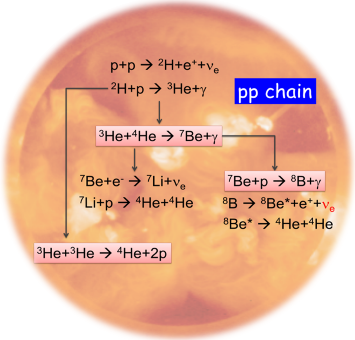
Ab initio calculations of reactions in the solar fusion chain

Mack C. Atkinson

Haverford College

^{3}He$(\alpha,\gamma)^7$Be important for solar-model predictions



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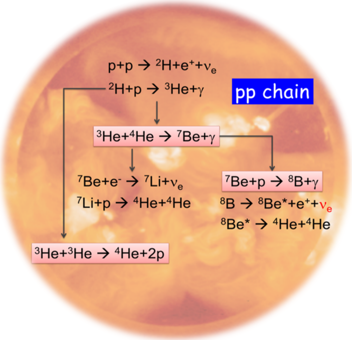

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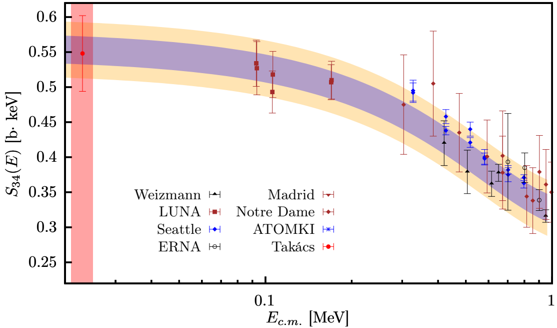
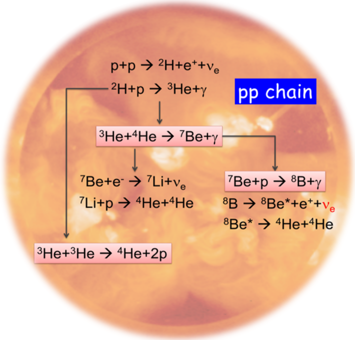


Acharya *et al.*, Rev Mod Phys **97** 035002 (2025)



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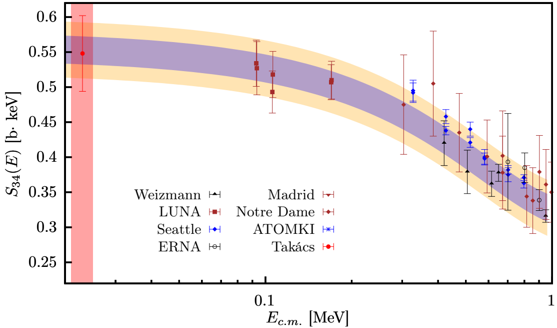

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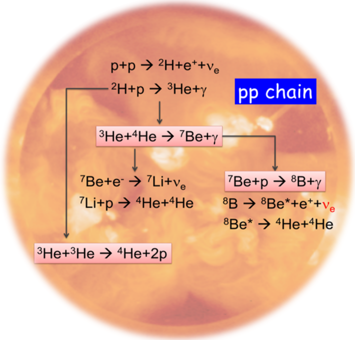

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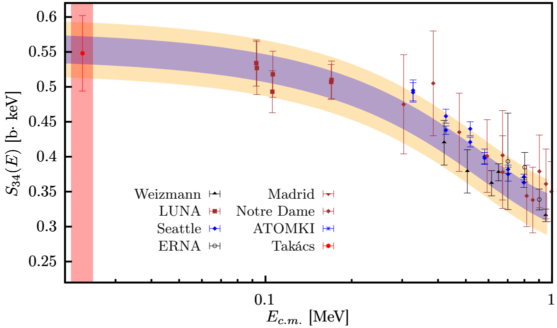

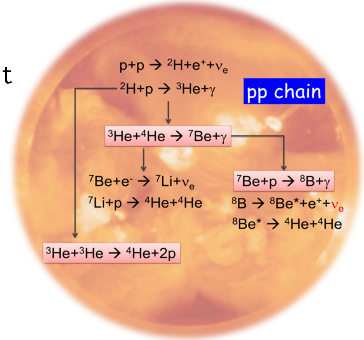

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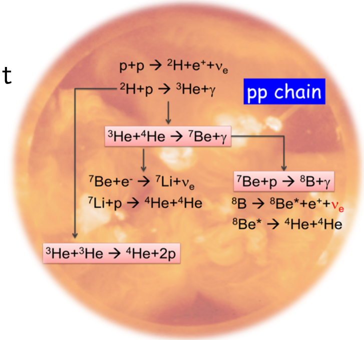
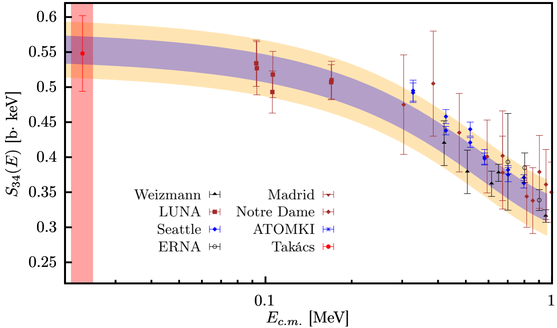
- Current evaluations depend on both theory and experiment
- Ideally, theory will accurately predict $S_{34}(E)$





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Current evaluation:

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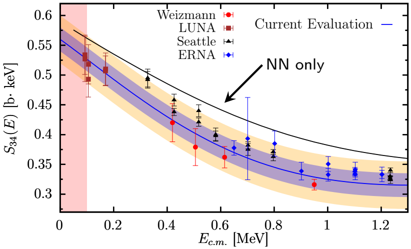

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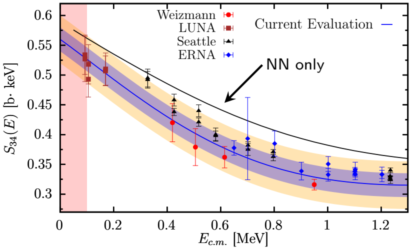

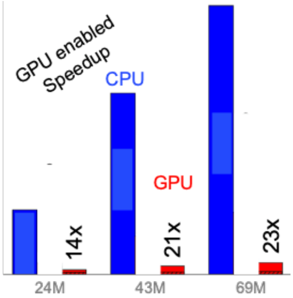

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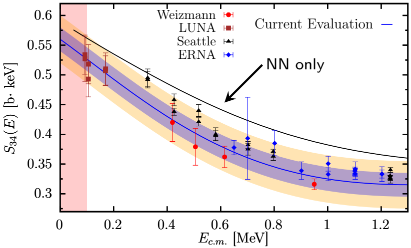

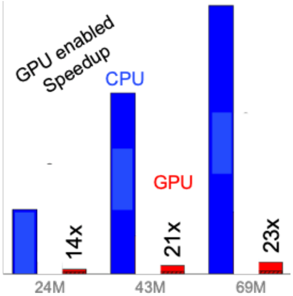

- GPU speedup $\implies$ NNN forces are now included

Ab initio reaction theory needed for capture calculations

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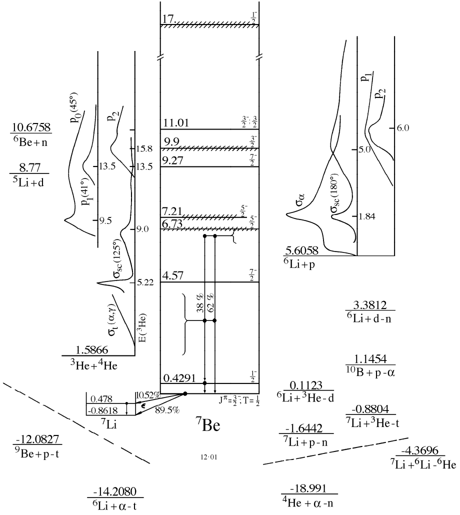

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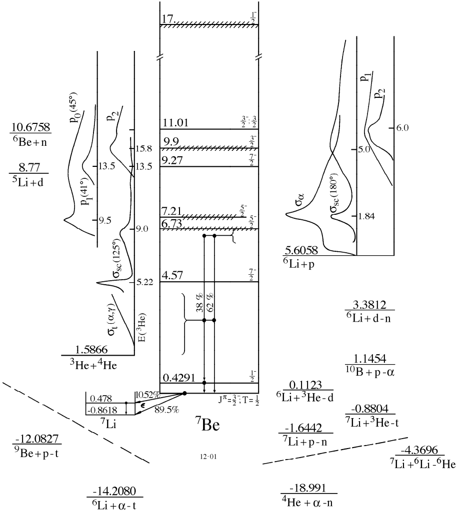
- Need a method to calculate ψ_{sc} and ψ_{bs} simultaneously



The *ab initio* method: from NCSM to NCSMC

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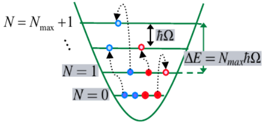

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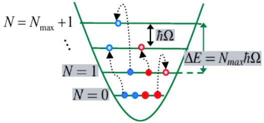

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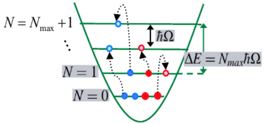

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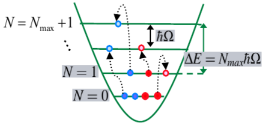

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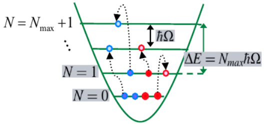

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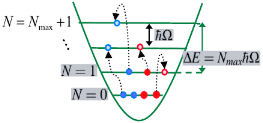

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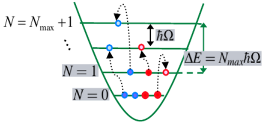

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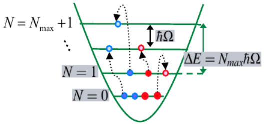

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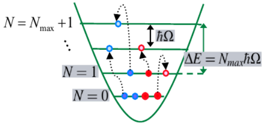

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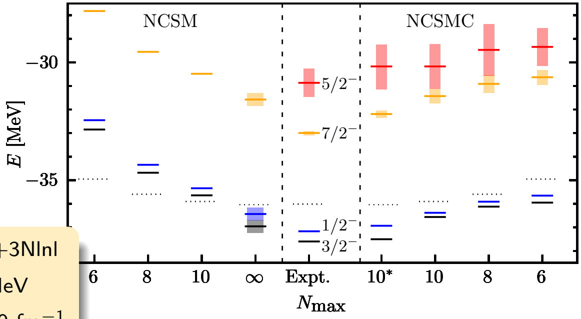
NCSMC Calculation of ^{3}He+^{4}He well-converged, levels need shifting



NN-N3LO+3NlnI

$\hbar\Omega = 20$ MeV

$\lambda_{\rm SRG} = 2.0$ fm^{-1}

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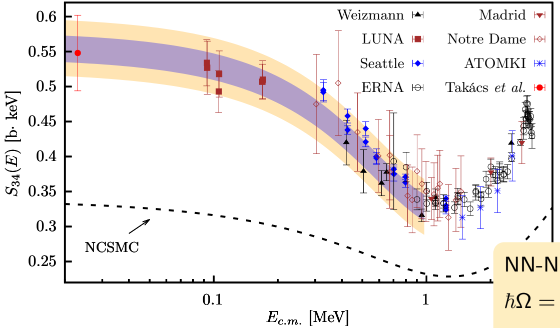

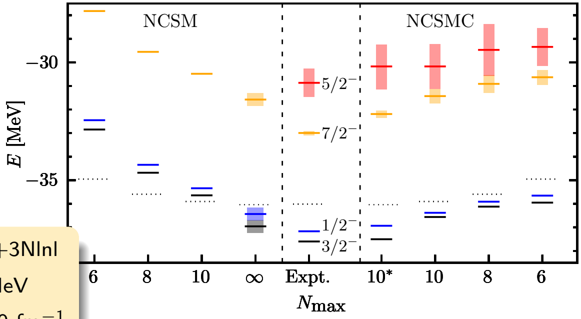

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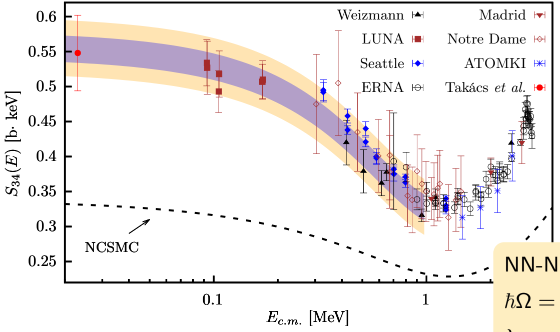

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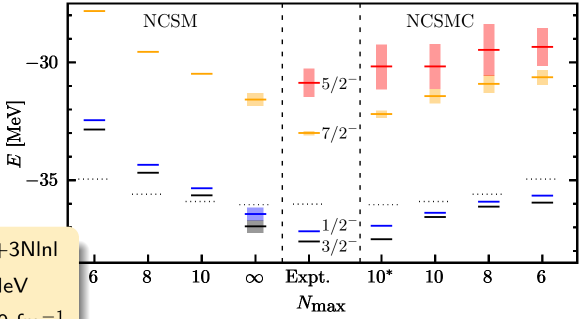

^{7}Be	NCSM	NCSMC	Expt.
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$\mathcal{C}_{3/2^-}$	-	3.46	-
$\mathcal{C}_{1/2^-}$	-	3.44	-
$r_{\rm ch}$	2.44	2.70	2.647(17)

- Capture rate accurate only if Expt. levels reproduced

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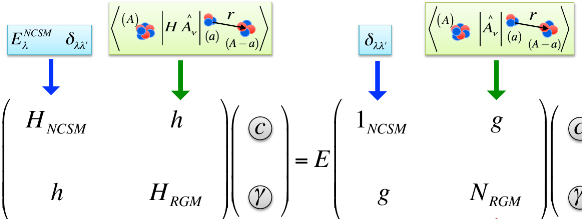

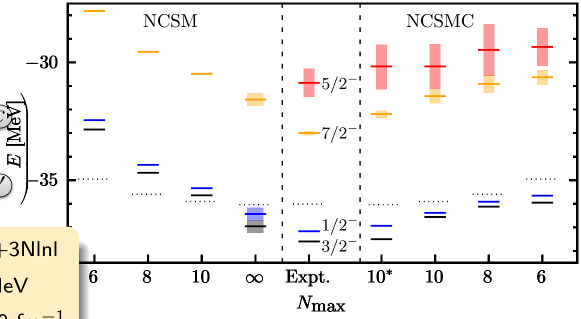

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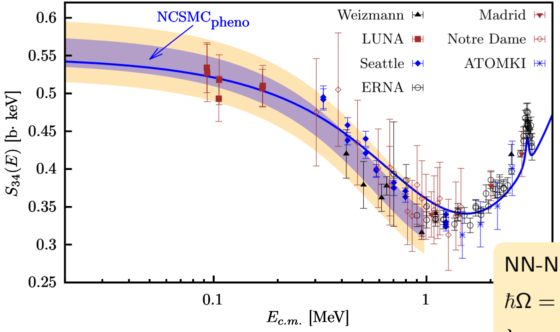

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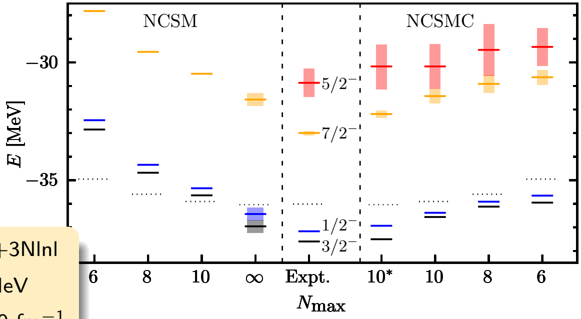
$\lambda_{\text{SRG}} = 2.0$ fm^{-1}



^{7}Be	NCSM	NCSMC	NCSMC$_{\text{pheno}}$	Expt.
$E_{3/2^-}$	0.261	-1.05	-1.587	-1.587
$E_{1/2^-}$	0.563	-0.874	-1.16	-1.16
$\mathcal{C}_{3/2^-}$	-	3.46	4.20	-
$\mathcal{C}_{1/2^-}$	-	3.44	3.79	-
r_{ch}	2.44	2.70	2.63	2.647(17)

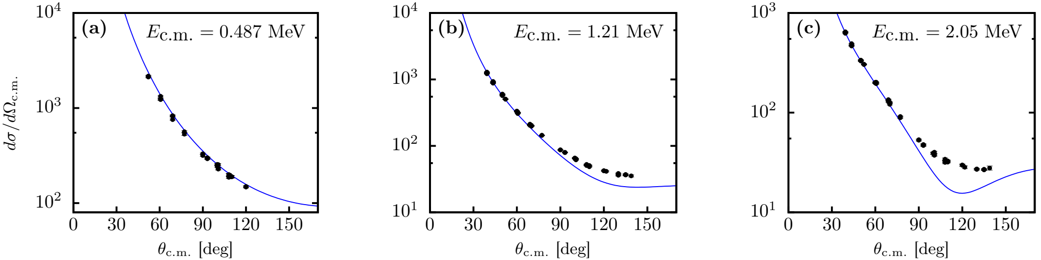
- Capture rate accurate only if Expt. levels reproduced

$$E_\lambda^{NCSM} \rightarrow E_\lambda^{NCSM} + \epsilon$$

M.C. Atkinson *et al.*, PLB **860** 139189 (2025)

Now, how about the scattering wave functions?

- Compare to elastic scattering results to further probe ψ_{sc}



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Paneru *et al.*, PRC **109** 015802 (2024)

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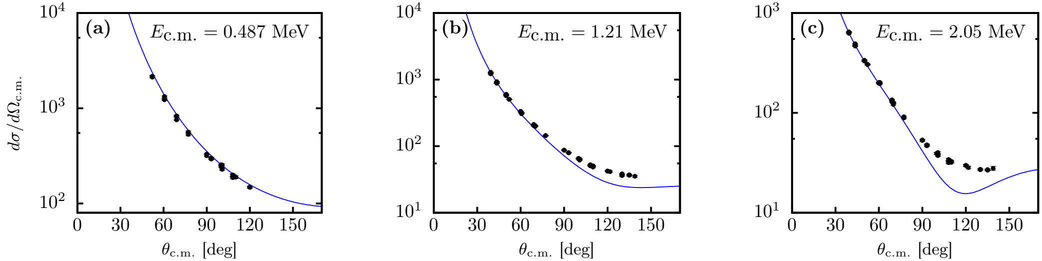

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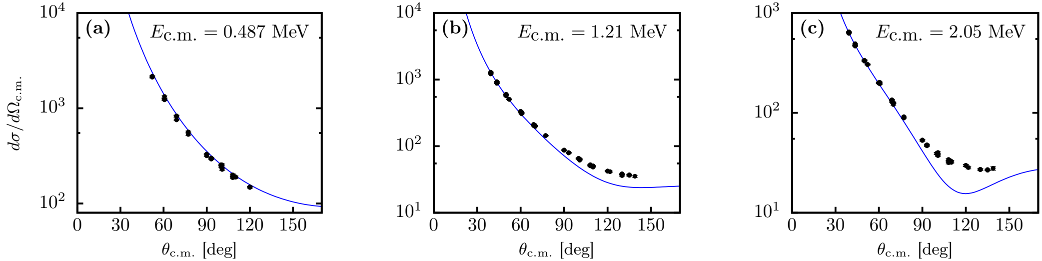

- What is the source of discrepancy at large angles?

NN-N3LO+3NlnI
$\hbar\Omega = 20$ MeV
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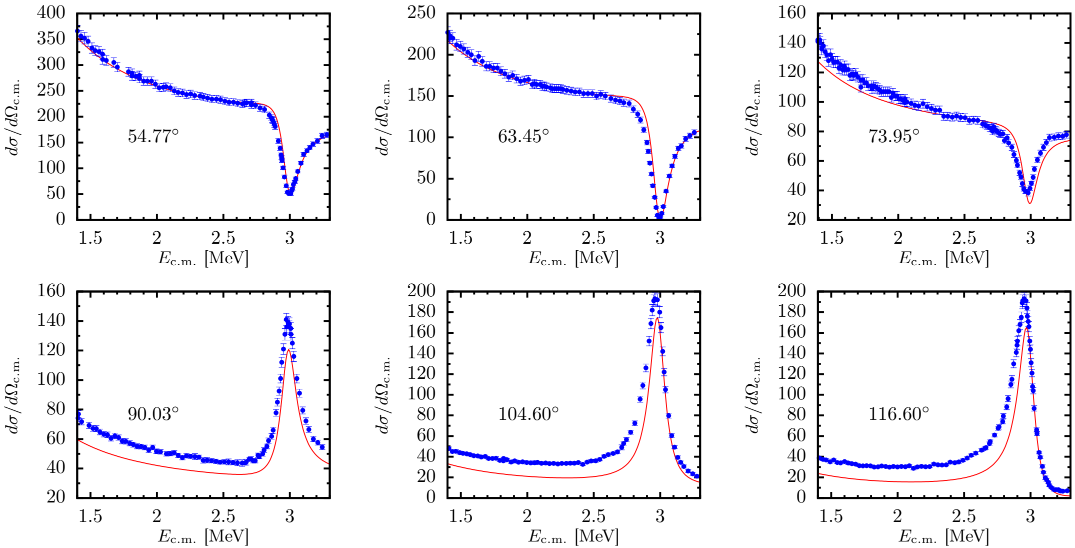
Paneru *et al.*, PRC **109** 015802 (2024)

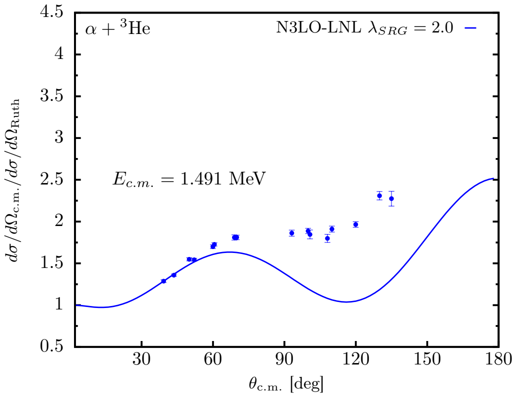
Same large-angle discrepancy when comparing to 1964 Barnard *et al.*



Diagnosing the discrepancy

- Rutherford obscures the fact that a constant shift accounts for the discrepancy

$$\frac{d\sigma}{d\Omega}_{\text{Ruth}} = \left(\frac{Z_1 Z_2 e^2}{8\pi\epsilon_0 m v^2 \sin^2\left(\frac{\theta}{2}\right)}\right)^2$$



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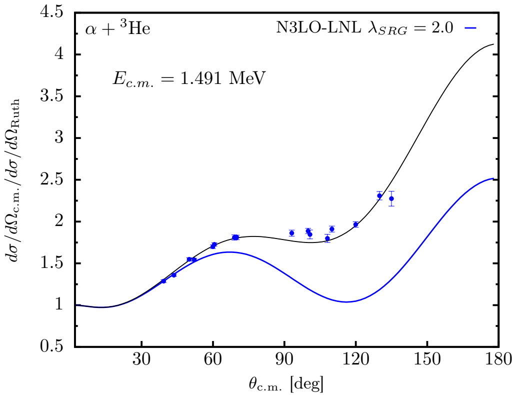

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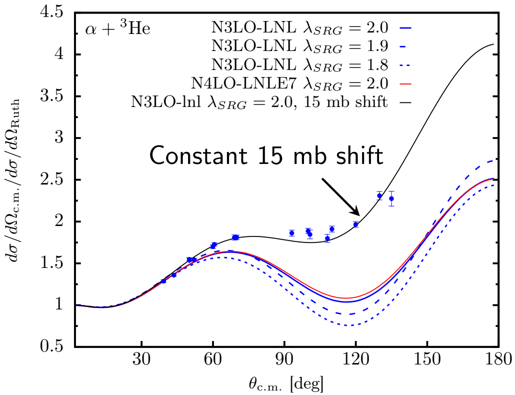

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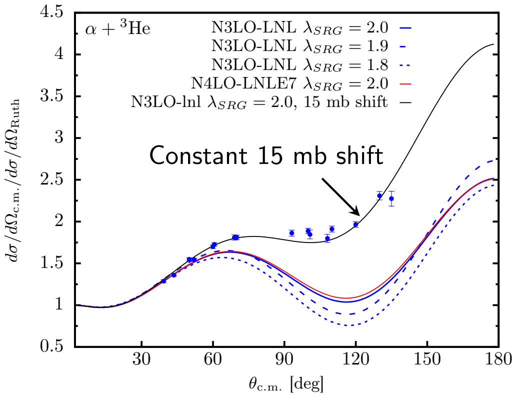
How can we emulate a constant shift?



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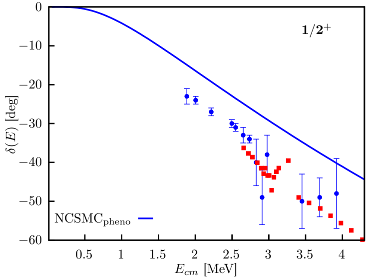

D. Hardy *et al.*, Nucl Phys A **195** 250 (1972) R.J. Spiger *et al.*, Phys Rev **163** 964 (1967) M.C. Atkinson *et al.*, PLB **860** 139189 (2025)

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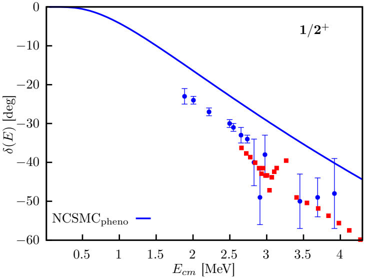

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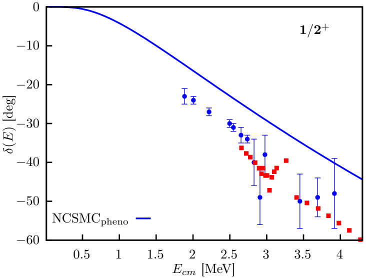

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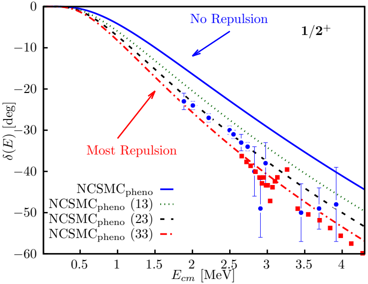

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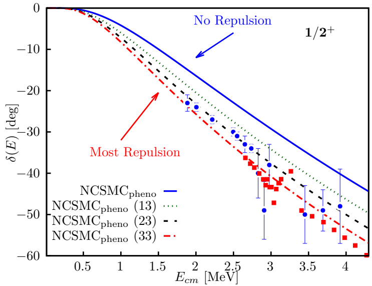

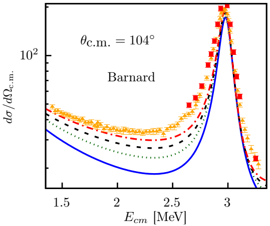

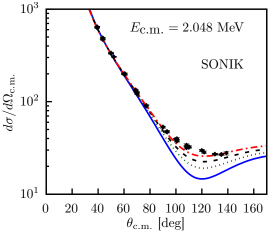

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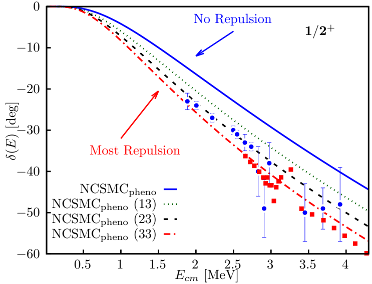

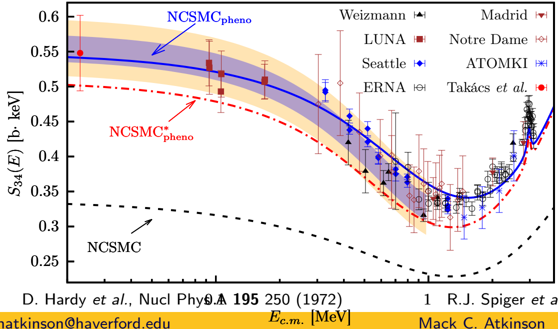

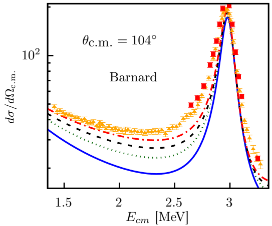

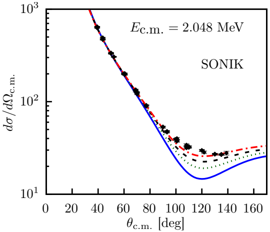

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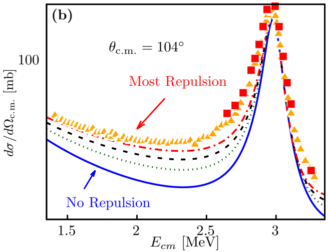
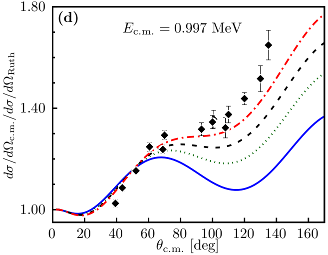
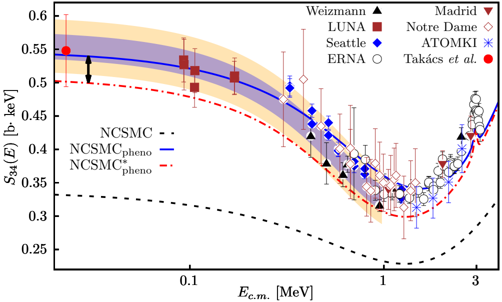
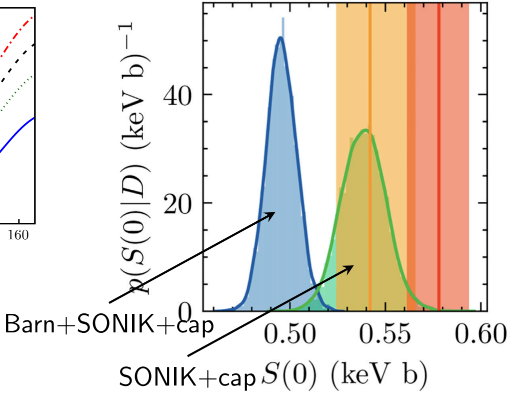
Tension in data sets also observed in R matrix analyses







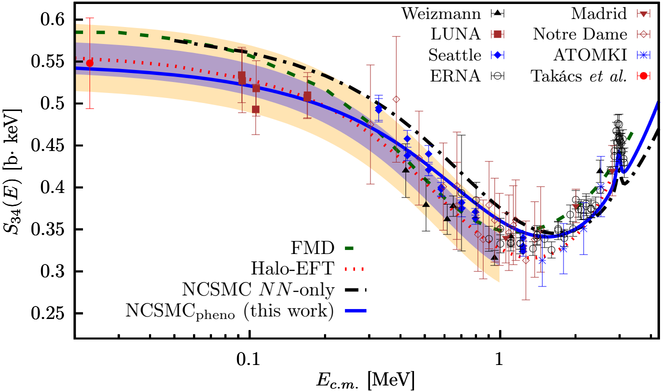


- Simultaneous R matrix fit of capture and elastic scattering

Odell *et al.*, Front. in Phys. **10** 888476 (2022)

Data-Informed S factor

- Tension between elastic and capture data dominates the uncertainty



Model	$S_{34}(0)$ [keV b]
NCSMC$_{\text{pheno}}$	0.545 ± 0.001
NCSMC$^{*}_{\text{pheno}}$	0.505
halo EFT [9]	$0.577^{+0.015}_{-0.016}$
halo EFT [10]	$0.558 \pm 0.008(\text{fit}) \pm 0.056(\text{EFT})$
R-matrix [60]	$0.539^{+0.011}_{-0.012}$
SF III [2]	$0.561 \pm 0.018(\text{exp}) \pm 0.022(\text{th})$

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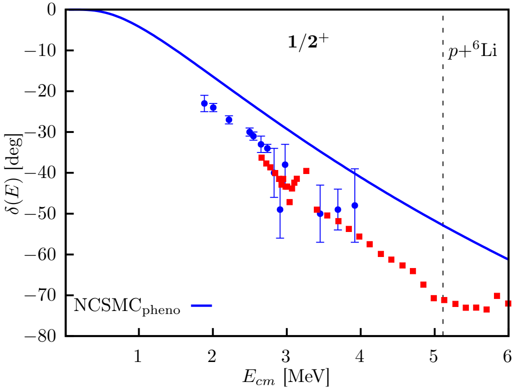

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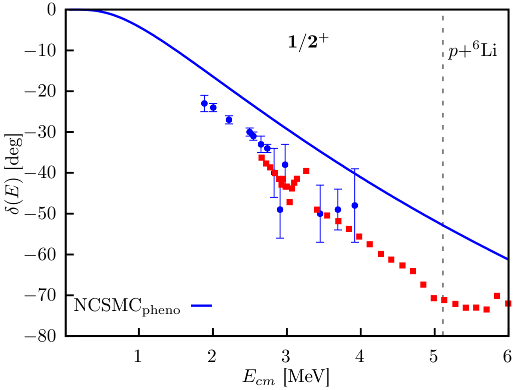
2. **Chiral interaction**
   - Phase shift shows some dependence on interaction
   - Need to compare more interactions



From bound to continuum: $^{11}\text{Be} \rightarrow (p + {}^{10}\text{Be}) + \beta + \nu$

Physics Letters B 732 (2014) 305–308

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D. Baye and E.M. Tursunov, PLB **696**, 4, 464-467 (2011)

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  2. There are unobserved dark decay modes

Editors' Suggestion

Direct Observation of Proton Emission in ^{11}Be

Y. Ayyad,[1,2,*] B. Olaizola,[3] W. Mittig,[2,4] G. Potel,[1] V. Zelevinsky,[1,2,4] M. Horoi,[5] S. Beceiro-Novo,[4] M. Alcorta,[3] C. Andreoiu,[6] T. Ahn,[7] M. Anholm,[3,8] L. Atar,[9] A. Babu,[3] D. Bazin,[2,4] N. Bernier,[3,10] S. S. Bhattacharjee,[3] M. Bowry,[3] R. Caballero-Folch,[3] M. Cortesi,[2] C. Dalitz,[11] E. Dunling,[3,12] A. B. Garnsworthy,[3] M. Holl,[3,13] B. Kootte,[3,8] K. G. Leach,[14] J. S. Randhawa,[2] Y. Saito,[3,10] C. Santamaria,[15] P. Šiurytė,[3,16] C. E. Svensson,[9] R. Umashankar,[3] N. Watwood,[2] and D. Yates[3,10]

PHYSICAL REVIEW LETTERS **123,** 082501 (2019)

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- Directly observed the protons from $^{11}\text{Be}(\beta p)^{10}\text{Be}$

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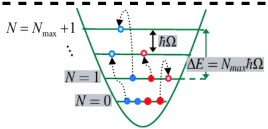
- Measured consistent branching ratio $b_p = 1.3(3) \times 10^{-5}$
  - Still orders of magnitude larger than theoretical predictions
- Predict the $(\frac{1}{2}^+, \frac{1}{2})$ proton resonance at 197 keV from the proton energy distribution

NCSMC calculation of ^{11}Be and ^{11}B



$$\Psi^{A} = \sum_{N=0}^{N_{\max}} \sum_{i} c_{Ni} \Phi^{A}_{Ni}$$

$$\hat{H} = \hat{T} + \hat{V}_{NN} + \hat{V}_{NNN}$$

$$\hat{H}\left|\Psi^{A}\right\rangle = E\left|\Psi^{A}\right\rangle$$

NCSM

NCSMC

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

$$\left|^{11}\mathrm{B}\right\rangle \qquad \left|p\right\rangle \otimes \left|^{10}\mathrm{Be}\right\rangle$$

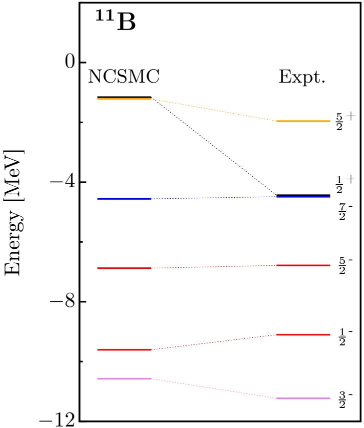
$$\left\langle \Psi_{sc}\left(p + {}^{10}\mathrm{Be}\right) \middle| \hat{\mathcal{M}}_{\mathrm{GT}} \middle| \Psi_{bs}\left({}^{11}\mathrm{Be}\right) \right\rangle$$

NCSMC Calculation of ^{11}B and ^{11}Be

NN-N4LO(500)+3NlnI

$\hbar\Omega = 18$ MeV, $N_{\max} = 7$

$\lambda_{\rm SRG} = 1.8$ fm^{-1}



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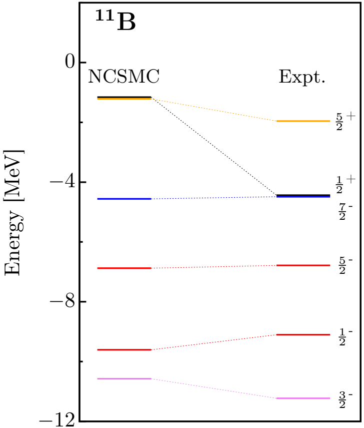

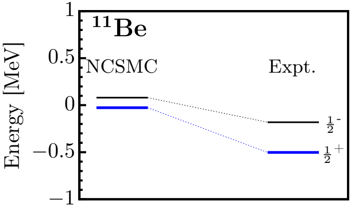

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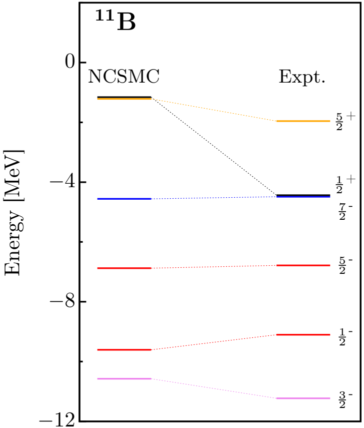

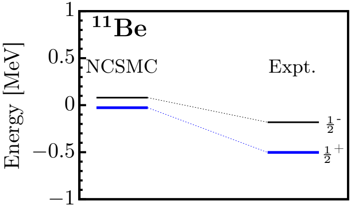

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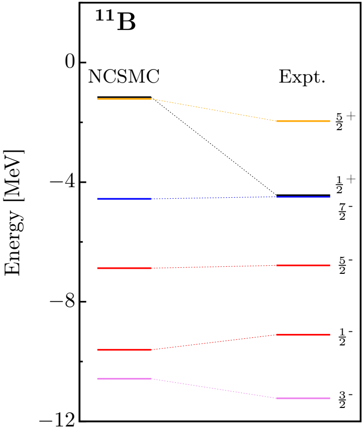

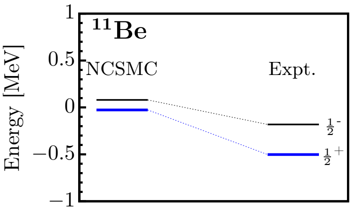

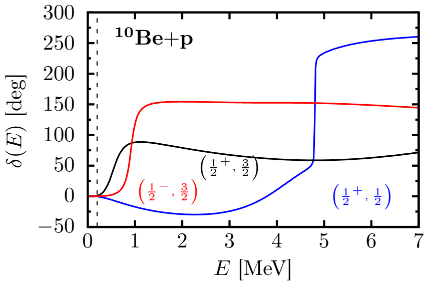

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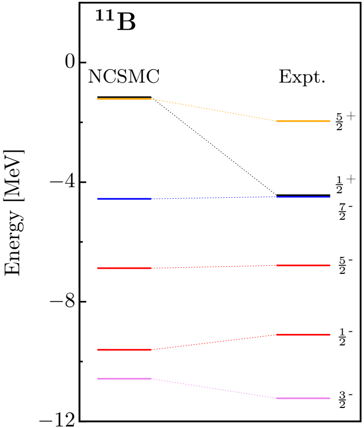

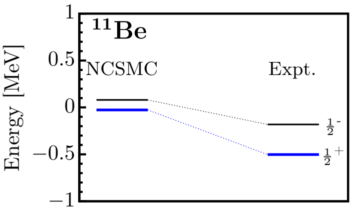

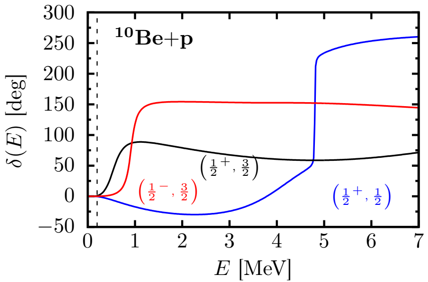

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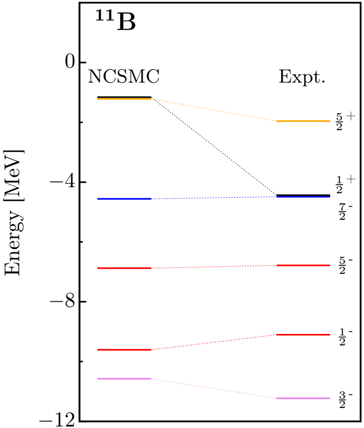

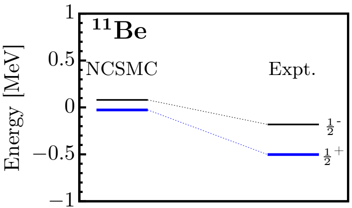

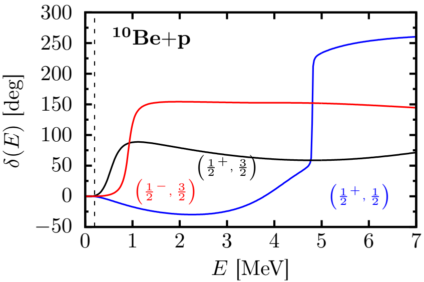

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NCSMC Calculation of ^{11}B and ^{11}Be

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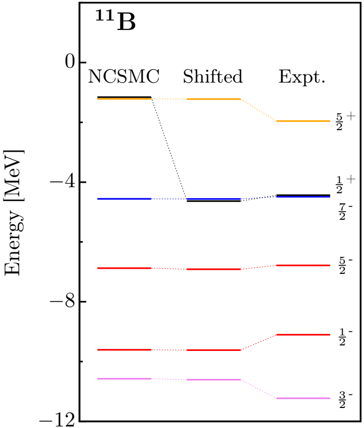

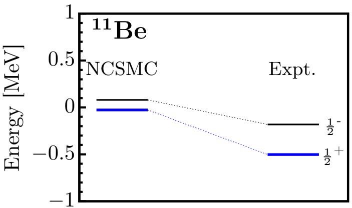

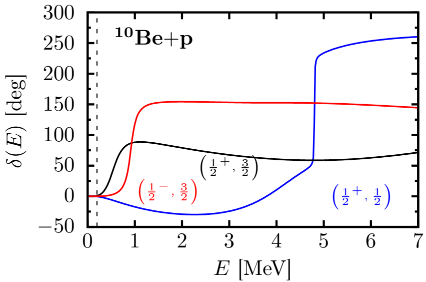

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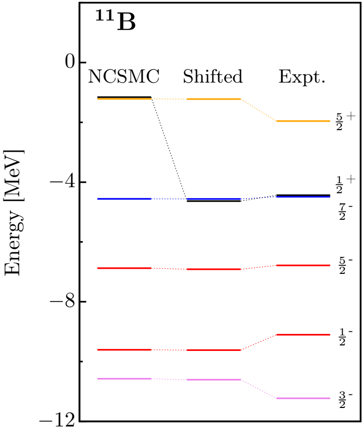

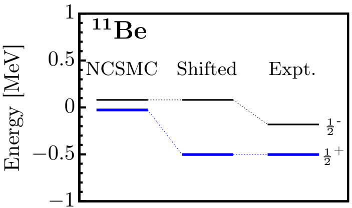

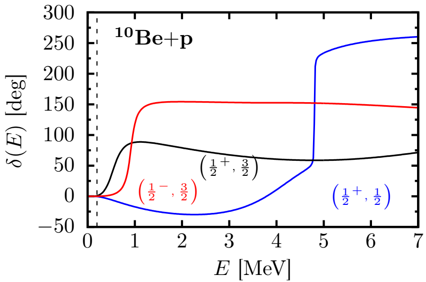

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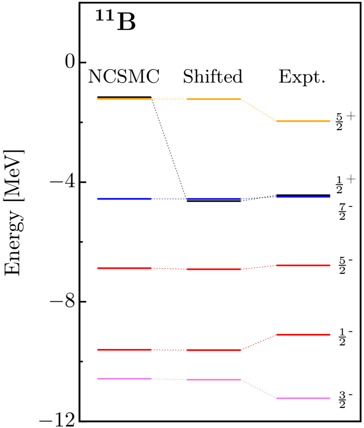

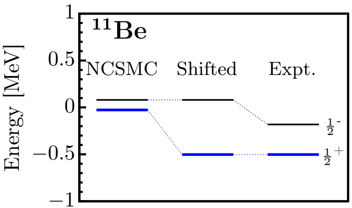

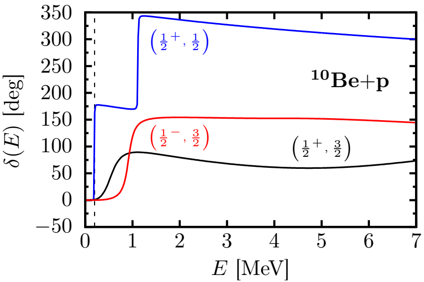

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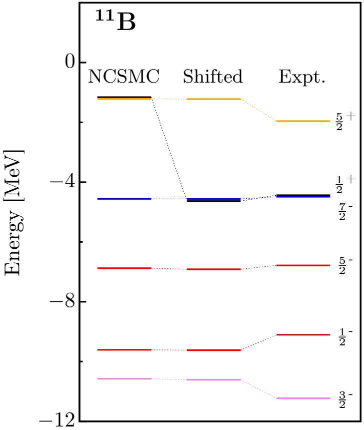

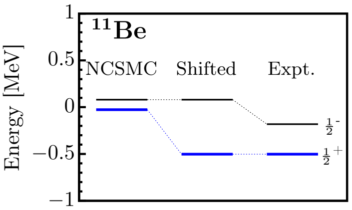

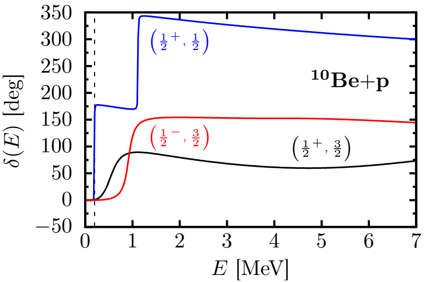

	NCSMC-shifted	Expt.
E [keV]	197	197(20)
Γ [keV]	10	12(5)

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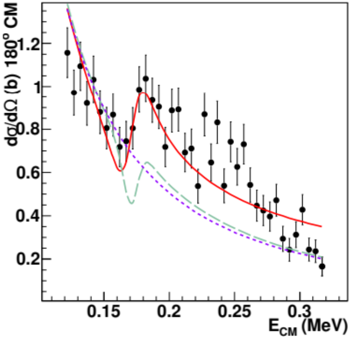
The $1/2^+$ resonance does enhance the branching ratio

Ayyad *et al.*, PRL **129** 012501 (2022)



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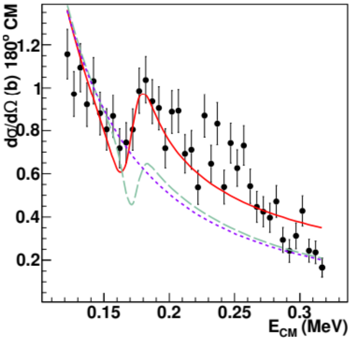

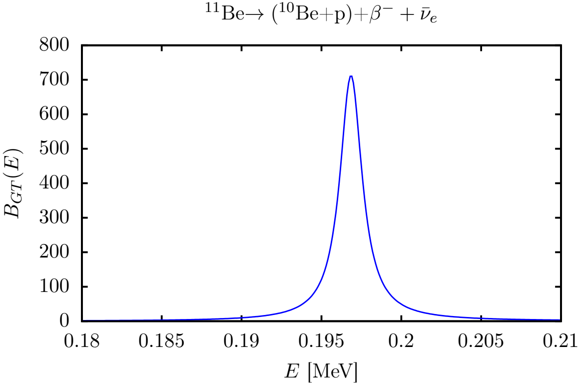

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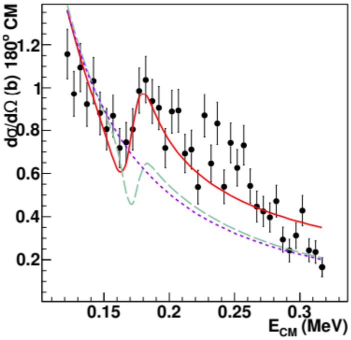

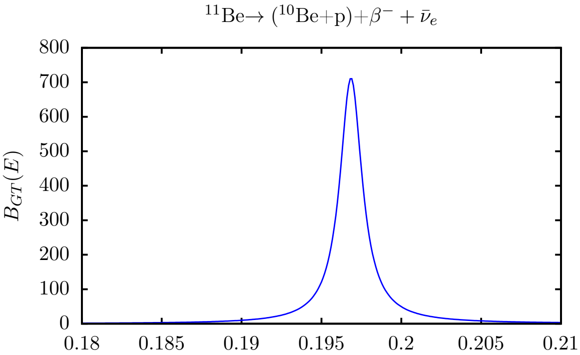

$(1/2^+, 1/2)$	$N_{\max}=5$		$N_{\max}=7$		Expt.
	NCSM	NCSMC$_{\text{pheno}}$	NCSM	NCSMC$_{\text{pheno}}$	
$B(\mathrm{GT})$	1.95	0.325	1.39	0.565	$5.5^{8.3}_{3.3}$
b_p	—	7.4×10^{-7}	—	1.3×10^{-6}	$1.3(3) \times 10^{-5}$

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Summary

- *Ab initio* calculation of ^{3}He$(\alpha,\gamma)^7$Be capture reaction using the NCSMC
- NCSMC results with $NN+3N$ quantitatively reproduce data
- Simultaneous analysis of elastic and capture data reveals tension
- Future: Explore lack of repulsion in $1/2^+$ channel
- Future: Include $p+{}^6$Li channel

Thanks!

Sofia Quaglioni

Kostas Kravvaris

(LLNL)

Guillame Hupin

(IN2P3)

Petr Navratil

(TRIUMF)