

Uncertainties in R -matrix extrapolations near reaction thresholds

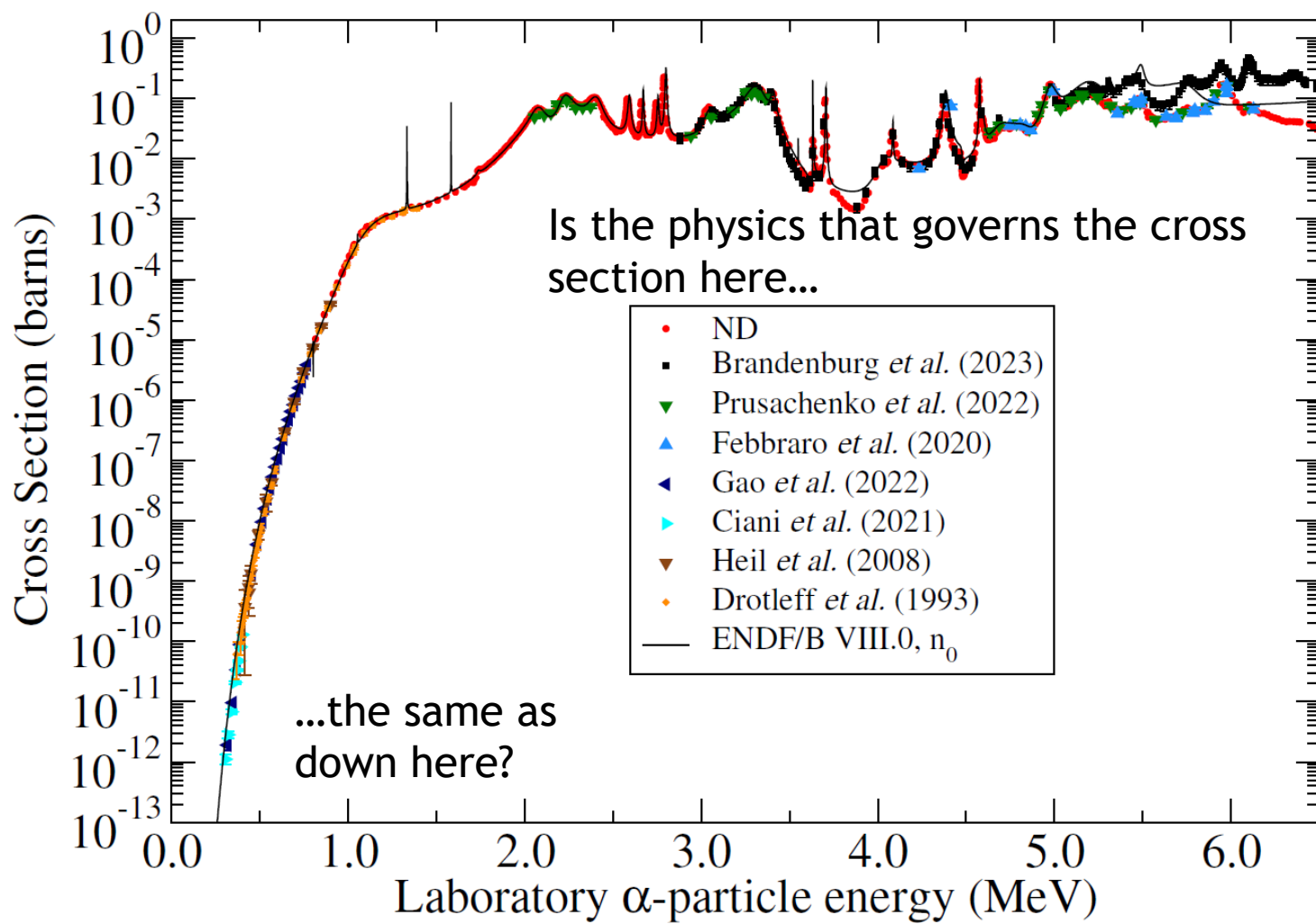
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CeNAM / IReNA Workshop on Atomic and Nuclear Quantum Effects Near Threshold



Extrapolation of cross sections over many orders of magnitude



Extrapolation
over 10 orders
of magnitude
in cross section

Phenomenological R-matrix

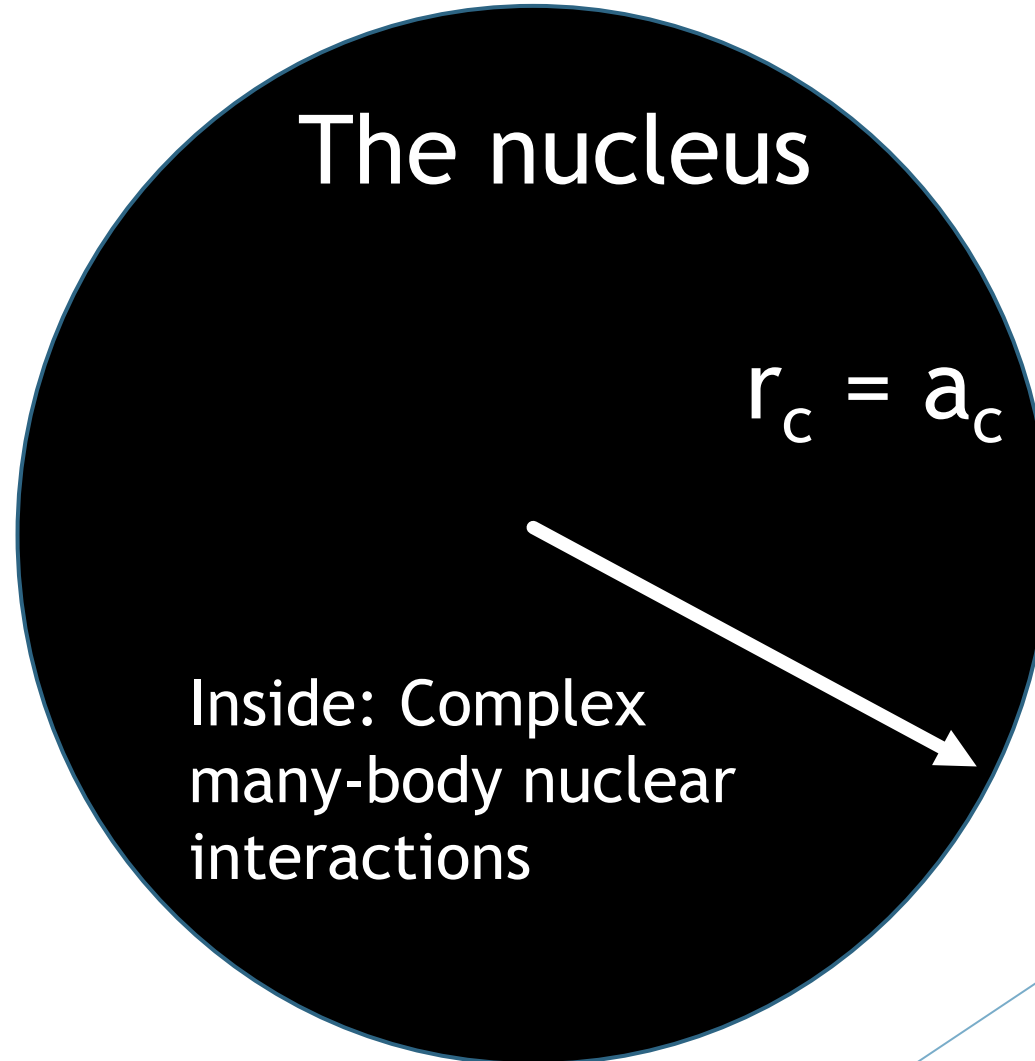
- ▶ A reaction framework where the energy dependence and interference between resonances is formally included (we believe and many verifications with data have shown)
- ▶ Specific levels and their properties are added to the calculations based on our best understanding (experiment, theory)
 - ▶ Advantage: very versatile, not limited by the levels that are only produced by one theory
 - ▶ Disadvantage: no fundamental **nuclear** physics guidance
- ▶ Low energy cross sections of charged particle reactions are dominated by the Coulomb barrier and therefore are very small, often too small to measure directly (sub picobarn)
- ▶ We must thus extrapolate from higher energies towards the threshold
- ▶ We rely on the structure at these higher energies to guide us, supposing that the physical conditions are essentially the same, only that the nuclear part of the cross section is suppressed by the Coulomb barrier
- ▶ We believe that we can accurately calculate the Coulomb penetrability

What could go wrong?

- ▶ Subthreshold states often dominate
 - ▶ Their strengths are characterized by Asymptotic Normalization Coefficients and γ -ray widths
 - ▶ How well do ANCs transfer between theories?
 - ▶ Akram Mukhamedzhonov
 - ▶ Is the γ -width really the total width for capture reactions? What about electron capture
- ▶ In R-matrix (maybe other theories too), usually the most ill-defined components are from background level contributions
- ▶ Masses
 - ▶ Nuclear or atomic?
- ▶ Experimental distortions of the experimental data
 - ▶ No cross section is a real cross section

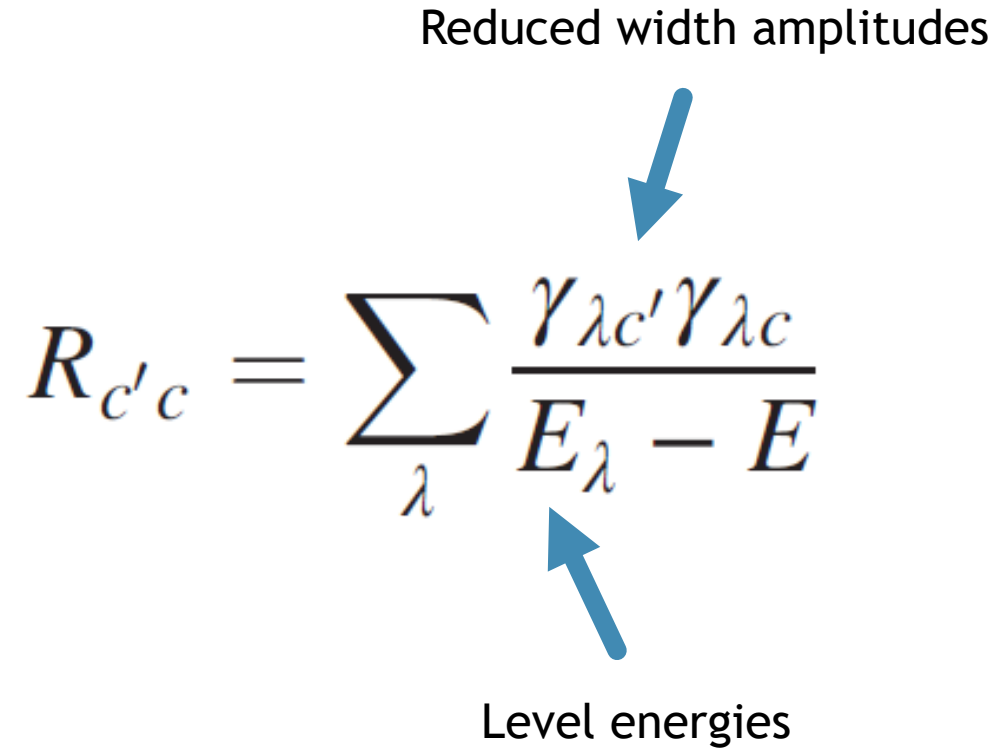
Basic Idea

Outside: two
particle clusters
that do not interact
except through the
Coulomb potential



R-matrix levels

Reduced width amplitudes



The diagram shows the R-matrix formula $R_{c'c} = \sum_{\lambda} \frac{\gamma_{\lambda c'} \gamma_{\lambda c}}{E_{\lambda} - E}$. A blue arrow points from the text 'Reduced width amplitudes' to the product of the reduced width amplitudes $\gamma_{\lambda c'} \gamma_{\lambda c}$ in the numerator. Another blue arrow points from the text 'Level energies' to the denominator $E_{\lambda} - E$, specifically pointing to E_{λ} .

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

Level energies

Essentially, ***R*** defines the logarithmic derivative of the radial wave function at the channel surfaces(s) as a function of energy.

R-matrix to cross section

Known stuff

$$I_c^+ = (G_c - iF_c) \exp(i\omega_c),$$

$$O_c^+ = (G_c + iF_c) \exp(-i\omega_c),$$

$$O_c^- = W(-\eta_\alpha, l + \frac{1}{2}; 2\rho_\alpha)$$

$$\omega_c \equiv \omega_{\alpha l} = \sigma_{\alpha l} - \sigma_{\alpha 0} = \sum_{n=1}^l \tan^{-1}(\eta_\alpha/n)$$

$$\eta_c = \eta_{\alpha l} = \frac{Z_{1\alpha} Z_{2\alpha} e^2}{\hbar v_\alpha},$$

$$L_c \equiv (\rho_c O_c' / O_c) r_c = a_c$$

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

$$\mathbf{U} = \rho^{\frac{1}{2}} \mathbf{O}^{-1} (\mathbf{1} - \mathbf{R} \mathbf{L}_0)^{-1} (\mathbf{1} - \mathbf{R} \mathbf{L}_0^*) \mathbf{I} \rho^{-\frac{1}{2}}$$

$$T_{cc'} = e^{2i\omega_c} \delta_{cc'} - U_{cc'}$$

$$\sigma_{\alpha\alpha'} = \frac{\pi}{k_{\alpha}^2} \sum_{Jl l' s s'} g_J |T_{cc'}^J|^2$$

$$(2s+1) \frac{k_{\alpha}^2}{\pi} \frac{d\sigma_{\alpha s, \alpha' s'}}{d\Omega_{\alpha'}}$$

$$\begin{aligned} &= (2s+1) |C_{\alpha'}(\theta_{\alpha'})|^2 \delta_{\alpha s, \alpha' s'} + \frac{1}{\pi} \sum_L B_L(\alpha s, \alpha' s') \\ &\quad \times P_L(\cos \theta_{\alpha'}) + \delta_{\alpha' s', \alpha s} (4\pi)^{-1/2} \sum_{Jl} (2J+1) \\ &\quad \times 2\text{Re}[i(T_{c'c}^J)^* C_{\alpha'}(\theta_{\alpha'}) P_l(\cos \theta_{\alpha'})]. \end{aligned} \quad ($$

Connection to the nuclear potential

External radial wave functions

$$\chi \sim r_\alpha^{-1} u_{\alpha sl}(r_\alpha) (i^l Y_m^{(l)}(\Omega_\alpha)),$$

$$\left[\frac{d^2}{dr_\alpha^2} - \frac{l(l+1)}{r_\alpha^2} - \frac{2M_\alpha}{\hbar^2} (V_{\alpha sl} - E_\alpha) \right] u_{\alpha sl}(r_\alpha) = 0$$

$$V_{\alpha sl} = Z_{\alpha 1} \tilde{Z}_{\alpha 2} e^2 / r_\alpha$$

Internal wave functions

(just the general property that they can be written as mutually orthogonal eigenfunctions)

$$\Psi_{JM} = \sum_{\lambda} A_{\lambda J} X_{\lambda JM},$$

Surface wave functions (matching wave functions at the channel surface $\mathcal{S}$)

$$\varphi_{\alpha sl \nu m} = r_\alpha^{-1} \psi_{\alpha s \nu} (i^l Y_m^{(l)})$$

$$\gamma_{\lambda c} \equiv V_{\lambda c} = (\hbar^2 / 2M_c a_c)^{\frac{1}{2}} \int \varphi_c^* X_{\lambda JM} dS,$$

No explicit internal potential is defined, instead only the values of the overlap integrals, which are related to the logarithmic derivatives at the channel surface that specify the boundary conditions to be satisfied by the $X_{\lambda JM}$ on $\mathcal{S}$. Thus the effect of the potential is parameterized in terms of poles $\gamma_{\lambda c}$ and amplitudes over some limited energy range.

R-matrix: scattering of s-wave neutrons by a square well potential

- ▶ Erich Vogt, RMP 34, 723 (1962)
- ▶ Take a case where we define a toy model so that we can actually write down a potential explicitly
- ▶ Definition of a specific potential then leads to specific values for the energies and reduced widths

$$-(\hbar/2m)d^2\phi/dr^2 + V\phi = E\phi$$

$$\begin{aligned} V &= -V_1 & r &\leq R_1 \\ &= 0 & r &> R_1 \end{aligned}$$

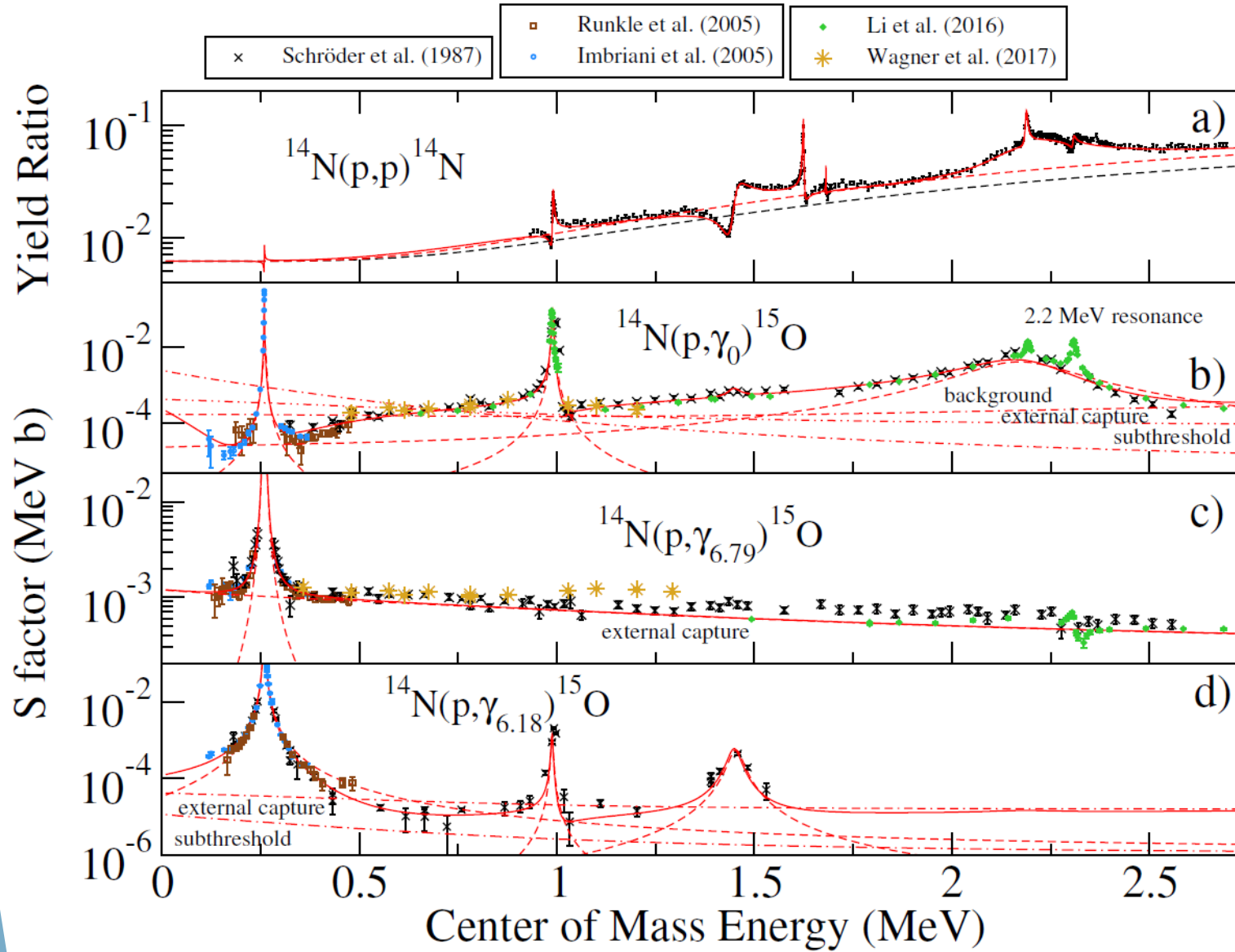


$$\gamma_\lambda^2 = \hbar^2/mR_1^2$$

Essentially the Wigner limit

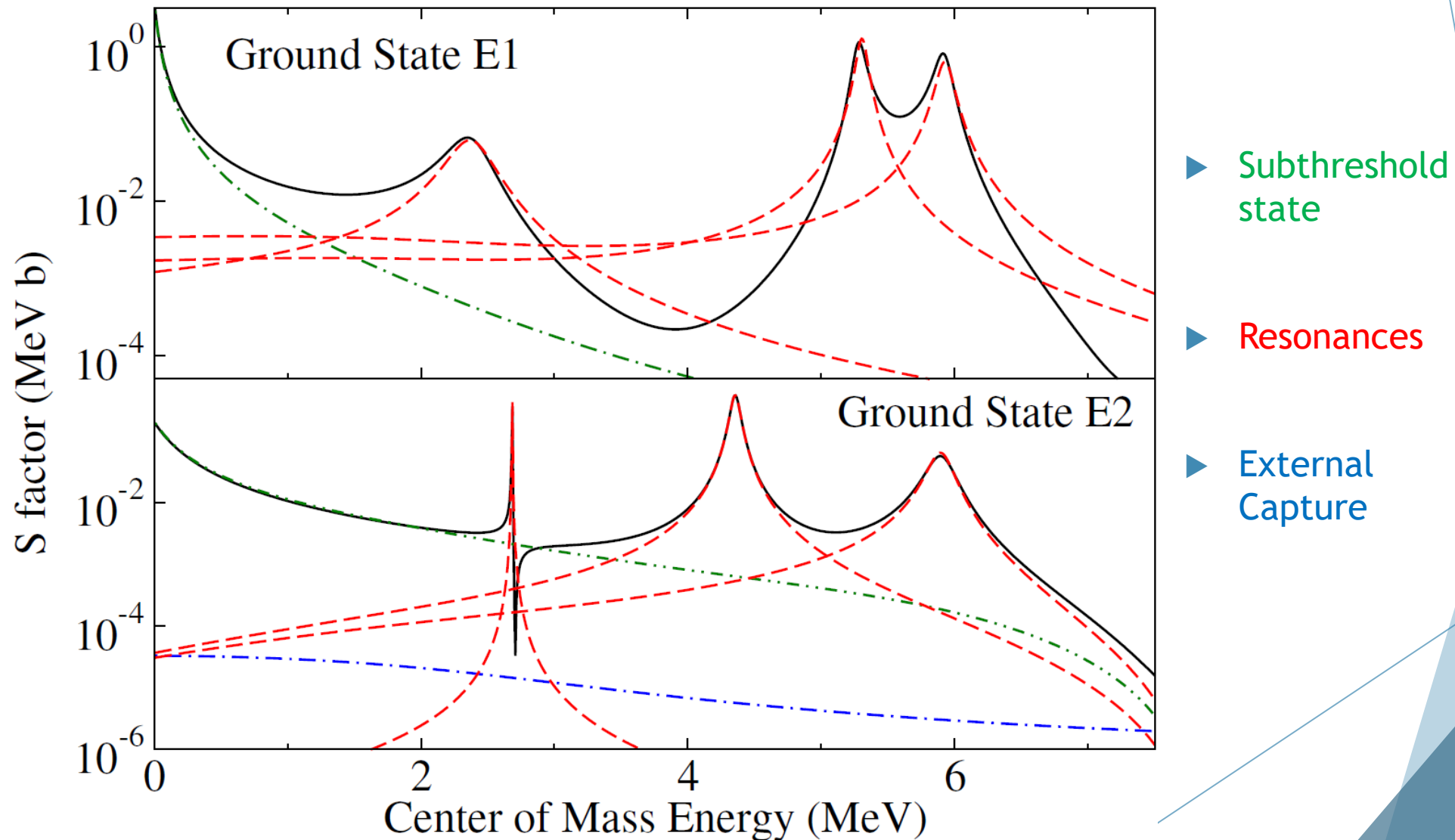
$$\gamma_W^2 = 3\hbar^2/2\mu a^2$$

Reaction components of R-matrix theory



- Resonances
- Subthreshold states
- Background levels
- Hard sphere phase shifts (scattering and external capture)

Subthreshold states: $^{12}\text{C}(\alpha,\gamma)^{16}\text{O}$



Subthreshold states

- ▶ How well do ANCs determined from transfer experiments translate from a DWBA model to an R-matrix model?
 - ▶ Model dependence should be less
 - ▶ SubCoulomb measurements claim they can get the uncertainty down to about 10%
- ▶ For α -particle ANCs for the bound states of ^{16}O , different transfer experiments seem to agree, but some uncertainties are very large
- ▶ Some issues with consistency of 2^+ bound state however
- ▶ Maybe we are underestimating uncertainties?

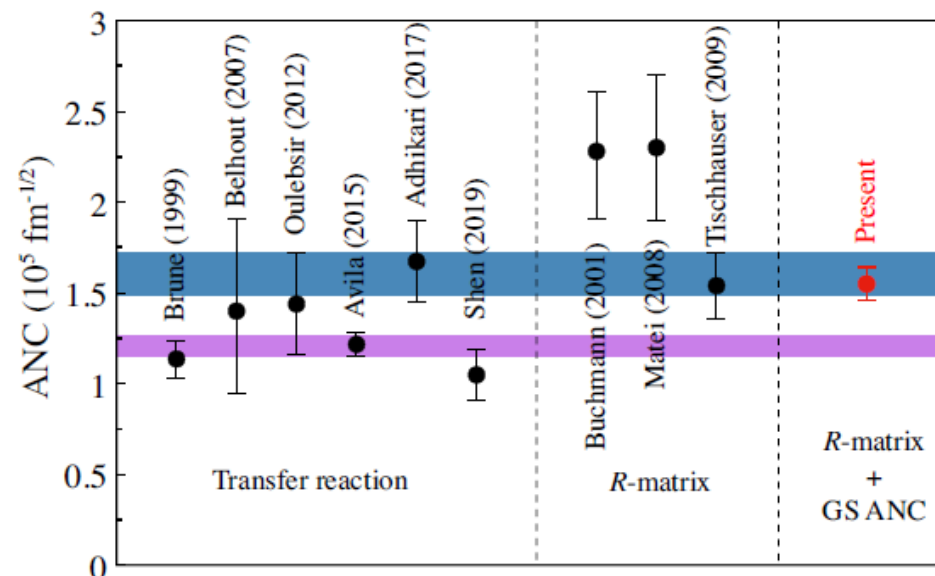


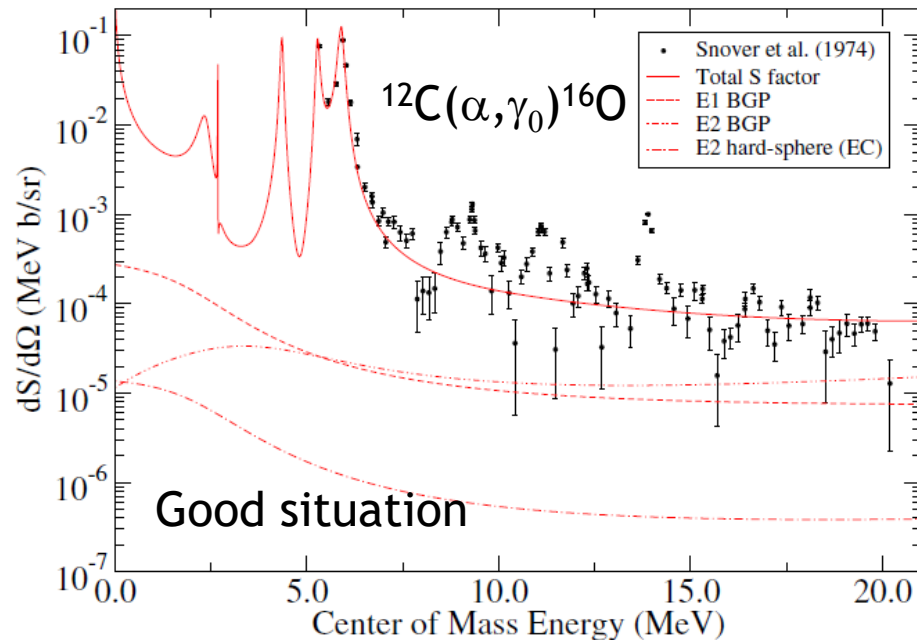
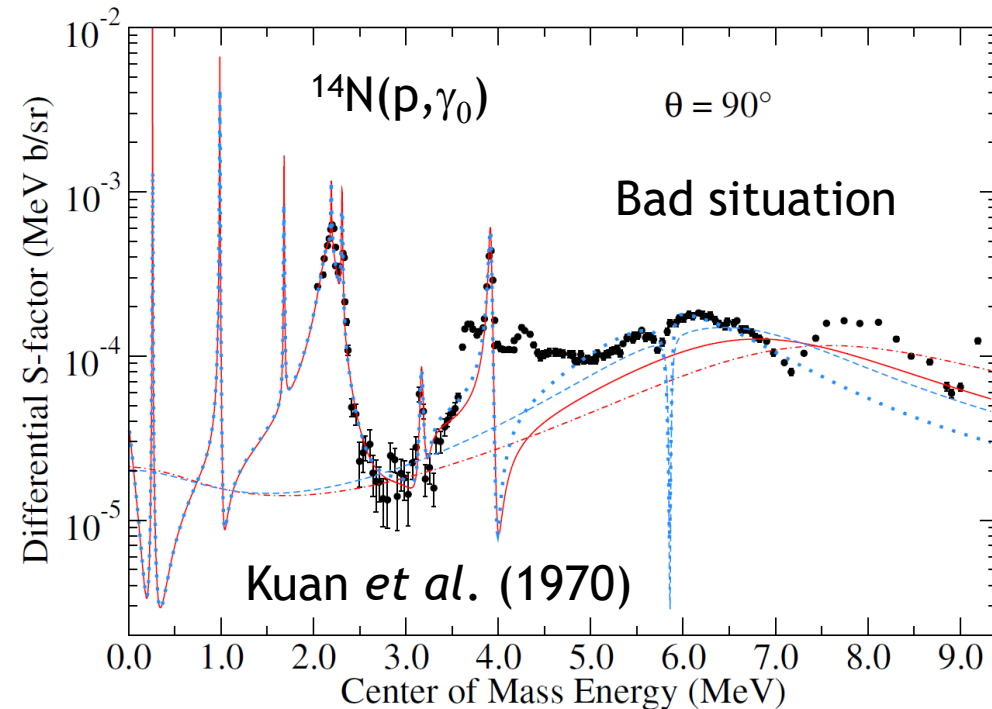
FIG. 4. Comparison of recent values of the 2^+ subthreshold ANC in ^{16}O obtained from R -matrix fits to $^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$ data [47], $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$ 6.92 MeV cascade data only [48] or global fitting [49], none of which include constraints on the ANCs from transfer measurements, or transfer reaction measurements using $^{12}\text{C}(^7\text{Li}, t)^{16}\text{O}$ [12,13,15,45], $^{12}\text{C}(^6\text{Li}, d)^{16}\text{O}$ [12,46], and $^{12}\text{C}(^{11}\text{B}, ^7\text{Li})^{16}\text{O}$ [17] reactions. The red point indicates the value deduced from the present GS ANC of ^{16}O and the low energy $E2$ capture data as discussed in the text. The blue and purple bands represent the weighted average of the ANCs from the R -matrix analyses including the present result and the one of the ANCs from six measurements of transfer reactions, respectively. See Table XIII of deBoer *et al.* [3] for comparisons to additional measurements that lack uncertainty estimates.

Background levels

- Are there broad resonances at higher energy whose low energy tails can have an influence on fitting and extrapolating into the low energy region?

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

Usually just one background level per J^{π}

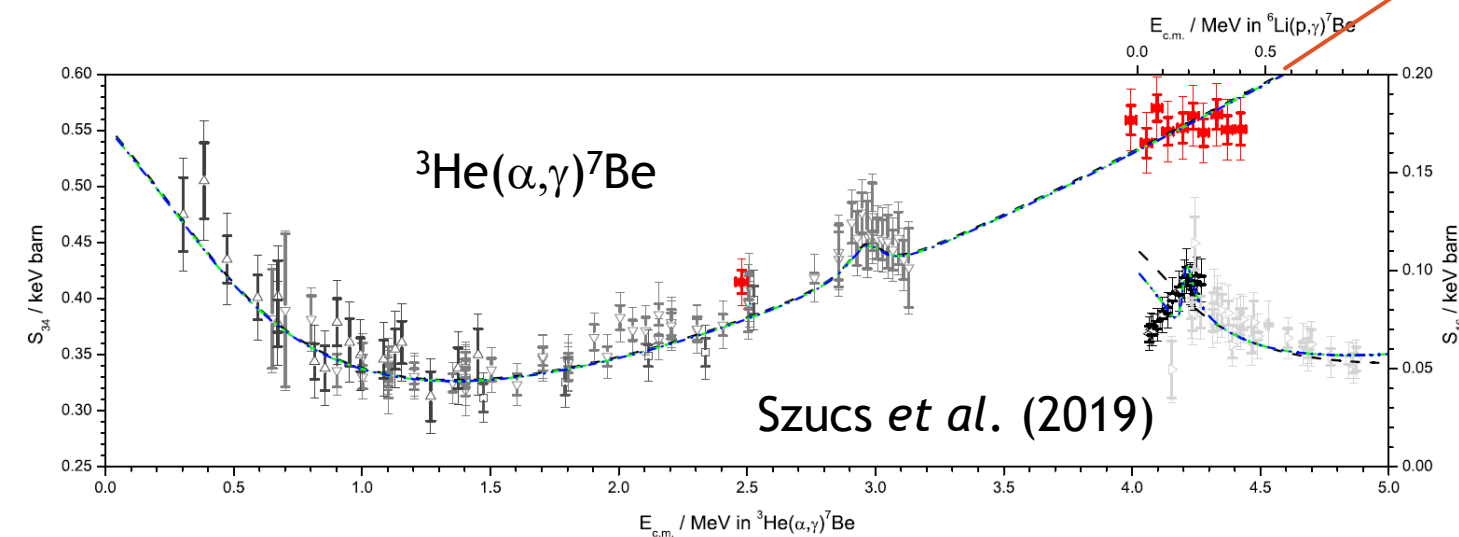


Background levels

- ▶ One of the most ambiguous parts of most R-matrix fits
- ▶ They often are needed
 - ▶ A real, broad, strong, resonance at energies just above your experimental data
- ▶ **Needed to augment the hard sphere phase shifts to fit scattering data**
 - ▶ This is where many are often needed

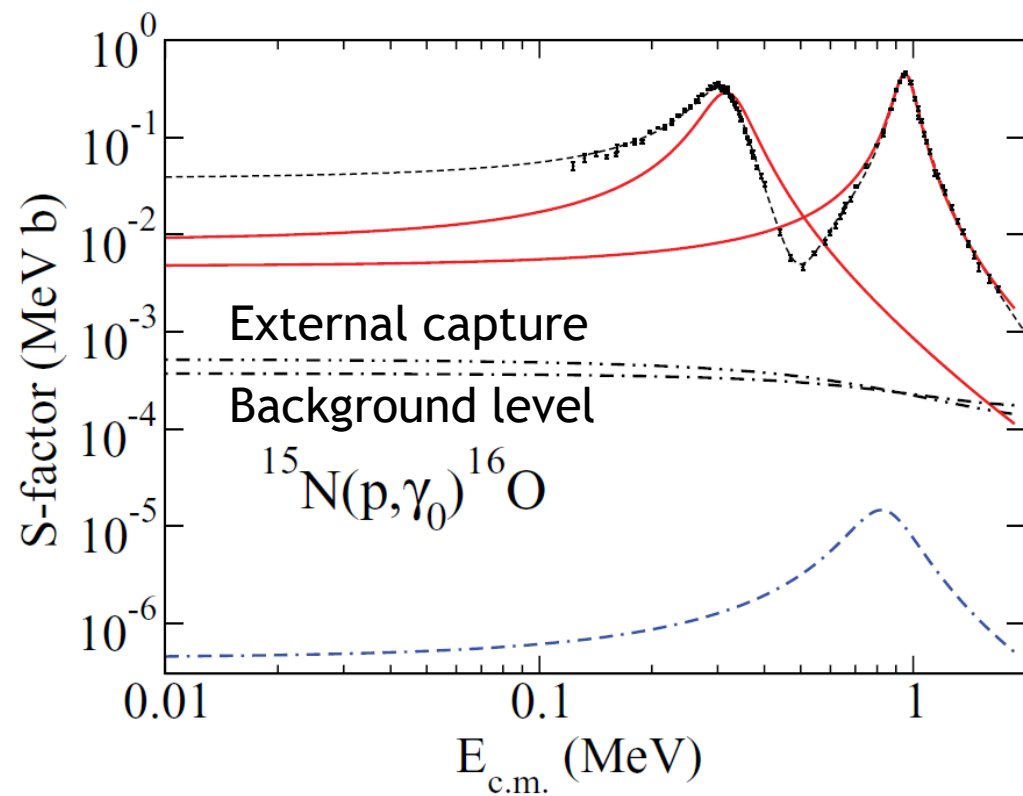
Broad high energy resonance?

Look for a new measurement soon from ATOMKI on this topic

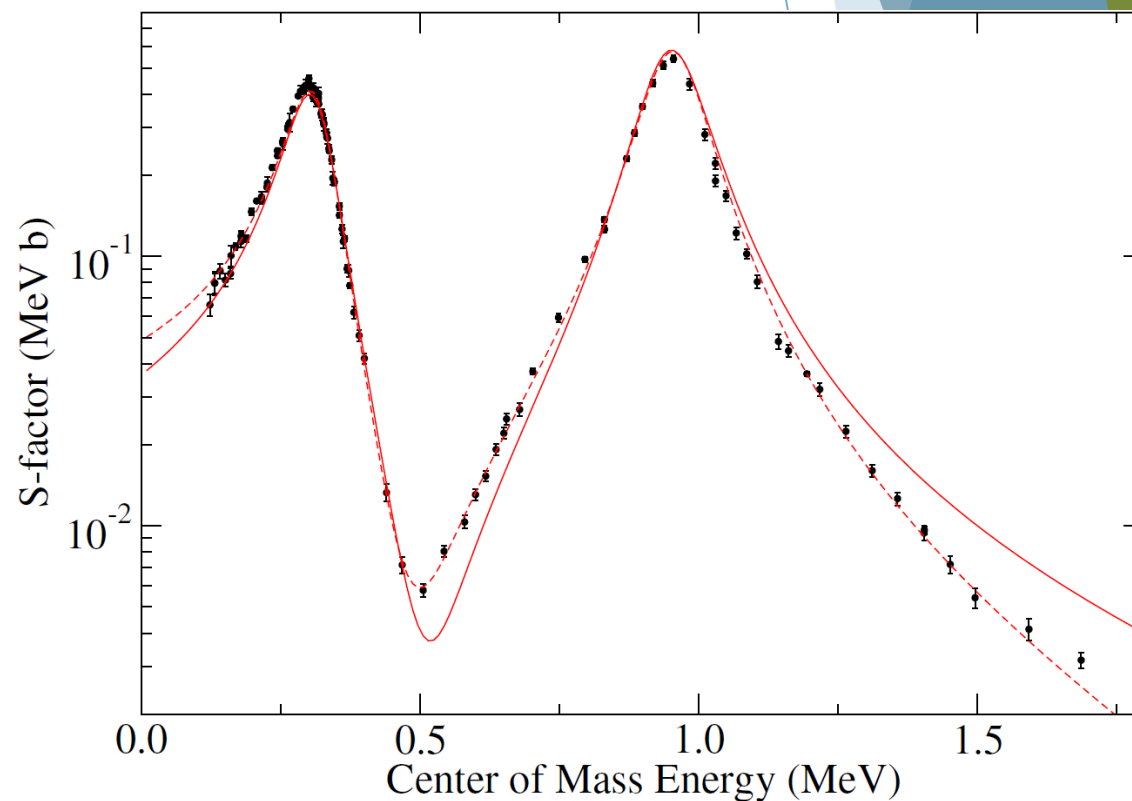


Cases that bug me

- ▶ $^{15}\text{N}(p,\gamma)^{16}\text{O}$, ground state transition
- ▶ No higher energy data
- ▶ Is this background real?

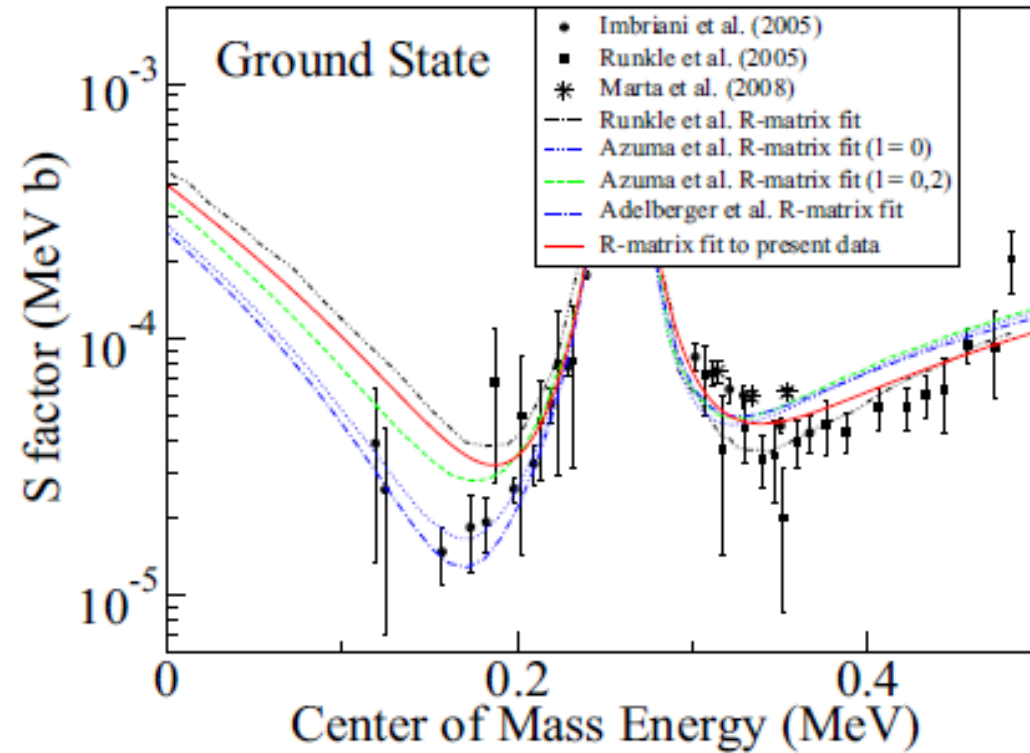
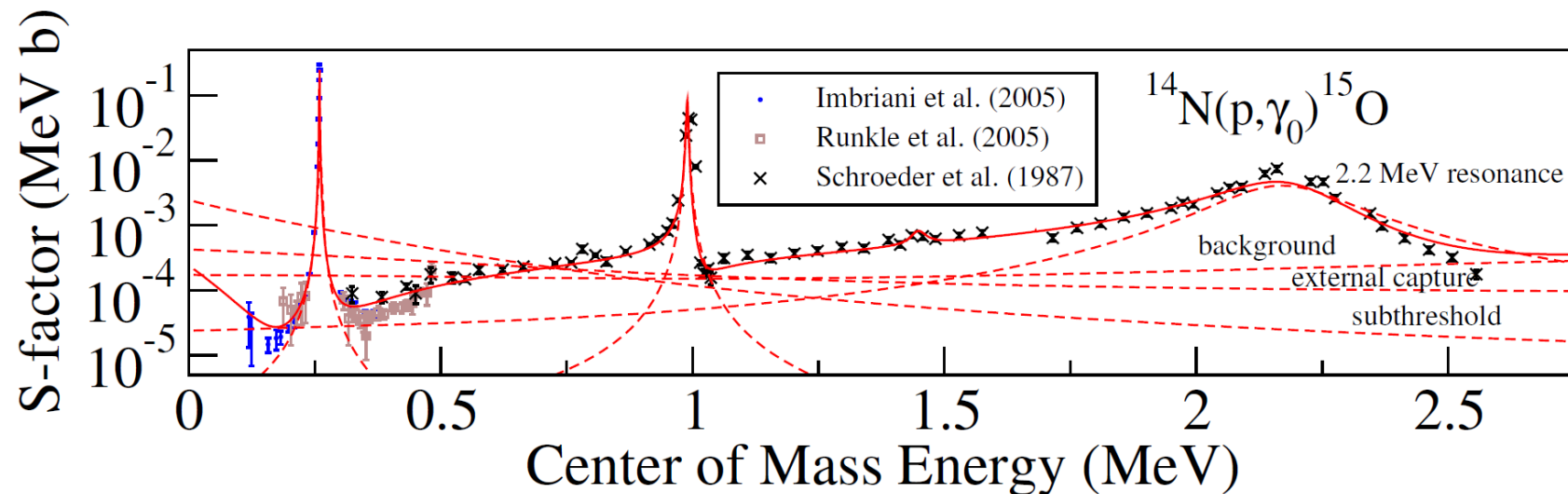


With and without
background level

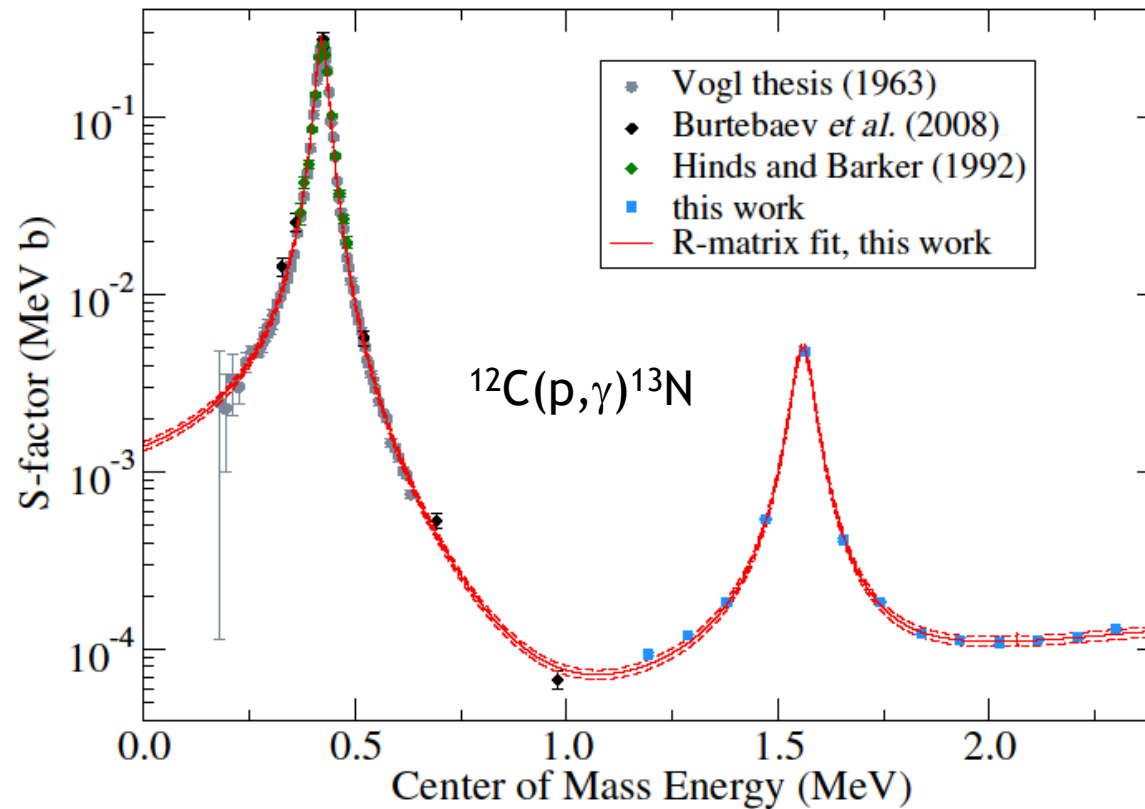


Cases that bug me

- ▶ $^{14}\text{N}(p,\gamma)^{15}\text{O}$ ground state transition



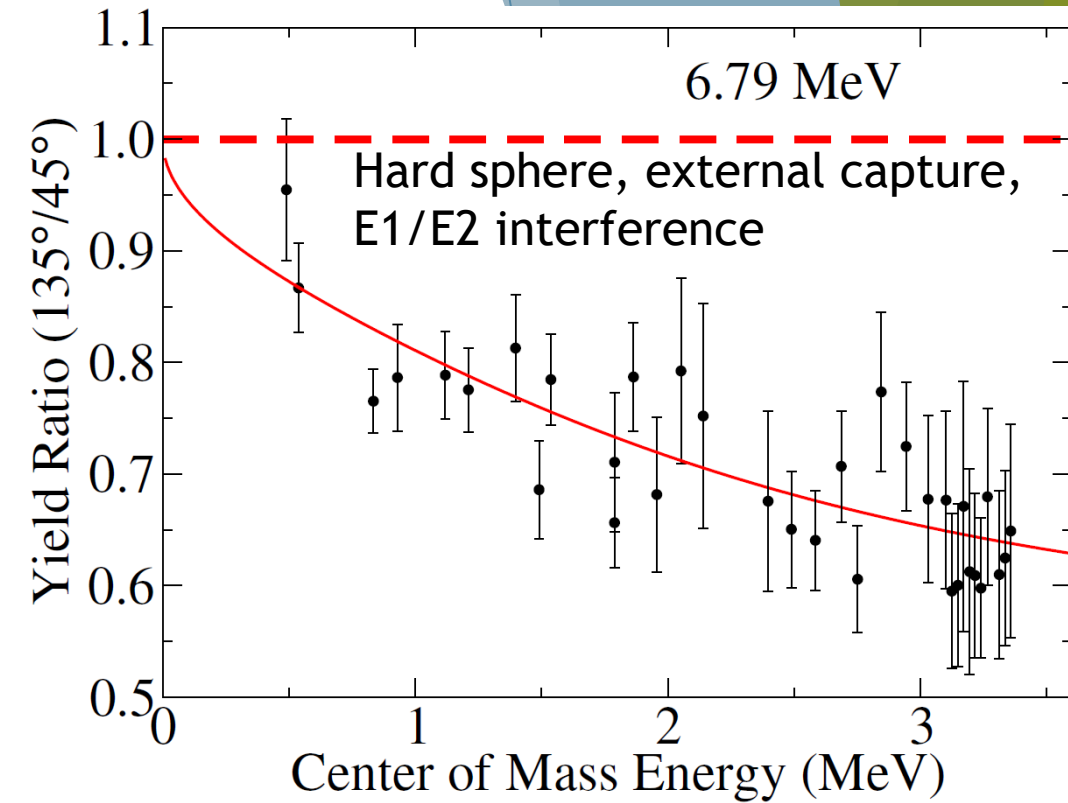
There are also lots of cases that work really well



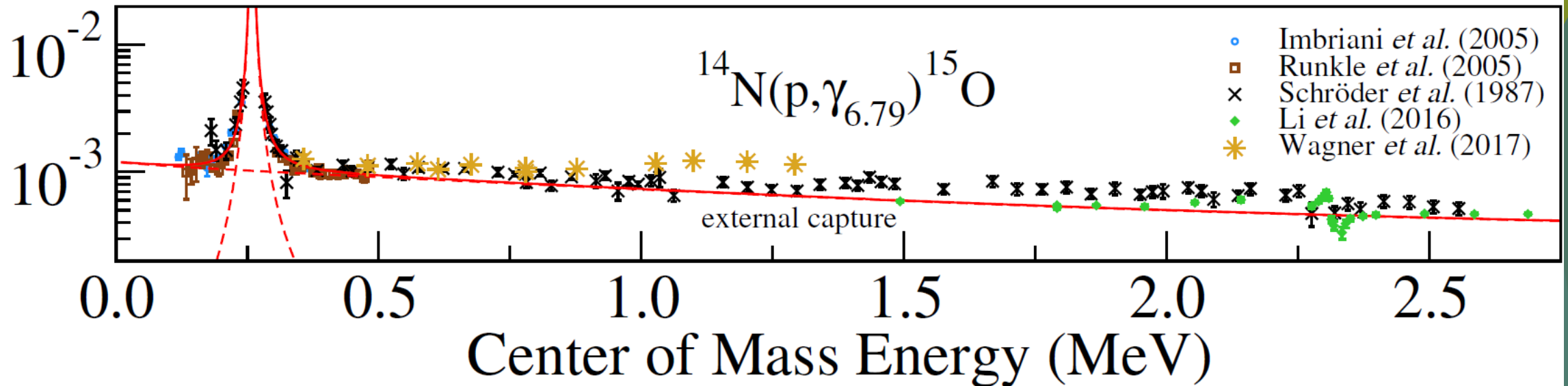
ANCs from $^{12}\text{C}(^7\text{Li}, ^6\text{He})^{13}\text{N}$ and $^{12}\text{C}(^{10}\text{B}, ^9\text{Be})^{13}\text{N}$ proton transfer experiments by Li et al. (2010) and Artemov et al. (2022): 1.64(11) and 1.63(13) fm^{-1/2}. R-matrix fit gives 1.615(52) fm^{-1/2}.

There are also lots of cases that work really well

- ▶ $^{14}\text{N}(p,\gamma)^{15}\text{N}$, 6.79 MeV transition
- ▶ ANC from transfer: 4.6(5) and 5.2(6) fm $^{-1/2}$ from Bertone *et al.* (2002) and Mukhamedzhanov *et al.* (2003), respectively
- ▶ ANC from R-matrix fit: 4.91(18) fm $^{-1/2}$ from Li *et al.* (2016)

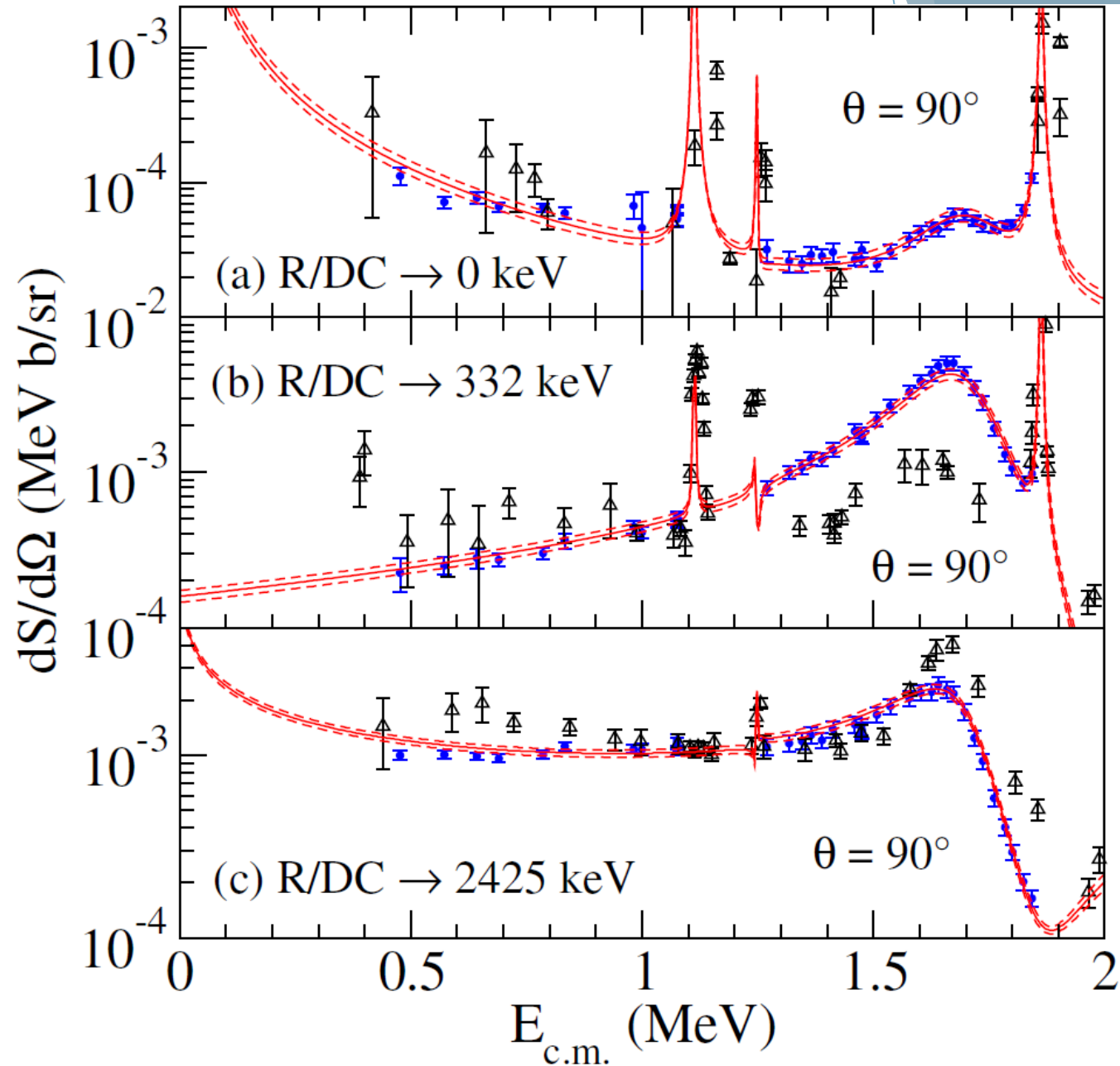


S factor (MeV b)



$^{20}\text{Ne}(p,\gamma)^{21}\text{Na}$

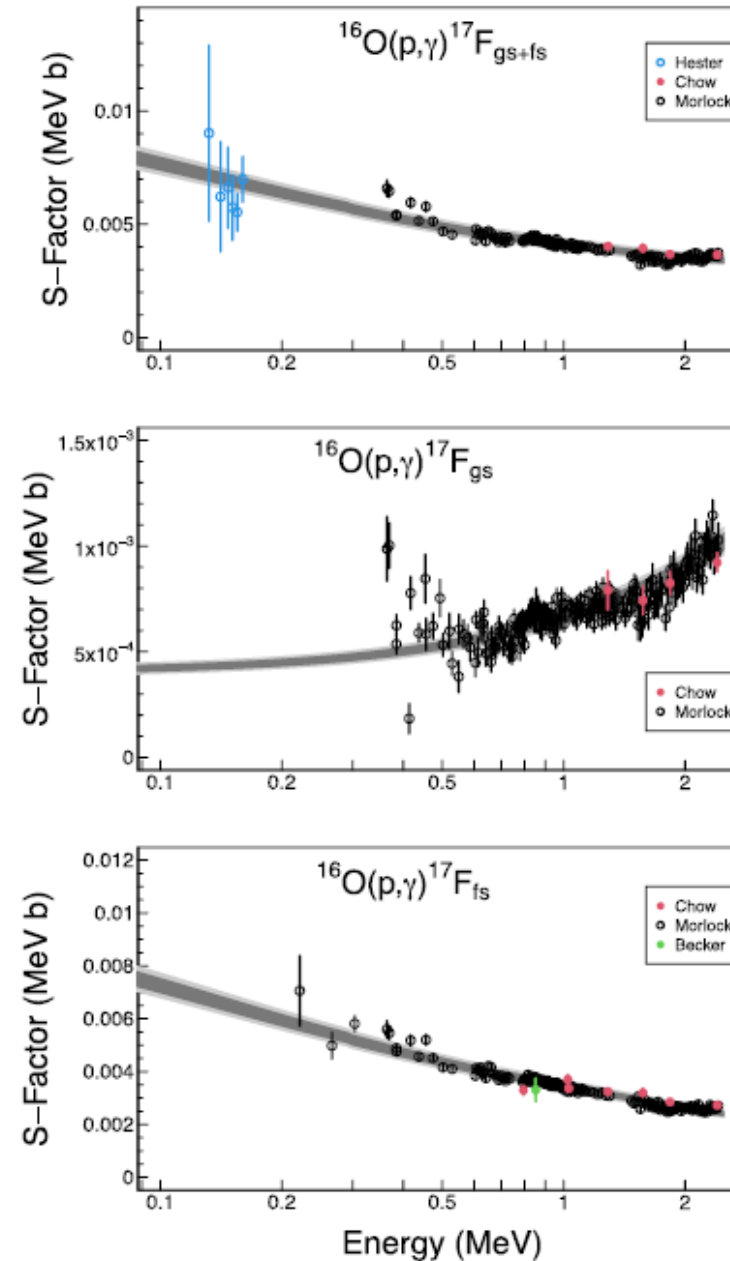
- ▶ Revised analysis of that presented in Lyons *et al.* (2018)
- ▶ Using a Bayesian MCMC analysis using BRICK
- ▶ 2425 keV state ANC: $8.1(4)\text{e}16$ vs $8.2(2)\text{e}16$ fm $^{-1/2}$ from transfer
- ▶ GS ANC: $0.53(5)$ vs $0.46(4)$ fm $^{-1/2}$
- ▶ 332 keV state ANC: $1.53(11)$ vs $1.4(1)$ fm $^{-1/2}$



$^{16}\text{O}(p,\gamma)^{17}\text{F}$

- ▶ Recent potential model analysis by Iliadis *et al.* (2022) using Bayesian MCMC sampler for uncertainty analysis
- ▶ For comparison, I've done the analysis using R-matrix using BRICK for the Bayesian uncertainty analysis
- ▶ Uncertainties are small! A few percent
- ▶ Look for this in SFIII

Iliadis *et al.* (2022)

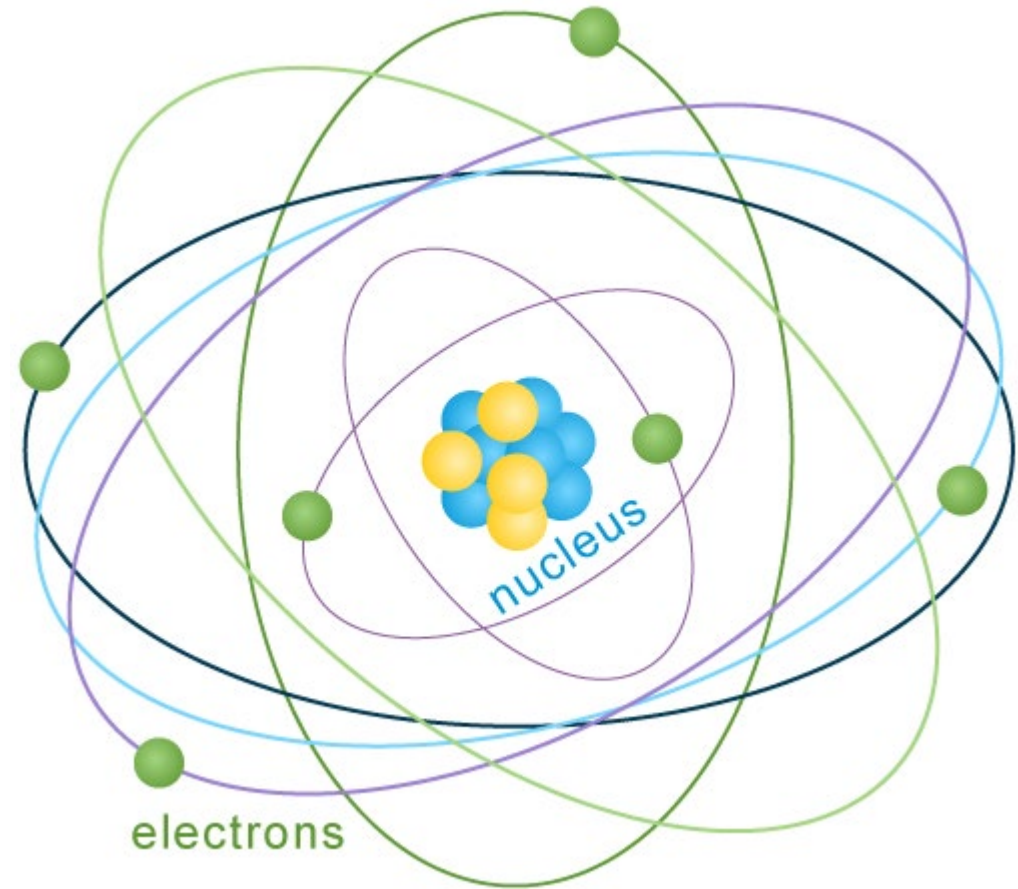


Struggling with consistency

- ▶ A nice case to compare
 - ▶ R-matrix and potential model
 - ▶ Different Bayesian samplers
- ▶ ANC: 84.1(17) R-matrix (me) vs 84.0(17) fm^{-1/2} potential model (Iliadis)
- ▶ Value and uncertainty is very similar
- ▶ Atomic masses give 82.8(17) fm^{-1/2}, a 1.5% difference. But the uncertainty in the cross section is then twice this, about 3%, which is now comparable to the overall cross section uncertainty of 4.2% found by Iliadis.

Masses

- ▶ Nuclear vs atomic mass
 - ▶ No electrons?
 - ▶ But in experiments we have electrons
 - ▶ Beam can be in different ionization states
 - ▶ Targets have all of their electrons (usually)
- ▶ Plasma environments like NIF and Omega
 - ▶ Particles are fully ionized

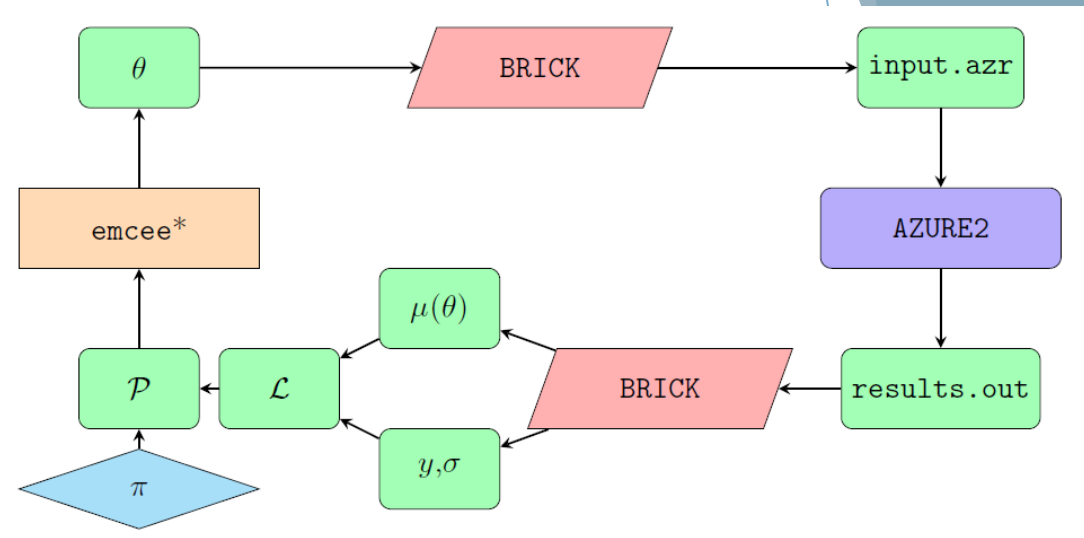
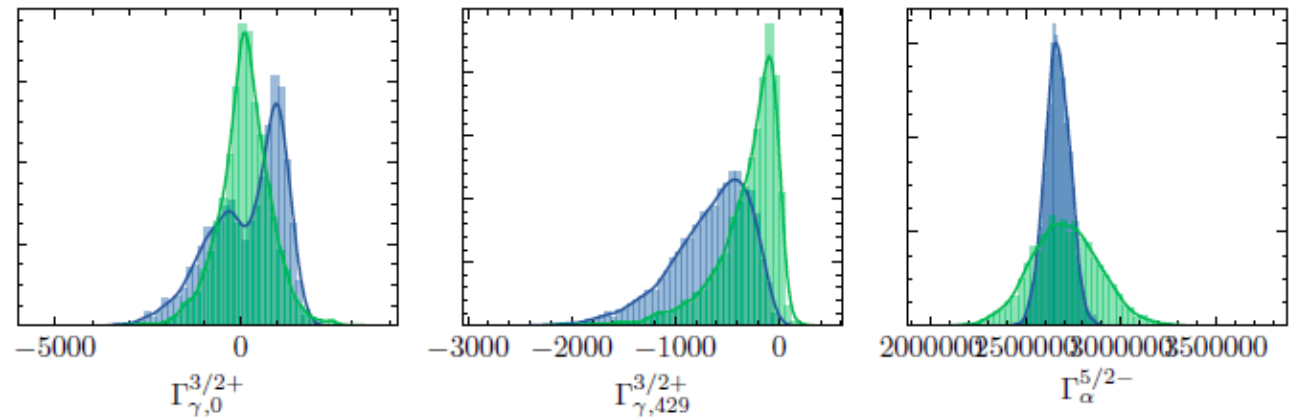


Bayesian MCMC uncertainty estimation

- ▶ A powerful tool for helping us better understand uncertainties
- ▶ Note a silver bullet, but it facilitates a better understanding of how the uncertainties are behaving
- ▶ The analysis produces the full posterior probability distributions for the parameters
 - ▶ That is, it gives the shape of the probability distribution for each fit parameter (and any other quantity, e.g. cross section) the results from the constraints of the experimental data, model, and priors
- ▶ Traditional χ^2 analysis tools only give “1 sigma” upper and lower uncertainty estimates for each fit parameter and the covariance matrix

Improving uncertainty estimation for R-matrix fits

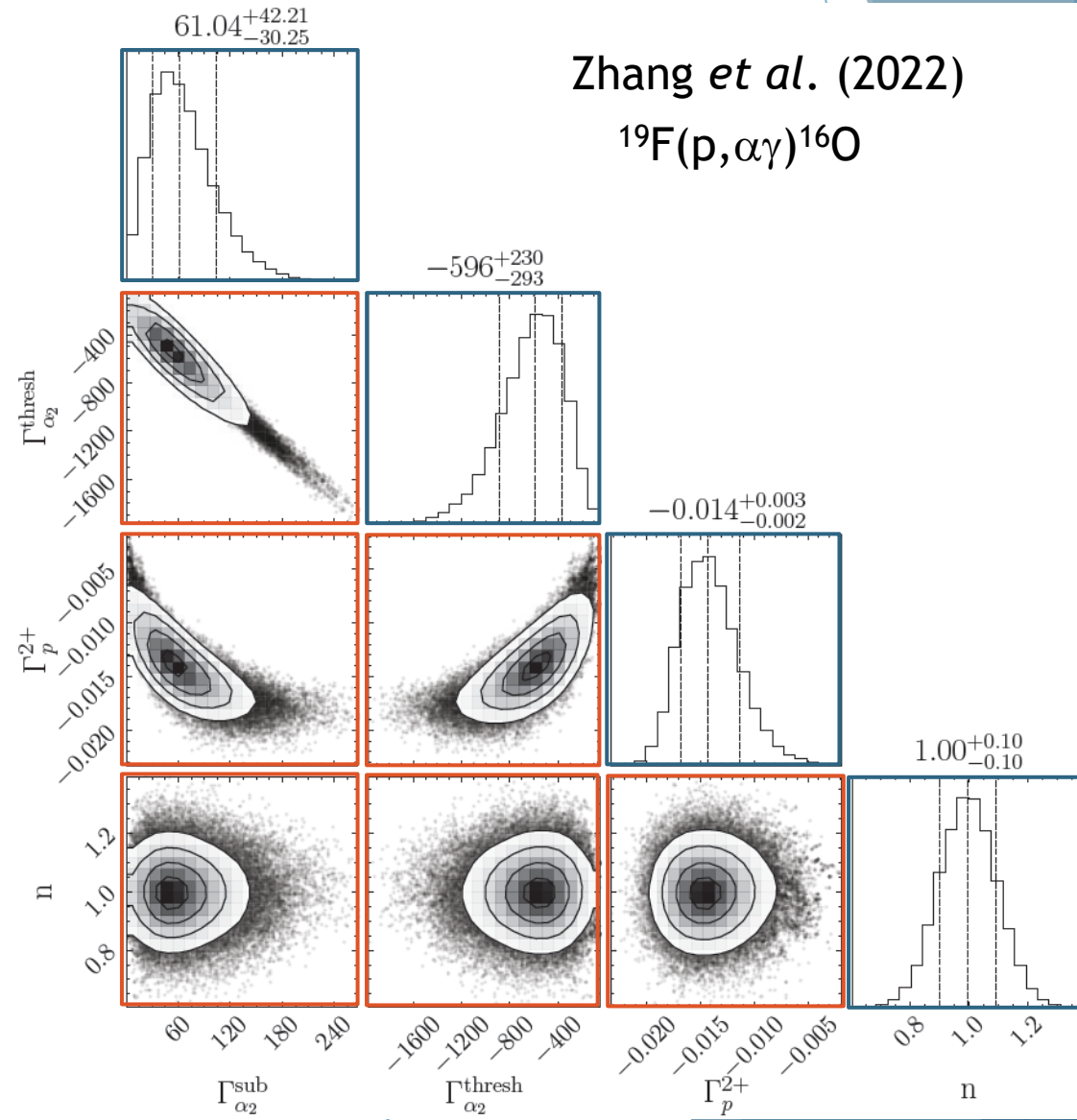
- ▶ A more general problem
- ▶ **Bayesian** methods provide a way to improve and gain more detailed information
- ▶ Computationally intensive, but probably doable
- ▶ **Daniel Odell** at Ohio University has developed the Bayesian R-matrix Inference Code Kit (**BRICK**) for use with the **AZURE2** R-matrix code
- ▶ Odell *et al.*, *Frontiers in Physics* **10**, 888476 (2022), special issue on uncertainty quantification



Figures courtesy of Daniel Odell

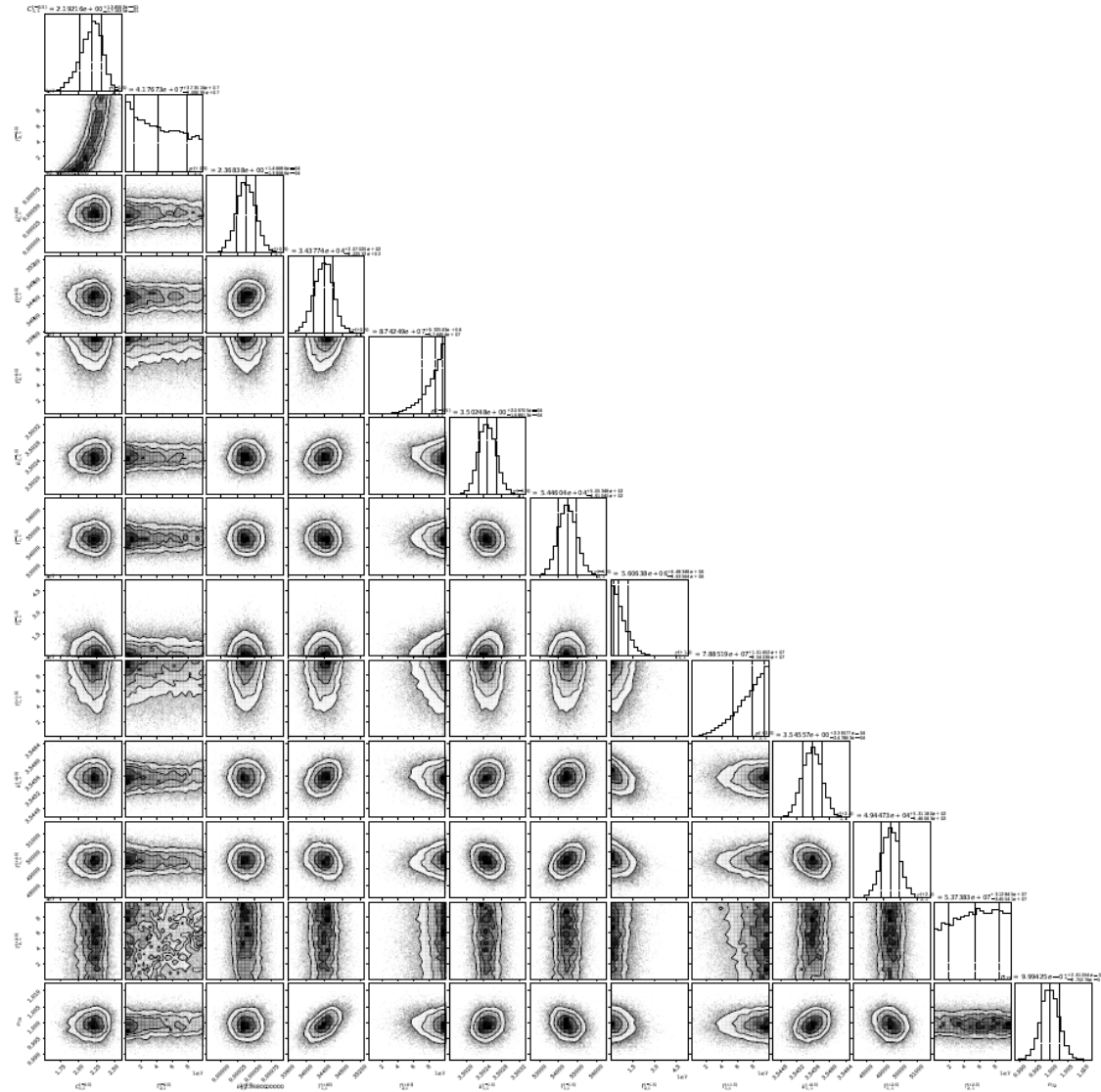
Why aren't traditional methods enough?

- ▶ Posterior distributions are often NOT Gaussian in shape when uncertainties are large
- ▶ Level parameters (fit parameters) PDFs
- ▶ Correlations



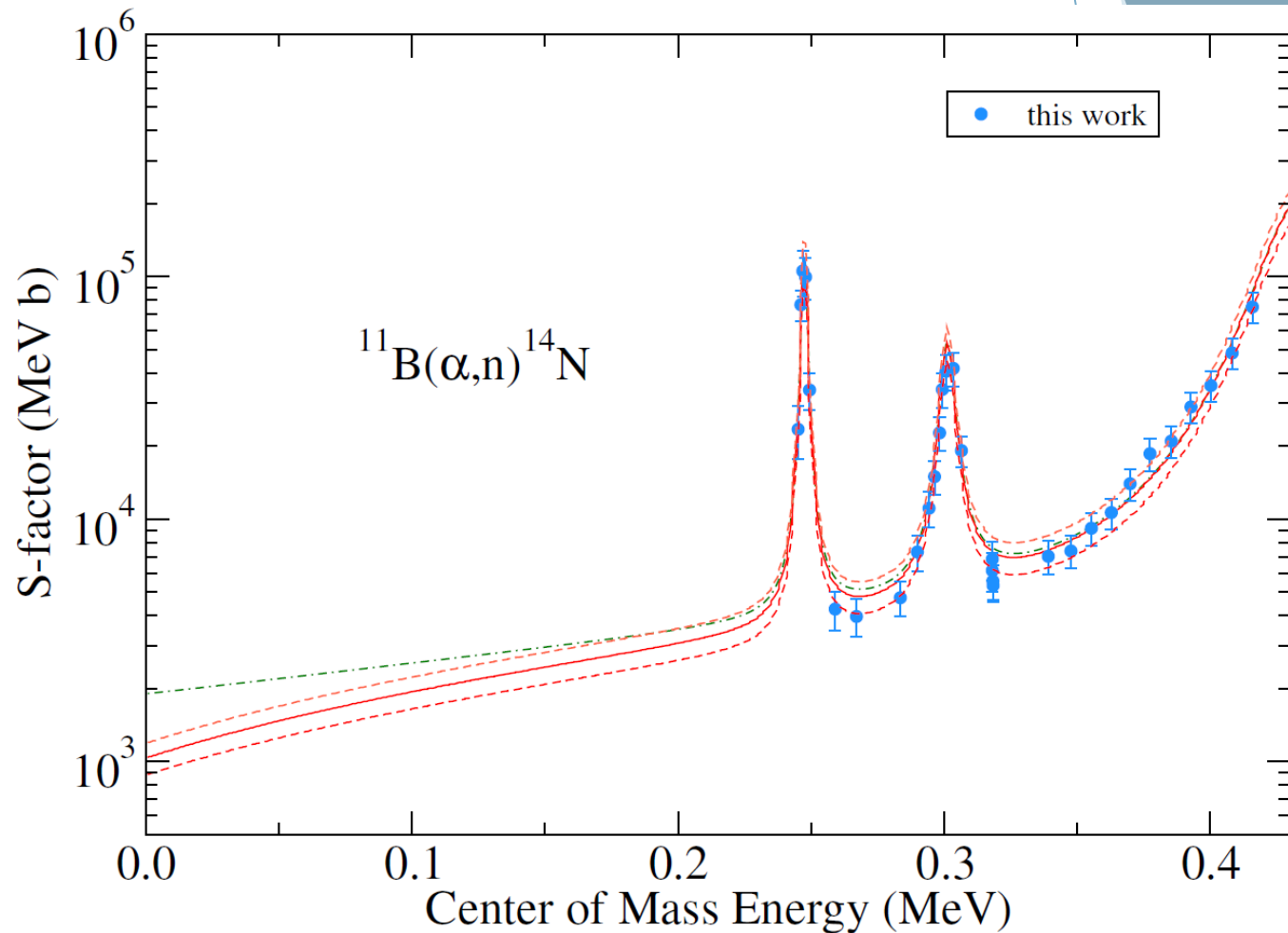
Those pesky background levels

- ▶ If posterior PDFs are not Gaussian, it helps us troubleshoot the calculation.
 - ▶ Is the parameter space just too small?
 - ▶ Do we have redundant fit parameters?
- ▶ Maybe what is more interesting, it can show us what background terms are unconstrained by the data, but still effect the extrapolation. This can then give a better idea of what data can be measured to help reduce this uncertainty.



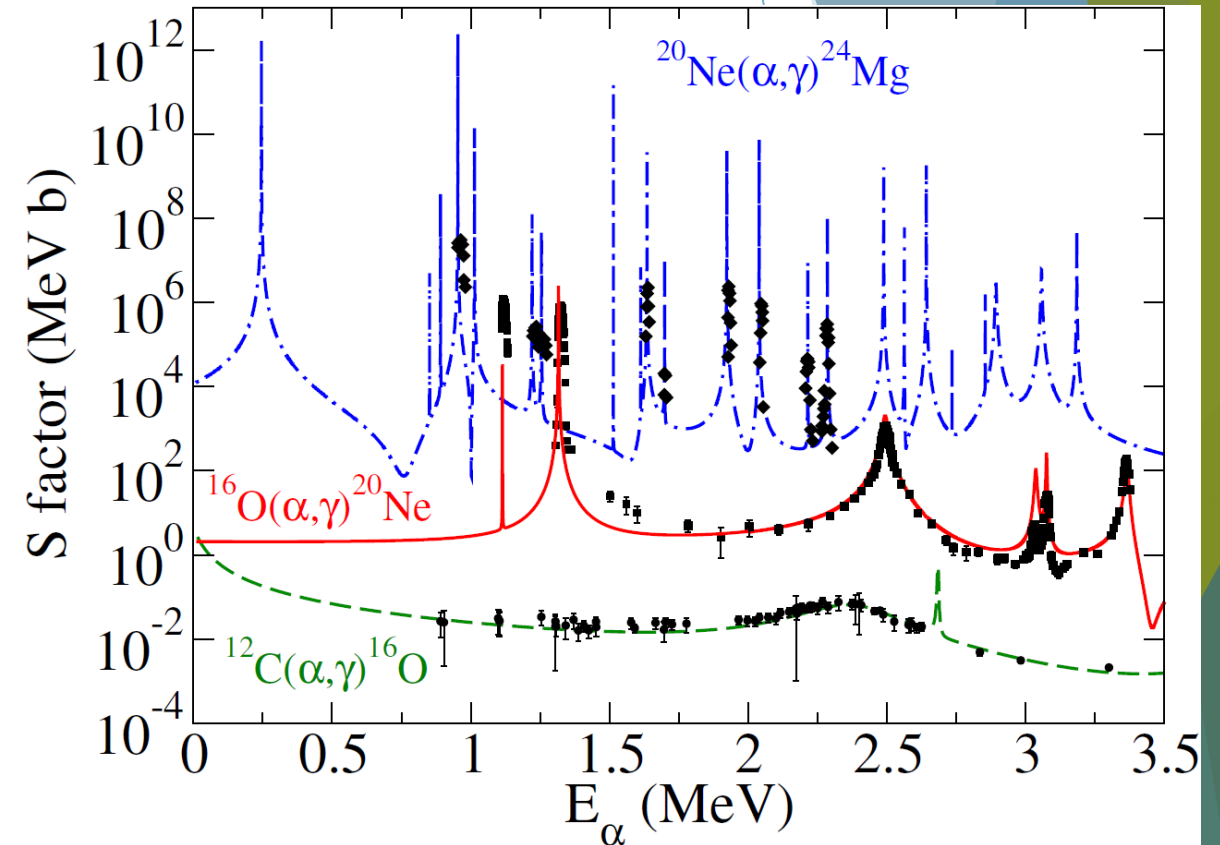
$^{11}\text{B}(\alpha, n)^{14}\text{N}$, an interesting extrapolation example

- ▶ Extrapolation uncertainty was very dependent on the background components that were included in the calculation.
- ▶ Many were not needed for a good fit to the data, but were found to influence the extrapolated S-factor.
- ▶ Effect is augmented because there are no low energy resonances, so the extrapolation depends on the tails of high energy resonances.
- ▶ In some ways a worst case scenario.



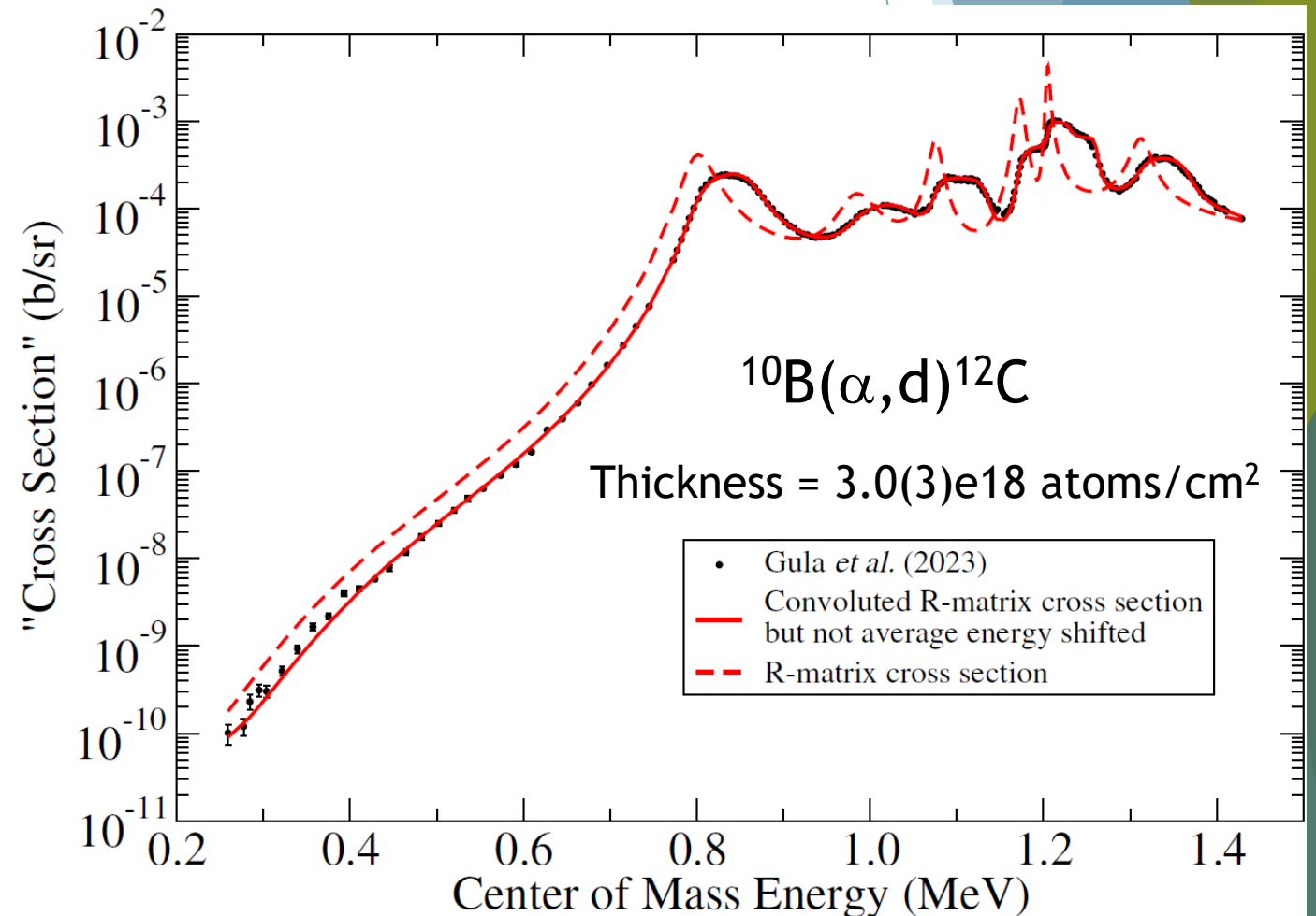
Experimental effects

- ▶ Very few data sets are completely free of experimental effects (to with the quoted uncertainties at least)
- ▶ For proton induced reactions the energy loss averaging over target thickness can be only a few keV or less, but for α -induced reactions its hard to get less than 10's of keV.
- ▶ If we have very narrow resonances, we don't care and purposely make our targets thick so we can perform thick-target yield scans
- ▶ For cross sections with very broad resonances (100's of keV), these effects can be negligible
- ▶ We run into problems when we have resonances in the 10's of keV region

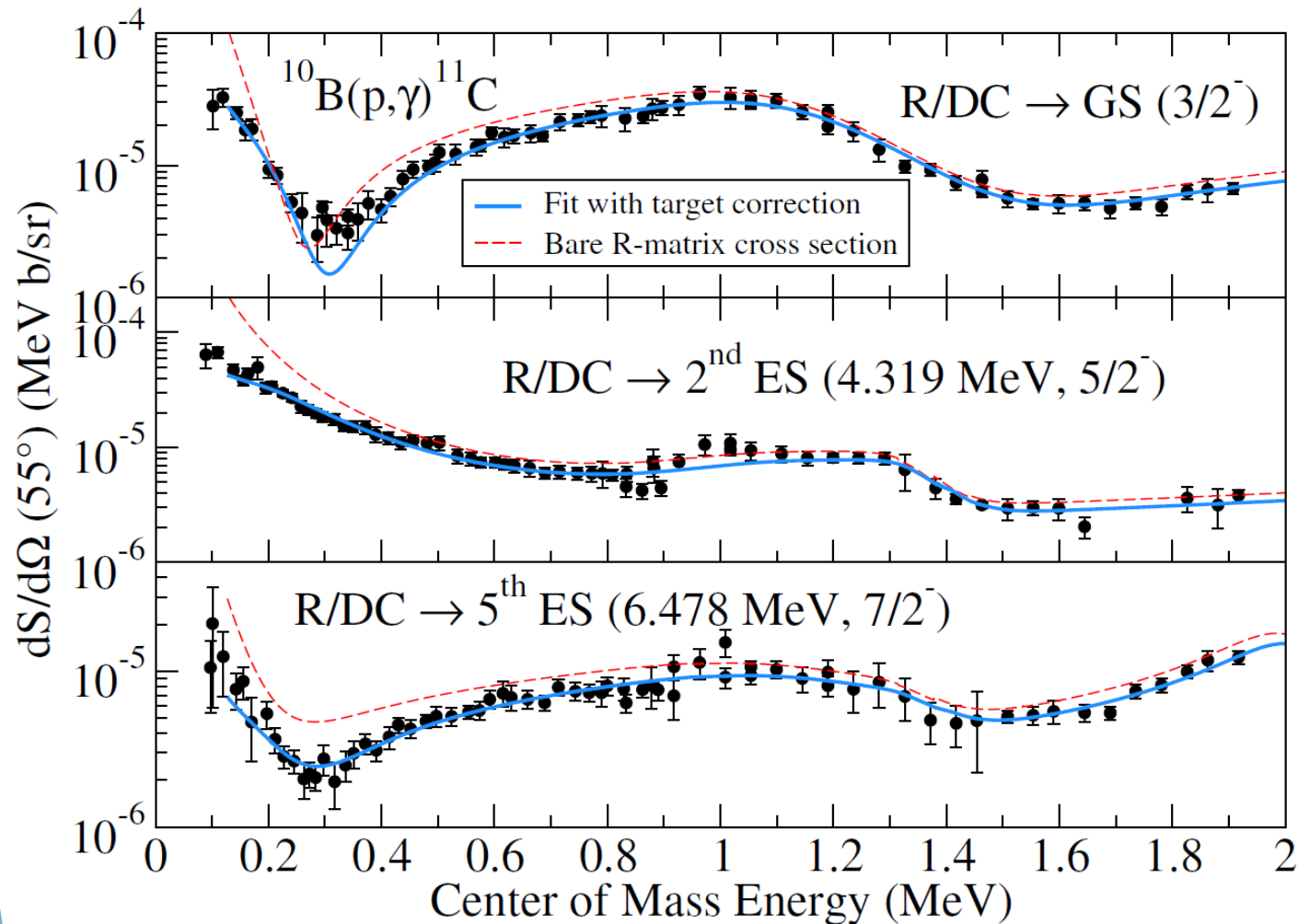


Experimental effect convolution of theoretical cross section

- ▶ Con: computationally very expensive
- ▶ Con: have to know the characteristics of the experimental effects, more information to track
- ▶ Pro: yield data are closer to actual measurements, can often retain uncorrelated point-to-point uncertainties
- ▶ Pro: convolution method can be improved later and original data is retained



Can strongly influence the low energy extrapolation



Vande Kolk *et al.* (2022)

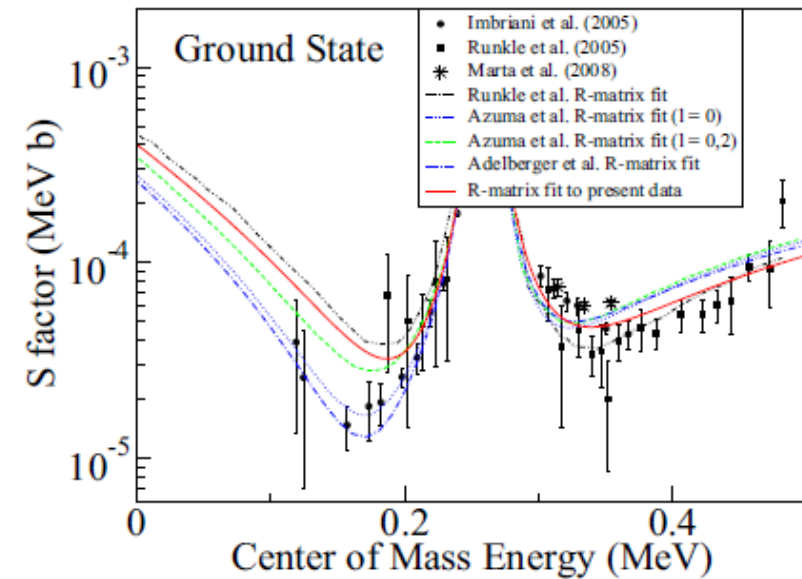
Data from Wiescher *et al.* (1983)

Thickness of 124 $\mu\text{g}/\text{cm}^2$

Fit simultaneously with $^{10}\text{B}(p,\alpha)^7\text{Be}$ and (p,p) data

Anecdotal observation

- ▶ R-matrix fitting often works really well for “transfer” type particle reactions
 - ▶ e.g. (p,α) , (α,n) , (p,γ) with negligible direct capture
 - ▶ It seems like difficulties more often arise with fitting scattering and (x,γ) reactions with a mix of resonance and direct capture
 - ▶ May trace back to the hard sphere phase shifts?



How can we move forward?

- ▶ Bayesian uncertainty analysis is helping to better understand the problem and improve the implementation of the uncertainty analysis
 - ▶ Doesn't crash when there are a lot of background contributions in the calculations
- ▶ Maybe something like a hybrid R-matrix / potential model calculation can help to better constrain background contributions (and modify phase shifts)
 - ▶ Higher energy data is also great
- ▶ The mass issue, not sure
- ▶ Faster computational implementations of
 - ▶ MCMC routine directly in the C++ AZURE2 code
 - ▶ convolution routines
- ▶ Can machine learning help?
 - ▶ Maybe it can speed up calculations?
 - ▶ It may be able to do things like identify levels when spin-parities are unknown?
 - ▶ Struggling to understand