R-matrix developments

James deBoer, ERC-NUCLEAR Kick-off Event - 15 May 2025

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E},$$

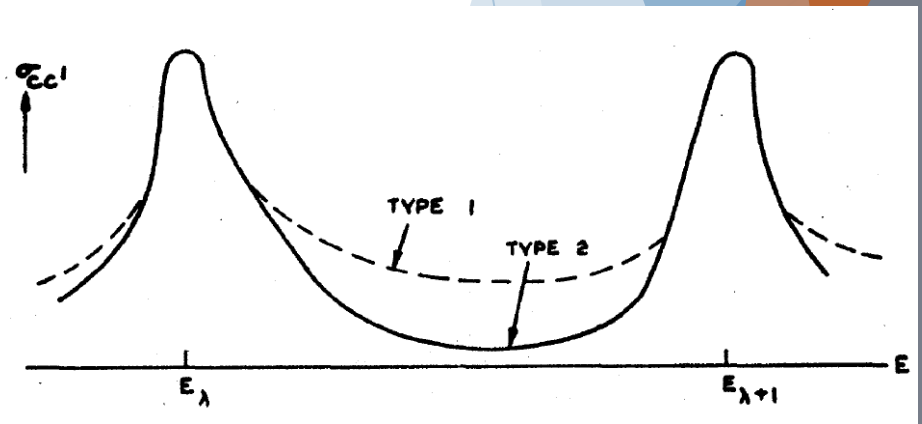
The parameters of the *R*-matrix are what we are normally varying as fit parameters to experimental data.

$\gamma_{\lambda c}$ Reduced width amplitudes

E_λ Pole energies

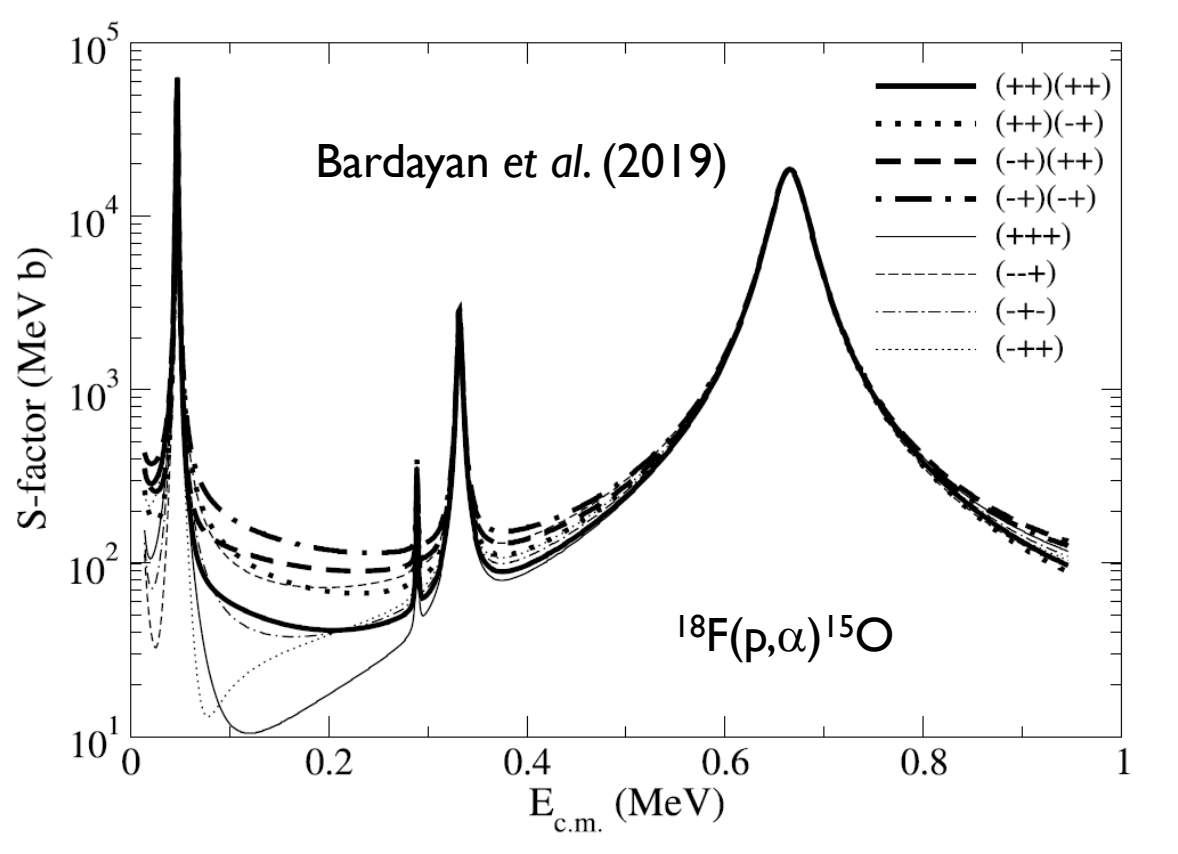
Remember λ is the level index and c is the channel index.

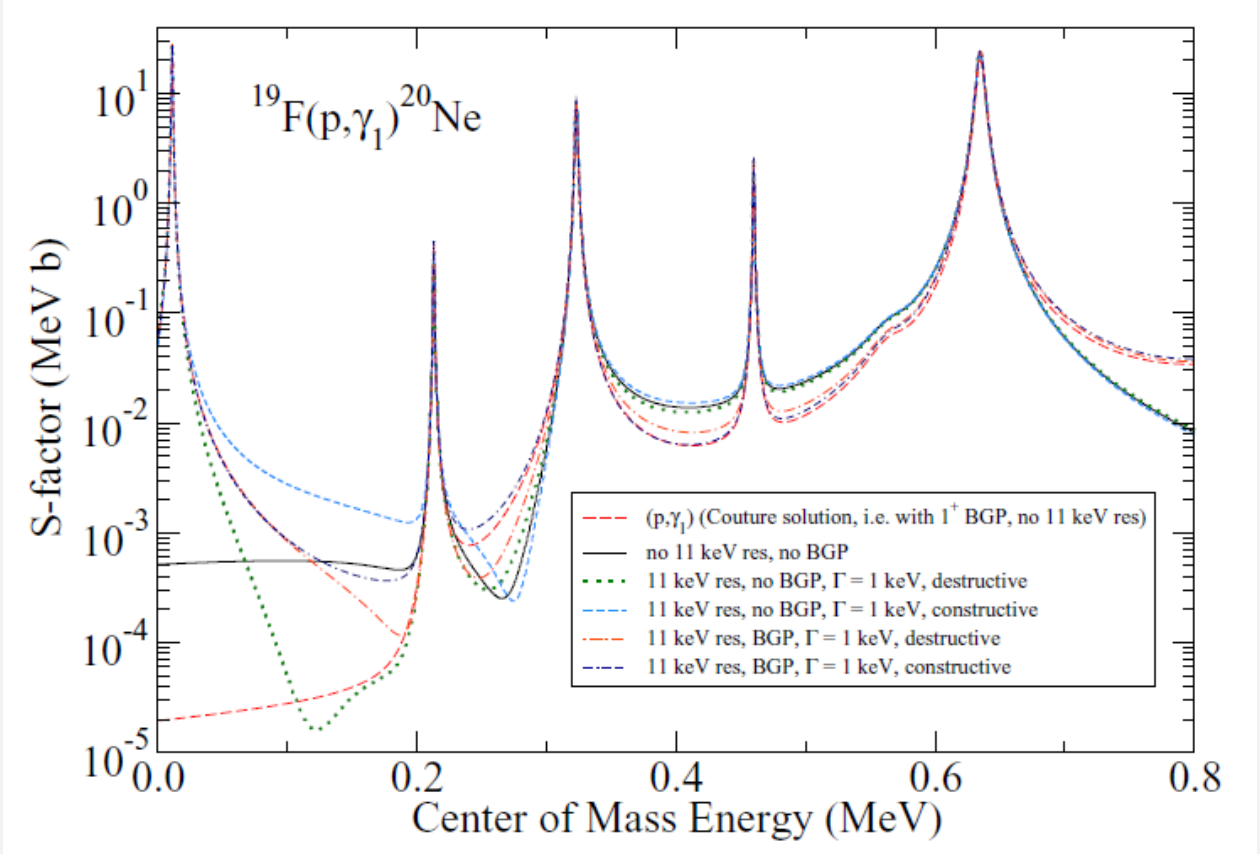
Also, $\gamma_{\lambda c}$ can be positive or negative and its sign determines the interference pattern between multiple resonances!



Lane and Thomas, **XII**.5

MULTI-RESONANCE INTERFERENCE

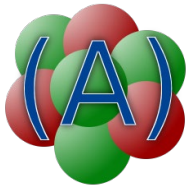




The AZURE2 code: an R-matrix code for nuclear astrophysics

- Originally developed by R.E. Azuma under the Joint Institute for Nuclear Astrophysics (JINA), published 2010

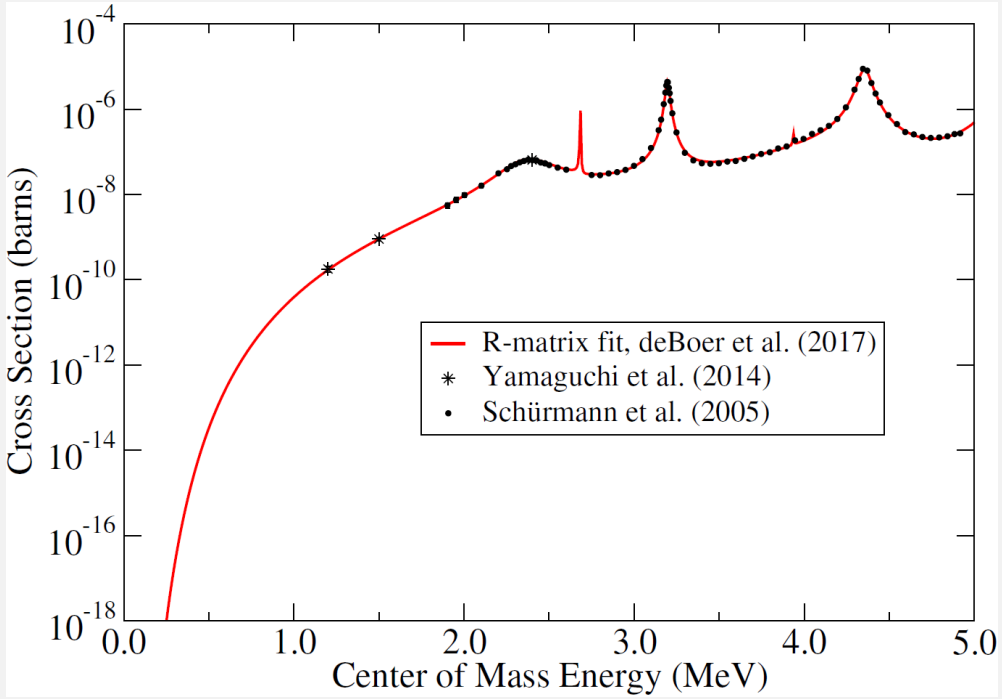
- AZURE2 developed by Ethan Uberseder, made publically available in 2012



- azure.nd.edu

- **Developed benchmark to increase the fidelity of R-matrix calculations in the community**

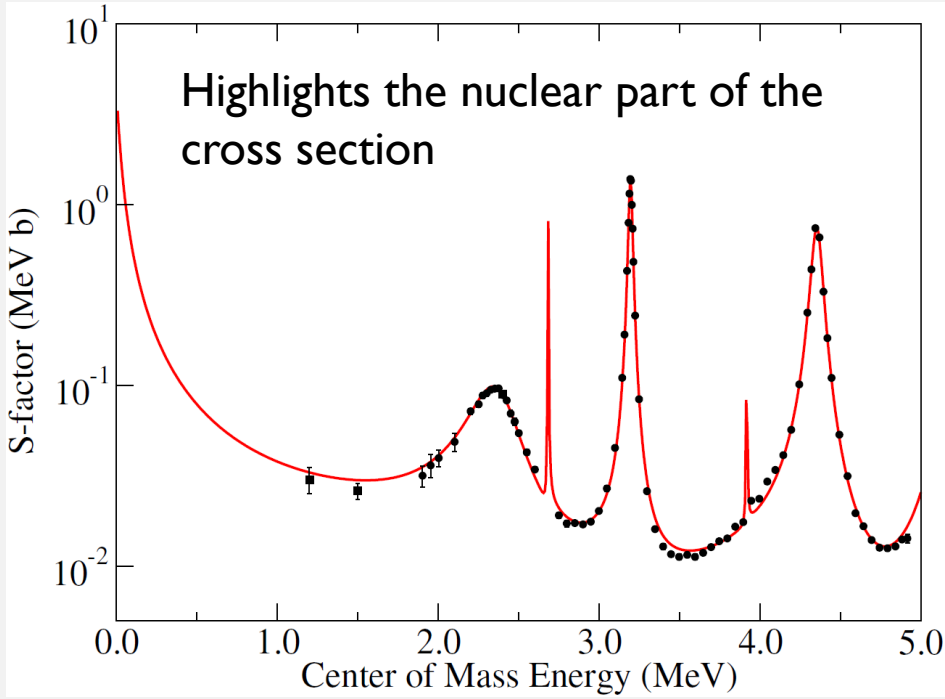
ASTROPHYSICAL S-FACTOR

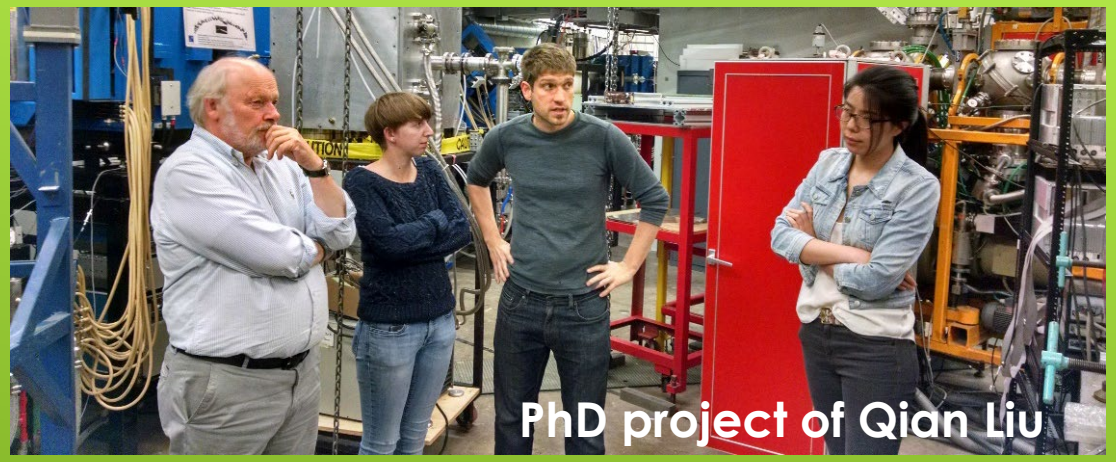


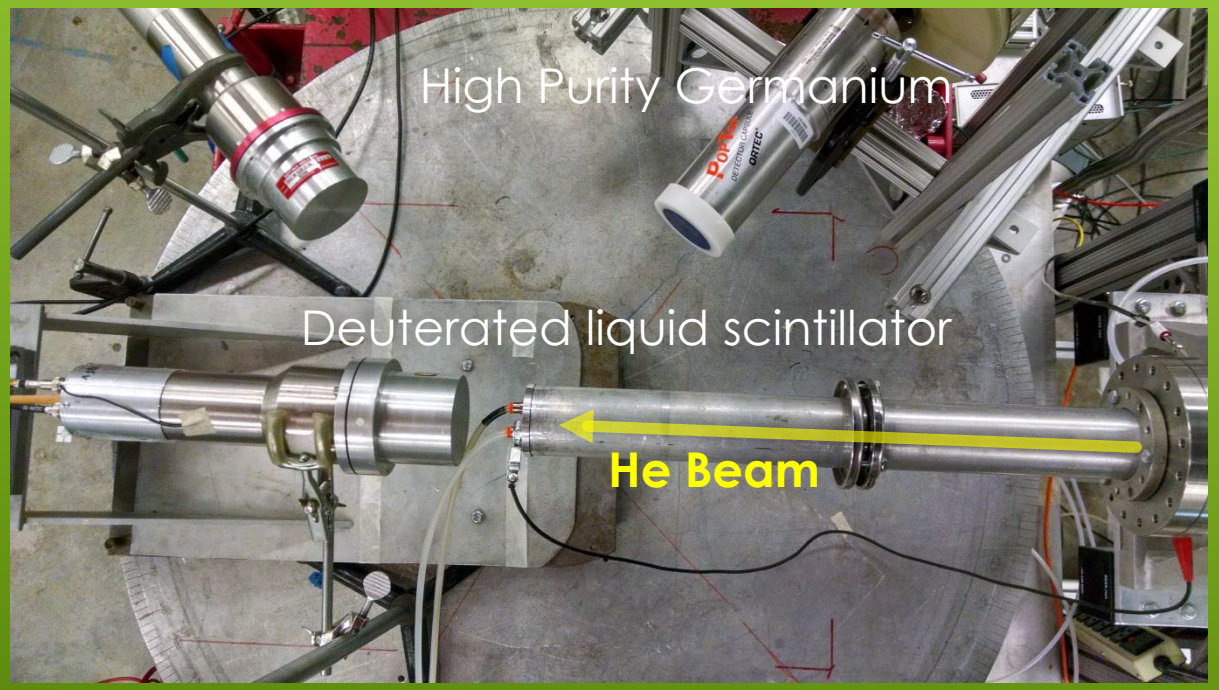
$$S(E) = E\,\sigma(E)\,e^{2\pi\eta}$$

$$\eta = \sqrt{\frac{\mu}{2E}}\frac{Z_1 Z_2 e^2}{\hbar^2}$$

Approximately dividing out the s-wave Coulomb penetrability (visualization / computational reasons only)

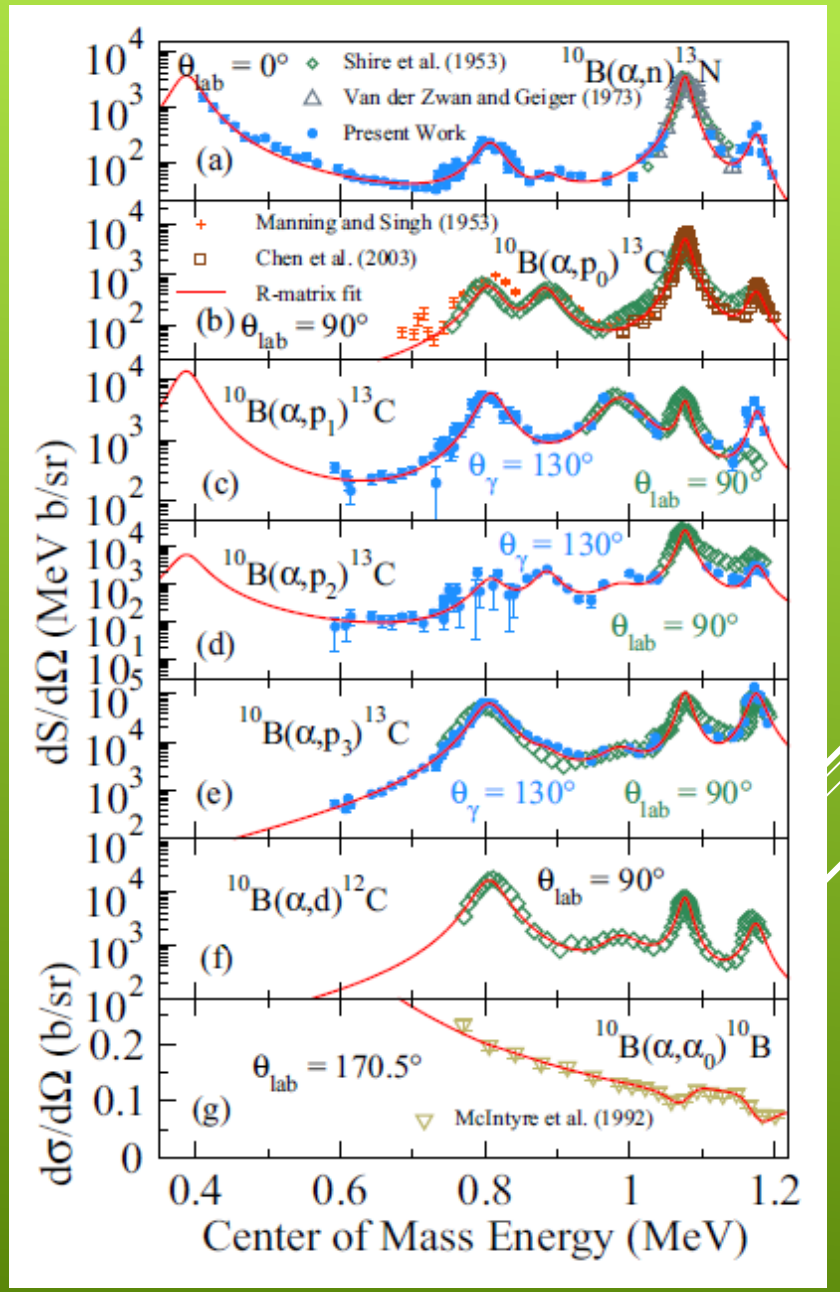


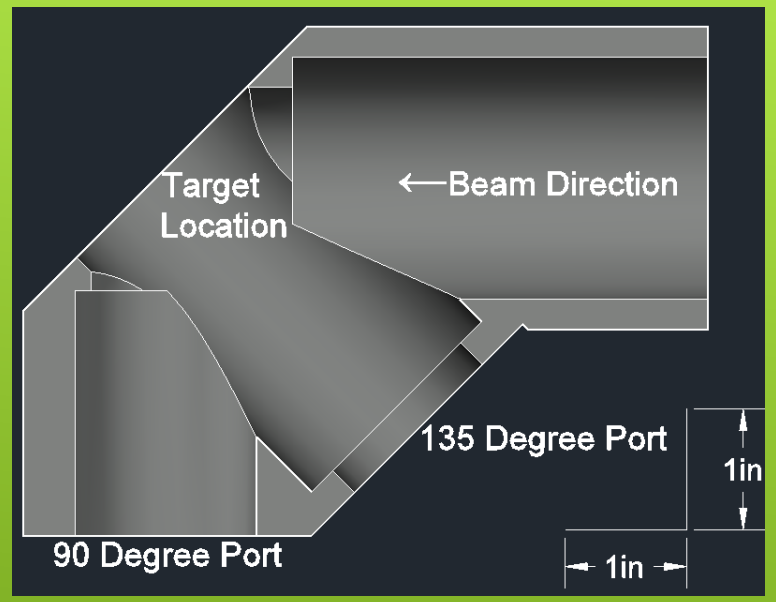


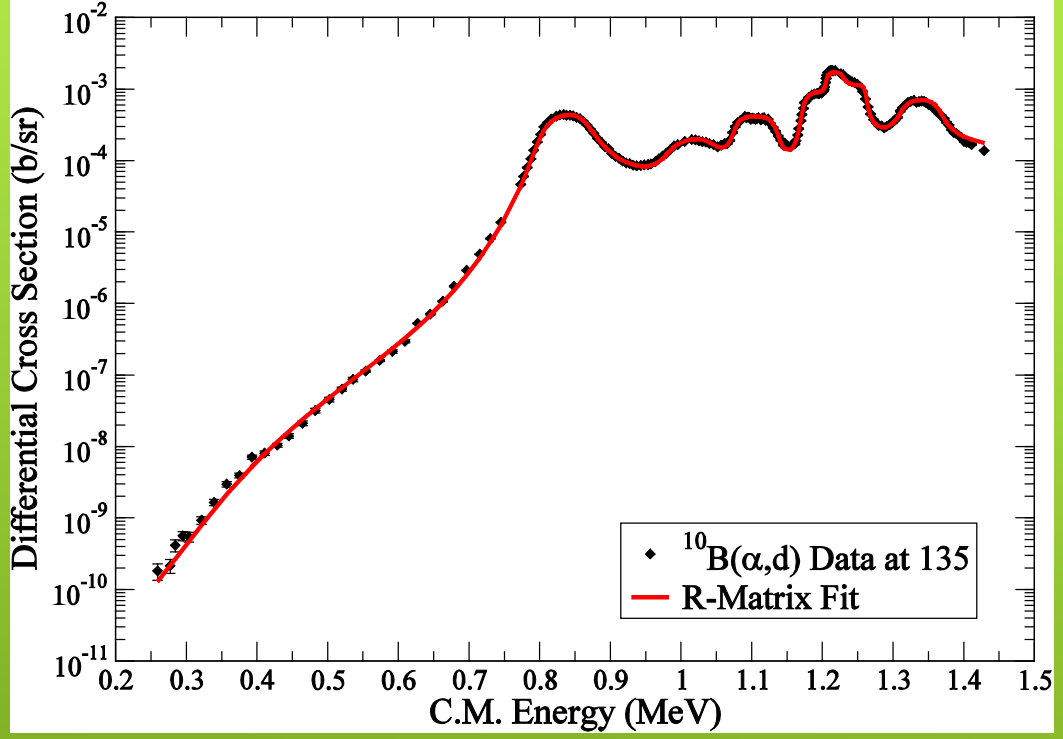


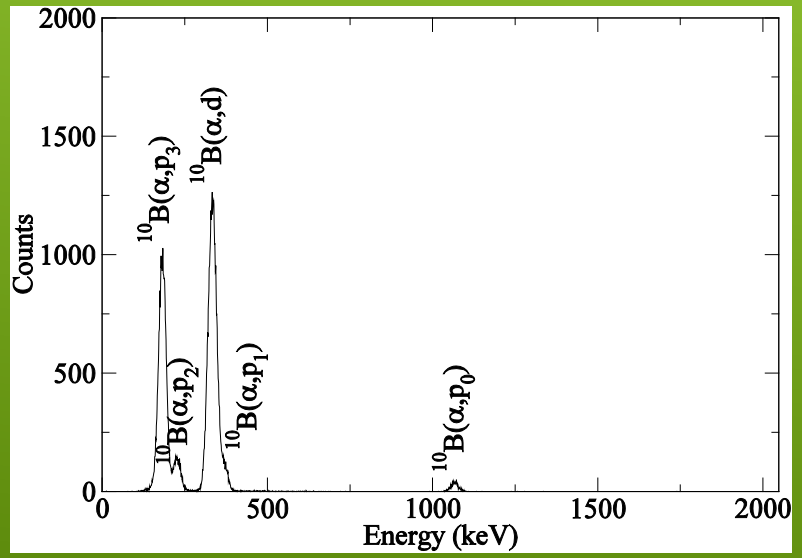
$^{10}B(\alpha,n)^{13}N$ MEASUREMENT

Liu et al. (2020) PRC

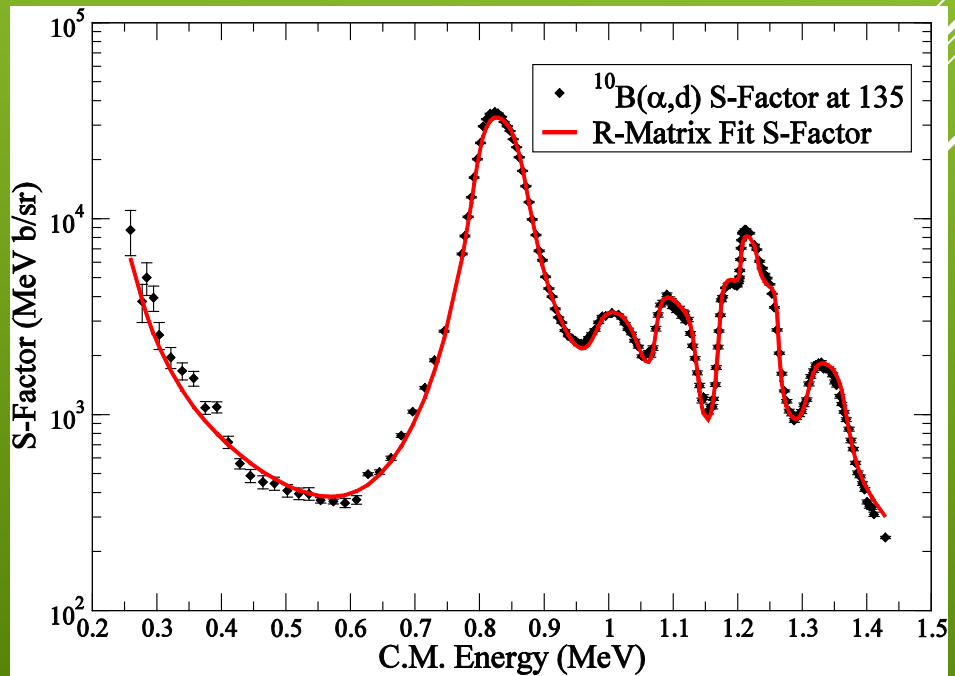




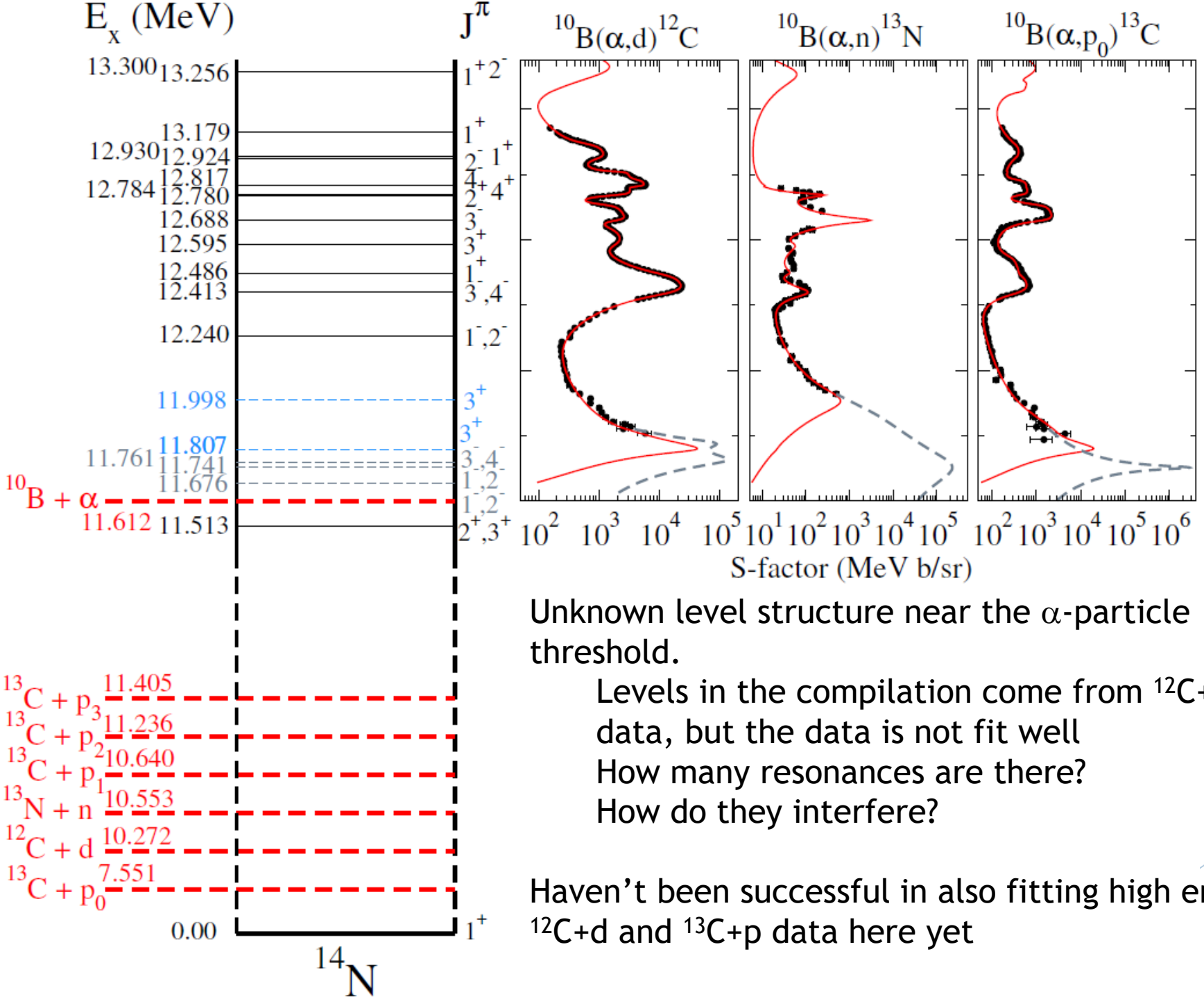




Lower energy measurements at LUNA?



^{10}B(α,d)^{12}C AND ^{10}B(α,p)^{13}C

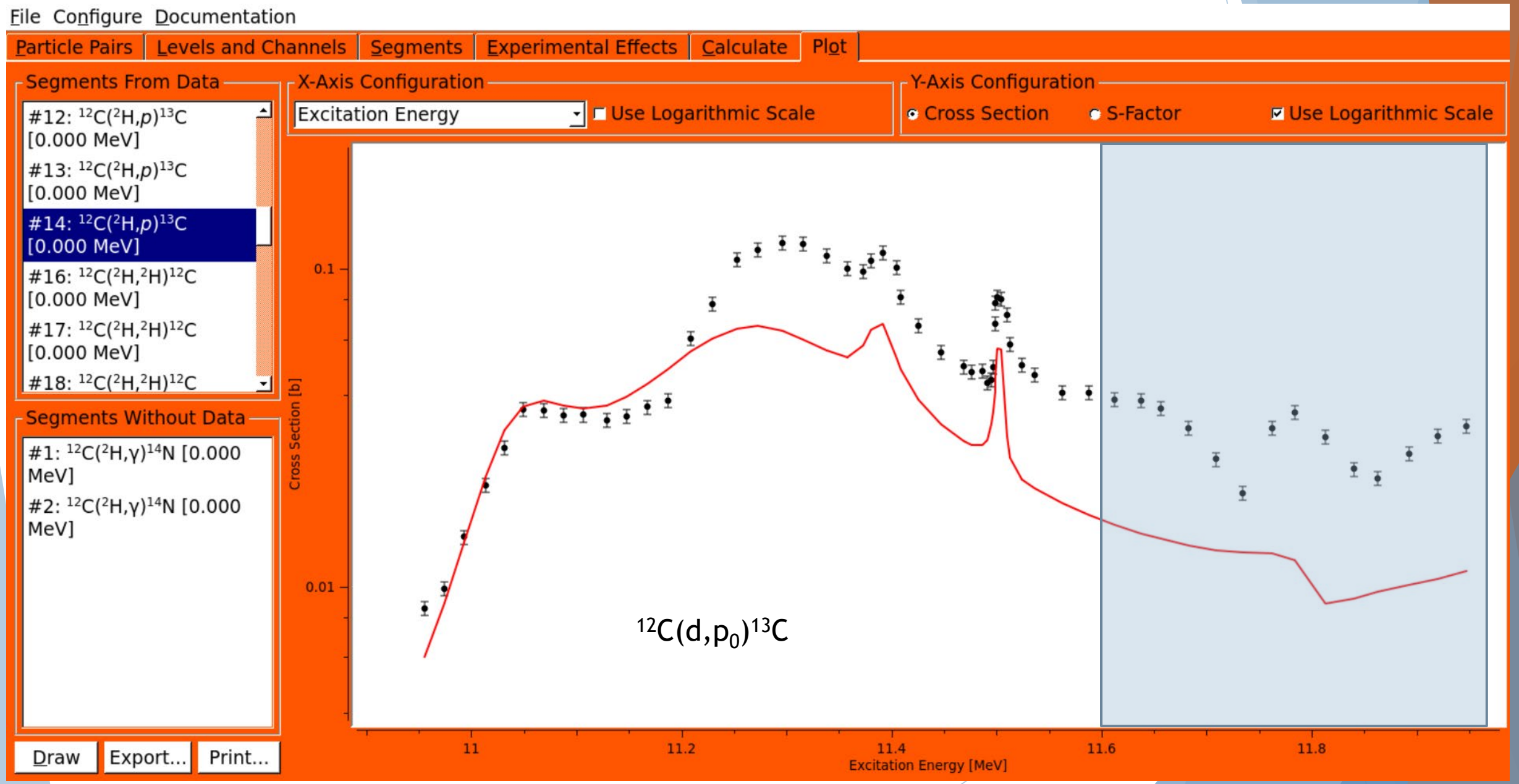


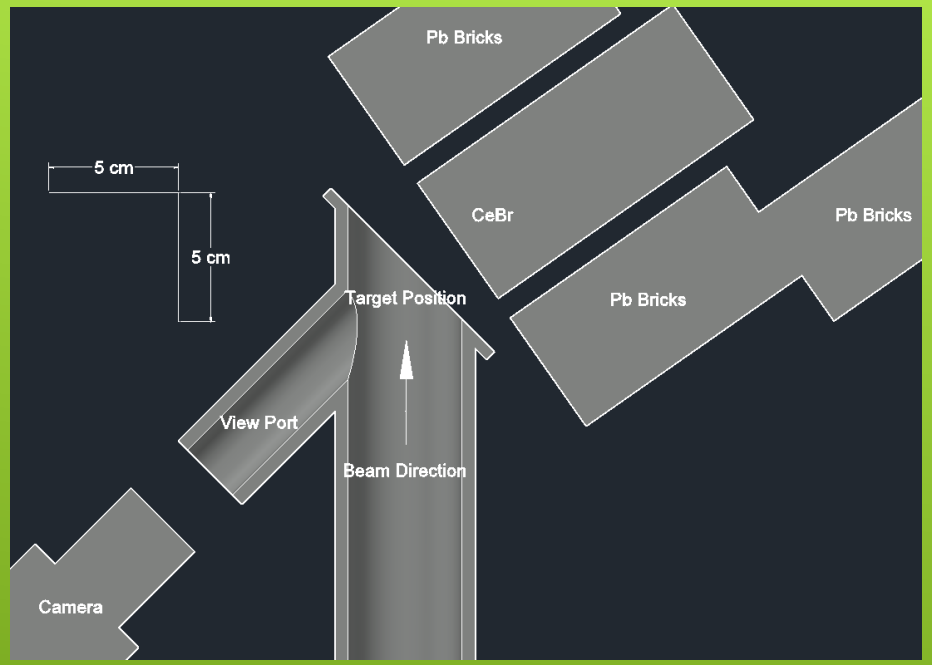
Unknown level structure near the α-particle threshold.

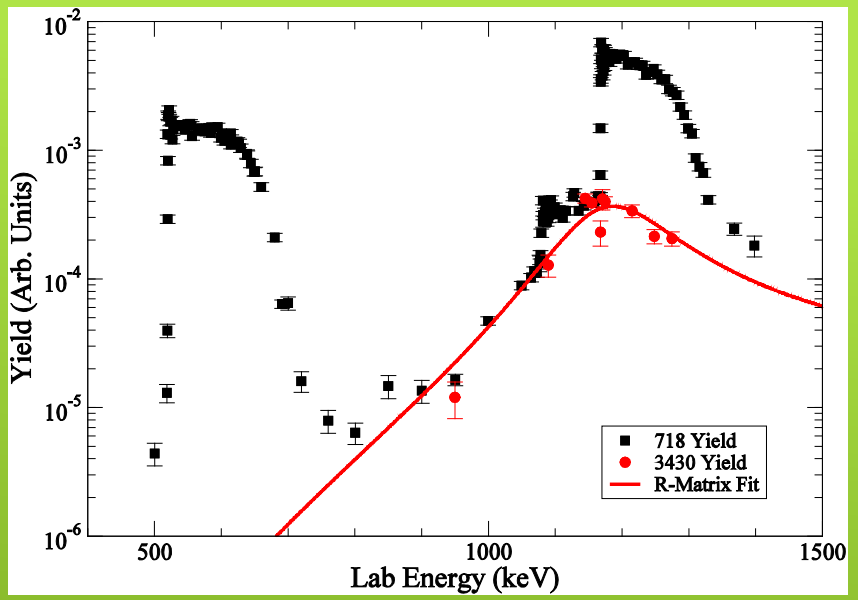
- Levels in the compilation come from ^{12}C+d data, but the data is not fit well
- How many resonances are there?
- How do they interfere?

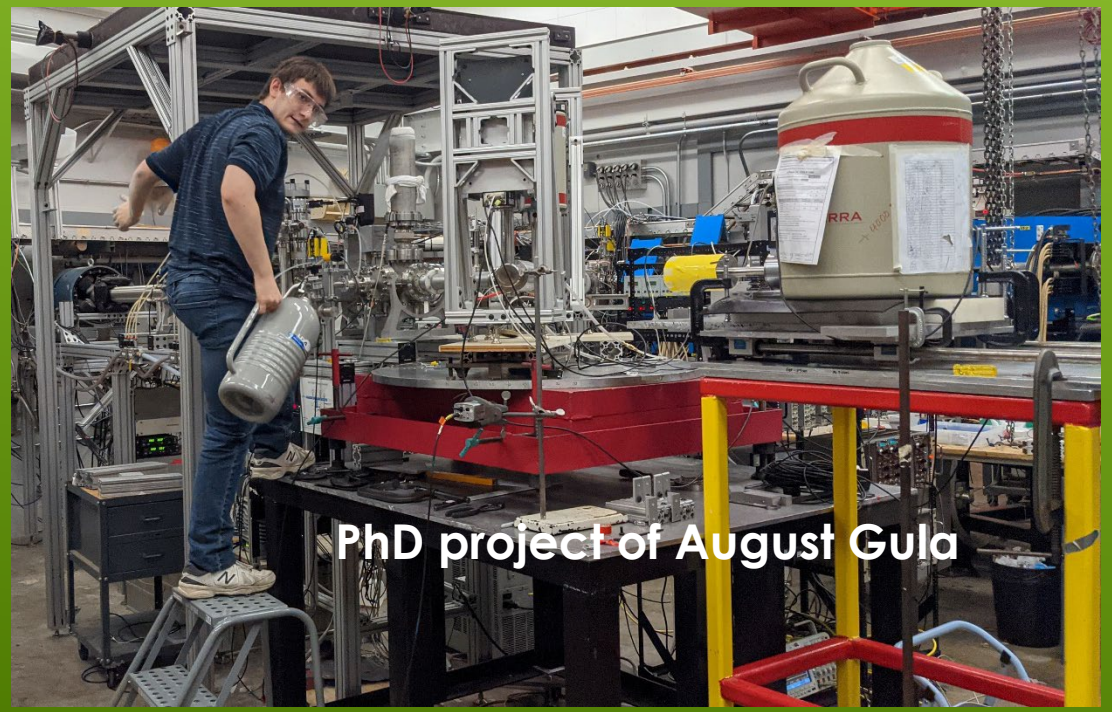
Haven't been successful in also fitting high energy ^{12}C+d and ^{13}C+p data here yet

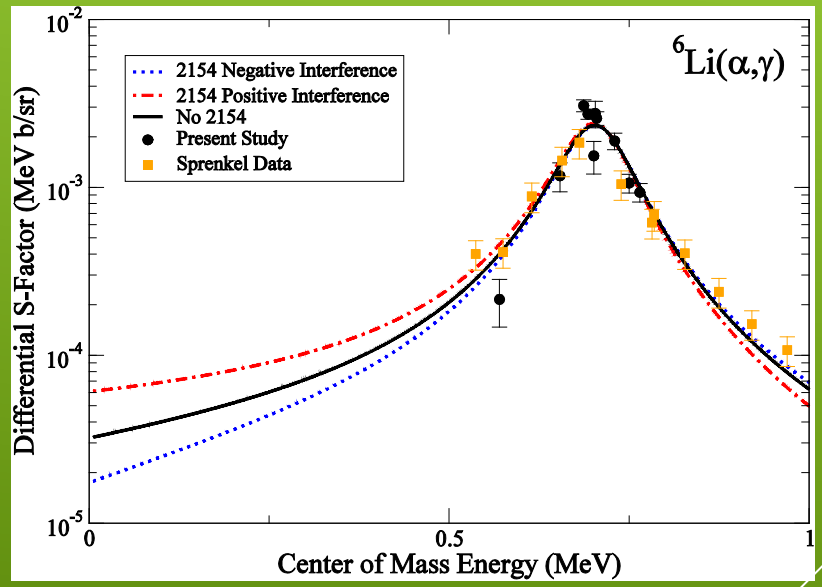
^{12}C+d data


File Configure Documentation
Particle Pairs
Levels and Channels
Segments
Experimental Effects
Calculate
Plot
Segments From Data
#12: 12C(2H,p)13C [0.000 MeV]
#13: 12C(2H,p)13C [0.000 MeV]
#14: 12C(2H,p)13C [0.000 MeV]
#16: 12C(2H,2H)12C [0.000 MeV]
#17: 12C(2H,2H)12C [0.000 MeV]
#18: 12C(2H,2H)12C
Segments Without Data
#1: 12C(2H,γ)14N [0.000 MeV]
#2: 12C(2H,γ)14N [0.000 MeV]
Draw
Export...
Print...
X-Axis Configuration
Excitation Energy
Use Logarithmic Scale
Y-Axis Configuration
Cross Section
S-Factor
Use Logarithmic Scale
0.1
0.01
Cross Section [b]
11
11.2
11.4
11.6
11.8
Excitation Energy [MeV]
12C(d,p0)13C





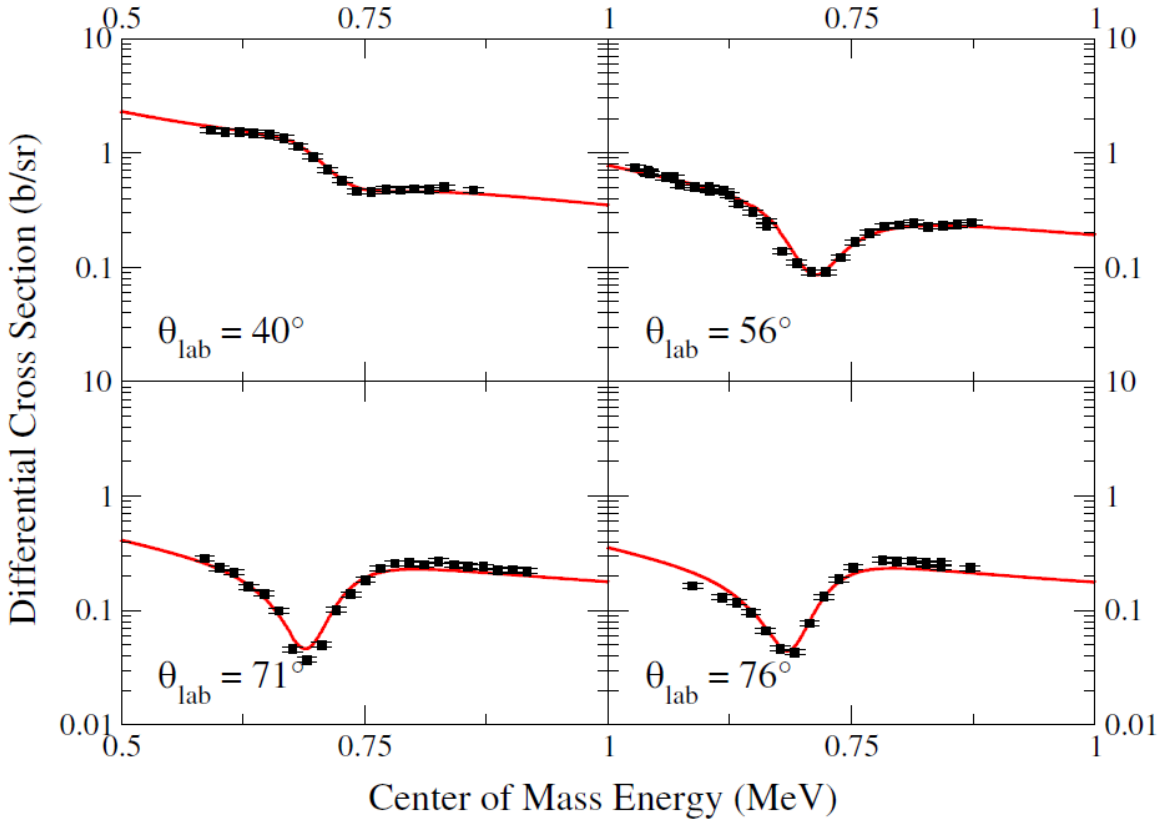


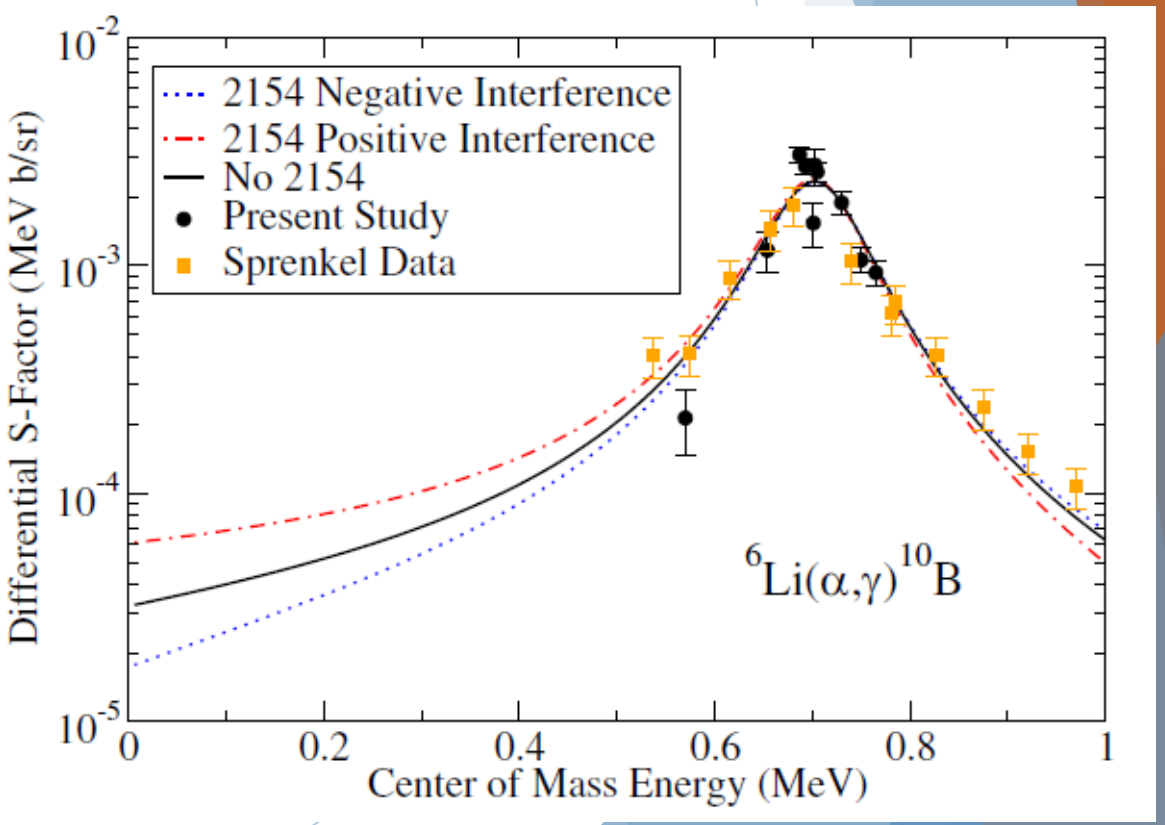


^{6}Li(α,γ)^{10}B MEASUREMENT

R-matrix fitting

- Pretty simple, no other open particle channels
- One scattering measurement by Dearnaley *et al.* (1962)
- One other radiative capture data set from Sprenkel *et al.* (1961)

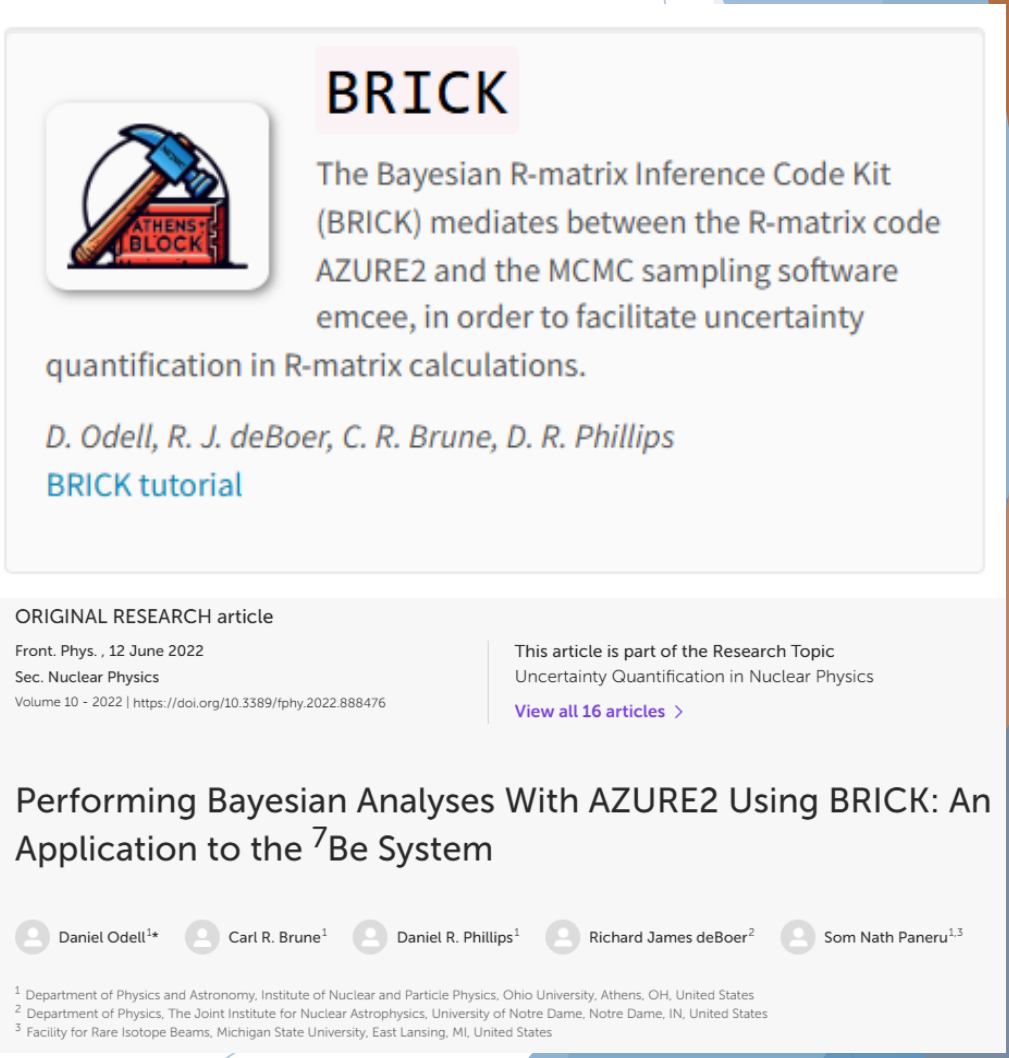




Improving uncertainty estimation for R-matrix fits

- **Bayesian** methods provide a way to improve and gain more detailed information
- See de **Souza et al. (2020)** for an application to $^{3}H(d,n)^{4}He$
- Computationally intensive, but probably doable
- **Daniel Odell** at Ohio University has developed the Bayesian R-matrix Inference Code Kit (**BRICK**) for use with the **AZURE2** R-matrix code

BAND
Bayesian Analysis of Nuclear Dynamics



BRICK

The Bayesian R-matrix Inference Code Kit (BRICK) mediates between the R-matrix code AZURE2 and the MCMC sampling software emcee, in order to facilitate uncertainty quantification in R-matrix calculations.

D. Odell, R. J. deBoer, C. R. Brune, D. R. Phillips

BRICK tutorial

ORIGINAL RESEARCH article

Front. Phys. , 12 June 2022
Sec. Nuclear Physics
Volume 10 - 2022 | https://doi.org/10.3389/fphy.2022.888476

This article is part of the Research Topic
Uncertainty Quantification in Nuclear Physics
View all 16 articles >

Performing Bayesian Analyses With AZURE2 Using BRICK: An Application to the ^{7}Be System

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[3] Facility for Rare Isotope Beams, Michigan State University, East Lansing, MI, United States

Improvements

- Current R-matrix process
  - Obtain experimental data
    - Literature
    - Databases (EXFOR)
  - Obtain level structure information
    - Literature
    - Databases (NNDC, TUNL Nuclear Data Project (up to mass 20))
  - Try to fit data using known level information
    - If this doesn't work, try to see if adding new levels can give better agreement
  - Compile all data that populate the same compound system and try to fit that all together
  - Perform all of these fits using χ^2 fitting
  - Perform refined uncertainty analysis using Bayesian uncertainty analysis using MCMC sampling

Improvements

- Recent improvements
  - Angular distributions for secondary γ-rays following particle emission (still not implemented in a released version of the code)
  - Bayesian uncertainty analysis using MCMC (BRICK)
  - Energy dependent convolution for neutron time of flight type studies
  - Various other small improvements that need to be incorporated into public version
- Wish list
  - Potential model hybrid calculations
    - Constrain background "potential" contribution to the low energy cross section
    - Ethan did it for $^{12}C(\alpha,\gamma)^{16}O$ but source code was lost
  - Energy fitting
    - χ^2 in AZURE2
    - Implemented in BRICK
  - Make BRICK more user friendly, GUI if possible?
  - Implement an electron screening term in AZURE2

Potential model / R-matrix hybrids

PHYSICAL REVIEW C VOLUME 7, NUMBER 2 FEBRUARY 1973

Unified R-Matrix-Plus-Potential Analysis for $^{16}O + n$ Cross Sections

C. H. Johnson
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830*
(Received 15 August 1972)

$^{12}C(\alpha,\gamma)^{16}O$ REVISITED

K. LANGANKE

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and

W.K. Kellogg Radiation Laboratory, California Institute of Technology, Pasadena, CA 91125, USA

and

S.E. KOONIN

W.K. Kellogg Radiation Laboratory, California Institute of Technology, Pasadena, CA 91125, USA

Received 19 October 1984
(Revised 2 January 1985)

PHYSICAL REVIEW C VOLUME 12, NUMBER 5 NOVEMBER 1975

R-matrix description of scattering from optical model potentials*

R. J. Philpott
Department of Physics, Florida State University, Tallahassee, Florida 32306
(Received 15 July 1975)

PHYSICAL REVIEW C VOLUME 4, NUMBER 2 AUGUST 1971

Potential Scattering and Spectroscopic Factors in R-Matrix Theory*

G. D. Westin and J. L. Adams
Department of Physics, Ohio University, Athens, Ohio 45701
(Received 29 April 1971)

Hybrid potential/R-matrix models for the $^{12}C + \alpha$ system

Jean-Marc Sparenberg[a]

[a]TRIUMF Theory Group, 4004 Wesbrook Mall, Vancouver, BC, Canada V6T 2A3

PHYSICAL REVIEW C **95**, 024616 (2017)

Internal and external radiative widths in the combined R-matrix and potential-model formalism

A. M. Mukhamedzhanov,[1,*] Shubhchintak,[2,†] C. A. Bertulani,[2,3,‡] and T. V. Nhan Hao[2,§]
[1]*Cyclotron Institute, Texas A&M University, College Station, Texas 77843, USA*
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[3]*Department of Physics and Astronomy, Texas A&M University, College Station, Texas 77843, USA*
(Received 28 October 2016; published 22 February 2017)

Potential model / R-matrix hybrids

I use the hybrid potential/R-matrix model presented in refs. [2,3]. The general principle is to calculate, for a given partial wave, the R-matrix corresponding to the potential model, $R_{\rm pot}(E)$, and to add to it phenomenological poles corresponding to discrete states. This leads to the total R-matrix

$$R(E) = R_{\rm pot}(E) + R_{\rm res}(E) = R_{\rm pot}(E) + \sum_{\lambda=1}^{L} \frac{\gamma_\lambda^2}{E_\lambda - E},$$

- Sparenburg (2004) and previous
- Short conclusion, there is actually a lot more literature here than I thought and I think I'm starting to understand it more.

The potential phase shifts can be expanded into hard sphere and "resonant" components familiar to the R-matrix theory[1, 2, 12];

$$\delta_{lJ} = \varphi_{lJ} + \delta_{lJ}^{R}, \qquad (5)$$

where

$$\tan\varphi_{lJ} = (F_{lJ}/G_{lJ})_{r=r_b} \qquad (6)$$

and

$$\tan\delta_{lJ}^{R} = \left.\frac{P_{lJ}R_{lJ}^{p}}{1 - S_{lJ}^{0}R_{lJ}^{p}}\right|_{r=r_b} \qquad (7)$$

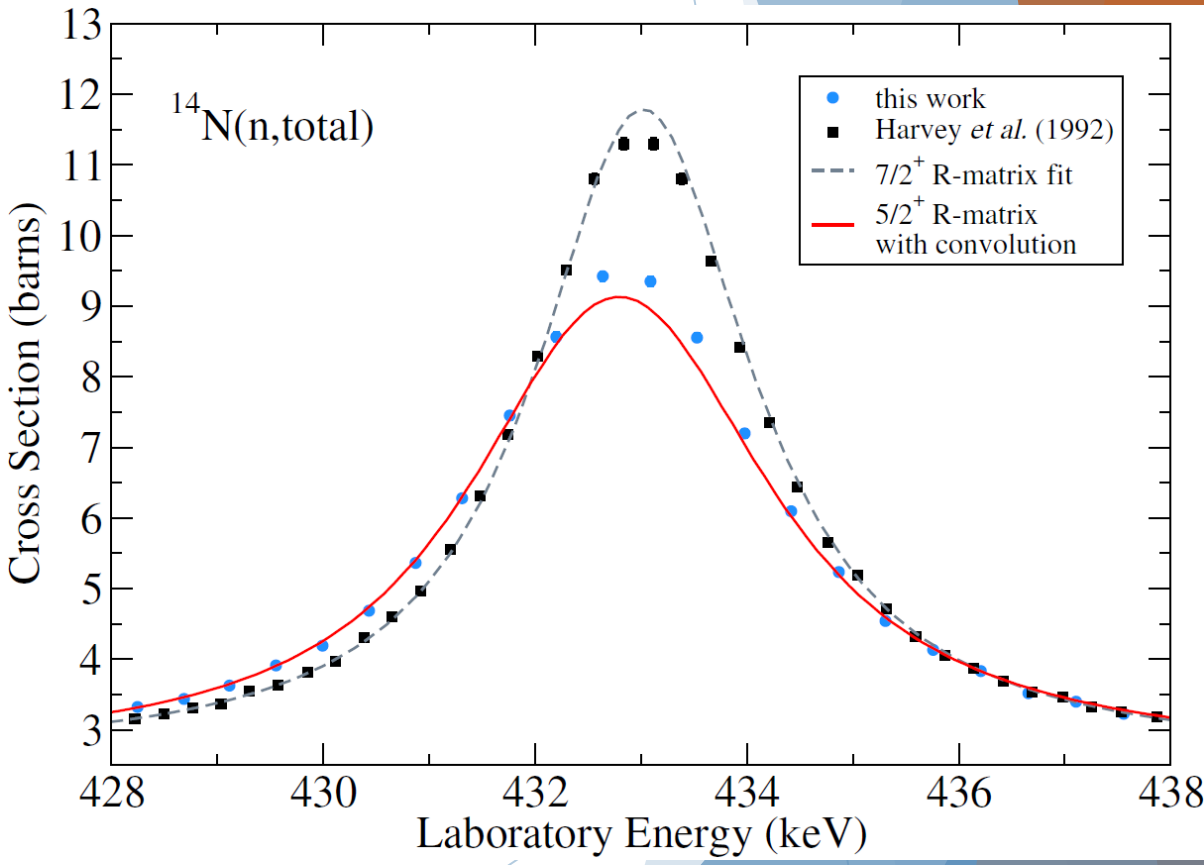
with $S_{lJ}^{0} = S_{lJ} - b_{lJ}$.

The potential R function is given by

$$R_{lJ}^{p} = (f_{lJ} - b_{lJ})^{-1},$$

Energy adjustments

- We currently allow the cross section to have an adjustable scaling factor but all data sets also have an energy uncertainty as well
- This can be a linear shift or something more complicated depending on how the experiment was performed
- Again, Ethan had implemented this once but never shared the source code with me so it was lost
- In principle it should be so difficult to implement the linear shift. Others are a little more complicated
- This should be high priority however!



BRICK upgrades

- Energy variation like in AZURE2 itself (probably easier)
- Graphical User Interface
  - Right now this is done through python input files or some python interface like Jupyter notebooks
- Jakub has been testing other uncertainty algorithms as well and has made some interesting finds

Native electron screening potential term in the code

- Should be pretty trivial
- This would just add an additional screening term to the cross section
- Also something that should be high priority