

MULTICHANNEL R-MATRIX EVALUATIONS

James deBoer

University of Notre Dame

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**UNIVERSITY OF
NOTRE DAME**



NNSA
National Nuclear Security Administration

R-MATRIX: NUCLEAR ASTROPHYSICS

REVIEWS OF MODERN PHYSICS, VOLUME 97, JULY–SEPTEMBER 2025

Solar fusion III: New data and theory for hydrogen-burning stars

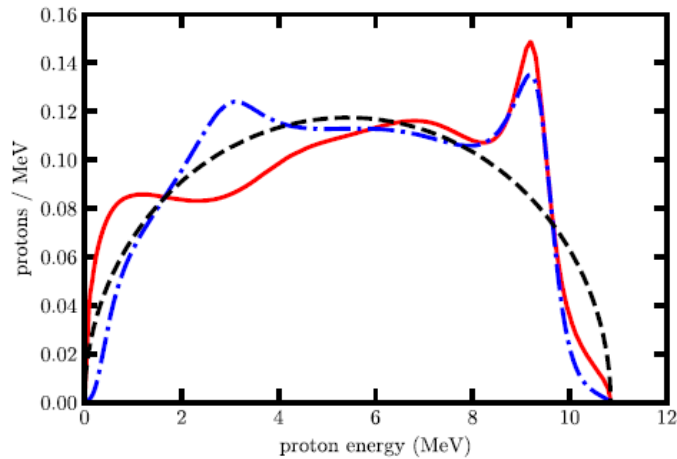
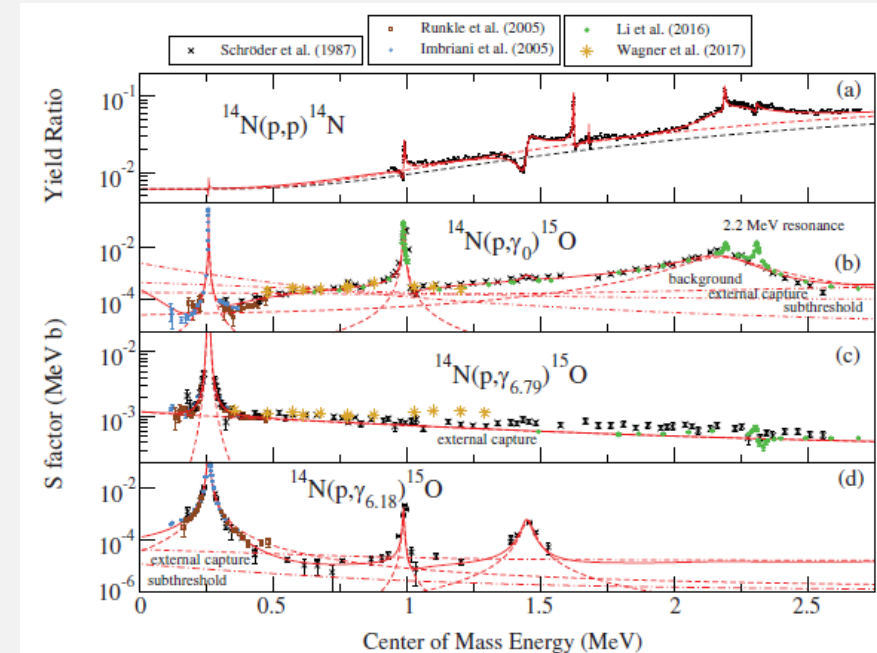
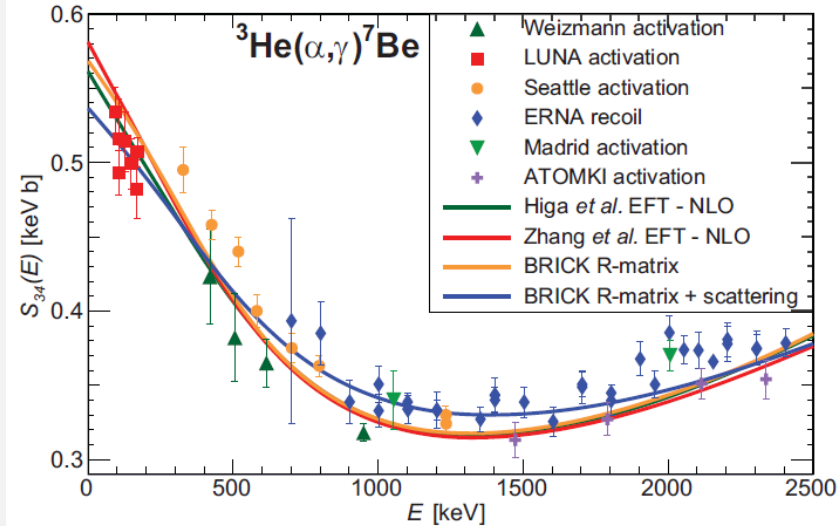
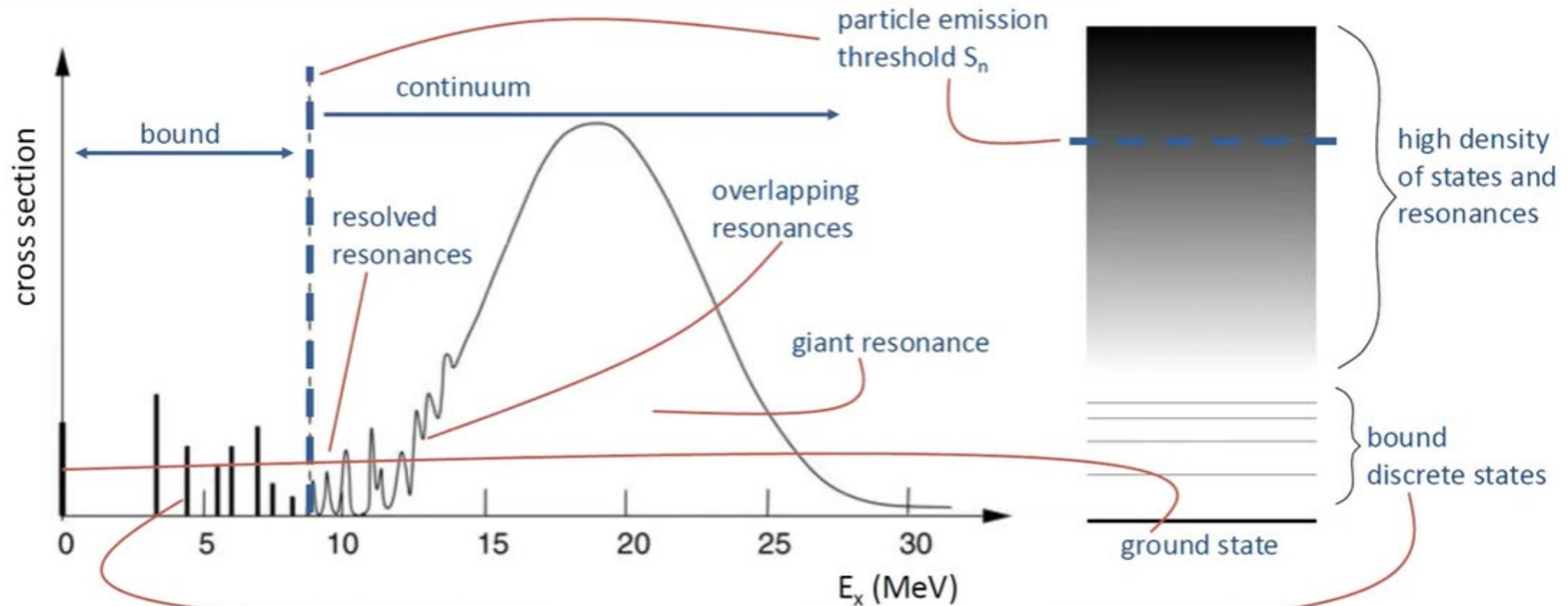


FIG. 6. Calculated proton energy spectra in the c.m. frame for the ${}^3\text{He}({}^3\text{He}, 2p){}^4\text{He}$ reaction at $E_{\text{c.m.}} = 165$ keV. The solid red and dot-dashed blue curves are models 1 and 2, respectively, from Fig. 3(a) of Zylstra *et al.* (2017). The dashed black curve is the elliptical spectrum. The spectra are normalized to unit area.



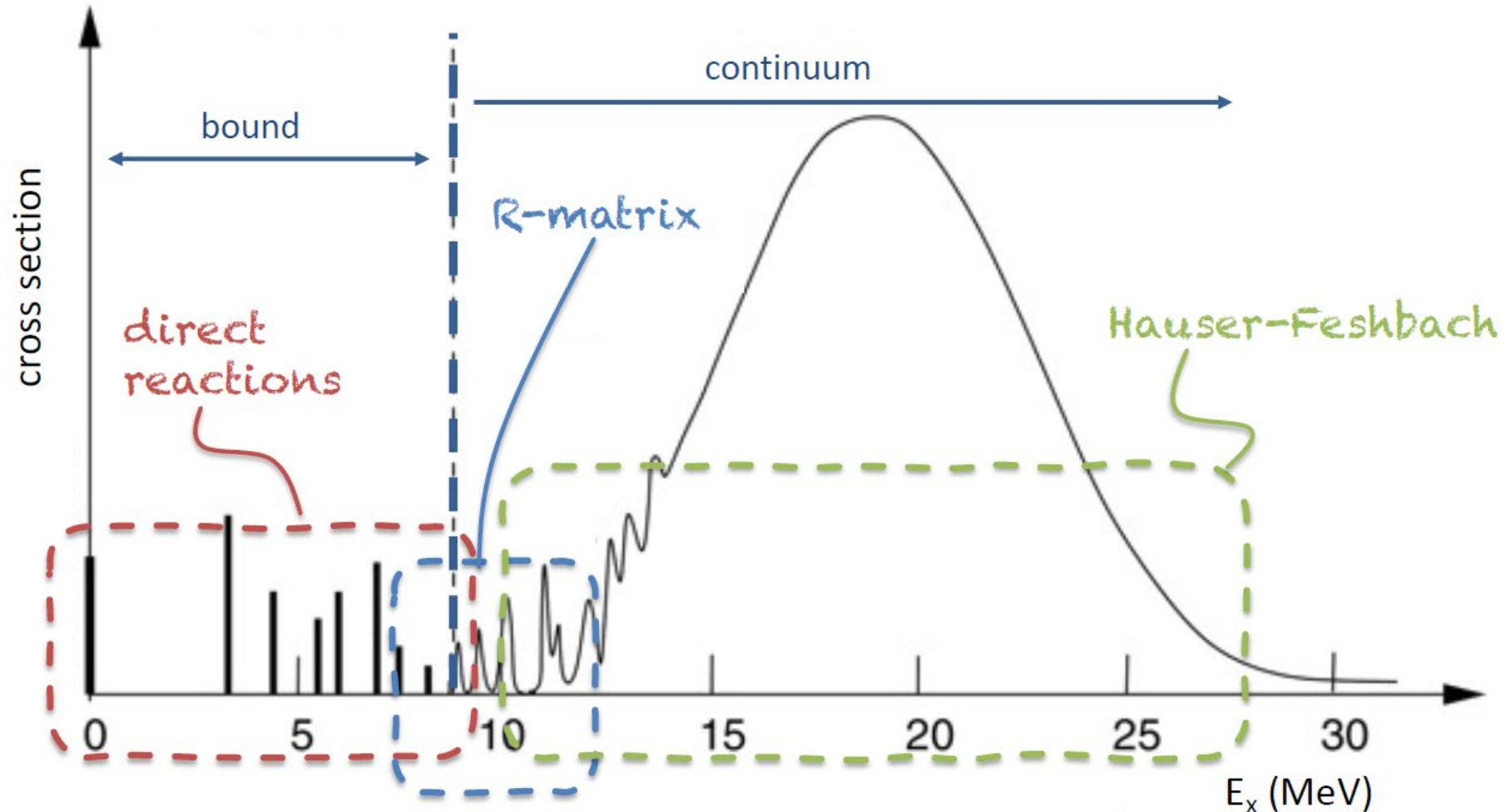
THE EVOLVING RESONANCE REGION

Features of nuclear spectra probed by nuclear reactions



Shamelessly stolen from a lecture by Gregory Potel

DIFFERENT THEORIES FOR DIFFERENT ENERGY RANGES

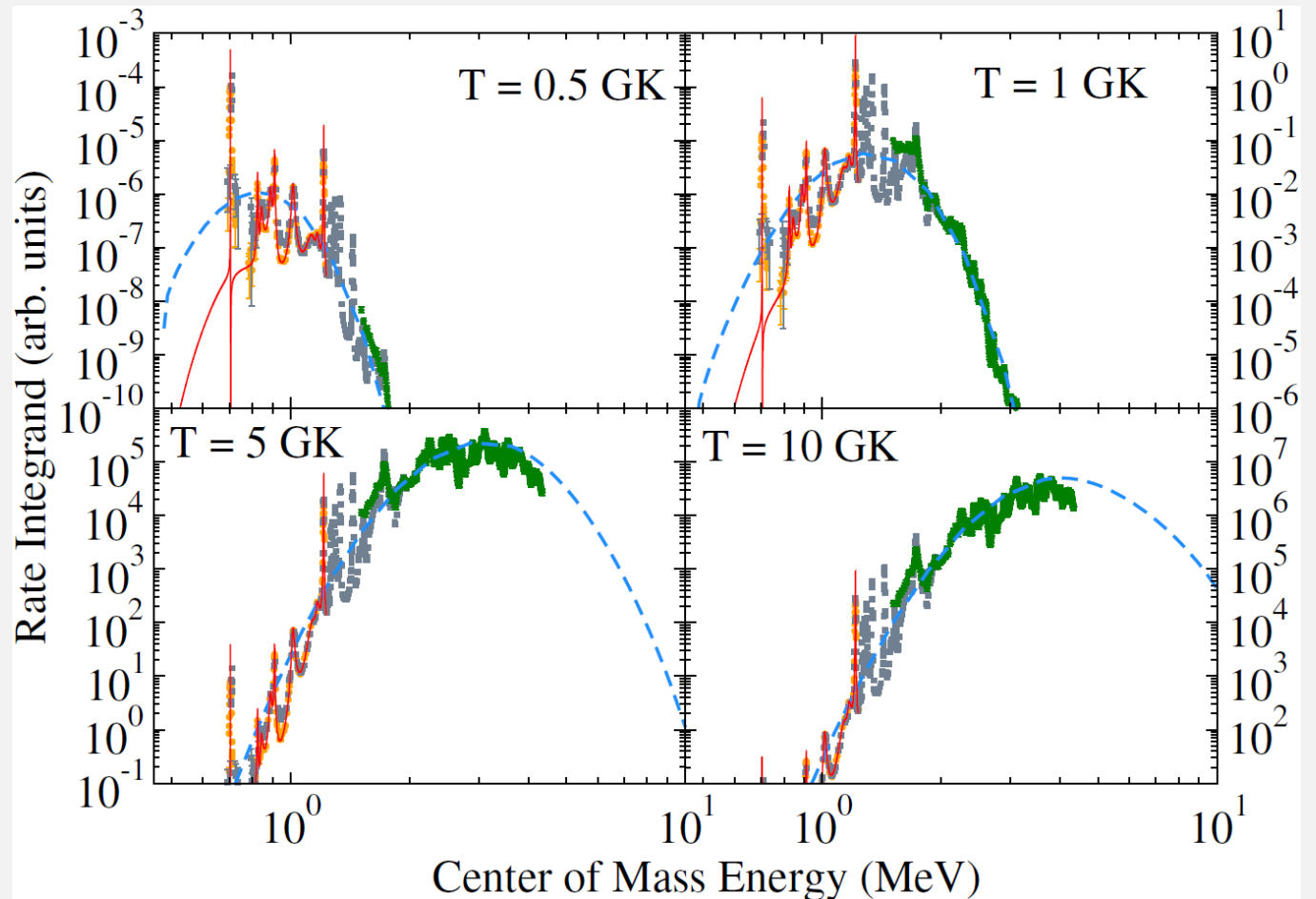
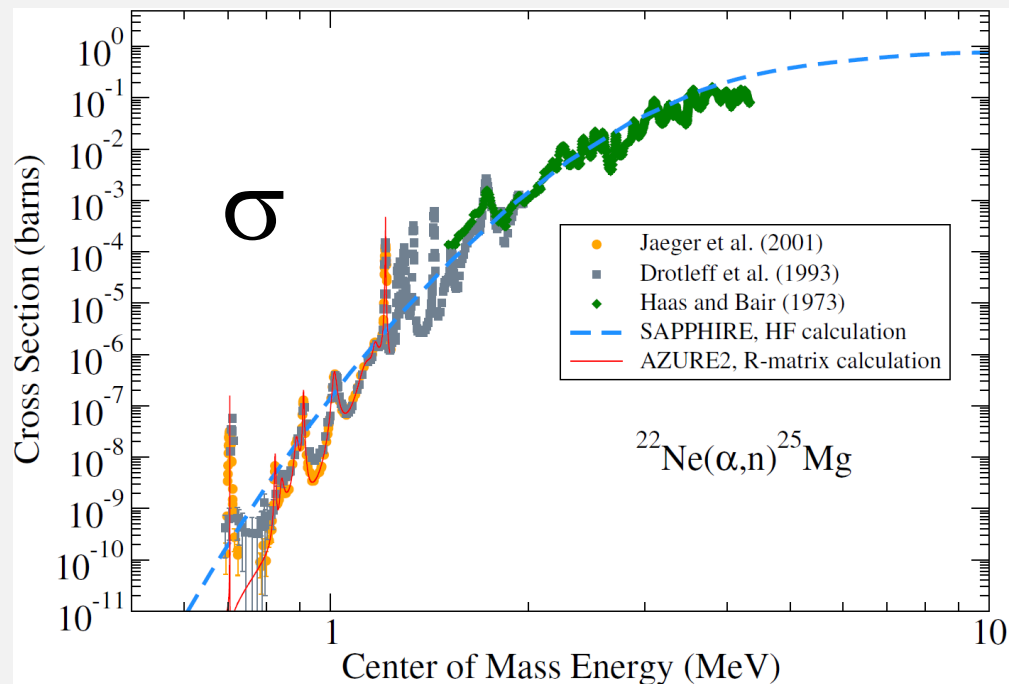


Shamelessly stolen from a lecture by Gregory Potel

NEAR THRESHOLD STATES ARE PARTICULARLY IMPORTANT FOR NUCLEAR ASTROPHYSICS

$$N_A \langle \sigma v \rangle = 3.7313 \times 10^{10} A^{-1/2} T_9^{-3/2} \int_0^{\infty} \sigma E \exp(-11.605 E/T_9) dE,$$

At the temperatures of stellar burning, the rates are often dominated by a few resonances

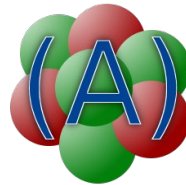


The AZURE2 code: an R-matrix code for nuclear astrophysics

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



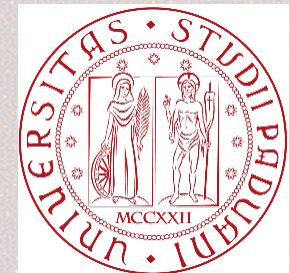
- AZURE2 developed by Ethan Uberseder, made publically available in 2012



- azure.nd.edu

- Jakub Skowronski** is working on many upgrades!

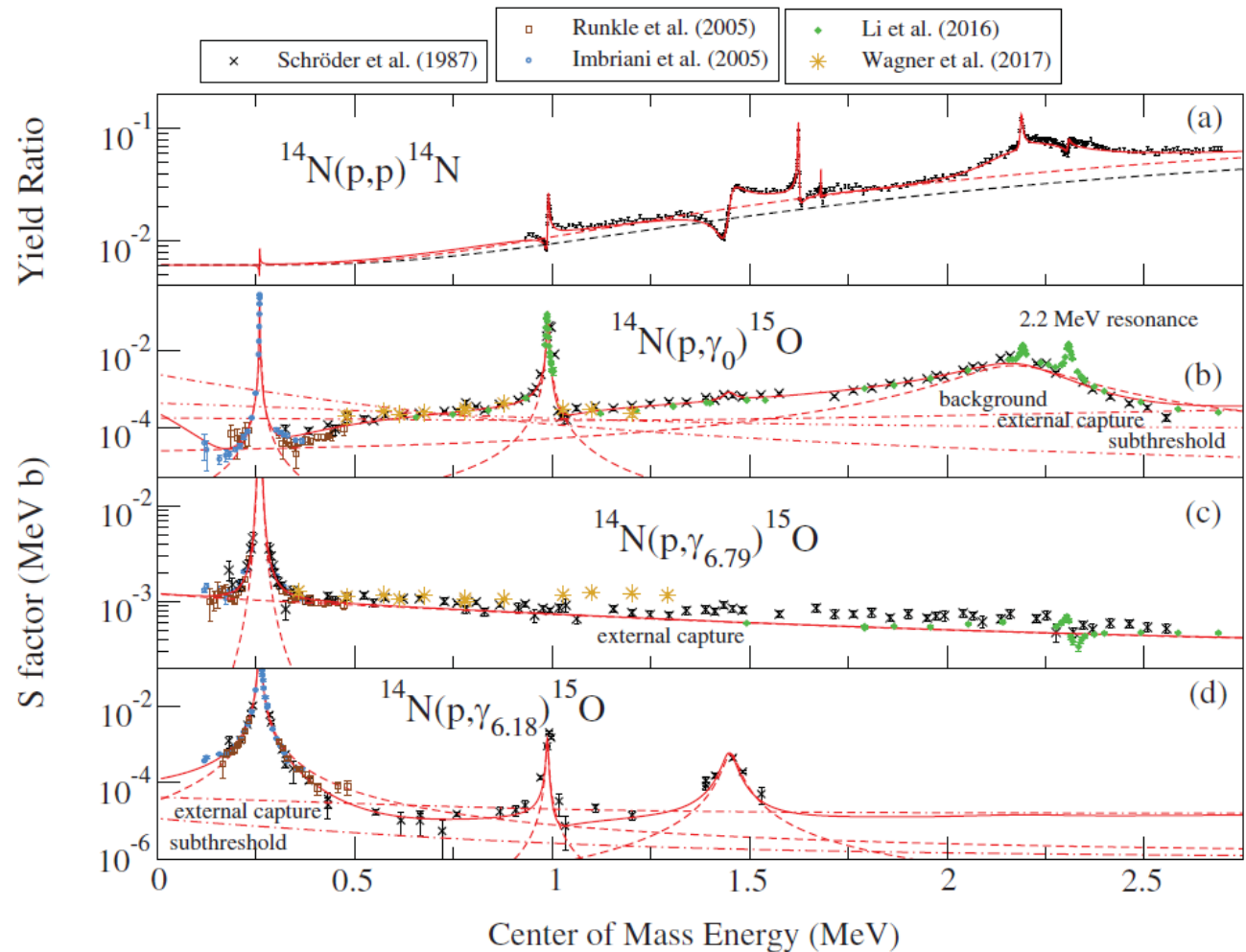
- <https://github.com/rdeboer1/AZURE2/>



RADIATIVE CAPTURE IN AZURE2

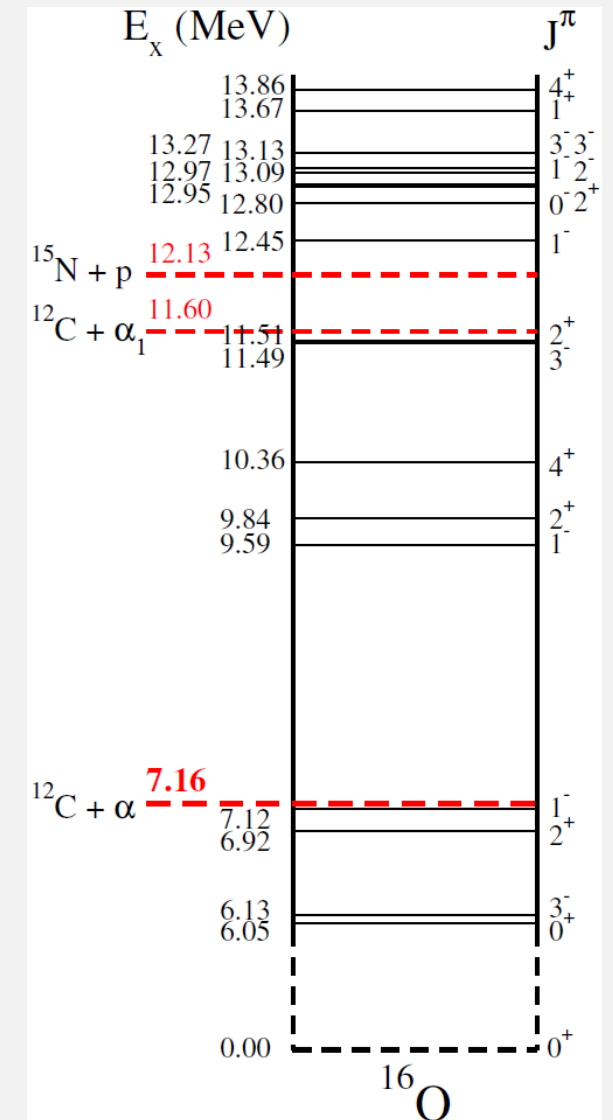
- Lane and Thomas give a perturbative approach for resonance (internal) radiative capture
- Unlike particle interactions, a **direct mechanism** is very significant for many radiative capture reactions even at low energies (external radiative capture)
 - **Holt et al.** (1978), Barker and Kajino (1991), Angulo and Descouvemont (2001), deBoer et al. (2017)
 - **Asymptotic Normalization Coefficient (ANC)** gives the magnitude of the direct capture
 - **See the many works by Akram Mukhamedzhanov**

$$C_{\lambda c} = \frac{(2m_{\alpha}a_c)^{1/2}}{\hbar W_c(a_c)} \frac{\gamma_{\lambda c}}{[1 + \sum_{c'} \gamma_{\lambda c'}^2 (dS_{c'}/dE)(E_{\lambda})]^{1/2}},$$



FUNDAMENTAL PHYSICS CONSTRAINTS AND THE LEVEL STRUCTURE

- The phenomenological R-matrix theory has limited (but sometimes powerful) physical constraints
 - **Momentum conservation (resonance interference)**
 - **Conservation of probability flux (unitarity)**
 - **Time reversal symmetry**
- Since limited nuclear physics constraint is present, we need to be very careful
 - Legitimate R-matrix criticism: you can fit any cross section you want to arbitrary precision if you use an arbitrarily large number of levels
 - It is therefore very important to have either a **well-known level structure** or a **LOT of constraining data**
 - If you don't have either of these things then it leads to **large uncertainties** that can be **difficult to quantify**
- The inclusion of additional information from nuclear structure / theory helps a lot
 - We should strive to better incorporate it into our analysis



PARAMETERIZATION

- The practical utility of the Brune parameterization is very consequential as it makes it much easier to maintain the full level structure of the system
- It provides a way to **fix** the **level energies** and **reduced widths** of any number of levels in a way that is impossible using the standard R-matrix parameterization
- Why this matters?
 - Bound state levels can now be fixed in energy, so that the bound state level structure can be included
 - ANC's of these levels can then be applied in a straightforward way
 - Background poles (levels) can be fixed in energy (stops them "running off" to undesired values)
 - Narrow resonances can be included more easily (rate calculations)

PHYSICAL REVIEW C **66**, 044611 (2002)

Alternative parametrization of *R*-matrix theory

C. R. Brune

Edwards Accelerator Laboratory, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701

(Received 15 July 2002; published 24 October 2002)

An alternative parametrization of *R*-matrix theory is presented which is mathematically equivalent to the standard approach, but possesses features that simplify the fitting of experimental data. In particular, there are no level shifts and no boundary-condition constants which allow the positions and partial widths of an arbitrary number of levels to be easily fixed in an analysis. These alternative parameters can be converted to standard *R*-matrix parameters by a straightforward matrix diagonalization procedure. In addition, it is possible to express the collision matrix directly in terms of the alternative parameters.

- Can do fits in terms of "observable" energies and reduced widths (E_r, γ_i)

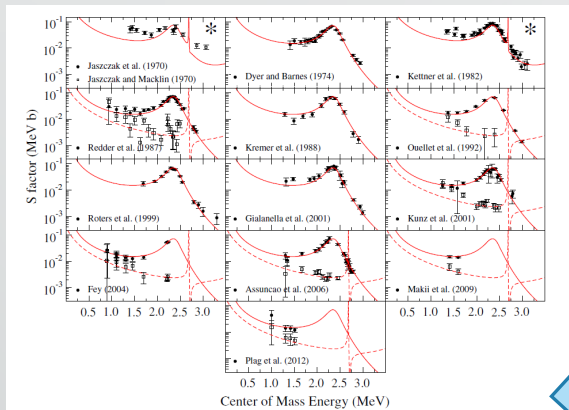
Unbound state

$$\Gamma_{ic} = \frac{2P_c \tilde{\gamma}_{ic}^2}{1 + \sum_c \tilde{\gamma}_{ic}^2 \left(\frac{dS_c}{dE} \right)_{\tilde{E}_i}}$$

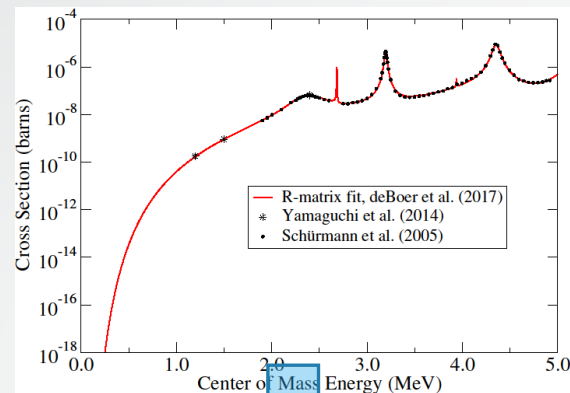
Bound state

$$C_{ic}^2 = \frac{2\mu_c a_c}{\hbar^2 O_c^2} \left[\frac{\tilde{\gamma}_{ic}^2}{1 + \sum_c \tilde{\gamma}_{ic}^2 \left(\frac{dS_c}{dE} \right)_{\tilde{E}_i}} \right]$$

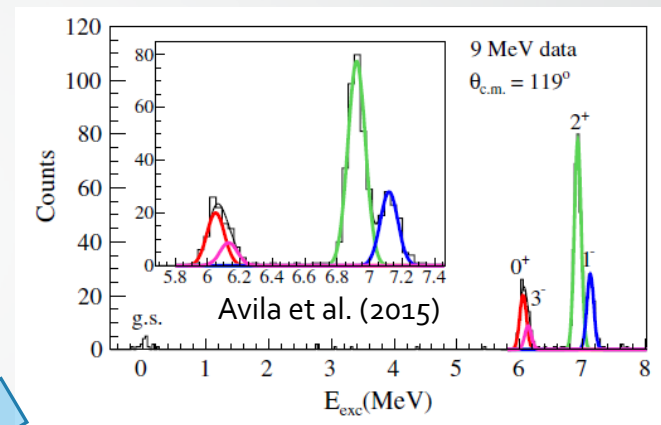
A methodology for combining data from many sources



Low energy $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$ data

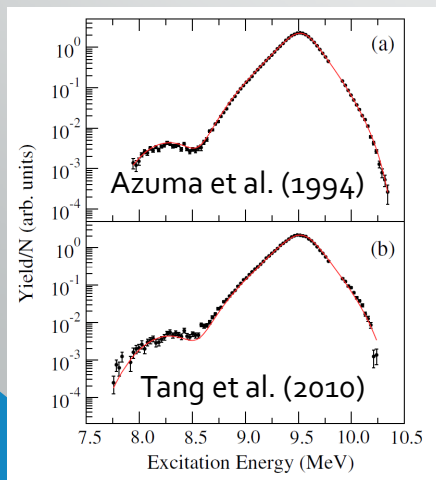


Total capture cross sections (recoils)

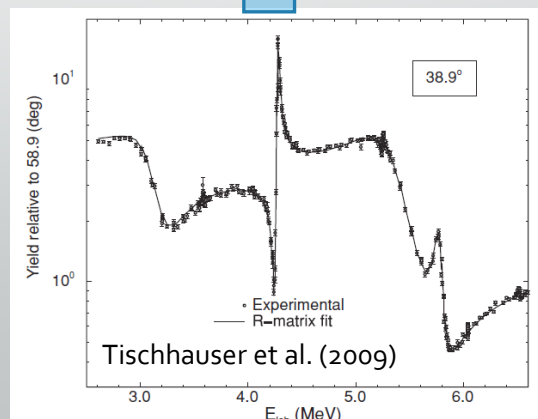


Transfer data (ANCs)

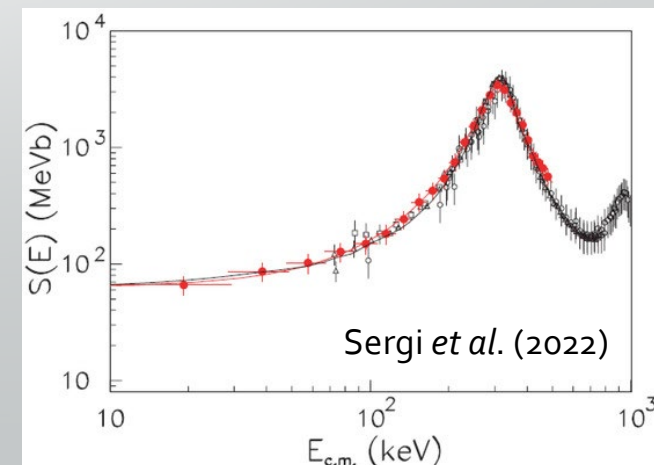
$^{16}\text{N}(\beta\alpha)^{12}\text{C}$ spectrum



$^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$ data



Trojan Horse



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

TRUNCATION OF MANY THINGS

- Theory has infinite sums over J^π , levels (for each J^π), channels, and angular momentum

$$R_{cc'} = \sum_{\lambda=1}^{\infty} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E}$$

λ = level index

- Drastic truncations are often made, how can this approach still work?
- Levels have a **local** (energy) effect on the cross section
 - If resonances have larger widths, data should cover a wider energy range
 - Can sometimes get by with just the levels in the energy range covered by your data
 - Sometimes need subthreshold states and/or background states

- At low energies, low angular momenta dominate

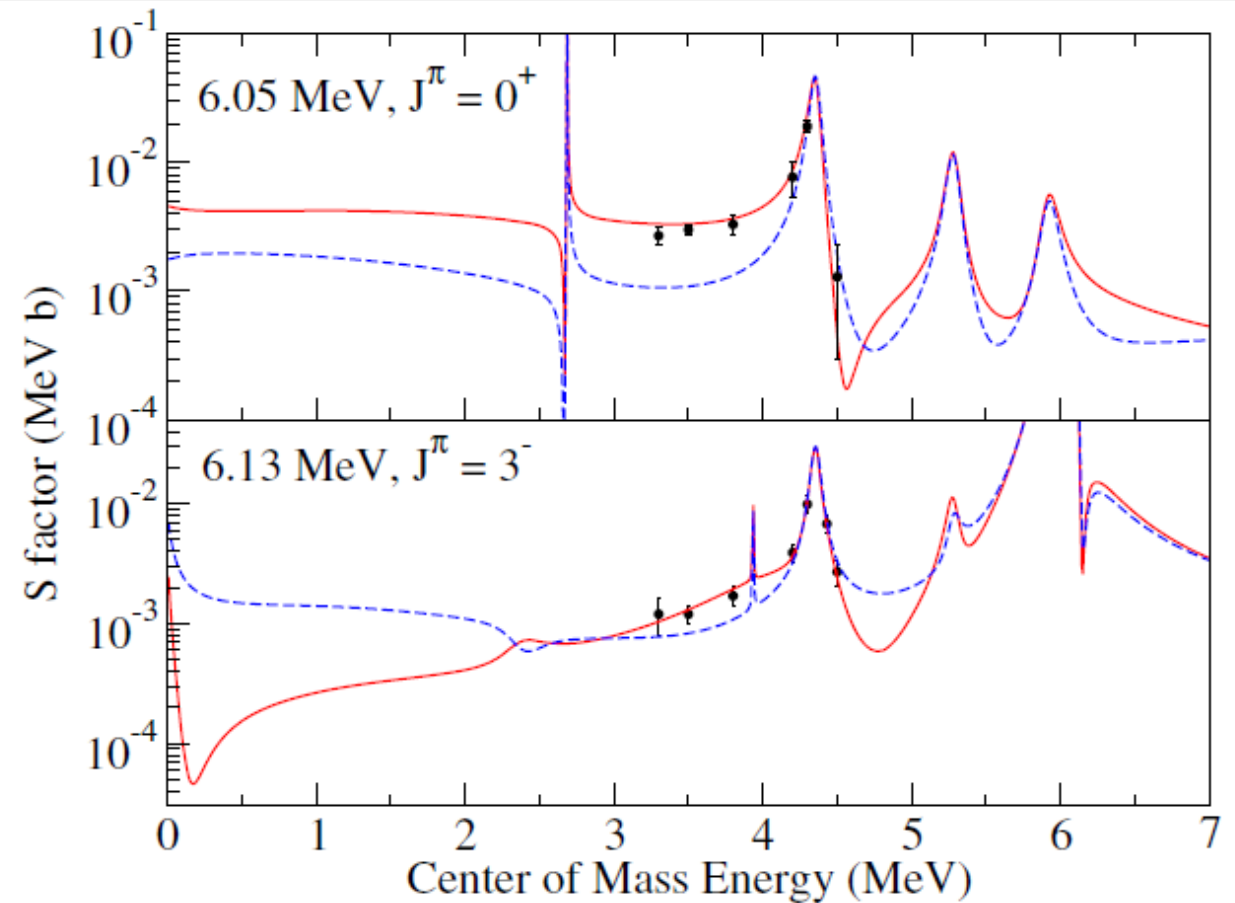
- **Penetrability, both orbital and Coulomb**

$$R_{cc'} = \sum_{\lambda}^{\# \text{ of real levels}} \left(\frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E} \right) + \sum_b^{\# \text{ of BG levels}} \left(\frac{\gamma_{bc} \gamma_{bc'}}{E_b - E} \right)$$

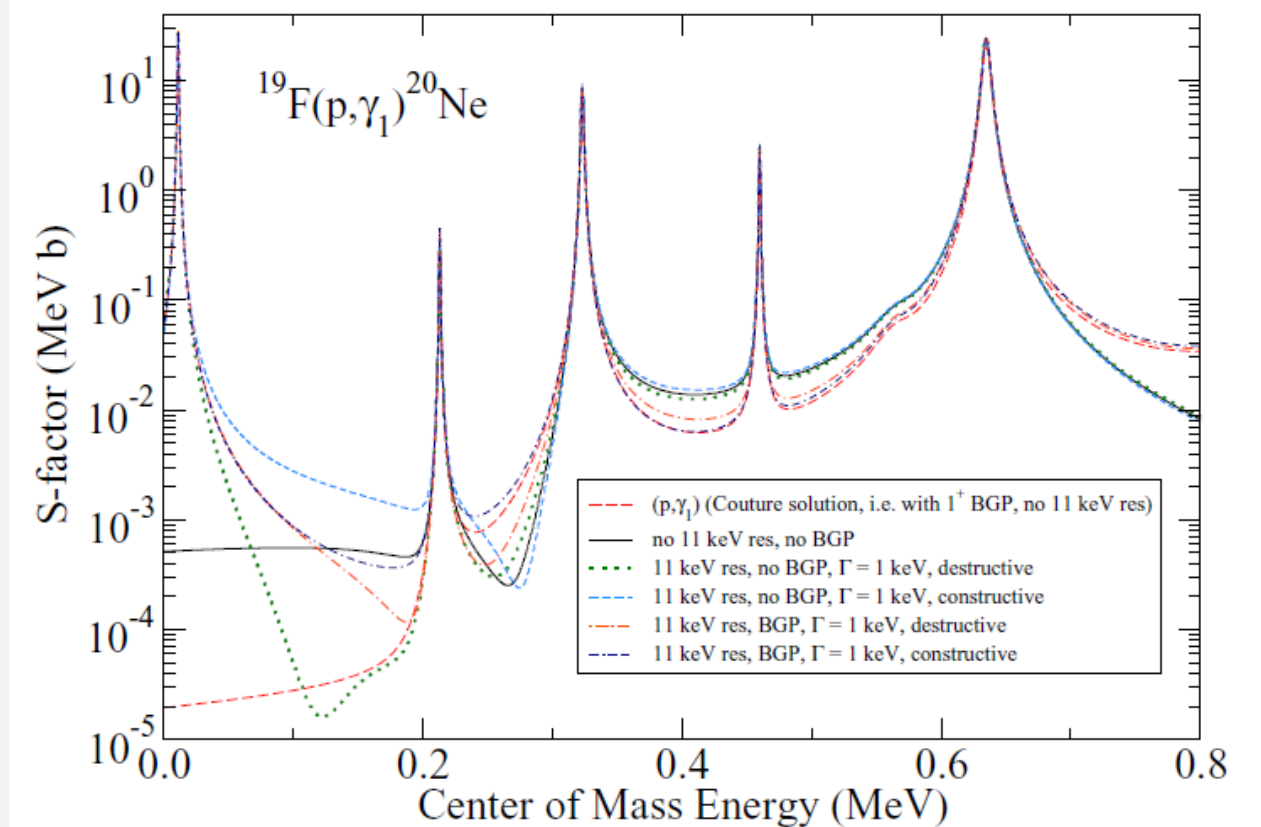
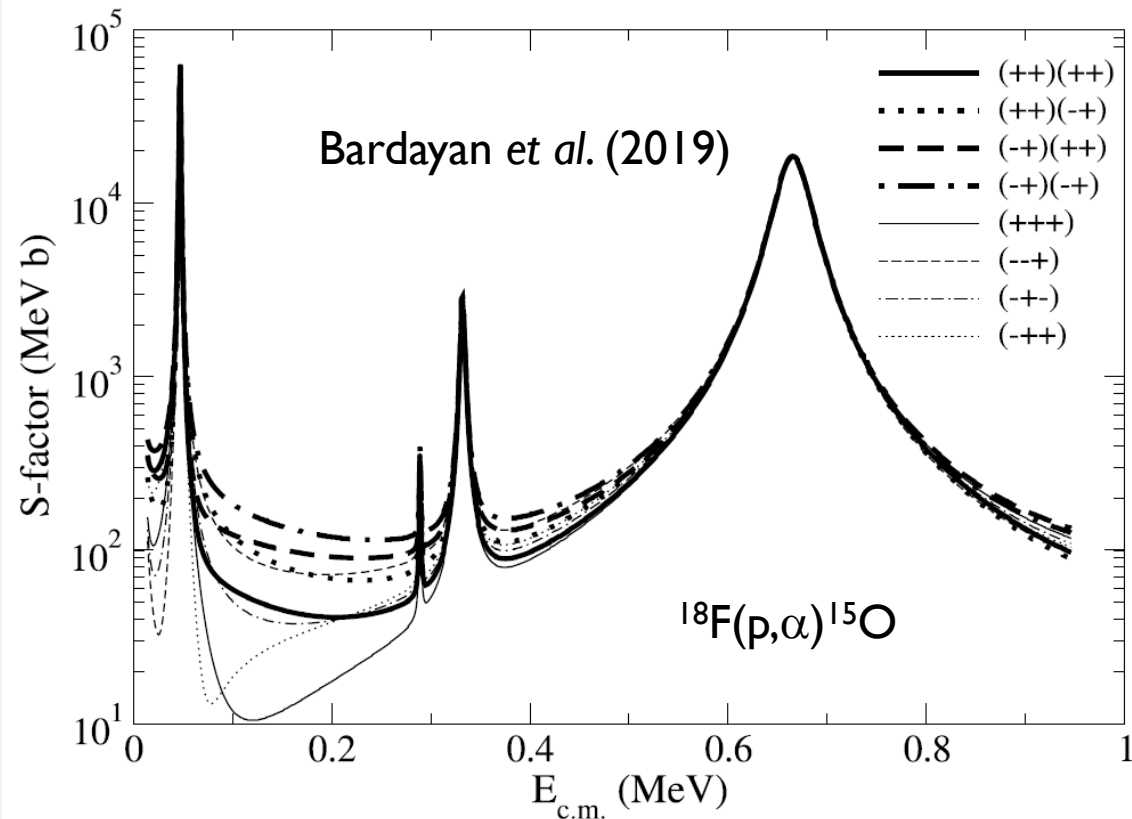
- Closed channels usually don't have much of an effect except near (above) thresholds
 - Can cause trouble for data sets that end at a particle threshold
 - Don't expect a good fit at the highest energies of your data

INTERFERENCE

- Included in the SHAPE of the cross section, is the correct modeling of the interference between resonances, which is very important for **EXTRAPOLATING** the cross section to low energy

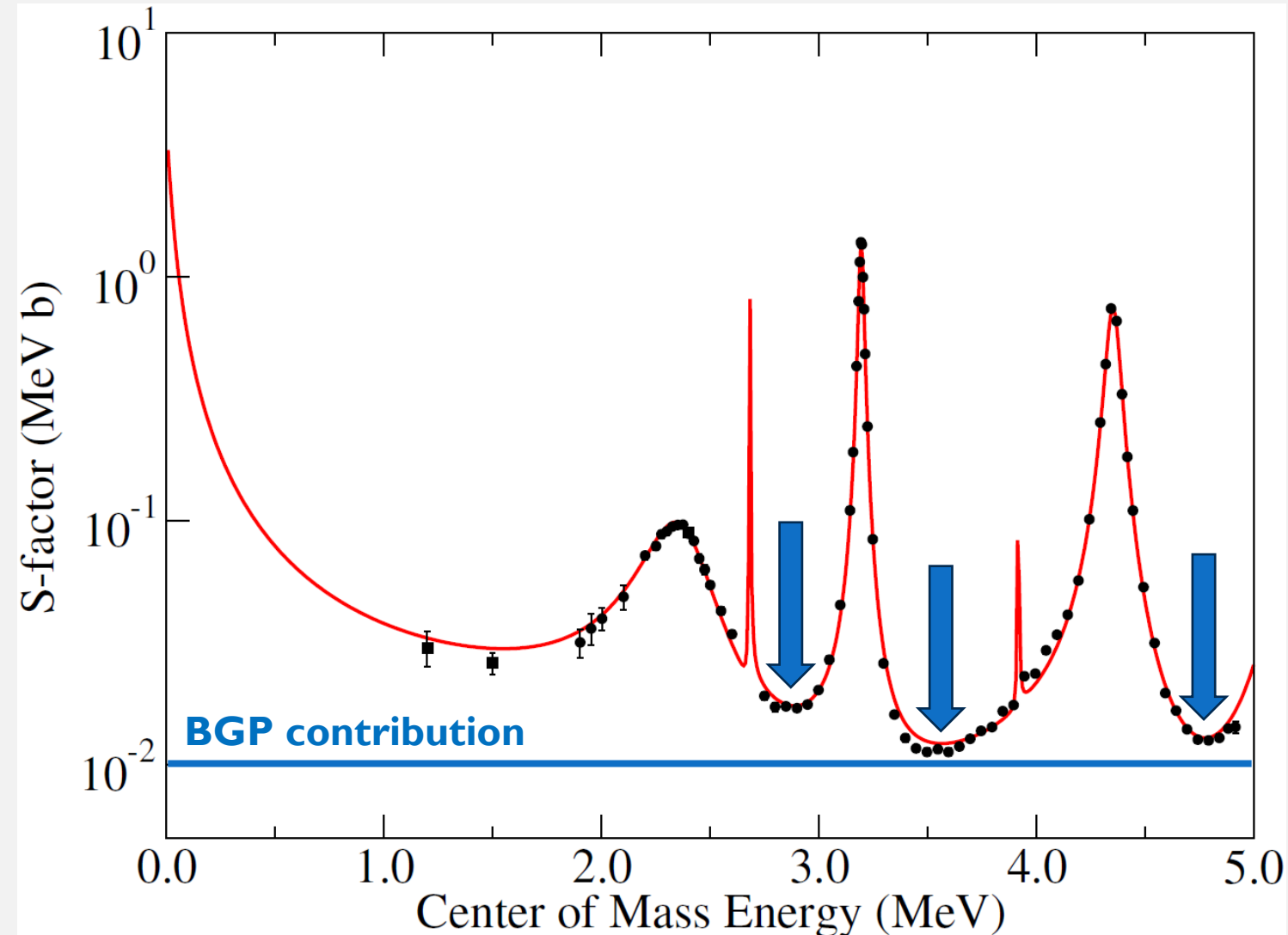


MULTI-RESONANCE INTERFERENCE



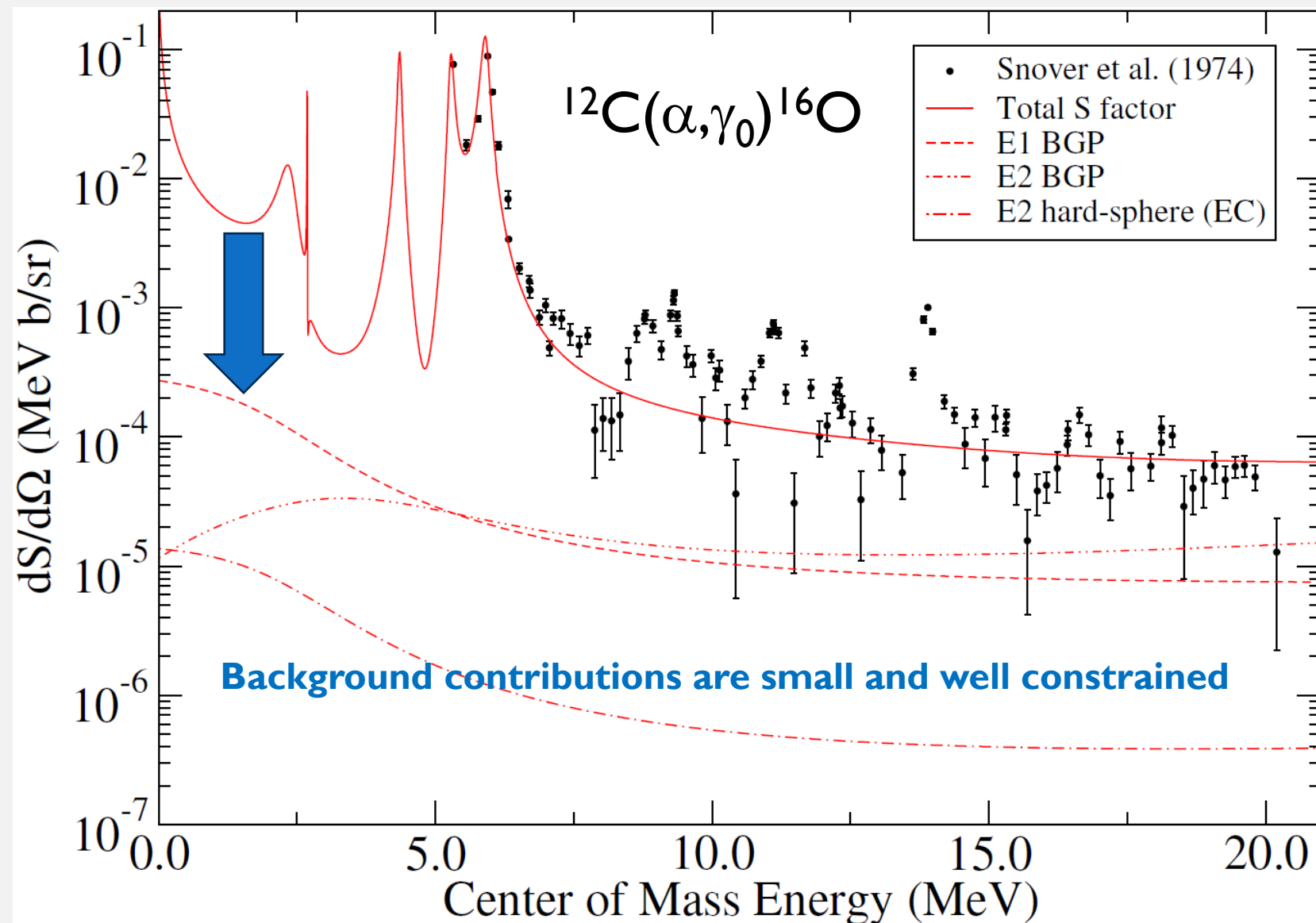
WHY OFF-RESONANCE MEASUREMENTS ARE SO IMPORTANT

- Off resonance regions are crucial for...
 - determining the interference patterns between resonances
 - limiting the strength of background poles (BGP) and direct capture (or the external capture model (EC) in R-matrix) contributions
- In the case of $^{12}\text{C}(\alpha,\gamma)^{16}\text{O}$, the higher energy data of Schürmann *et al.* were extremely constraining for the above reasons



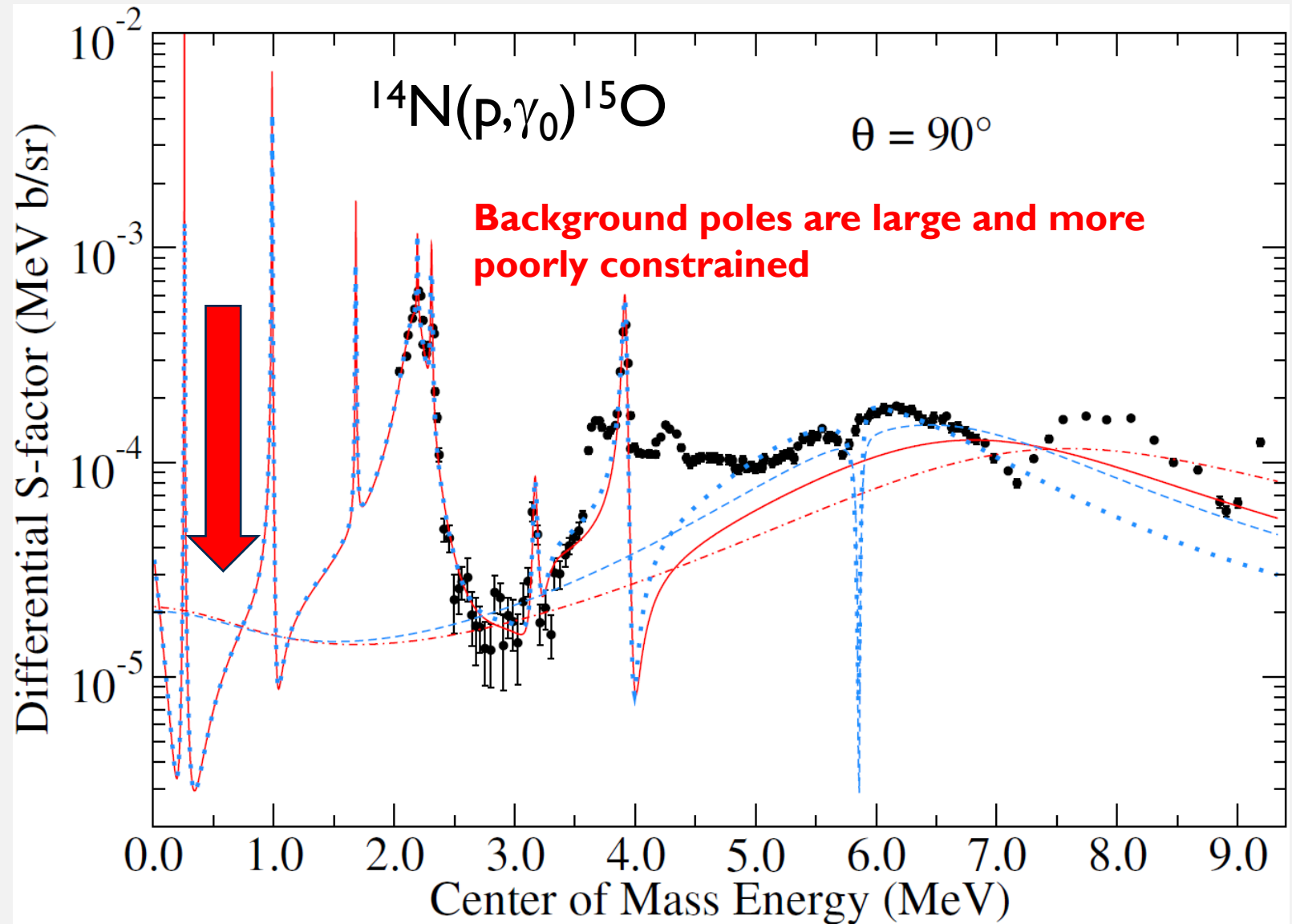
BGPS CONTINUED

- A good situation
- BGP is at 40 MeV
- Contribution is relatively flat as a function of S-factor
- Higher energy resonances are weak
- High energy data constrains the magnitude of the BGP contribution well
- BGP and EC contributions are similar in energy dependence!

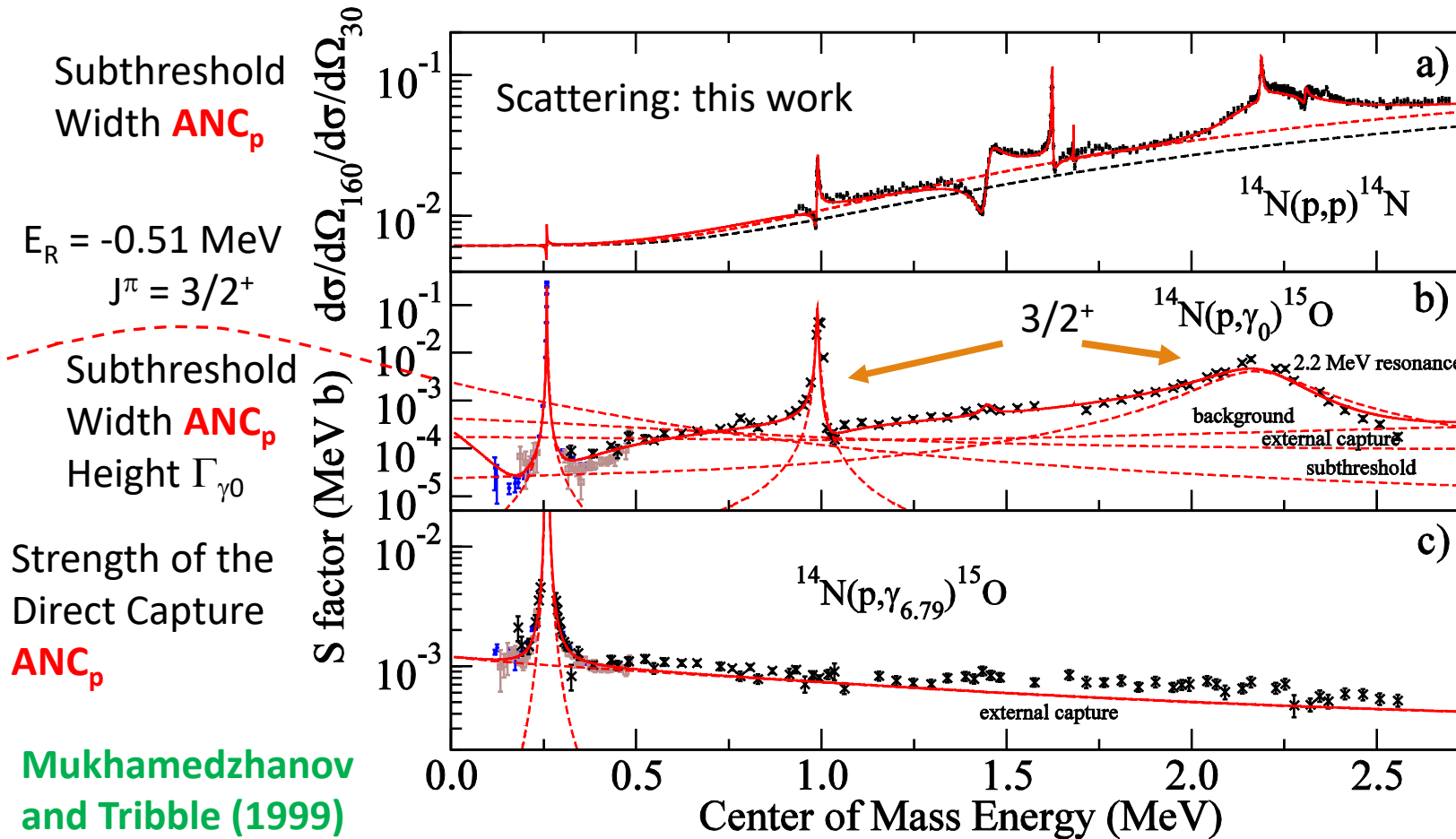


BGPS CONTINUED

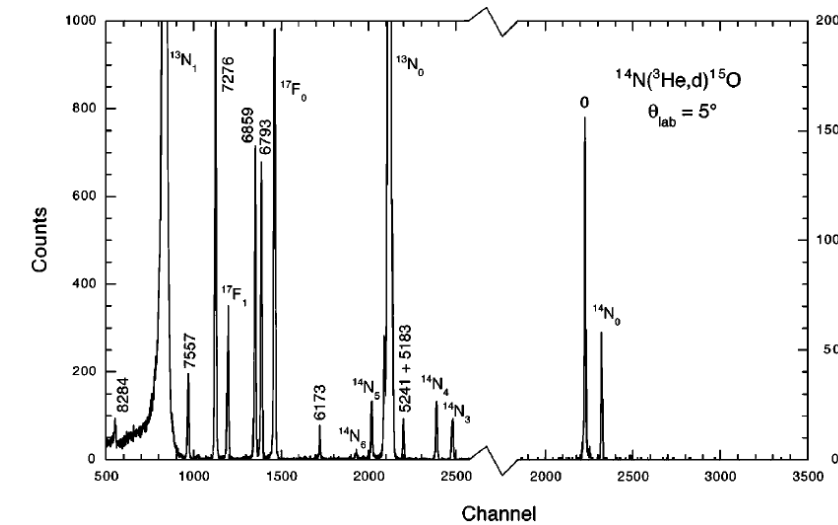
- A bad situation
- Broad, strong, resonances are present at these higher energies
- Could the tails of these broad, higher energy resonances contribute to the low energy cross section?
- Fit to the high energy data not accomplished satisfactorily
- BGPs definitely needed, but not constrained so well



The ANC connection

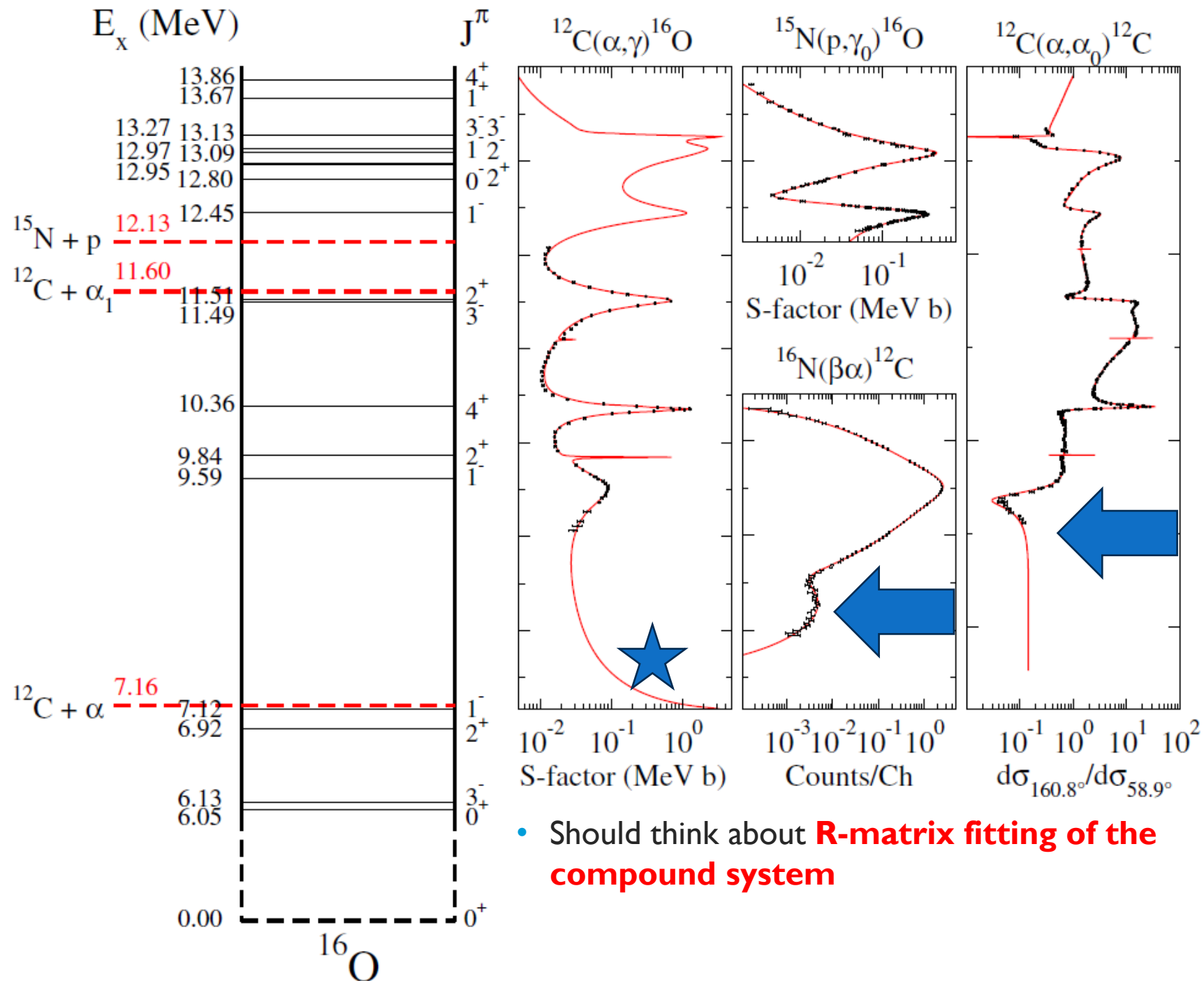


Transfer reactions



THE CLASSIC NUCLEAR ASTROPHYSICS EXAMPLE

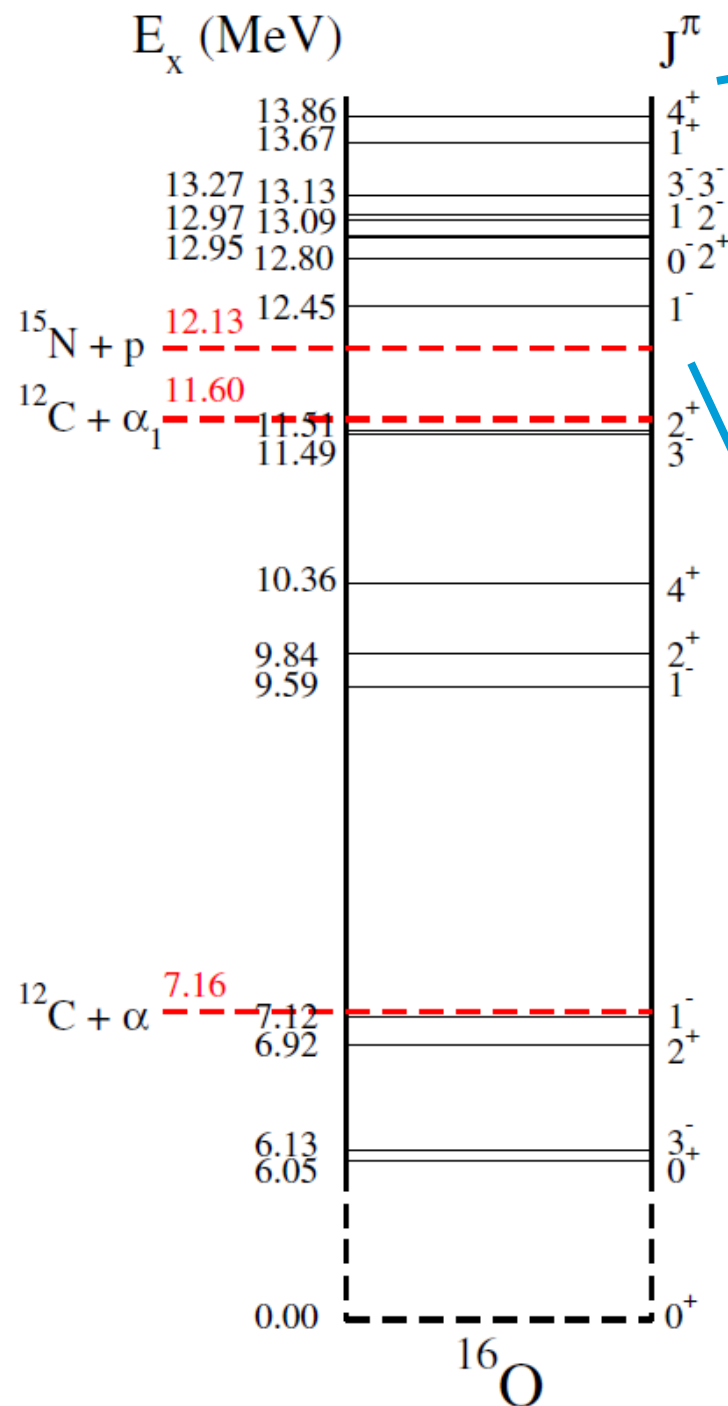
- Multichannel R-matrix fit was done by Fred Barker as early as 1971
- Well known level structure
- $^{12}\text{C}+\alpha$ places limits on the number of populated levels to natural parity states
- **$^{12}\text{C}(\alpha,\alpha)^{12}\text{C}$ data provides the backbone**
- Low energy $^{16}\text{N}(\beta\alpha)^{12}\text{C}$ spectra and $^{12}\text{C}(\alpha,\alpha)^{12}\text{C}$ data provide constraints on ANCs
- (subCoulomb) α -transfer data give further constraints



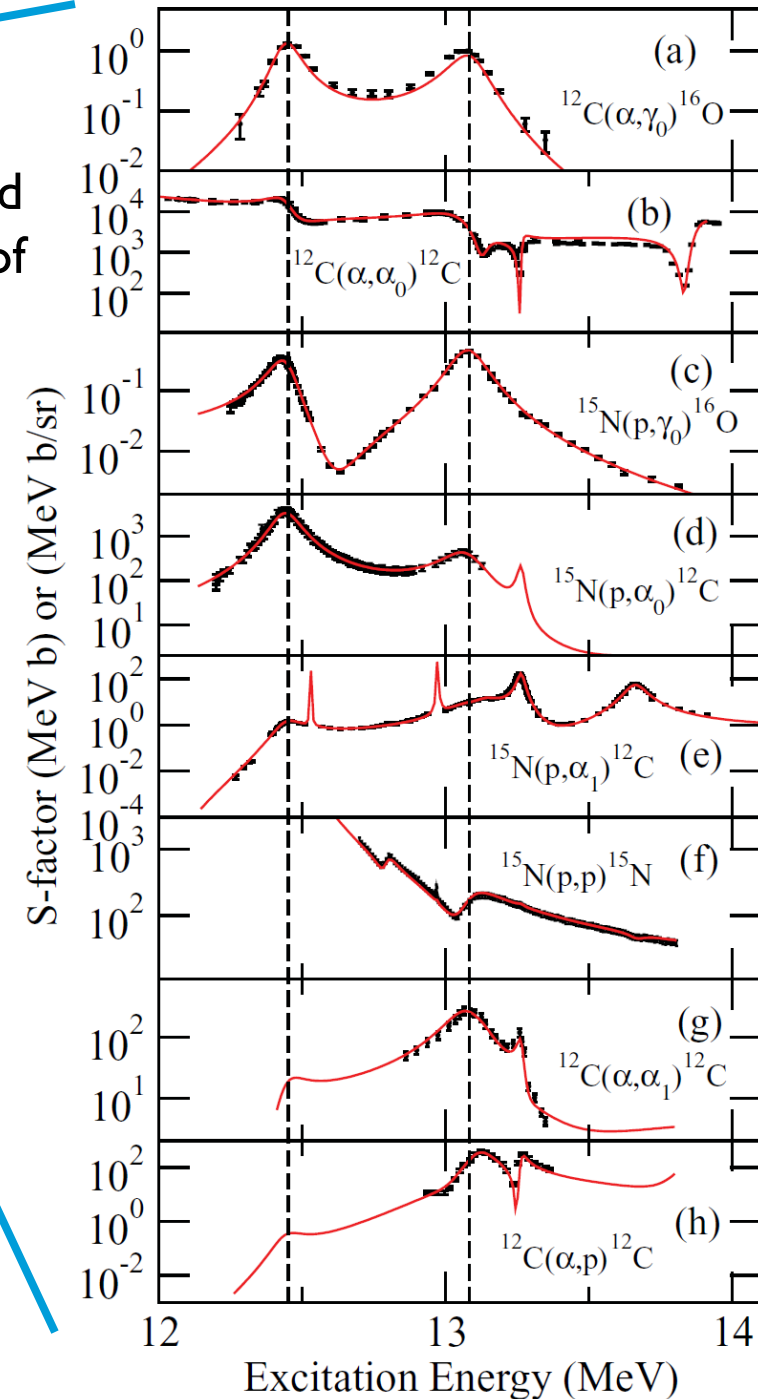
- Should think about **R-matrix fitting of the compound system**

HIGHER ENERGY: $^{15}\text{N}+p$

- Higher energy region
- Constrains the background for $^{12}\text{C}(\alpha, g)^{16}\text{O}$
- Simultaneously used to fit / extrapolate the $^{15}\text{N}(p, \alpha)^{12}\text{C}$ and $^{15}\text{N}(p, \gamma)^{16}\text{O}$ cross sections

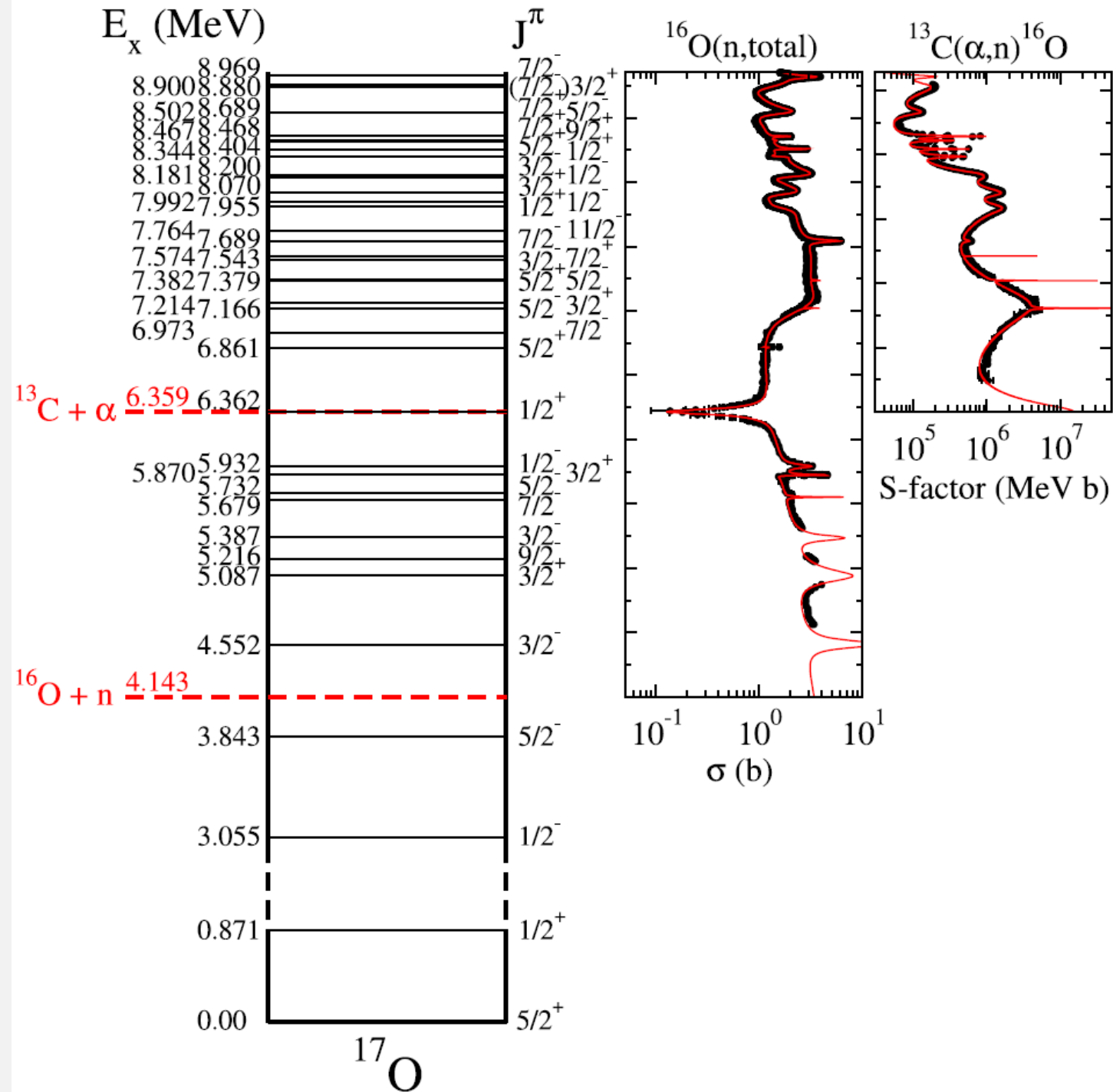


Same level parameters used to describe all of the data simultaneously!

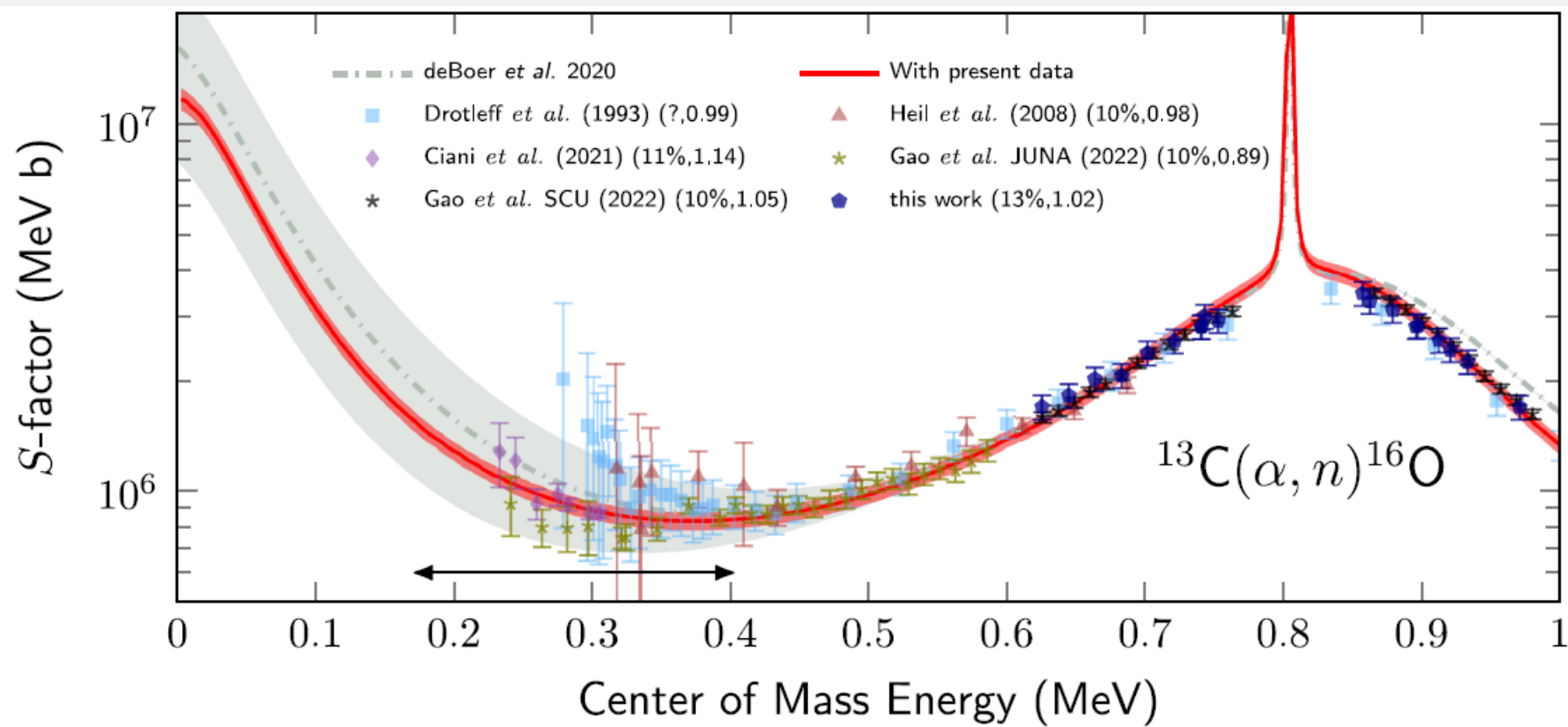


$^{13}\text{C}(\alpha, n)^{16}\text{O}$ AND $^{16}\text{O}(n, \alpha)^{13}\text{C}$

- Total neutron cross section measurements form the backbone of this analysis
- LANL, Gerry Hale *et al.* have put in a lot of excellent work on this analysis to get it to where it is today → look at the number of levels involved!
- Problematic data sets for $^{13}\text{C}(\alpha, n)^{16}\text{O}$ have led to a lot of confusion in recent years, but recent measurements are proving to be much more consistent
 - Gerry's R-matrix fit gave the right answer, but experimentalists are stubborn ☺
- Trying to push this to higher energies where excited state channels open in both $^{13}\text{C}+\alpha$ and $^{16}\text{O}+n$, but there isn't much data (see later talk)

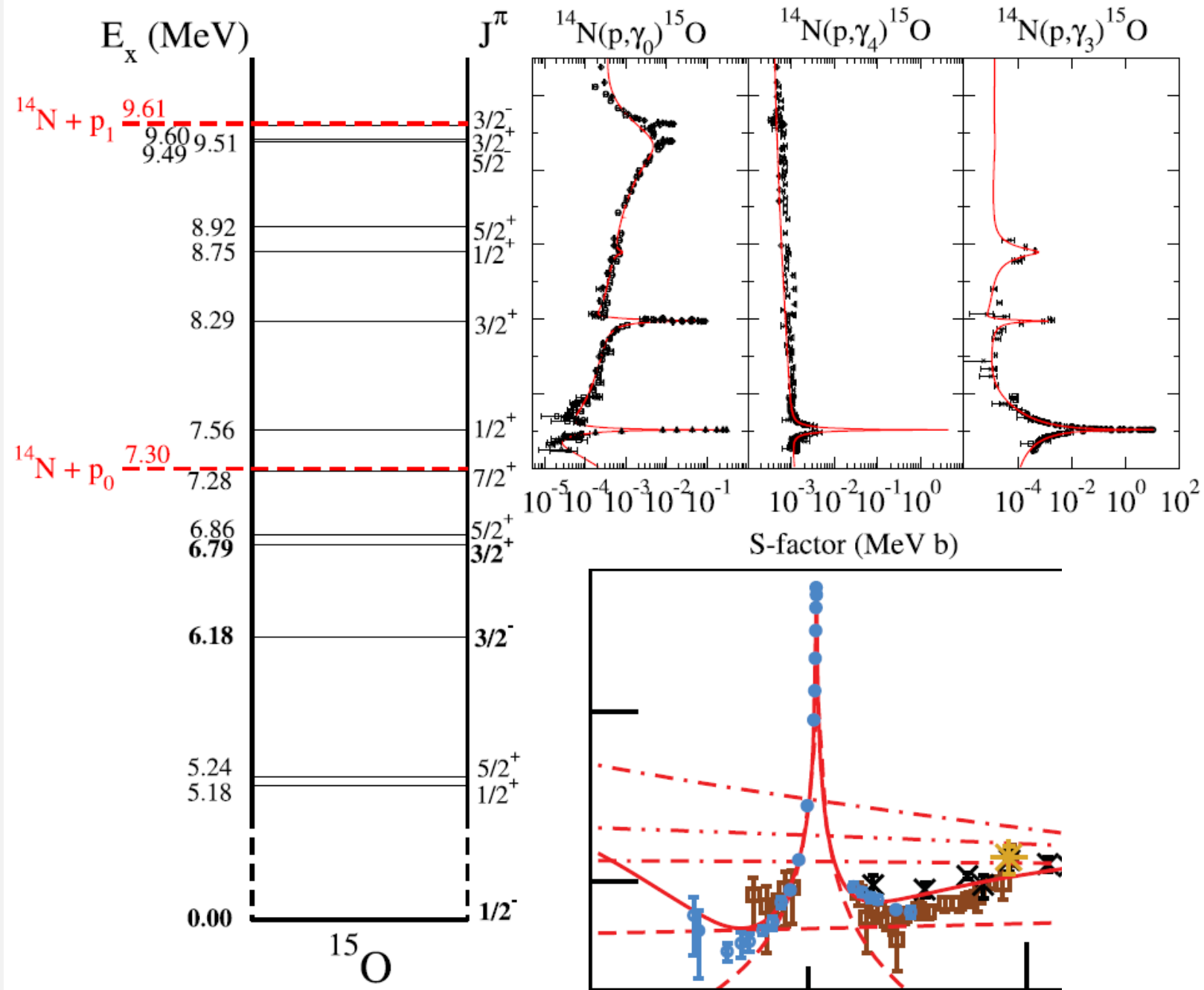


A LOT OF IMPROVEMENT AT LOW ENERGIES



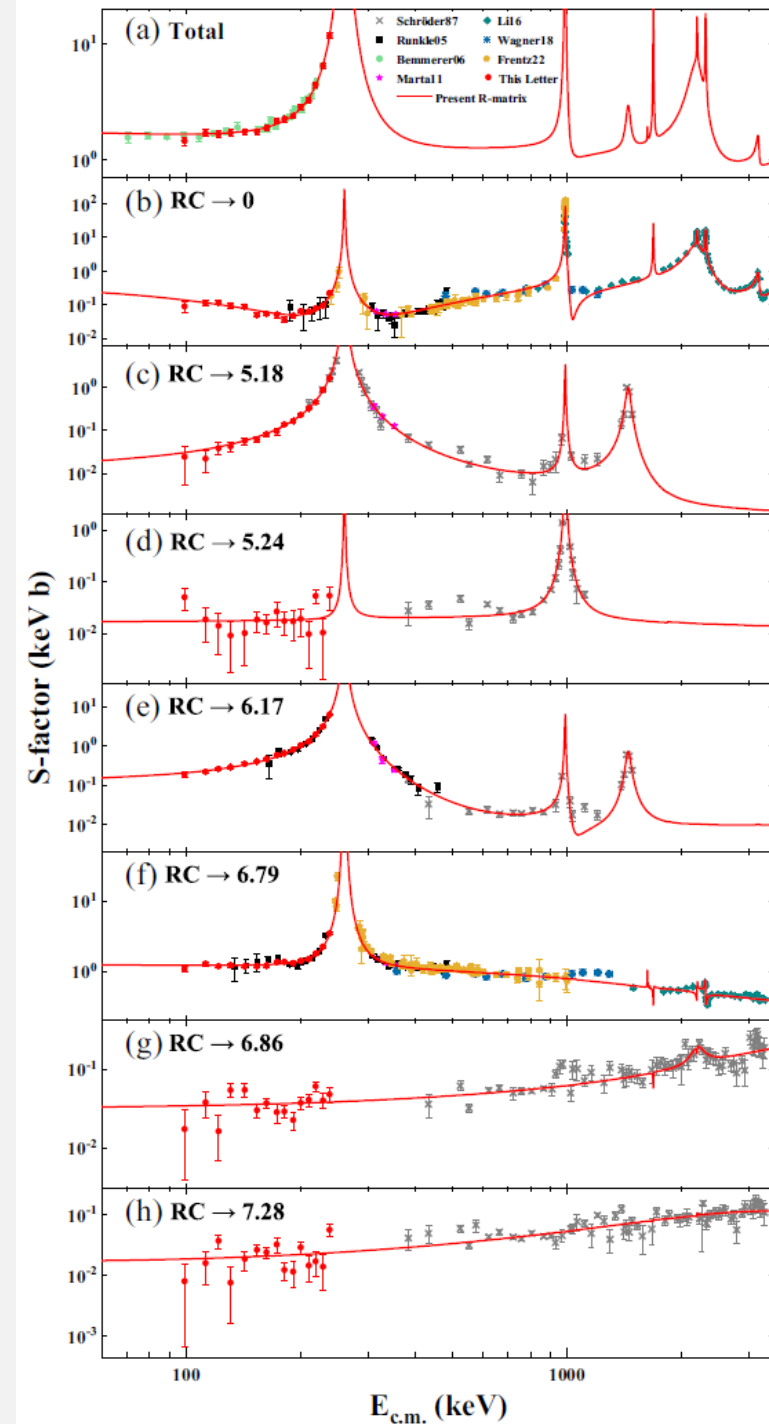
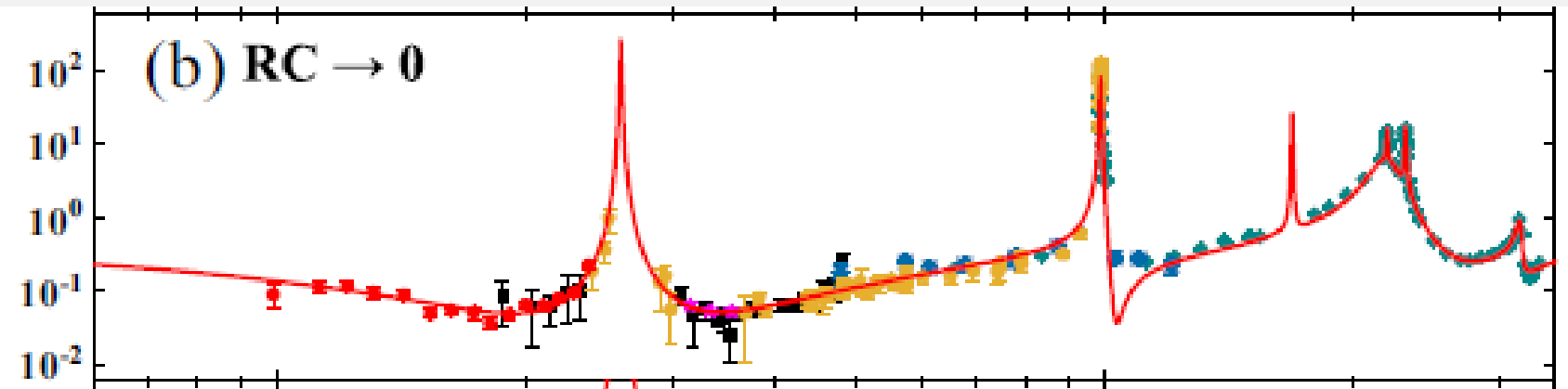
ANOTHER R-MATRIX DATA DISAGREEMENT

- The low energy S-factor in the ground state transition $^{14}\text{N}(p,\gamma_0)^{15}\text{O}$ has been hotly debated since the publication of Imbriani *et al.* (2005) --- LUNA
- The R-matrix fit consistently overestimates the S-factor data, and there is no way to make it lower given the constraints imposed by the level structure and the higher energy data



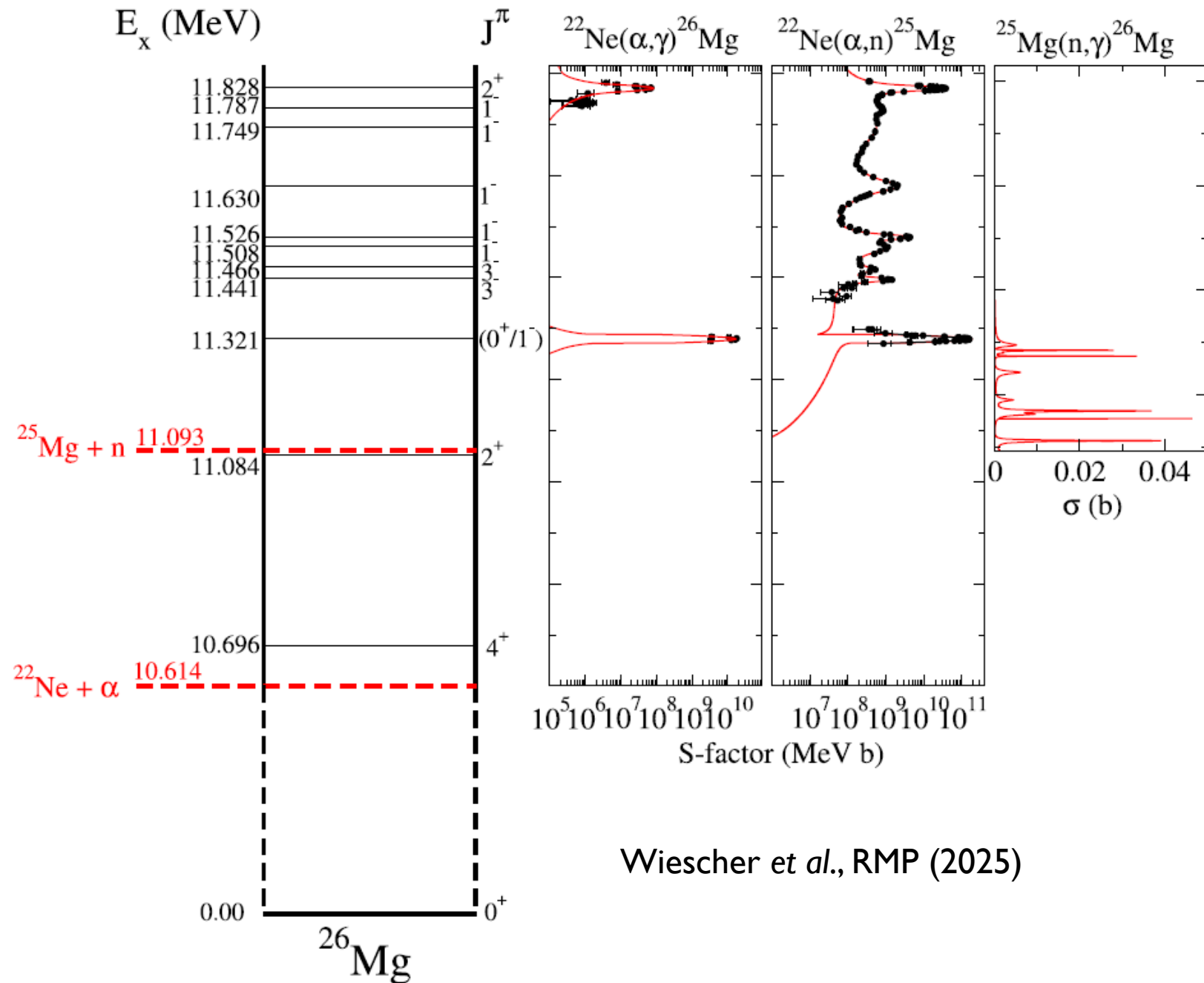
SOME INTERESTING NEW RESULTS

- New measurement by **Chen et al. (2025)** PRL now reports a larger low energy S-factor, in agreement with the R-matrix prediction
- Other parties are also looking to investigate!
- Also a nice demonstration of how data at higher energies strongly constrain the low energy extrapolation

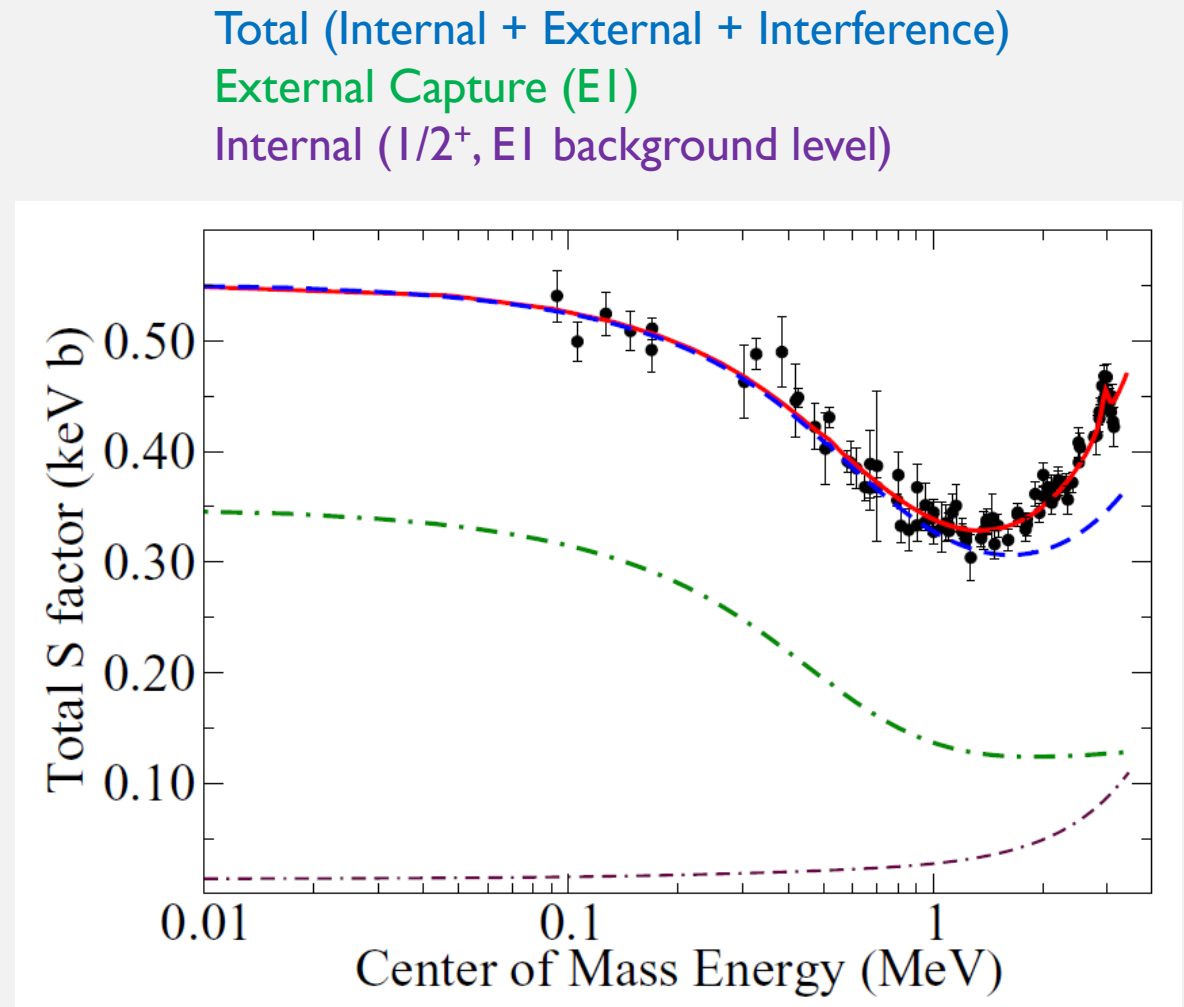
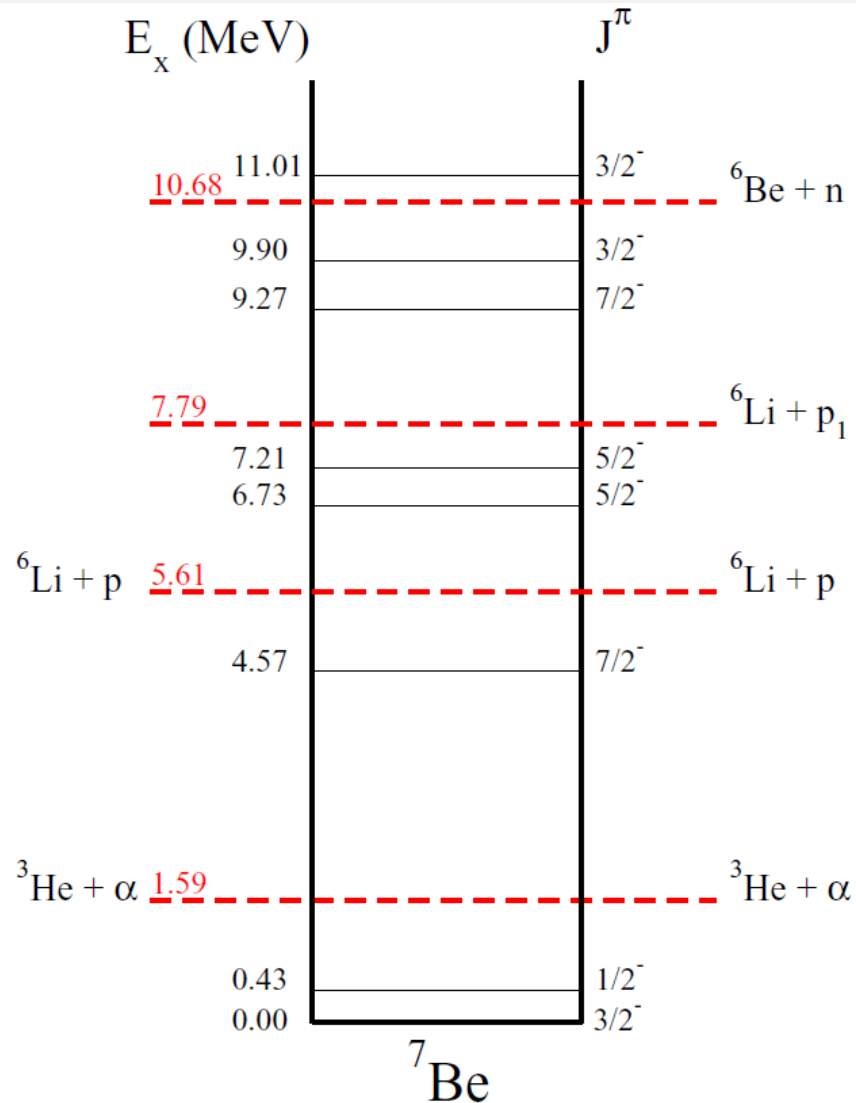


A DISAPPOINTING SITUATION

- Another seemingly good multichannel system is for $^{22}\text{Ne}+\alpha$ and $^{25}\text{Mg}+n$ reactions
- However, experimental challenges with $^{25}\text{Mg}+n$ and a high level-density have made it difficult to establish correspondence between the resonances in the different cross sections and the underlying nuclear levels

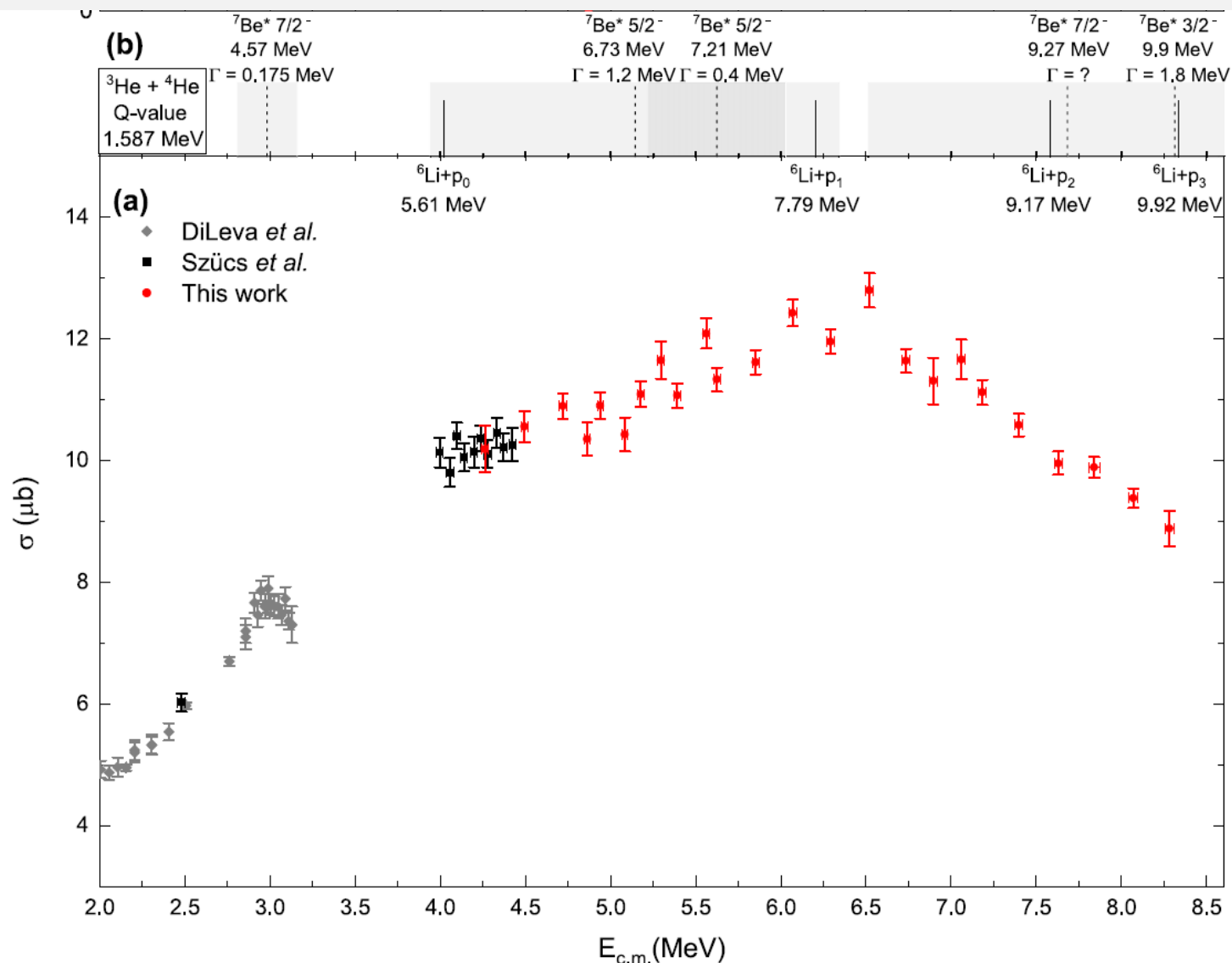
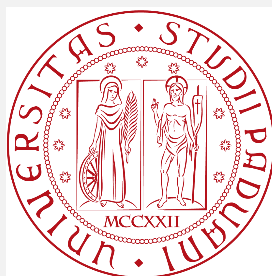


${}^3\text{He}(\alpha, \gamma){}^7\text{Be}$, HIGH ENERGY QUESTIONS



WHERE DOES THIS INTERNAL PART COME FROM?

- Toth *et al.* (2023) extend the $^3\text{He}(\alpha, \gamma)^7\text{Be}$ measurements to high energy and find a large cross section with a broad width
- But none of the states in ^7Be can describe this structure!
 - Widths are too narrow
 - Note EI decays
- Jakub Skowronski has found a solution



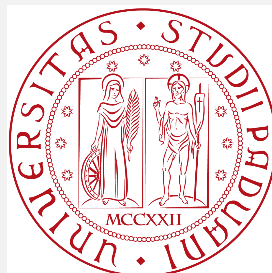
INDEN-LE (IAEA) EVALUATION OF THE ^7Be SYSTEM

- International Nuclear Data Evaluation Network – Light Elements
- Vivian Dimitriou (IAEA)
- Includes many R-matrix researchers
- We have been using the ^7Be system as a benchmark for about the last 10 years



CONVOLUTION OF DATA WITH EXPERIMENTAL RESOLUTION

- No data is really “cross section data”, there is always some distortion in the observed yields due to experimental resolution
- Energy loss through targets for charged particles
- Energy resolution from time-of-flight and detector thickness for neutron induced
- Angular resolution
- Etc.
- Resolution is significant for both the present measurements and many of the $^{14}\text{N}+n$ measurements from the literature
- Computationally expensive! ☹️



Example: TOF resolution function

$$Y(E) = \int_{-\infty}^{\infty} f(\epsilon) \cdot g(E - \epsilon) d\epsilon$$

$$g(E - \epsilon) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(E - \epsilon)^2}{2\sigma_b^2(E - \epsilon)}}$$

ToF resolution approximation

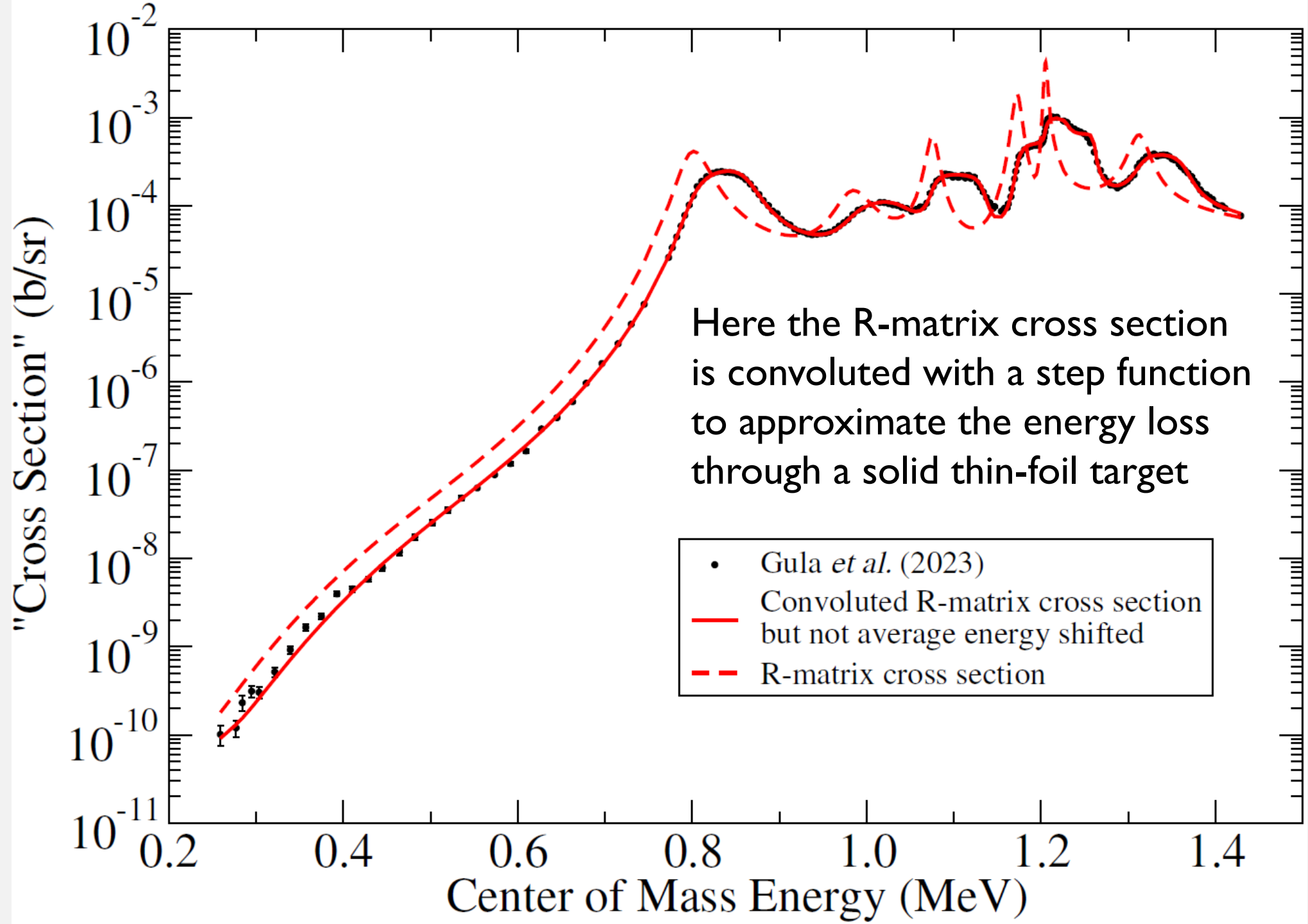
$$\sigma_b(E - \epsilon) = 2(E - \epsilon) \left(\left(\frac{dL}{L} \right)^2 + \left(\frac{dt}{L} \right)^2 \left(\frac{2c^2}{m_n c^2} \right) (E - \epsilon) \right)^{1/2}$$

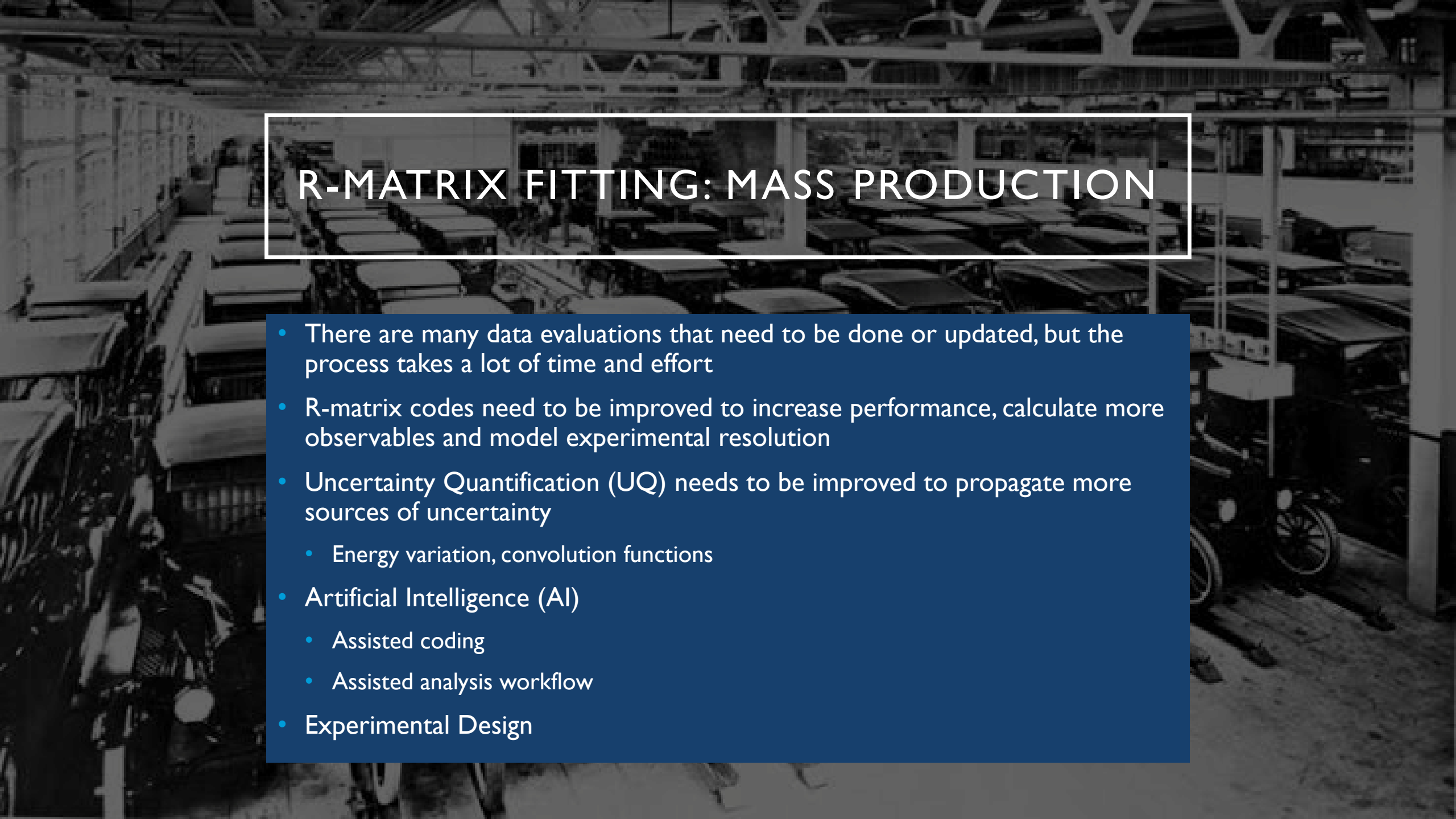
$$g(\epsilon) = \begin{cases} \frac{1}{\epsilon_{sp}(\epsilon)}, & (E - \Delta) < \epsilon < E \\ 0 & \text{otherwise} \end{cases}$$

Charged particle energy loss plus straggling

$$\sigma_{str}(E) = \alpha_{str} \sqrt{E_0 - E}$$

Amy Roberts, Garrett Arquette (undergrad), Jakub Skowronski (postdoc at Padova)





R-MATRIX FITTING: MASS PRODUCTION

- There are many data evaluations that need to be done or updated, but the process takes a lot of time and effort
- R-matrix codes need to be improved to increase performance, calculate more observables and model experimental resolution
- Uncertainty Quantification (UQ) needs to be improved to propagate more sources of uncertainty
 - Energy variation, convolution functions
- Artificial Intelligence (AI)
 - Assisted coding
 - Assisted analysis workflow
- Experimental Design

AI ASSISTED R-MATRIX

James doing R-matrix



Jakub doing R-matrix with AI



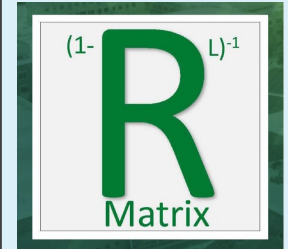
FUNDING ACKNOWLEDGMENTS



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R-MATRIX SCHOOL 2027



- A series of three R-matrix schools organized by **Marco Pigni** (ORNL), Carl Brune (OU) and myself (UND)
- **Hosted by the University of Notre Dame, taking place at the University of Northern Michigan in Marquette, MI from May 17 to 21**
- First school took place at ORNL back in 2025 and a third school will take place in 2029 at Ohio University
- **A hands-on school to teach researchers how to use the SAMMY and AZURE2 R-matrix codes**

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