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No-core shell model with continuum applications to nuclear astrophysics

SYMPOSIUM
“Developments of Physics of Unstable Nuclei (YKIS2022b)”
23-27 May 2022

Petr Navratil

TRIUMF

2022-06-09

Discovery, accelerated

Nuclear reactions in astrophysics

- Nuclear reactions play important role in astrophysics and cosmology
  - Light nuclei synthesized in Big Bang
  - Heavier nuclei up to iron produced by fusion, transfer, radioactive capture in the stars
  - Still heavier nuclei produced by s-, i-, r-, rp-processes

- Thermonuclear reaction rate $r_{12} = \langle \sigma v \rangle\, n_1\, n_2$

$$\langle \sigma v \rangle = \left(\frac{8}{\mu\pi}\right)^{1/2} (kT)^{-3/2} \int_0^\infty E\sigma(E)\exp(-E/kT)\, dE$$

- S-factor

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

Sommerfeld parameter $\eta = Z_1 Z_2 e^2/\hbar v$

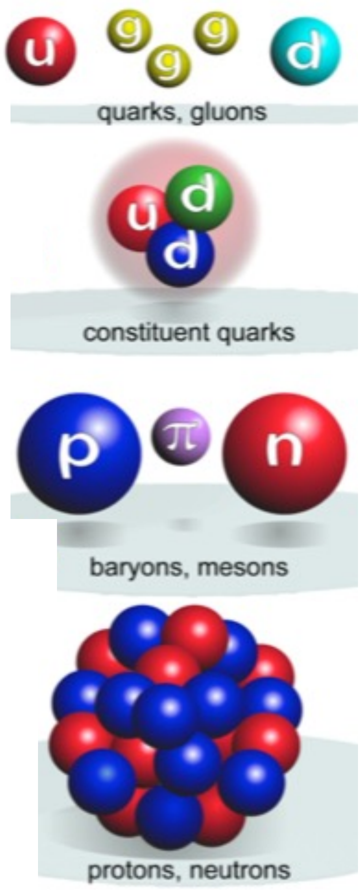
$$\langle \sigma v \rangle = \left(\frac{8}{\mu\pi}\right)^{1/2} (kT)^{-3/2} \int_0^\infty S(E)\exp(-E/kT - d/E^{1/2})\, dE$$

$d = (2\mu)^{1/2}\pi Z_1 Z_2 e^2/\hbar$

- Gamow window – narrow energy range; frequently inaccessible to experiments – **theory important**

First principles or *ab initio* nuclear theory

Quantum Chromodynamics (QCD)



Genuine *Ab Initio*

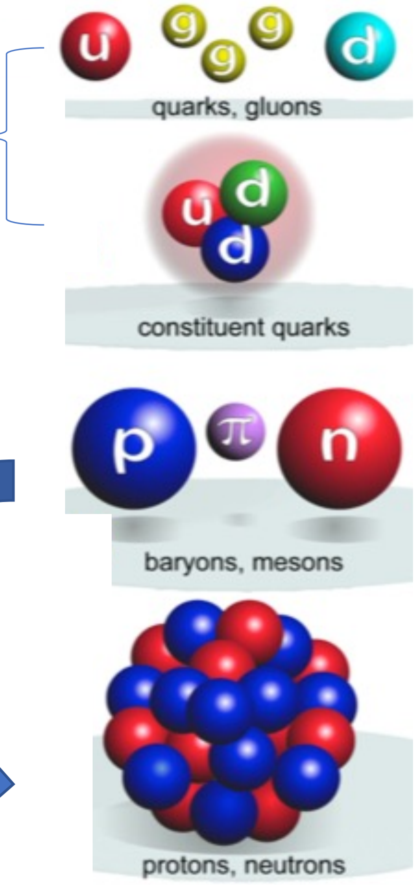
First principles or *ab initio* nuclear theory – what we do at present

Quantum Chromodynamics (QCD)

Chiral Effective Field Theory (parameters fitted to NN data)

Current *ab anitio* nuclear theory

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

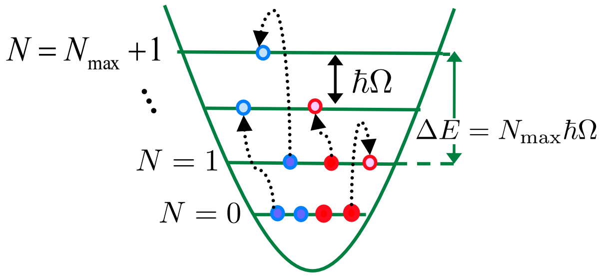


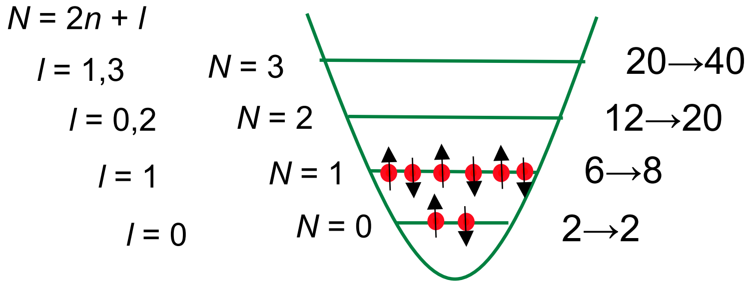
Progress in Particle and Nuclear Physics 69 (2013) 131–181
Contents lists available at SciVerse ScienceDirect
Progress in Particle and Nuclear Physics
journal homepage: www.elsevier.com/locate/ppnp
ELSEVIER
Review
Ab initio no core shell model
Bruce R. Barrett[a], Petr Navrátil[b], James P. Vary[c,*]

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





$$E = (2n + l + \tfrac{3}{2})\hbar\Omega$$

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

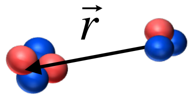
$$\Psi^A_{SD} = \sum_{N=0}^{N_{max}} \sum_j c^{SD}_{Nj} \Phi^{HO}_{SD\,Nj}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = \Psi^A \varphi_{000}(\vec{R}_{CM})$$

Ab Initio Calculations of Reactions Important for Astrophysics
Unified approach to bound & continuum states: NCSMC

- 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

- Combine the above: *ab initio* no-core shell model with continuum (NCSMC)

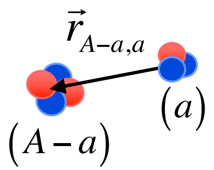
NCSMC

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

Unknowns

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

Binary cluster basis



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

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

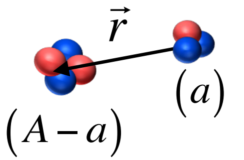
Target — Projectile

- 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

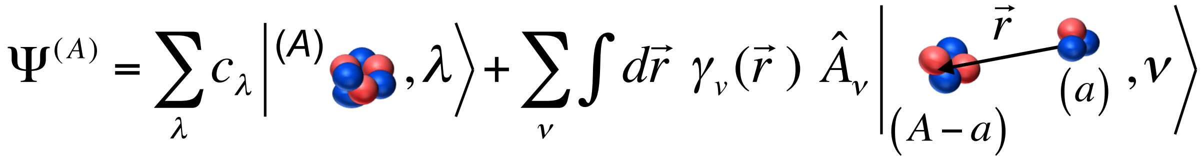
$$\sum_\nu \int d\vec{r}\ \gamma_\nu(\vec{r})\ \hat{A}_\nu \Big|$$

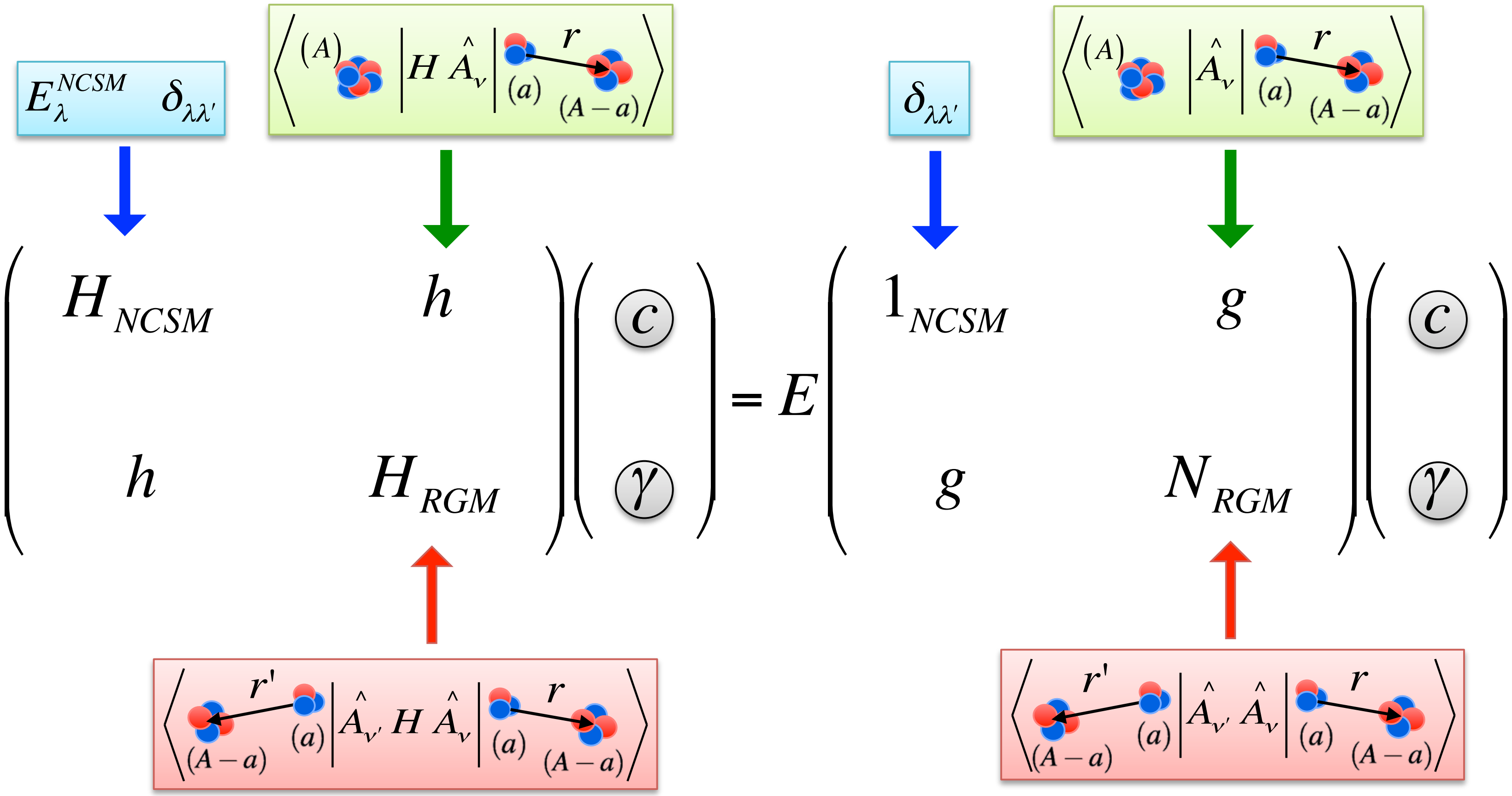


$$,\nu\Big\rangle$$

Coupled NCSMC equations

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





IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta
Phys. Scr. **91** (2016) 053002 (38pp) doi:10.1088/0031-8949/91/5/053002

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]

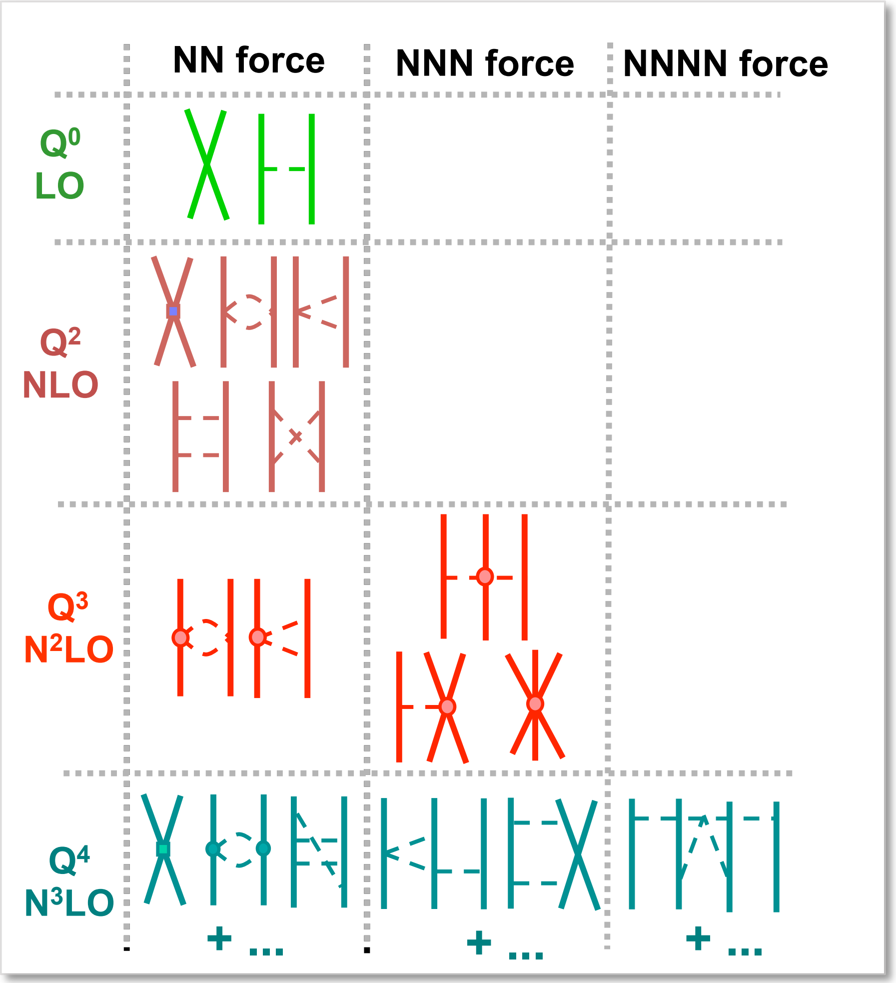
Radiative capture calculations in NCSMC

- Typically, E1 transitions the most important
  - Operator $$\hat{D} = e\sum_{i=1}^{A}\frac{1+\tau_i^z}{2}(\mathbf{r}_i - \mathbf{R}^{(A)}_{\text{c.m.}})$$
  - NCSMC wave function $$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda^{J^\pi T}|AJ^\pi T\rangle + \sum_\nu \int drr^2\frac{\gamma_\nu^{J^\pi T}(r)}{r}\mathcal{A}_\nu|\Phi_{\nu r}^{J^\pi T}\rangle$$
  - Matrix element $$\langle\Psi_f^{J_f^{\pi_f}T_f}{}_{M_{T_f}}||\hat{\mathcal{O}}^{(\kappa\tau)}_{\mu_\tau}||\Psi_i^{J_i^{\pi_i}T_i}{}_{M_{T_i}}\rangle = \sum_{\lambda_i\lambda_f}\tilde{c}^*_{\lambda_f}\tilde{c}_{\lambda_i}\langle A\lambda_f J_f T_f M_{T_f}||\hat{\mathcal{O}}^{(\kappa\tau)}_{\mu_\tau}||A\lambda_i J_i T_i M_{T_i}\rangle$$
$$+\sum_{\lambda_f\nu_i}\tilde{c}^*_{\lambda_f}\int_0^\infty drr^2\tilde{\chi}_{\nu_i}(r)\tfrac{1}{r}\langle A\lambda_f J_f T_f M_{T_f}||\hat{\mathcal{O}}^{(\kappa\tau)}_{\mu_\tau}\hat{\mathcal{A}}_{\nu_i}||\Phi_{\nu_i r}^{J_i T_i M_{T_i}}\rangle$$
$$+\textstyle\sum_{\lambda_i\nu_f}\tilde{c}_{\lambda_i}\int_0^\infty drr^2\tilde{\chi}^*_{\nu_f}(r)\tfrac{1}{r}\langle\Phi_{\nu_f r}^{J_f T_f M_{T_f}}||\hat{\mathcal{A}}_{\nu_f}\hat{\mathcal{O}}^{(\kappa\tau)}_{\mu_\tau}||A\lambda_i J_i T_i M_{T_i}\rangle$$
$$+\textstyle\sum_{\nu_f\nu_i}\int_0^\infty dr'r'^2\tilde{\chi}^*_{\nu_f}(r')\tfrac{1}{r'}\int_0^\infty drr^2\tilde{\chi}_{\nu_i}(r)\tfrac{1}{r}\langle\Phi_{\nu_f r'}^{J_f T_f M_{T_f}}||\hat{\mathcal{A}}_{\nu_f}\hat{\mathcal{O}}^{(\kappa\tau)}_{\mu_\tau}\hat{\mathcal{A}}_{\nu_i}||\Phi_{\nu_i r}^{J_i T_i M_{T_i}}\rangle$$
  - Express operator as target, projectile, and relative motion parts

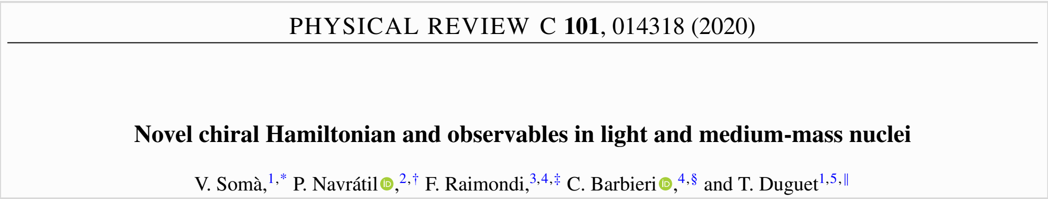
$$\hat{D} = e\sum_{i=1}^{A-a}\frac{1+\tau_i^z}{2}(\mathbf{r}_i - \mathbf{R}^{(A-a)}_{\text{c.m.}}) + e\sum_{i=A-a+1}^{A}\frac{1+\tau_i^z}{2}(\mathbf{r}_i - \mathbf{R}^{(a)}_{\text{c.m.}}) + e\frac{Z_{(A-a)}a - Z_{(a)}(A-a)}{A}\mathbf{r}_{A-a,a}$$

Input for NCSMC calculations:
Nuclear forces from chiral Effective Field Theory

- Approach taking advantage of the separation of scales
  - 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


PHYSICAL REVIEW C **101**, 014318 (2020)

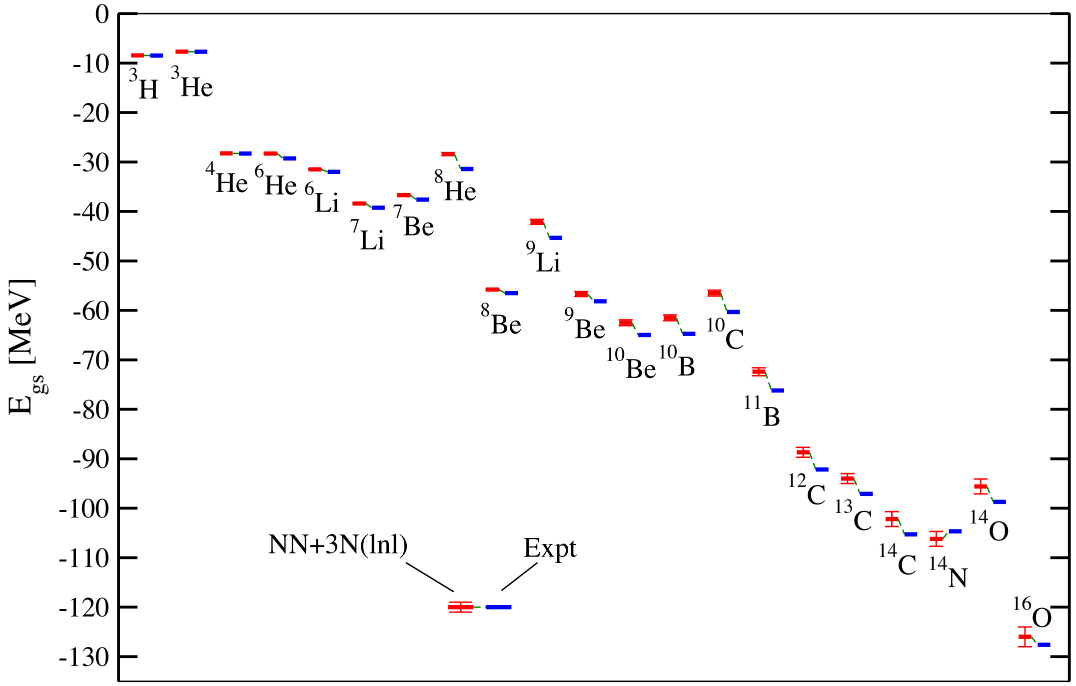
Novel chiral Hamiltonian and observables in light and medium-mass nuclei

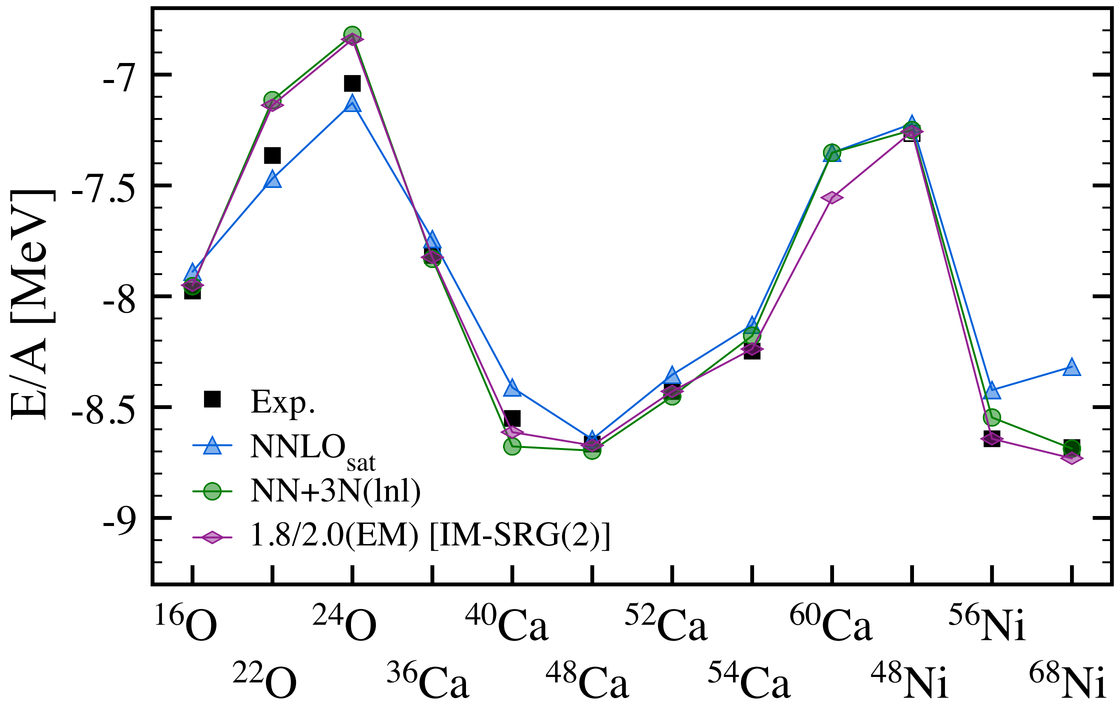
V. Somà,[1,*] P. Navrátil,[2,†] F. Raimondi,[3,4,‡] C. Barbieri,[4,§] and T. Duguet[1,5,∥]

Binding energies of light and selected medium mass nuclei from chiral NN+3N forces

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - **The Hamiltonian fully determined in *A*=2 and *A*=3,4 systems**
    - Nucleon–nucleon scattering, deuteron properties, ^{3}H and ^{4}He binding energy, ^{3}H half life
  - Light nuclei – NCSM
  - Medium mass nuclei – Self-Consistent Green's Function method

NN N^{3}LO (Entem-Machleidt 2003)
3N N^{2}LO w local/non-local regulator





1.8/2.0 (EM) results: J. Simonis, S. R. Stroberg, K. Hebeler, J. D. Holt, and A. Schwenk, Phys. Rev. C 96, 014303 (2017).

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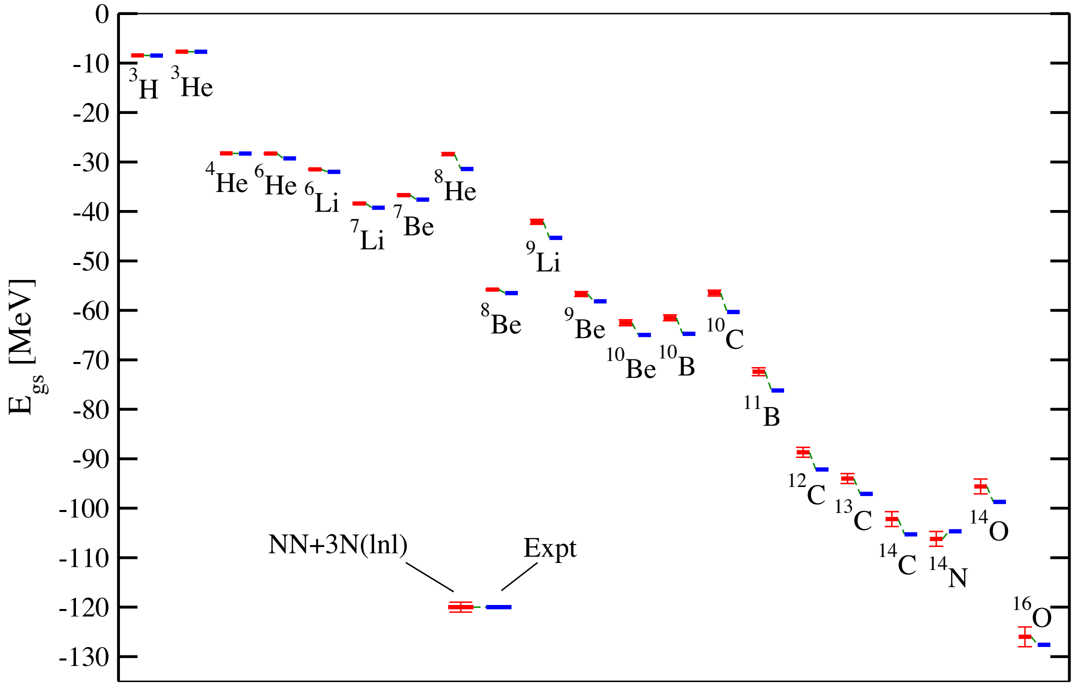
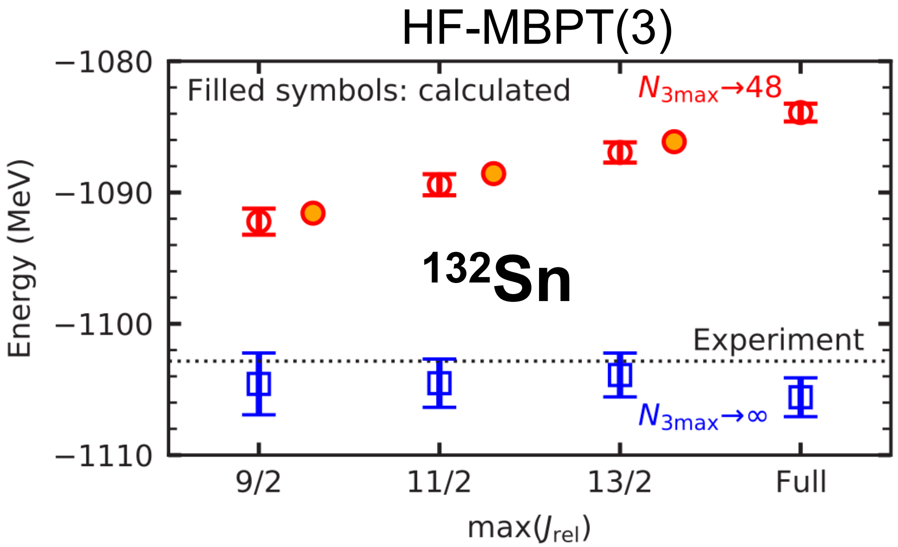




PHYSICAL REVIEW C **105**, 014302 (2022)

Converged *ab initio* calculations of heavy nuclei

T. Miyagi,[1,*] S. R. Stroberg,[2,†] P. Navrátil,[1,‡] K. Hebeler,[3,4,5,§] and J. D. Holt[1,6,‖]

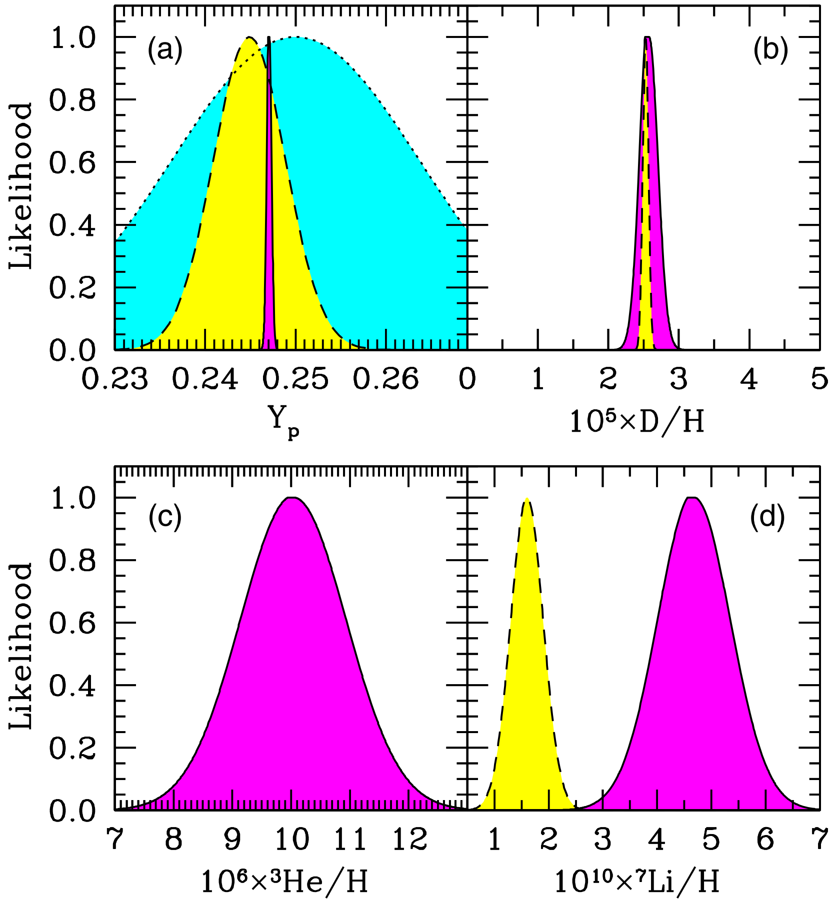
Big Bang Nucleosynthesis

- Primordial nucleosynthesis – 10 s to 20 min after the Big Bang
  - Helium 25% of the mass of the Universe
  - Prediction depends on
    - Baryon-to-photon ratio – CMB Planck data
    - Nuclear reaction rates

$n(p,\gamma)^2H$	$^2H(p,\gamma)^3He$	$^2H(d,\gamma)^4He$	$^2H(d,n)^3He$	$^2H(d,p)^3H$	$^3He(n,p)^3H$
$^3H(d,n)^4He$	$^3He(d,p)^4He$	$^2H(\alpha,\gamma)^6Li$	$^6Li(p,\gamma)^7Be$	$^6Li(p,\alpha)^3He$	$^6Li(n,\alpha)^3H$
$^3H(\alpha,\gamma)^7Li$	$^3He(\alpha,\gamma)^7Be$	$^7Li(p,\alpha)^4He$	$^7Li(p,\gamma)^8Be$	$^7Be(n,p)^7Li$	

- D and ^{4}He in agreement with observations
- ^{3}He – reliable measurements do not exist
- ^{7}Li – predictions three times higher than observations
- ^{6}Li?

Yellow - observations
Purple – BBN predictions

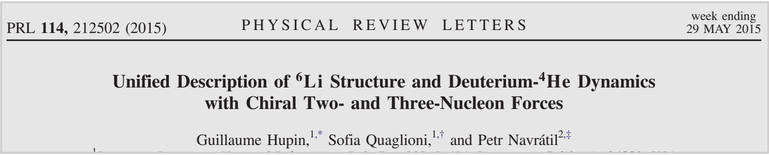


Rev. Mod. Phys. **88**:015004 (2016)

Radiative capture of deuterons on ^{4}He

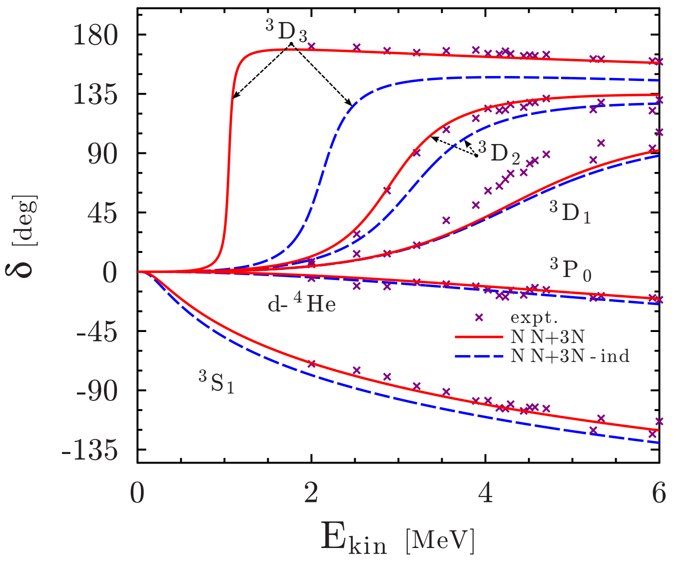
- Reaction ^{4}He(d,γ)^{6}Li responsible for ^{6}Li production in BBN
- Three orders of magnitude discrepancy between BBN predictions and observations
  - Problem with our understanding of the reaction rate?
  - New physics?
  - Problem with astronomical observations?

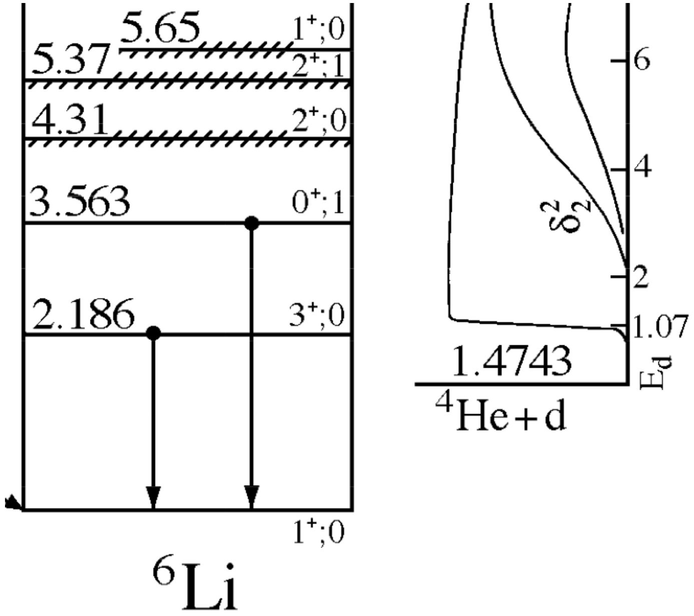
^{6}Li ↔ ^{4}He+d investigated within NCSMC in the past


PRL 114, 212502 (2015) PHYSICAL REVIEW LETTERS week ending 29 MAY 2015

Unified Description of ^{6}Li Structure and Deuterium-^{4}He Dynamics with Chiral Two- and Three-Nucleon Forces

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





Ab initio prediction of the $^4He(d,\gamma)^6Li$ big-bang radiative capture

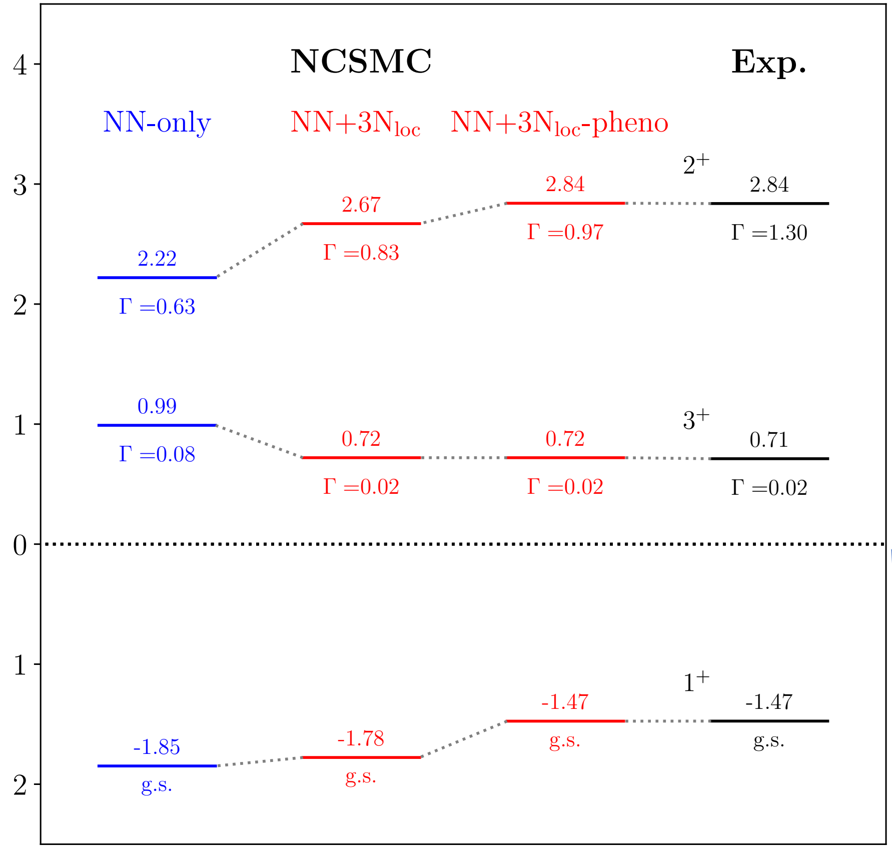
C. Hebborn,[1,2,*] G. Hupin,[3] K. Kravvaris,[2] S. Quaglioni,[2] P. Navrátil,[4] and P. Gysbers[4,5]

arXiv: 2203.15914

Radiative capture of deuterons on ^{4}He

- NCSMC calculations with chiral NN+3N interaction

Structure of ^{6}Li



^{4}He+d threshold

Ground state properties:
Energy
Asymptotic normalization constants
Magnetic moment

	NN-only	NCSMC	NCSMC-pheno	Exp. or Eval.
$E_{g.s.}$ [MeV]	-1.848	-1.778	-1.474	-1.4743
$\mathcal{C}_0$ [fm$^{-1/2}$]	2.95	2.89	2.62	2.28(7)
$\mathcal{C}_2$ [fm$^{-1/2}$]	-0.0369	-0.0642	-0.0554	-0.077(18)
$\mathcal{C}_2/\mathcal{C}_0$	-0.013	-0.022	-0.021	-0.025(6)(10)
μ [μ_N]	0.85	0.84	0.84	0.8220473(6)

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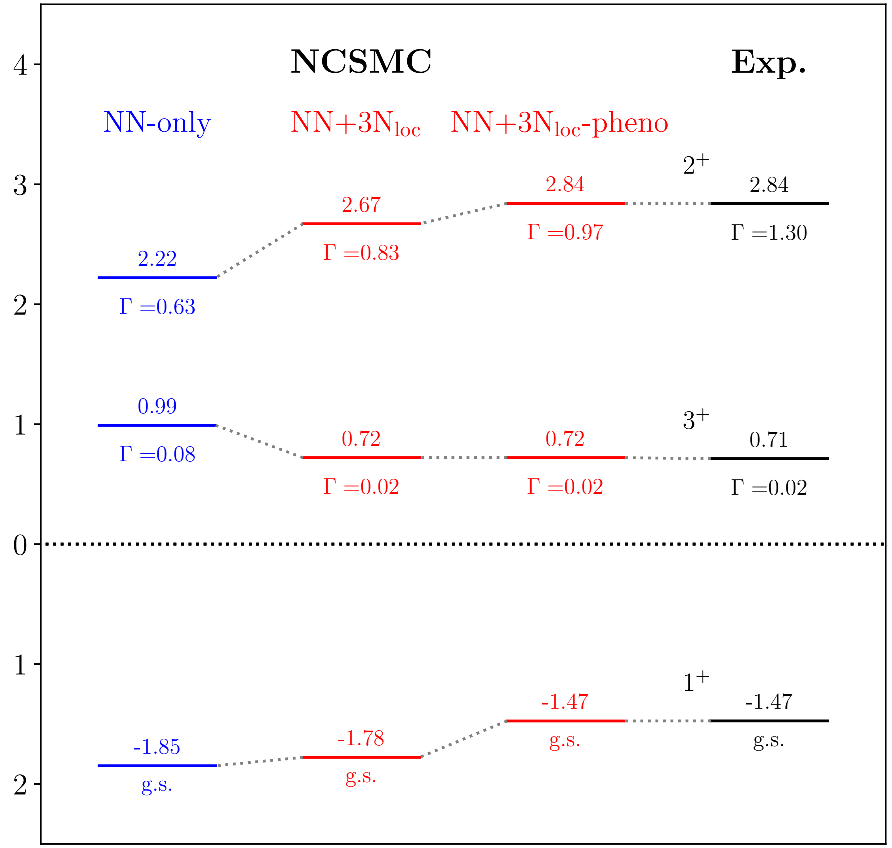
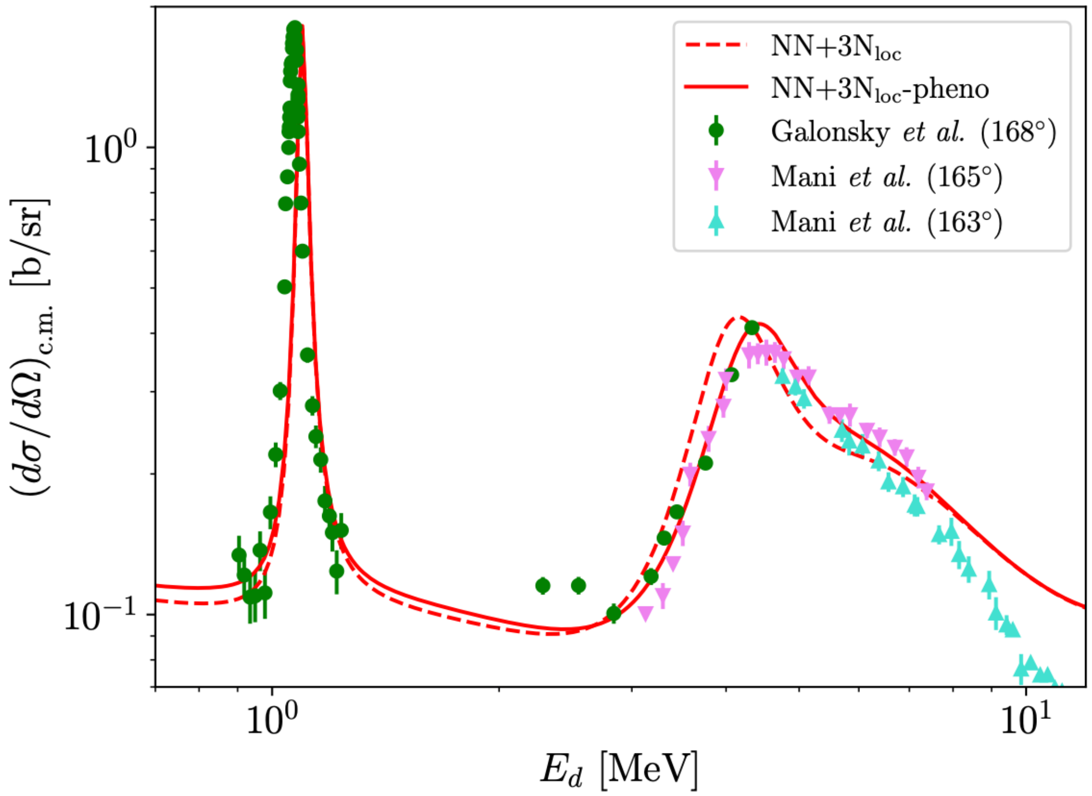


Elastic scattering ^{4}He$(d,d)^4$He cross section at the deuteron back scattered angle 164°



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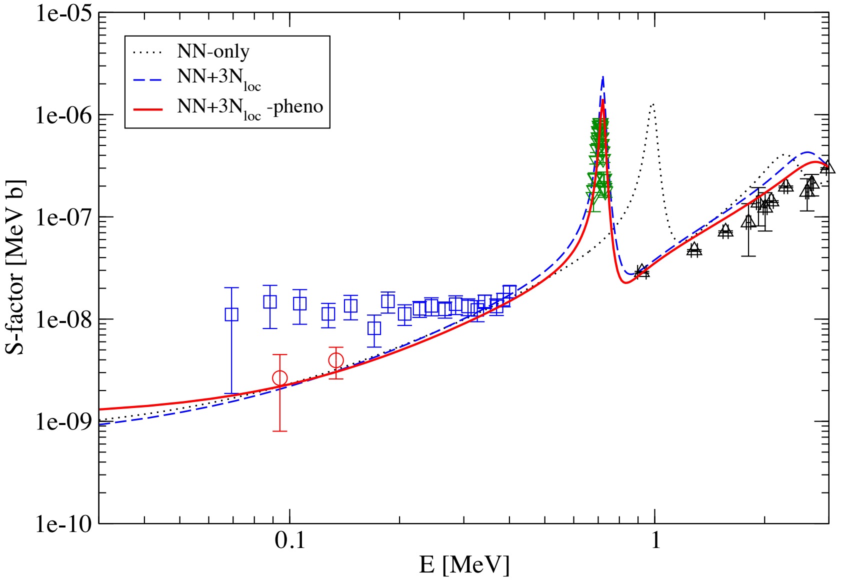
Radiative capture of deuterons on ^{4}He

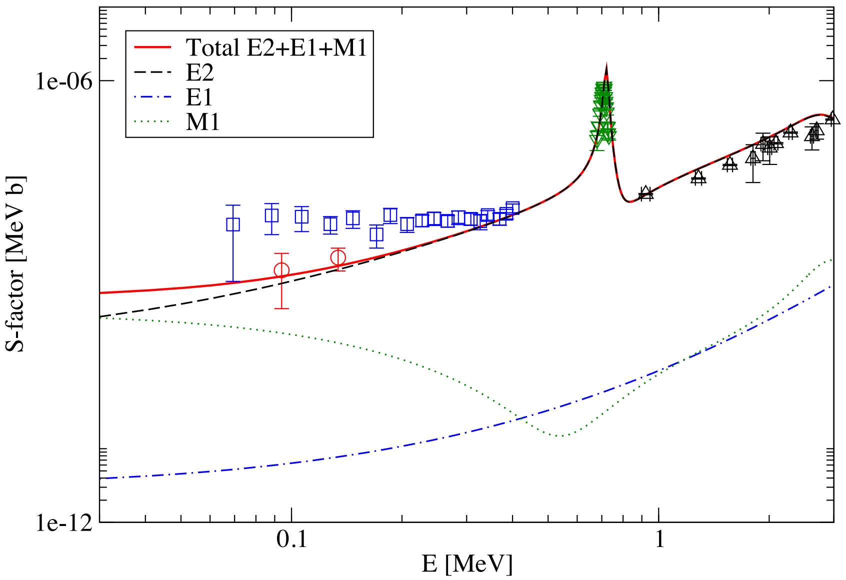
- NCSMC calculations with chiral NN+3N interaction
  - Capture S-factor

Dominated by E2
M1 significant at low energy
E1 negligible – isospin supressed (T=0 → T=0)

$$\mathcal{M}^{E\lambda} = e\sum_{j=1}^{A}\frac{1+\tau_{jz}}{2}[\boldsymbol{r}_j - \boldsymbol{R}_{cm}^{(A)}]^\lambda$$

$$\mathcal{M}^{M1} = \frac{\mu_N}{\hbar c}\sqrt{\frac{3}{4\pi}}\sum_{j=1}^{A}(g_{lj}L_j + g_{sj}S_j)$$





Low energy S-factor consistent with LUNA data, below the ^{6}Li Coulomb breakup data

$Ab\ initio$ prediction of the ^{4}He$(d,\gamma)^6$Li big-bang radiative capture

C. Hebborn,[1,2,*] G. Hupin,[3] K. Kravvaris,[2] S. Quaglioni,[2] P. Navrátil,[4] and P. Gysbers[4,5]

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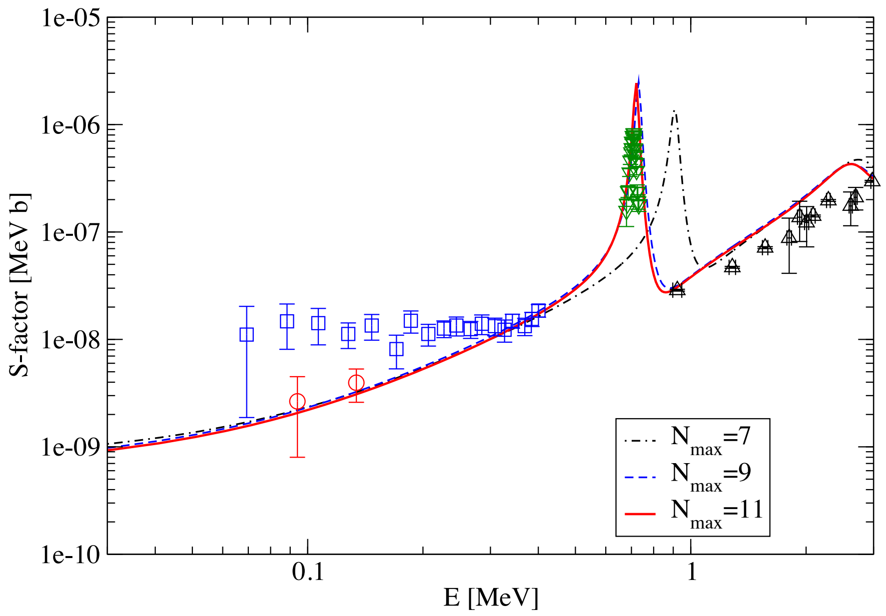
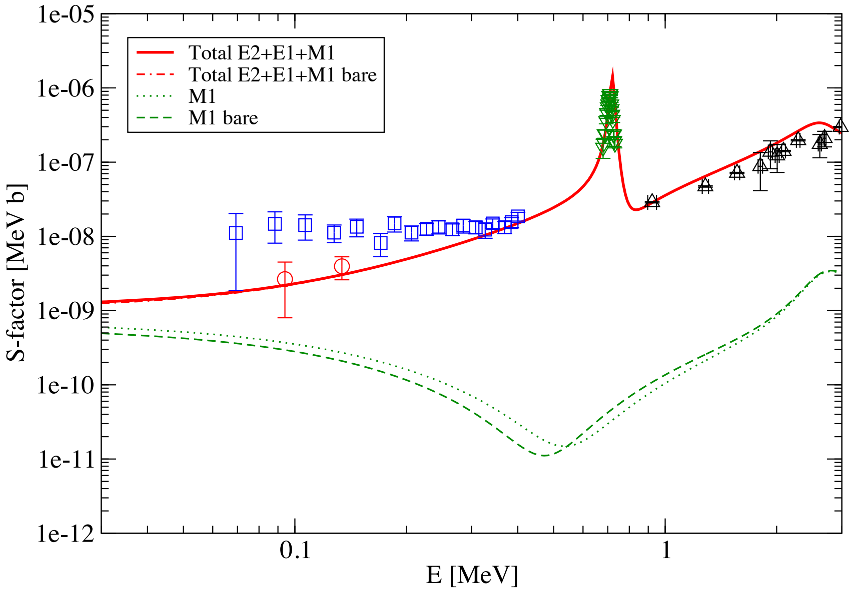
Radiative capture of deuterons on ^{4}He

- NCSMC calculations with chiral NN+3N interaction
  - Capture S-factor

Convergence of the S-factor with N_{max}



SRG renormalization of the M1 operator



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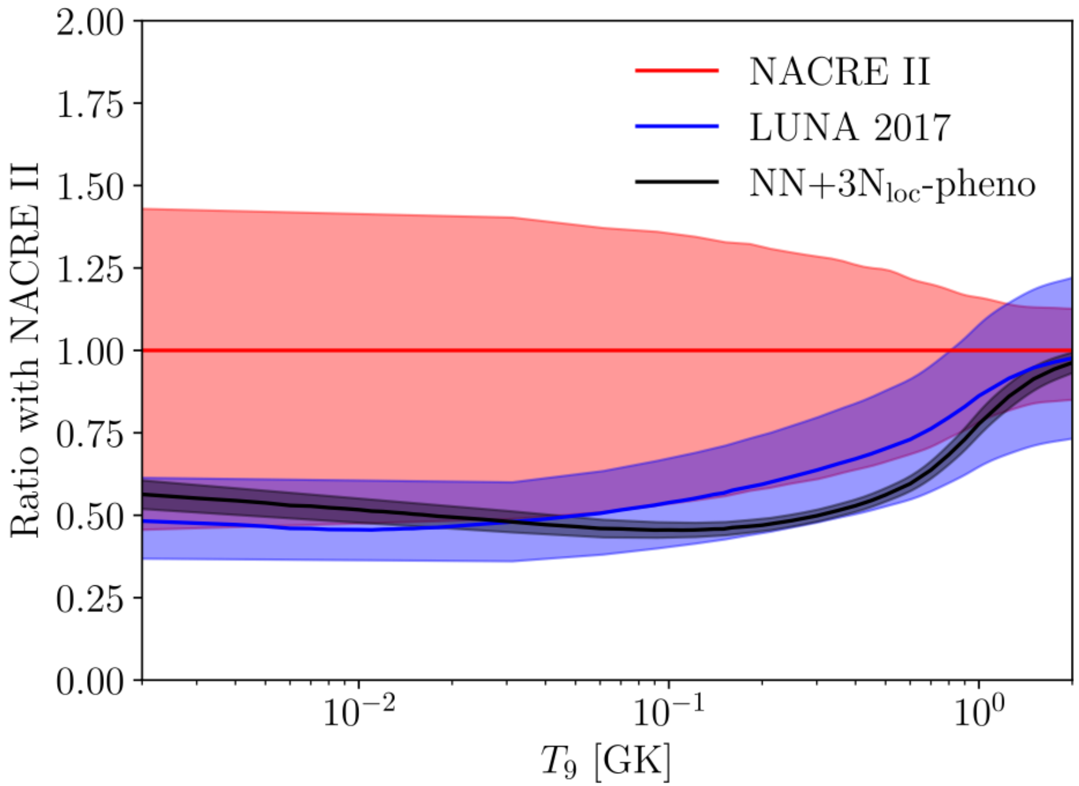
Radiative capture of deuterons on ^4He

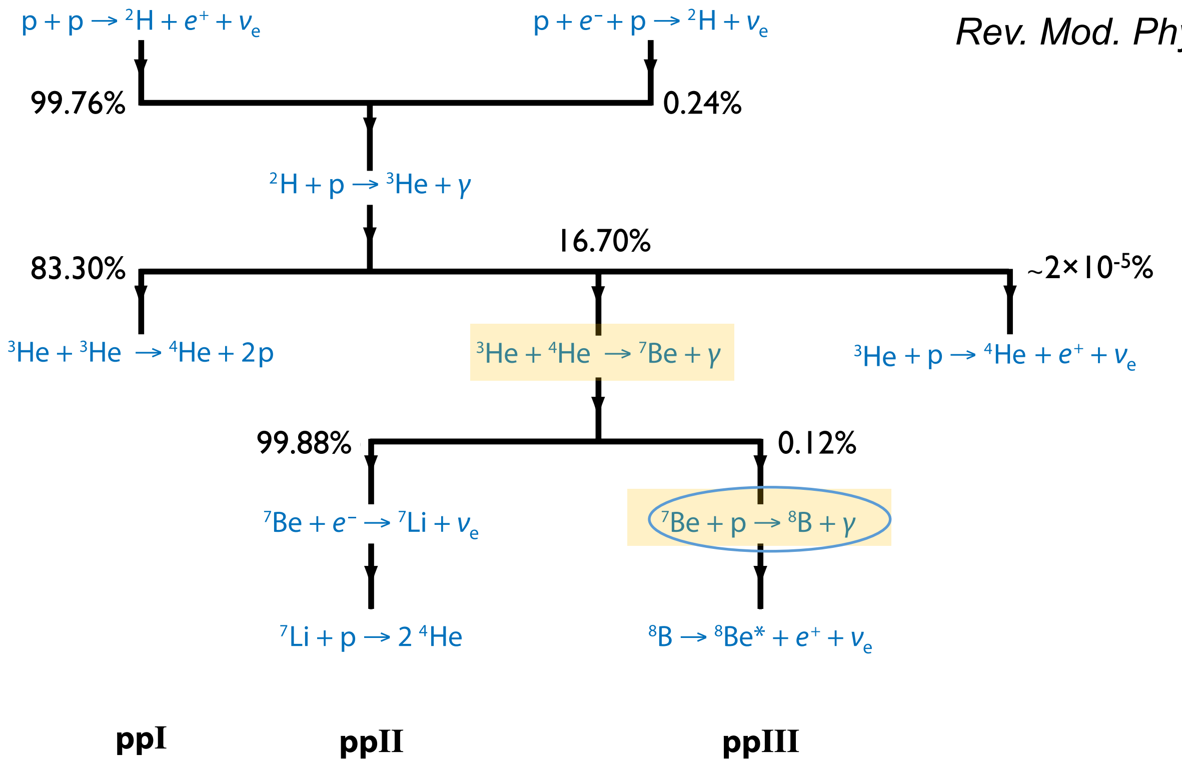
- NCSMC calculations with chiral NN+3N interaction
  - Thermonuclear reaction rate



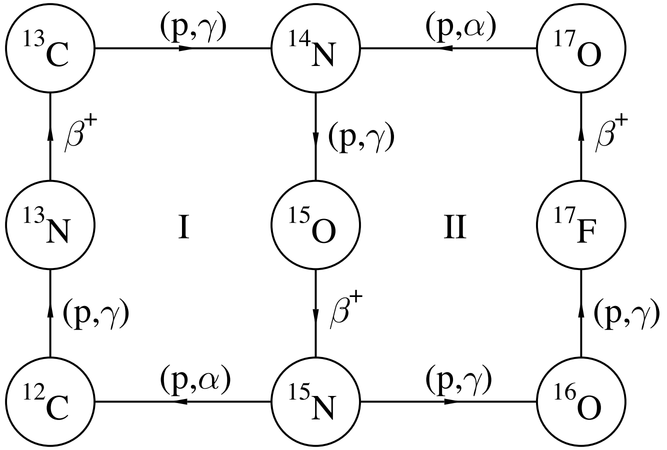
Thermonuclear reaction rate smaller than NACRE II evaluation, agreement with LUNA result with less uncertainty

Stellar burning

- Hydrogen burning – converting 4 protons to ^{4}He
  - pp chain
  - CNO cycles



Rev. Mod. Phys. **83,**195–245 (2011)



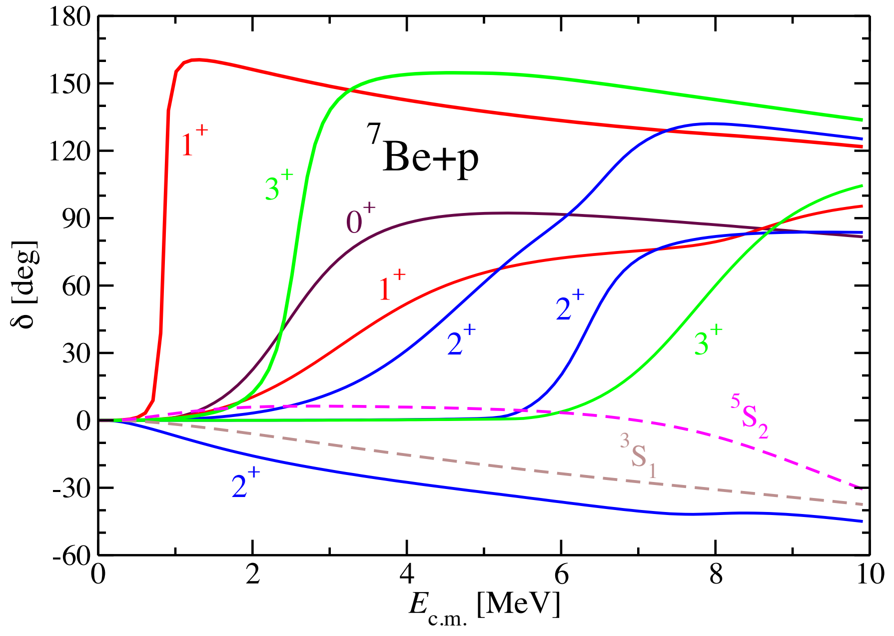
- Helium burning $\alpha + \alpha \rightarrow {}^{8}\mathrm{Be}$ $\quad {}^{8}\mathrm{Be}(\alpha,\gamma){}^{12}\mathrm{C}$ $\quad {}^{12}\mathrm{C}(\alpha,\gamma){}^{16}\mathrm{O}$

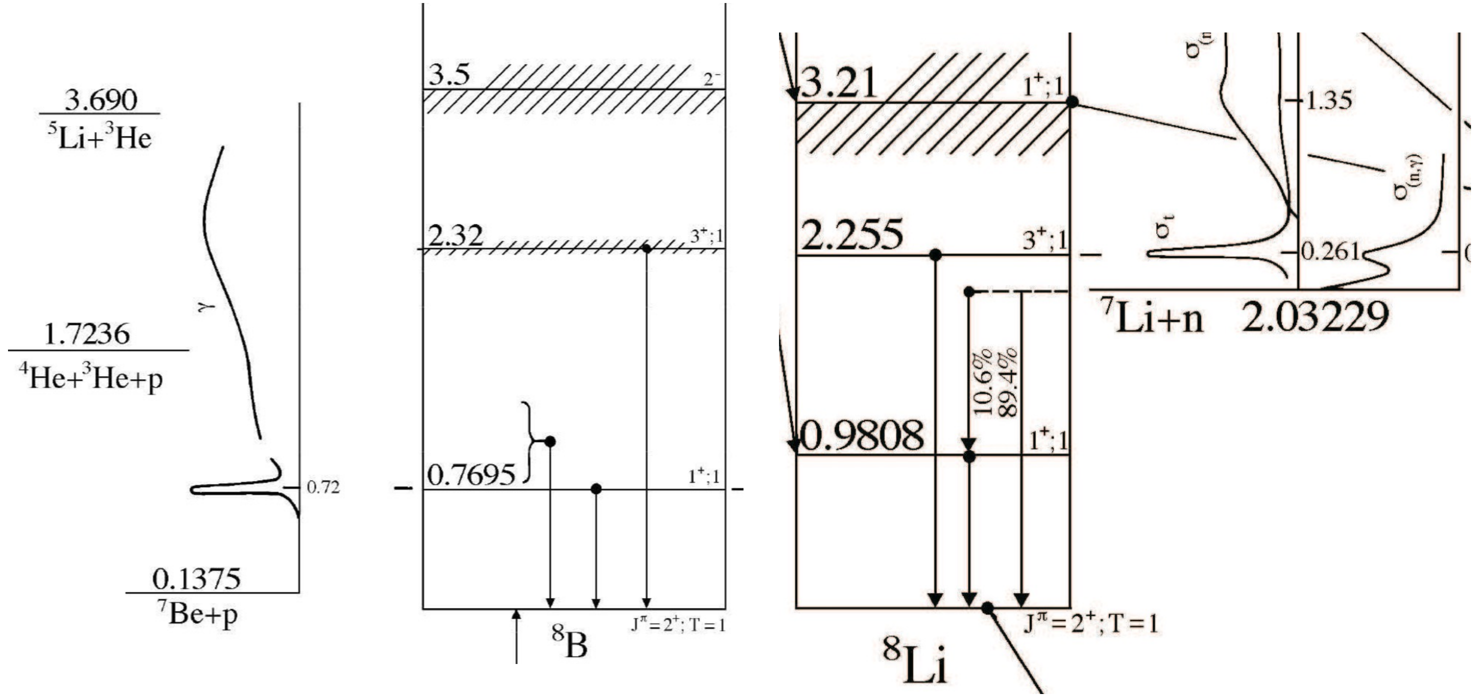
Ab initio prediction for the radiative capture of protons on ^{7}Be
K. Kravvaris,[1] P. Navrátil,[2] S. Quaglioni,[1] C. Hebborn,[3,1] and G. Hupin[4]
arXiv: 2202.11759

Radiative capture of protons on ^{7}Be

- Solar pp chain reaction, solar ^{8}B neutrinos
- NCSMC calculations with a set of chiral NN+3N interactions as input

- Example of ^{8}B structure results

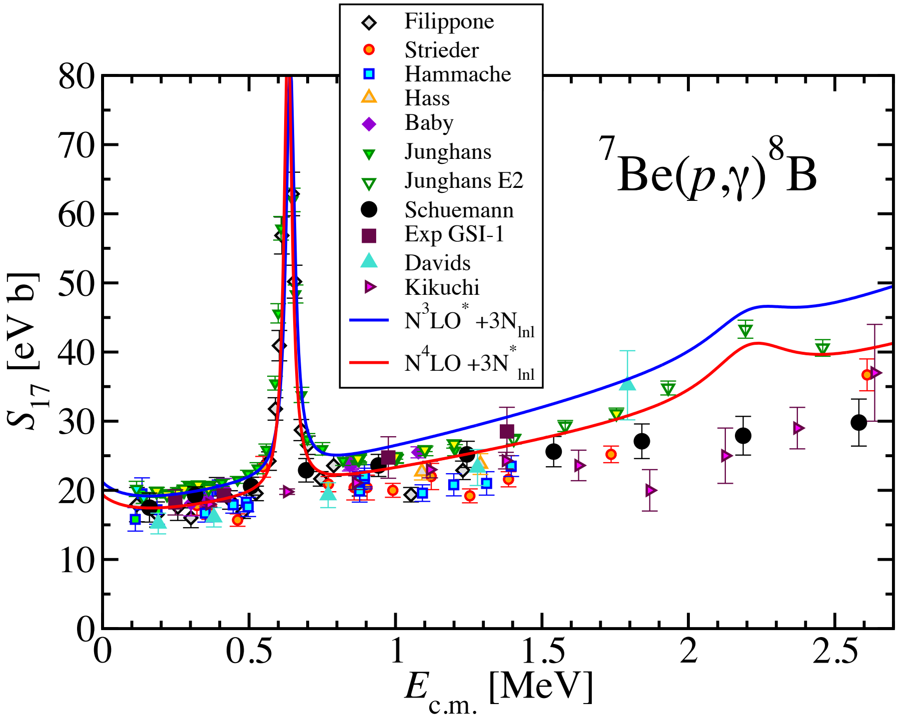


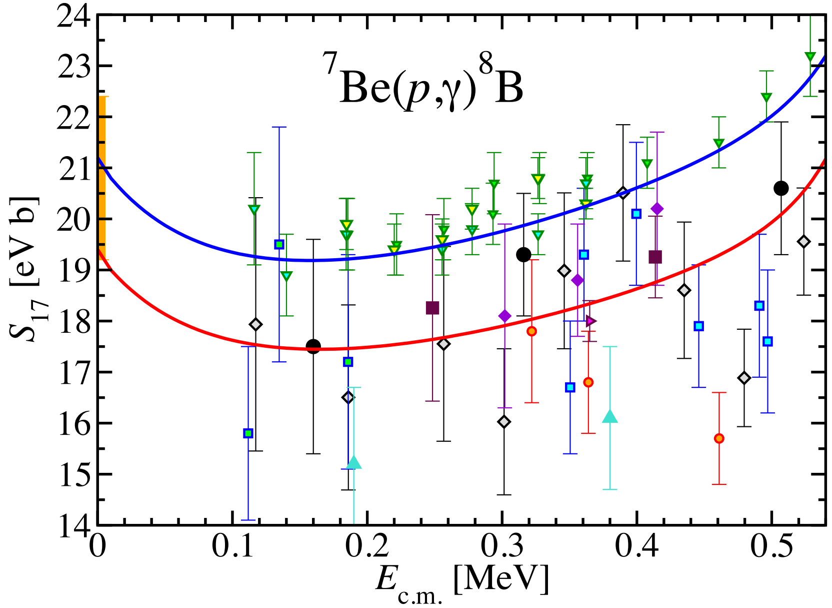


Radiative capture of protons on ^{7}Be

- NCSMC S-factor results

	$C_{p_{1/2}}$	$C_{p_{3/2}}$	a_1	a_2	$S_{17}(0)$
N^2LO+3N_{lnl}	0.384	0.691	4.4(1)	-0.5(1)	23.9
N^3LO+3N_{lnl}	0.390	0.678	1.3(1)	-4.7(1)	23.5
N^4LO+3N_{lnl}	0.354	0.669	1.6(1)	-4.4(1)	22.0
$N^4LO+3N^*_{lnl}$	0.343	0.621	1.3(1)	-5.0(1)	19.3
$N^3LO^*+3N_{lnl}$	0.334	0.663	0.1(1)	-7.7(1)	21.1
$N^3LO^*+3N_{loc}$	0.308	0.584	2.5(1)	-3.6(2)	16.8
Ref. [41]	0.315(9)	0.66(2)	$17.34^{+1.11}_{-1.33}$	$-3.18^{+0.55}_{-0.50}$	





E1 non-resonant, M1/E2 at 1⁺ and 3⁺ resonances

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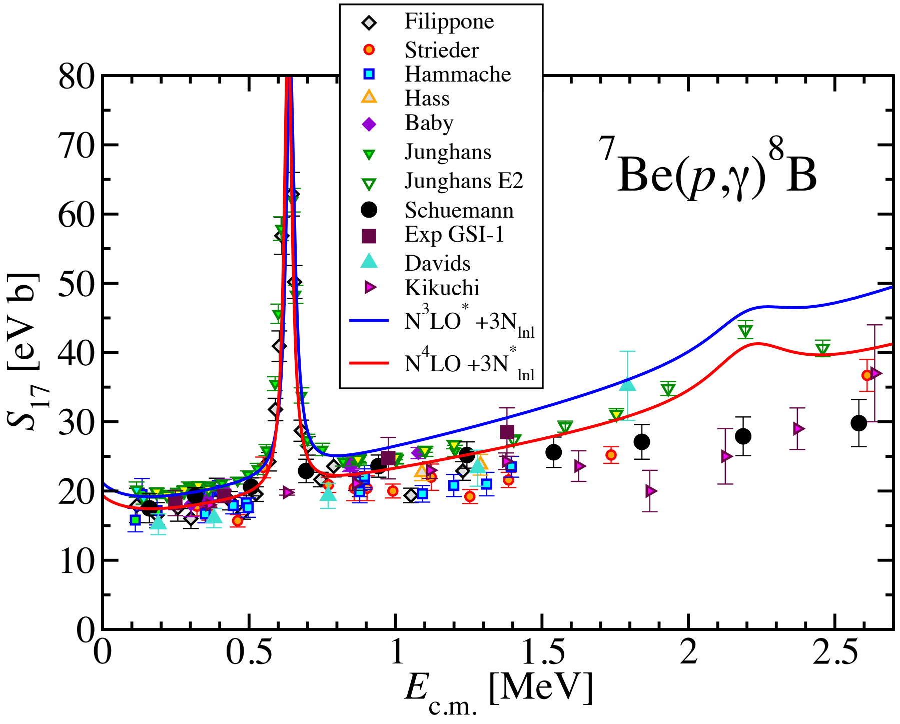

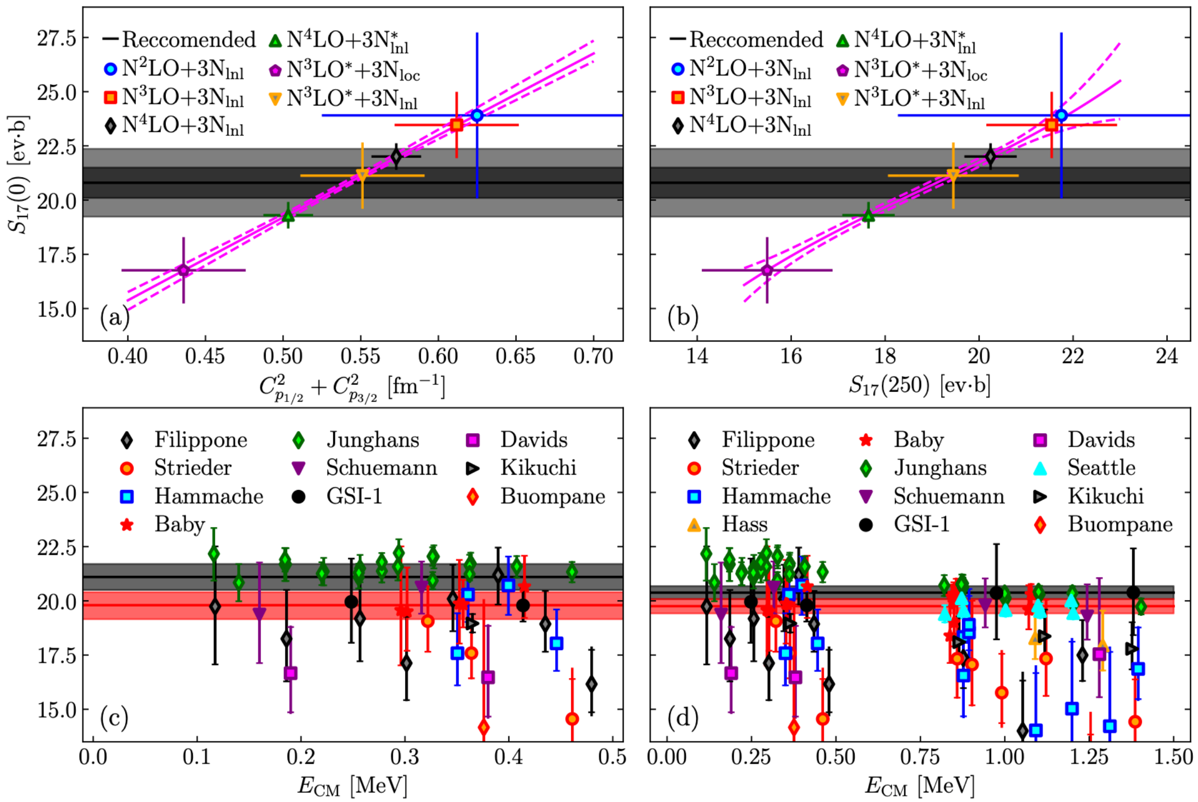

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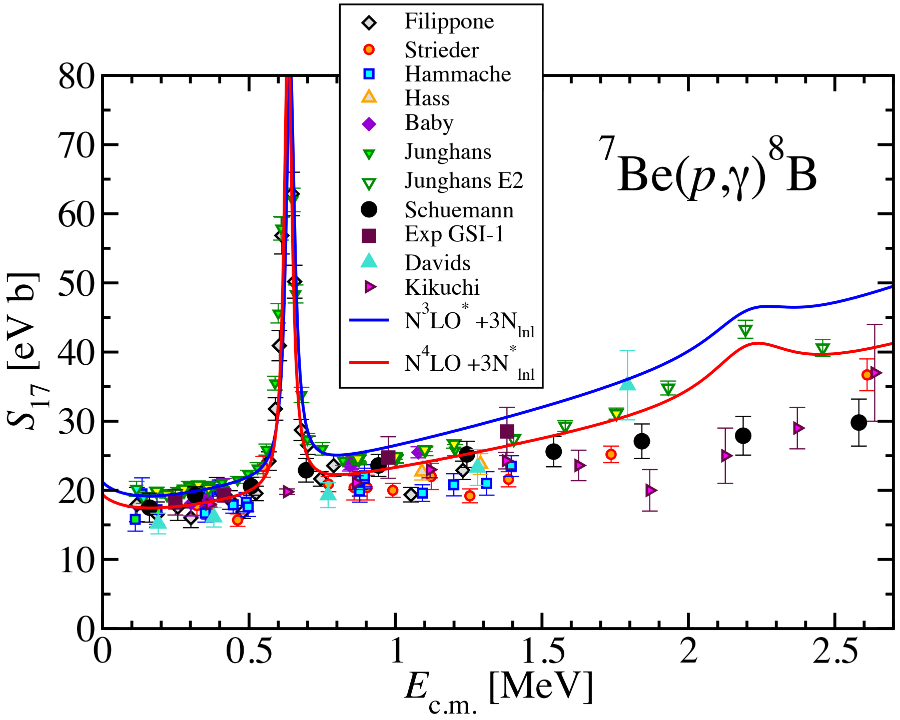

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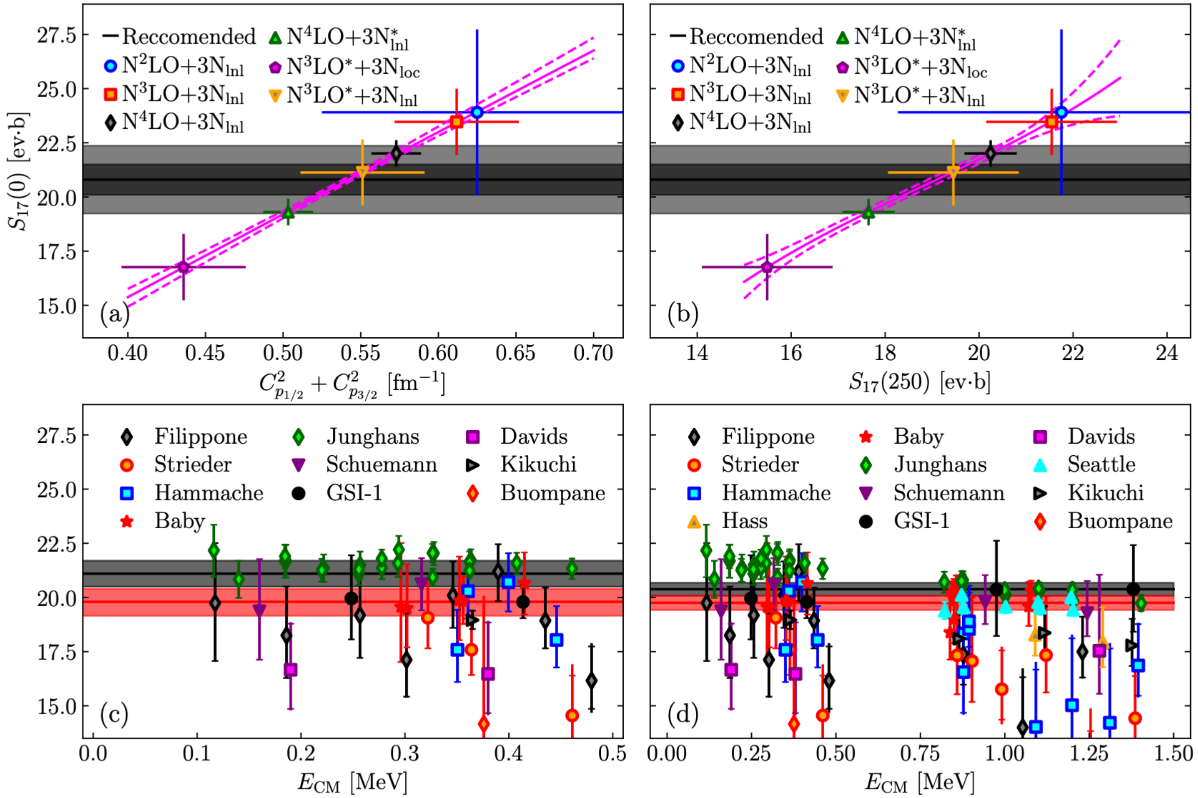

Recommended value $S_{17}(0)$ ~ 19.8(3) eV b

Latest evaluation in *Rev. Mod. Phys.* **83**,195–245 (2011):
$S_{17}(0)$ = 20.8 ± 0.7(expt) ± 1.4(theory) eV b

Conclusions

- *Ab initio* calculations of nuclear structure and reactions becoming feasible beyond the lightest nuclei
  - Make connections between the low-energy QCD, many-body systems, and nuclear astrophysics

- Applications of *ab initio* theory to nuclear reactions important for astrophysics
  - ^{4}He(d,γ)^{6}Li – importance of M1 contribution at very low energies
  - ^{7}Be(p,γ)^{8}B – new evaluation with significantly reduced uncertainty

- *Ab initio* nuclear theory essential for precision applications such as tests of fundamental symmetries
  - Quenching of g_A
  - Double beta decay matrix elements
  - Isospin mixing correction δ_C
  - Nuclear anapole moment, electric dipole moment
  - …

In synergy with experiments, *ab initio* nuclear theory is the right approach to understand low-energy properties of atomic nuclei

TRIUMF

Thank you!

Merci!

ありがとうございました

Discovery, accelerated