FRIB

Ab Initio Calculations of Radiative Capture

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INT-26-2b - Quantum Physics of Stars
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Acknowledgements

- TRIUMF: Petr Navrátil, Jakub Herko
  - University of Victoria: Roan Stafford, Marshall Kodar
- LLNL: Sofia Quaglioni, Kostas Kravvaris
- IJCLab: Guillaume Hupin

Outline

- No-Core Shell Model with Continuum (NCSMC)
- Proton Capture: Extensions to Electron-Positron Pair Production
  - $^{7}\mathrm{Li}(p,\gamma/e^{+}e^{)}\,^{8}\mathrm{Be}$
  - $^{11}\mathrm{B}(p,\gamma/e^{+}e^{-})^{12}\mathrm{C}$
- Applications to the CNO-Cycle
  - $^{12}\mathrm{C}(p,\gamma)^{13}\mathrm{N}$
  - $^{14}\mathrm{N}(p,\gamma)^{15}\mathrm{O}$

Ab Initio Calculations of Many-Nucleon Systems

Find the eigenstates of a realistic nuclear Hamiltonian

$$H^A \left|\Psi_\lambda\right\rangle = E_\lambda \left|\Psi_\lambda\right\rangle \text{, where } H^A = \sum_i^A T_i + \sum_{i<j} V_{ij}^{NN} + \sum_{i<j<f} V_{ijf}^{3N}$$

- e.g. NN(N^3LO) + 3N$_{lnl}(N^2LO)$ interaction: [PRC **101**, 014318 (2020)]
- Low-energy constants determined in $A = 2, 3, 4$ systems

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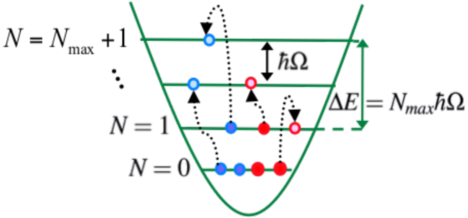
No-Core Shell Model (NCSM)

$$\left|{}^{(A)}\,,\lambda\right\rangle = \sum_{N=0}^{N_{\text{max}}} \sum_j c_{Nj}^{\lambda} \left|\Phi_{Nj}\right\rangle$$



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No-Core Shell Model with Continuum (NCSMC)

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

NCSMC Equations

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

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

$$\boxed{E_{\lambda}^{NCSM}\;\delta_{\lambda\lambda'}} \qquad \boxed{\left\langle {}^{(A)} \middle| H\,\hat{A}_{\nu} \middle| \underset{(a)}{}\overset{r}{\longrightarrow}\underset{(A-a)}{}\right\rangle} \qquad \boxed{\delta_{\lambda\lambda'}} \qquad \boxed{\left\langle {}^{(A)} \middle| \hat{A}_{\nu} \middle| \underset{(a)}{}\overset{r}{\longrightarrow}\underset{(A-a)}{}\right\rangle}$$

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

$$\boxed{\left\langle \underset{(A-a)}{}\overset{r'}{\longleftarrow}\underset{(a)}{} \middle| \hat{A}_{\nu'}\,H\,\hat{A}_{\nu} \middle| \underset{(a)}{}\overset{r}{\longrightarrow}\underset{(A-a)}{}\right\rangle} \qquad \boxed{\left\langle \underset{(A-a)}{}\overset{r'}{\longleftarrow}\underset{(a)}{} \middle| \hat{A}_{\nu'}\,\hat{A}_{\nu} \middle| \underset{(a)}{}\overset{r}{\longrightarrow}\underset{(A-a)}{}\right\rangle}$$

NCSMC for $^7\mathrm{Li}(p,\gamma)^8\mathrm{Be}$

$$\left|\Psi^{(8)}_{\text{NCSMC}}\right\rangle = \sum_\lambda c_\lambda \left|^8\mathrm{Be},\lambda\right\rangle + \sum_\nu \int \mathrm{d}r \gamma_\nu(r) \hat{A}_\nu \left|^7\mathrm{Li}+p,\nu\right\rangle + \sum_\mu \int \mathrm{d}r \gamma_\mu(r) \hat{A}_\mu \left|^7\mathrm{Be}+n,\mu\right\rangle$$

Process:

- Solve NCSM for each constituent nucleus: $^8\mathrm{Be}$, $^7\mathrm{Li}$ and $^7\mathrm{Be}$
  - 15 (+) and 15 (-) eigenstates from $^8\mathrm{Be}$
  - 5 eigenstates each from $^7\mathrm{Li}$ and $^7\mathrm{Be}$
- Solve NCSMC for $c_\lambda(E)$, $\gamma_\nu(r,E)$, $\gamma_\mu(r,E) \to |\Psi(E)\rangle$
  - R-matrix on a Lagrange mesh
- Reaction cross-sections depend on transition matrix elements: e.g. $\left\langle\Psi(E_f)\right| M1 \left|\Psi(E_i)\right\rangle$

Results

The NCSMC allows simultaneous calculation of many observables

● ${}^{8}\mathrm{Be}$ Structure

○ Scattering: ${}^{7}\mathrm{Li}(p,p){}^{7}\mathrm{Li}$, ${}^{7}\mathrm{Be}(n,n){}^{7}\mathrm{Be}$

○ Transfer Reactions: ${}^{7}\mathrm{Li}(p,n){}^{7}\mathrm{Be}$, ${}^{7}\mathrm{Be}(n,p){}^{7}\mathrm{Li}$

● Radiative Capture: ${}^{7}\mathrm{Li}(p,\gamma){}^{8}\mathrm{Be}$

● Search for new physics: ${}^{7}\mathrm{Li}(p,e^{+}e^{-}){}^{8}\mathrm{Be}$, ${}^{7}\mathrm{Li}(p,X){}^{8}\mathrm{Be}$

PHYSICAL REVIEW C **110**, 015503 (2024)

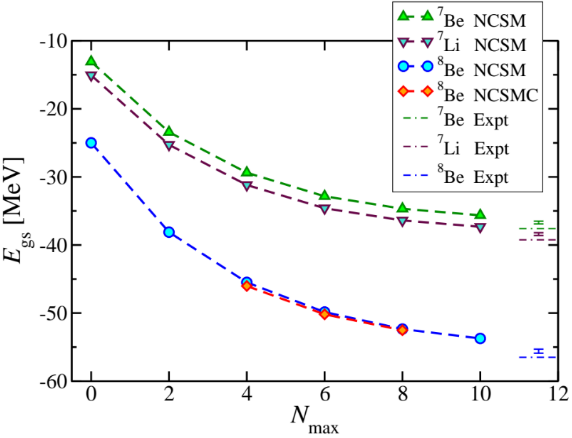
Editors' Suggestion

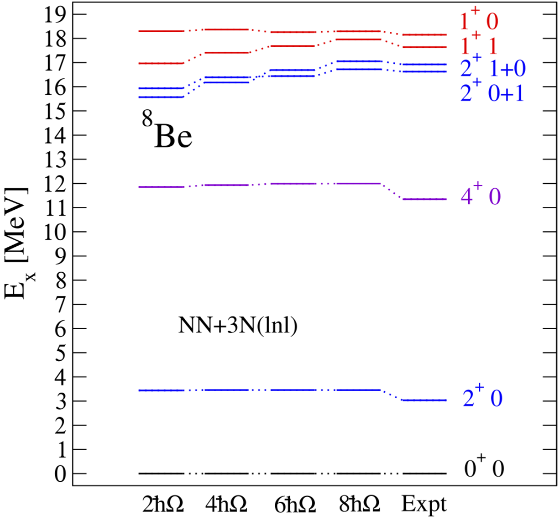
***Ab initio* investigation of the ${}^{7}\mathrm{Li}(p,e^{+}e^{-}){}^{8}\mathrm{Be}$ process and the X17 boson**

P. Gysbers,[1,2,3] P. Navrátil,[1,4] K. Kravvaris,[5] G. Hupin,[6] and S. Quaglioni[5]

NCSM Convergence

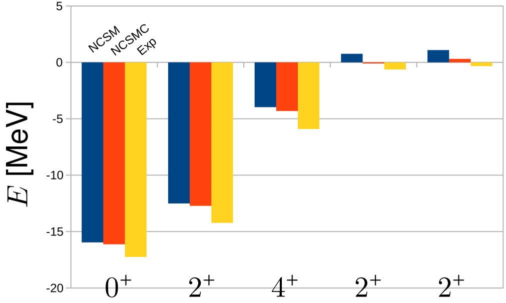
$\lambda_{SRG} = 2.0\text{fm}^{-1}$, $\hbar\Omega = 20\text{MeV}$

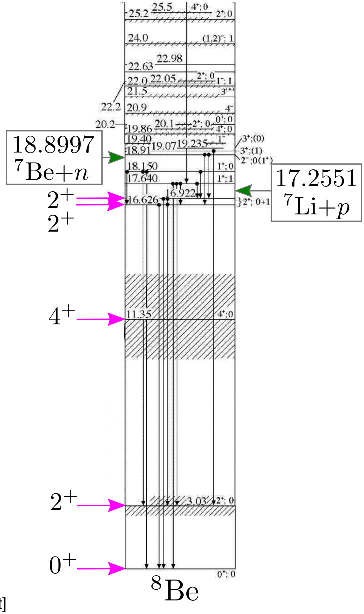




^{8}Be Structure

Calculations of ^{8}Be “bound” states (w.r.t. $^{7}\text{Li} + p$ threshold) are improved by inclusion of the continuum ($N_{max} = 8$)





- Energies likely too high due to neglected $\alpha + \alpha$ breakup
- Matches experiment well, except the 3rd 2^+ is still slightly above the $^{7}\text{Li} + p$ threshold

[TUNL Nuclear Data Evaluation Project]

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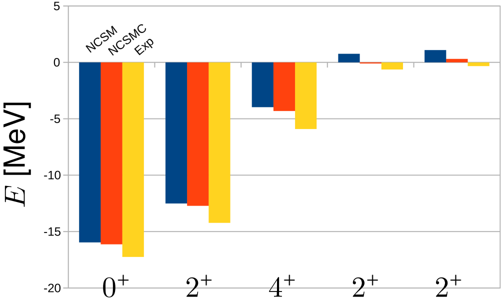

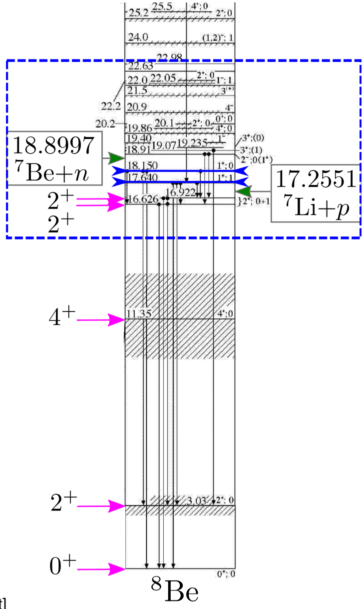

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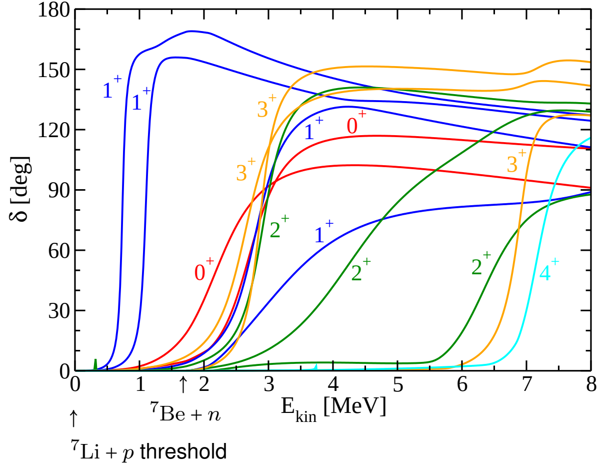
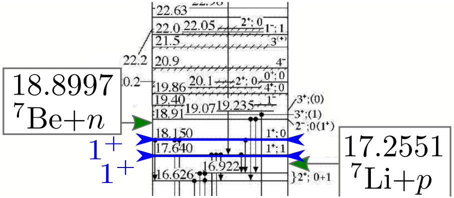
[TUNL Nuclear Data Evaluation Project]

Eigenphase-shift Results (positive parity)



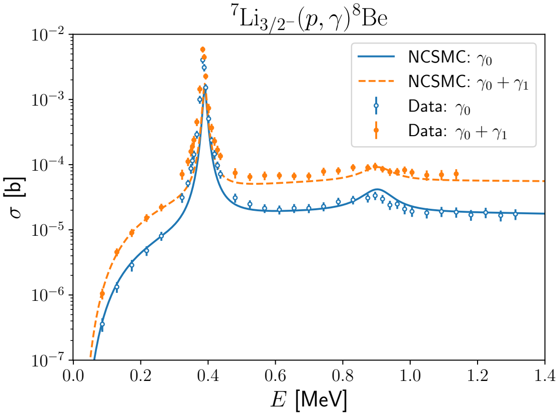


Additional resonances are seen compared to TUNL data evaluation

Radiative Capture (γ)

$$\hat{O}_\gamma = E1 + M1 + E2$$

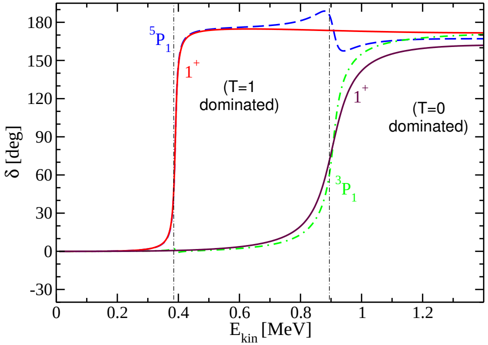
$${}^{2S+1}P_J : \left[\left(\left| {}^7\mathrm{Li} \right\rangle |p\rangle \right)^{(S)} Y_L(\hat{r}) \right]^J \quad P : L = 1$$



γ_0: decay to ground state (0^+)

γ_1: decay to first excited (2^+)

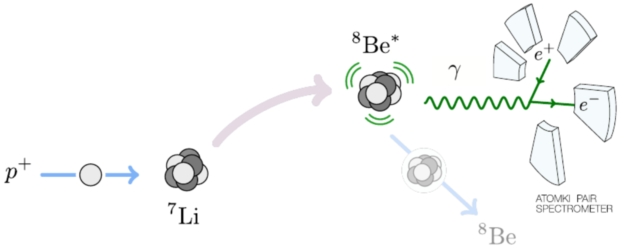
[Data: Zahnow et al
Z.Phys.A **351** 229-236 (1995)]



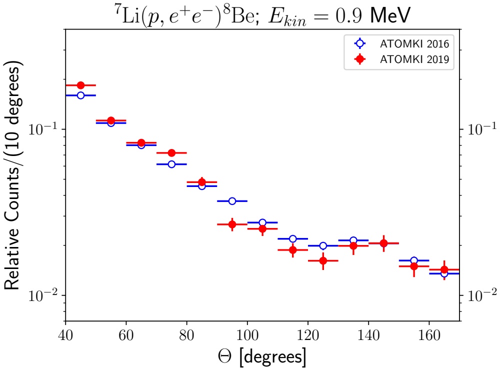
Phenomenological adjustment: fit threshold and resonance positions to match experiment

The X17 Anomaly in $p + {}^7\mathrm{Li} \to {}^8\mathrm{Be} + e^+e^-$

- ${}^7\mathrm{Li}(p, e^+e^-)^8\mathrm{Be}$ @ATOMKI (Hungary) [PRL **116** 042501 (2016)]
- Decay of composite ${}^8\mathrm{Be}$ produces electron-positron pairs



[Feng PRD **95**, 035017 (2017)]



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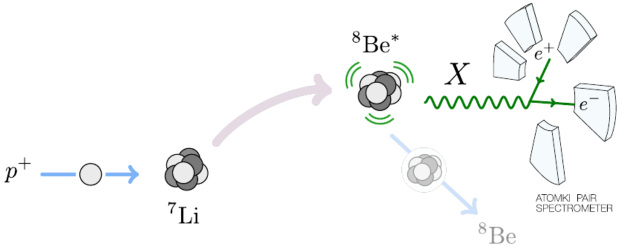
- Decay of composite ${}^8\mathrm{Be}$ produces electron-positron pairs
- Anomaly in pair distribution implies an intermediate particle of mass 17 MeV



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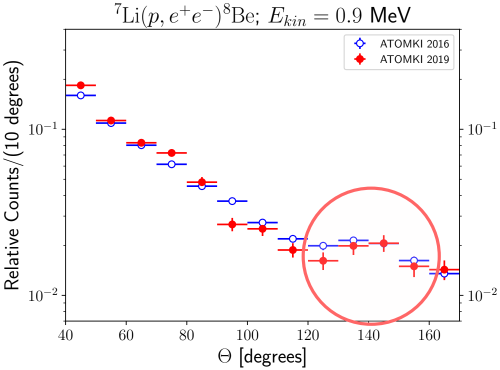
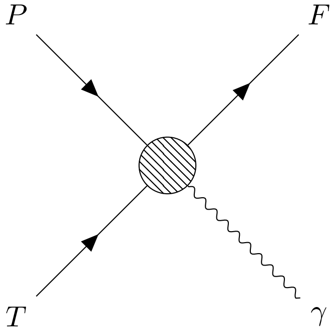
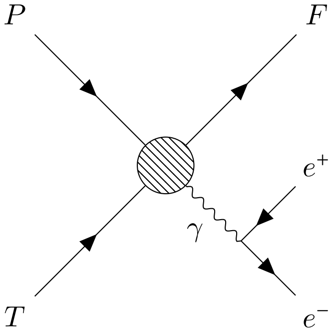


Radiative Capture: $P + T \to F + \gamma/e^+e^-$



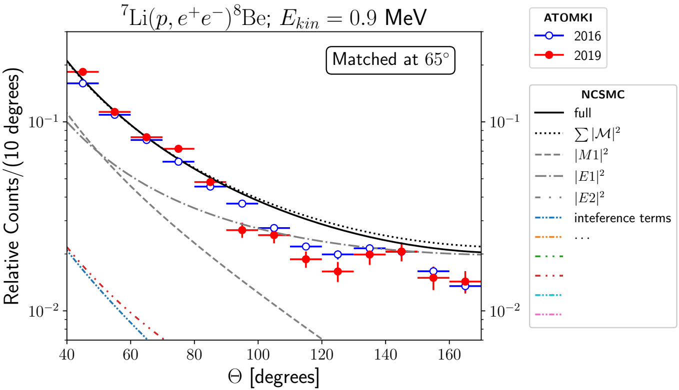


$$\mathrm{d}\sigma \sim \mathrm{d}q_\gamma |\langle\psi(P+T)|\hat{O}_\gamma|\psi(F)\rangle|^2$$

$$\mathrm{d}\sigma \sim \mathrm{d}p_+\mathrm{d}p_- \int \frac{\mathrm{d}q}{q^4} |\langle\psi(P+T)|\hat{O}_{e^+e^-}|\psi(F)\rangle|^2$$

Radiative Capture (e^+e^-)

- Counts $\propto$ partially integrated differential cross section
- $E1$ and $M1$ are dominant



(electron-positron separation angle)

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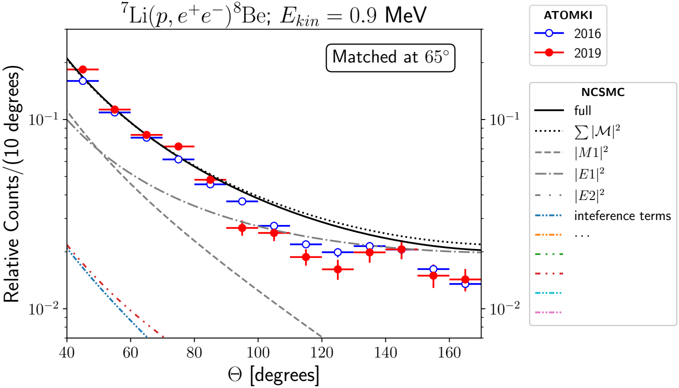
- But theory and data still inconsistent - possible $M1$ contamination from lower resonance



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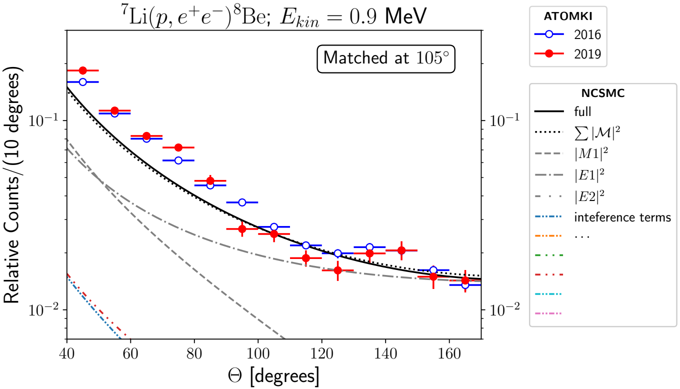
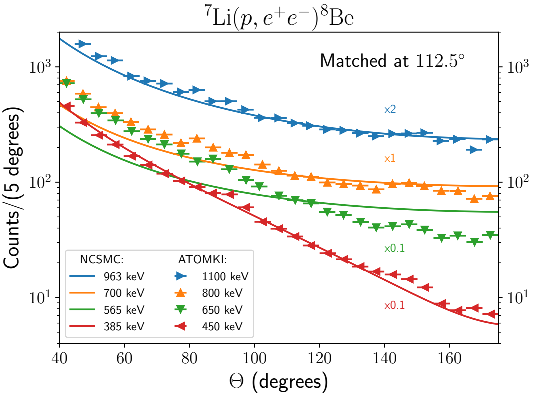
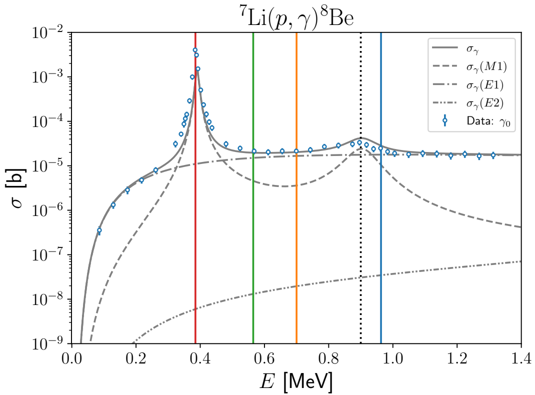


(electron-positron separation angle)

More Recent Results





- Updated ATOMKI data (2022) arXiv:2205.07744
- Data in-between resonances seems to be contaminated by $M1$ from first resonance

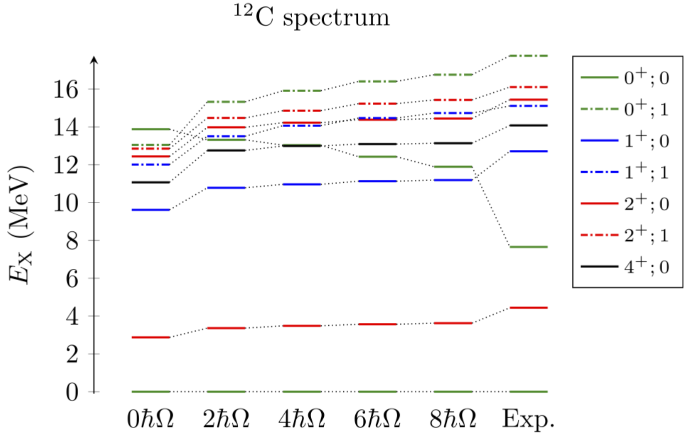
NCSMC for $^{11}\mathrm{B}(p,\gamma)^{12}\mathrm{C}$ and $^{11}\mathrm{B}(p,e^+e^-)^{12}\mathrm{C}$

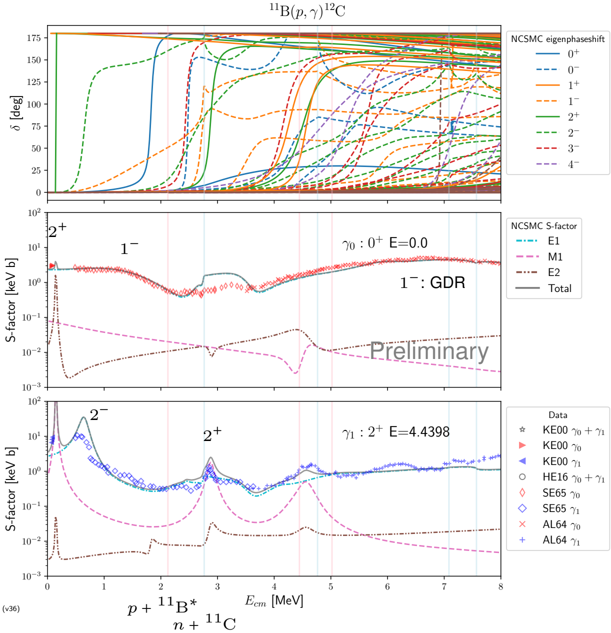
$$\left|\Psi^{(12)}_{\text{NCSMC}}\right\rangle = \sum_\lambda c_\lambda \left|^{12}\mathrm{C},\lambda\right\rangle + \sum_\nu \int \mathrm{d}r\gamma_\nu(r)\hat{A}_\nu \left|^{11}\mathrm{B}+p,\nu\right\rangle + \sum_\mu \int \mathrm{d}r\gamma_\mu(r)\hat{A}_\mu \left|^{11}\mathrm{C}+n,\mu\right\rangle$$

Process:

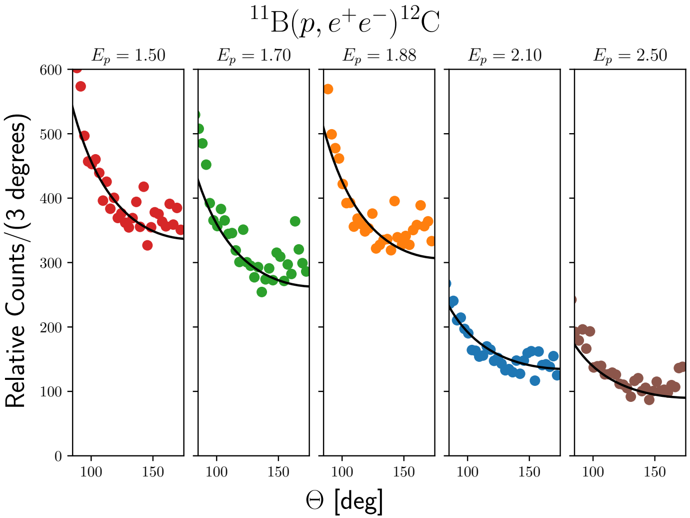
- Solve NCSM for each constituent nucleus: $^{12}\mathrm{C}$, $^{11}\mathrm{B}$ and $^{11}\mathrm{C}$
  - 40 (-) and 13 (+) eigenstates from $^{12}\mathrm{C}$ ($E_{ex} \lesssim 24$ MeV)
  - 4 eigenstates each from $^{11}\mathrm{B}$ and $^{11}\mathrm{C}$
  - $N_{max} = 6,7$
- Interaction: NN(N^4LO) + 3N$_{lnlE7}(N^2LO+)$
  includes additional subleading 3N term [PRC **84**, 014001 (2011)]

NCSM predicts most bound states (except excited 0^+)

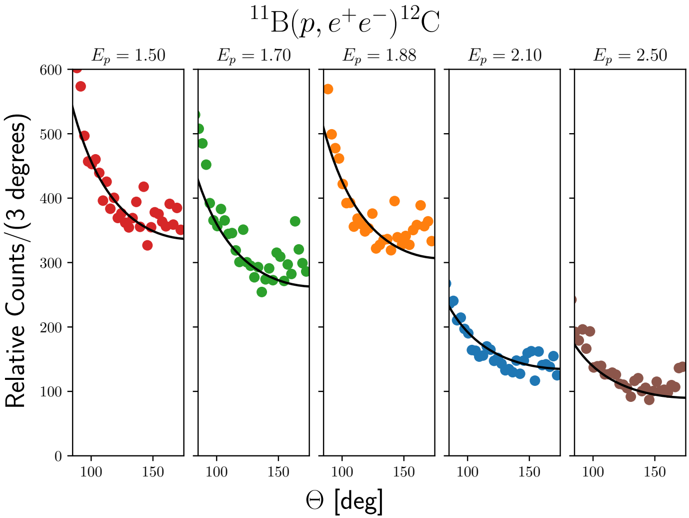




- Capture to 0^+ ground state and 2^+ first excited well produced
- Some pheno-adjustment required for resonance positions
  - 2-4 MeV region difficult to fit
  - Many ambiguous states in TUNL evaluation



- Experiment: PRC **106** L061601 (2022)
- E1 component completely dominates
- New development: E0
  - but contribution is very small



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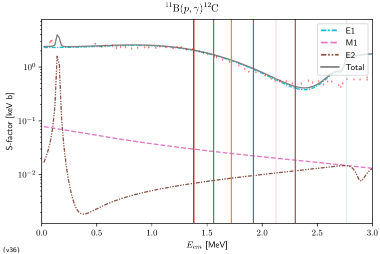
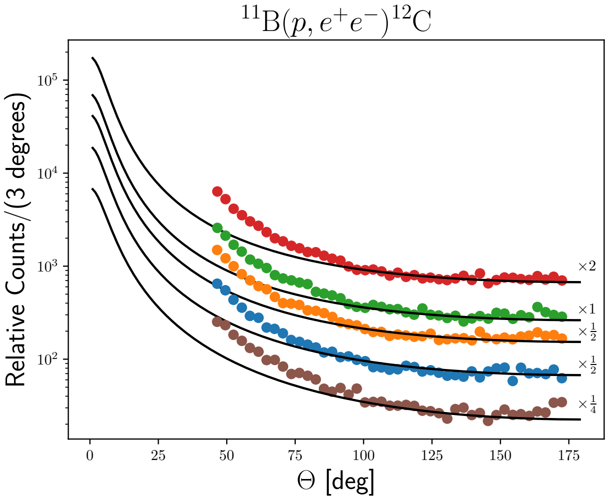
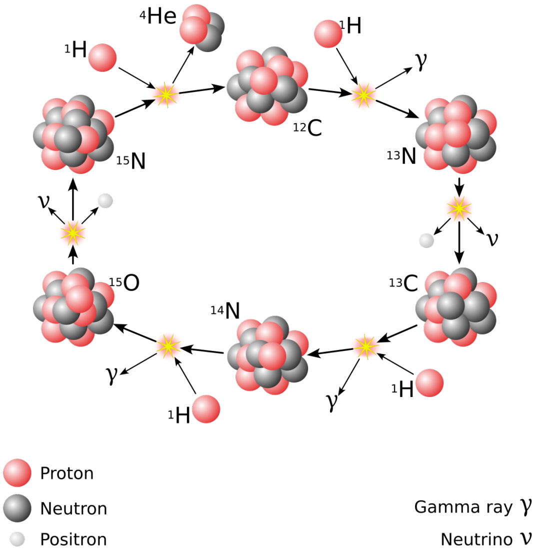




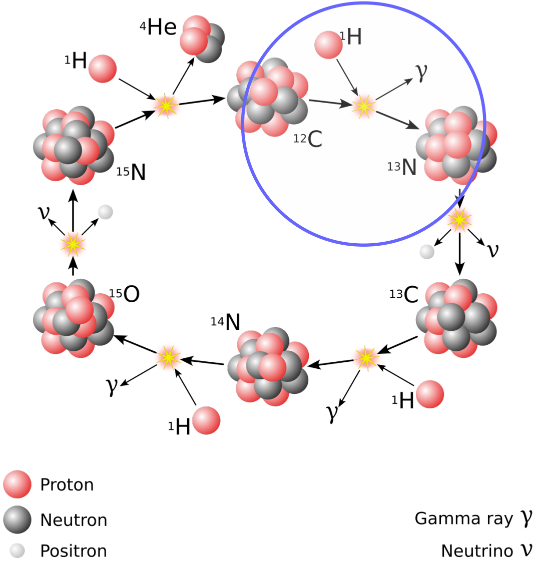
- Experiment: PRC **106** L061601 (2022)
- E1 component completely dominates
- New development: E0
  - but contribution is very small
- Counts too high below $\Theta \simeq 90°$
  - M1 contamination again?
  - No resonance looks like a culprit

CNO cycle



4He
1H
1H
γ
12C
15N
13N
ν
ν
15O
13C
14N
γ
γ
1H
1H
Proton
Neutron
Positron
Gamma ray γ
Neutrino ν

CNO cycle



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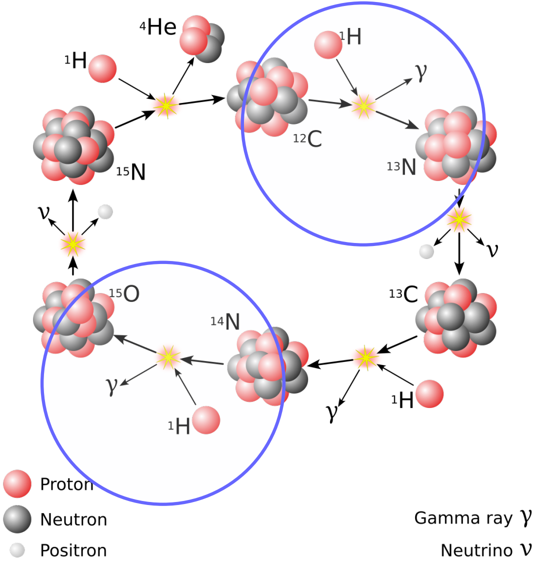

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Proton
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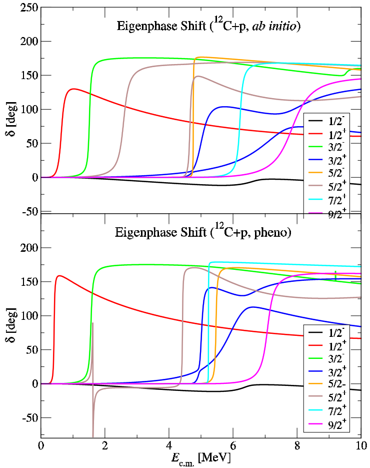
$^{12}\mathrm{C}(p,\gamma)^{13}\mathrm{N}$

- Only one physical bound state ($\frac{1}{2}^-$)
-

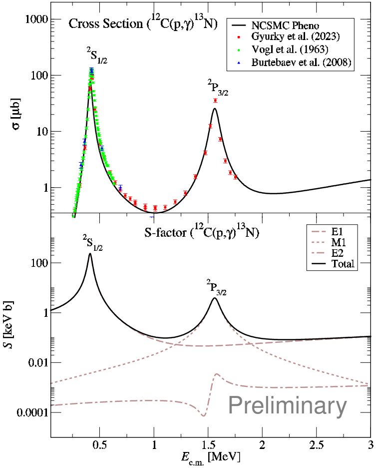
$$\left|\Psi^{(13)}_{\text{NCSMC}}\right\rangle = \sum_\lambda c_\lambda \left|^{13}\mathrm{N},\lambda\right\rangle + \sum_\nu \int \mathrm{d}r \gamma_\nu(r) \hat{A}_\nu \left|^{12}\mathrm{C}+p,\nu\right\rangle$$

  - $^{13}\mathrm{N}$: 15 (+) and 15 (-) eigenstates
  - $^{12}\mathrm{C}$: 2 eigenstates (0^+, 2^+)
  - $N_{max} = 6, 7$



$^{12}\mathrm{C}(p,\gamma)^{13}\mathrm{N}$

- Only one physical bound state ($\frac{1}{2}^-$)
- $$\left|\Psi^{(13)}_{\text{NCSMC}}\right\rangle = \sum_\lambda c_\lambda \left|^{13}\mathrm{N},\lambda\right\rangle + \sum_\nu \int \mathrm{d}r \gamma_\nu(r) \hat{A}_\nu \left|^{12}\mathrm{C}+p,\nu\right\rangle$$
  - $^{13}\mathrm{N}$: 15 (+) and 15 (-) eigenstates
  - $^{12}\mathrm{C}$: 2 eigenstates (0^+, 2^+)
  - $N_{max} = 6, 7$



$^{14}\mathrm{N}(p,\gamma)^{15}\mathrm{O}$

- 7 bound states
- $$\left|\Psi^{(15)}_{\text{NCSMC}}\right\rangle = \sum_{\lambda} c_\lambda \left|^{15}\mathrm{O},\lambda\right\rangle + \sum_{\nu}\int \mathrm{d}r\gamma_\nu(r)\hat{A}_\nu \left|^{14}\mathrm{N}+p,\nu\right\rangle + \sum_{\mu}\int \mathrm{d}r\gamma_\mu(r)\hat{A}_\mu \left|^{14}\mathrm{O}+n,\mu\right\rangle$$
  - $^{15}\mathrm{O}$: 9 (+) and 12 (-) eigenstates
  - $^{14}\mathrm{N}$: 1^+, 0^+, 1^+
  - $^{14}\mathrm{O}$: 0^+
  - $N_{max} = 6,7$

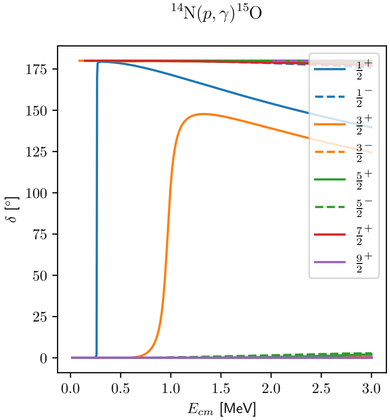
$^{14}N(p,\gamma)^{15}O$

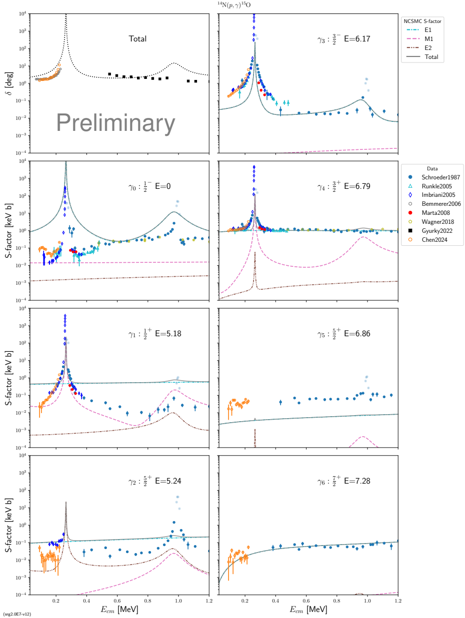
- 7 bound states
-

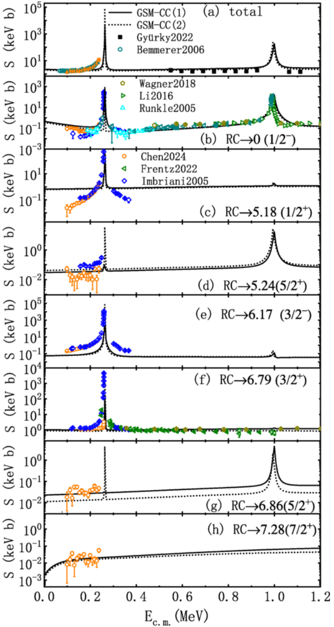
$$\left|\Psi^{(15)}_{\text{NCSMC}}\right\rangle = \sum_\lambda c_\lambda \left|^{15}\text{O},\lambda\right\rangle + \sum_\nu \int dr \gamma_\nu(r)\hat{A}_\nu \left|^{14}\text{N}+p,\nu\right\rangle + \sum_\mu \int dr \gamma_\mu(r)\hat{A}_\mu \left|^{14}\text{O}+n,\mu\right\rangle$$

  - ^{15}O: 9 (+) and 12 (-) eigenstates
  - ^{14}N: $1^+, 0^+, 1^+$
  - ^{14}O: 0^+
  - $N_{max} = 6, 7$

- Only 1 bound state ($\frac{1}{2}^-$) in *ab initio*
- Pheno-adjustment required to move resonances below threshold







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Summary and Outlook

- NCSMC can reproduce low-lying spectra and proton capture cross sections
  - some fine-tuning required for comparison to experiment
- Further CNO reactions with NCSMC
  - $^{13}\mathrm{N} \rightarrow {}^{13}\mathrm{C}$ beta decay
    - inc. $^{12}\mathrm{C} + n$ continuum
- The X17 remains unconfirmed
  - unresolved discrepancy with theory below $\Theta \sim 90$
  - independent experimental tests in progress (NewJEDI, PADME, MEGII)

Backup Slides

NCSM Scaling