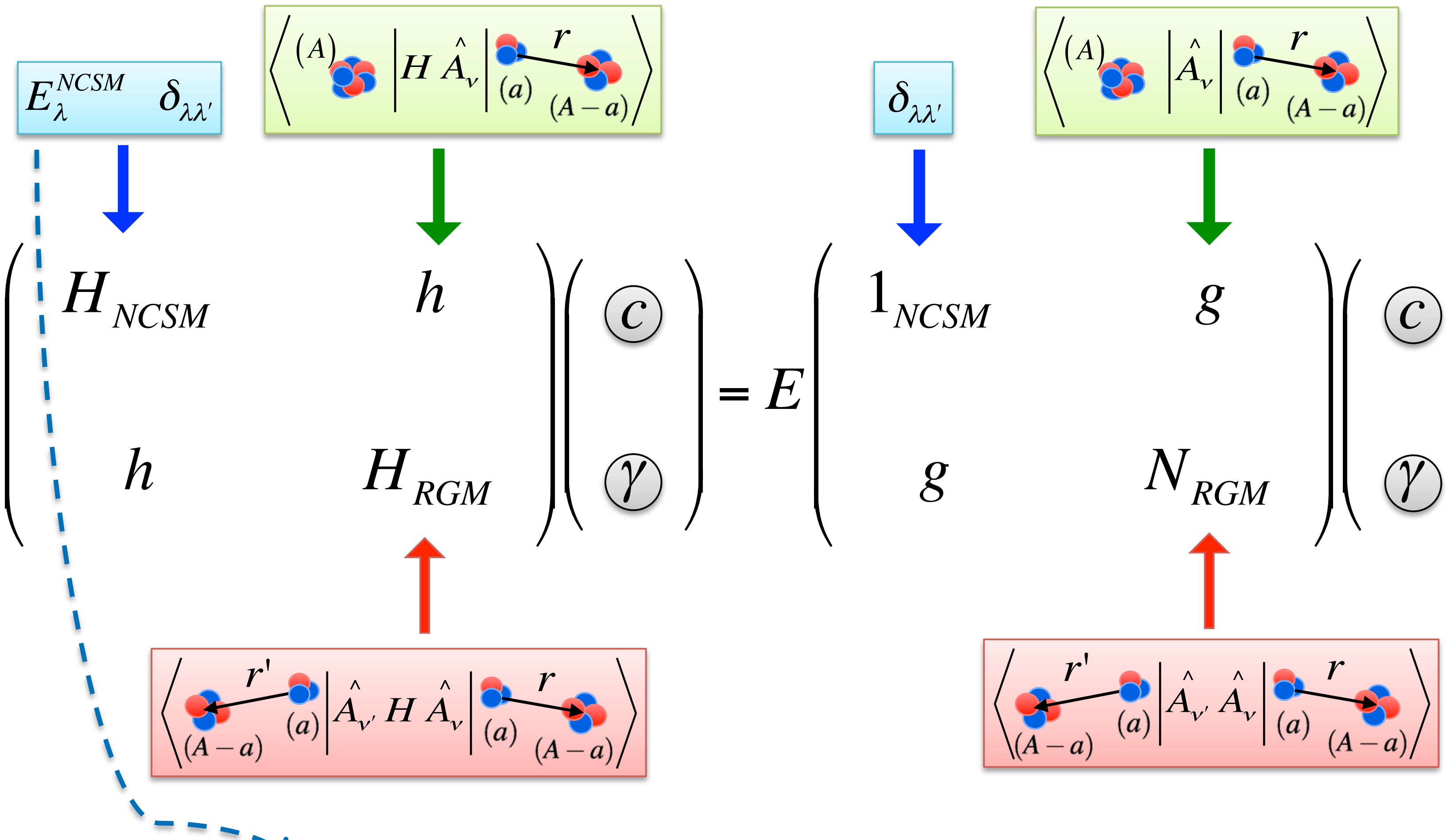
$$\vec{E}1 = e \sum_{i=1}^{A-a} \frac{1+\tau_i^{(3)}}{2} \left(\vec{r}_i - \vec{R}^{(A-a)}_{\mathrm{c.m.}} \right) + e \sum_{j=A-a+1}^{A} \frac{1+\tau_j^{(3)}}{2} \left(\vec{r}_i - \vec{R}^{(a)}_{\mathrm{c.m.}} \right) + e \frac{Z_{(A-a)} a - Z_{(a)} (A-a)}{A} \vec{r}_{A-a,a} \,.$$

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

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)

NCSMC phenomenology



E_λ^{NCSM} energies treated as adjustable parameters

Cluster excitation energies set to experimental values

TRIUMF

Photo-disassociation of ^{11}Be

Bound to bound	NCSM	NCSMC-phenom	Expt.
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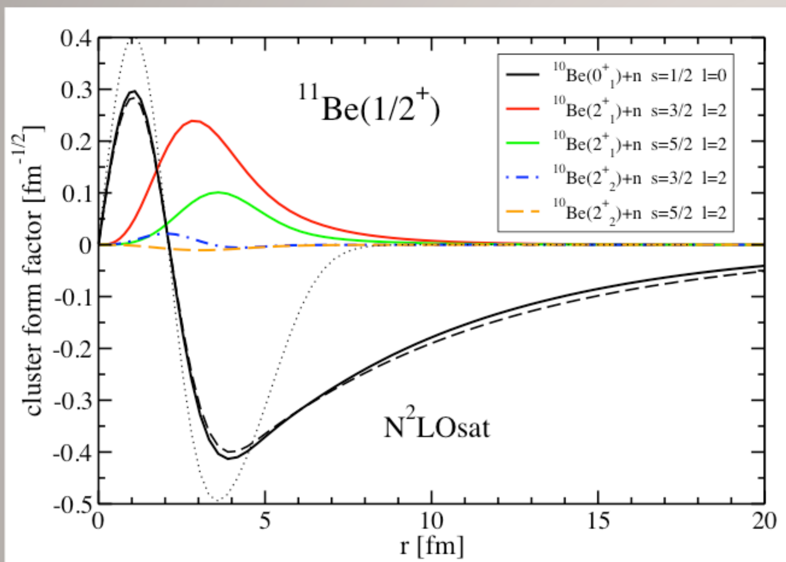
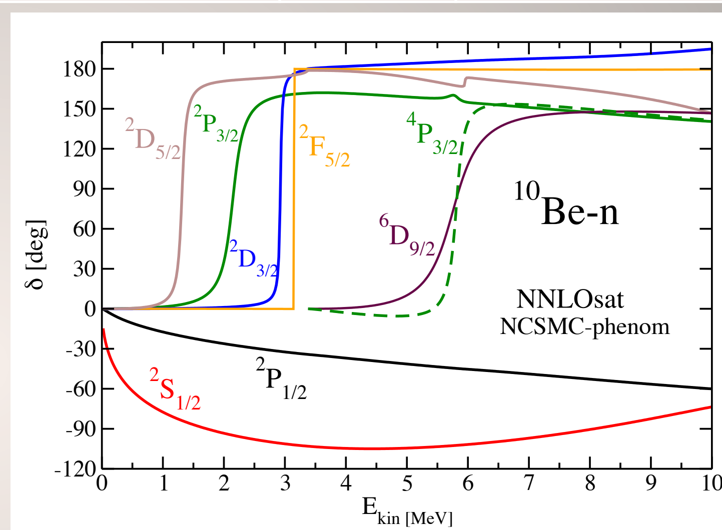
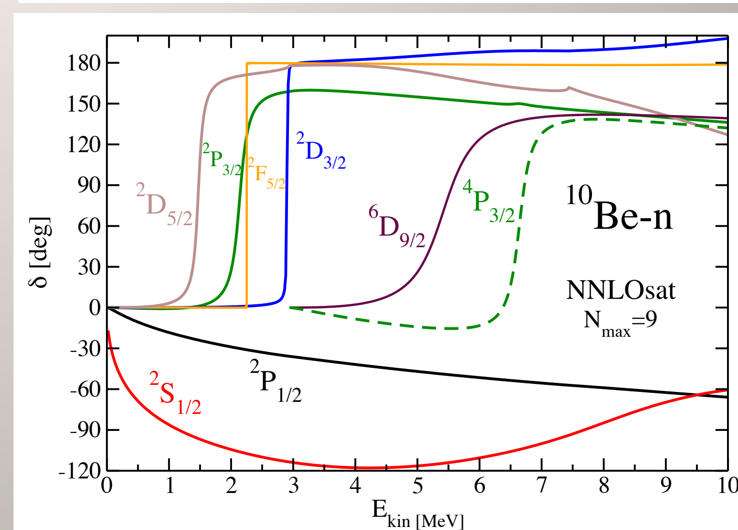
Halo structure







cluster form factor

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

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

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

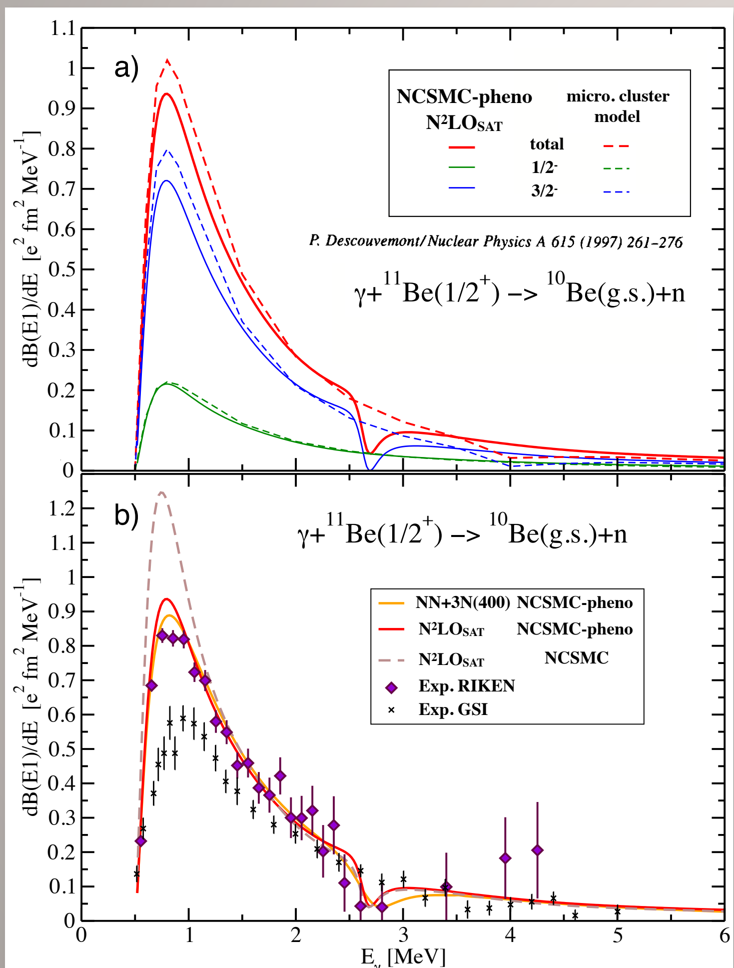
Can *Ab Initio* Theory Explain the Phenomenon of Parity Inversion in ^{11}Be?

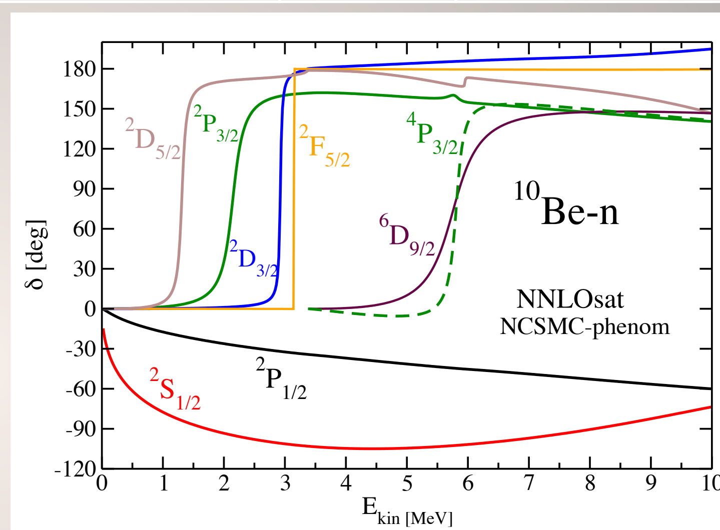
Angelo Calci,[1,*] Petr Navrátil,[1,†] Robert Roth,[2] Jérémy Dohet-Eraly,[1,‡] Sofia Quaglioni,[3] and Guillaume Hupin[4,5]

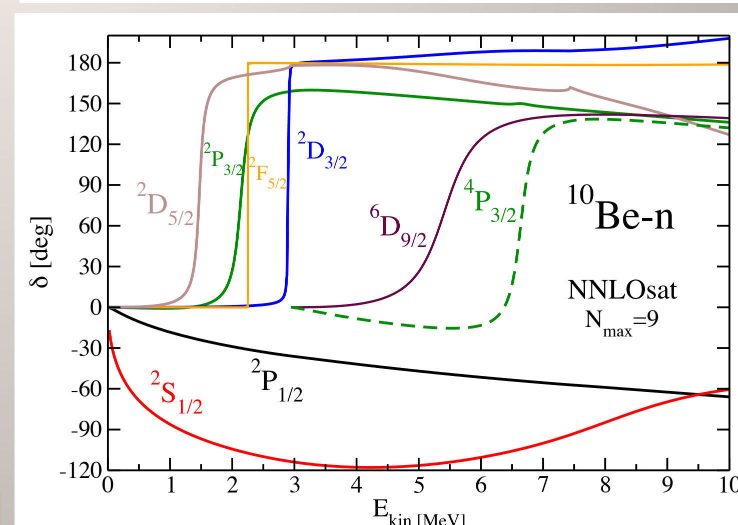
Photo-disassociation of ^{11}Be

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)

Bound to continuum







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

TRIUMF

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

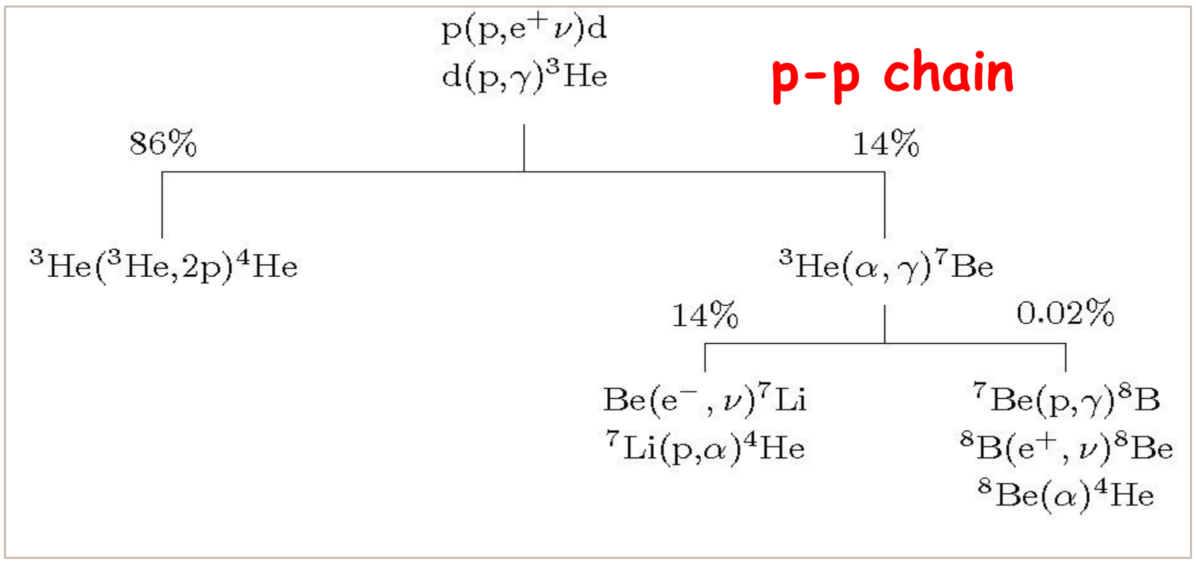
- Measurement of ^{11}C(p,p) resonance scattering planned at TRIUMF
  - TUDA facility
  - ^{11}C beam of sufficient intensity produced

- 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

Next: 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



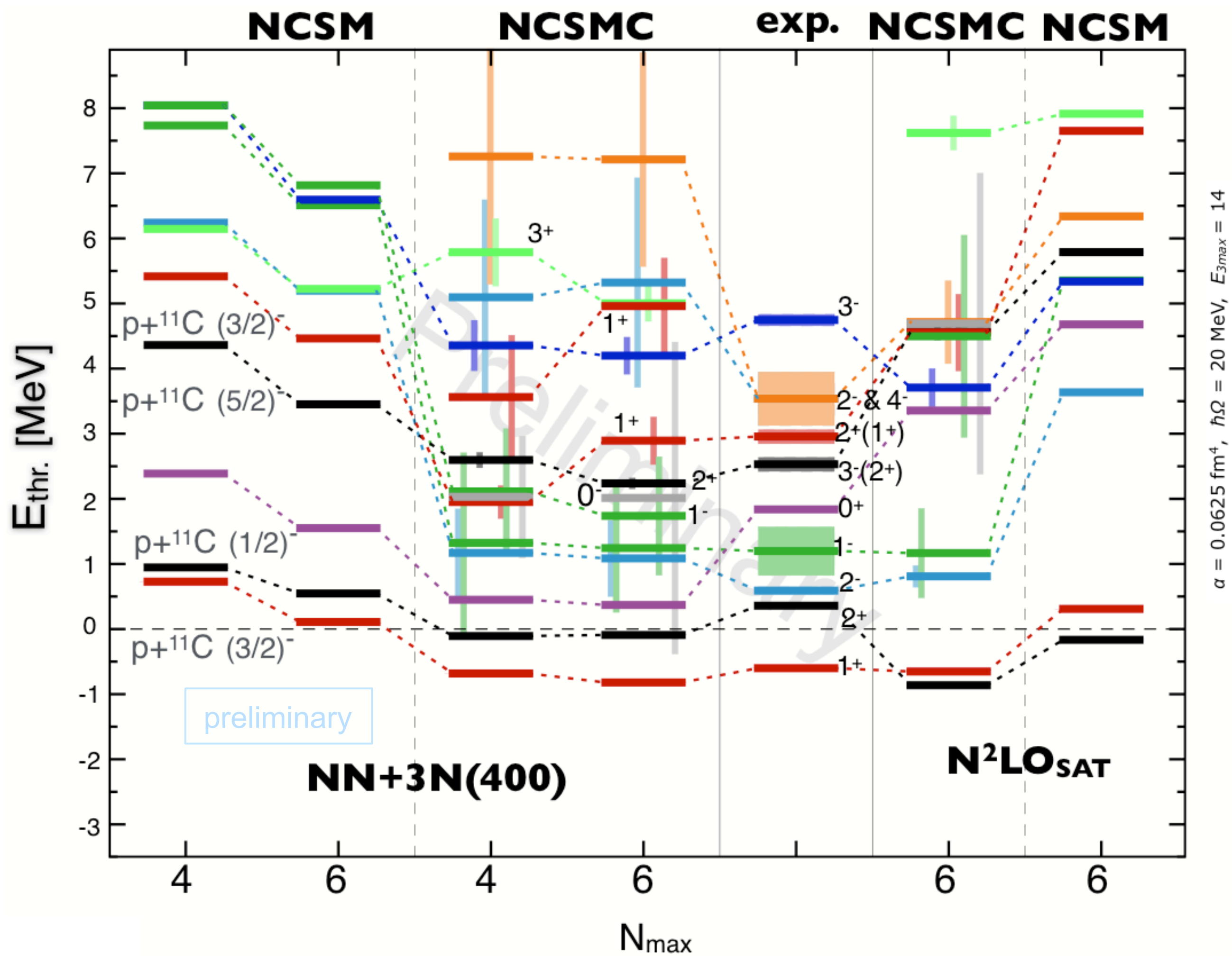
$$^{3}He(\alpha,\gamma)^{7}Be(\alpha,\gamma)^{11}C(p,\gamma)^{12}N(p,\gamma)^{13}O(\beta^{+},\nu)^{13}N(p,\gamma)^{14}O$$

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

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

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



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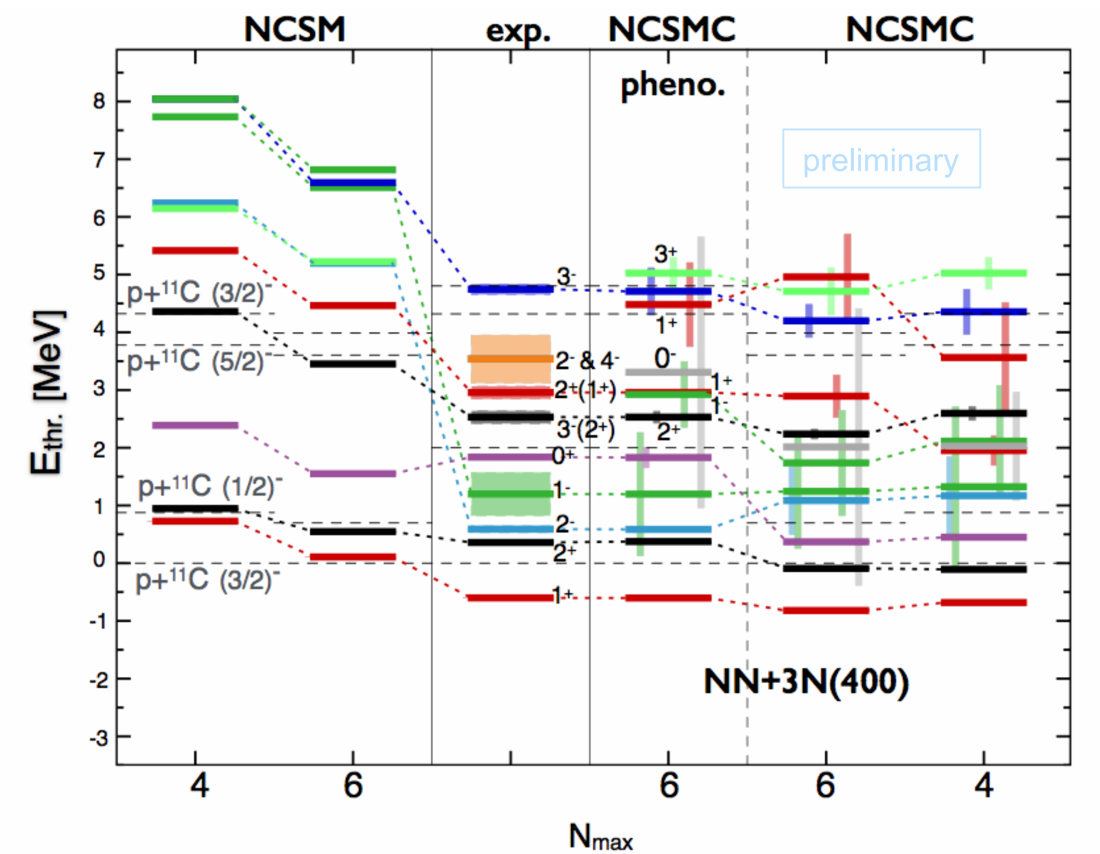

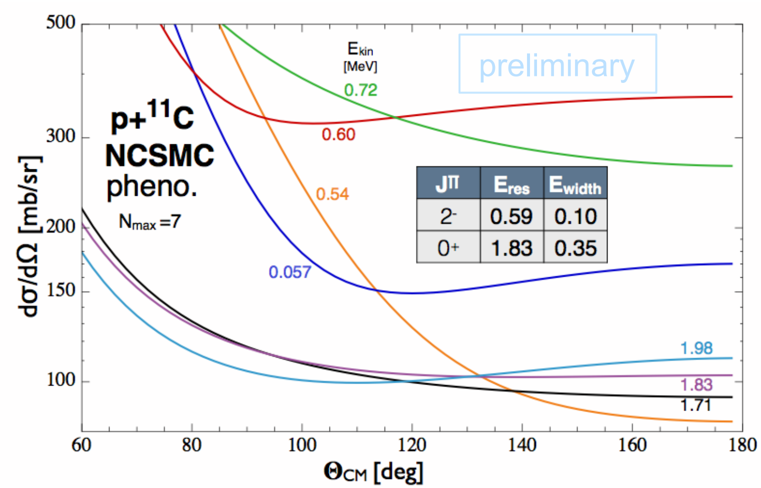

NCSMC calculations to be validated by measured cross sections and applied to calculate the ^{11}C(p,γ)^{12}N capture

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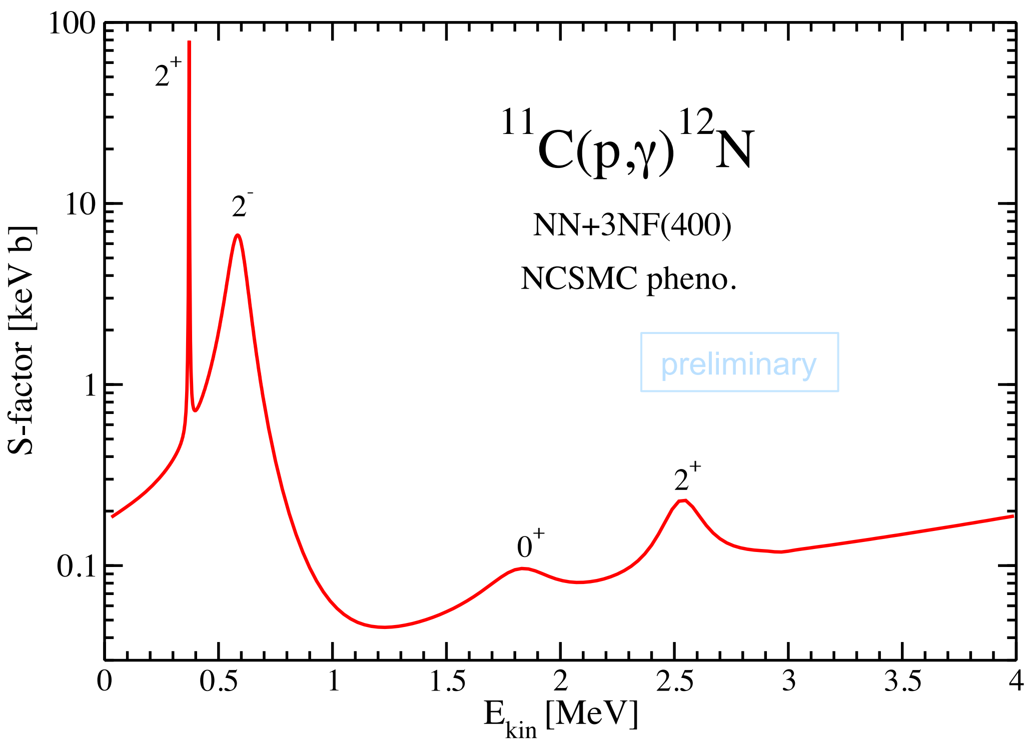
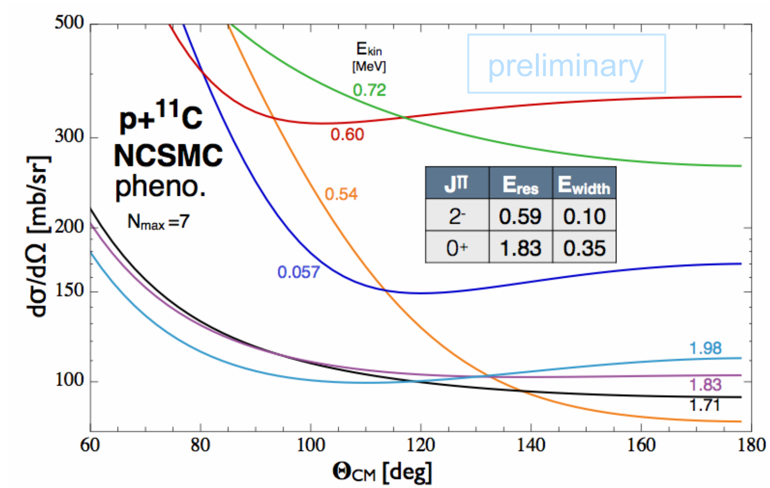




NCSMC calculations to be validated by measured cross sections and applied to calculate the ^{11}C(p,γ)^{12}N capture

TRIUMF

Conclusions and Outlook

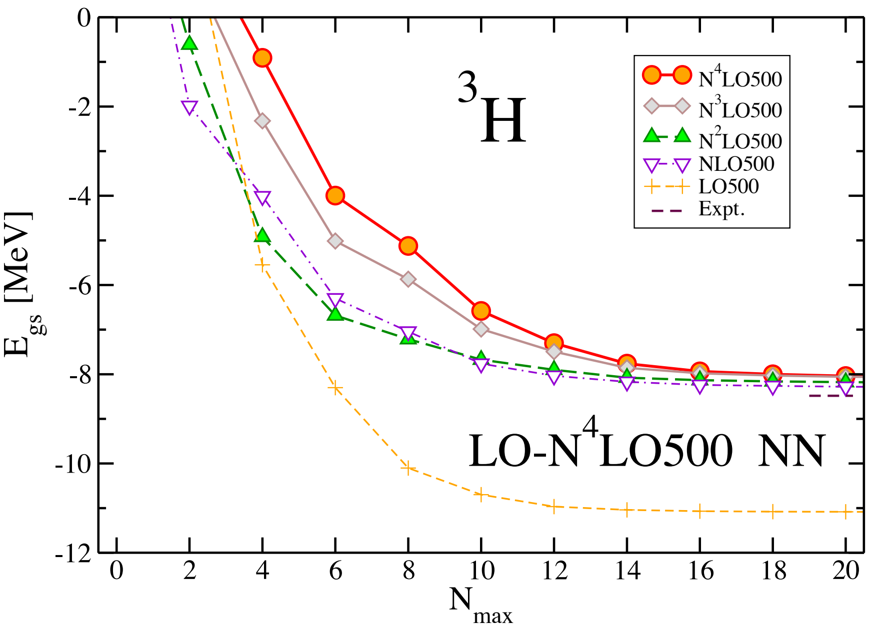
- *Ab initio* calculations of nuclear structure and reactions is a dynamic field with significant advances
- We developed a new unified approach to nuclear bound and unbound states
  - Merging of the NCSM and the NCSM/RGM = **NCSMC**
  - Inclusion of three-nucleon interactions in reaction calculations for *A*>5 systems
  - Extension to three-body clusters (^{6}He ~ ^{4}He+n+n): NCSMC in progress
- Ongoing projects:
  - Transfer reactions
  - Applications to capture reactions important for astrophysics
  - Bremsstrahlung
- Outlook
  - Alpha-clustering (^{4}He projectile)
    - ^{12}C and Hoyle state: ^{8}Be+^{4}He
    - ^{16}O: ^{12}C+^{4}He

TRIUMF

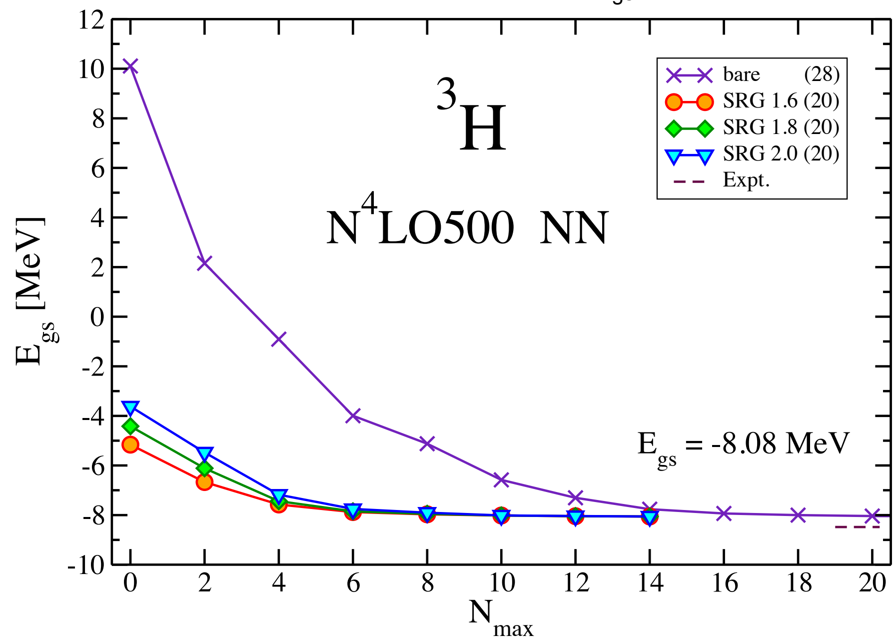
Backup slides

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, to be published.



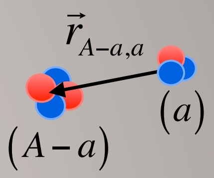
Original EM 2003 N^3LO NN E_{gs}=-7.85 MeV



Binary cluster Resonating Group Method

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

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



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

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

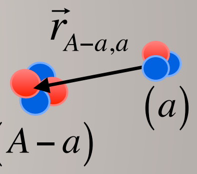
  - Allows to bring the wave function of the relative motion in front of the antisymmetrizer

Binary cluster Resonating Group Method

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

- 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:

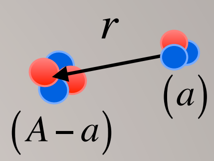
$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r} \underbrace{\hat{A}_\nu \left[\left(\left| A-a\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle \left| a\ \alpha_2 I_2^{\pi_2} T_2 \right\rangle \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi T)} \frac{\delta(r - r_{A-a,a})}{r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

$\left|\Phi_{\nu r}^{J^\pi T}\right\rangle$ (Jacobi) channel basis

TRIUMF

Binary cluster RGM equations

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



- Projecting the Schrödinger equation on the channel basis yields:

$$\sum_\nu \int \left[H_{\nu'\nu}^{J^\pi T}(r',r) - E\ N_{\nu'\nu}^{J^\pi T}(r',r) \right] \frac{g_\nu^{J^\pi T}(r)}{r}\ r^2\, dr = 0$$

$$\left\langle \Phi_{\nu' r'}^{J^\pi T} \middle| \hat{A}_{\nu'} H \hat{A}_\nu \middle| \Phi_{\nu r}^{J^\pi T} \right\rangle$$

Hamiltonian kernel

$$\left\langle \Phi_{\nu' r'}^{J^\pi T} \middle| \hat{A}_{\nu'} \hat{A}_\nu \middle| \Phi_{\nu r}^{J^\pi T} \right\rangle$$

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

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

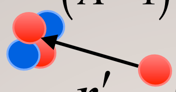
Note that this is OK,
in particular when the sum
is truncated,
ONLY for localized
parts of the kernels

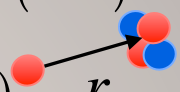
  - We call them Jacobi channel states because they describe only the internal motion
    - Target and projectile wave functions are both translational invariant NCSM eigenstates calculated in the Jacobi coordinate basis

Norm kernel (Pauli principle)

Single-nucleon projectile

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

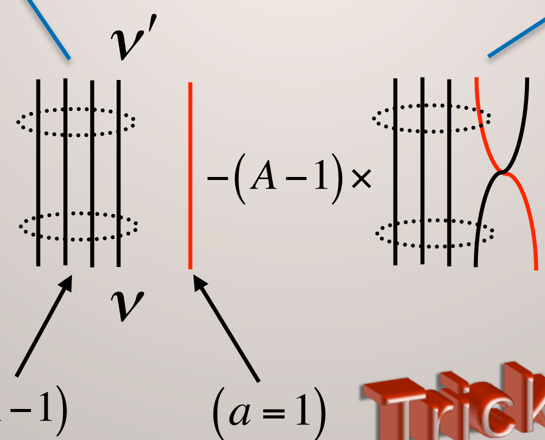




$$N^{J^\pi T}_{\nu'\nu}(r',r) = \delta_{\nu'\nu} \frac{\delta(r'-r)}{r'r} - (A-1) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

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

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)

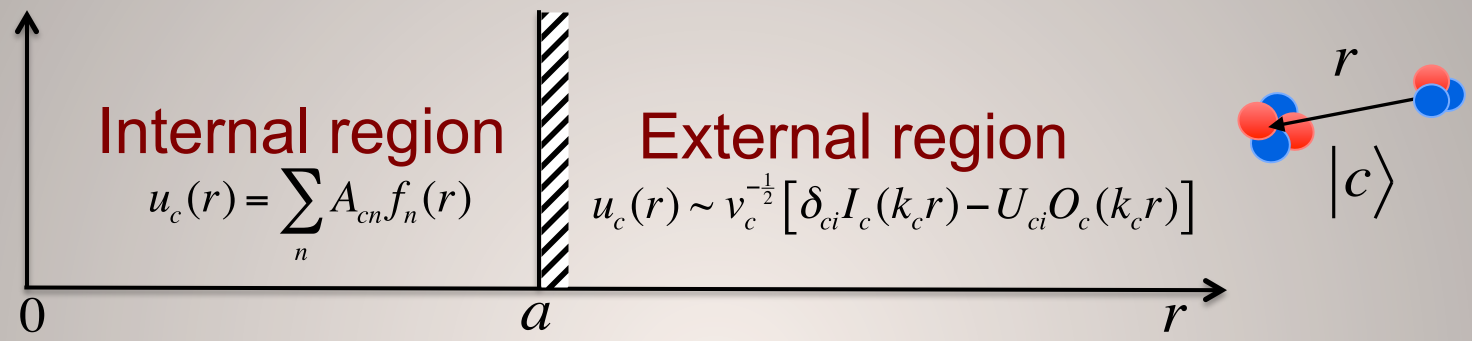
Trick #1 $$\frac{\delta(r - r_{A-a,a})}{r\, r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

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

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: $L_c = \dfrac{\hbar^2}{2\mu_c}\delta(r-a)\left(\dfrac{d}{dr}-\dfrac{B_c}{r}\right)$
  - 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

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

Bound state — Scattering state

Scattering matrix (U_{ci})