

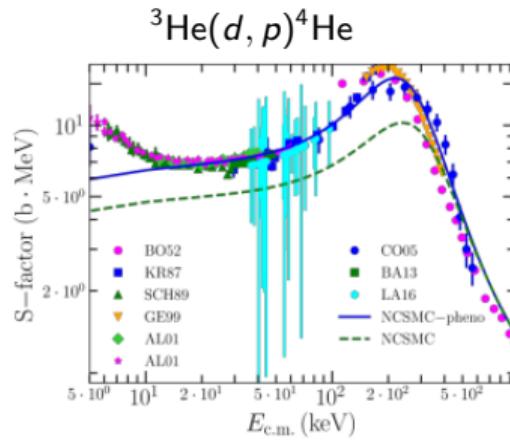
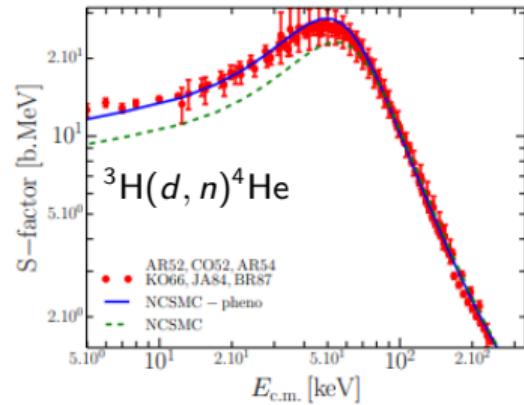
# *Ab initio* reactions: from continuum to bound states and back

Mack C. Atkinson



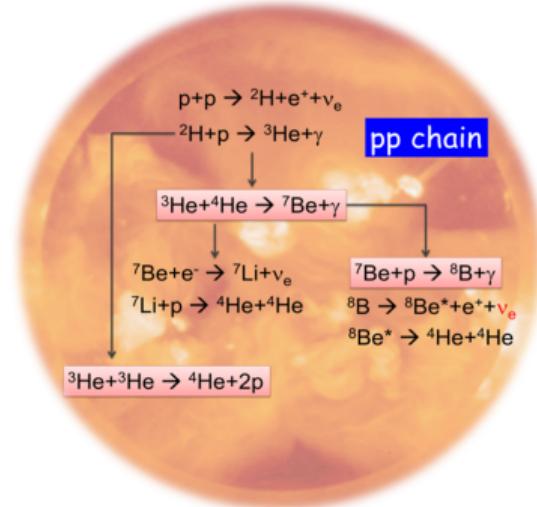
# Introduction

- Huge progress in *ab initio* calculations of bound properties
- *Ab initio* calculations of continuum properties are limited to much lighter nuclei
- While this is a limited region of the nuclear chart, there is an abundance of interesting reactions involving light nuclei that can be studied
- Simultaneous description of bound and scattering states leads to a better understanding of fusion rates, constraints on BSM physics, etc.

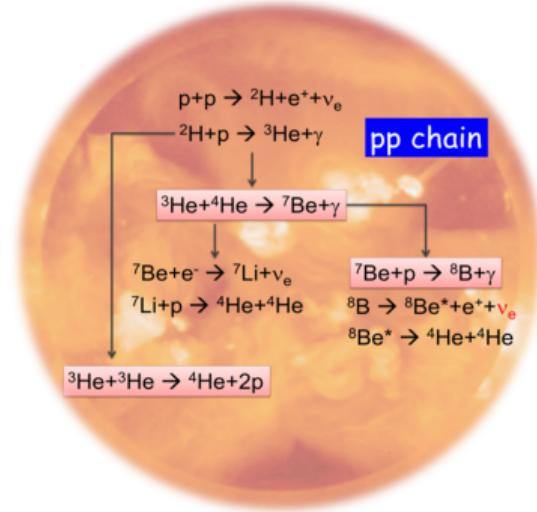


From continuum to bound:  ${}^3\text{He}(\alpha, \gamma){}^7\text{Be}$

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

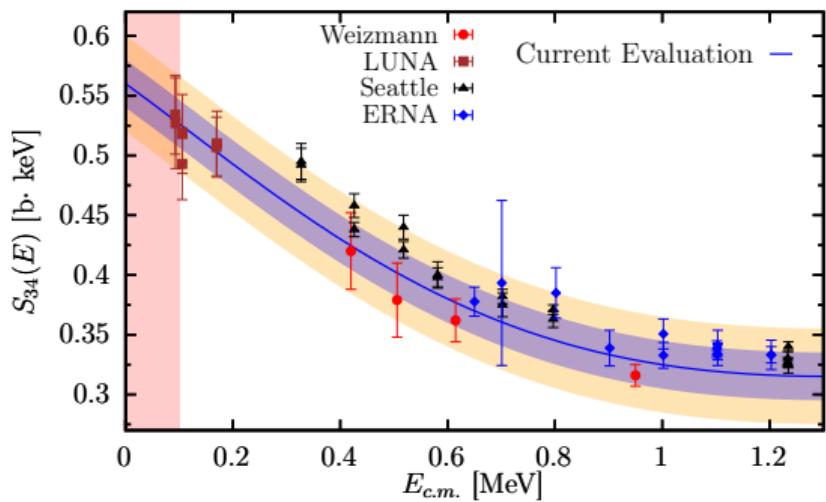


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$$\sigma(E) = \frac{S_{34}(E)}{E} \exp \left\{ -\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2E/m}} \right\}$$

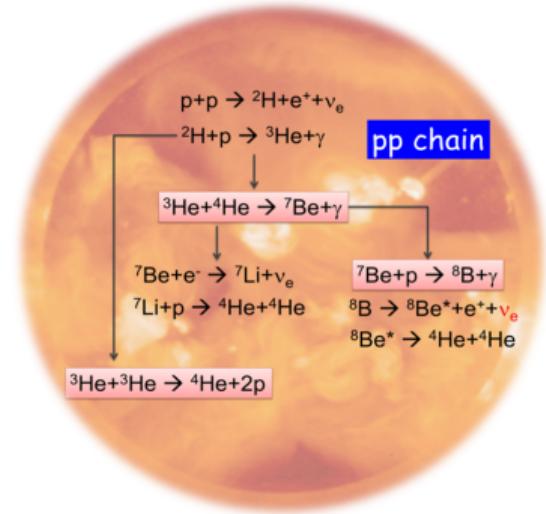
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Adelberger *et al.*, Rev Mod Phys 83 195 (2011)

atkinson27@llnl.gov

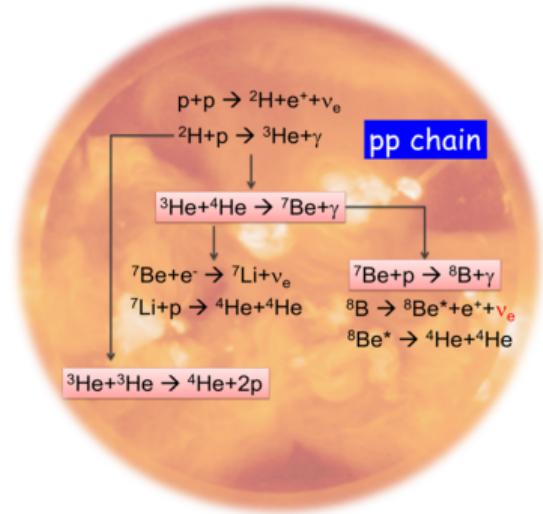
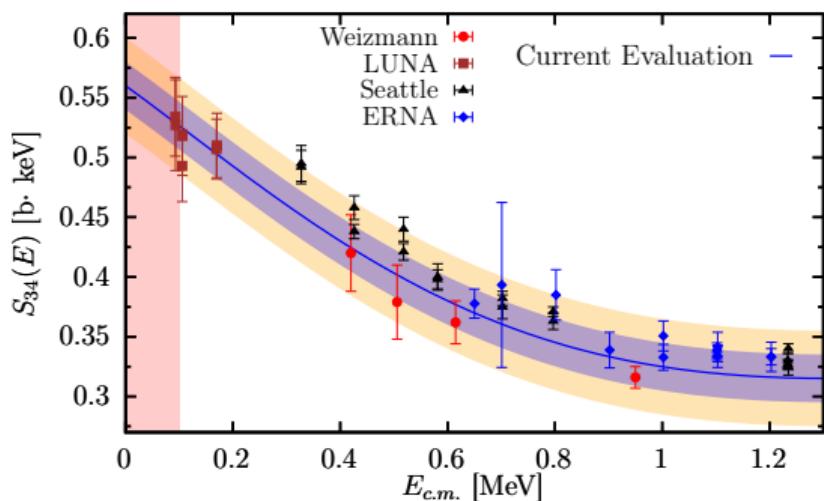
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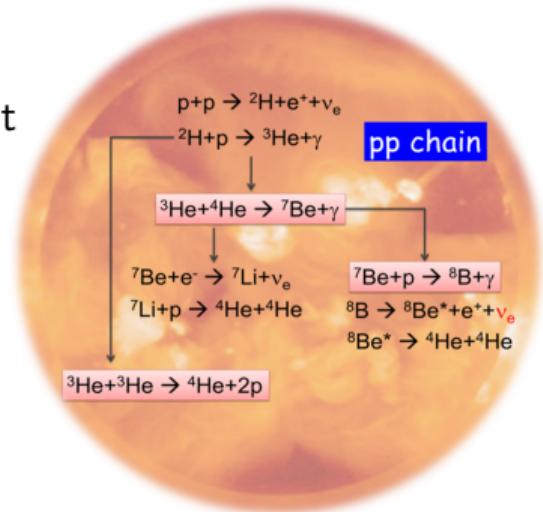
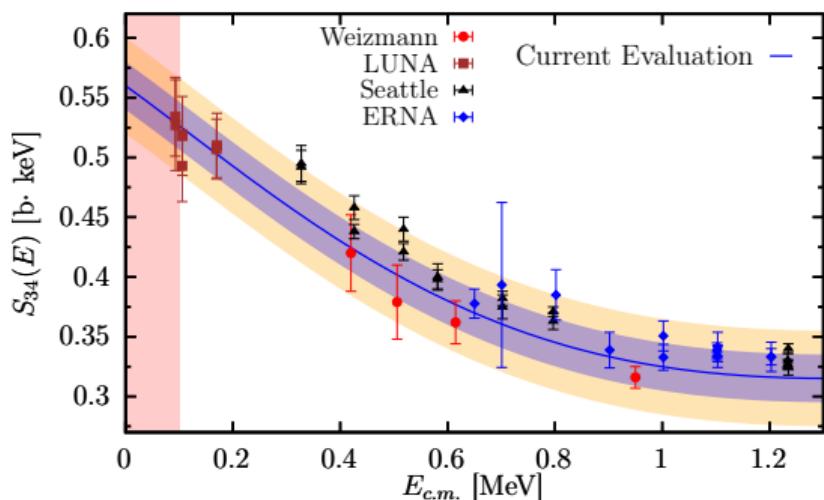
- Reaction rates too low at solar energies in the lab



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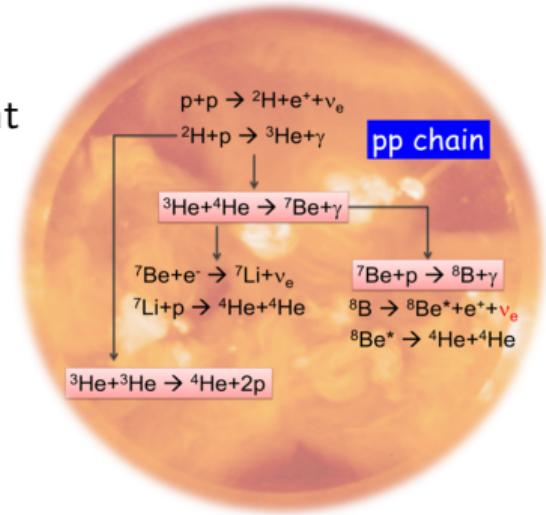
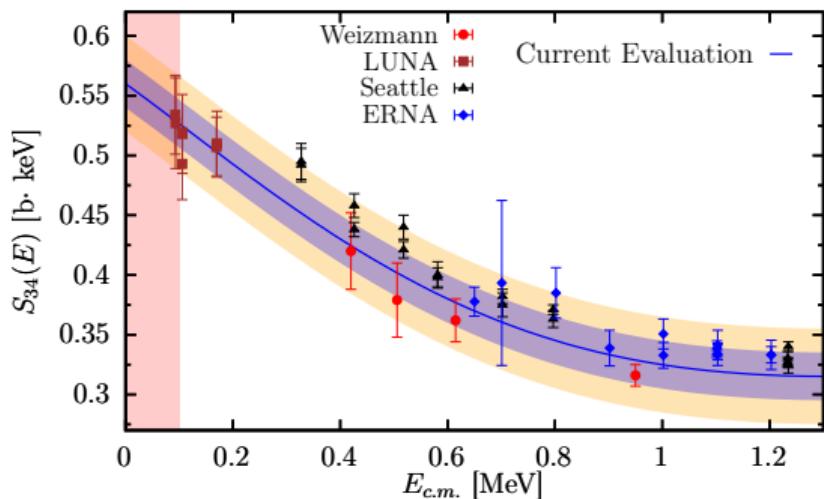
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- Current evaluations depend on both theory and experiment



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- Reaction rates too low at solar energies in the lab
- Current evaluations depend on both theory and experiment
- Ideally, theory will accurately predict  $S_{34}(0)$



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# The *ab initio* method: from NCSM to NCSMC

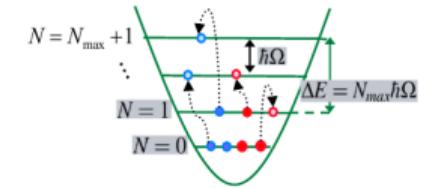
$$\left\langle \Psi_{bs} ({}^7\text{Be}) \mid \hat{\mathcal{M}}_{\text{EM}} \mid \Psi_{sc} ({}^3\text{He} + \alpha) \right\rangle$$

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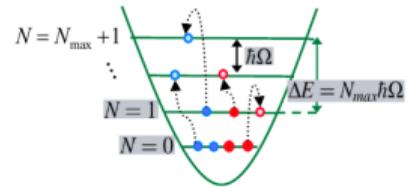


$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

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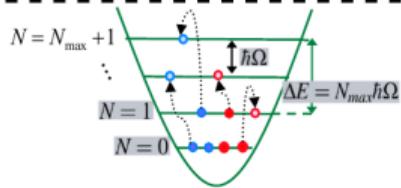
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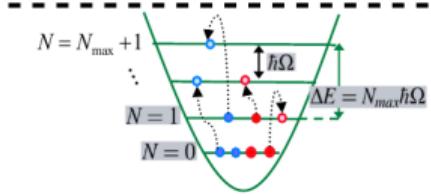
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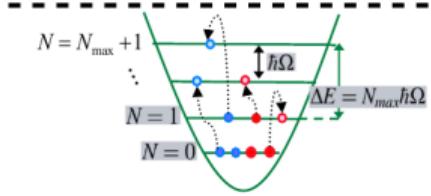
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$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} |(A) \text{ nuclei}, \lambda \rangle + \sum_v \int d\vec{r} \gamma_v(\vec{r}) \hat{A}_v \left|_{(A-a)} \text{ nuclei}, v \right\rangle$$

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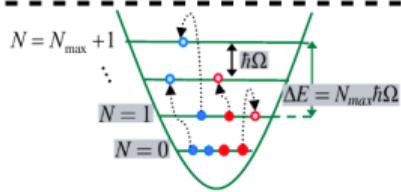
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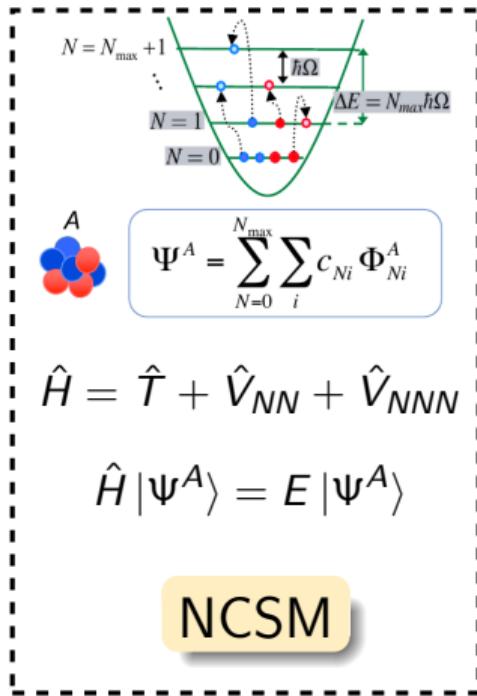
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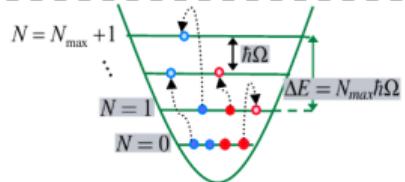
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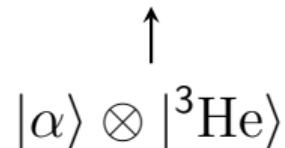
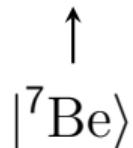
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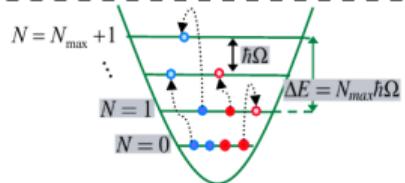
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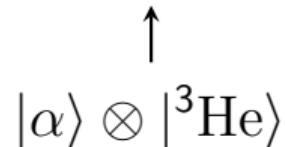
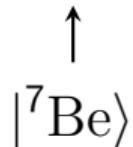
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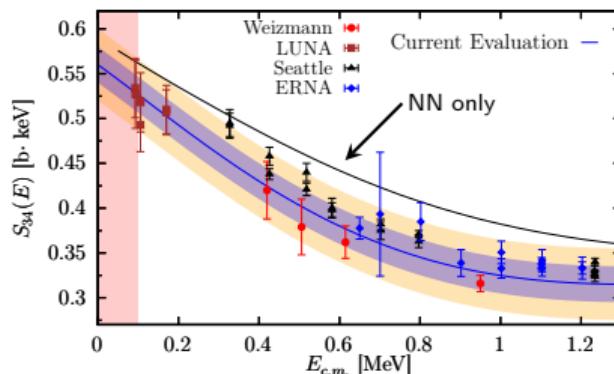
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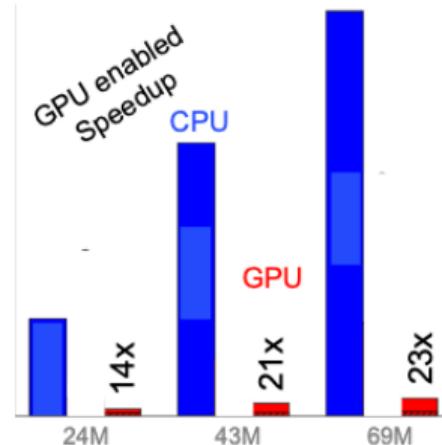
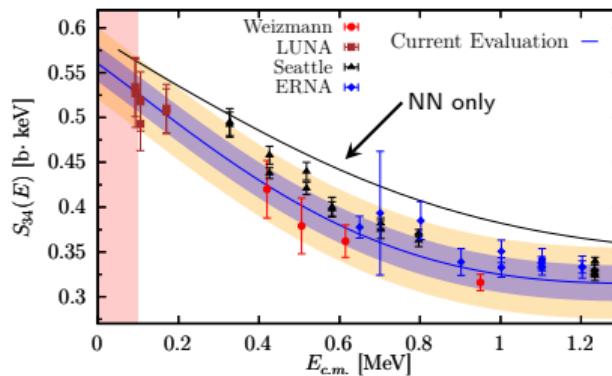


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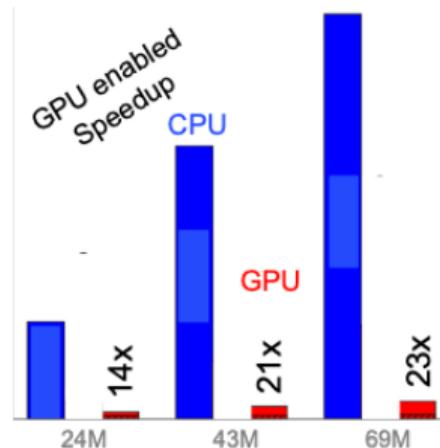
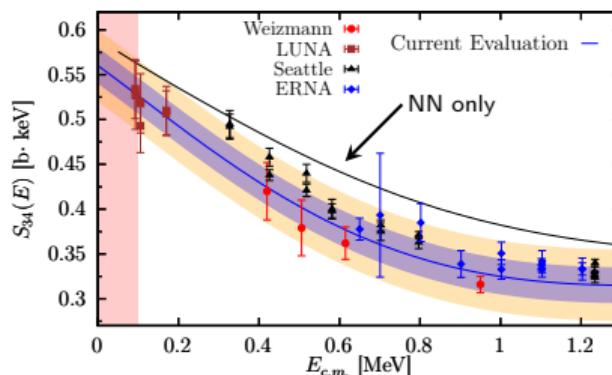


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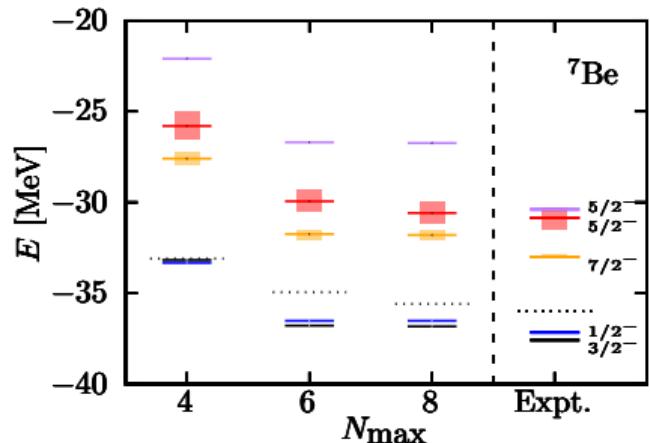
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- GPU speedup  $\implies$  NNN forces are now included

# NCSMC Calculation of $^3\text{He} + ^4\text{He}$ shows reasonable agreement with data



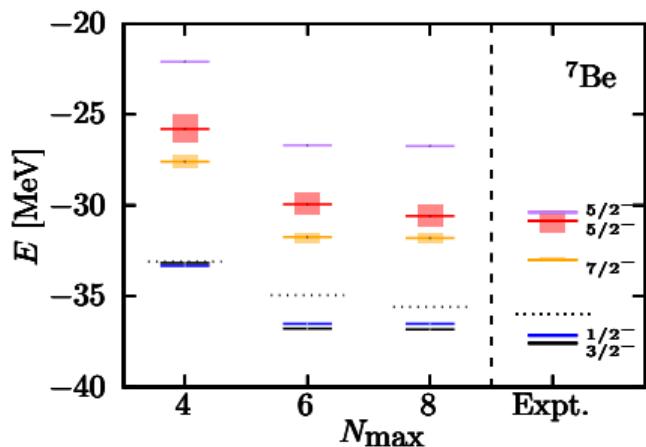
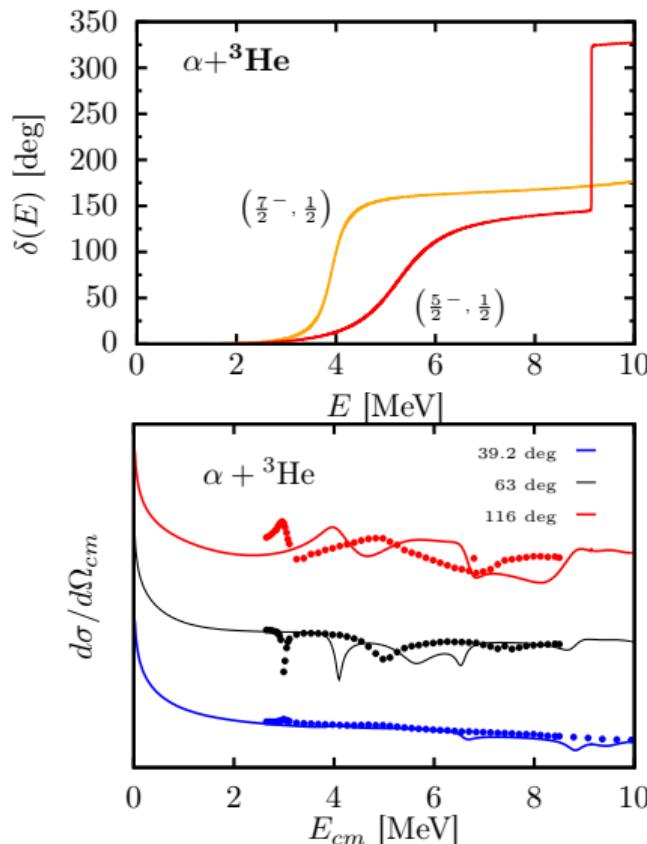
NN-N3LO+3Nlnl

$\hbar\Omega = 20 \text{ MeV}$

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

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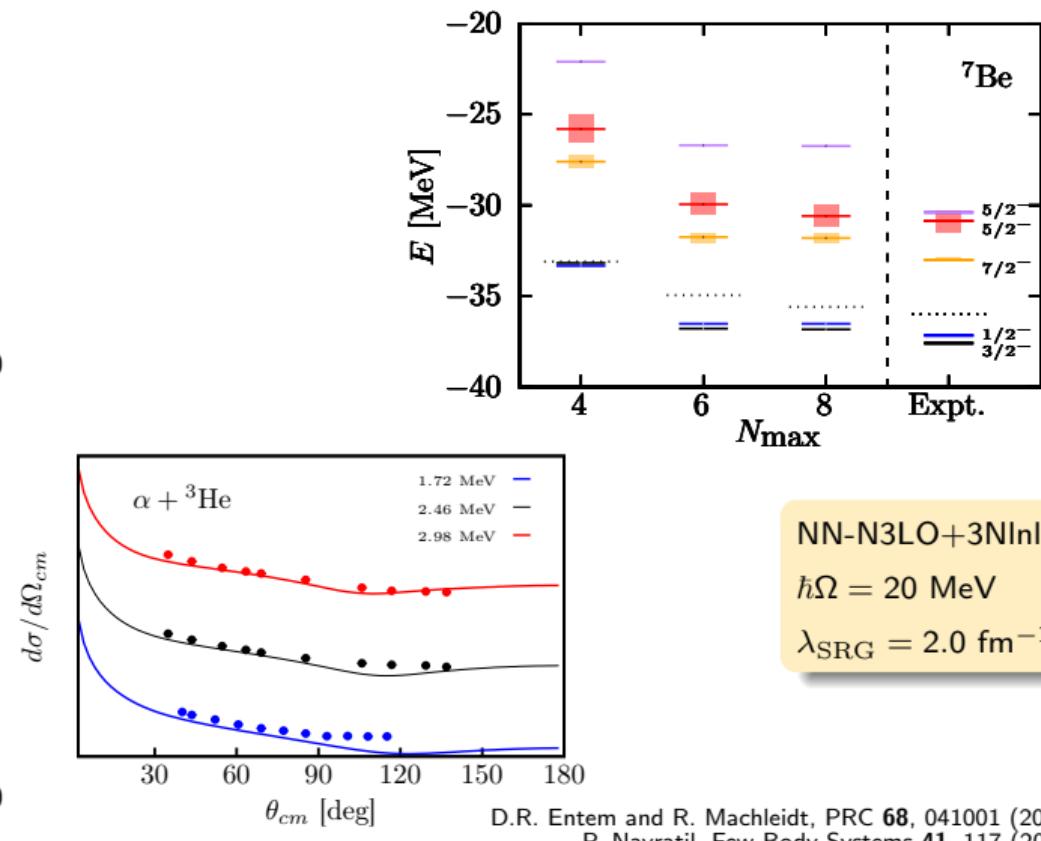
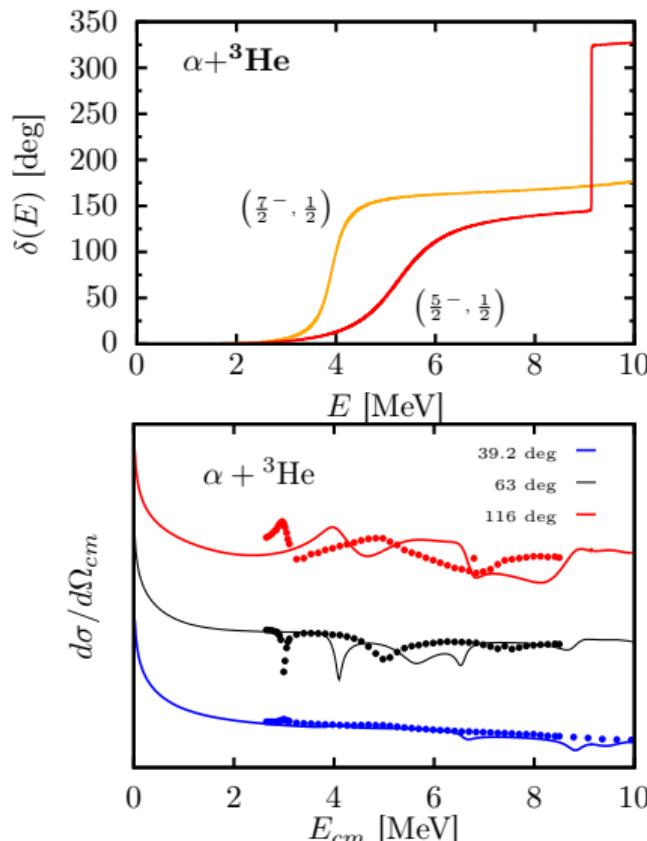
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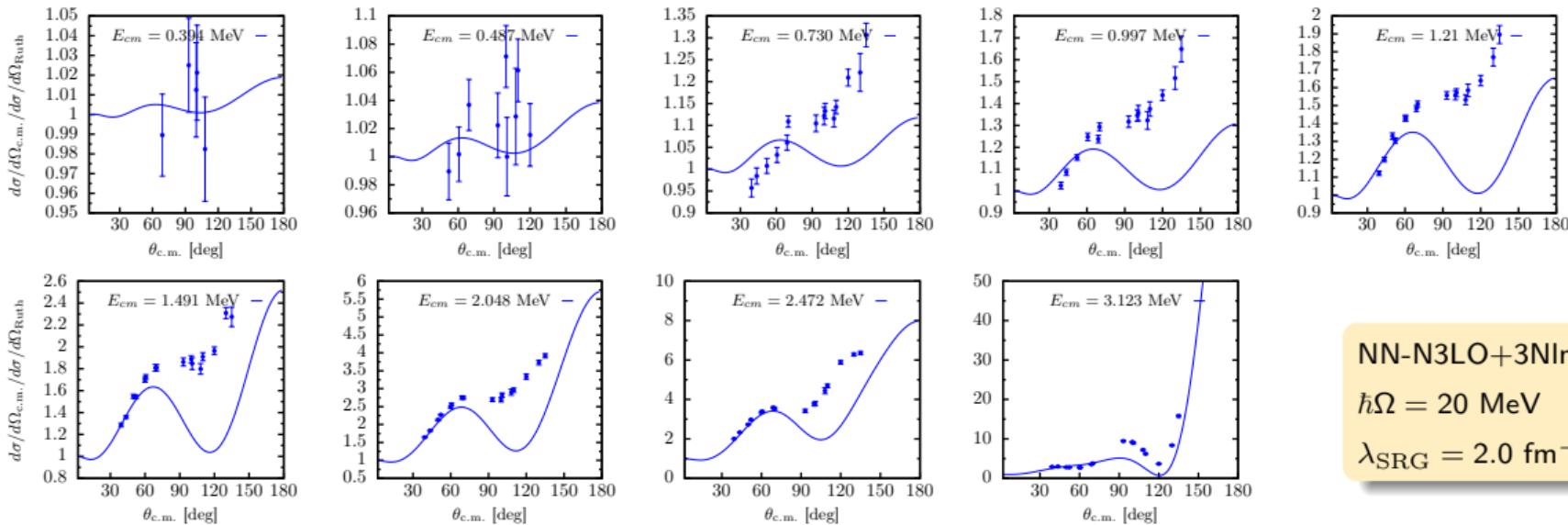
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# SONIK $^3\text{He} + ^4\text{He}$ elastic scattering ratio to Rutherford

- Experiment done at TRIUMF in 2022



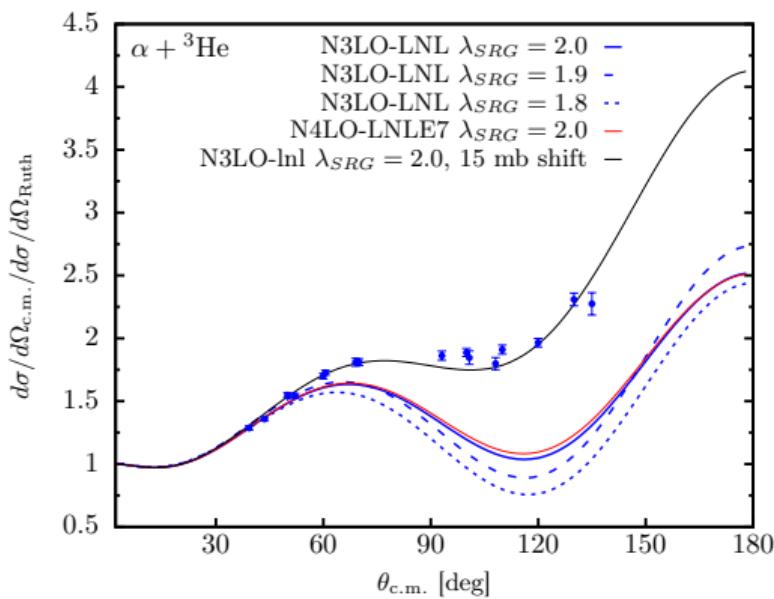
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## Discrepancy in NCSMC results

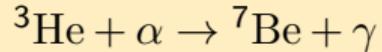
- Lack of strength in cross section ratio to Rutherford appears at high angles
  - Rutherford obscures the fact that a constant shift accounts for the discrepancy

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

- Varied properties of the interaction
  - Nothing in the NCMSC appears to reproduce the 15 mb shift



Results are promising but convergence needs to be explored

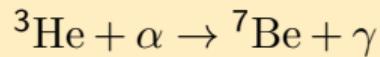
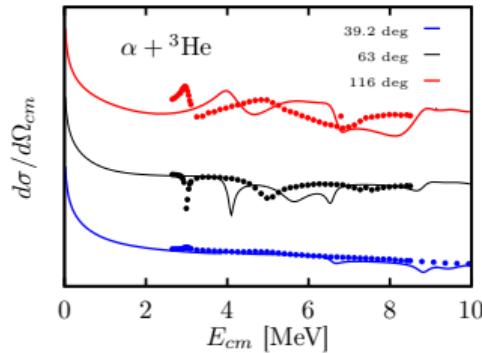


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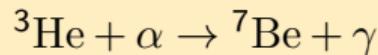
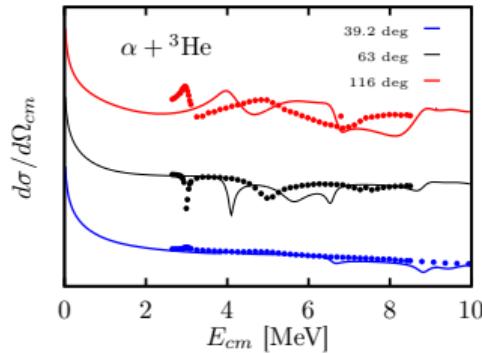
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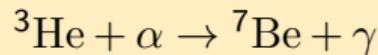
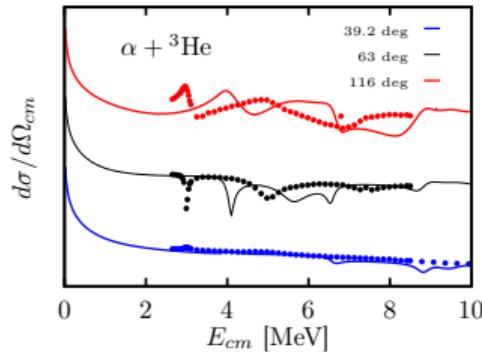
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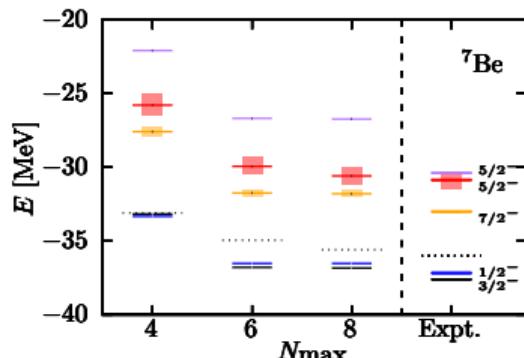
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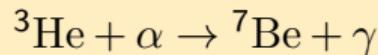
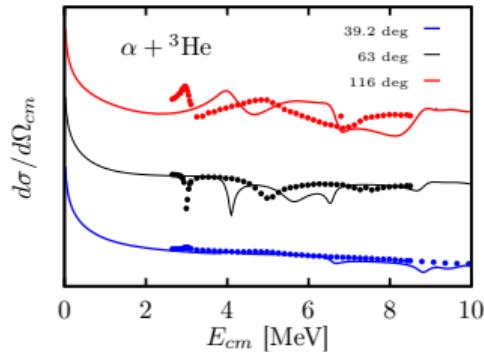
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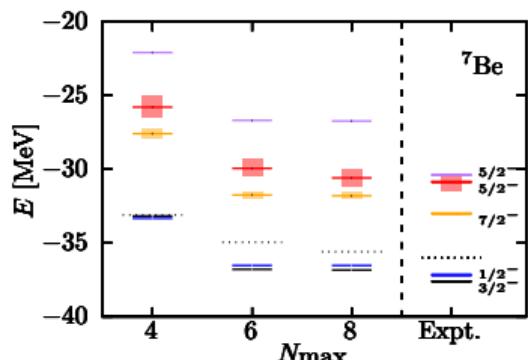
NN-N3LO+3Nlnl  
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 $\lambda_{SRG} = 2.0$  fm $^{-1}$



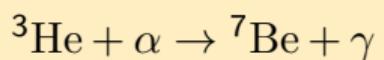
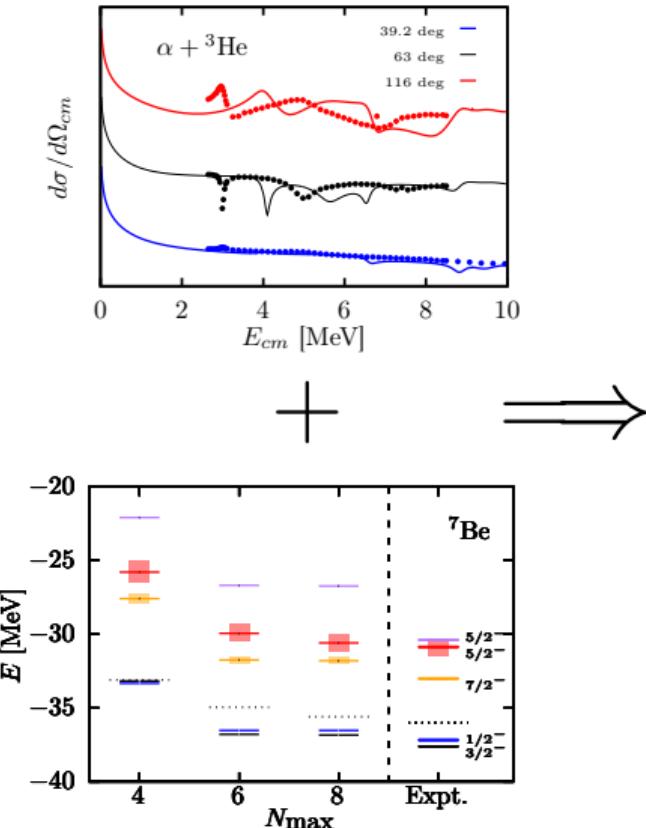
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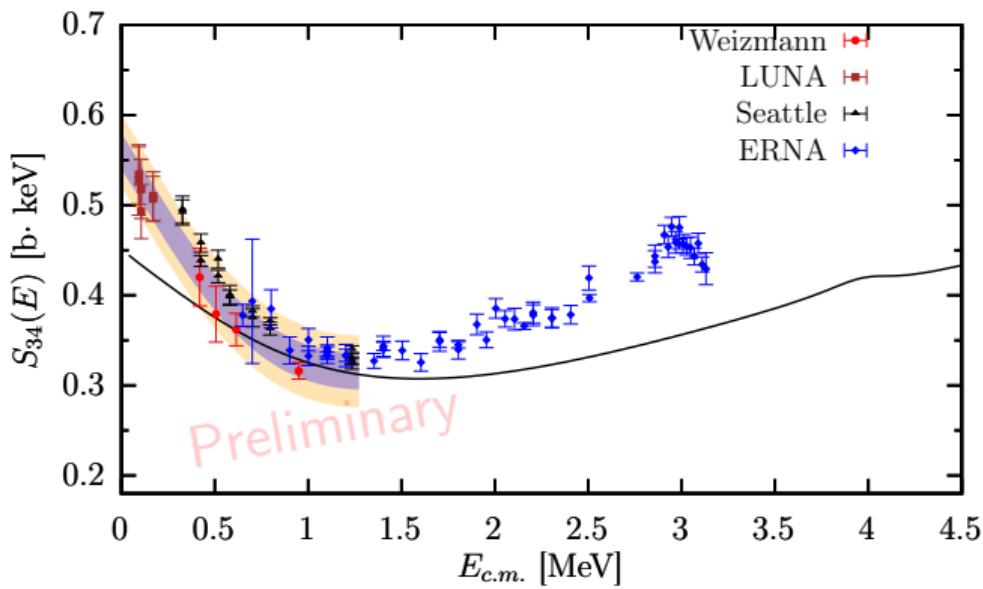
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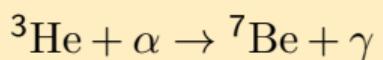
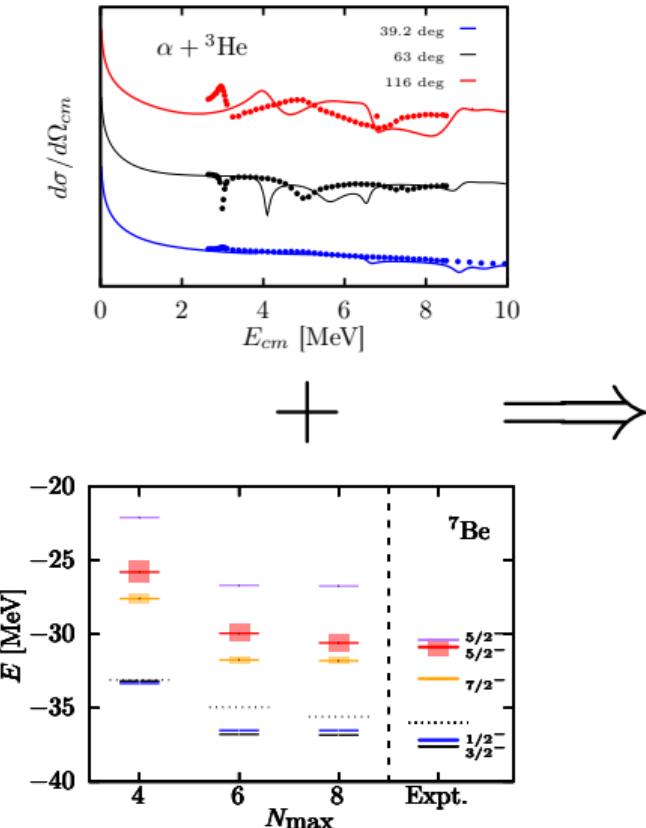
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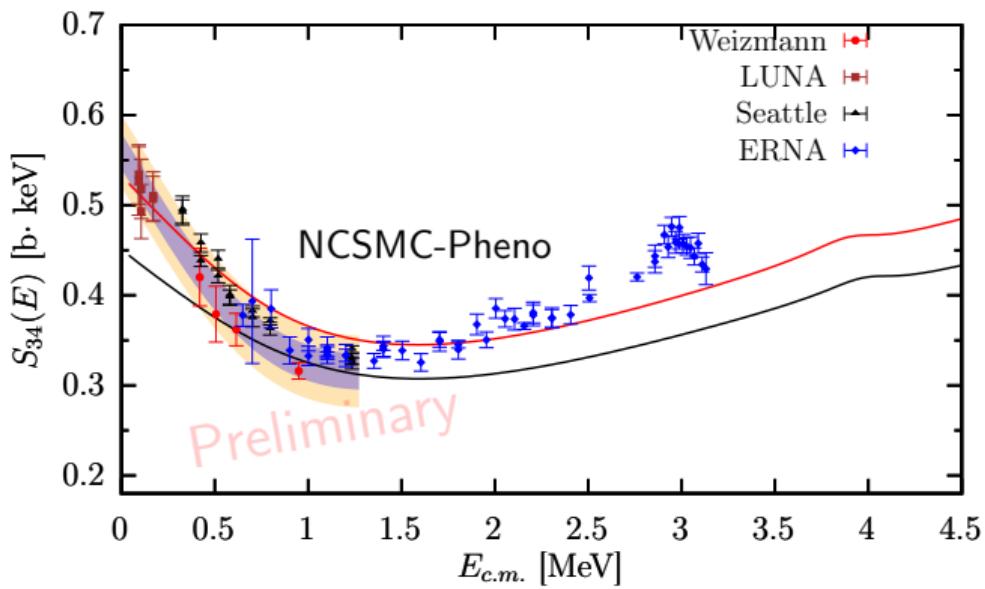
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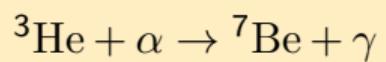
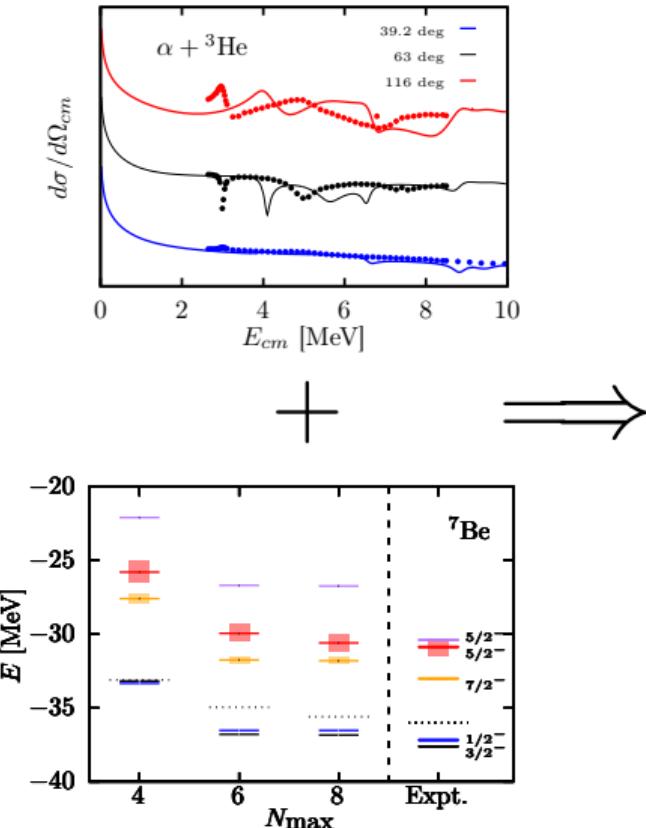
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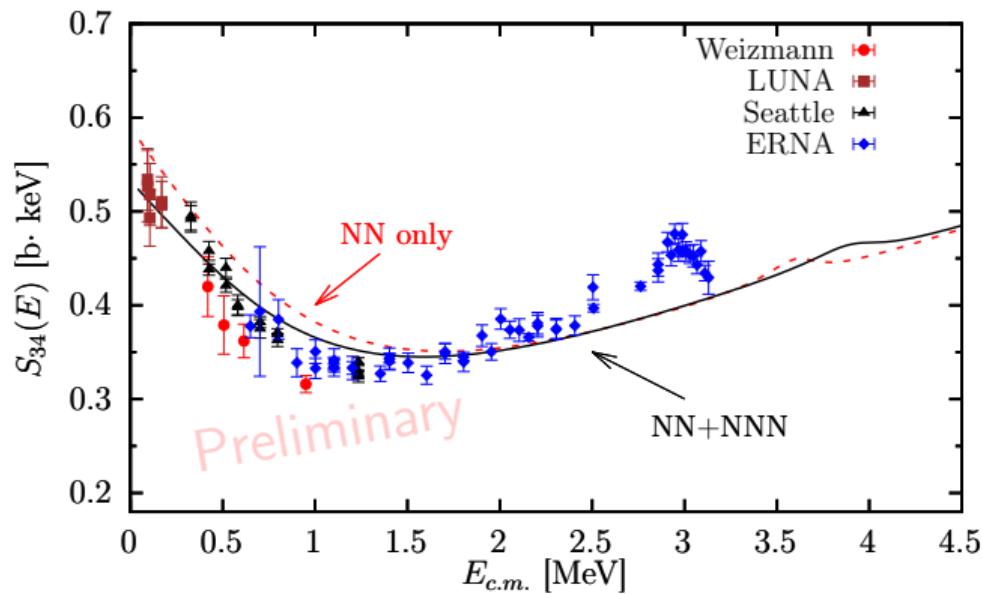
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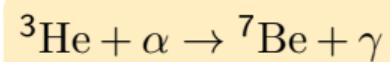
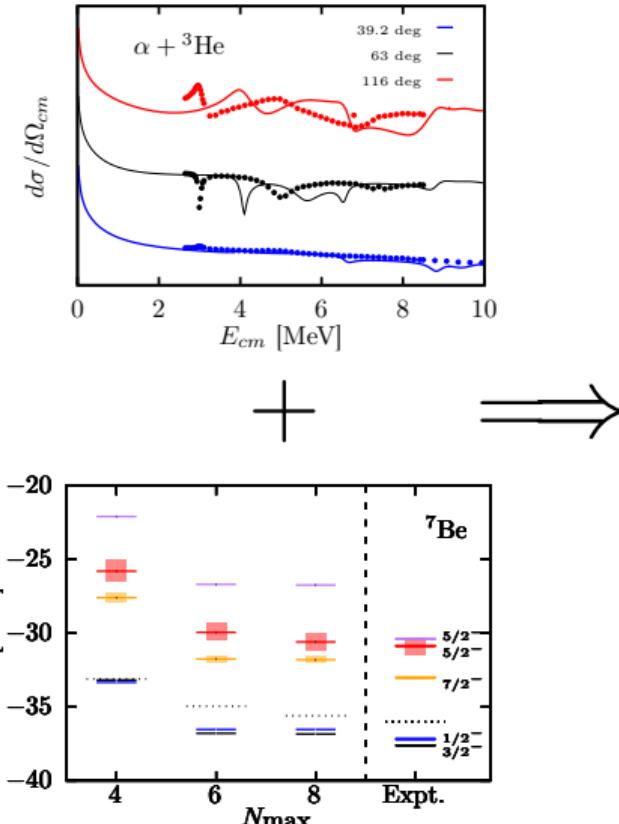
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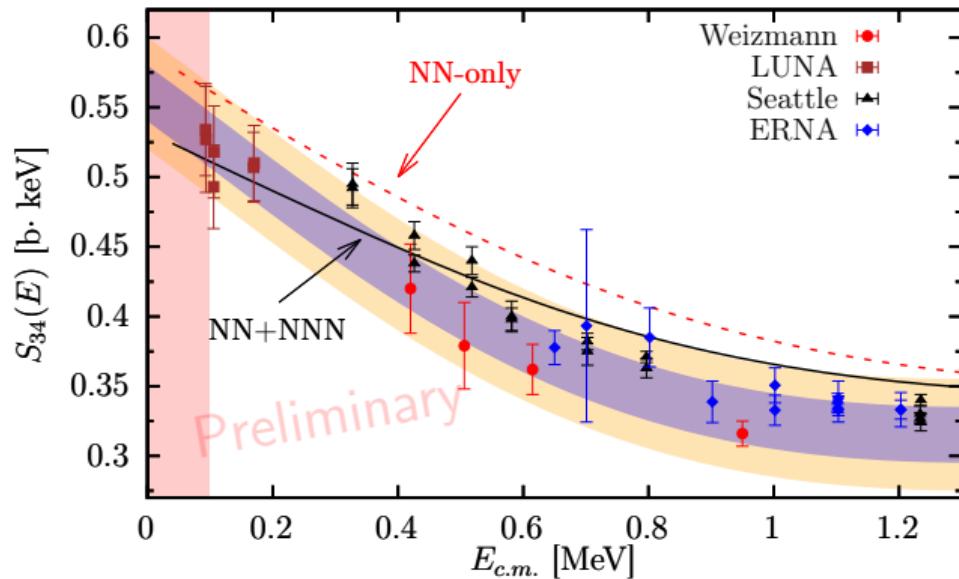
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From bound to continuum:  $^{11}\text{Be} \rightarrow (p + ^{10}\text{Be}) + \beta + \nu$



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



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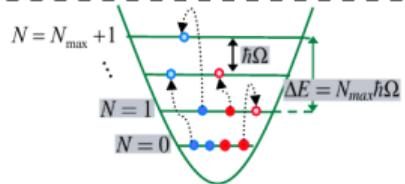
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- Predict the  $(\frac{1}{2}^+, \frac{1}{2})$  proton resonance at 197 keV from the proton energy distribution

# NCSMC calculation of $^{11}\text{Be}$ and $^{11}\text{B}$



$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

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

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

NCSM

NCSMC

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} |(A) \text{ nuclei}, \lambda\rangle + \sum_v \int d\vec{r} \gamma_v(\vec{r}) \hat{A}_v |(A-a), \vec{r}, (a), v\rangle$$

$$|^{11}\text{B}\rangle$$

$$|p\rangle \otimes |^{10}\text{Be}\rangle$$

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

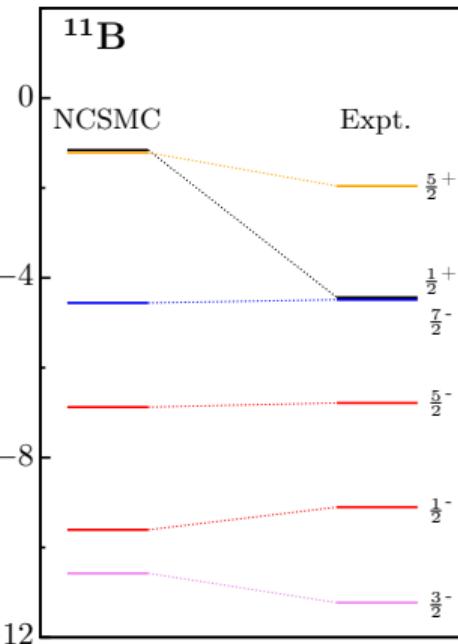


# NCSMC Calculation of $^{11}\text{B}$ and $^{11}\text{Be}$

NN-N4LO(500)+3Nlnl

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

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



P. Navratil, *Few-Body Systems* **41**, 117 (2007)

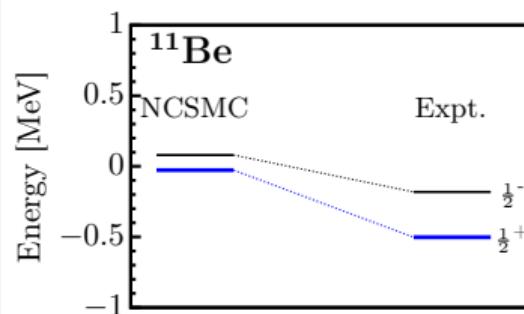
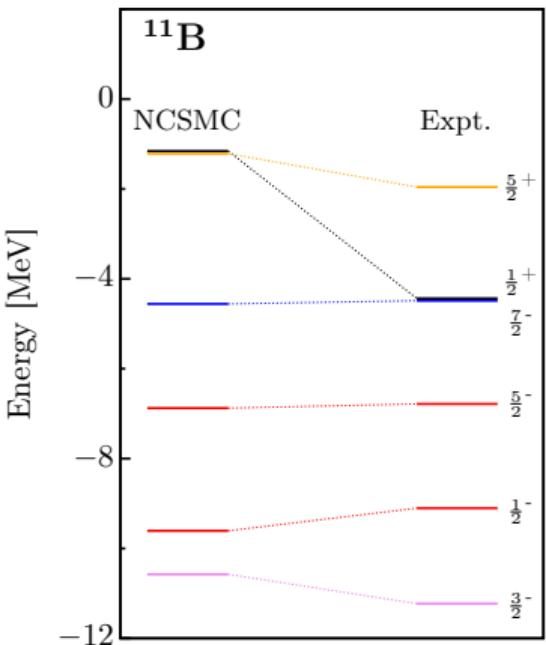
D.R. Entem et al., *Phys. Rev. C* **91**, 014002 (2015)

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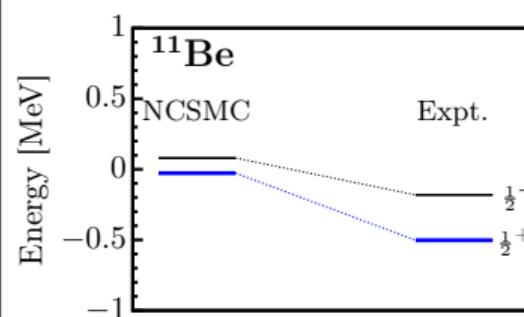
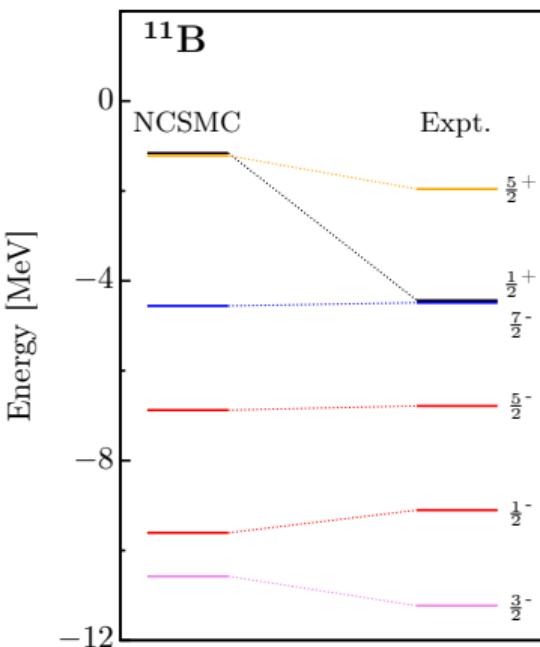
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- Parity inversion reproduced



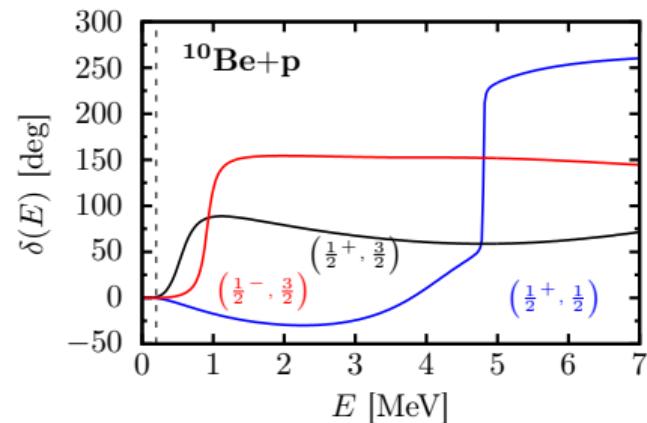
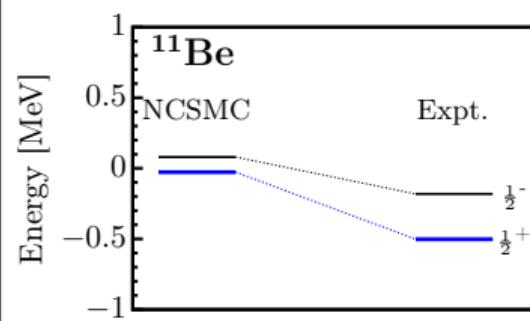
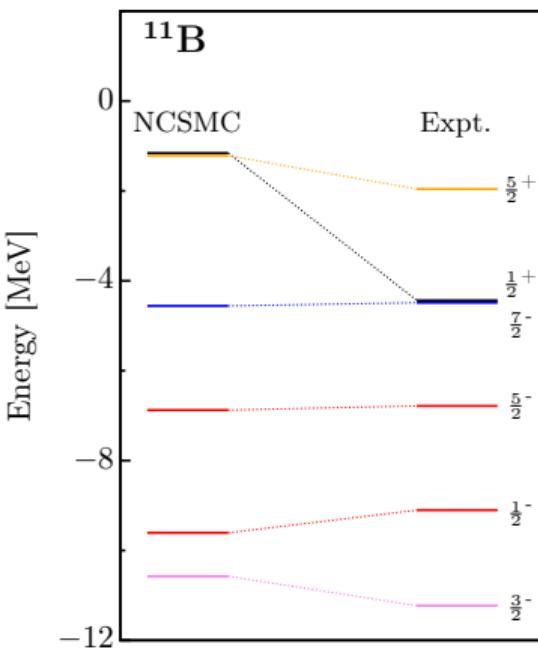
# NCSMC Calculation of $^{11}\text{B}$ and $^{11}\text{Be}$

NN-N4LO(500)+3Nlnl

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

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

- Parity inversion reproduced



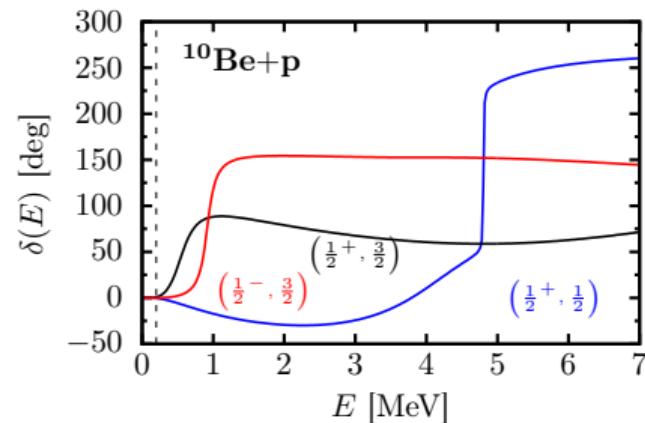
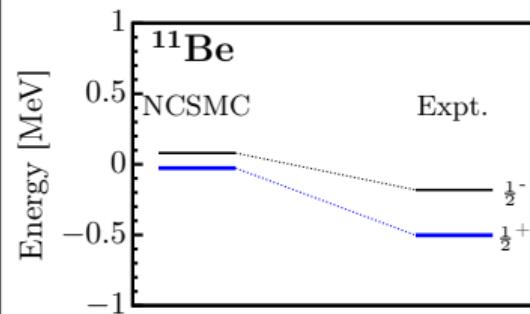
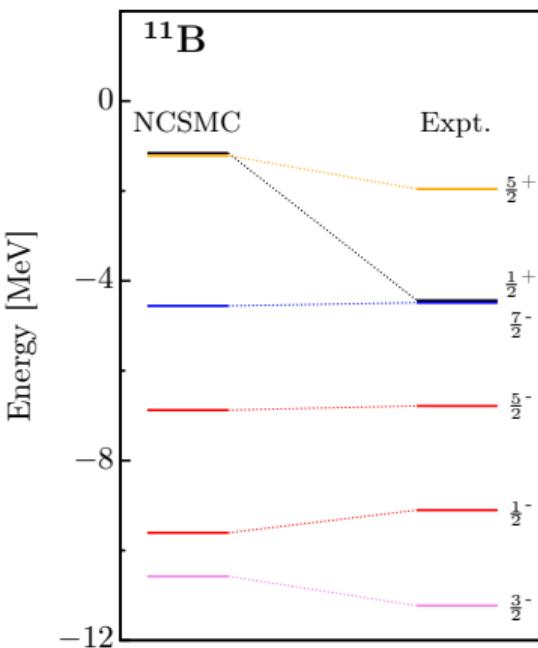
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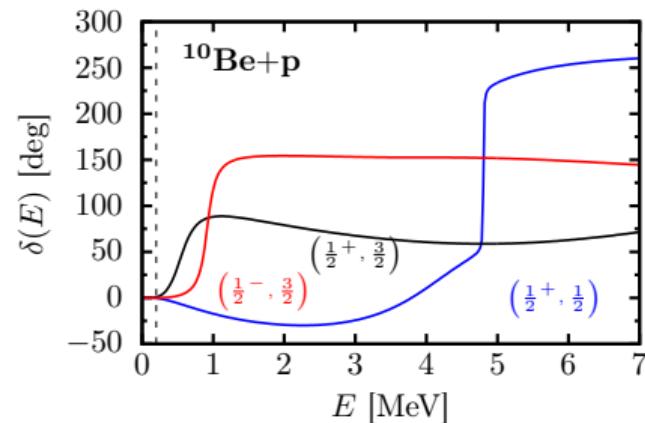
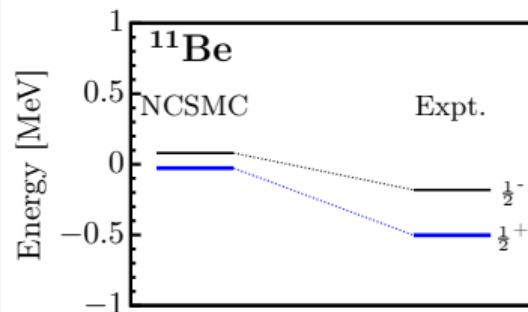
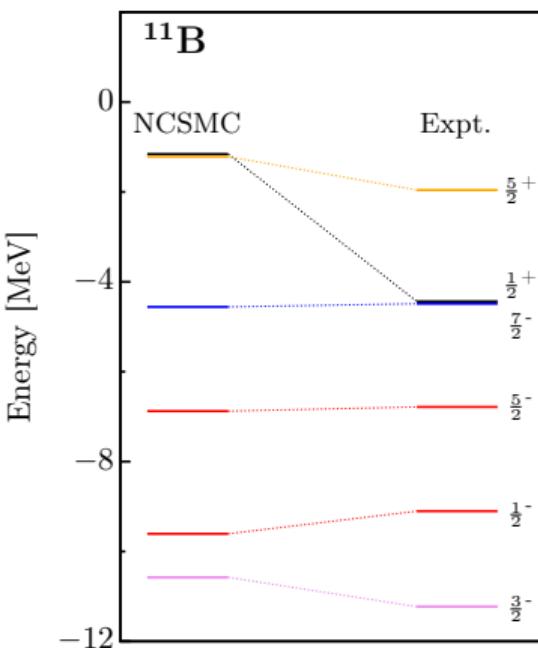
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- Phenomenologically shift levels to calculate  $\beta$ -decay



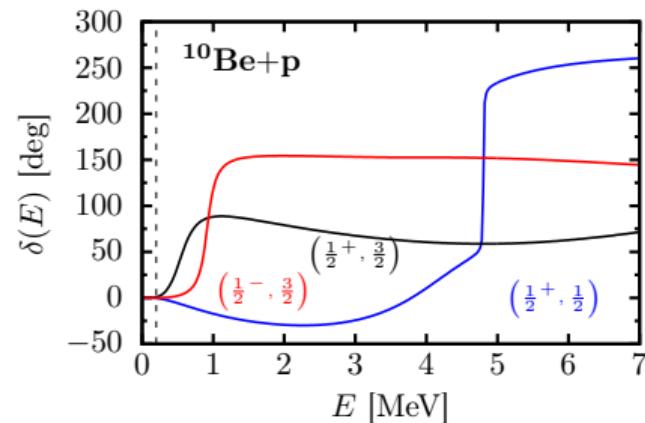
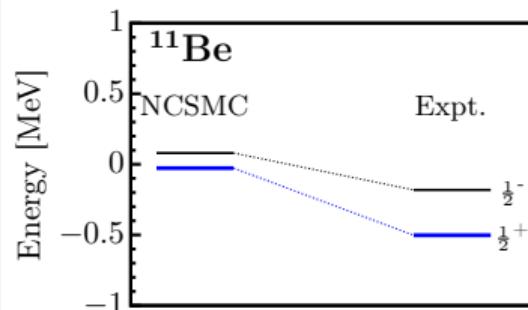
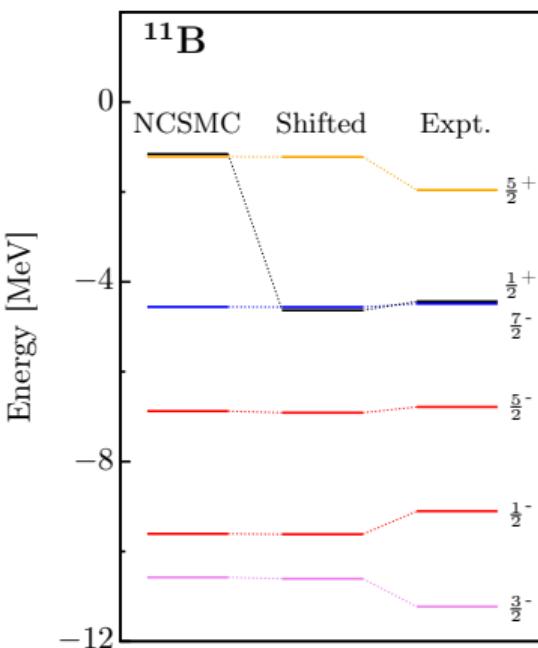
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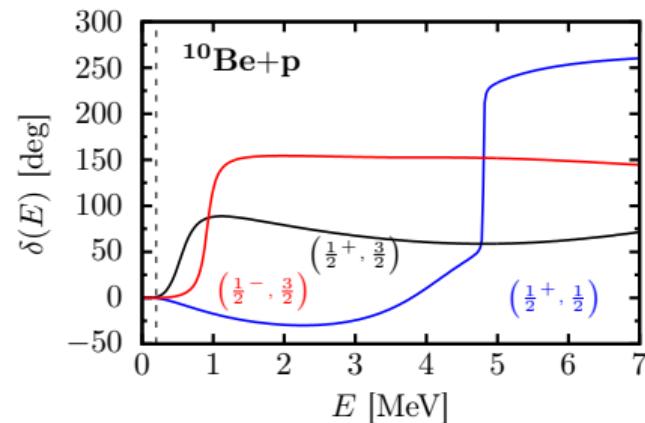
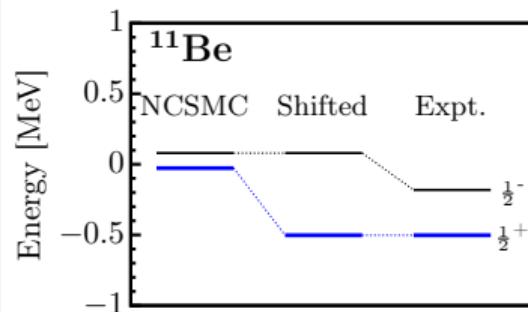
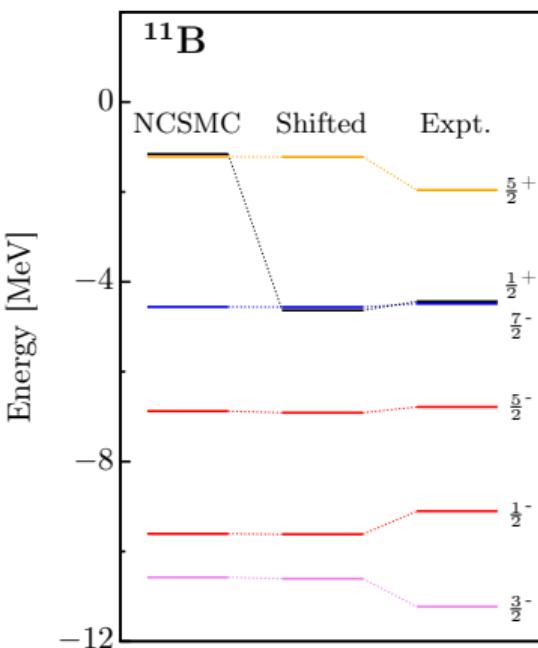
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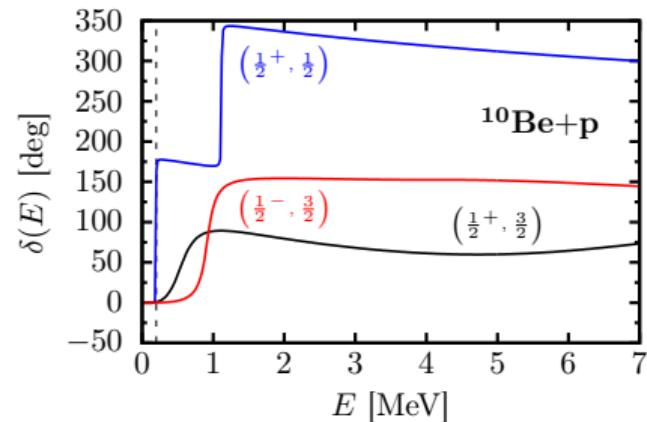
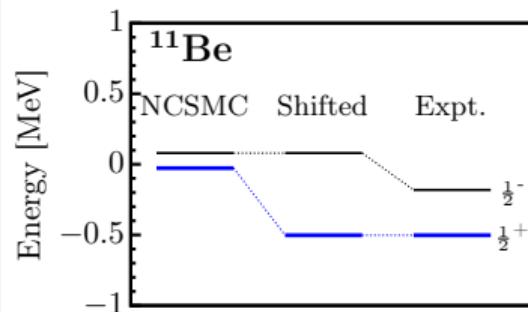
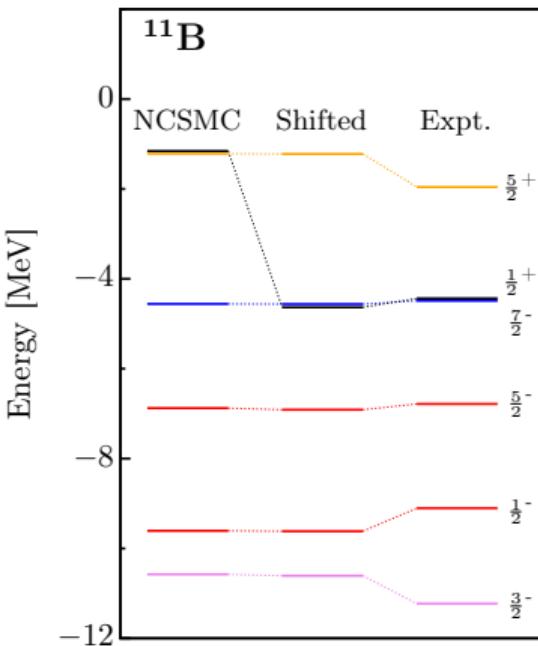
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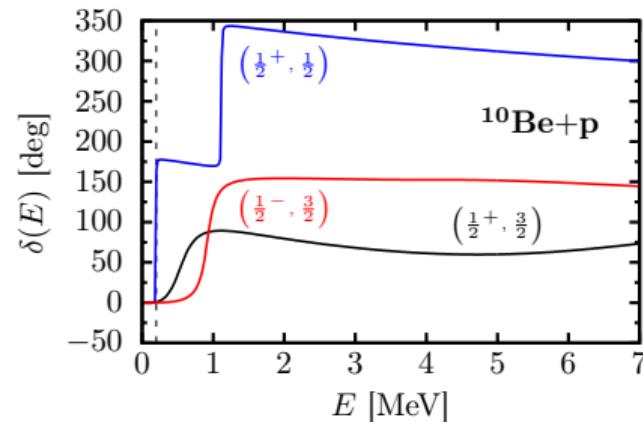
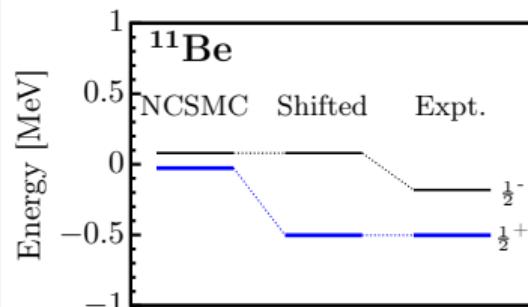
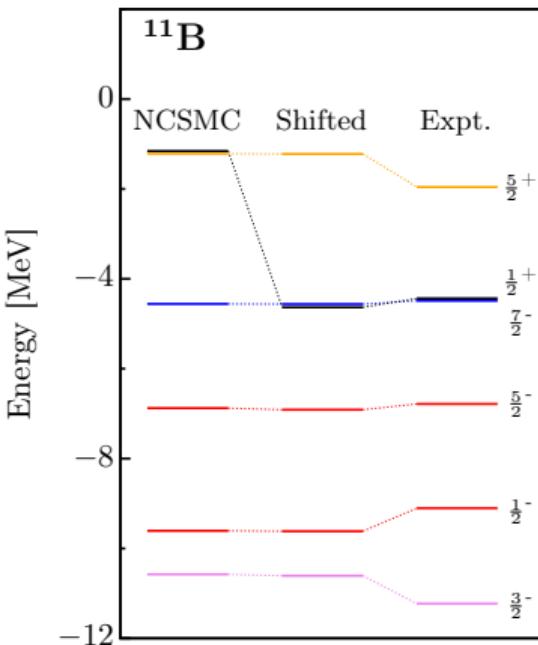
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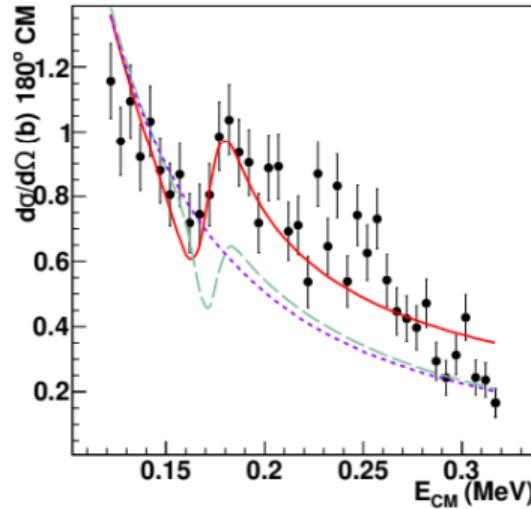
- Parity inversion reproduced
- Resonance found, but not at expt. energy
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	NCSMC-shifted	Expt.
$E$ [keV]	197	197(20)
$\Gamma$ [keV]	10	12(5)

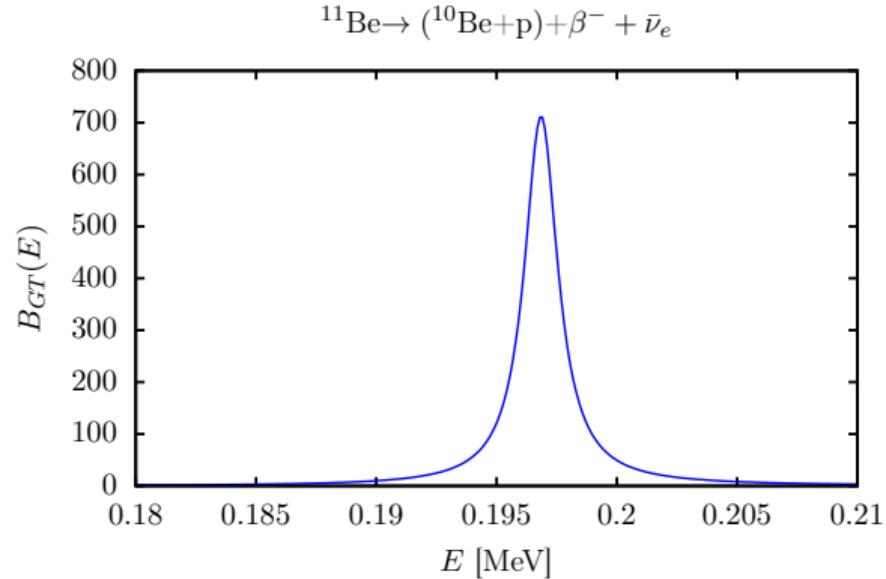
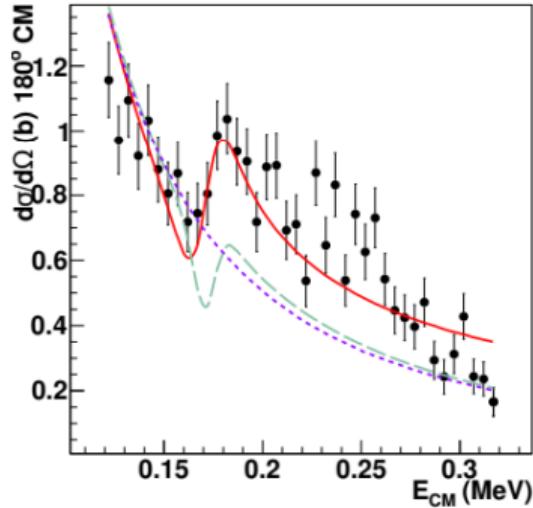
# $\beta$ -Decay to Resonant State

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



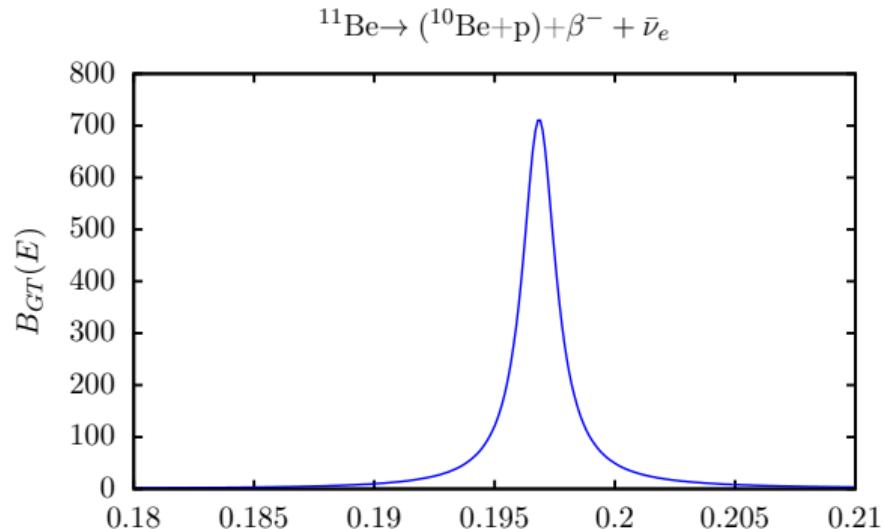
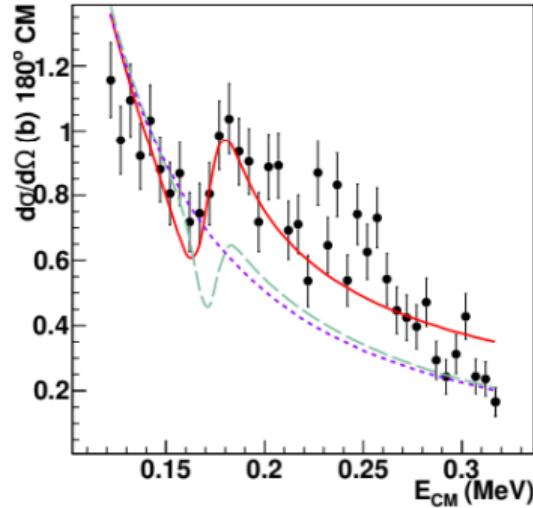
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Ayyad *et al.*, PRL 129 012501 (2022)



# $\beta$ -Decay to Resonant State

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

## Conclusions and Outlook

- The NCSMC provides a simultaneous description of bound and scattering states
- We can now include the  $NNN$  force in  ${}^3\text{He}(\alpha,\gamma){}^7\text{Be}$
- Our calculation of  ${}^{11}\text{B}$  confirms the existence of the  $1/2^+$  resonacne
- The corresponding  $B(GT)$  explains the large branching ratio observed in experiment
- Future: include the  $\alpha + {}^7\text{Li}$  channel in  ${}^{11}\text{B}$  calculation
- Future: include the  $p + {}^6\text{Li}$  channel in  $S_{34}(E)$  calculation

# Thanks



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Kostas Kravvaris



Guillame Hupin



Petr Navratil

(LLNL)

(IN2P3)

(TRIUMF)