Nuclear structure and dynamics from *ab initio* theory

1st APCTP-TRIUMF JOINT WORKSHOP on

Understanding Nuclei from Different Theoretical Approaches

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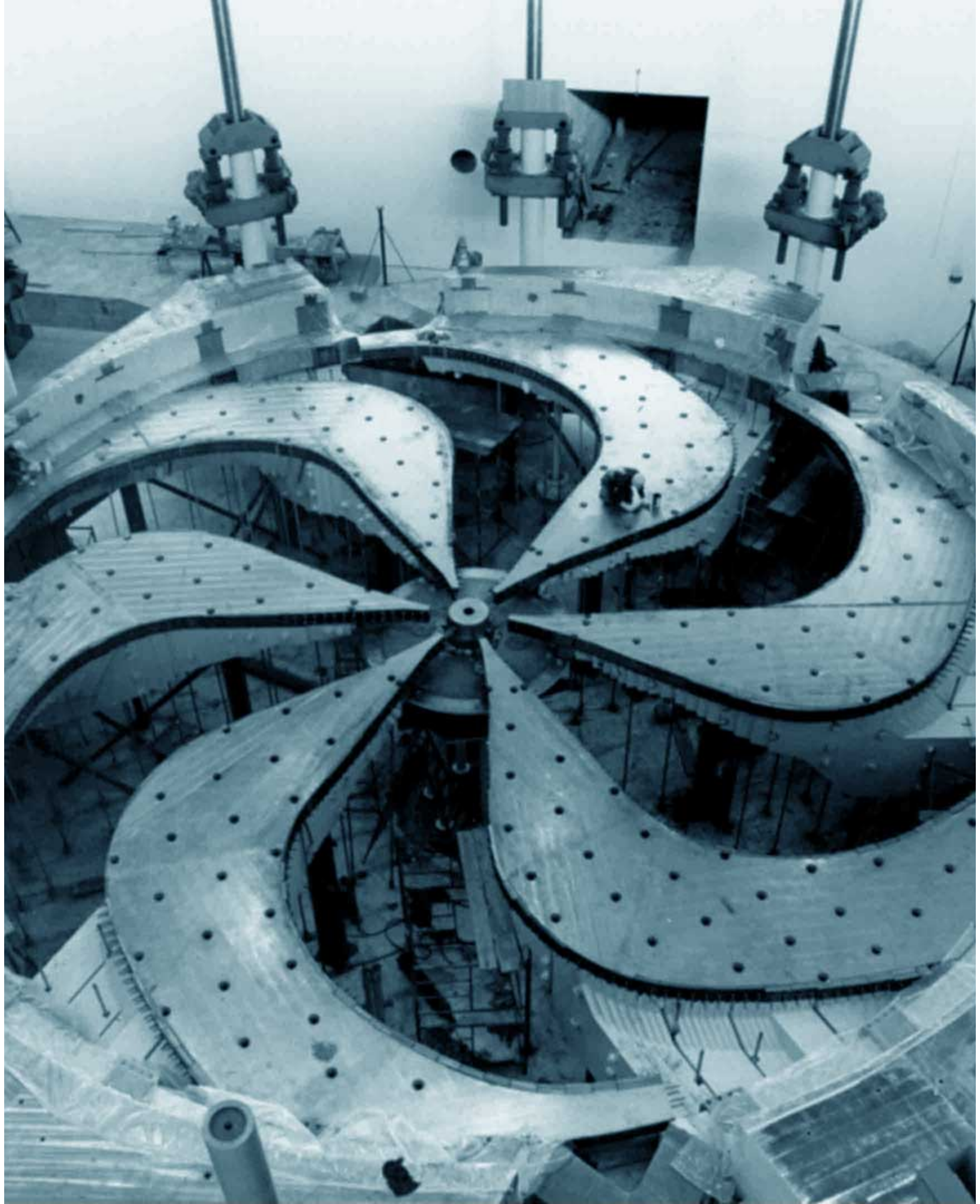
2018-09-18



Discovery, accelerated

Outline

- Nuclear structure and reactions from first principles
- New chiral NN N^4LO + 3N
  - Beta decays of light nuclei in NCSM
- No-Core Shell Model with Continuum (NCSMC)
- n-^{4}He scattering and D+T fusion
- ^{11}Be parity inversion in low-lying states, photo-dissociation
- 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

What is meant by *ab initio* in nuclear physics?

- **First principles for Nuclear Physics:**

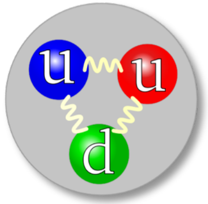
  QCD

  - Non-perturbative at low energies
  - Lattice QCD in the future

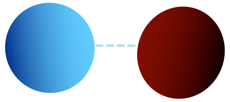
- Degrees of freedom: NUCLEONS
  - Nuclei made of nucleons
  - Interacting by nucleon-nucleon and three-nucleon potentials

- *Ab initio*
  - ✧ All nucleons are active
  - ✧ Exact Pauli principle
  - ✧ Realistic inter-nucleon interactions
    - ✧ Accurate description of NN (and 3N) data
  - ✧ Controllable approximations

From QCD to nuclei

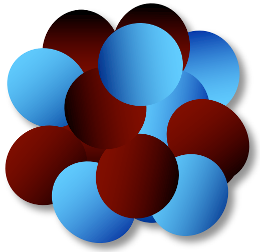


Low-energy QCD



NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

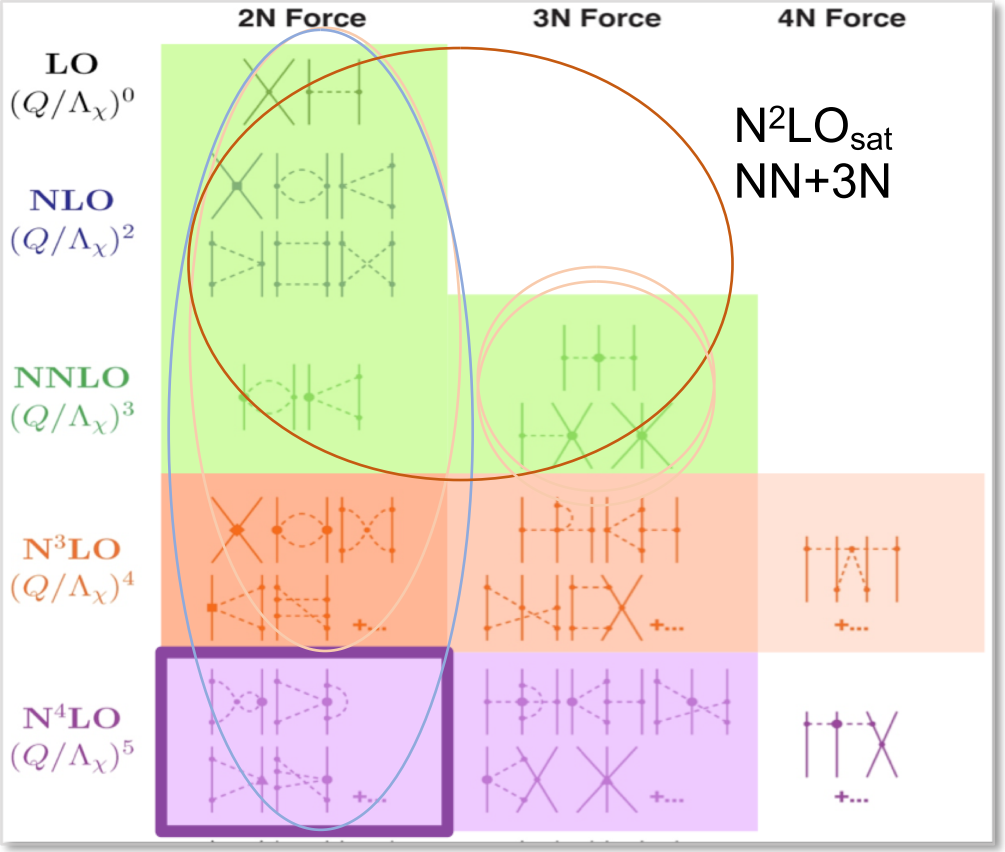


Nuclear structure and reactions

Chiral Effective Field Theory

- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order (Q/Λ_χ)
  - Hierarchy
  - Consistency
  - Low energy constants (LEC)
    - Fitted to data
    - Can be calculated by lattice QCD

Λ_χ~1 GeV :
Chiral symmetry breaking scale



N^4LO500 NN + N^2LO 3N

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

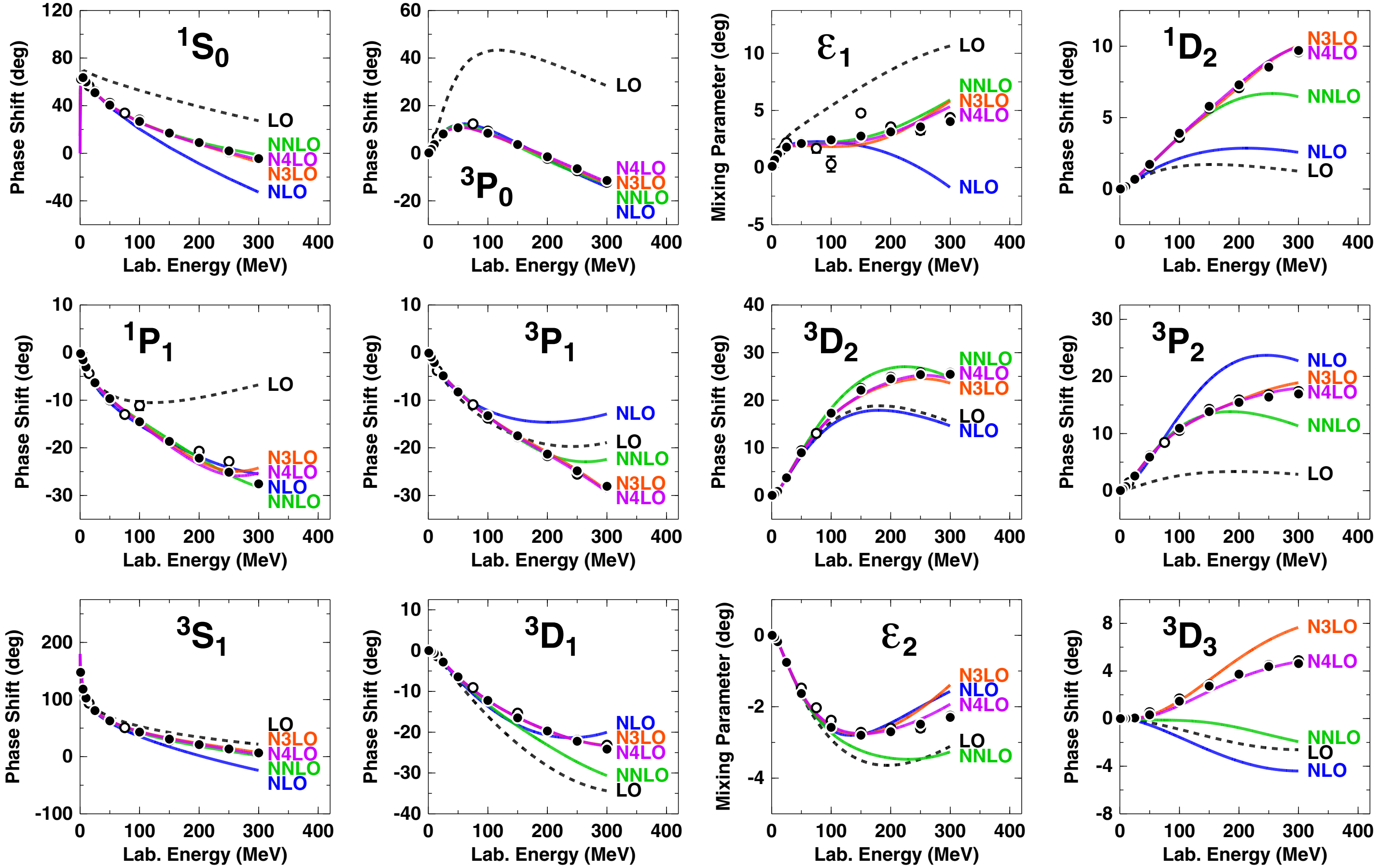
The NN interaction from chiral EFT

PHYSICAL REVIEW C **96**, 024004 (2017)

High-quality two-nucleon potentials up to fifth order of the chiral expansion

D. R. Entem,[1,*] R. Machleidt,[2,†] and Y. Nosyk[2]

- Chiral NN potential up to N^{4}LO
- Set of five potentials constructed
  - Sequence of LO, NLO,…,N^{4}LO
  - Uncertainty quantification
- At N^{3}LO and N^{4}LO:
  - 24 LECs fitted to the *np* scattering data and the deuteron properties
    - Including c_i LECs (i=1-4) from pion-nucleon scattering
- N^{4}LO NN fitted to data up to pion production threshold with χ^2/datum~1.15



Currents in chiral EFT

- Meson-exchange current

PHYSICAL REVIEW C **67**, 055206 (2003)

Parameter-free effective field theory calculation for the solar proton-fusion and hep processes

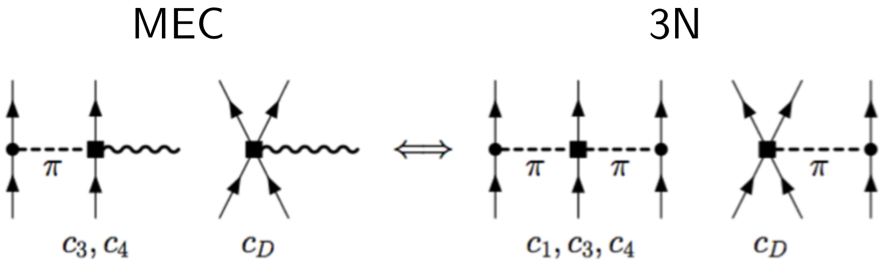
T.-S. Park,[1,2,3] L. E. Marcucci,[4,5] R. Schiavilla,[6,7] M. Viviani,[5,4] A. Kievsky,[5,4] S. Rosati,[5,4] K. Kubodera,[1,2]
D.-P. Min,[8] and M. Rho[1,9]

  - weak axial current
    - one-body: LO - Gamow-Teller

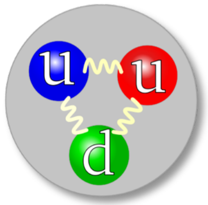
$$\boldsymbol{A}_l = -g_A \tau_l^- e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_l}\left[\boldsymbol{\sigma}_l + \frac{2(\bar{\boldsymbol{p}}_l \boldsymbol{\sigma}_l\cdot\bar{\boldsymbol{p}}_l - \boldsymbol{\sigma}_l \bar{\boldsymbol{p}}_l^2) + i\boldsymbol{q}\times\bar{\boldsymbol{p}}_l}{4m_N^2}\right]$$

    - two-body: MEC

$$\boldsymbol{A}_{12} = \frac{g_A}{2m_N f_\pi^2}\frac{1}{m_\pi^2+k^2}\Bigg[-\frac{i}{2}\tau_\times^- \boldsymbol{p}(\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2)\cdot\boldsymbol{k} + 4\hat{c}_3 \boldsymbol{k}\boldsymbol{k}\cdot(\tau_1^-\boldsymbol{\sigma}_1+\tau_2^-\boldsymbol{\sigma}_2) + \left(\hat{c}_4+\frac{1}{4}\right)\tau_\times^- \boldsymbol{k}\times[\boldsymbol{\sigma}_\times\times\boldsymbol{k}]\Bigg] + \frac{g_A}{m_N f_\pi^2}[2\hat{d}_1(\tau_1^-\boldsymbol{\sigma}_1+\tau_2^-\boldsymbol{\sigma}_2)+\hat{d}_2\tau_\times^a\boldsymbol{\sigma}_\times],$$



From QCD to nuclei



Low-energy QCD

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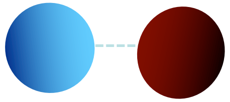
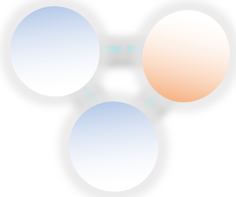


NN+3N interactions from chiral EFT

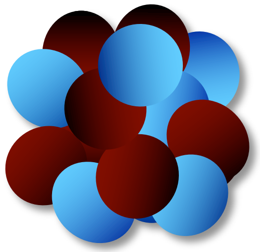
…or accurate meson-exchange potentials

↓



Unitary/similarity transformations

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



Nuclear structure and reactions

Similarity Renormalization Group (SRG) evolution

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

$$\frac{dH_\alpha}{d\alpha} = \frac{dU_\alpha}{d\alpha} H U_\alpha^+ + U_\alpha H \frac{dU_\alpha^+}{d\alpha} = \frac{dU_\alpha}{d\alpha} U_\alpha^+ U_\alpha H U_\alpha^+ + U_\alpha H U_\alpha^+ U_\alpha \frac{dU_\alpha^+}{d\alpha}$$

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

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

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 $H_{\alpha=0} = H_{\lambda=\infty} = H$ $\quad \lambda^2 = 1/\sqrt{\alpha}$
- **Induces many-body forces**
  - **In applications to chiral interactions three-body induced terms large, four-body small**

SRG evolution for *A*-nucleon system

- Evolution induces many-nucleon terms (up to *A*)

$$\tilde{H}_\alpha = \tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]} + \tilde{H}_\alpha^{[3]} + \tilde{H}_\alpha^{[4]} + \ldots + \tilde{H}_\alpha^{[A]}$$

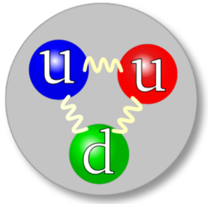
- SRG "magic" – $\tilde{H}_\alpha^{[2]}$ determined completely in A=2 system, $\tilde{H}_\alpha^{[3]}$ determined completely in A=3 system, etc.

- In actual calculations so far only terms up to $\tilde{H}_\alpha^{[3]}$ kept

- Three types of SRG-evolved Hamiltonians used
  - **NN only**: Start with initial T+V_{NN} and keep $\tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]}$
  - **NN+3N-induced**: Start with initial T+V_{NN} and keep $\tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]} + \tilde{H}_\alpha^{[3]}$
  - **NN+3N-full**: Start with initial T+V_{NN}+V_{NNN} and keep $\tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]} + \tilde{H}_\alpha^{[3]}$

α variation (Λ variation) provides a diagnostic tool to asses the contribution of omitted many-body terms, tests the unitarity of the SRG transformation

From QCD to nuclei



Low-energy QCD

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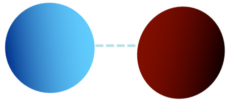

NN+3N interactions from chiral EFT — …or accurate meson-exchange potentials

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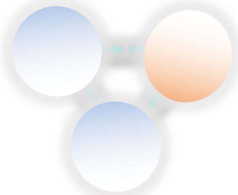


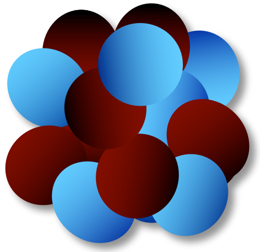
Unitary/similarity transformations — Identity or SRG or OLS or UCOM … Softens NN, induces 3N

⇩

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

Many-Body methods — NCSM, NCSMC, CCM, SCGF, IM-SRG, GFMC, HH, Nuclear Lattice EFT…

⇩

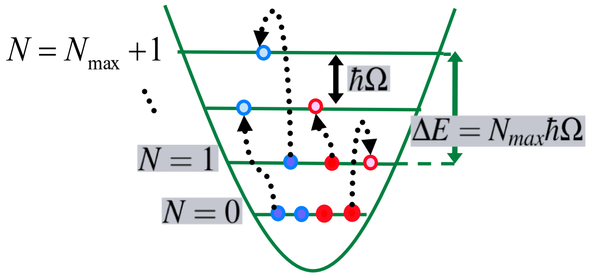


Nuclear structure and reactions

Conceptually simplest *ab initio* method: No-Core Shell Model (NCSM)

NCSM

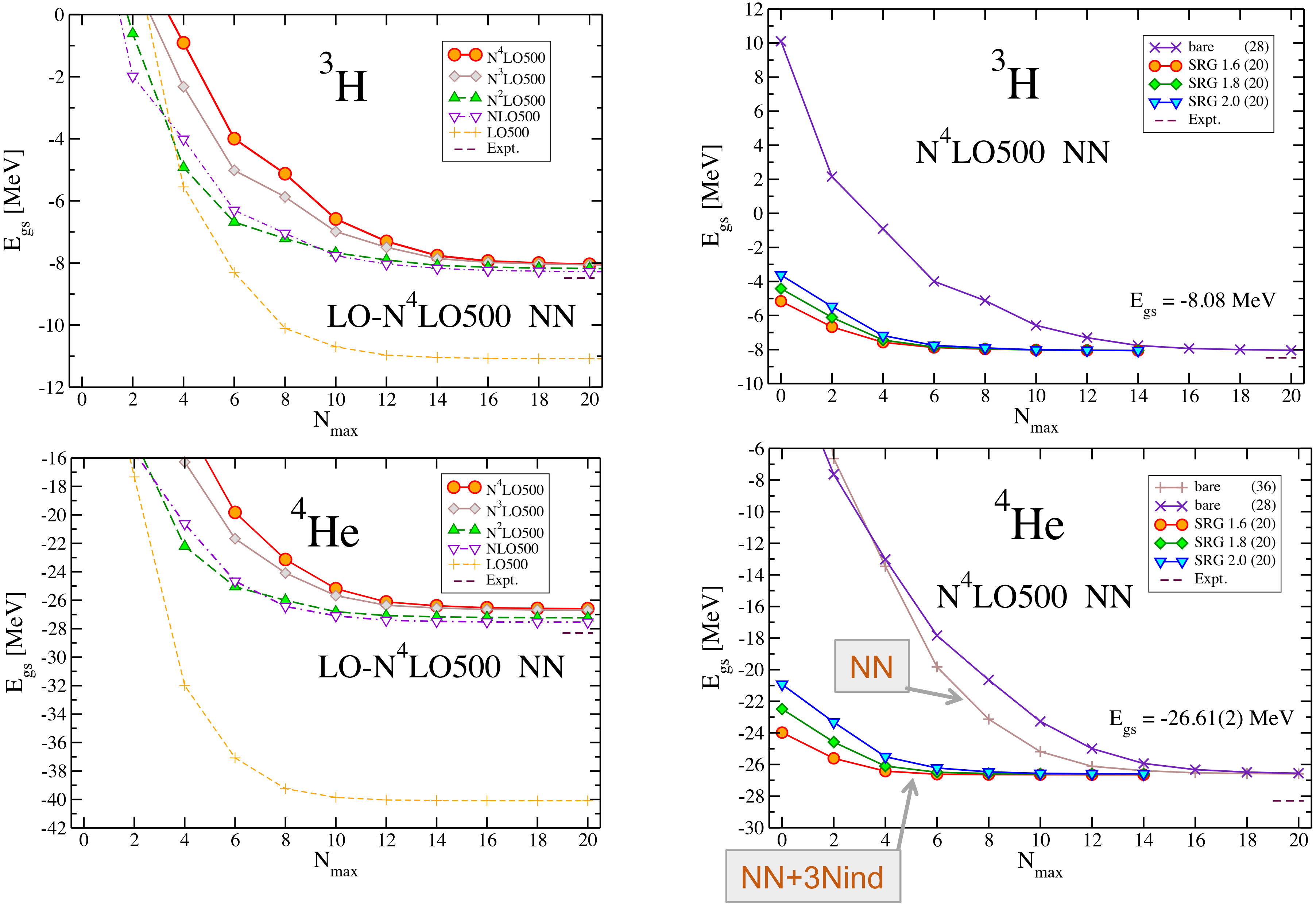
- Basis expansion method
  - Harmonic oscillator (HO) basis truncated in a particular way ($N_{\max}$)
  - Why HO basis?
    - Lowest filled HO shells match magic numbers of light nuclei (2, 8, 20 – ^{4}He, ^{16}O, ^{40}Ca)
    - Equivalent description in relative-coordinate and Slater determinant basis
- Short- and medium range correlations
- Bound-states, narrow resonances



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

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

^{3}H and ^{4}He with chiral EFT interactions up to N^{4}LO



$^3H \rightarrow {}^3He$ β decay

$$\hat{O} = GT^{(1)} \rightarrow \hat{O}_\alpha = GT^{(1)} + GT^{(2)}_\alpha + \ldots$$

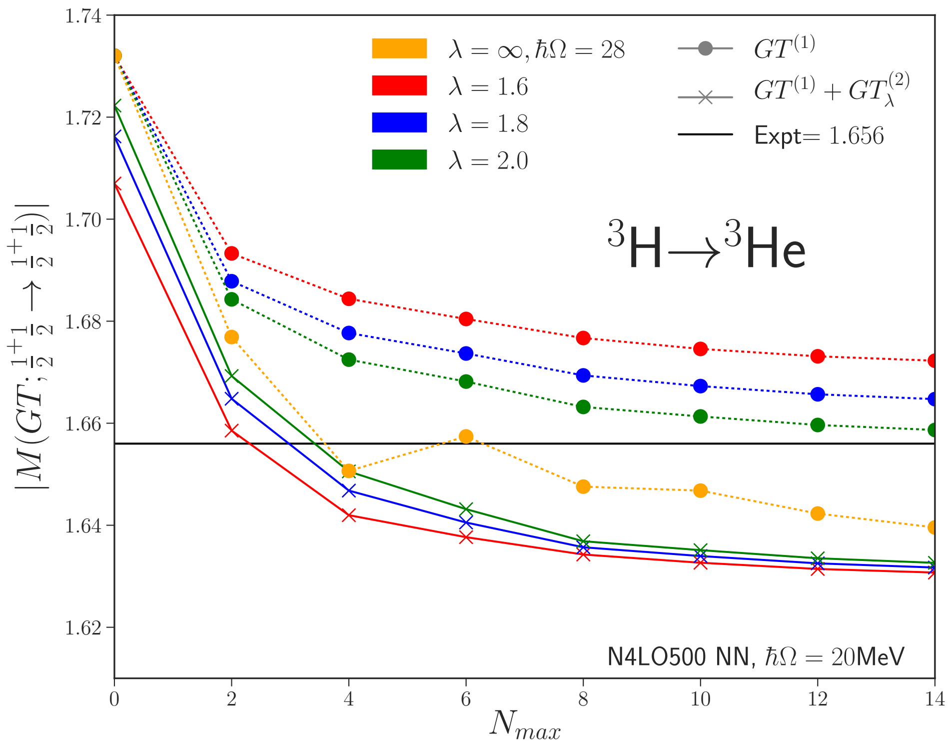
Operator:

Gamow-Teller (1-body)

$\langle GT^{(2)}_\alpha \rangle_{A=2} = \langle (GT^{(1)})_\alpha \rangle_{A=2} - \langle GT^{(1)} \rangle_{A=2}$

Potential: "N^{4}LO NN"

- chiral NN @ N^{4}LO, Machleidt PRC96 (2017), 500MeV cutoff



Hamiltonian:
chiral NN with SRG 2- and 3-body induced
(except orange line: bare chiral NN)

$^3H \rightarrow {}^3He$ β decay

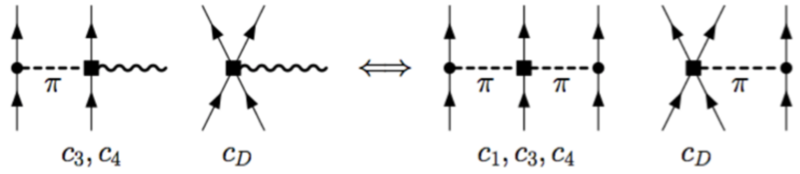
$$\hat{O} = GT^{(1)} + MEC^{(2)} \rightarrow \hat{O}_\alpha = GT^{(1)} + GT^{(2)}_\alpha + MEC^{(2)}_\alpha + \ldots$$

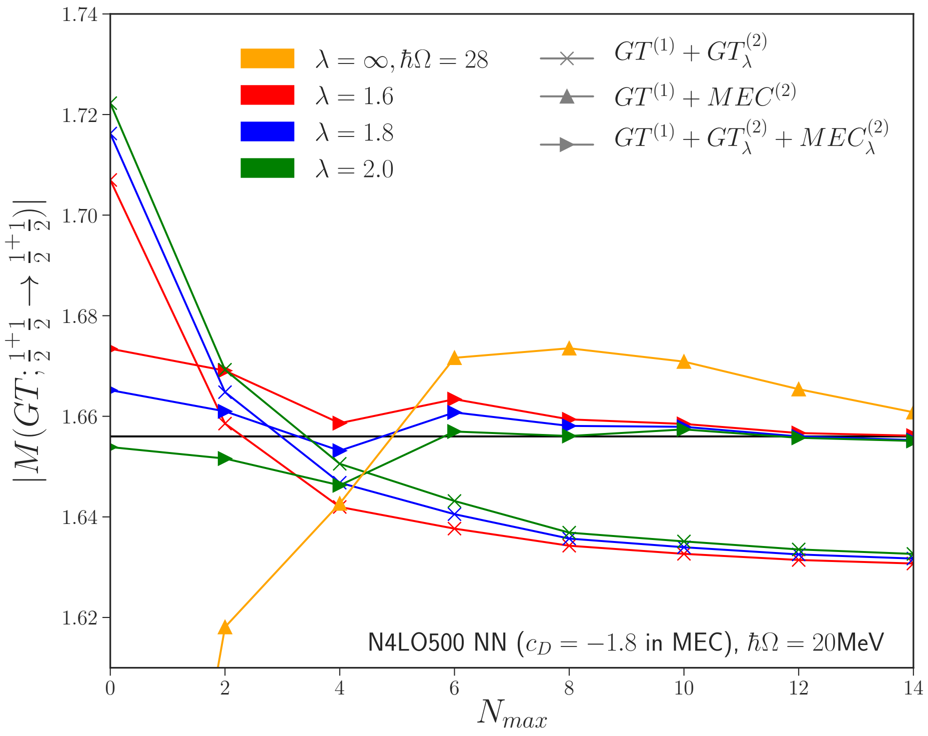
Operator:

Gamow-Teller (1-body) + chiral meson exchange current (2-body) Park (2003)

Potential: "N^{4}LO NN"

- chiral NN @ N^{4}LO, Machleidt PRC96 (2017), 500MeV cutoff
- LEC $c_D = -1.8$ determined





Original EM 2003 N^{3}LO NN c_D=+0.8 (3N repulsive)

⇔

Determination of the c_D parameter relevant to chiral 3N force c_D=-1.8 (3N attractive)

^{6}He→^{6}Li β decay

$$\hat{O} = GT^{(1)} + MEC^{(2)} \rightarrow \hat{O}_\alpha = GT^{(1)} + GT^{(2)}_\alpha + MEC^{(2)}_\alpha + \dots$$

Operator:

Gamow-Teller (1-body) + chiral meson exchange current (2-body) Park (2003)

Potential: "N^{4}LO NN"

- chiral NN @ N^{4}LO, Machleidt PRC96 (2017), 500MeV cutoff
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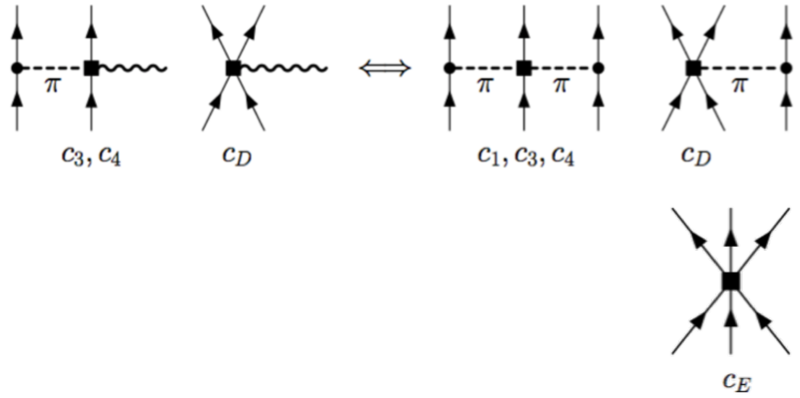
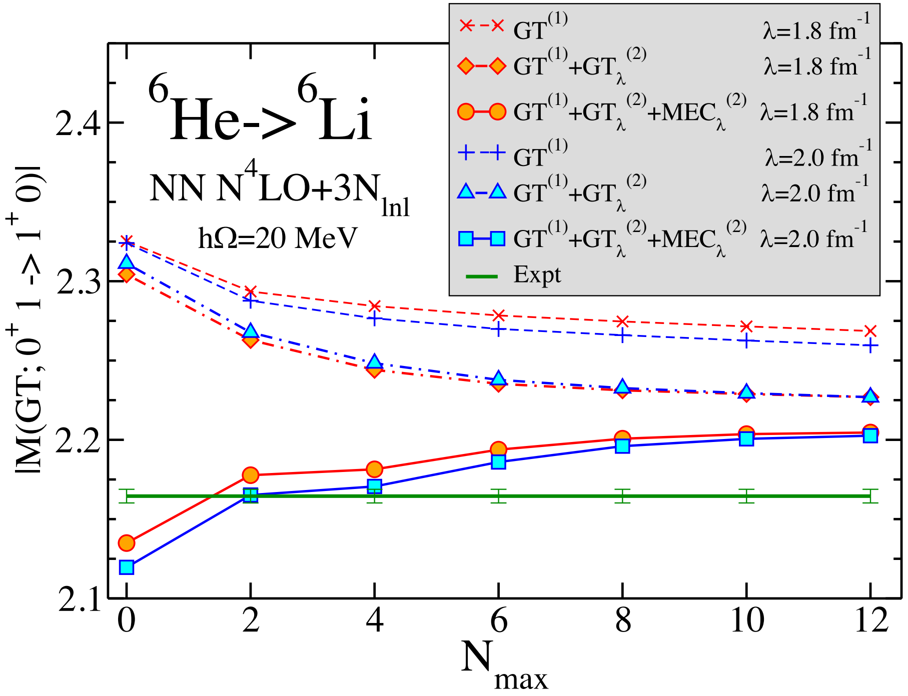


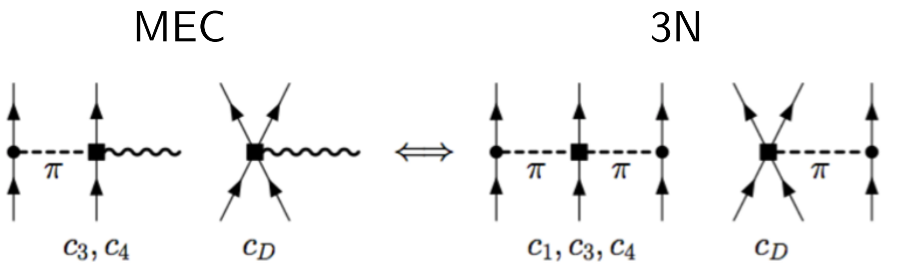


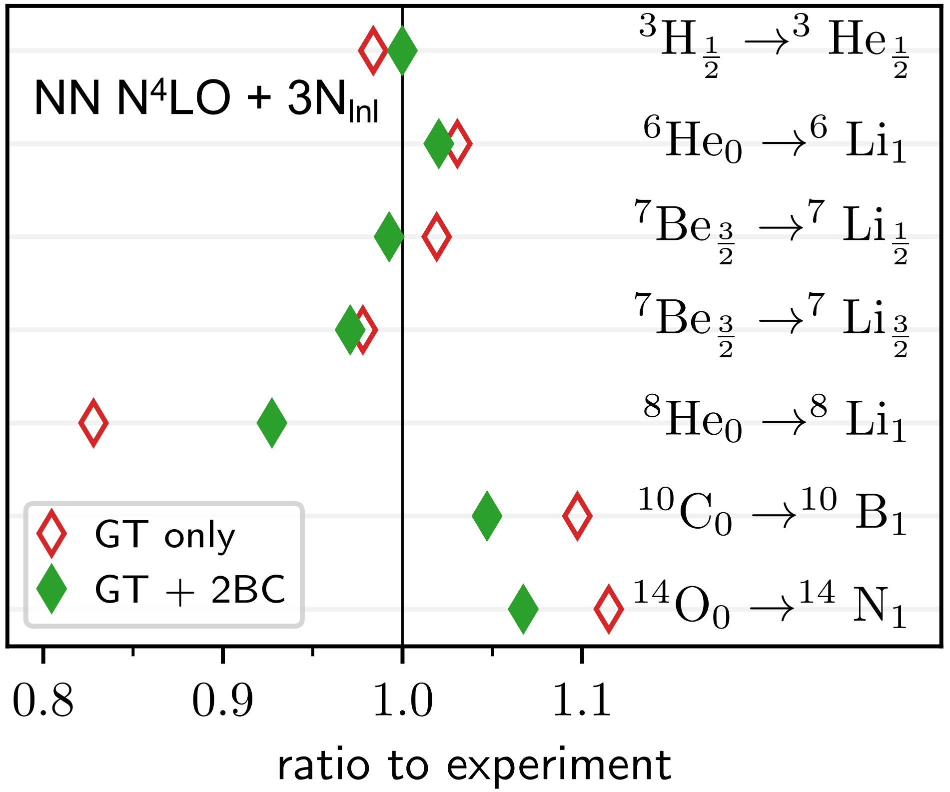
Determination of the c_D parameter from ^{3}H beta decay
c_D=-1.8 (3N D-term attractive)
c_E from ^{3}H binding energy
c_E=-0.31 (3N E-term repulsive)

Applications to β decays in p-shell nuclei and beyond

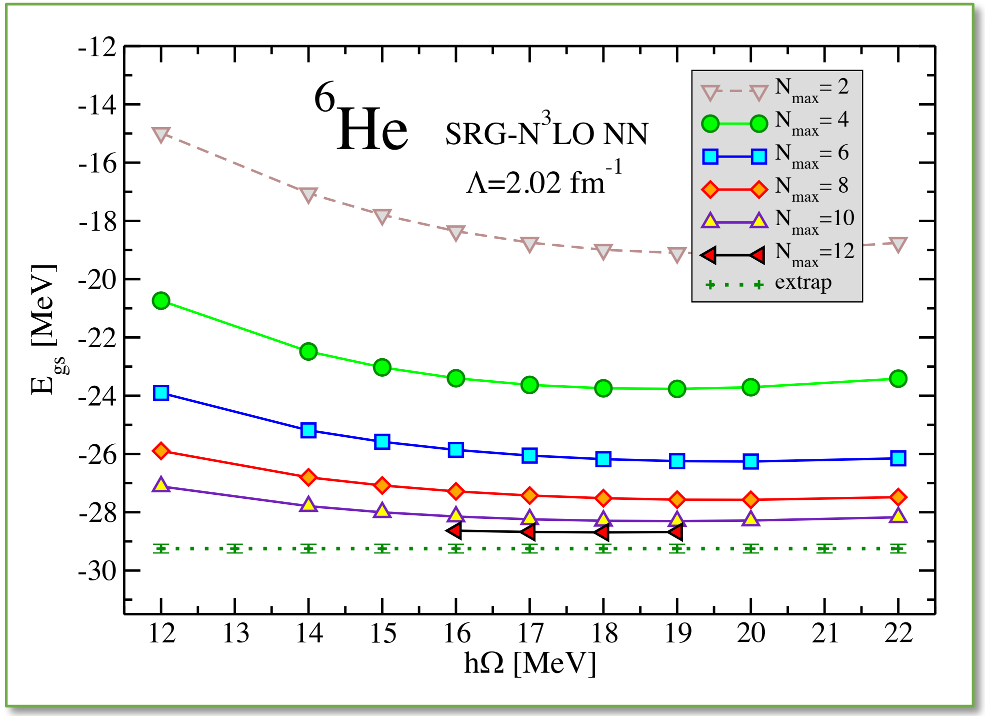
- Does inclusion of the MEC explain g_A quenching?
- In light nuclei correlations present in *ab initio* (NCSM) wave functions explain almost all of the quenching compared to the standard shell model
  - MEC inclusion overall improves agreement with experiment
- The effect of the MEC inclusion is greater in heavier nuclei
- SRG evolved matrix elements used in coupled-cluster and IM-SRG calculations (up to ^{100}Sn)

Hollow symbols – GT
Filled symbols – GT+MEC
Both Hamiltonian and operators SRG evolved
Hamiltonian and current consistent parameters





NCSM calculations of ^{6}He g.s. energy



Dependence on:

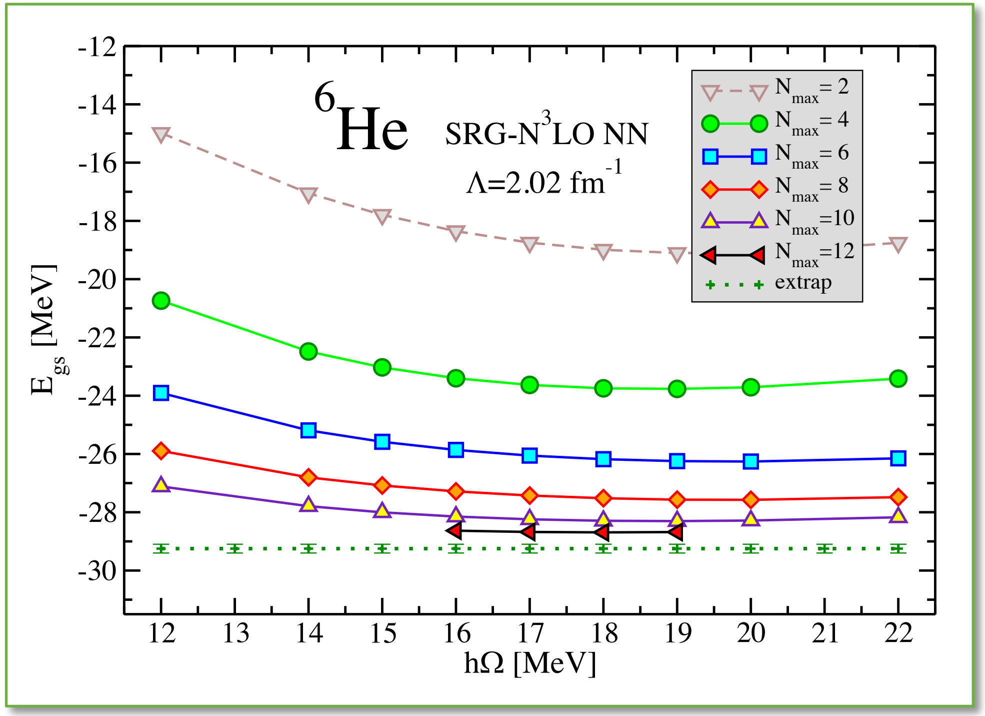
Basis size – N_{max}

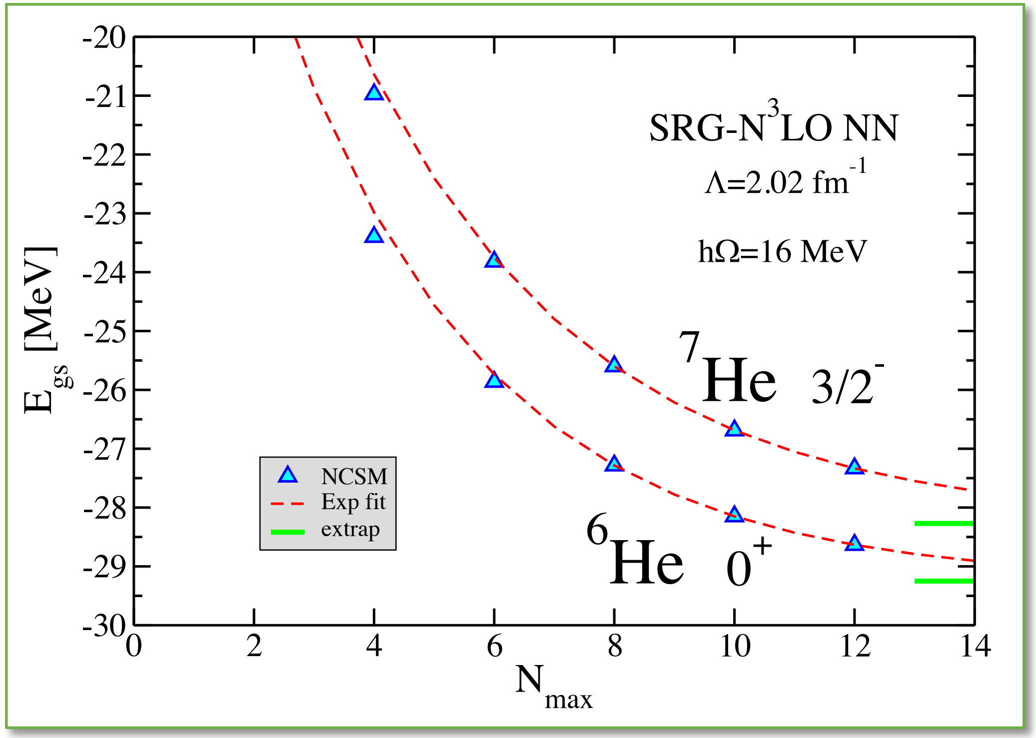
HO frequency – hΩ

$E_{g.s.}$ [MeV]	^{4}He	^{6}He
NCSM N_{max}=12	-28.05	-28.63
NCSM extrap.	-28.22(1)	-29.25(15)
Expt.	-28.30	-29.27

- Soft SRG evolved NN potential
  - ✓ N_{max} convergence OK
  - ✓ Extrapolation feasible

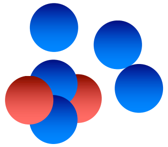
NCSM calculations of ^{6}He and ^{7}He g.s. energies





- ^{7}He unbound
  - Expt. E_{th}=+0.430(3) MeV: NCSM E_{th}≈ +1 MeV
  - Expt. width 0.182(5) MeV: **NCSM no information about the width**

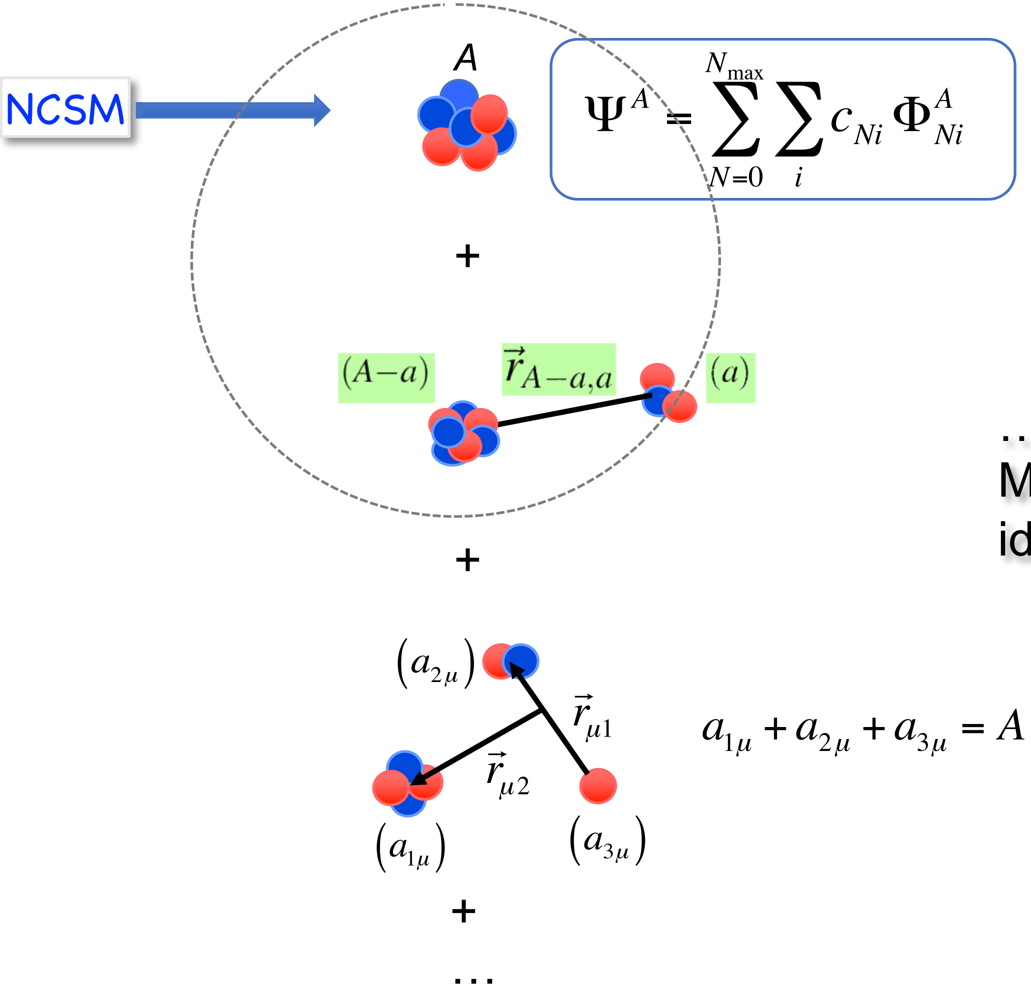
$E_{g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84



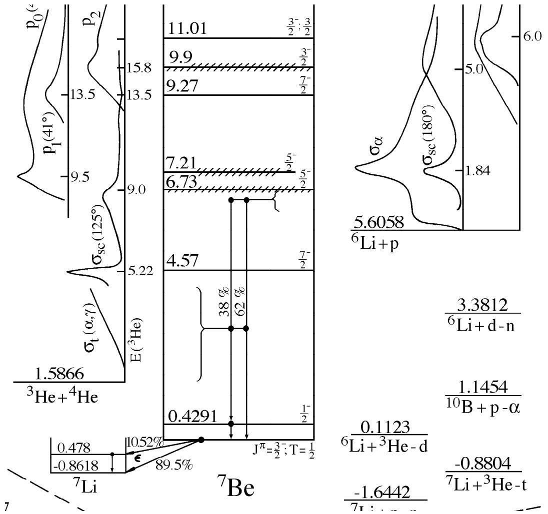
^{7}He unbound

Extending no-core shell model beyond bound states

Include more many nucleon correlations…



…using the Resonating Group Method (RGM) ideas

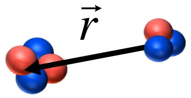


Unified approach to bound & continuum states; to nuclear structure & reactions

- No-core shell model (NCSM)
  - *A*-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - short- and medium range correlations
  - Bound-states, narrow resonances

NCSM

- NCSM with Resonating Group Method (NCSM/RGM)
  - cluster expansion, clusters described by NCSM
  - proper asymptotic behavior
  - long-range correlations



NCSM/RGM

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

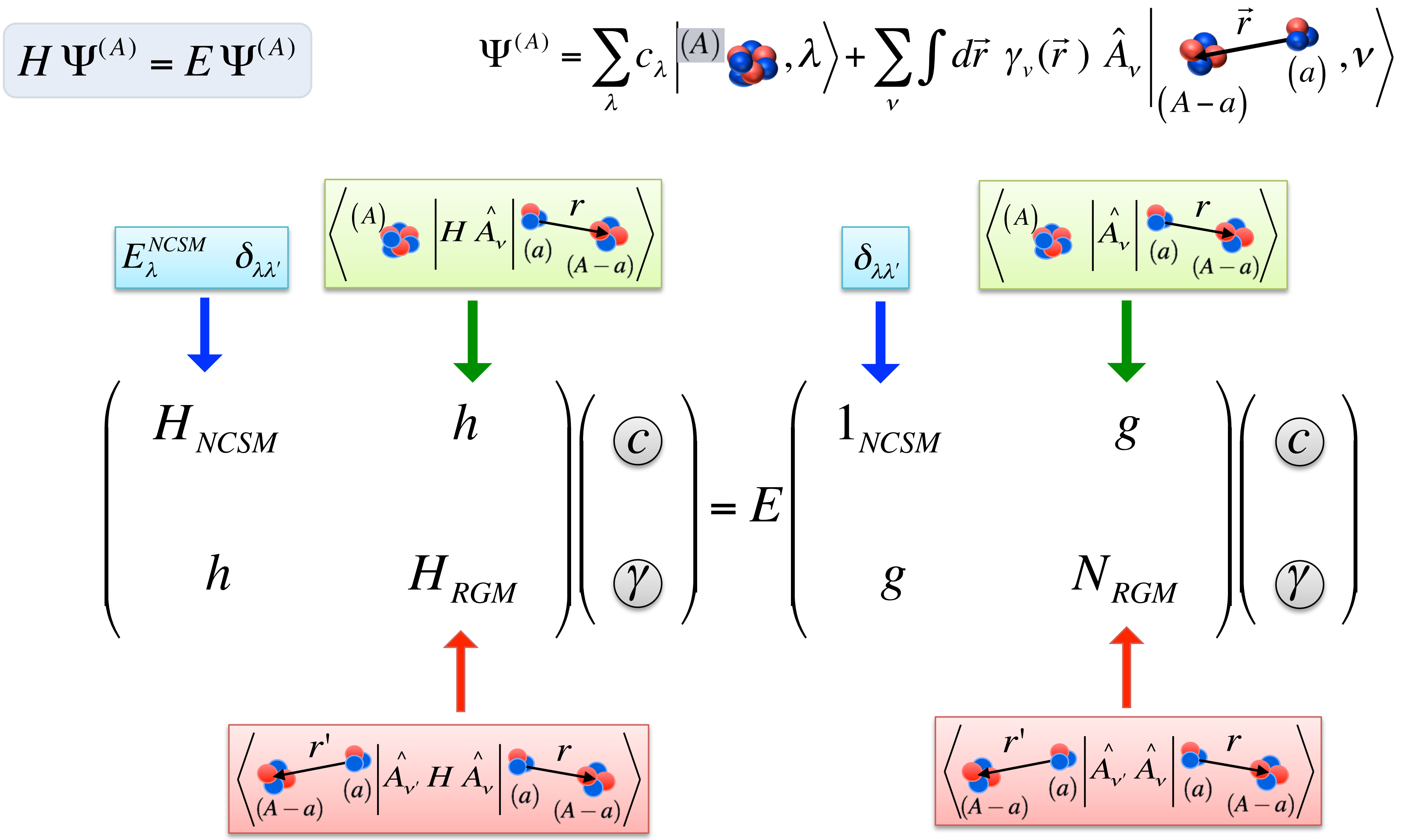
NCSMC

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

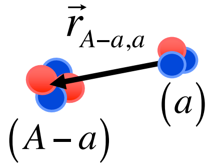
Unknowns

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

Coupled NCSMC equations



Binary cluster basis



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

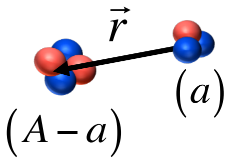
$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \hat{A}_\nu \left[\left(\underbrace{\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle}_{\text{Target}} \underbrace{\left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle}_{\text{Projectile}} \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi T)} \frac{g_\nu^{J^\pi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

- 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

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



$$, \nu \Big\rangle$$

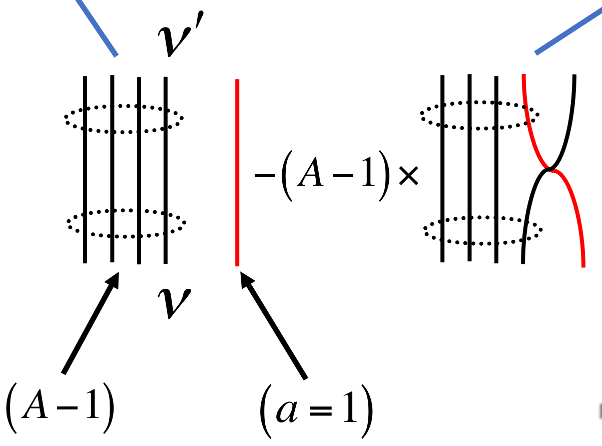
Norm kernel (Pauli principle): Single-nucleon projectile

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

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

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

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



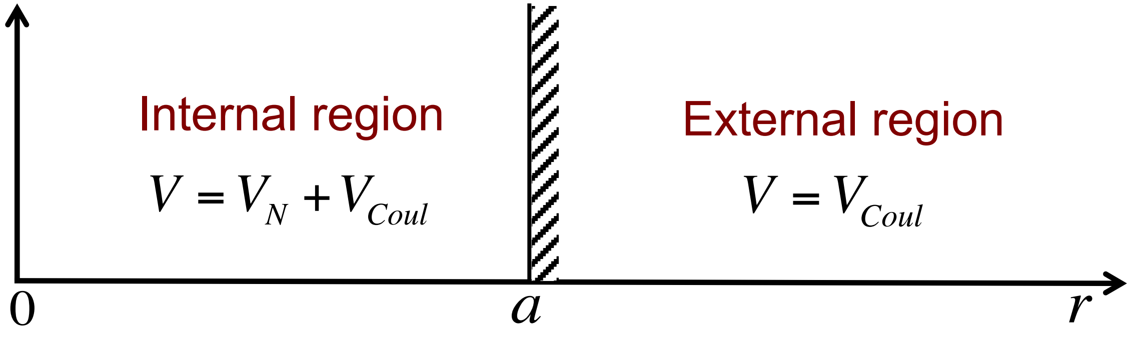
Exchange term:
Obtained in the model space!
(Many-body correction due to
the exchange part of the inter-cluster antisymmetrizer)

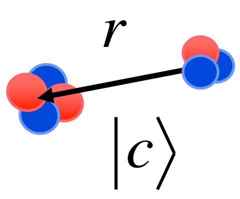
Trick #1 $$\frac{\delta(r - r_{A-a,a})}{r\, r_{A-a,a}} = \sum_{n} R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

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

Microscopic R-matrix theory on a Lagrange mesh – Coupled channels

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





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

Bound state $u_c(r) \sim C_c W(k_c r)$

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

Scattering matrix

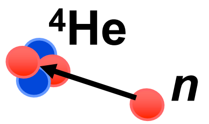
Lagrange basis associated with Lagrange mesh:

$$\{ax_n \in [0,a]\}$$

$$\int_0^1 g(x)dx \approx \sum_{n=1}^{N} \lambda_n g(x_n)$$

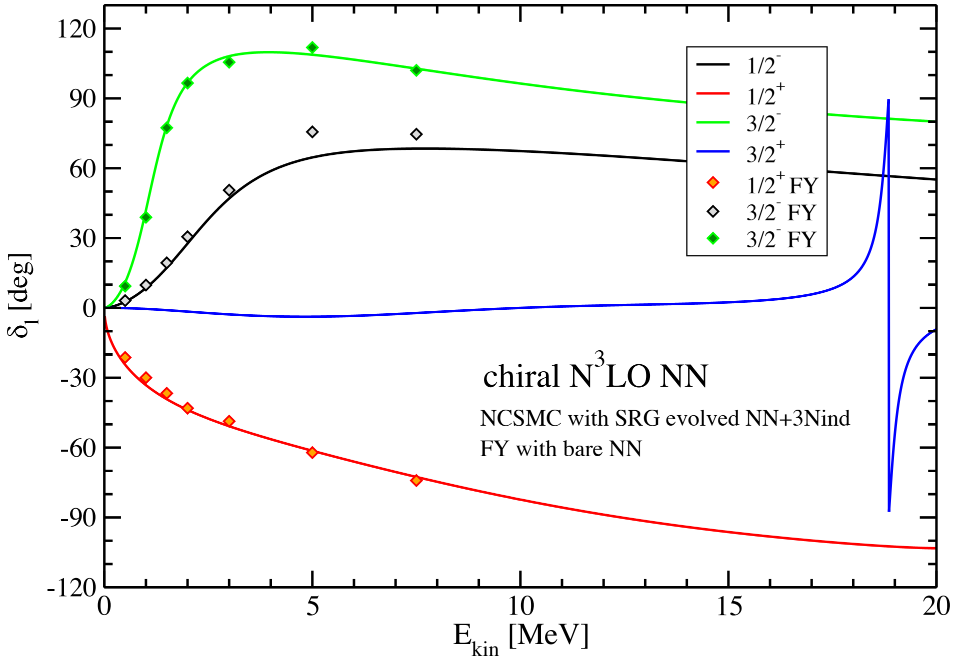
$$\int_0^a f_n(r) f_{n'}(r) dr \approx \delta_{nn'}$$

n-^{4}He scattering within NCSMC



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

chiral NN



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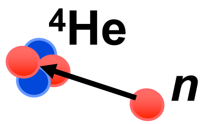
Phys. Scr. 00 (2016) 000000 (37pp)

Invited Comment

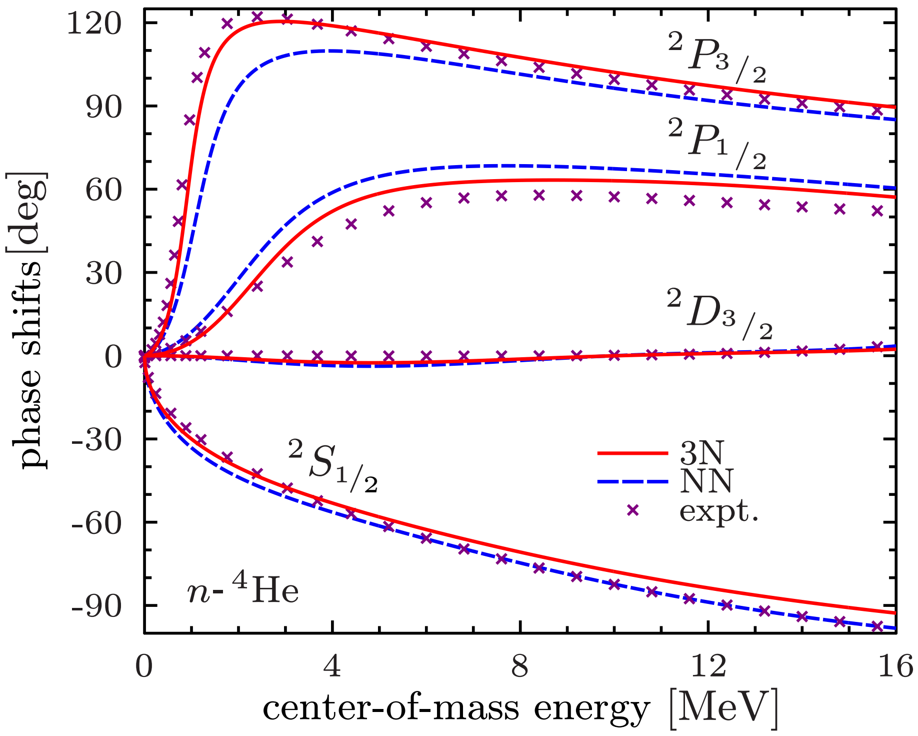
Unified *ab initio* approaches to nuclear structure and reactions

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

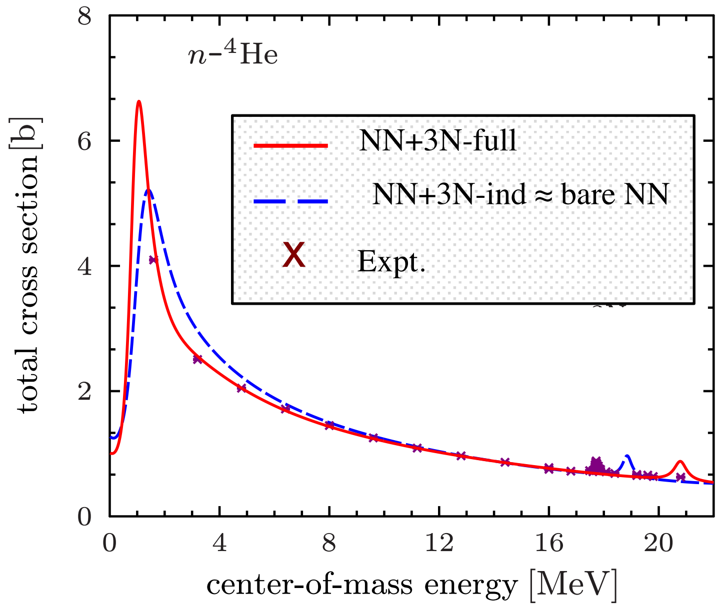
n-^{4}He scattering within NCSMC



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 $1/2^- \leftarrow\rightarrow 3/2^-$ splitting: Essential at low energies!

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,¶]

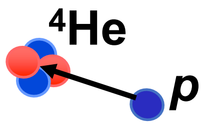
IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta
Phys. Scr. 00 (2016) 000000 (37pp)

Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

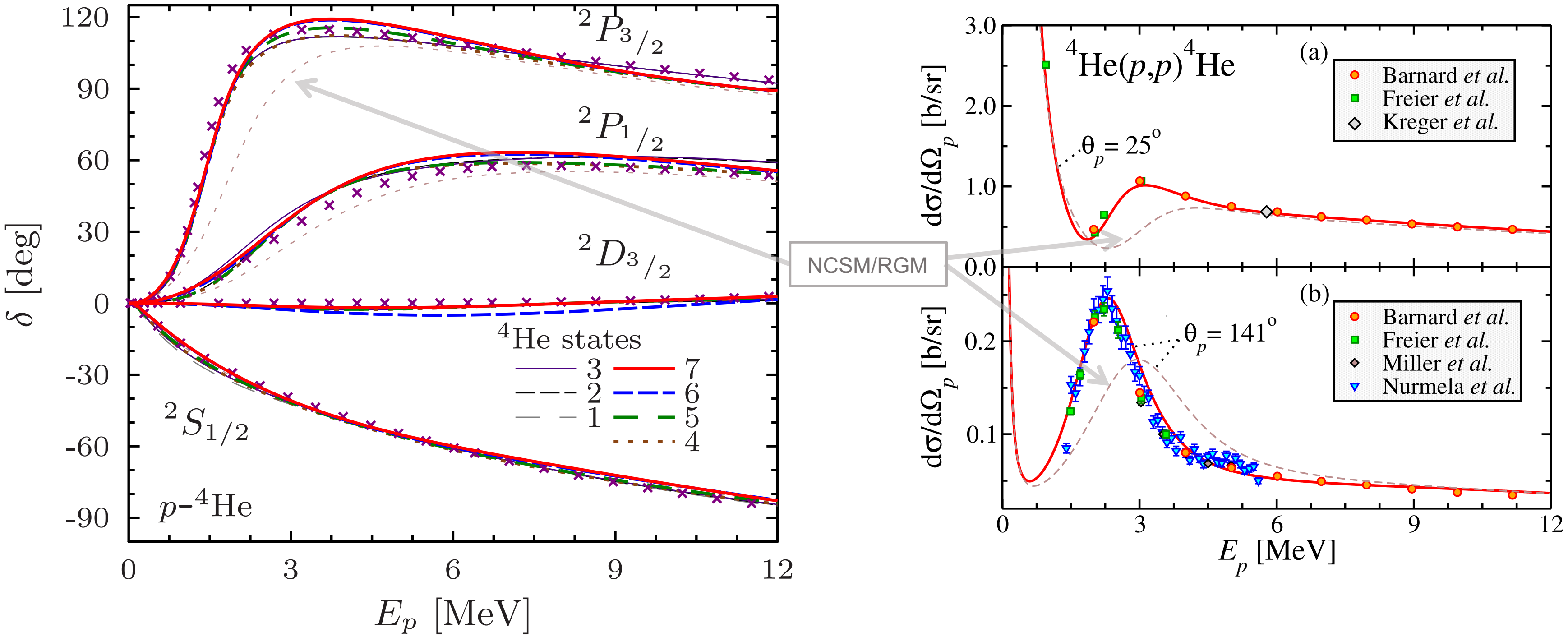
Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]

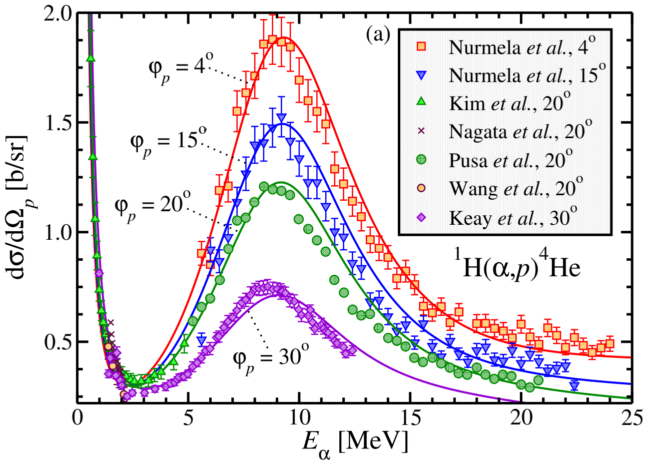
p-^{4}He scattering within NCSMC



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

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





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

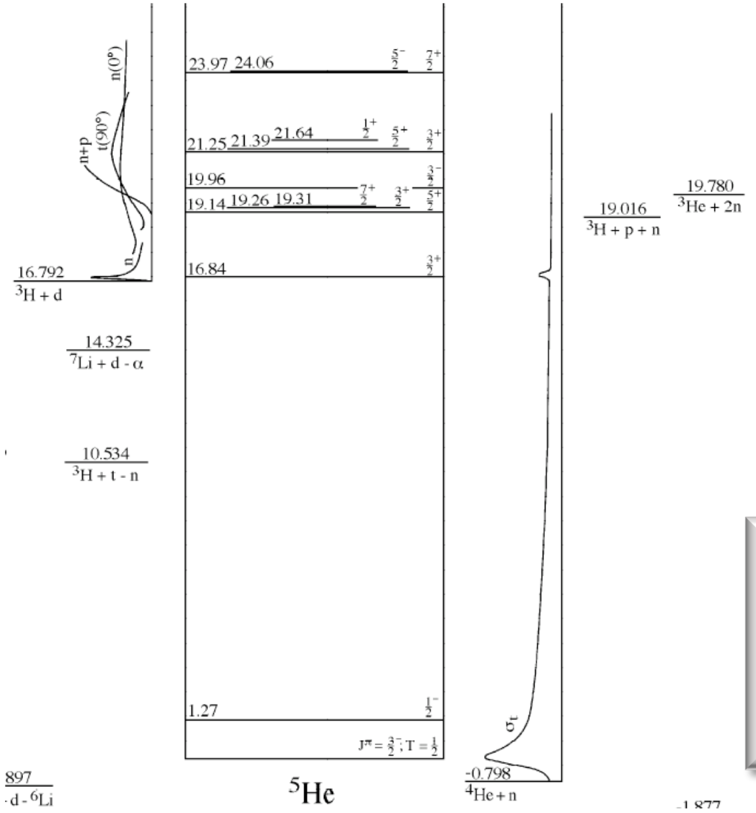
Predictive theory for elastic scattering and recoil of protons from ^{4}He

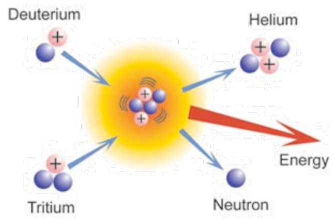
Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

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

Deuterium-Tritium fusion

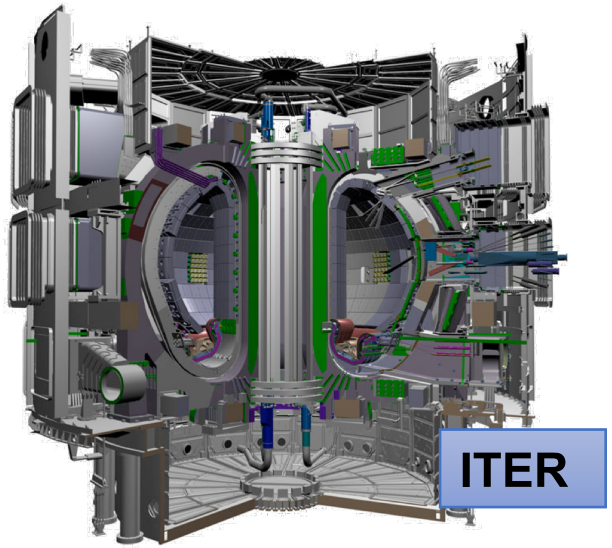
- The $d+{}^3H \rightarrow n+{}^4He$ reaction
  - The most promising for the production of fusion energy in the near future
  - Used to achieve inertial-confinement (laser-induced) fusion at NIF, and magnetic-confinement fusion at ITER
  - With its mirror reaction, ${}^3He(d,p){}^4He$, important for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



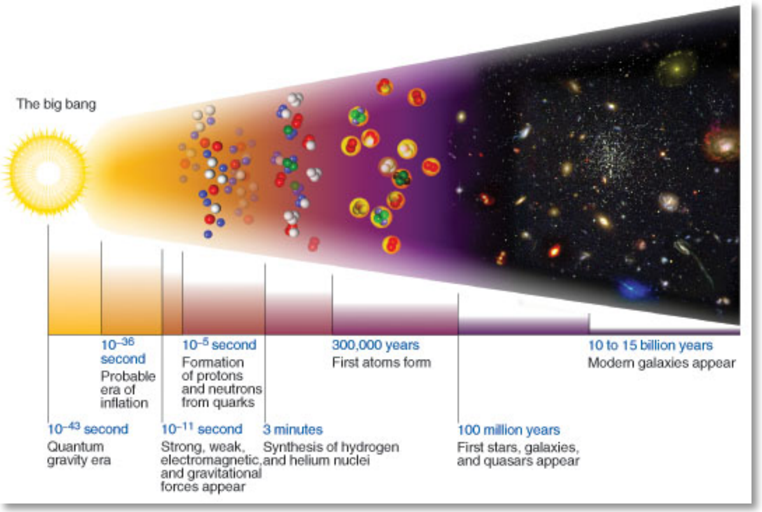


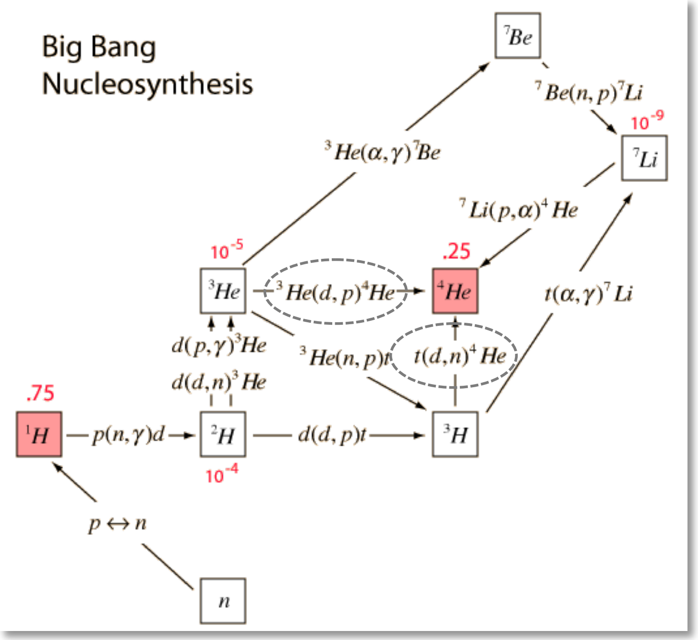
Resonance at E_{cm} =48 keV (E_d=105 keV) in the J=3/2$^+$ channel
Cross section at the peak: 4.88 b

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

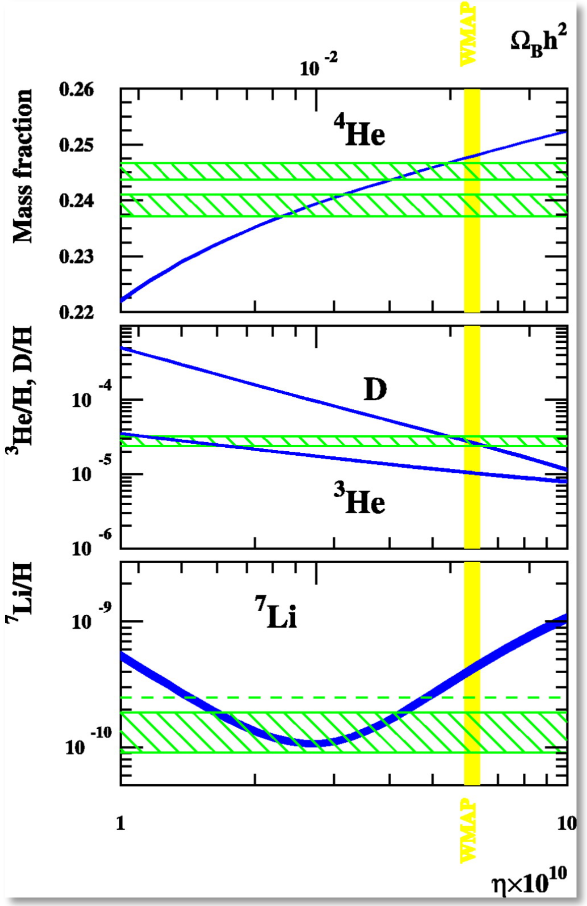


Big Bang nucleosynthesis



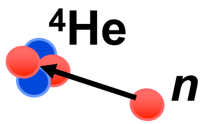


Key reactions



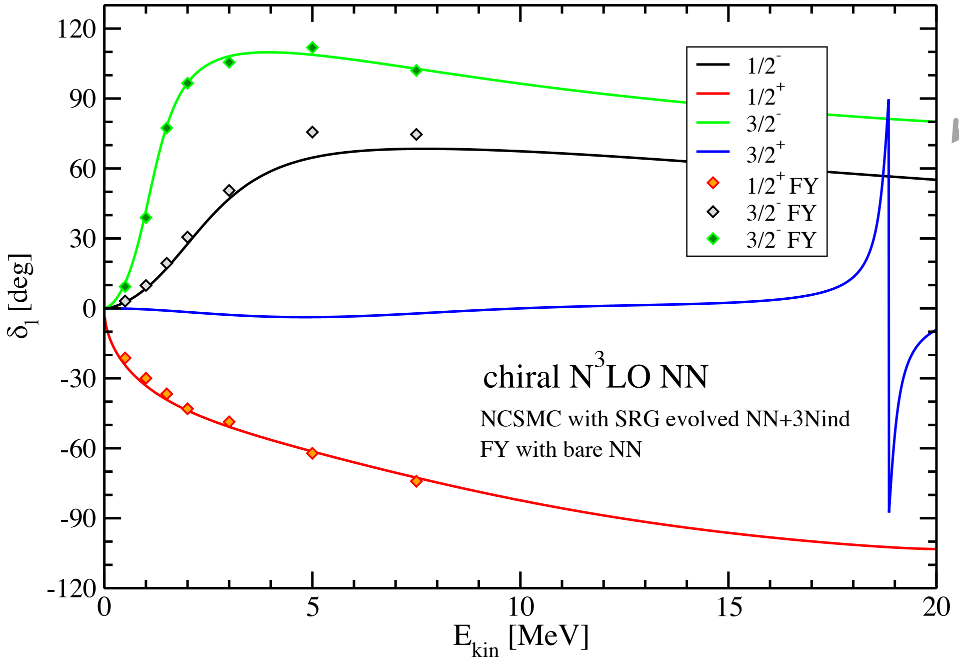
^{7}Li puzzle

n-^{4}He scattering and ^{3}H+d fusion within NCSMC



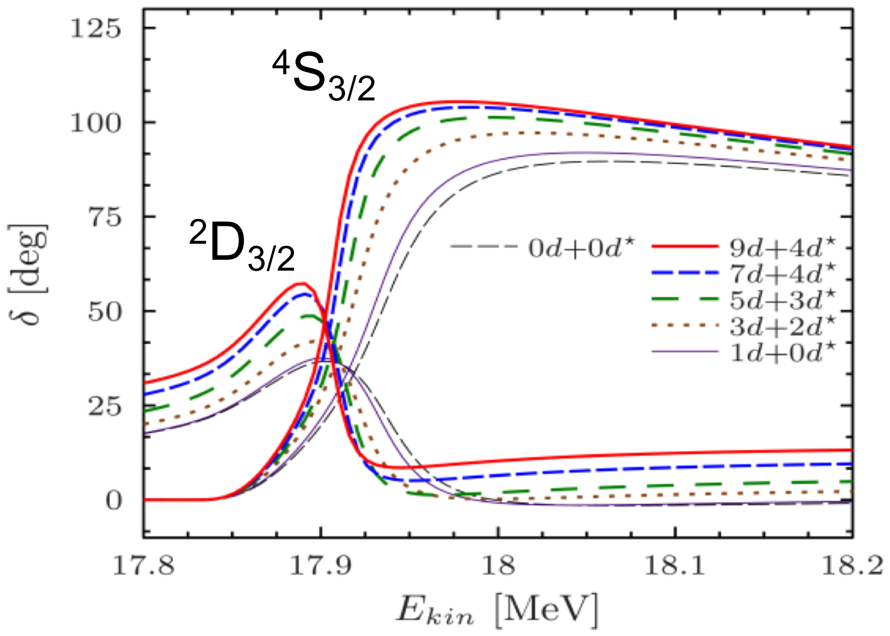
n-^{4}He scattering phase-shifts for chiral NN

^{4}He+n



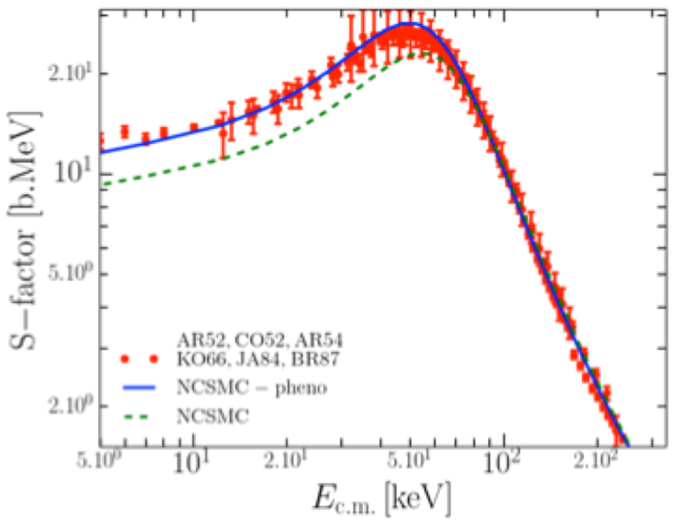
FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

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



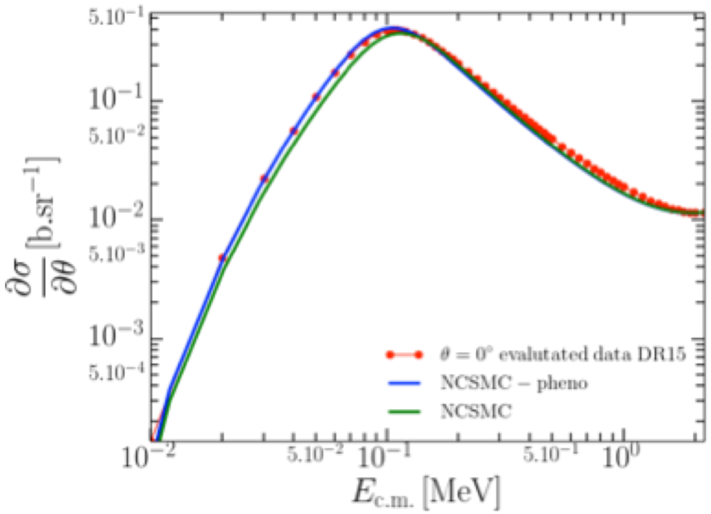
The *d*-^{3}H fusion takes place through a transition of *d*+^{3}H is *S*-wave to *n*+^{4}He in *D*-wave: Importance of the **tensor and 3N force**

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



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

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

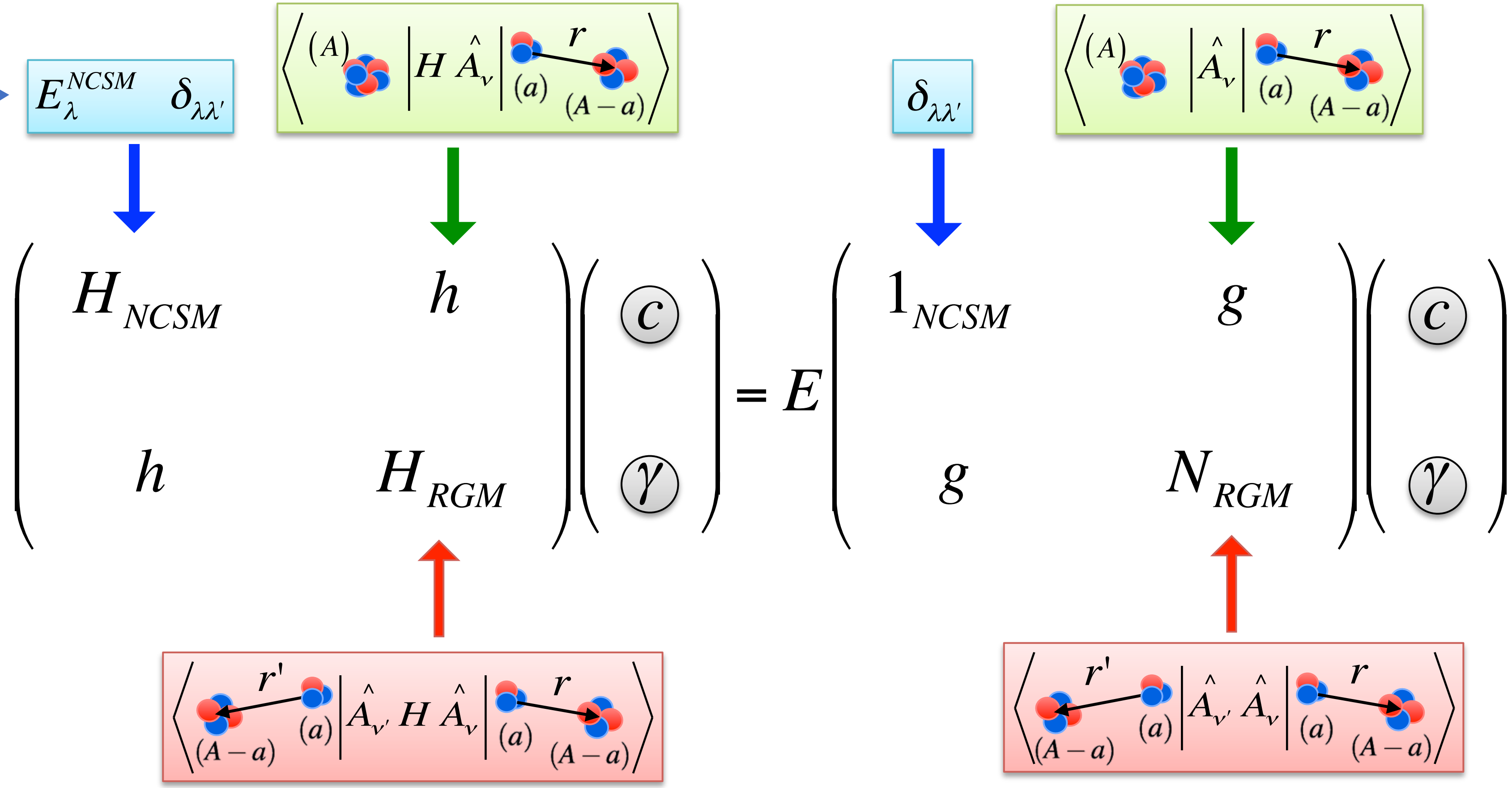


NCSMC phenomenology

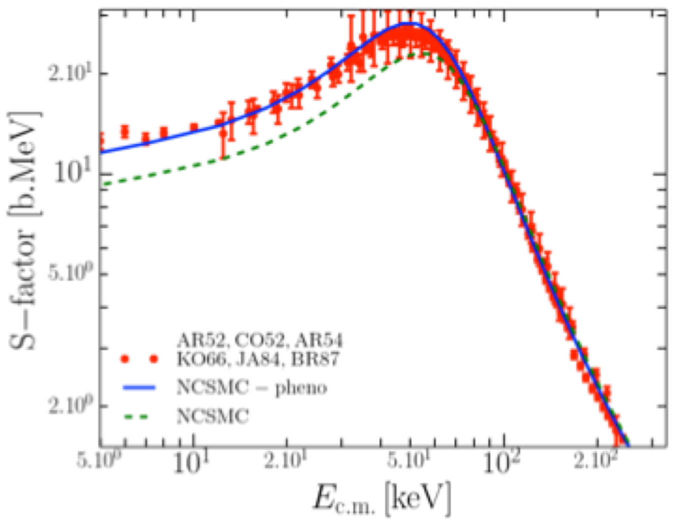
$$H\,\Psi^{(A)} = E\,\Psi^{(A)} \qquad \Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| (A), \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r})\; \hat{A}_{\nu} \left| (A-a)\; \vec{r}\; (a), \nu \right\rangle$$

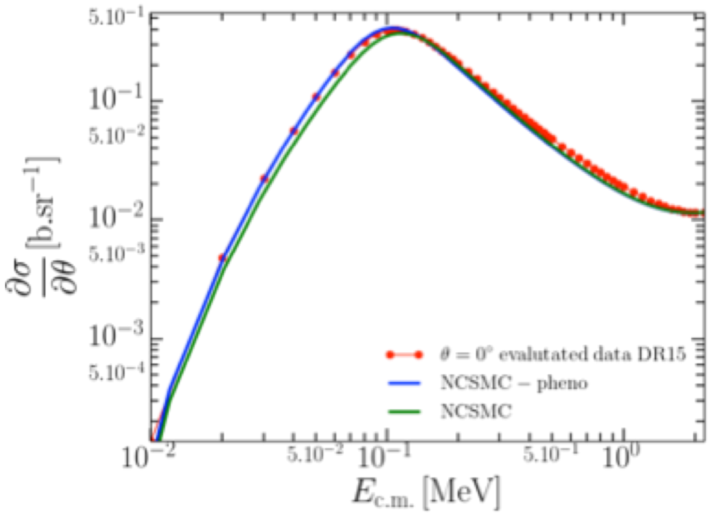
E_{λ}^{NCSM} energies treated as adjustable parameters

Cluster excitation energies set to experimental values



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





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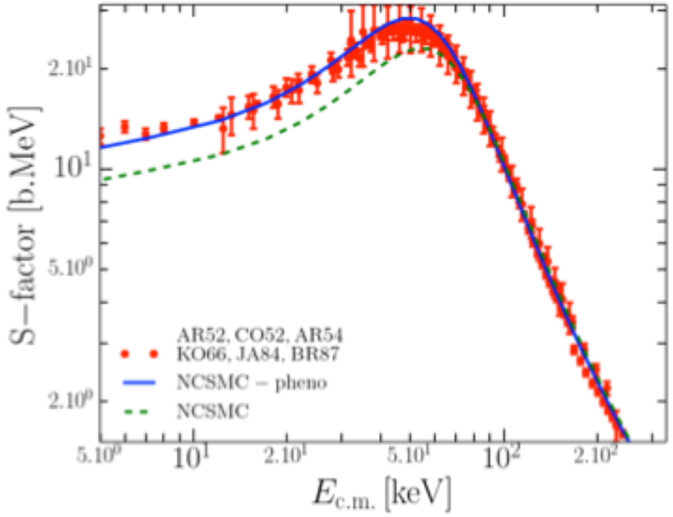
***Ab initio* predictions for *polarized* DT thermonuclear fusion**
arXiv:1803.11378
Guillaume Hupin[1,2,3], Sofia Quaglioni[3] and Petr Navrátil[4]

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

Polarized fusion

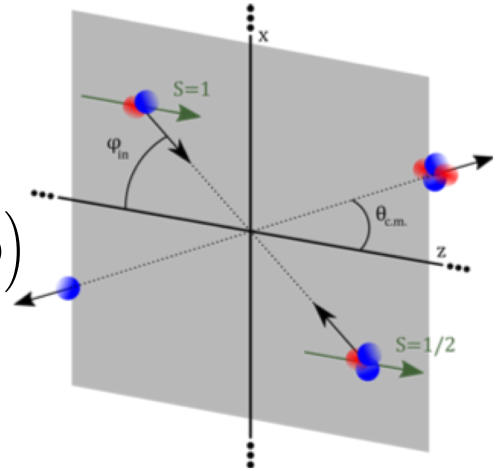


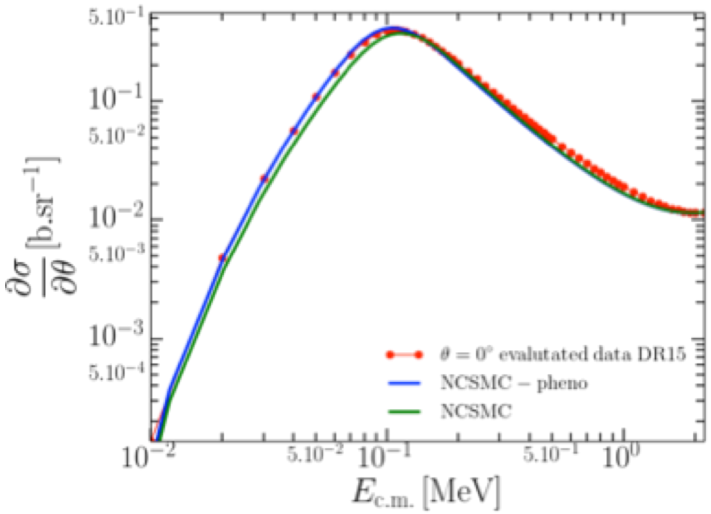
$$S(E) = E\sigma(E)\exp[2\pi\eta(E)]$$

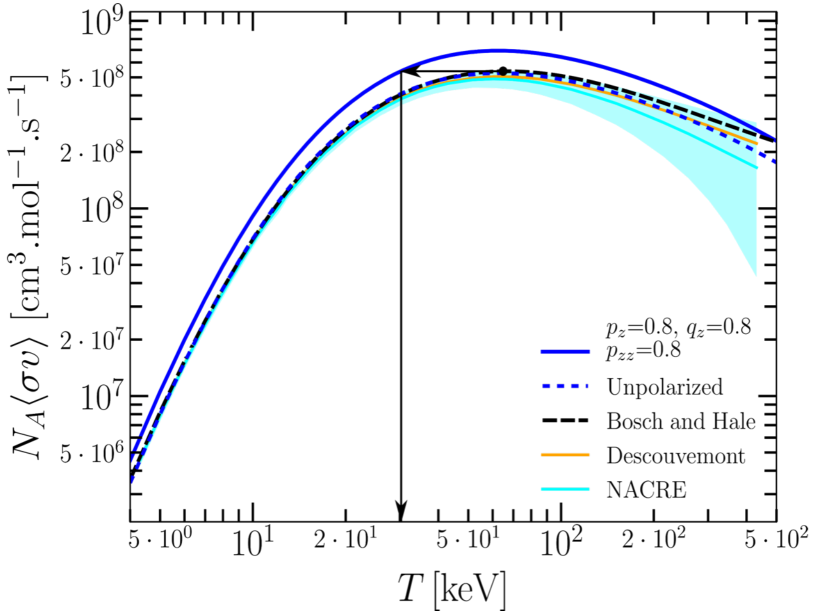
$$\eta(E) = Z_{A-a}Z_a e^2 / \hbar v_{A-a,a}$$

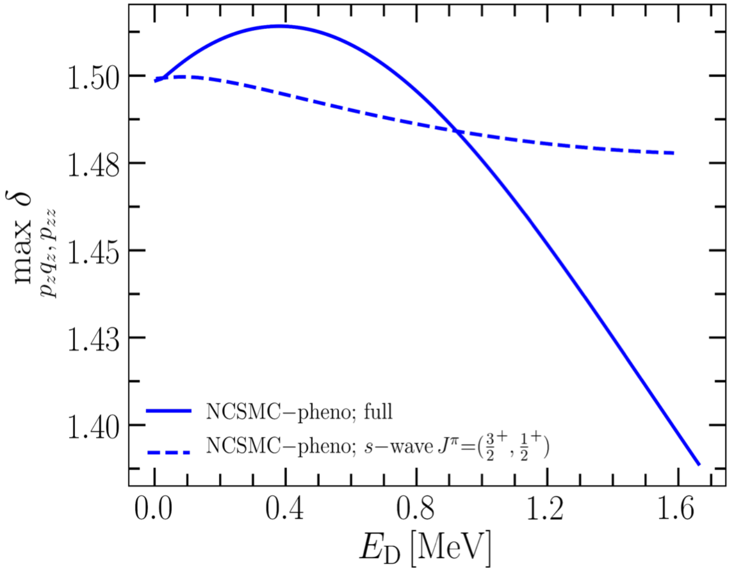
$$\frac{\partial\sigma_{pol}}{\partial\Omega_{c.m.}}(\theta_{\text{c.m.}}) = \frac{\partial\sigma_{unpol}}{\partial\Omega_{c.m.}}(\theta_{\text{c.m.}})\left(1 + \frac{1}{2}p_{zz}A_{zz}^{(b)}(\theta_{\text{c.m.}}) + \frac{3}{2}p_z q_z C_{z,z}(\theta_{\text{c.m.}})\right)$$

$$\langle\sigma v\rangle = \sqrt{\frac{8}{\pi\mu(k_bT)^3}}\int_0^\infty S(E)\ exp\left(-\frac{E}{k_bT} - \sqrt{\frac{E_g}{E}}\right)dE,$$









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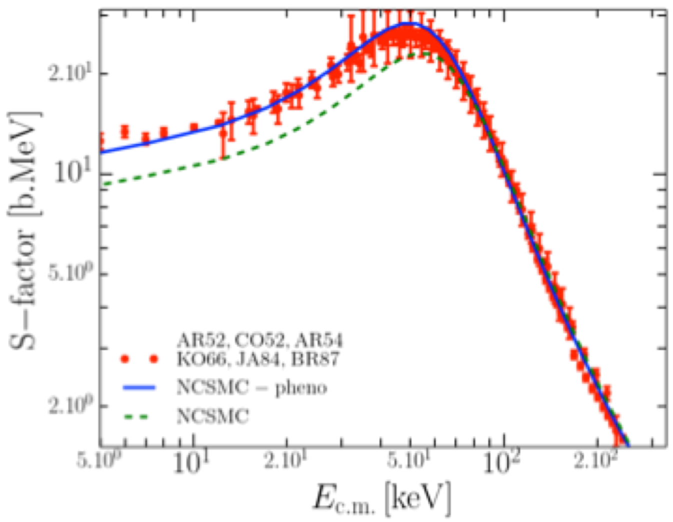

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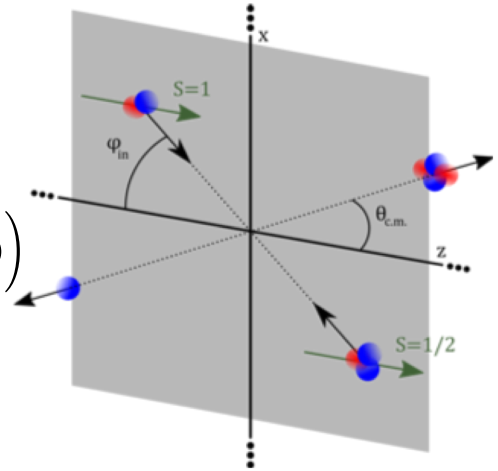
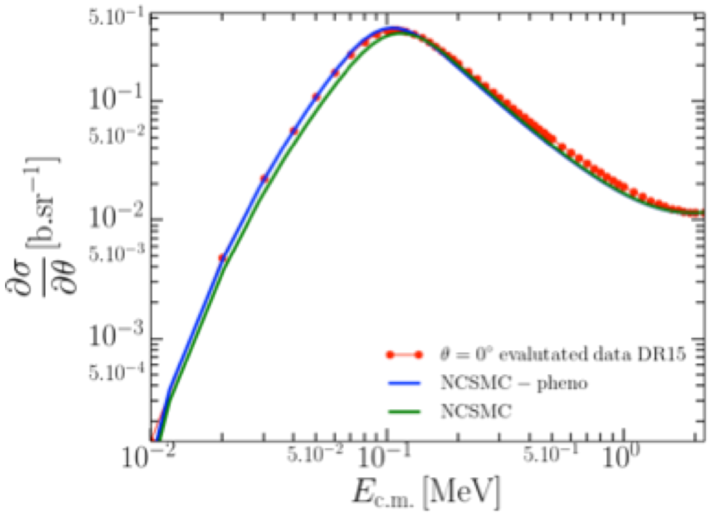
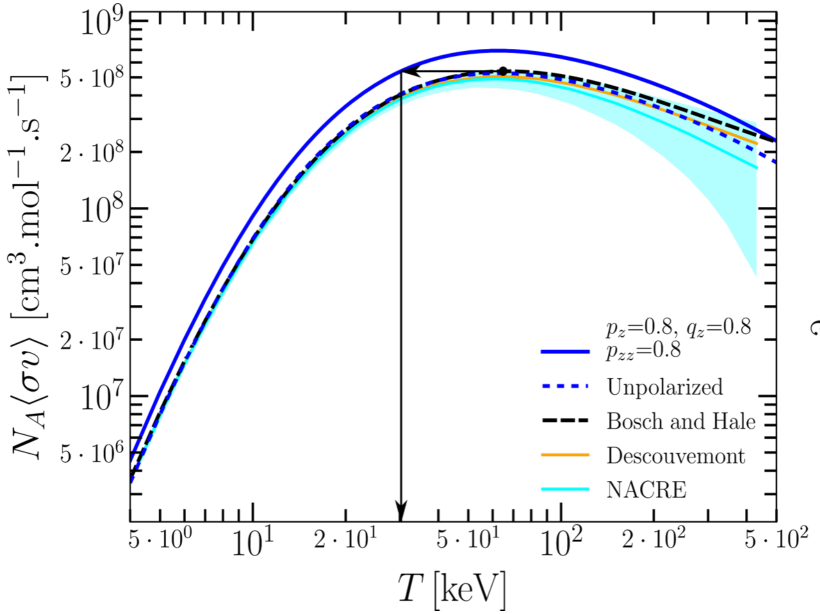
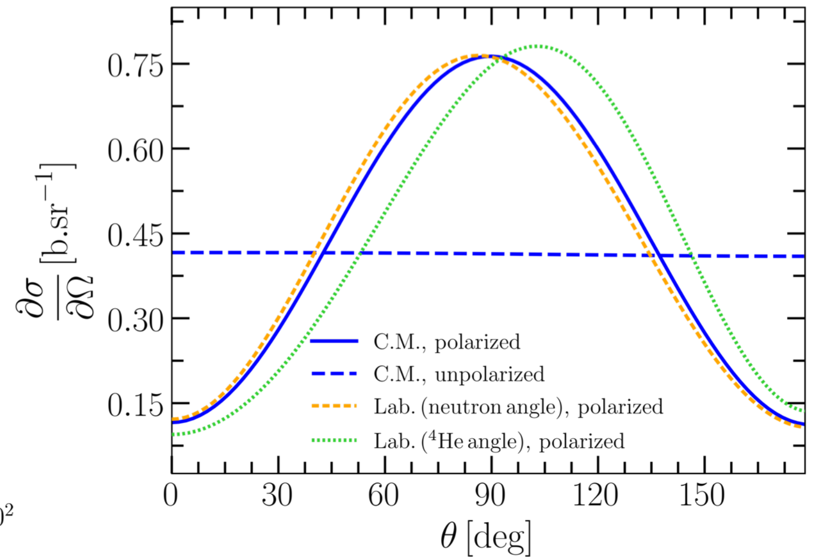
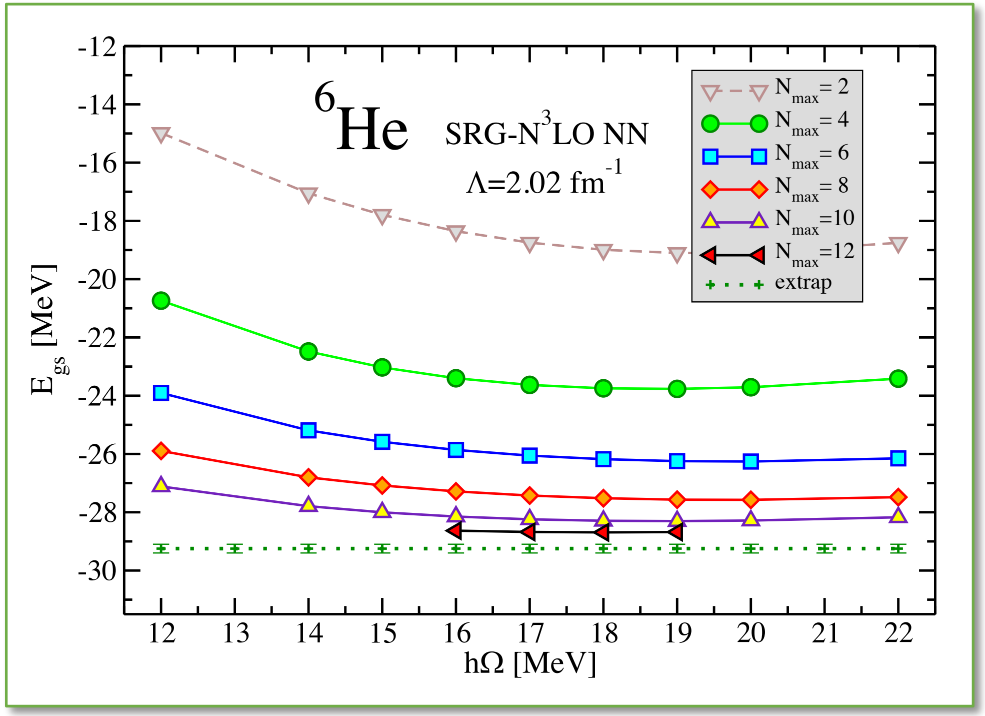


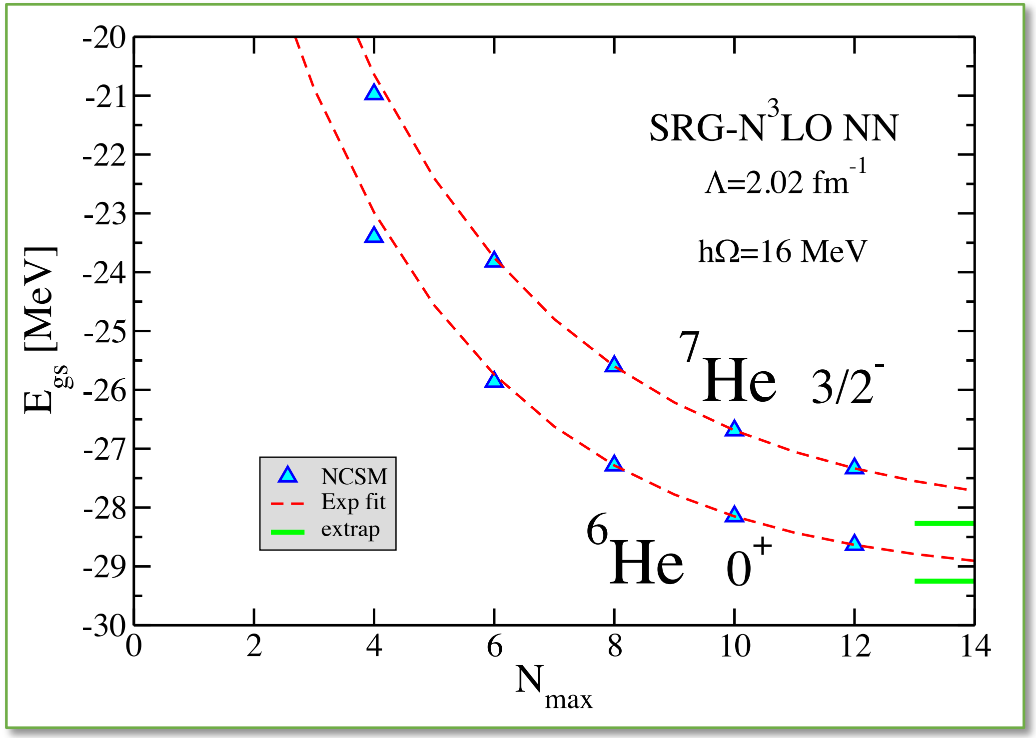






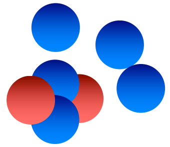
NCSM calculations of ^{6}He and ^{7}He g.s. energies





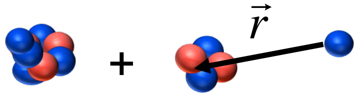
- ^{7}He unbound
  - Expt. E_{th}=+0.430(3) MeV: NCSM $E_{th}\approx$ +1 MeV
  - Expt. width 0.182(5) MeV: **NCSM no information about the width**

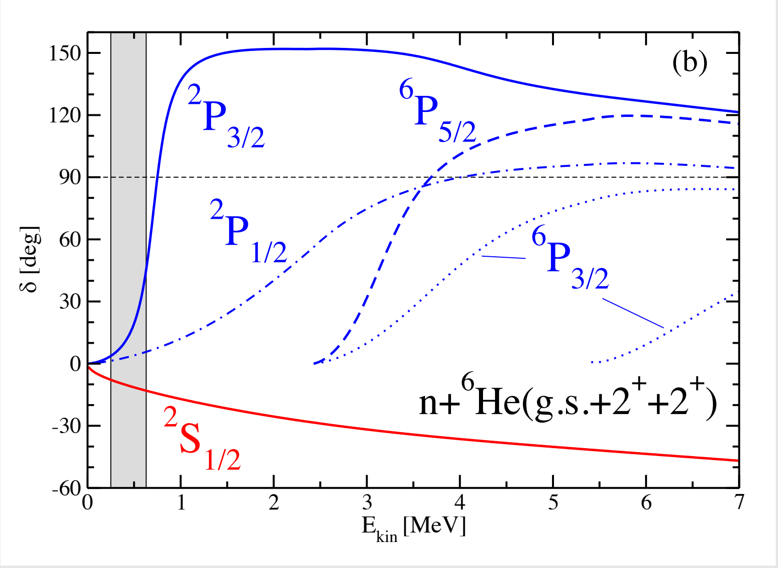
$E_{g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84



^{7}He unbound

NCSM with continuum: ^{7}He ⟷ ^{6}He+*n*





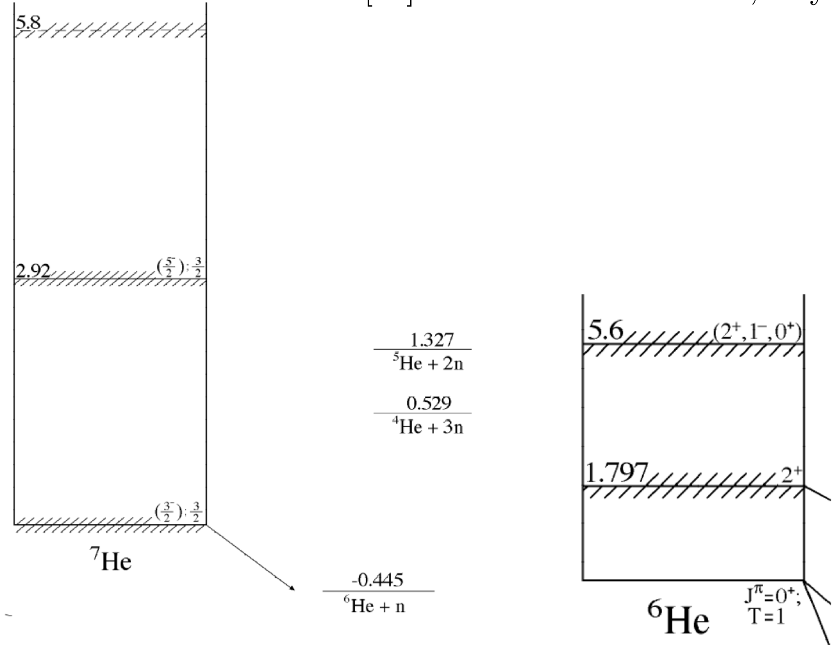
J^π	experiment			NCSMC	
	E_R	Γ	Ref.	E_R	Γ
$3/2^-$	0.430(3)	0.182(5)	[2]	0.71	0.30
$5/2^-$	3.35(10)	1.99(17)	[40]	3.13	1.07
$1/2^-$	3.03(10)	2	[11]	2.39	2.89
	3.53	10	[15]		
	1.0(1)	0.75(8)	[5]		

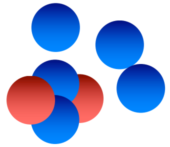
[11] A. H. Wuosmaa *et al.*, Phys. Rev. C **72**, 061301 (2005).

Experimental controversy:
Existence of low-lying 1/2$^-$ state
… not seen in these calculations

$$\Gamma = \frac{2}{\partial\delta(E_{kin})/\partial E_{kin}}\Bigg|_{E_{kin}=E_R}$$

NCSMC
with three ^{6}He states
and ten ^{7}He eigenstates
More **7-nucleon correlations**
Fewer ^{6}He-core states needed



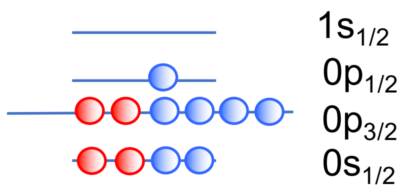


^{7}He unbound

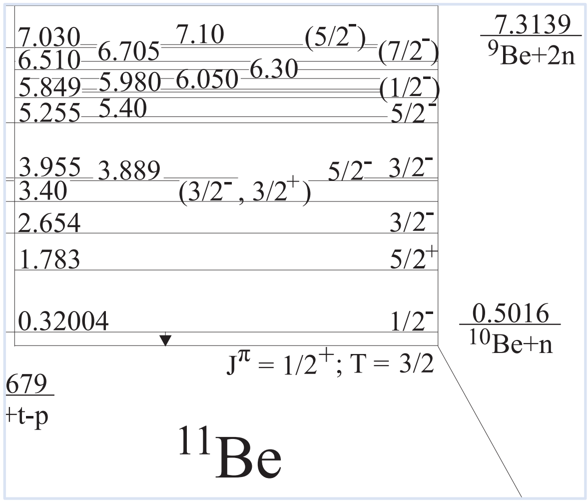
S. Baroni, P. N., and S. Quaglioni, PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

Neutron-rich halo nucleus ^{11}Be

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



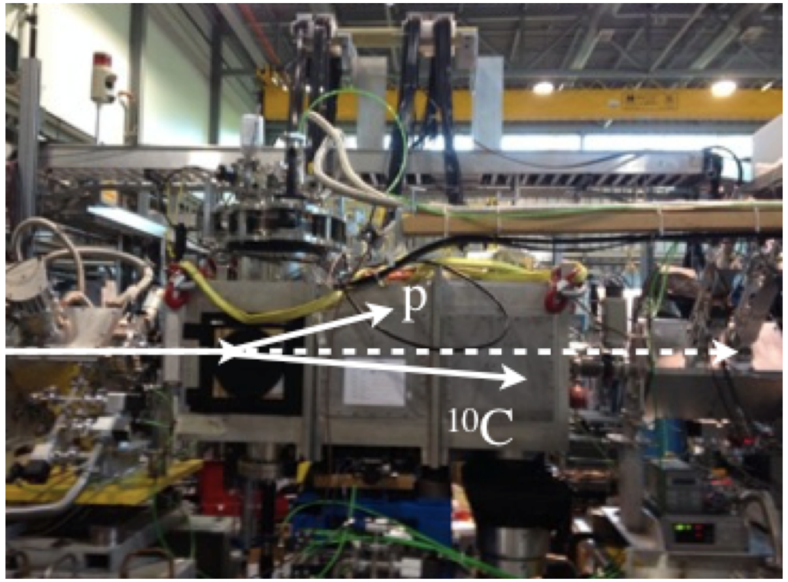
- Can we describe ^{11}Be in *ab initio* calculations?
  - Continuum must be included
  - Does the 3N interaction play a role in the parity inversion?

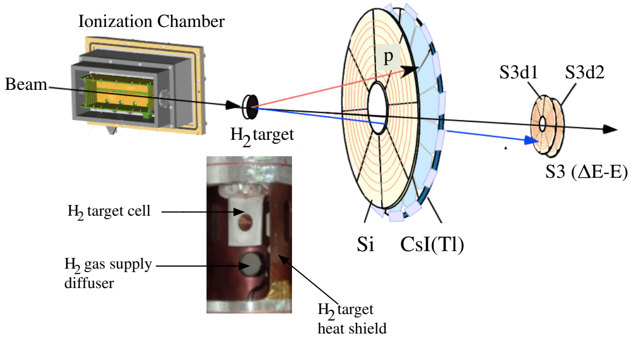


$^{10}C(p,p)$ @ IRIS with solid H_2 target

- 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

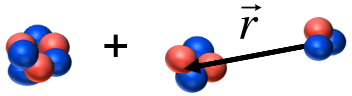




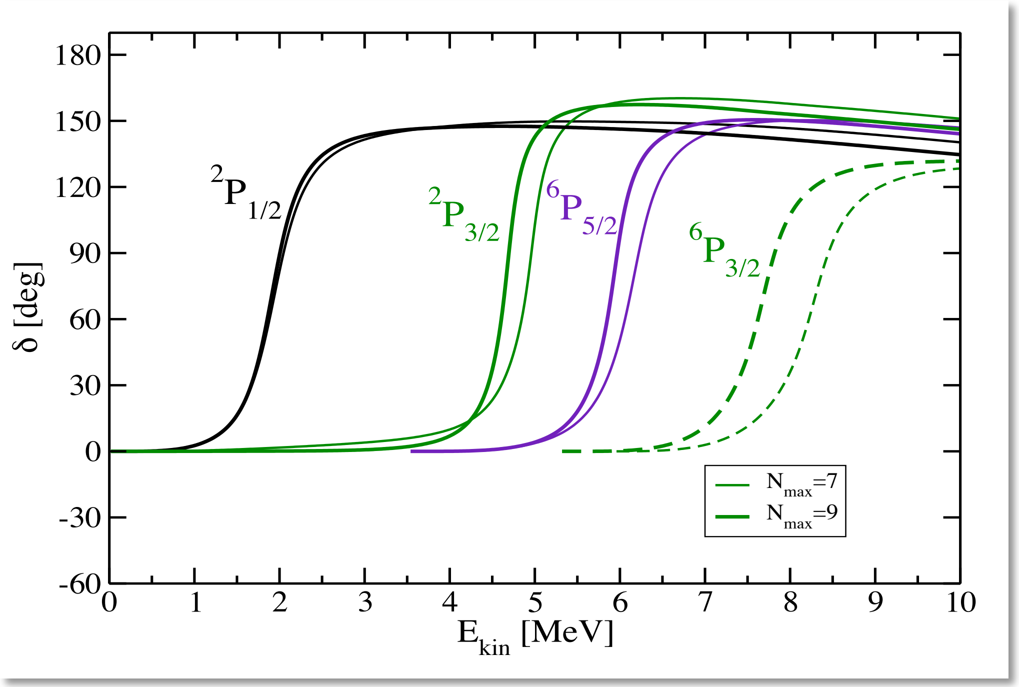
IRIS collaboration:
A. Kumar, R. Kanungo, A. Sanetullaev *et al.*

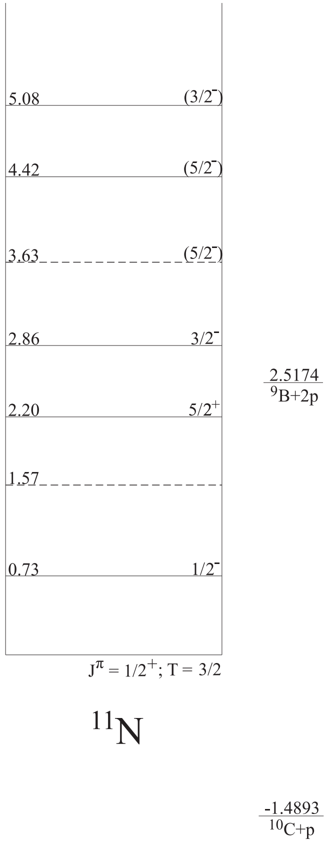
p+^{10}C scattering: structure of ^{11}N resonances

- NCSMC calculations with **chiral NN+3N** (N^{3}LO NN+N^{2}LO 3NF400, NNLOsat)
  - 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





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

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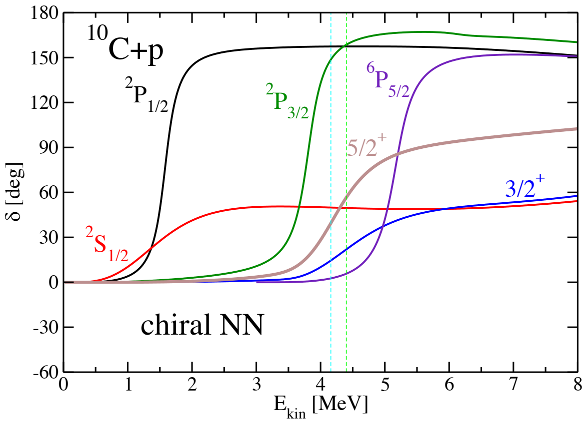

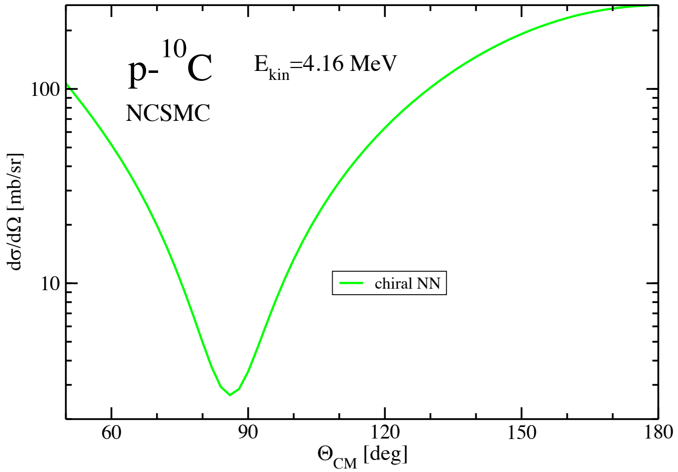

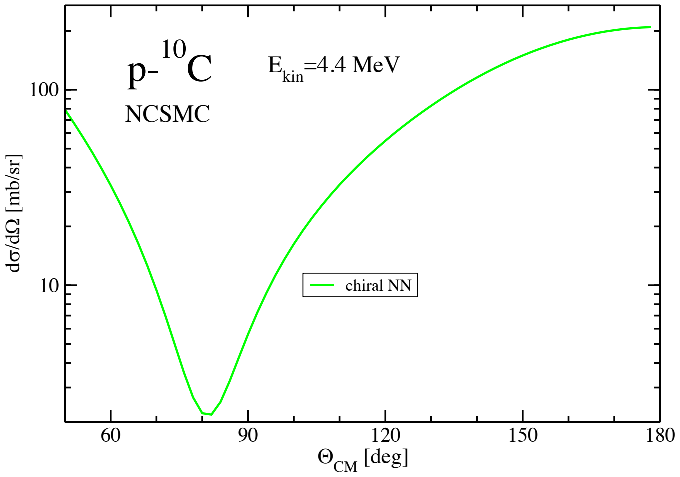

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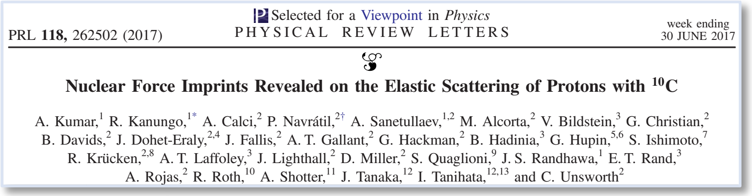
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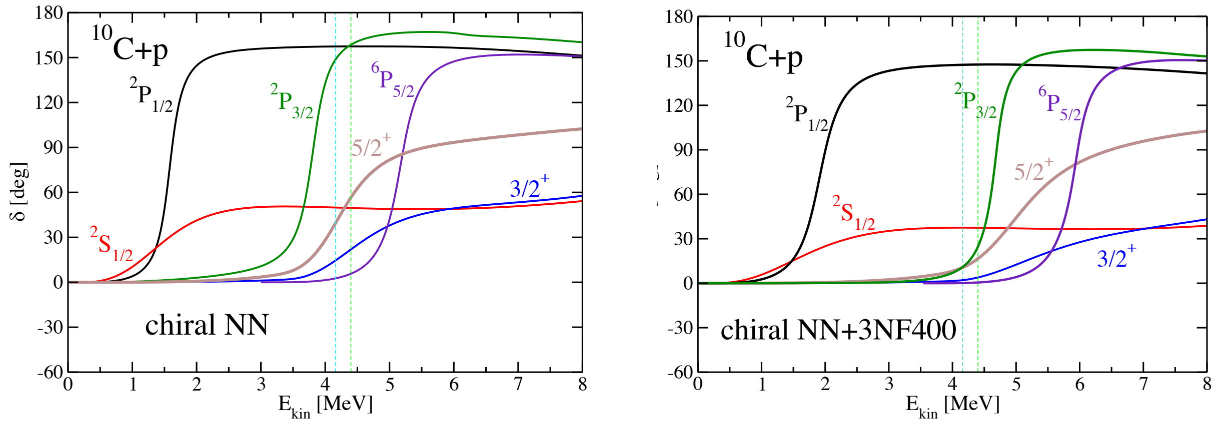

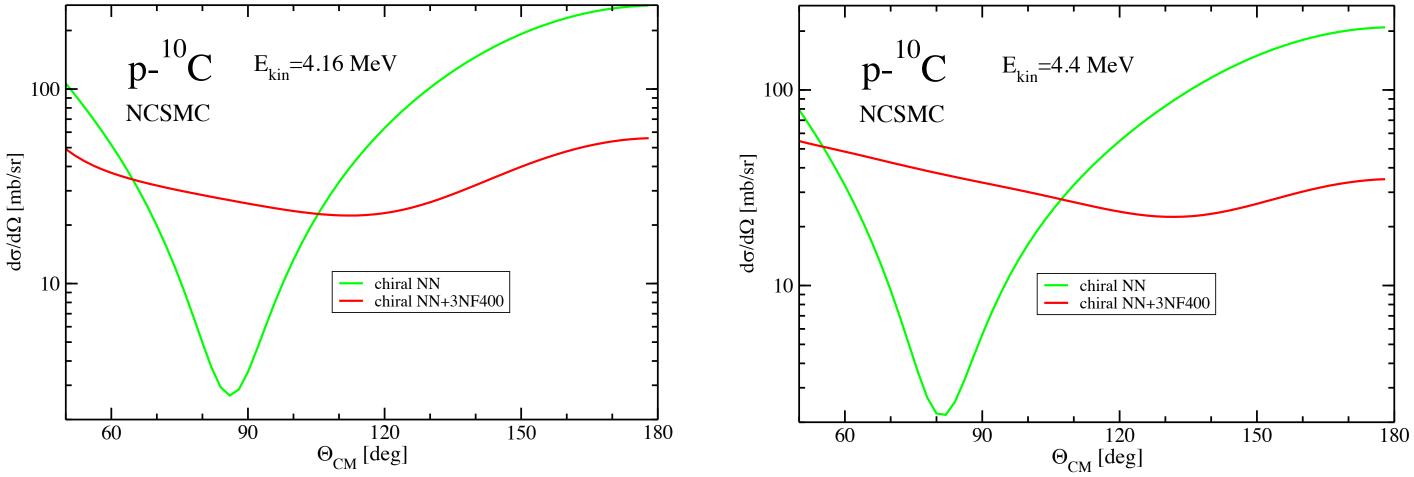

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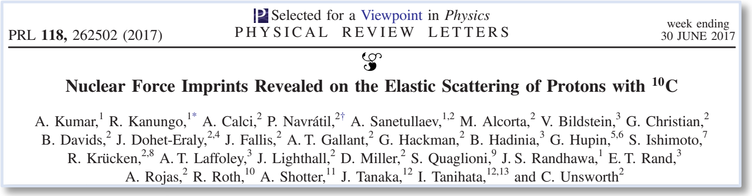
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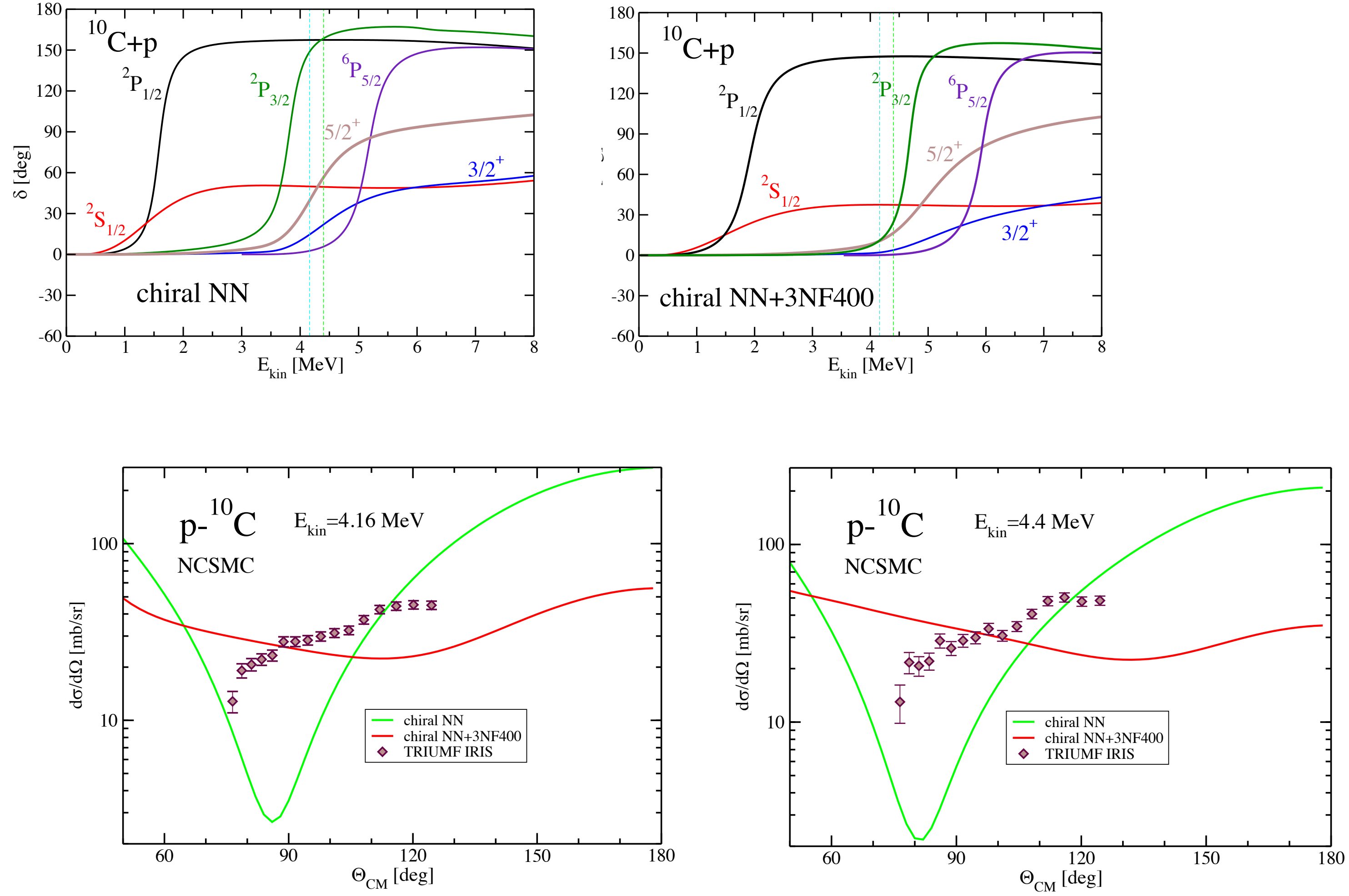
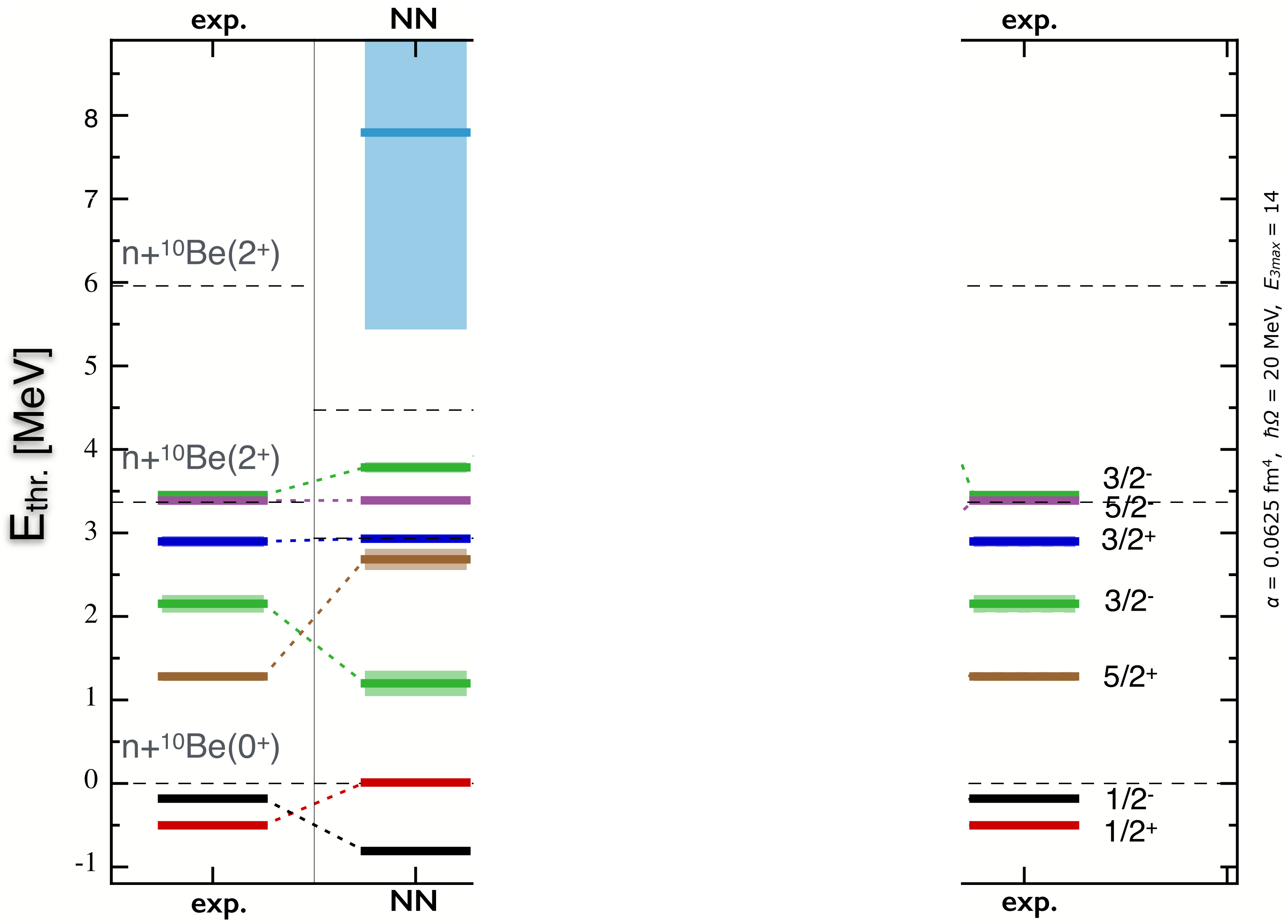


^{11}Be within NCSMC: Discrimination among chiral nuclear forces



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

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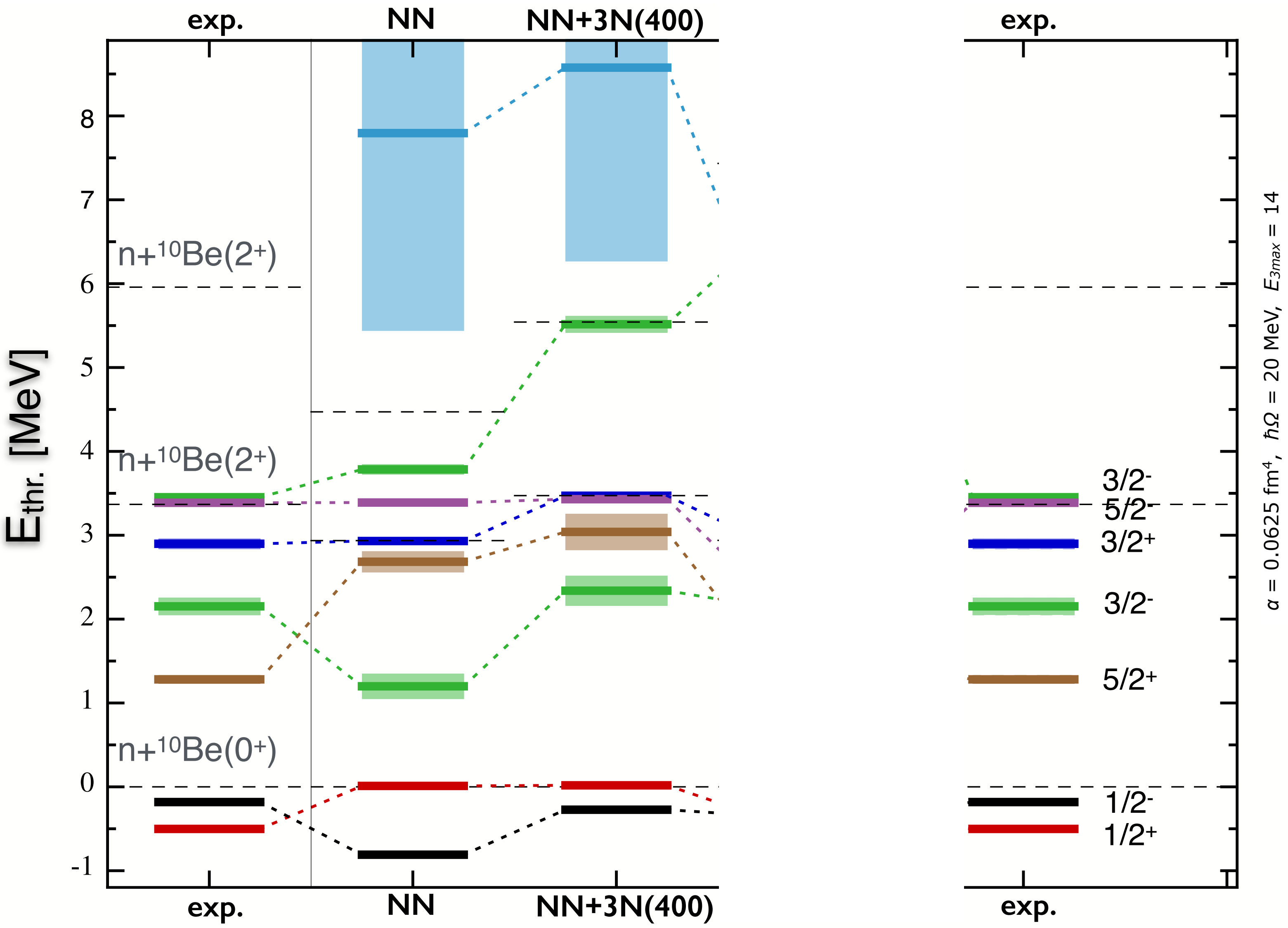

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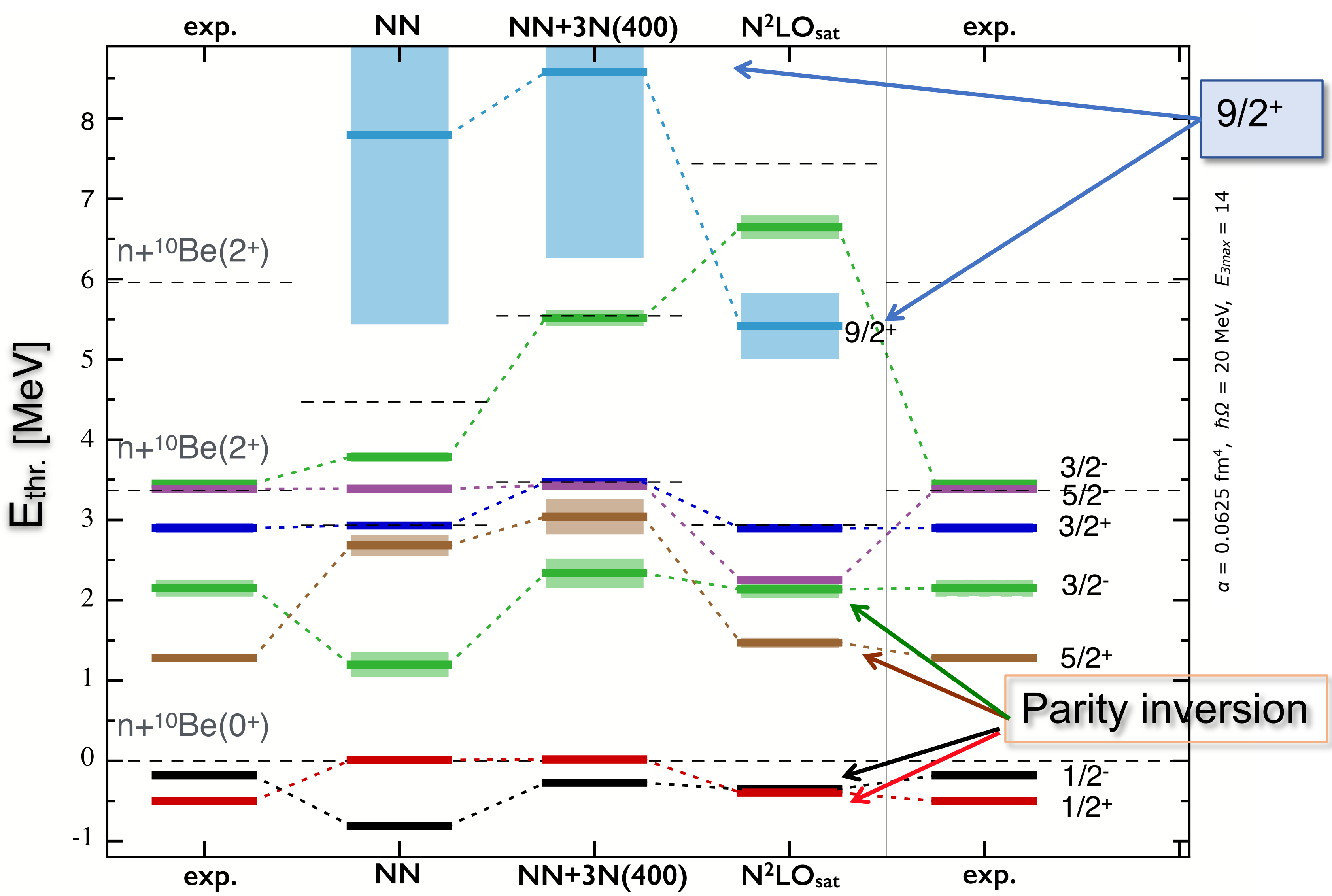

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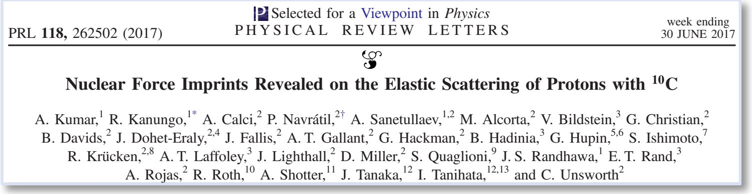
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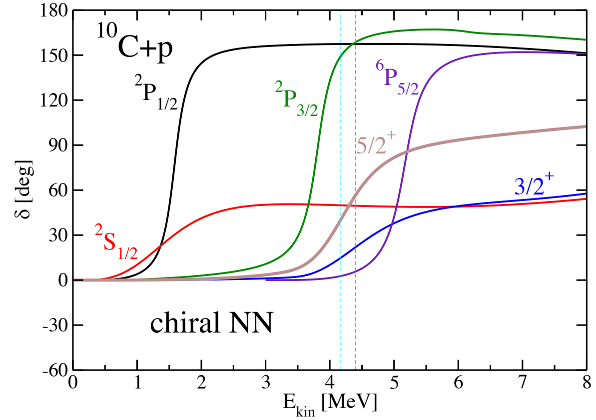

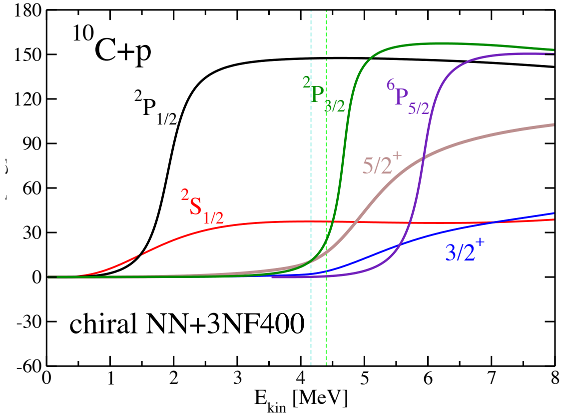

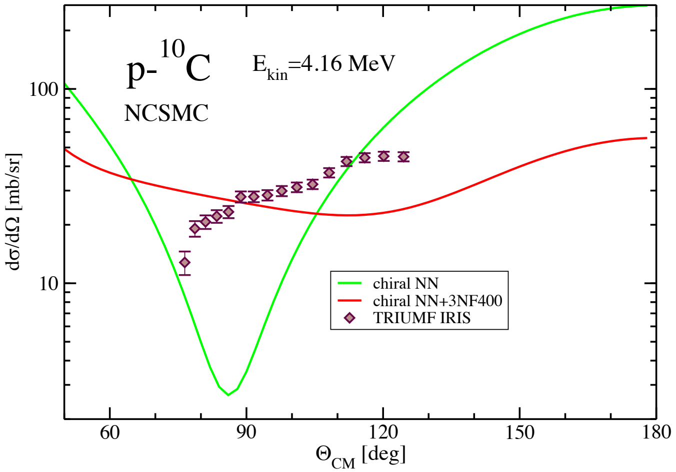

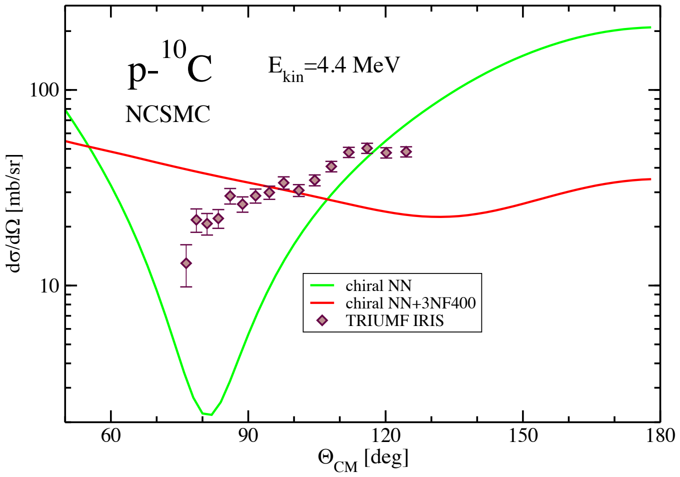

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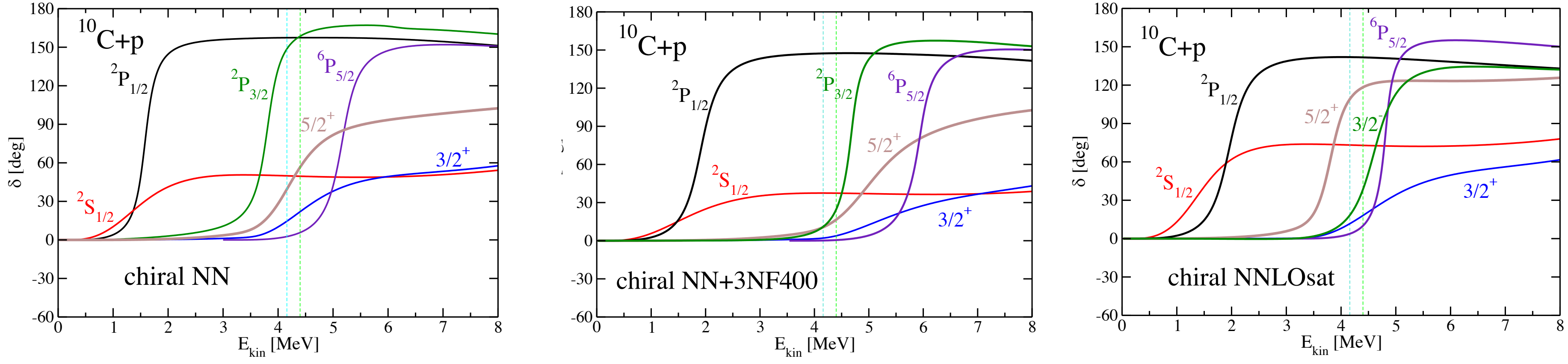

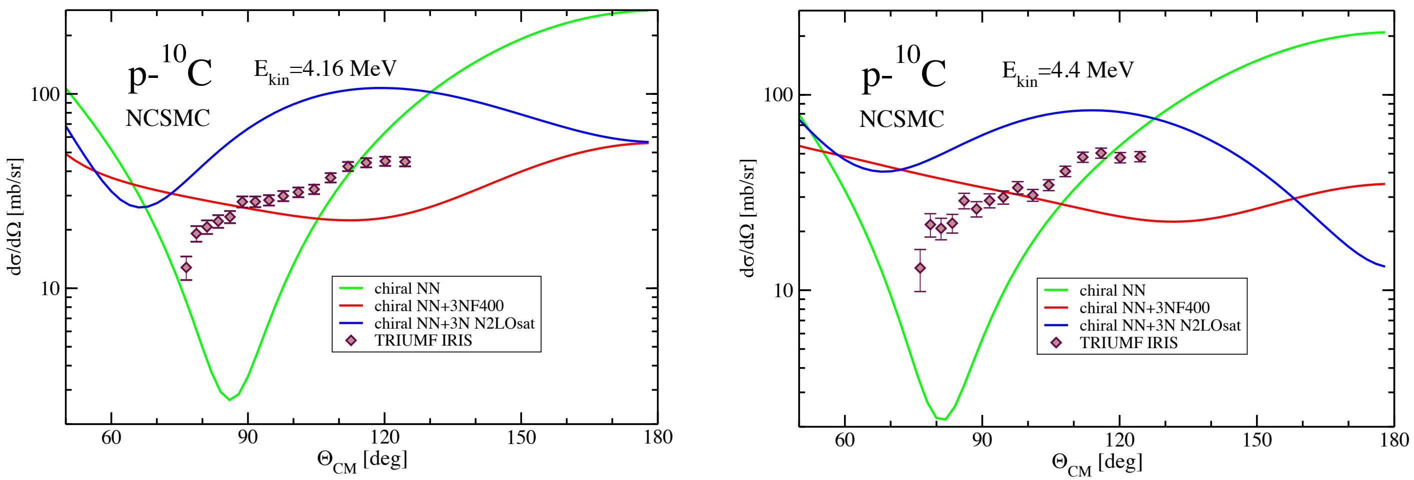

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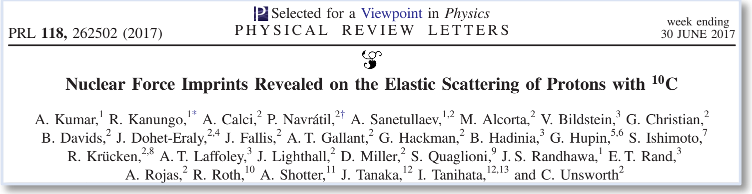
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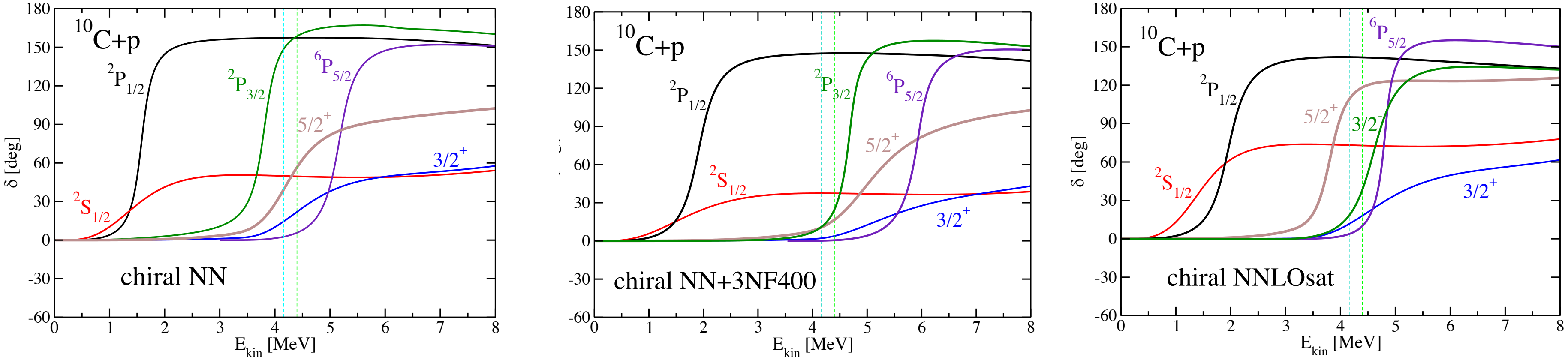
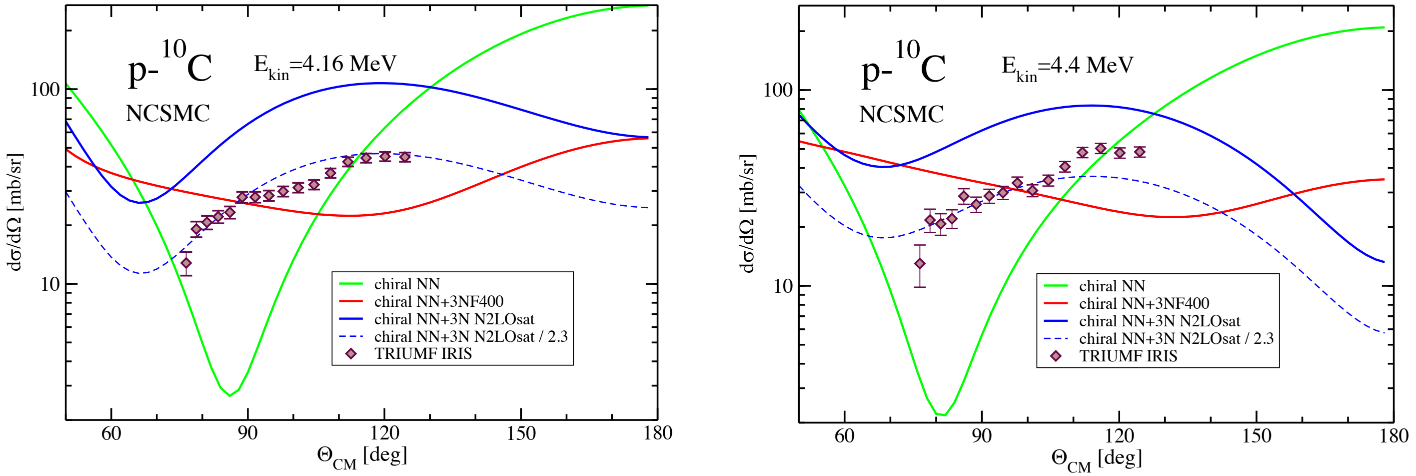
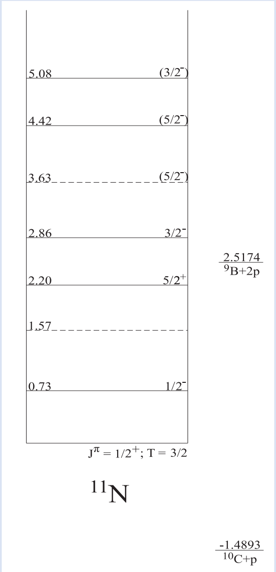


Discrimination among chiral nuclear forces





E1 transitions in NCSMC

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

$$\vec{E1} = e \sum_{i=1}^{A-a} \frac{1+\tau_i^{(3)}}{2} \left(\vec{r}_i - \vec{R}^{(A-a)}_{\text{c.m.}} \right) + e \sum_{j=A-a+1}^{A} \frac{1+\tau_j^{(3)}}{2} \left(\vec{r}_i - \vec{R}^{(a)}_{\text{c.m.}} \right) + e \frac{Z_{(A-a)} a - Z_{(a)}(A-a)}{A} \vec{r}_{A-a,a}\,.$$

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

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)

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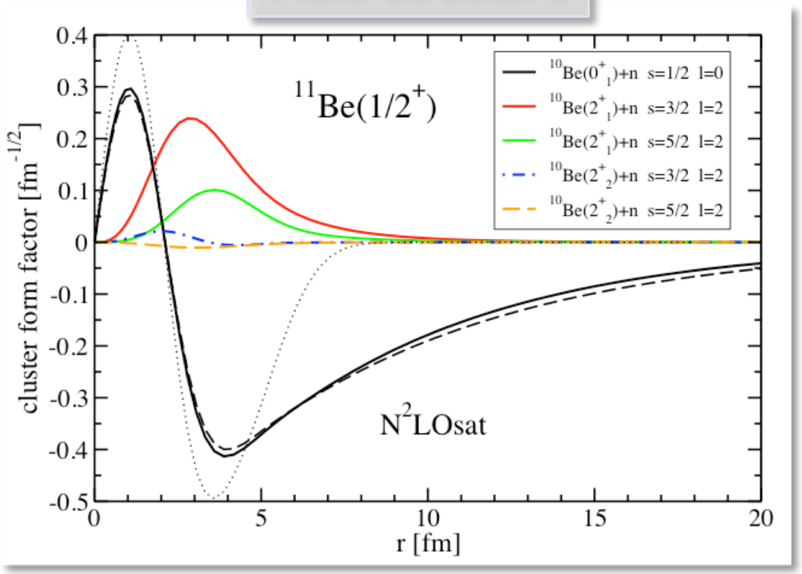
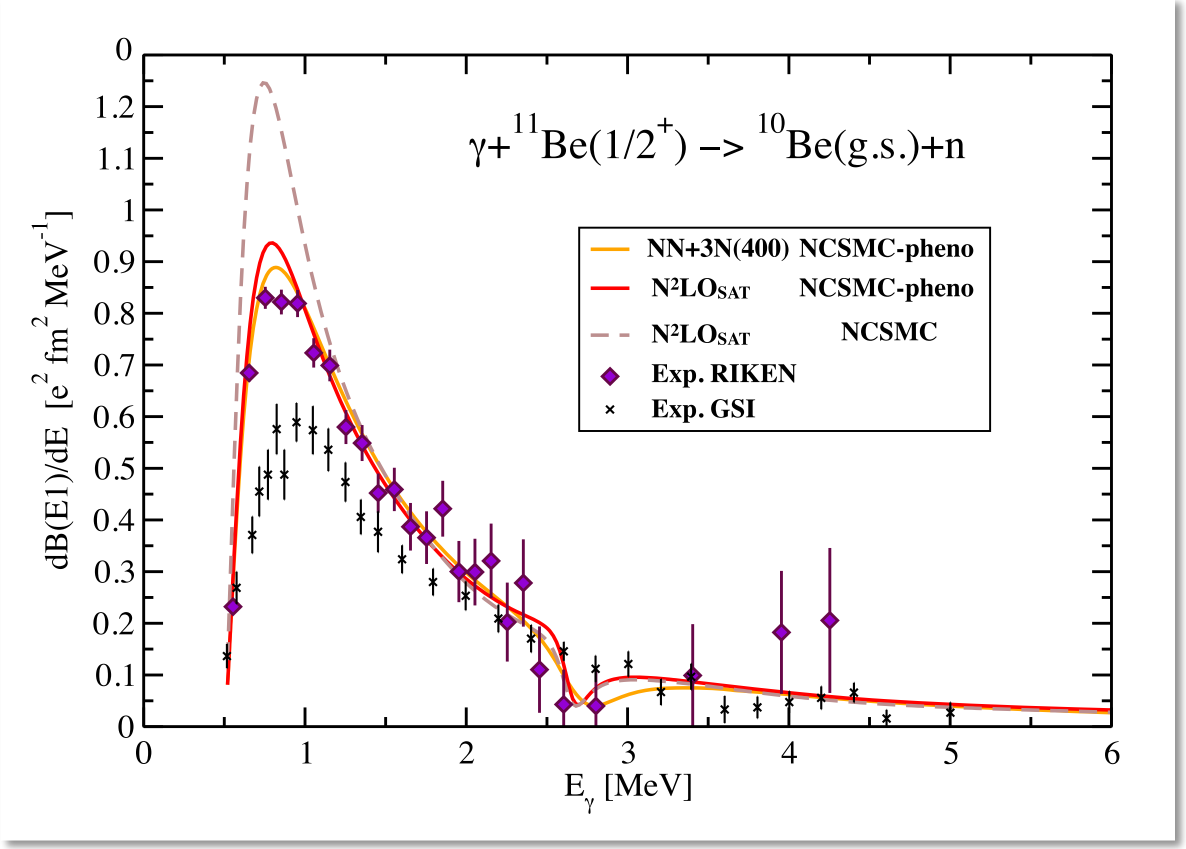
Bound to bound	NCSM	NCSMC-phenom	Expt.
B(E1; $1/2^+ \rightarrow 1/2^-$) [e^2 fm^2]	0.0005	0.117	0.102(2)

Halo structure



Bound to continuum



cluster form factor

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

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

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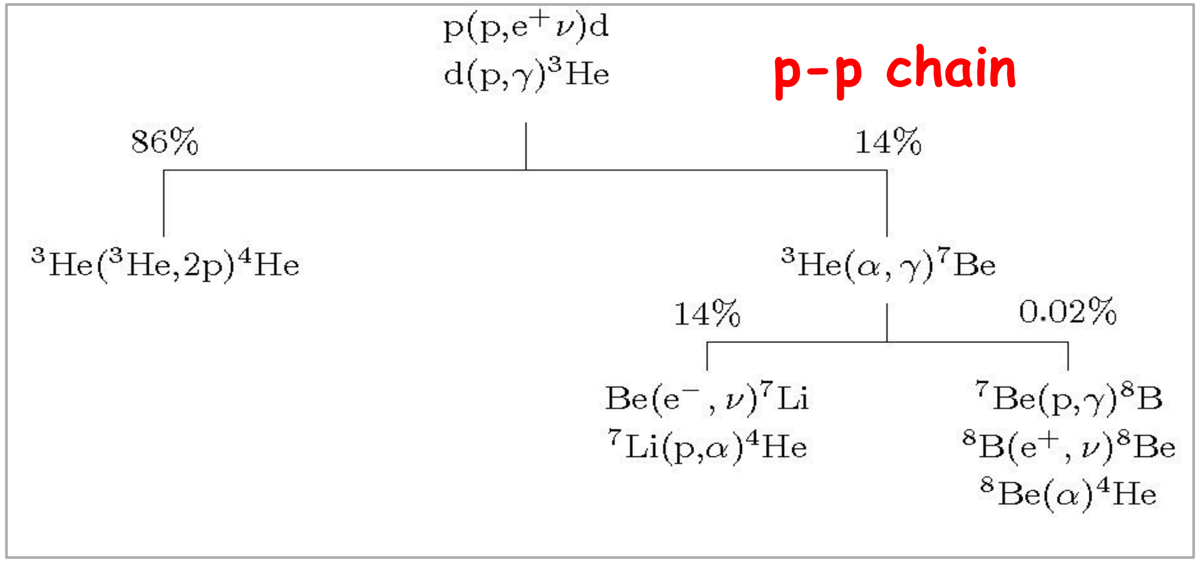
p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

- ^{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



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

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

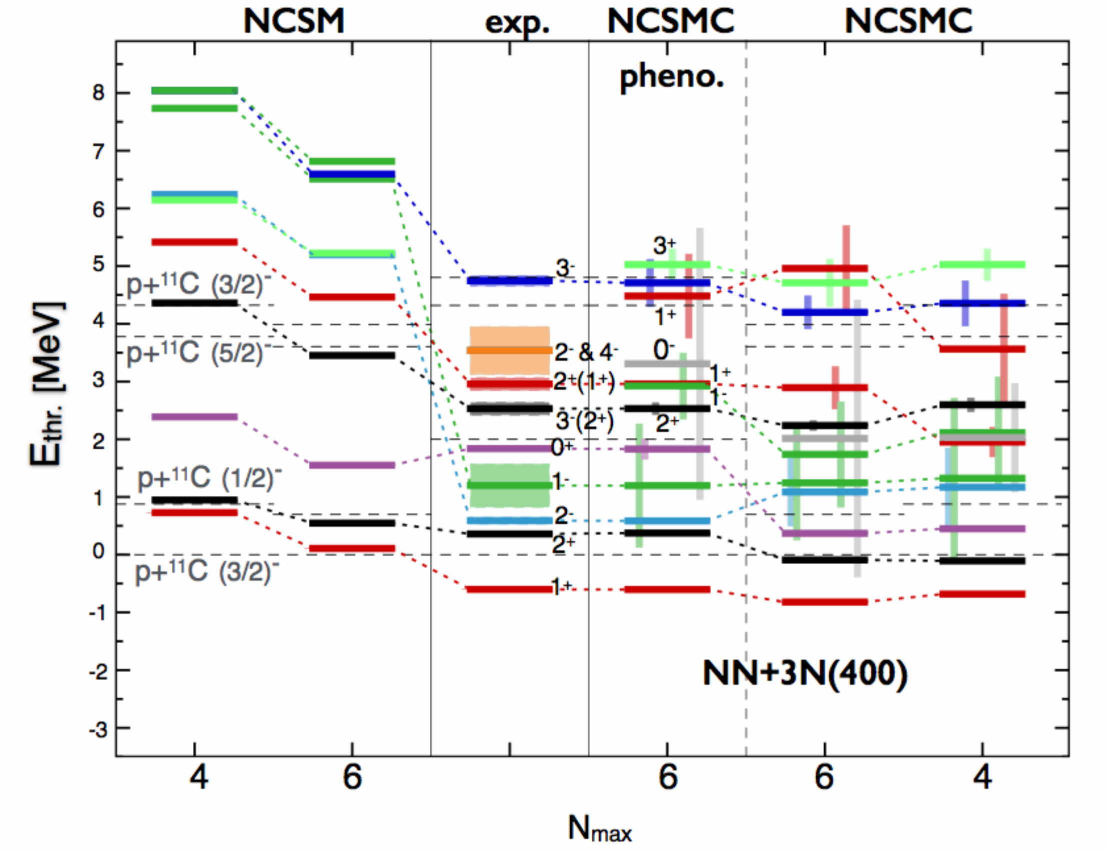
$$^{11}\mathrm{C}(\beta^{+}\ \nu)^{11}\mathrm{B}(p,\alpha)^{8}\mathrm{Be}(^{4}\mathrm{He},^{4}\mathrm{He})$$

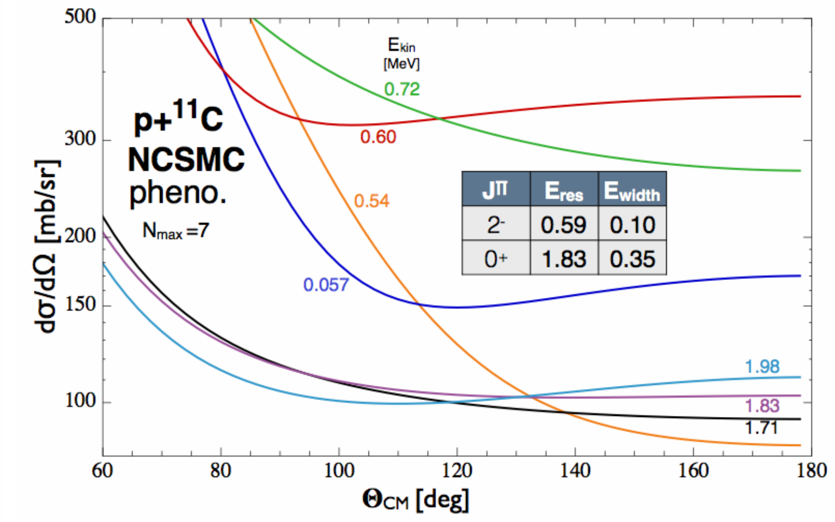
p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

- 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

- 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

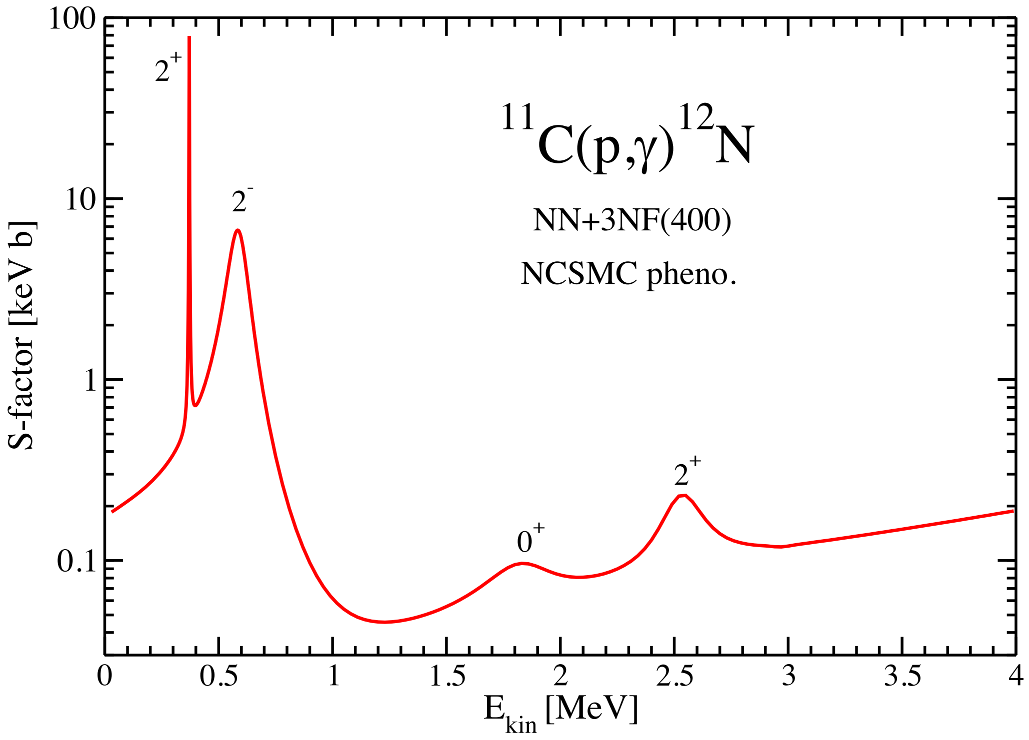


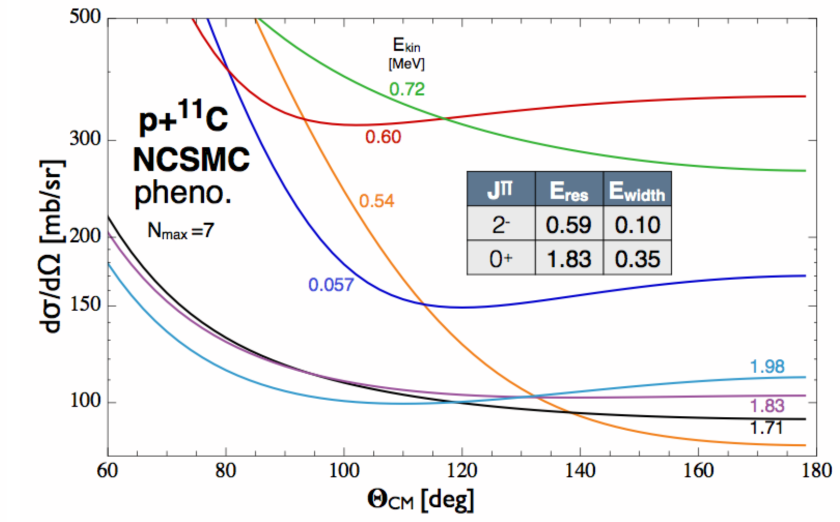


NCSMC calculations to be validated by measured cross sections and applied to calculate the ^{11}C(p,γ)^{12}N capture

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





Jπ	Eres	Ewidth
2-	0.59	0.10
0+	1.83	0.35

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

Conclusions and outlook

- *Ab initio* calculations of nuclear structure and reactions with predictive power becoming feasible beyond the latest nuclei

- *Ab initio* structure calculations can even reach (selected) medium & medium-heavy mass nuclei

- These calculations make the connection between the low-energy QCD, many-body systems, and nuclear astrophysics

TRIUMF

Thank you!

Merci!

Discovery,
accelerated