EXPERIMENTAL NUCLEAR REACTIONS

James deBoer

University of Notre Dame

Exotic Beam Summer School, Oak Ridge National Laboratory, June 22 to 26, 2026

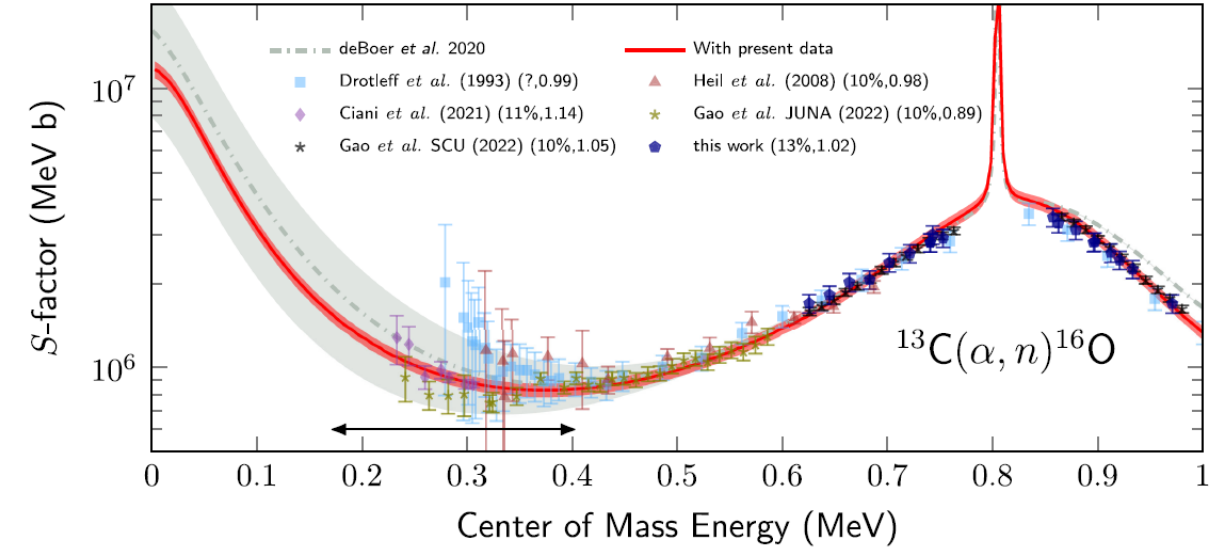
MY BACKGROUND

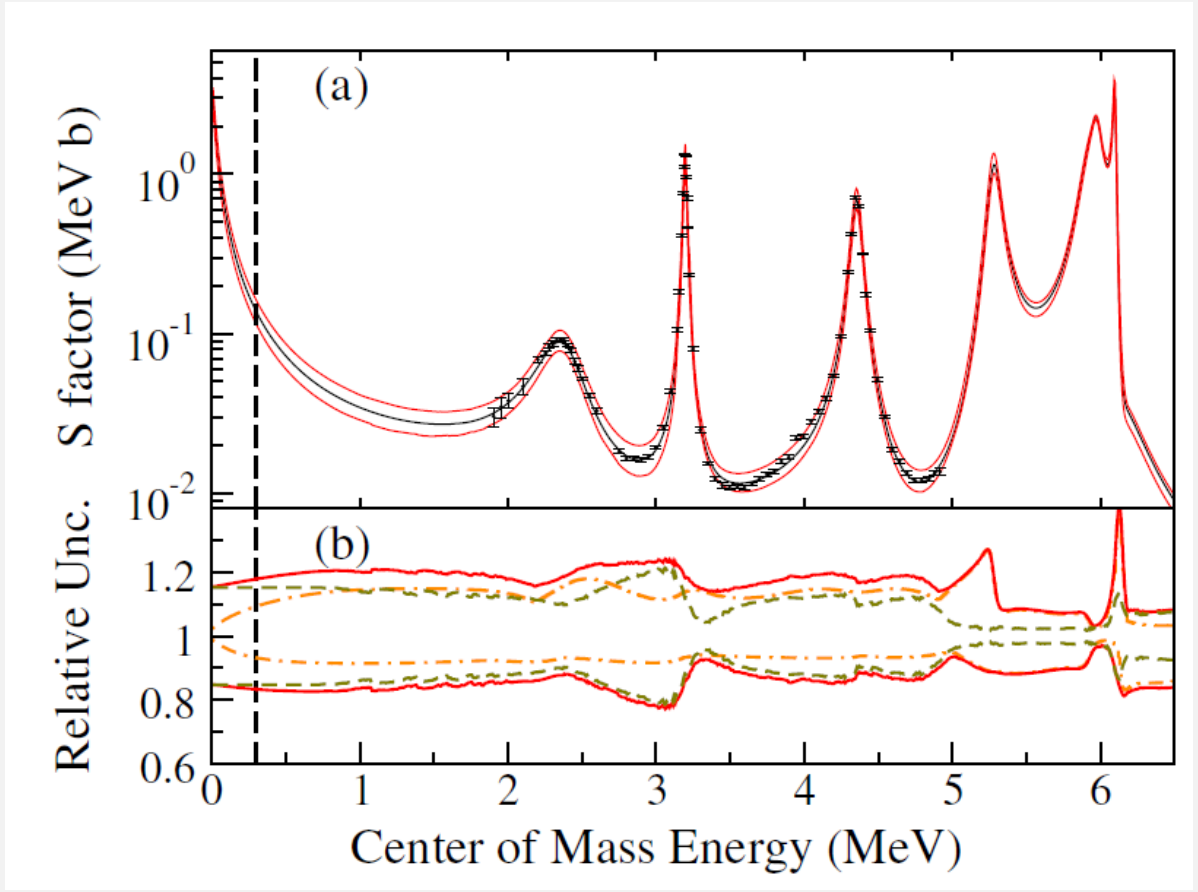
- Research faculty at the University of Notre Dame

- Nuclear astrophysics
- Energy and safeguards

- Low mass reactions with broad interfering resonances

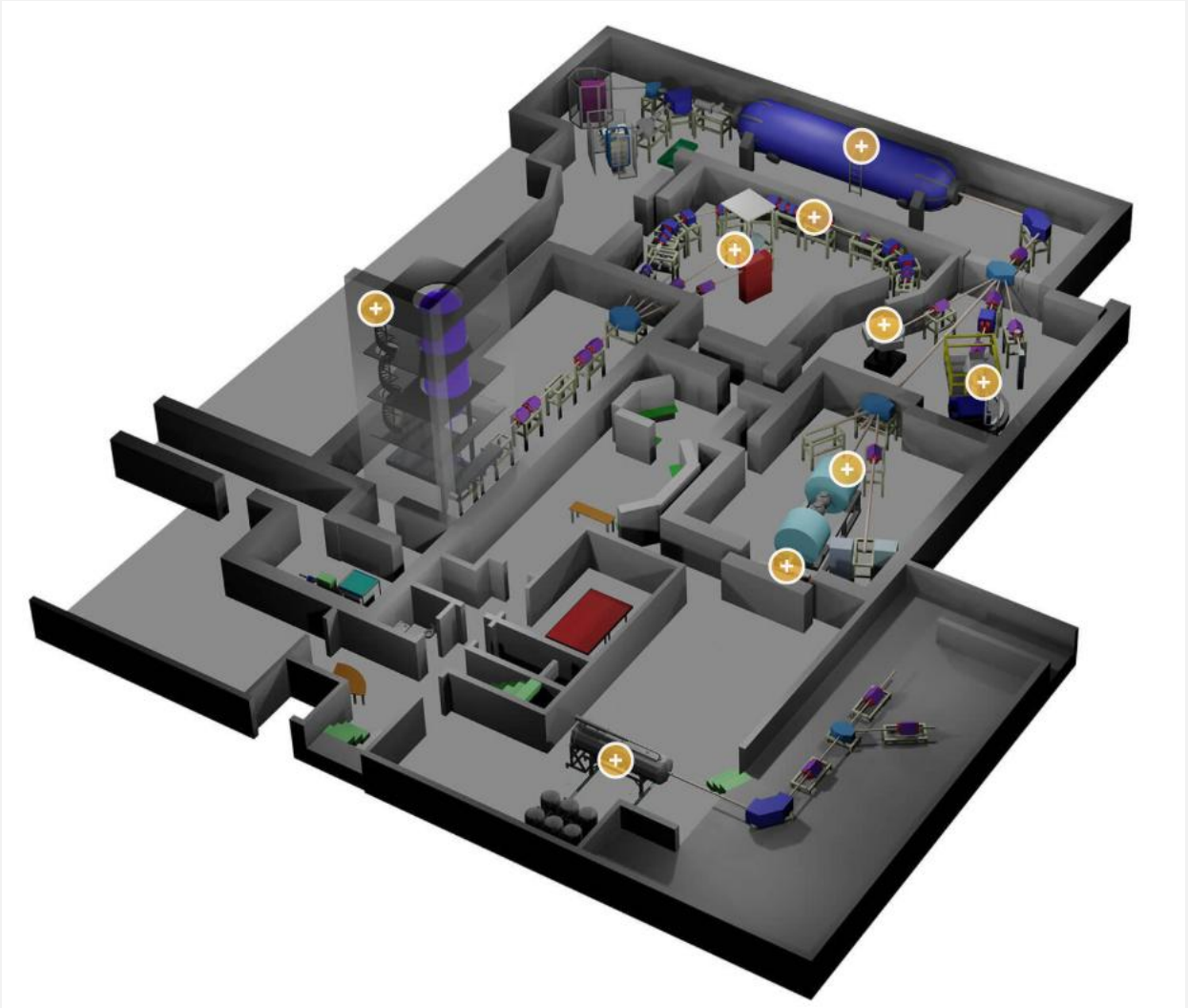
- Phenomenological R-matrix and uncertainty quantification





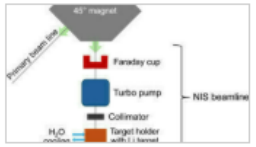
THE UNIVERSITY OF NOTRE DAME NUCLEAR SCIENCE LABORATORY

- "Midscale" nuclear physics laboratory
- Low energy nuclear reactions
  - Nuclear astrophysics
  - Nuclear Structure
  - Energy and Safeguards
- Particle accelerators
  - 5MV single ended machine
  - 10MV Tandem
  - 3MV Tandem



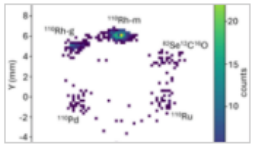
WE DO LOTS OF MEASUREMENTS!

Research Highlights



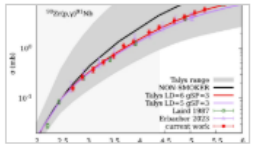
Neutron Irradiation Station at the NSL

June 2025 Simon-Robertson
M. Matney



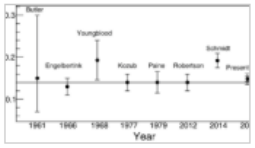
Longest Odd-Odd Chain of Nuclei with 1+ Ground States

March 2025 Brodeur
B. Liu



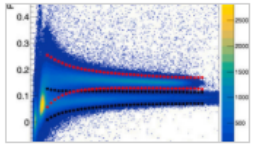
Resolving discrepancies in Zr-90(p,γ)Nb-91 data

March 2025 Simon-Robertson
A. Simon-Robertson



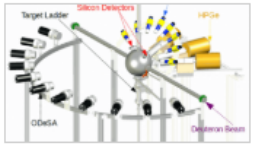
Strength measurements of Ca-40(p,γ)Sc-41 reaction

February 2025 Wiescher
R.S. Sidhu, R.J. deBoer



Light response of PEN to neutrons

December 2024 Wiescher
B. Hackett, R.J. deBoer

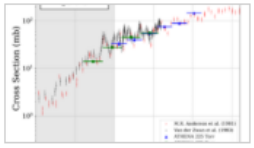


Comprehensive study of d+Li-6

October 2024 Wiescher
S.N. Paneru, R.J. deBoer

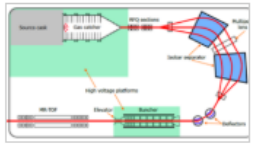
Enge Spectrometer Used in First Experiment

October 2024 Bardayan
S. Carmichael



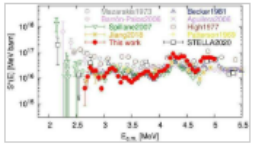
First Measurement of 25,26Mg(a,n) via Direct Recoil Detection

October 2024 Bardayan
D. Blankstein



Machine Learning Mass Modeling and Precise Mass Measurements

September 2024 Brodeur
W.S. Porter

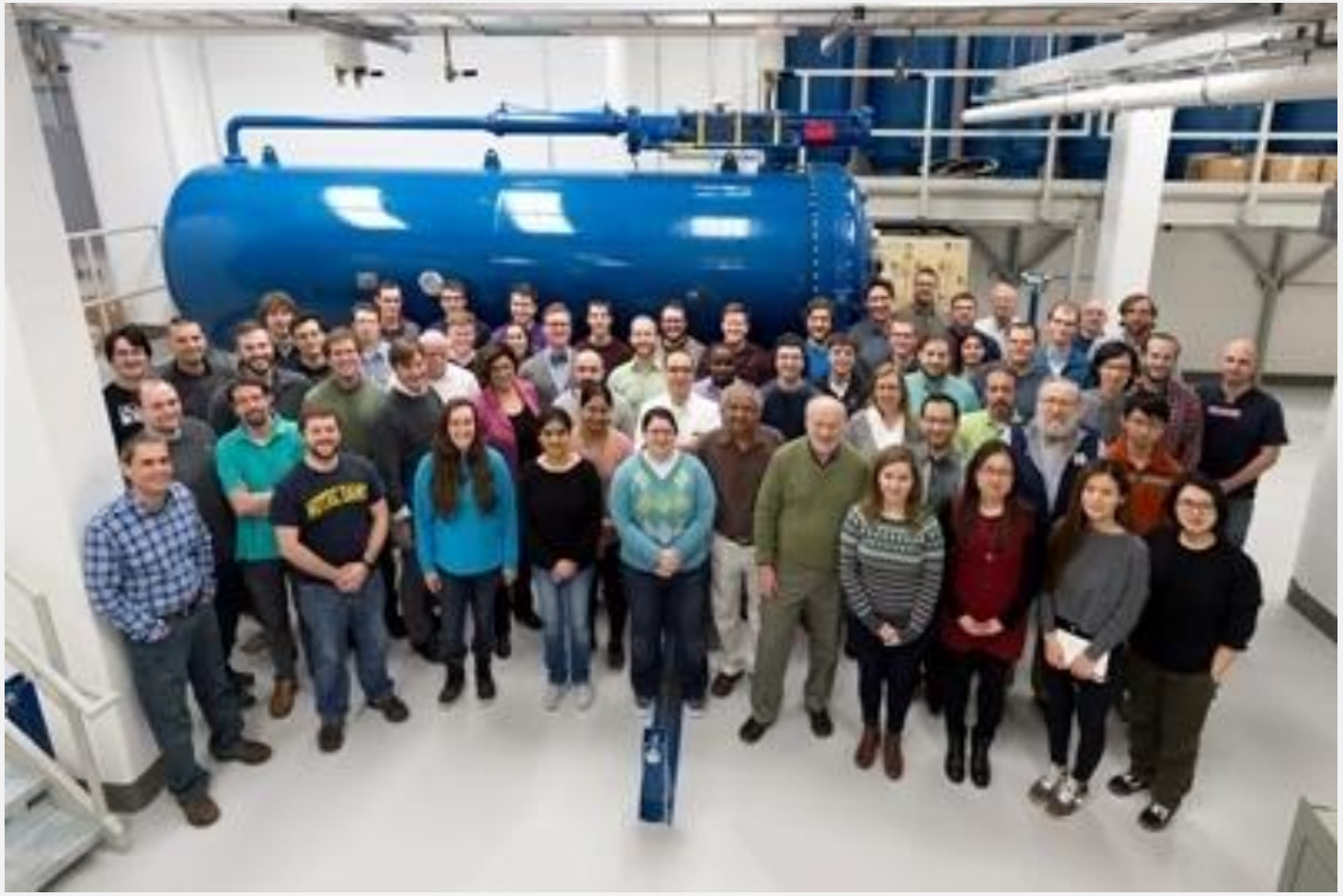


Coincident Measurement of the 12C+12C Fusion Cross Section via Differential Thick Target Technique

September 2024 Wiescher
W. Tan

PEOPLE

- Around 30 graduate students
- 19 faculty
  - 10 tenure track faculty
  - 7 research faculty
  - 2 theory



LECTURE OUTLINE

- Lecture I: Nuclear Models and Introduction to R-matrix theory
- Lecture II: Phenomenological R-matrix and uncertainty quantification

LECTURE 1: NUCLEAR MODELS AND R-MATRIX THEORY

REACTION MECHANISMS

Direct reaction

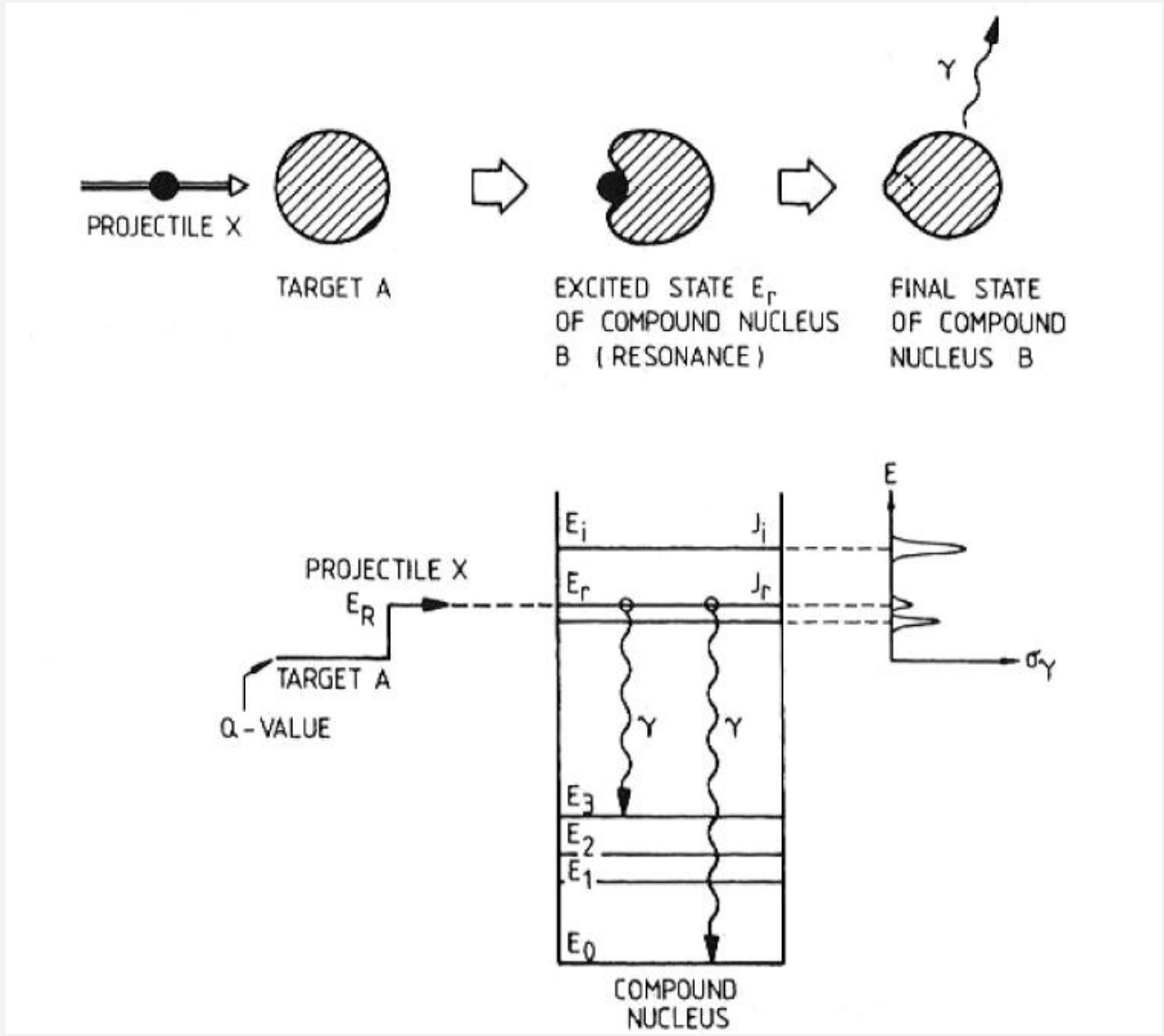
- Very fast --- time scale of 10^{-22} s
- No intermediate state

Compound Nucleus

- Significantly slower --- 10^{-15} to 10^{-19} s
- Intermediate state that has time to thermally equilibrate

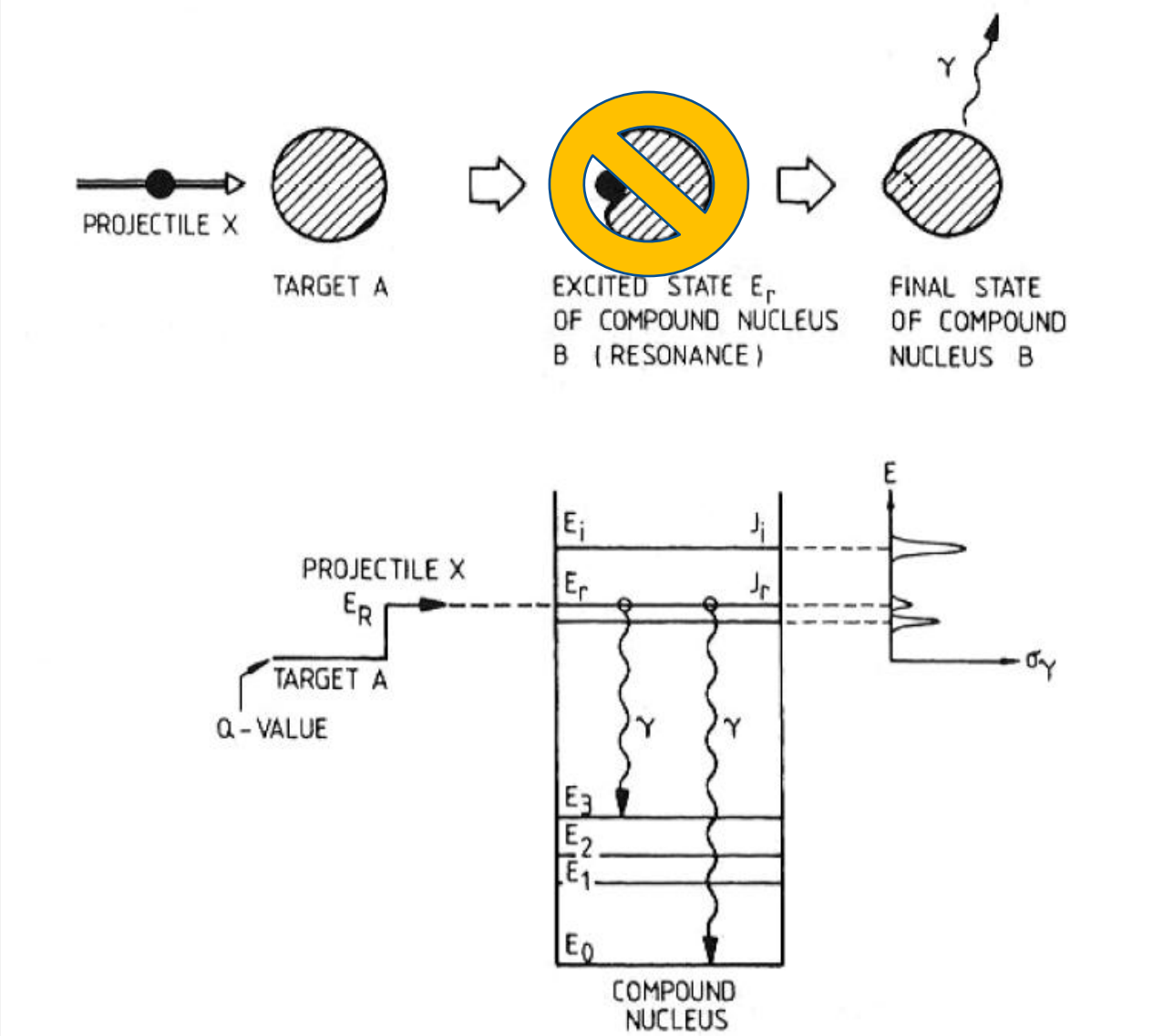
THE COMPOUND NUCLEUS

- A nuclear system that has intrinsic properties that **do not depend on how it was created**
  - Level energies, decay widths
- Dominates at low energies

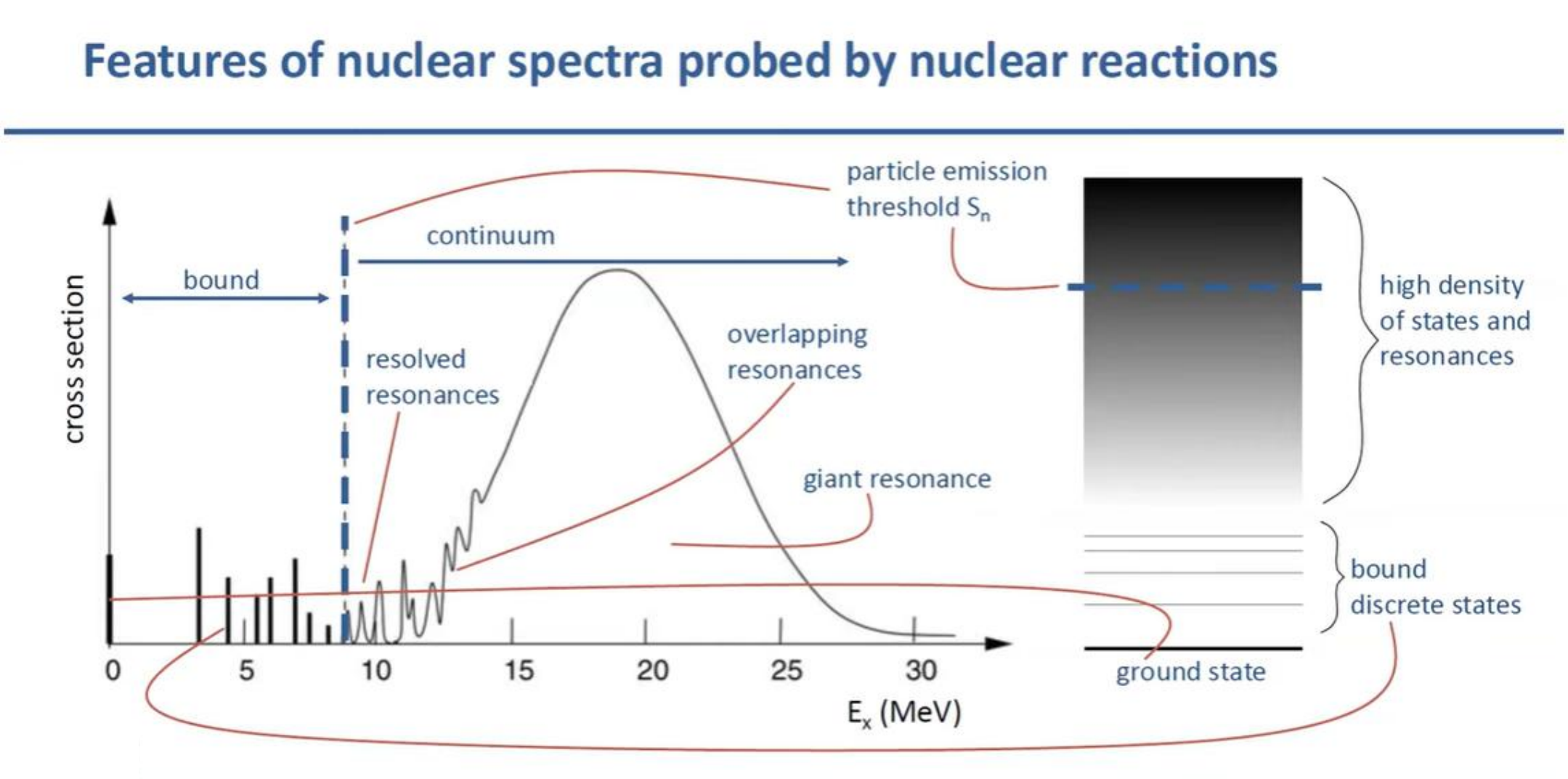


DIRECT REACTION

- No intermediate state
- Dominates at high energy

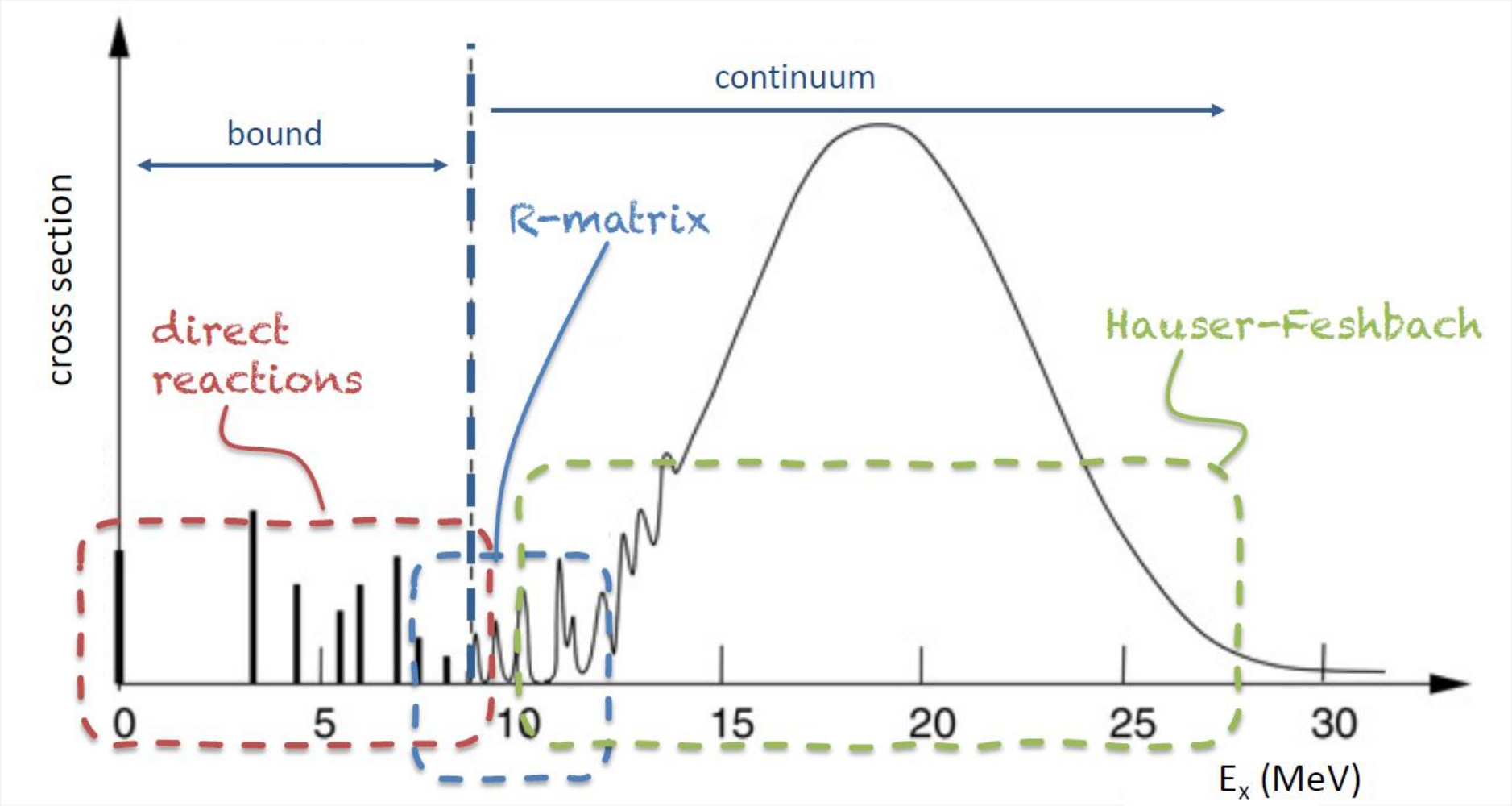


THE EVOLVING RESONANCE REGION



Shamelessly stolen from a lecture by Gregory Potel

DIFFERENT THEORIES FOR DIFFERENT ENERGY RANGES

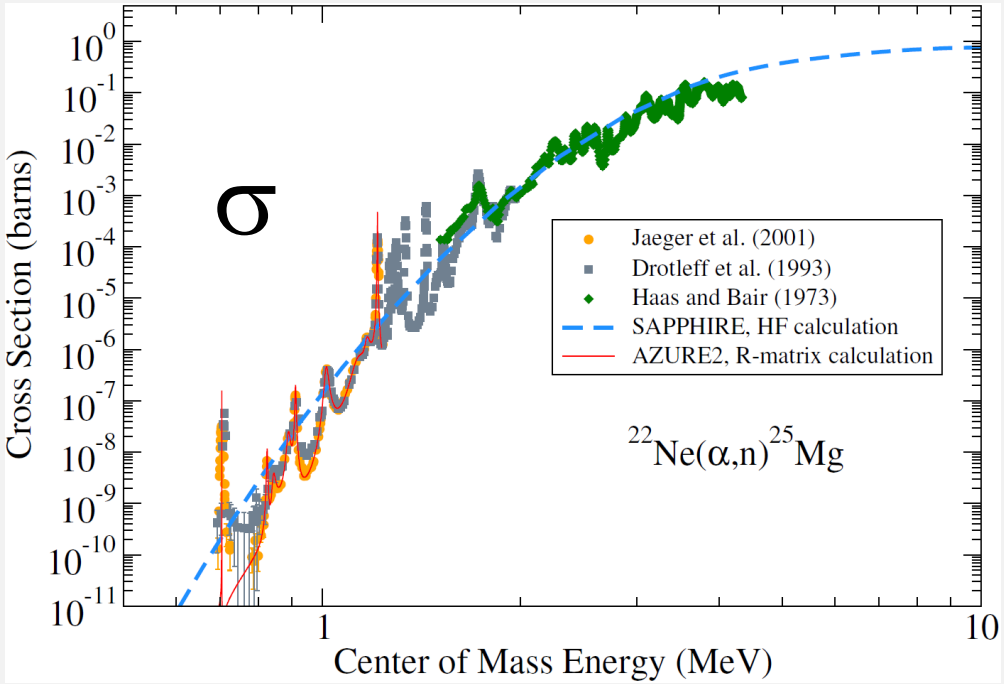


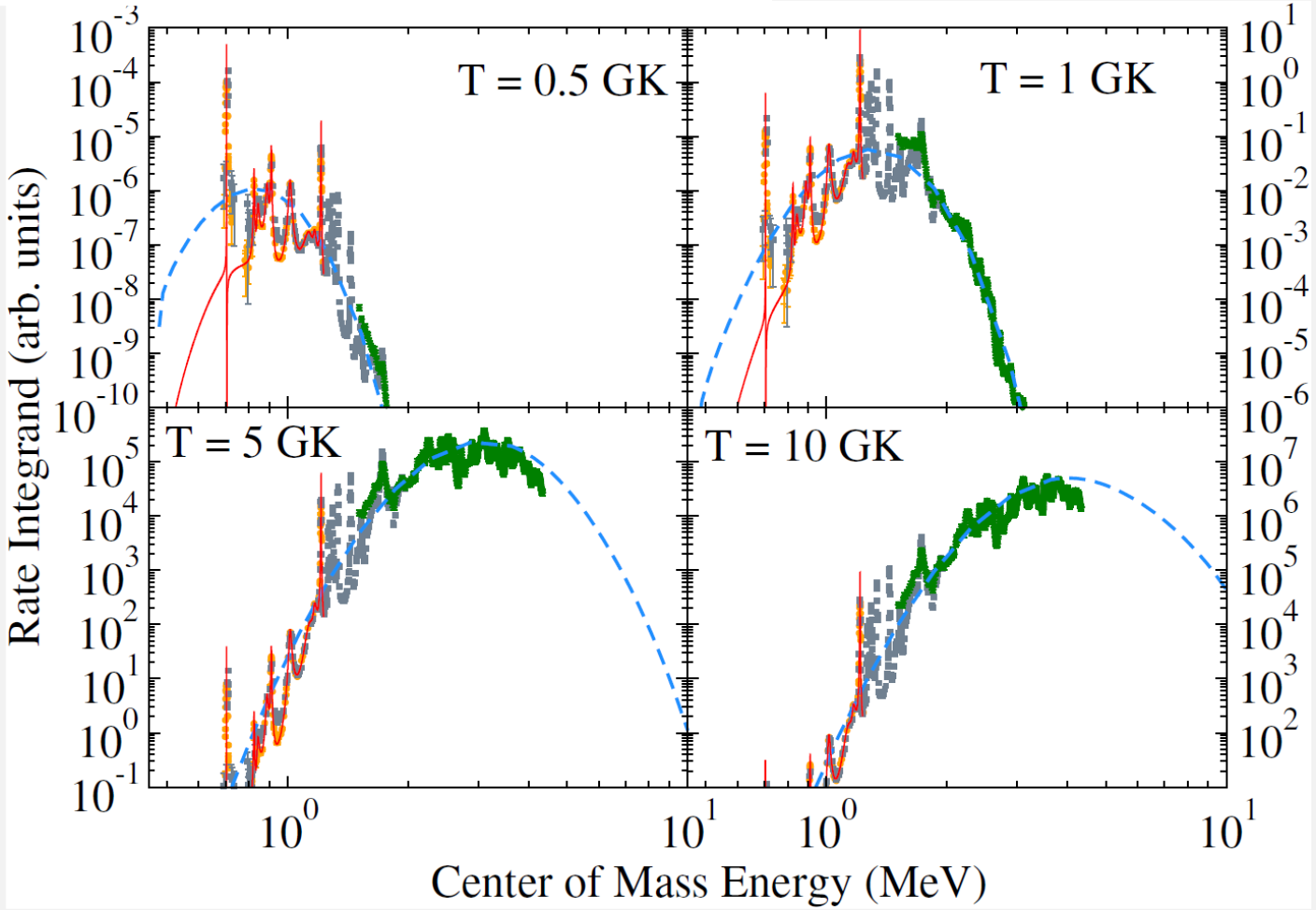
Shamelessly stolen from a lecture by Gregory Potel

NEAR THRESHOLD STATES ARE PARTICULARLY IMPORTANT FOR NUCLEAR ASTROPHYSICS

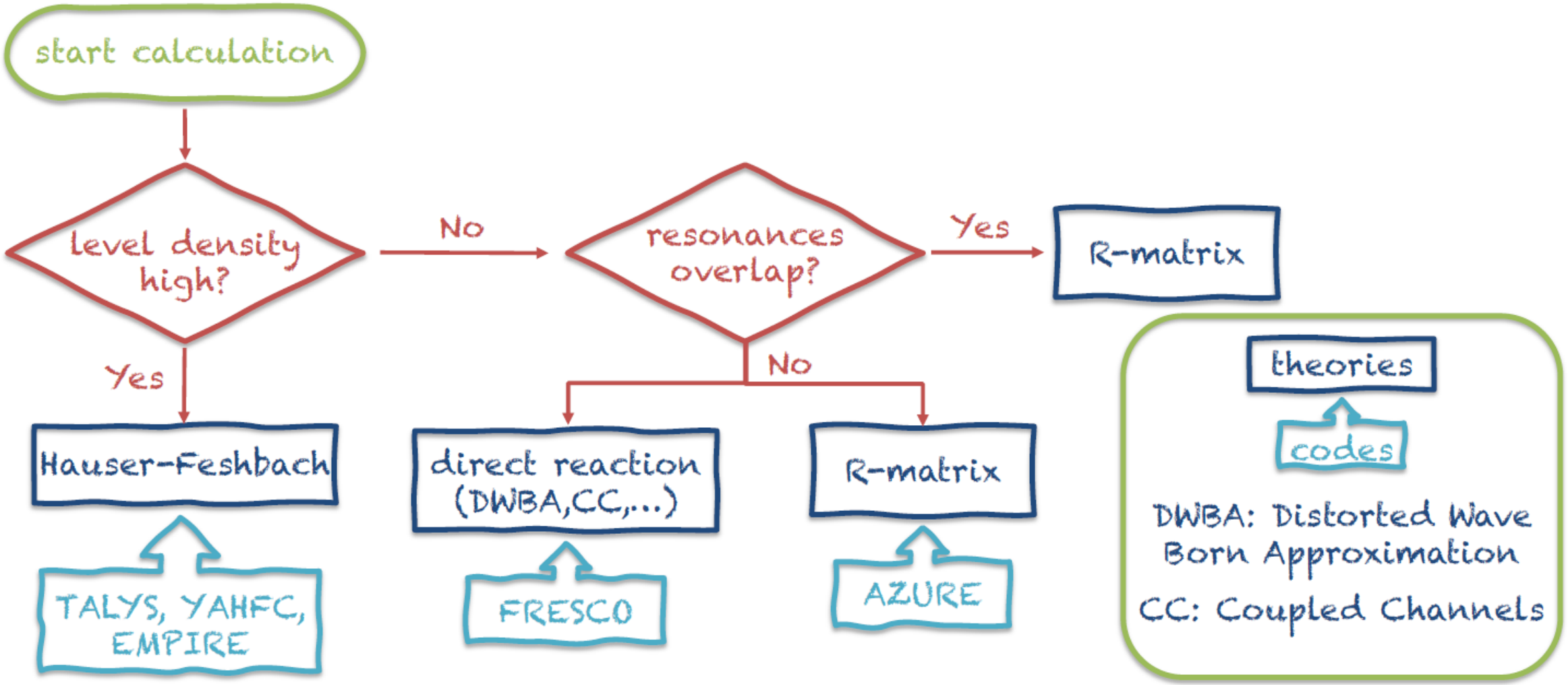
$$N_A\langle\sigma v\rangle = 3.7313 \times 10^{10} A^{-1/2} T_9^{-3/2} \int_0^\infty \sigma E \exp(-11.605E/T_9)\, dE,$$

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





Nuclear reaction theorist's roadmap



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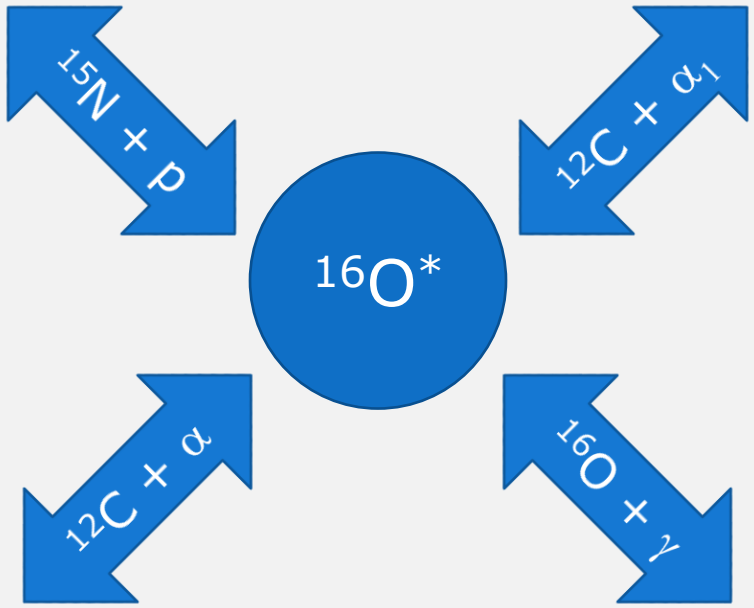
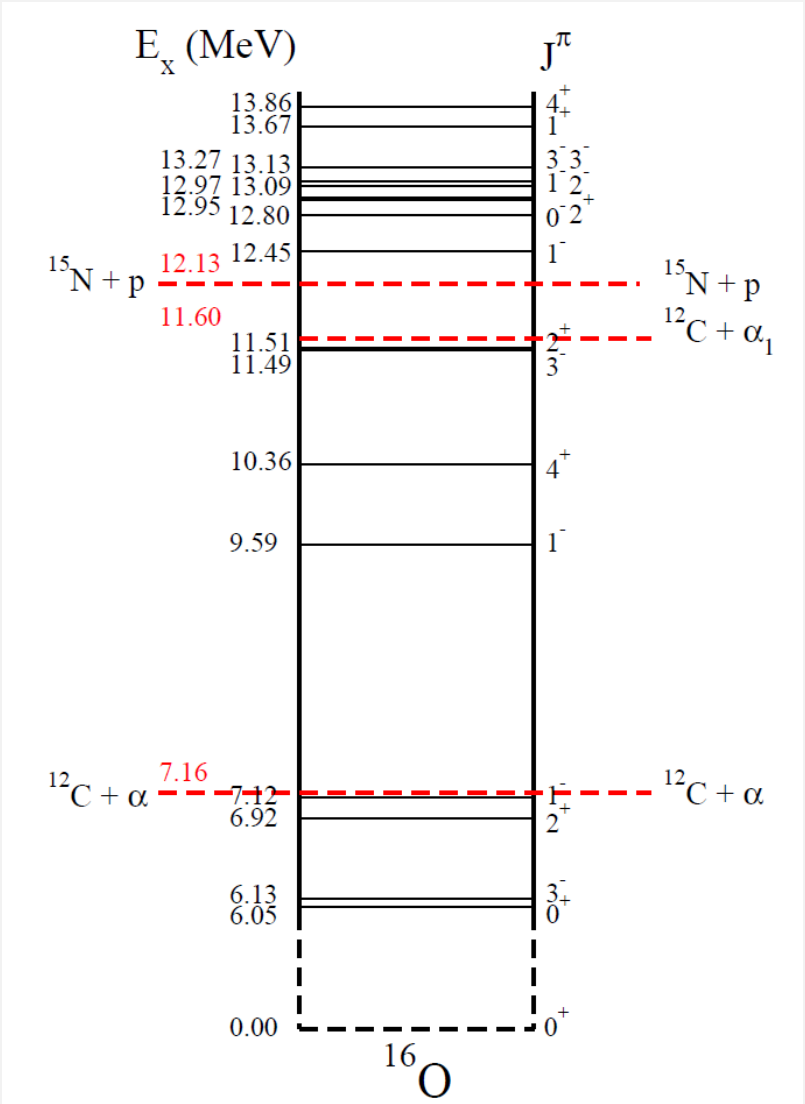
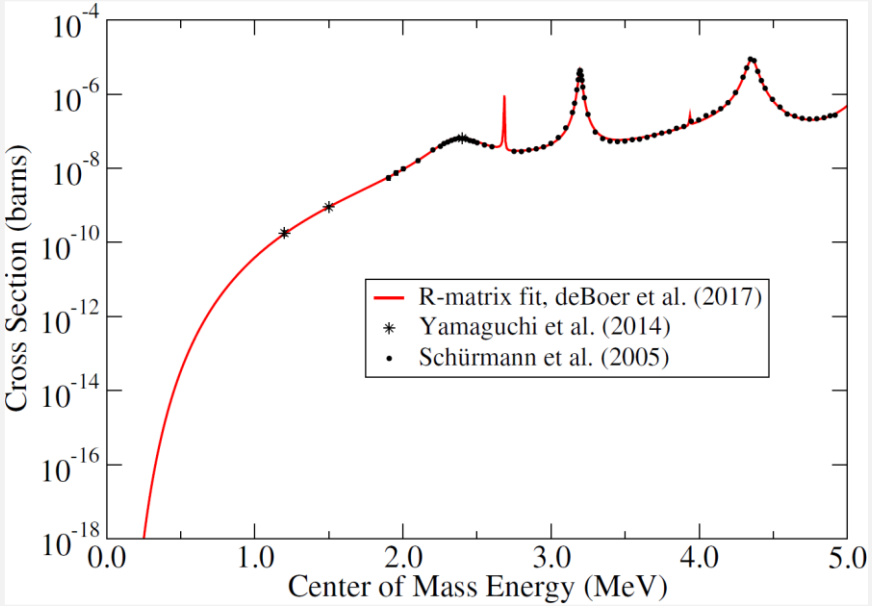
THE COMPOUND NUCLEUS HAS INTRINSIC PROPERTIES



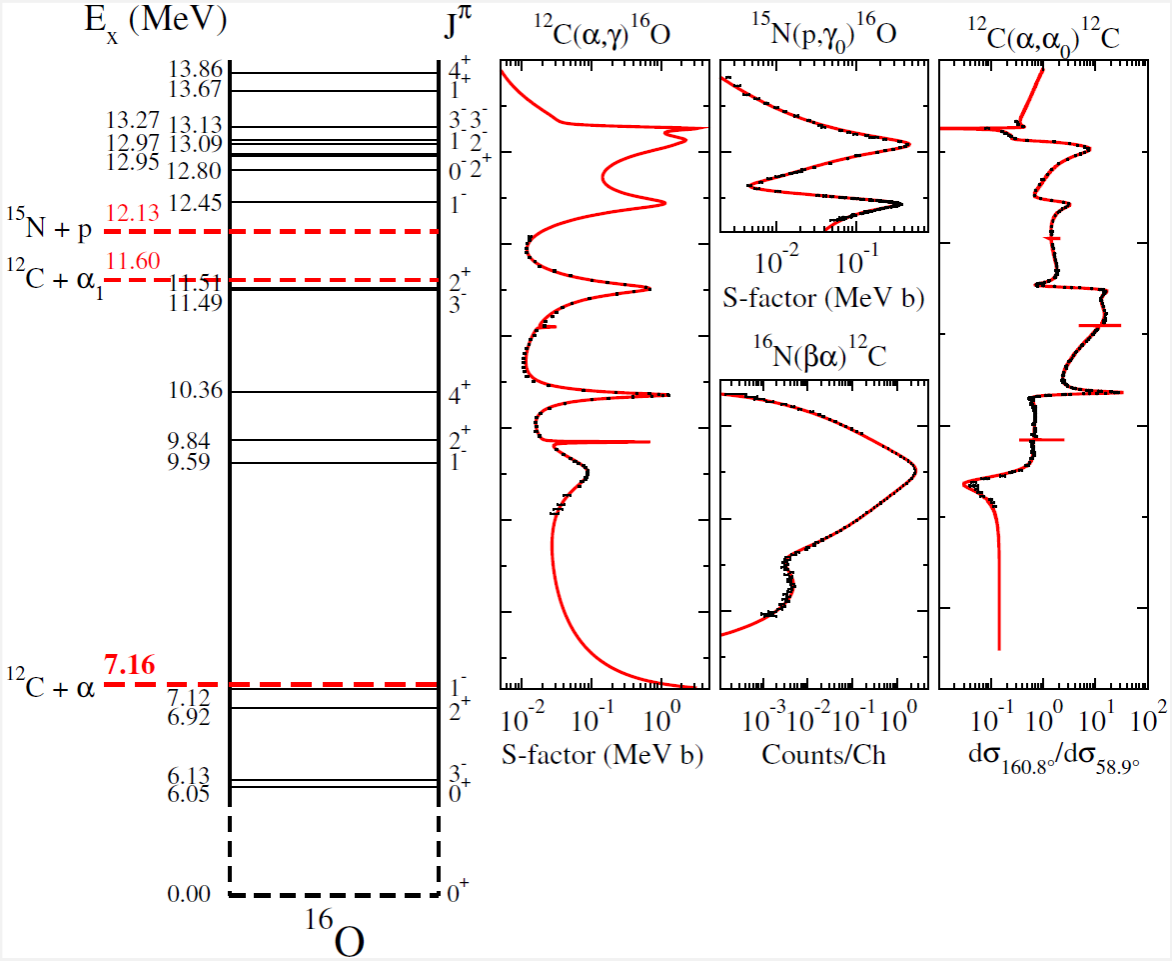


- Each level has a spin-parity (J^π), energy (E_x) and a set of partial decay widths (Γ_i)
- It doesn't matter what reaction is used to create the compound nucleus; these properties are always the same
- That means that we can use many different types of reactions to learn about the properties of a compound system
- It also means that any mathematical model must be self consistent when describing the cross section of the different reactions

CONNECTION BETWEEN THE ENERGIES OF REACTIONS AND THE LEVELS OF THE COMPOUND NUCLEUS



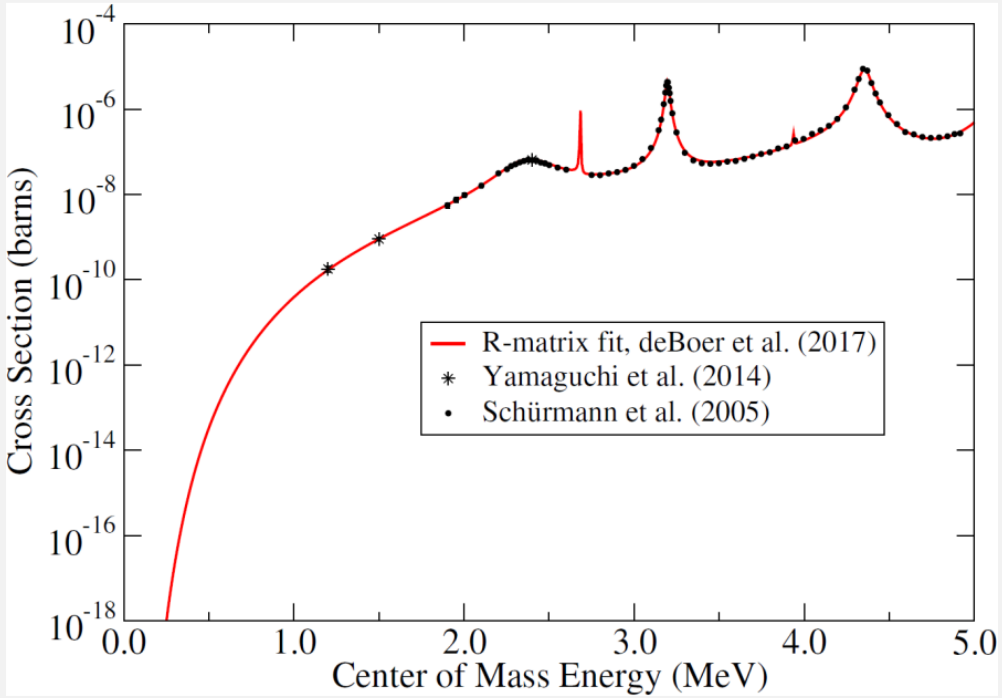
$E_x = E_{c.m.} + S_i$



$E_{c.m.} = E_{lab} \times M_H / (M_H + M_L)$
(when M_L is the beam particle)
M_l = mass of light particle
M_H = mass of heavy particle
E_{lab} = beam energy in the lab frame
$E_{c.m.}$ = energy in the center of mass frame

E_x = excitation energy
S_i = separation energy

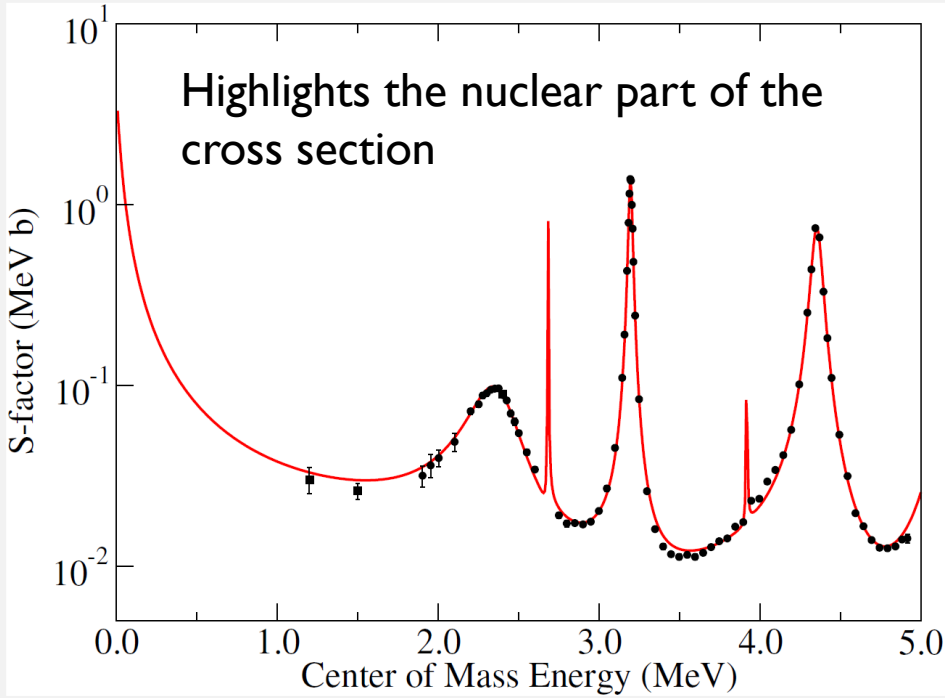
ASTROPHYSICAL S-FACTOR



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

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

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



SEPARATION ENERGIES

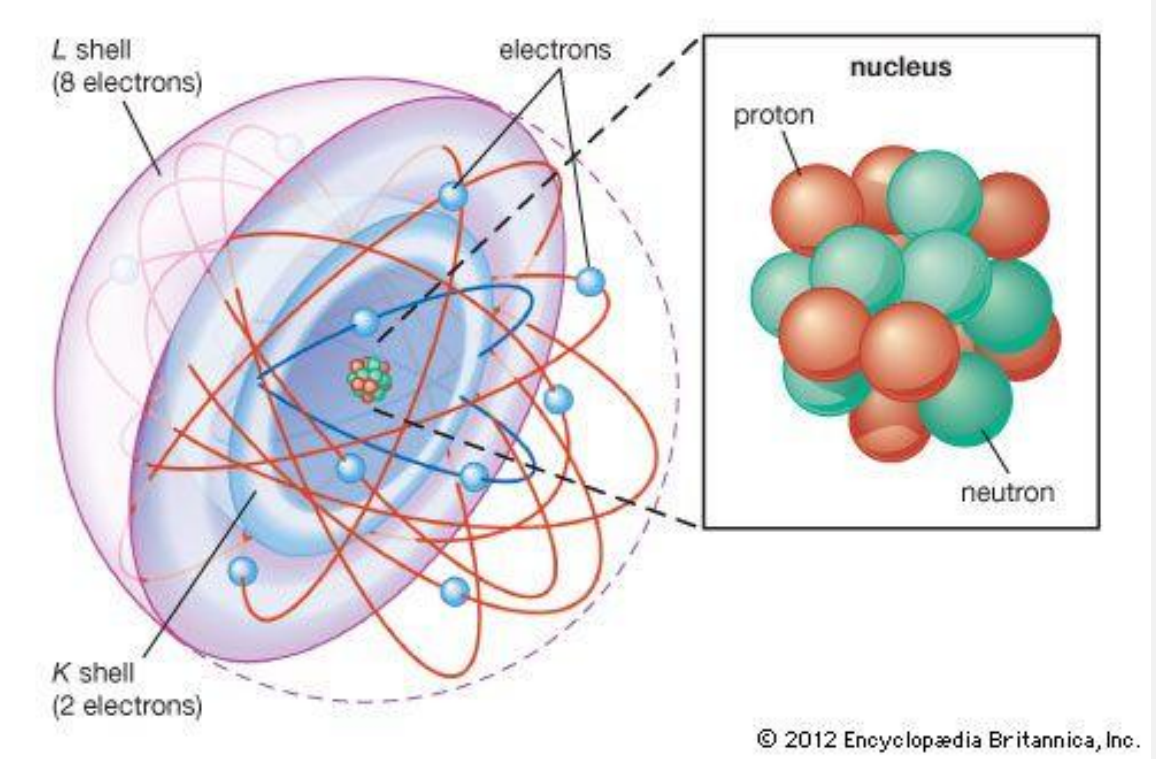
- How much energy it takes to pull a nucleus apart into smaller pieces
- Its just the difference in mass between the two individual particles and the compound nucleus
- Example: $^{12}C + \alpha$ separation energy in ^{16}O,
  - M(^{16}O) = 15.994914619257(319) amu
  - M(^{12}C) = 12 amu
  - M(^{4}He) = 4.002603254130(158) amu
  - 1 amu = 931.502 MeV/c^2
- [M(^{12}C) + M(^{4}He)] - M(^{16}O) = 7.16198 MeV

ITS HARD TO MODEL THE NUCLEAR POTENTIAL

- Many-body interactions are very hard to model
  - Essentially, if you have more than two interacting particles at the same time, the theory becomes extremely difficult
  - Modeling the nucleus is exactly this problem
  - Each nucleon in the nucleus interacts with the others simultaneously
- This is much different from, say, atomic physics, where the electrons are far from the nuclear core and their interactions can be treated independently (perturbatively)

Atomic interactions (long range)

Nuclear interactions (short range)



AB INITIO MODELS

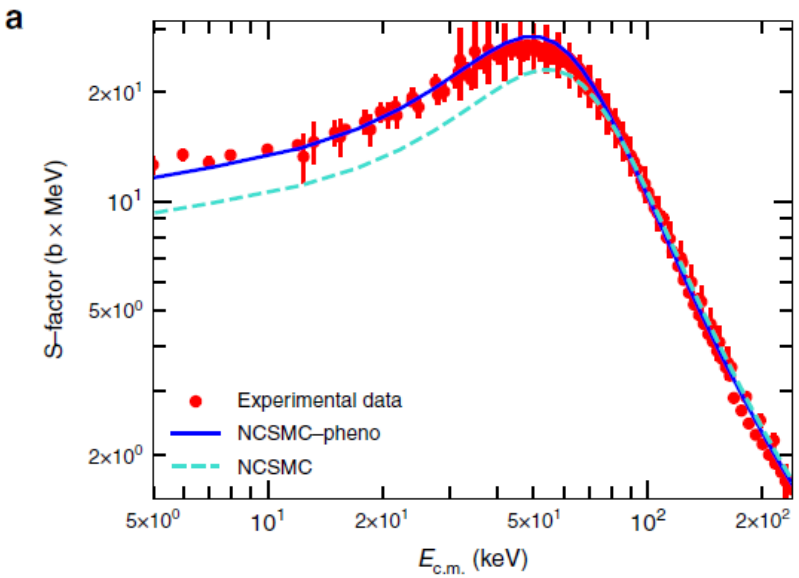
- Models that try to model nuclear interactions from as basic of a level as possible
  - Quantum chromodynamics (QCD) (quarks and gluons) --- not yet
  - Nucleon-nucleon interactions, with the many-body problem solved numerically up to some controlled approximation
  - Its always improving and that is part of the definition of it.
  - Examples for light mass reactions: Faddeev-Yakubovsky, hyperspherical harmonics, no-core shell model and quantum Monte Carlo lead to “exact” solutions to the many-body Schrödinger equation

EXAMPLE: d(t,n)^{3}He

Hupin *et al.*, Nature Communications (2019), https://doi.org/10.1038/s41467-018-08052-6

Ab initio no-core shell model with continuum to solve the five nucleon problem and chiral effective field theory to make approximations that streamline the computations

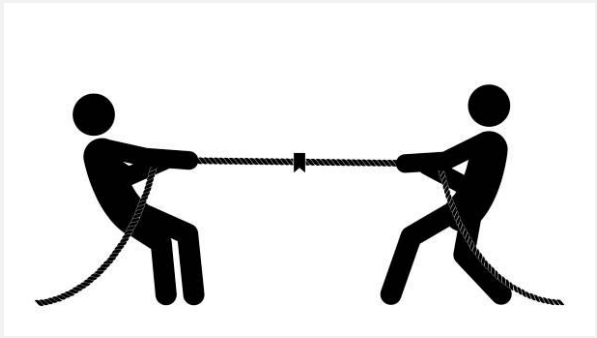
A small phenomenological correction still had to be applied to the resonance energy



WHY PHENOMENOLOGICAL MODELS?

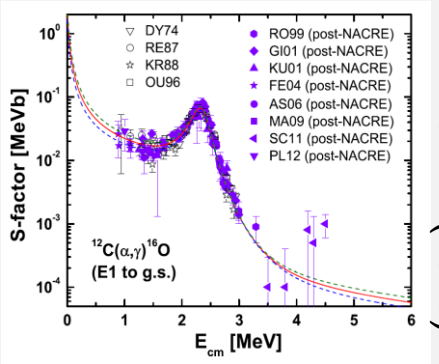
- We want to use nuclear cross sections as inputs for other applications
  - Nuclear astrophysics --- modeling energy production and nucleosynthesis in stellar environments
  - Applied physics --- modeling nuclear reactors, nuclear fuel storage and nuclear weapons
- We need a model that is flexible enough that it can both **very accurately** describe data but have enough **physical constraint** so that it can be used for extrapolation to unmeasured regions

match experimental data

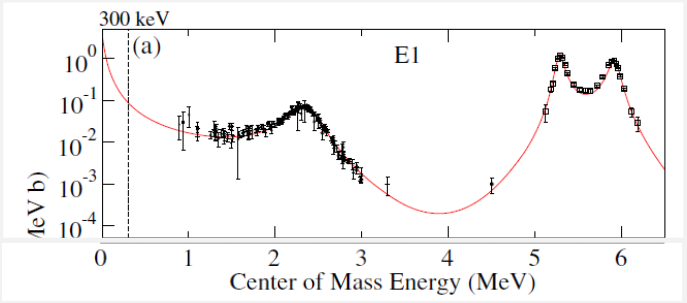


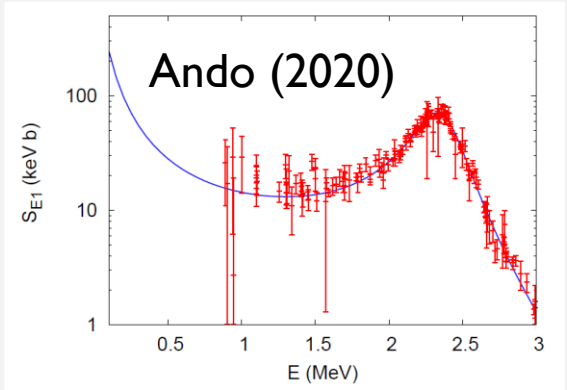
fundamental physics constraint

EXAMPLE PHENOMENOLOGICAL MODELS



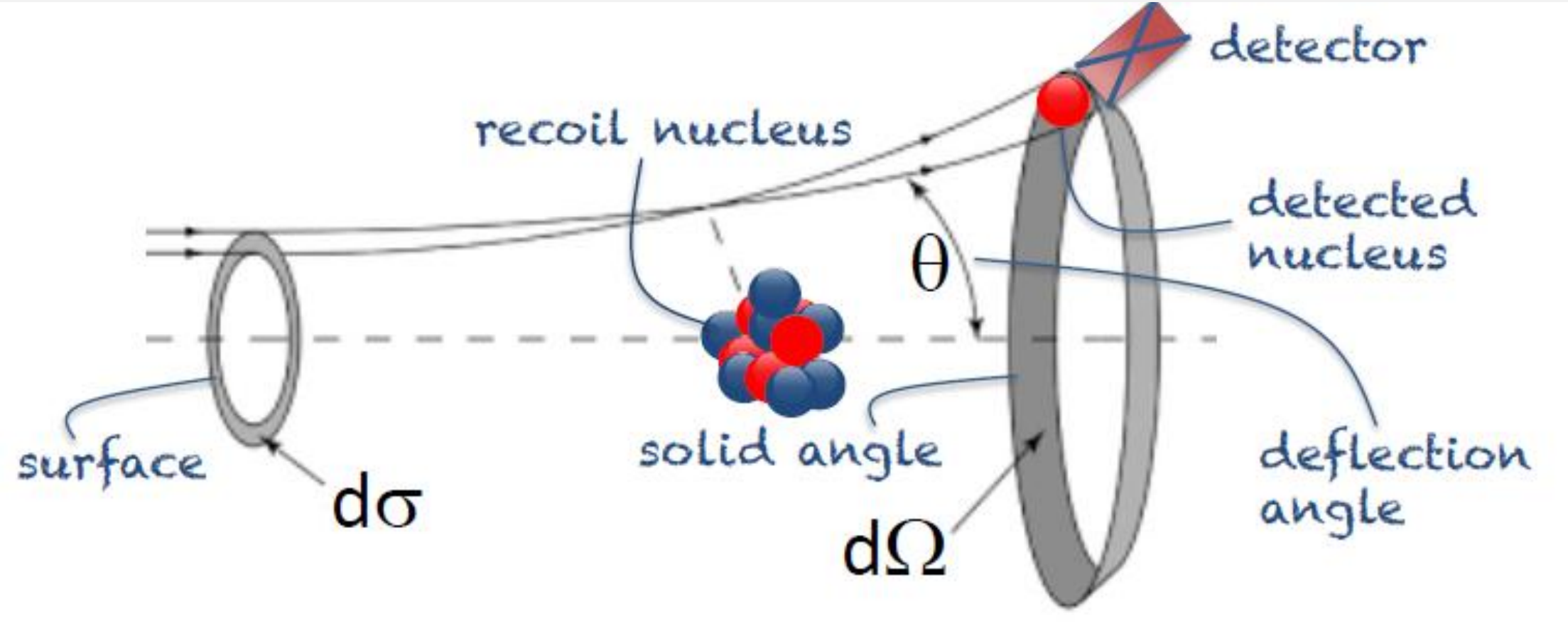
NACRE2 (2013)





- Potential models
  - Different (simple) functional forms for the potential are used
  - Often uses a Coulomb part plus Woods-Saxon potential and a surface absorption term
  - **Reproduces many resonances and direct part of the cross section directly from the potential**
  - **Additional resonances may have to be added ad hoc using individual Breit-Wigner functions**
  - **If an absorption term is used, it doesn't conserve unitarity. Usually just fits one reaction at a time.**
  - Tunable parameters: potential strengths (V_i), radii (r_i) and diffuseness (a_i) and possibly BR parameters as well
- R-matrix models
  - No specific potential is defined
  - **Allows for maximum flexibility to fit data**
  - **In the ideal case, all channels are modeled data from each is fit and unitarity is conserved**
  - **All resonances are added ad hoc**
  - **Resonance interference is accurately modeled**
  - **Background terms need to be included to model direct reaction part**
  - Each resonance has a tunable energy (E), reduced width amplitude (γ_i) and each channel has a radius parameter (a_c)
- Effective field theory
  - Derived as an expansion of momentum, where the momentum is small compared to the binding energies of the interacting particles
  - **Model accuracy (uncertainty) in the calculation can be estimated from the number of terms used in the expansion**
  - Fit parameters are the effective range parameters (ERP). **Some of these ERPs, can be related to fit parameters of other theories, such as level energies and asymptotic normalization coefficients (ANCs)**
  - **Still under development**

GOAL: SOLVE THE NUCLEAR SCATTERING PROBLEM



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"STANDARD SCATTERING THEORY"

Cross section and Schrödinger equation in 3D

the partial wave components $\phi_l(r)$ of the 3D wavefunction $\phi(\mathbf{r})$ satisfy a 1D Schrödinger equation:

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r) - E\right)\phi(\mathbf{r}) = 0; \qquad \phi_m(\mathbf{r}) = \sum_\ell \phi_\ell(r)\, Y_m^\ell(\hat{r}),$$

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + V(r) - E\right)\phi_\ell(r) = 0$$

if $V(r)$ has a short range (such as the nuclear interaction), it can be shown that:

scattering amplitude

deflection angle

solution for V(r)=0

$$\phi(\mathbf{r}) = \phi_0(\mathbf{r}) + \frac{e^{ikr}}{r} f(\theta); \qquad (r \to \infty)$$

cross section

$$\frac{d\sigma(\theta)}{d\Omega} = |f(\theta)|^2$$

Legendre polynomial

$$f(\theta) = -\frac{i}{2k}\sum_\ell (2\ell+1)(e^{2i\delta_\ell} - 1)P_\ell(\cos\theta)$$

phase shift

equivalent goal: obtain either
1. phase shifts, or
2. scattering amplitude

to get cross section

- **R-matrix, DWBA, whatever, this is the problem we are trying to solve**
- **The difference is how we handle V(r)**

Shamelessly stolen from a talk by Gregory Potel

THE GENERAL ABSTRACT SOLUTION

Review of the integral equation solution

Start with the time-independent Schrödinger equation

$$E\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

we rewrite it using the substitutions

$$Q = \left(\nabla^2 + k^2\right)\psi$$

$$k \equiv \frac{\sqrt{2mE}}{\hbar}, \quad Q \equiv \frac{2m}{\hbar^2}V\psi$$

this can be solved for an abitrary driving function ($Q \propto V\psi$) by solving for the Green's function, $G(\vec{r})$, which is the solution for a delta function source then the solution to the actual source, Q, becomes

$$\delta^3(\vec{r}) = \left(\nabla^2 + k^2\right) G(\vec{r})$$

$$\psi(\vec{r}) = \int G(\vec{r} - \vec{r}_0)\, Q(\vec{r}_0)\, d^3\vec{r}_0$$

the Green's function solution can be expressed as a Fourier transfom

$$G(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\vec{s}\cdot\vec{r}} g(\vec{s})\, d^3\vec{s}$$

the solution is obtained by using Cauchy's formula and contour integration

$$G(\vec{r}) = \frac{1}{(2\pi)^3} \int e^{i\vec{s}\cdot\vec{r}} \frac{1}{(k^2 - s^2)}\, d^3\vec{s} = -\frac{e^{ikr}}{4\pi r}$$

THE GENERAL ABSTRACT SOLUTION

General solution

The solution just obtained is not unique as it is possible to prove that the general solution is $G'(\vec{r}) = G(\vec{r}) + G_0(\vec{r})$, where $G_0(\vec{r})$ is any solution to the homogeneous Helmholtz equation

$$(\nabla^2 + k^2) G_0(\vec{r}) = 0$$

the general solution to the Schrödinger equation is thus

$$\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{m}{2\pi\hbar^2} \int \frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|} V(\vec{r}_0)\psi(\vec{r}_0)\, d\vec{r}_0$$

- **No matter the assumptions, we can start with a general solution based on Green's function method**

with $\psi_0(\vec{r})$ being the solution of the free particle Schrödinger equation

$$(\nabla^2 + k^2)\, \psi_0(\vec{r}) = 0$$

note that the wave function appears on both sides of this equation, requiring prior knowledge of the wave function to obtain an exact solution!

however, it is possible to use the integral equation for an approximation method called the Born approximation

DIFFERENT ASSUMPTIONS FOR DIFFERENT PROBLEMS

- Compound nucleus, R-matrix
  - There are a complete set of **orthonormal internal wave functions**, which can be associated with **intermediate states in the compound nucleus**
  - Incoming plane waves, outgoing spherical waves
  - Limited by truncation of infinite expansions: momentum, levels, channels

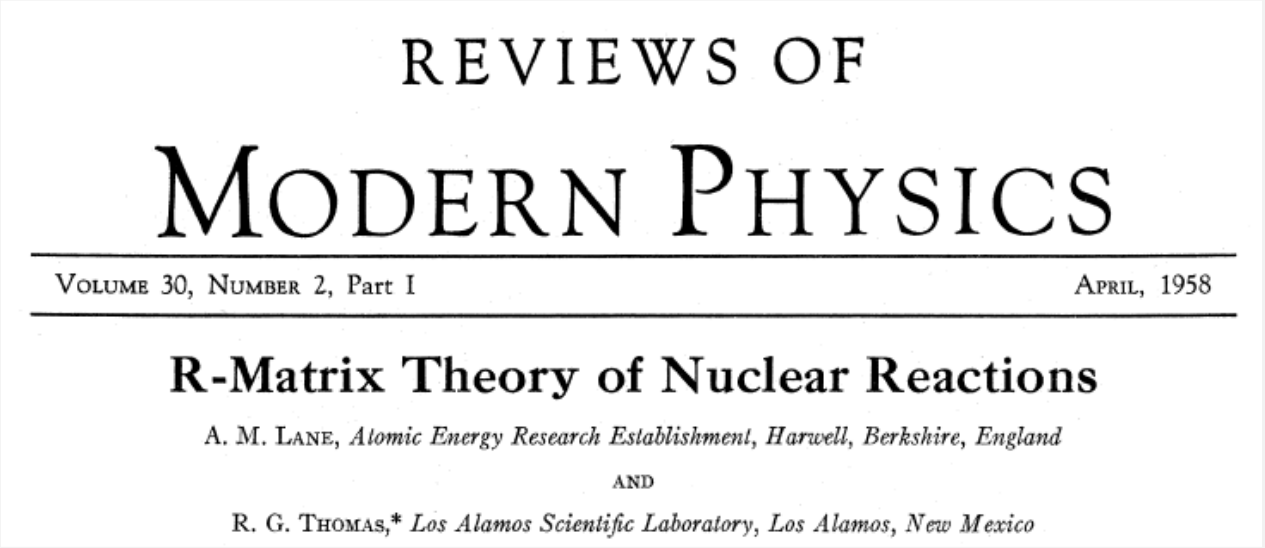
- Direct reactions, Distorted wave born approximation
  - The scattering is weak, incoming plane wave is **not significantly altered by the potential**
  - Incoming plane waves, outgoing plane waves

PHENOMENOLOGICAL R-MATRIX

- Includes "fundamental" quantum mechanics information

Descouvemont and Baye (2010)

deBoer *et al.* (2017), R-matrix theory section by Carl Brune



REVIEWS OF

MODERN PHYSICS

VOLUME 30, NUMBER 2, Part I — APRIL, 1958

R-Matrix Theory of Nuclear Reactions

A. M. LANE, *Atomic Energy Research Establishment, Harwell, Berkshire, England*

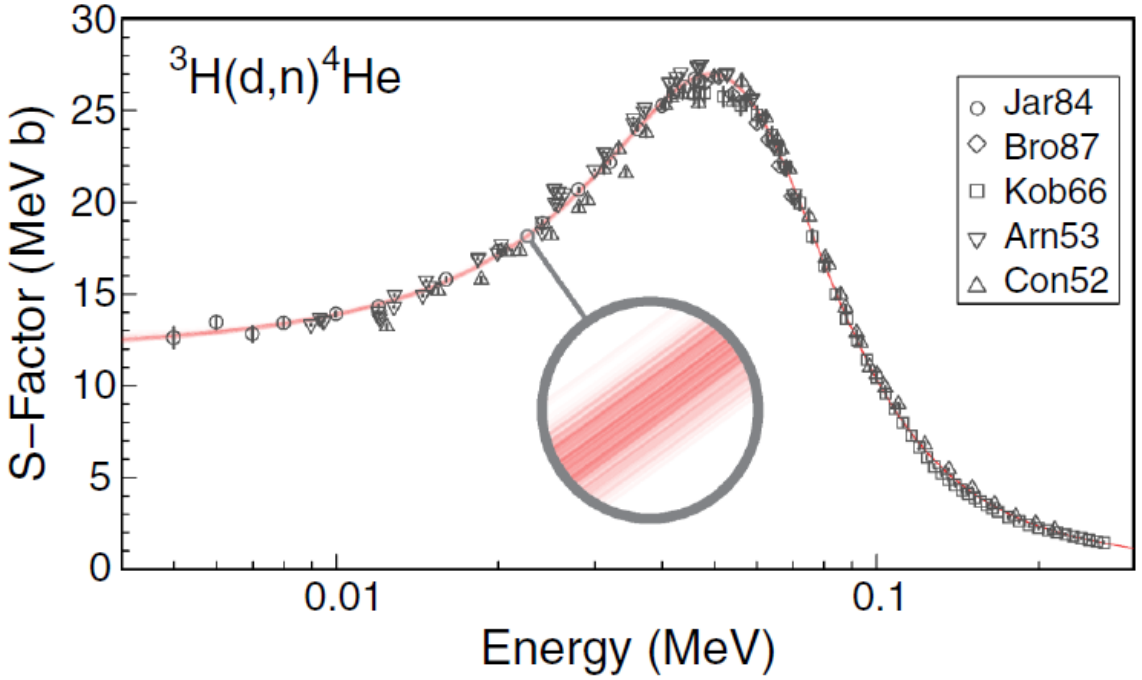
AND

R. G. THOMAS,* *Los Alamos Scientific Laboratory, Los Alamos, New Mexico*

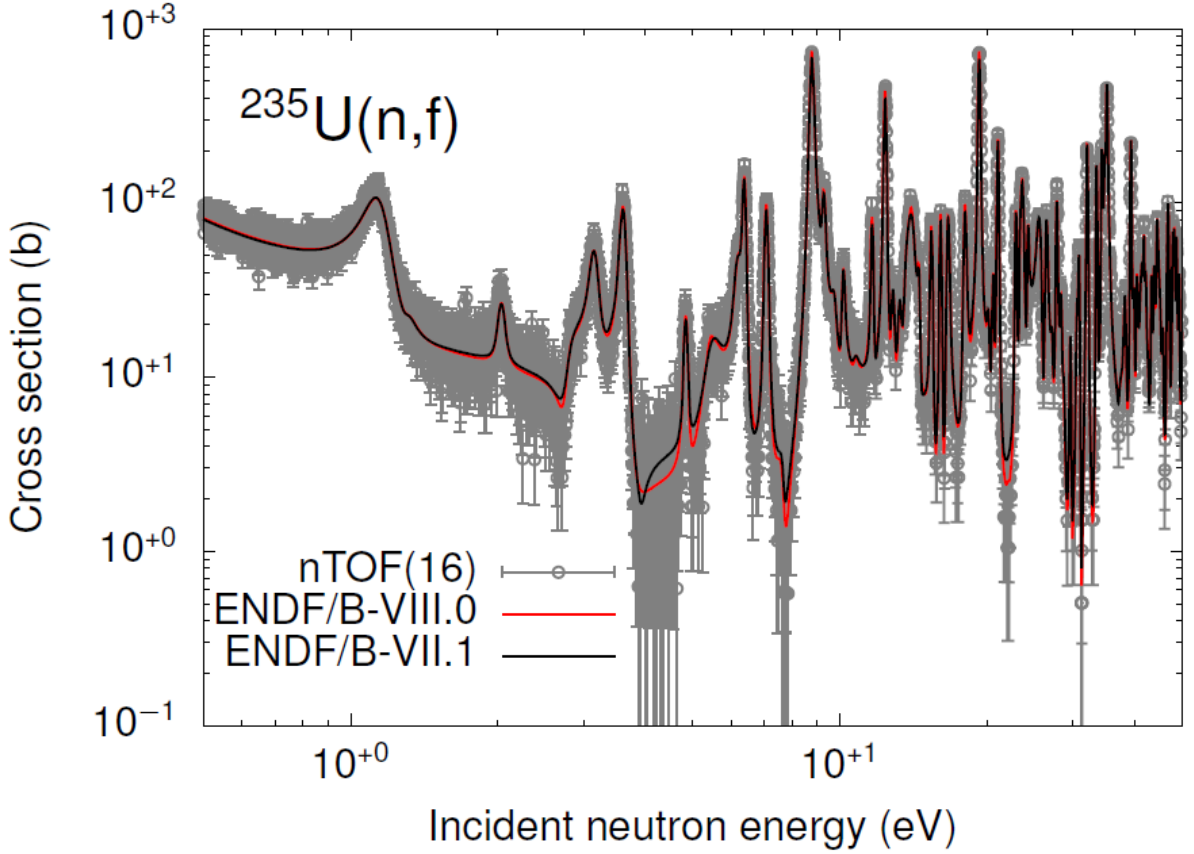
R-matrix bible

What is R-matrix used for?

- It's a **nuclear reaction theory framework**, primarily suited for resonance dominated cross sections
  - That usually means, low energy nuclear reactions, but can extend high up in mass
- Parameterize and evaluate nuclear data to determine cross sections



de Souza *et al.* (2024)



Brown *et al.* (2018), ENDF/B VIII.0

What is it used to for?

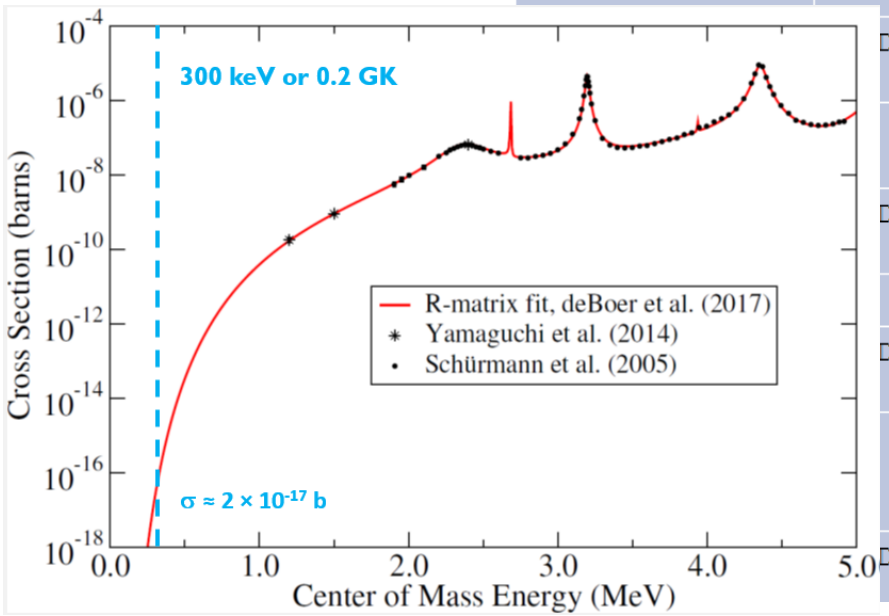
- Nuclear resonance parameters
  - Nuclear structure
- Evaluated cross sections
  - ENDF/B
  - Nuclear reaction particle transport codes (e.g. scale, GEANT4, MCNP, etc.)
- Extrapolate cross sections to near-threshold values
  - Stellar reaction rates

MCNP® MONTE CARLO N-PARTICLE

scale

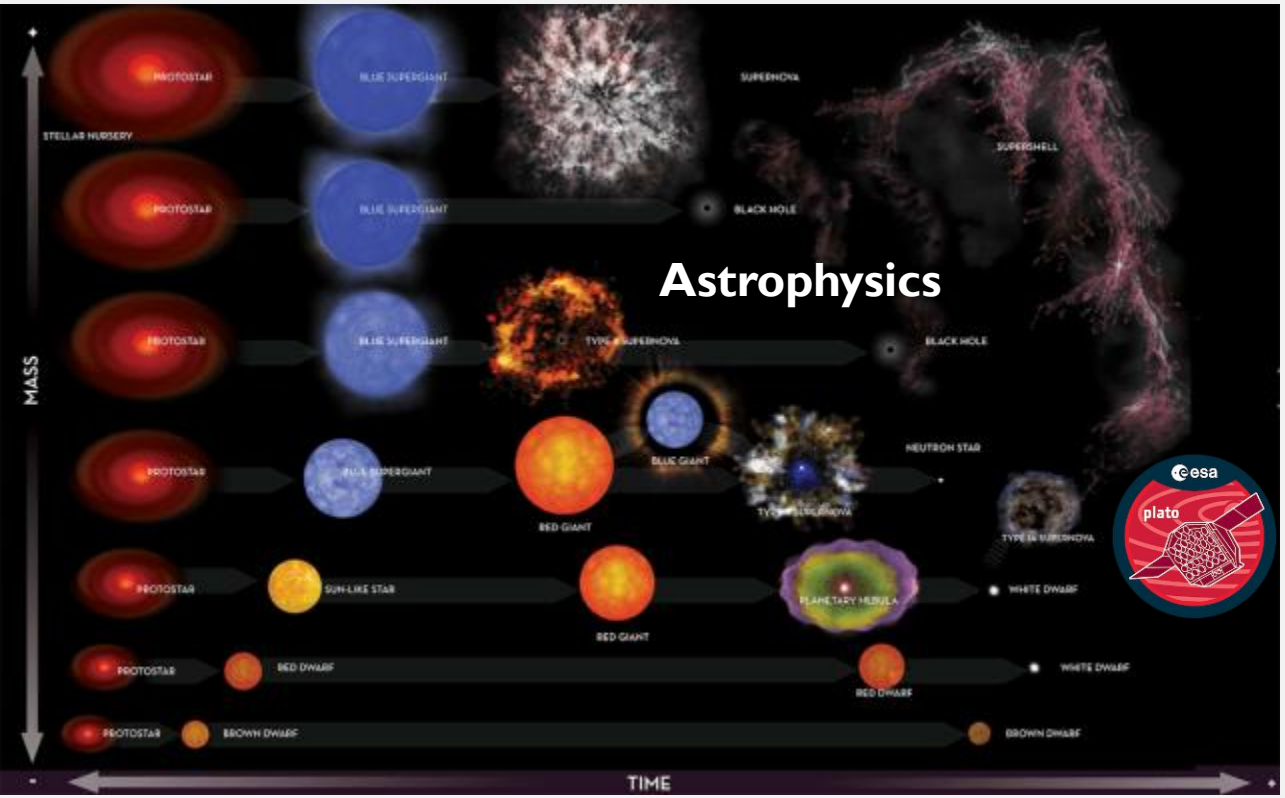
GEANT4 A SIMULATION TOOLKIT

E_{level} (keV)	XREF	Jπ	$T_{1/2}$
0.0	A DE GHIJKLM	1/2-	9.965 m *4* % ε = 100
2364.9 *6*	DEFGHI K	1/2+	31.7 keV *8* % IT = 0.00158 *13* % p = 100
3502 *2*	A DEFGHIJK	3/2-	62 keV *4* % IT = 0.0011 % p = 100
3547 *4*	D FGHI K	5/2+	47 keV *7* % p = 100 % IT < 4.3E-6
6364 *9*	CD FGH KL	5/2+	11 keV % p = 100
6886 *8*	CD FGH K	3/2+	115 keV *5* % p = 100
7155 *5*	CD FGH K	7/2+	9.0 keV *5* % p = 100
	D FGHIJKL	5/2-	75 keV *5* % p = 100
	FG	3/2+	≈ 1500 keV % p = 100
	D FG IJ L	1/2-	230 keV % p = 100
	GH J	9/2+	280 keV *30*
	D FGH J	3/2-	30 keV % p = 100
	E	(1/2+)	≈ 280 keV % IT = ? % p = ?
	D FGH	5/2-	

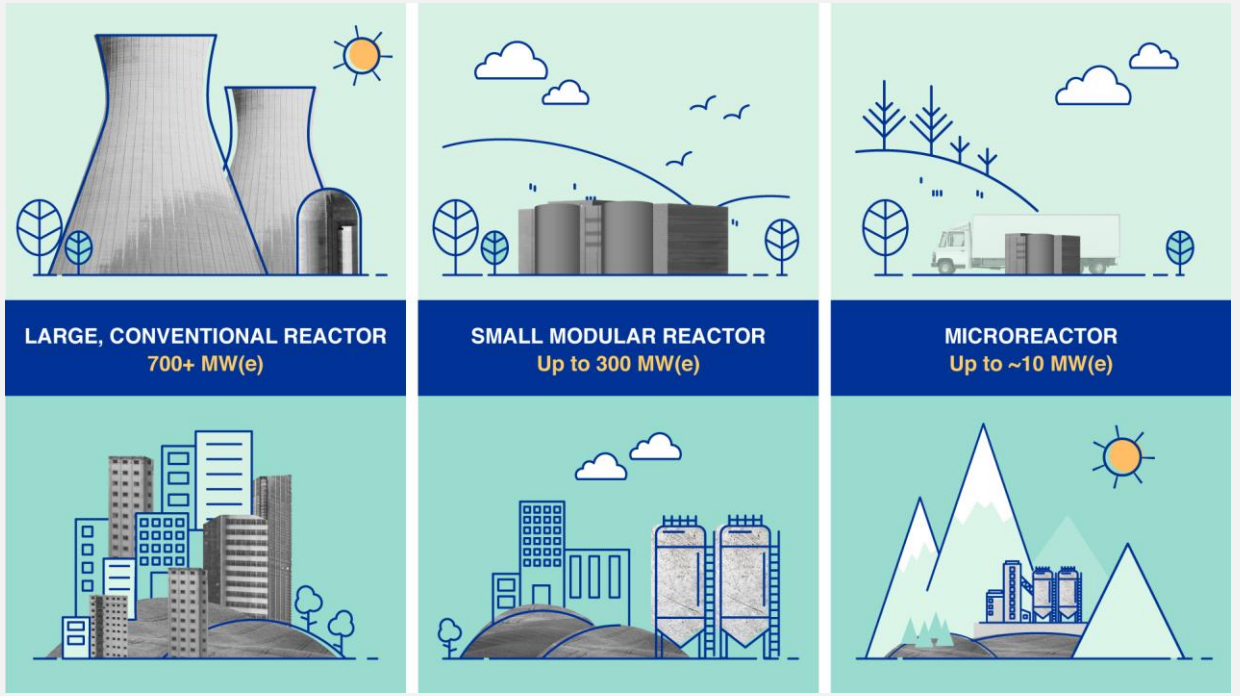


NNDC.BNL.GOV

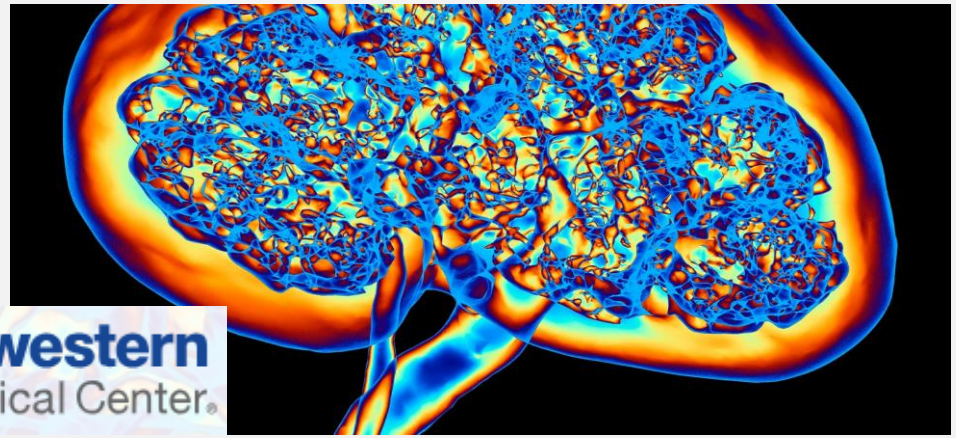
NUCLEAR DATA END USES



Nuclear Energy



Nuclear Medicine



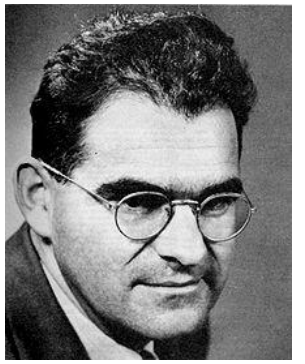
UT Southwestern Medical Center

IAEA
International Atomic Energy Agency
Atoms for Peace and Development

Nuclear Safeguards

A bit of history

- Very early nuclear theory was constructed in an *ad hoc* fashion with the assumption that the reactions proceeded by the compound nucleus mechanism first described by Bohr and Bethe around 1937
  - The only theory at that time that seemed relevant was Weisskopf and Wigner's theory for **an atomic system**
  - In 1938 Kapur and Peierls developed a rigorous nuclear theory (perturbation theory) that **did not depend on an assumed underlying reaction mechanism**
  - It can be easily associated with the **compound nucleus** theory if states that are far away in energy are ignored
- In the 1940's Wigner and Eisenbud then reworked Kapur and Peierls theory to make the energy dependence of different quantities more explicit, and this became R-matrix theory.
- In 1958 Lane and Thomas wrote the "bible" of R-matrix theory by pulling together all of this previous work. This is largely what is still used today.

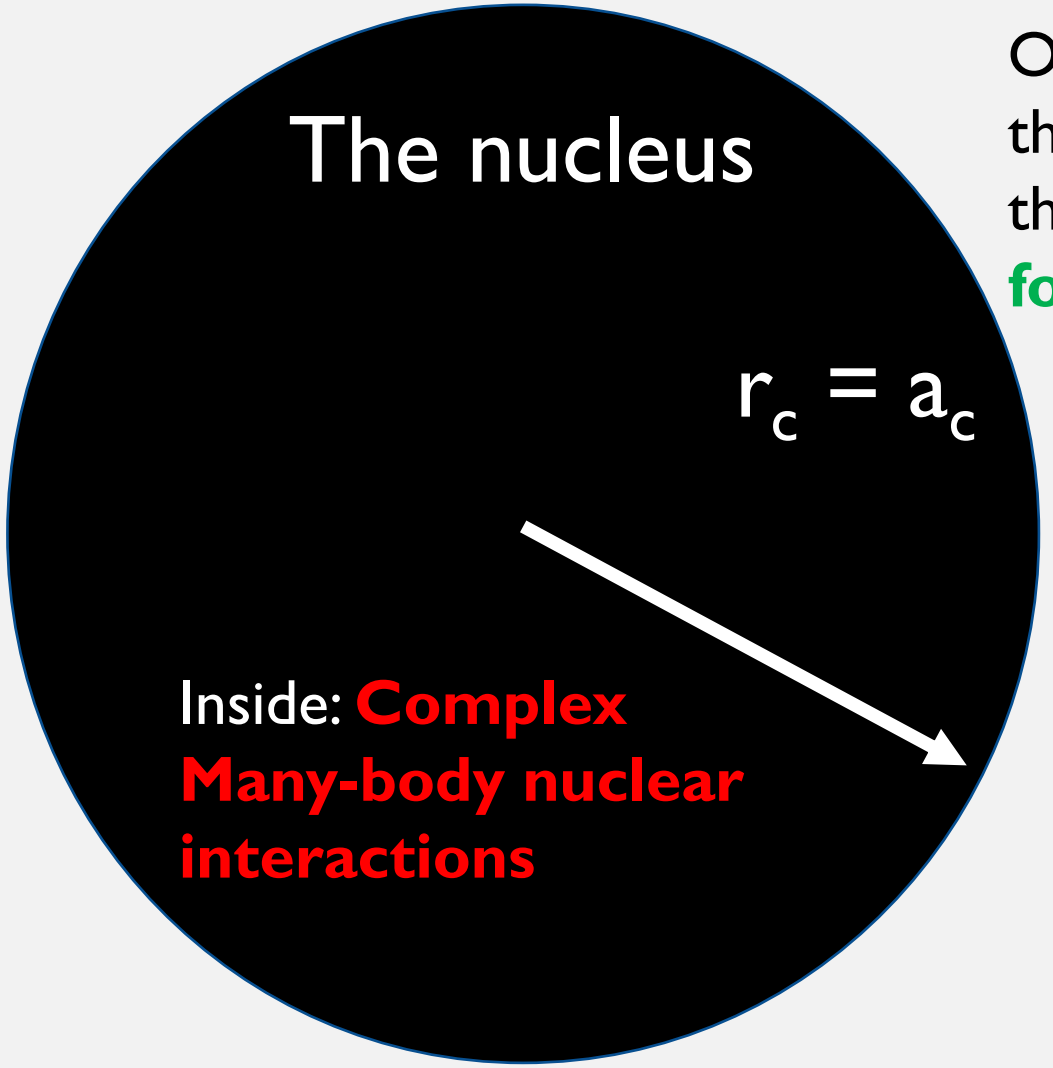


Weisskopf

Wigner

Peierls

CLASSIC BOUNDARY VALUE PROBLEM



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

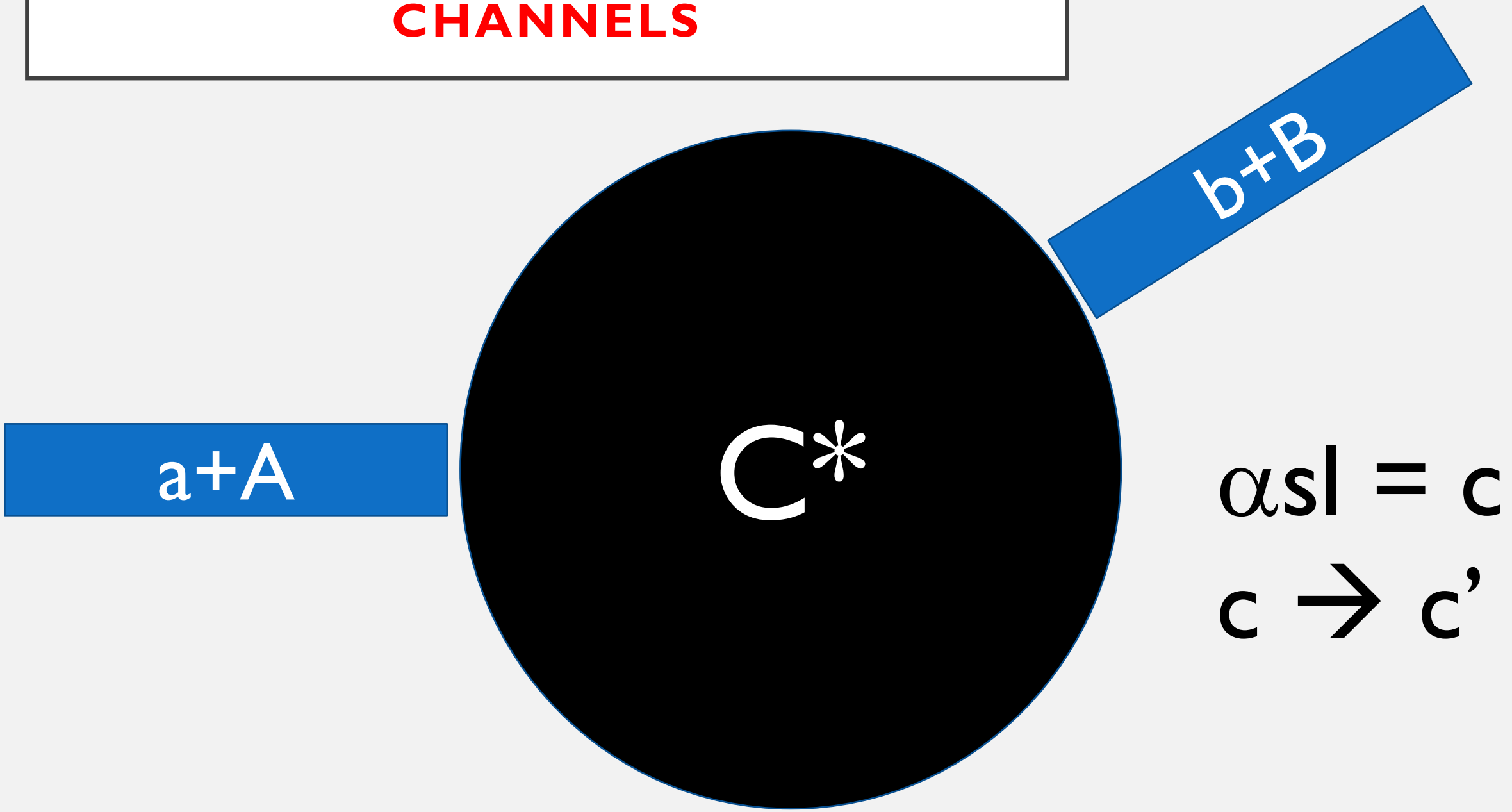
At $r_c > a_c$

$V = V_{Coulomb}$

At $r_c < a_c$

$V = V_?$

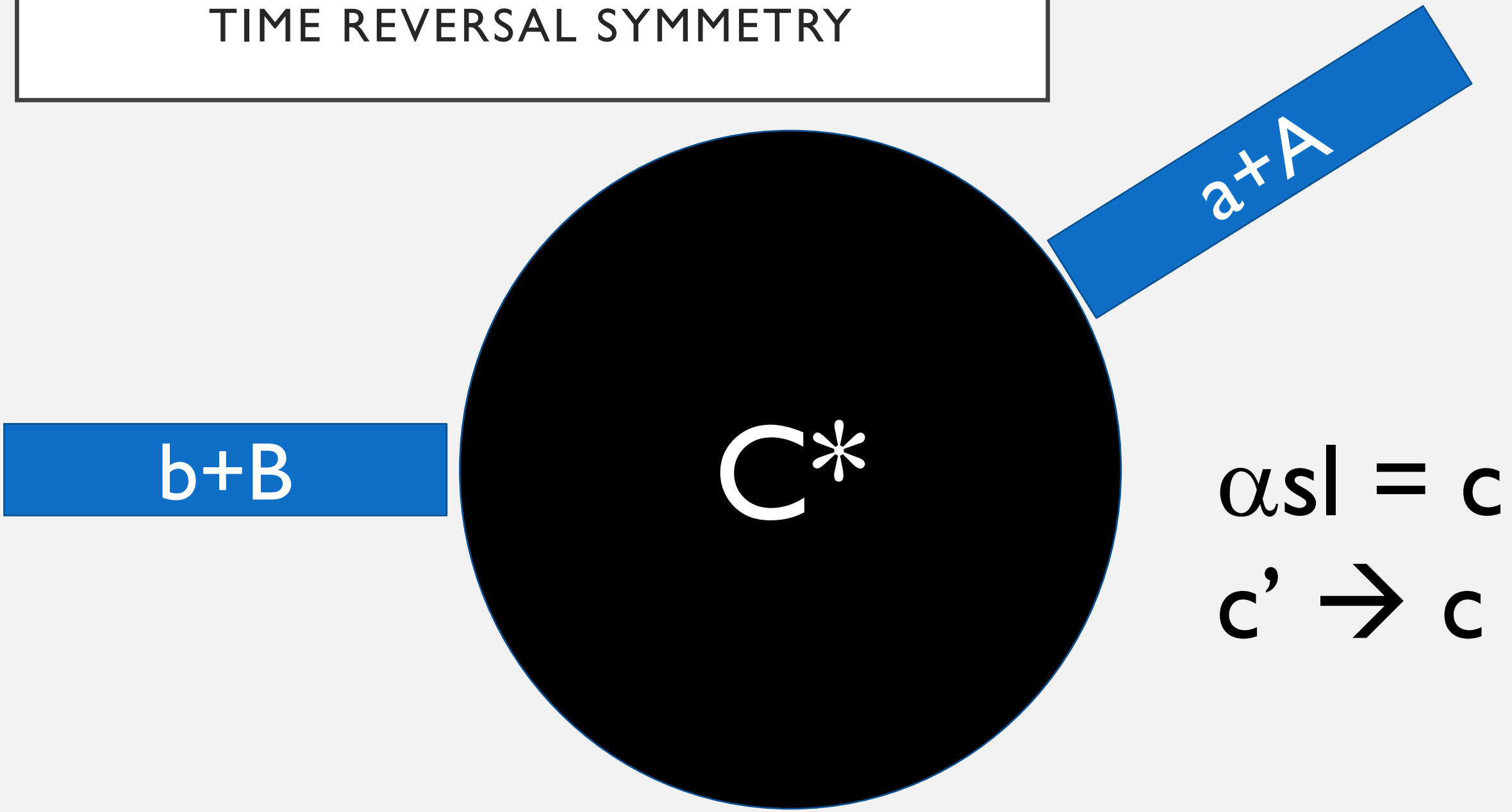
CHANNELS



$\alpha s l = c$

$c \rightarrow c'$

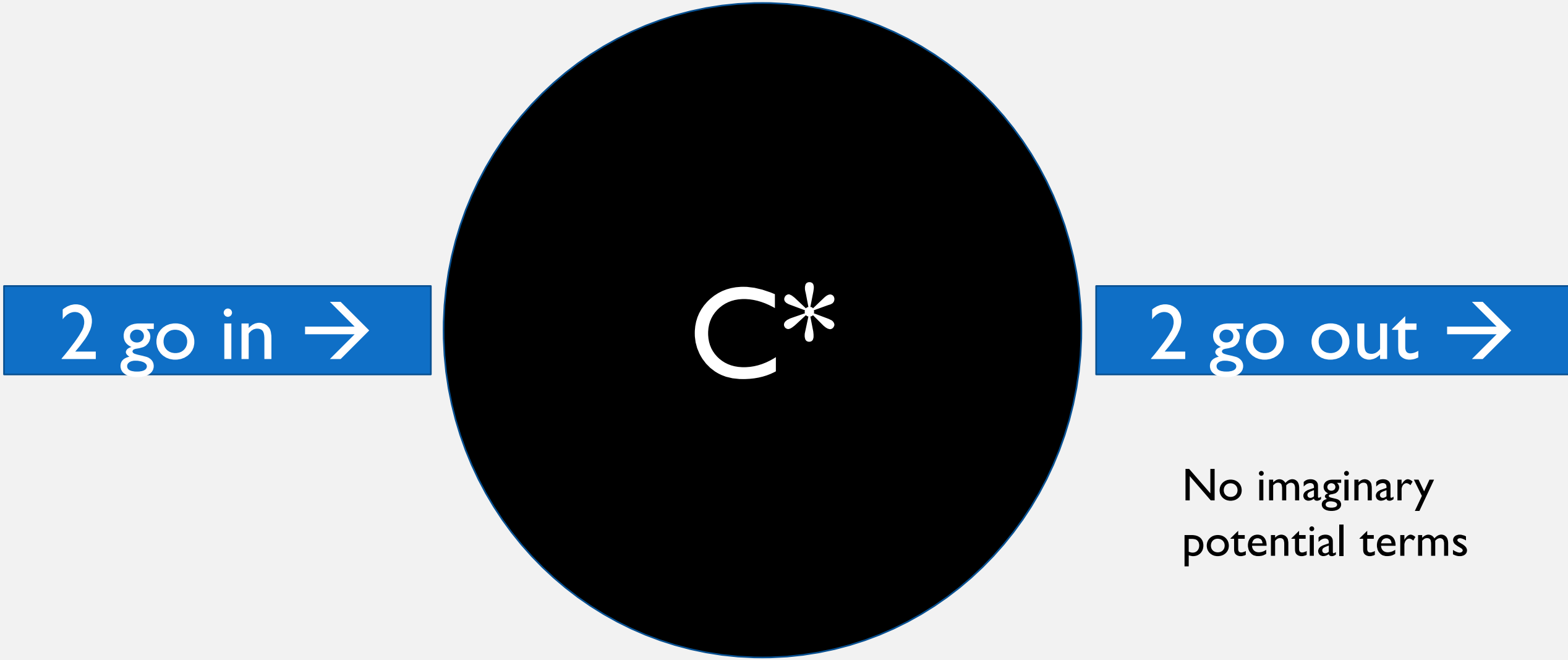
TIME REVERSAL SYMMETRY



$\alpha s l = c$

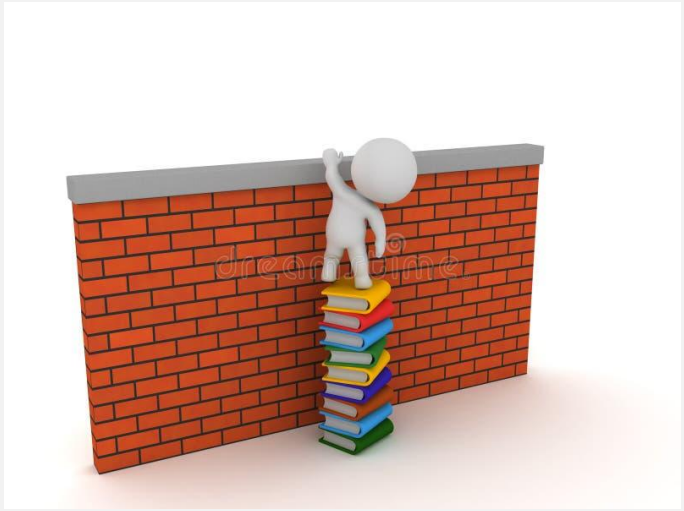
$c' \rightarrow c$

UNITARITY: CONSERVATION OF PROBABILITY
TWO BODY REACTIONS ONLY



No imaginary potential terms

LOTS OF DEFINITIONS



$E_c \equiv E_\alpha$, the energy of relative motion of the particles of the pair c;

$$M_c \equiv M_\alpha = \frac{M_{\alpha 1} M_{\alpha 2}}{M_{\alpha 1} + M_{\alpha 2}}, \text{ the reduced mass;}$$

$$k_c \equiv k_\alpha = \left(\frac{2M_\alpha |E_\alpha|}{\hbar^2} \right)^{\frac{1}{2}}, \text{ the wave number;}$$

$v_c \equiv v_\alpha = \hbar k_\alpha / M_\alpha$, the relative velocity;

$$\eta_c = \eta_{\alpha l} = \frac{Z_{1\alpha} Z_{2\alpha} e^2}{\hbar v_\alpha}, \text{ the Coulomb field parameter;}$$

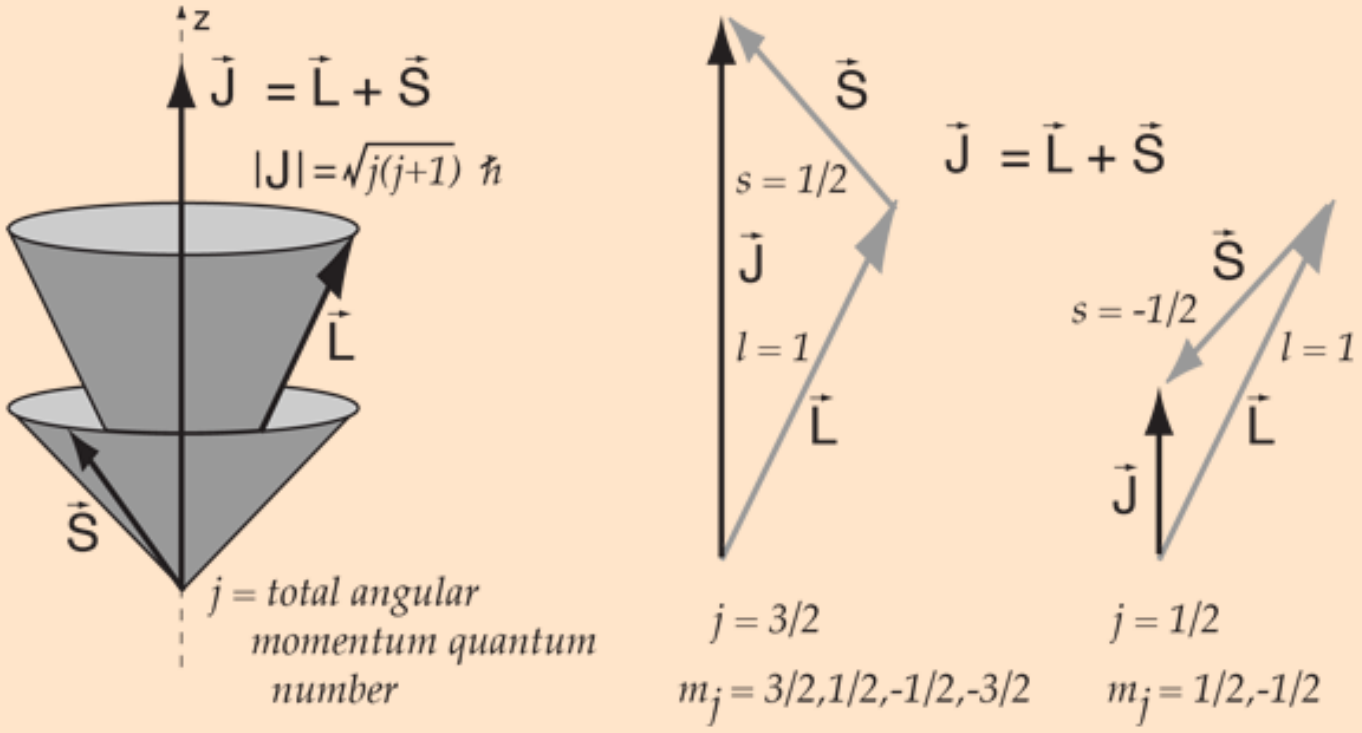
$\sigma_c \equiv \sigma_{\alpha l} = \arg\Gamma(1 + l_c + i\eta_c)$, the Coulomb phase shift;

$\rho_c \equiv \rho_\alpha = k_\alpha r_\alpha$.

VECTOR (SPIN-ORBIT) COUPLING

$$\mathbf{J = L + S}$$

This kind of combination is visualized in terms of a vector model of angular momentum.



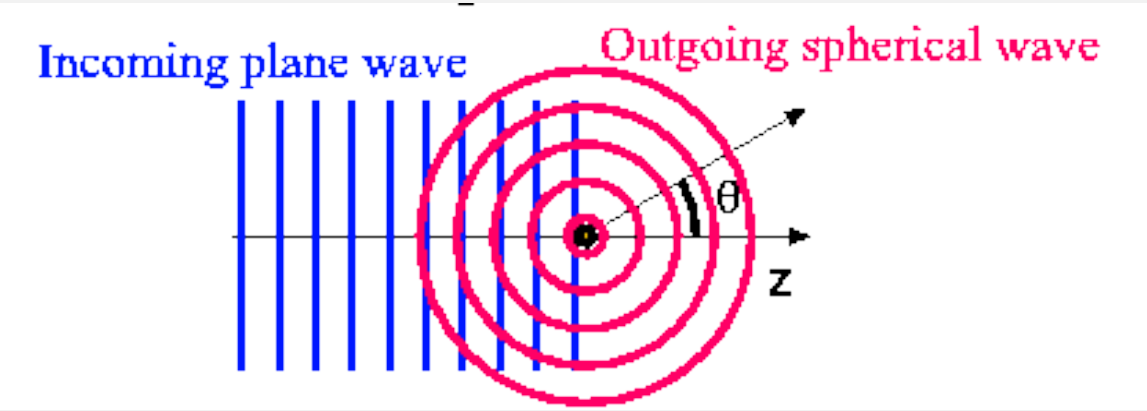
hyperPhysics.phys-astr.gsu.edu

TERMINOLOGY

- Partition (α) --- group of two particles that the system can be decomposed into (ex. $^{12}C+\alpha$). Outside of *R*-matrix theory, a partition is often called a channel, which can lead to some confusion.
- Channel ($c = \alpha s l$) --- a partition with a specific channel spin and angular momentum
- Channel spin (s) --- $s = s_1+s_2$
- Relative orbital angular momentum (l) --- the relative angular momentum of a channel
- Channel radius (a_c) --- phenomenological parameter, somewhat arbitrary division of the internal and external space, does **NOT** correspond to a real nuclear radius
- reduced width amplitude (γ_c) --- phenomenological parameter related to the width of a level (γ_c^2 is the reduced width)
- resonance pole energy (E_l) --- parameter associated with the energy of a level (does not necessarily correspond to the observed energy of a level in the formal theory)
- Boundary condition (B_c) --- phenomenological parameter, can be eliminated using the alternative Brune parameterization

OUTLINE OF THE R-MATRIX METHOD

- The problem assumes
  - Point like particles, 3D
  - Two particles in, two particles out (unitarity)
  - Angular momentum and parity conservation
  - Long-range Coulomb interaction
  - Time-reversal invariance
  - **No potential specified!**



Wave functions of relative motion

$$H_c\chi = \mathcal{E}\chi,$$

The wave function of relative motion has the form

$$\chi \sim r_\alpha^{-1} u_{\alpha sl}(r_\alpha)(i^l Y_m^{(l)}(\Omega_\alpha)), \qquad (2.5)$$

We need to derive the radial wave function $u_{\alpha sl}$

Solve the radial Schrödinger equation

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

At $r_c > a_c$

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

INCOMING AND OUTGOING PARTIAL WAVE EXPANSION IN THE EXTERNAL REGION

- The solution to the Schrödinger equation in the **external** region
  - At positive energies in a Coulomb field

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

where G_c and F_c are the irregular and regular **Coulomb functions**, respectively, and

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

ω_c are the nuclear phase shifts.

The condition of continuity for the wavefunction at the boundaries gives:

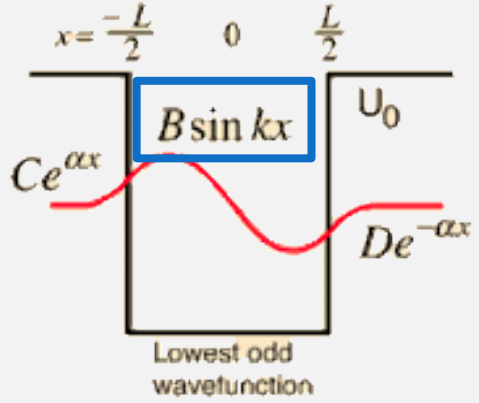
$$Ce^{-\alpha L/2} = B\sin(-kL/2) \quad \text{so} \quad C = -D$$
$$De^{-\alpha L/2} = B\sin(kL/2)$$

The condition of continuity for the derivative of the wavefunction gives:

$$\alpha Ce^{-\alpha L/2} = kB\cos(-kL/2)$$
$$-\alpha De^{-\alpha L/2} = kB\cos(kL/2)$$

Dividing either of these two sets gives:

$$\alpha = \frac{-k}{\tan\frac{kL}{2}} = \sqrt{\beta^2 - k^2}$$



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Remember a square well potential? The solution to the wave functions in the box are sin and cos, which are just another pair of special functions

INCOMING AND OUTGOING PARTIAL WAVE EXPANSION IN THE EXTERNAL REGION

- The solution to the Schrödinger equation in the external region
  - At negative energies in a Coulomb field

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

where W is the **Whittaker function**, and

- Now we can write down the complete external (channel) wave functions

$$\mathcal{I}_{\alpha s l v m}^{+} = (i^l Y_m^{(l)}) \frac{I_{\alpha l}^{+}}{v_\alpha^{\frac{1}{2}} r_\alpha} \psi_{\alpha s v}$$

$$\mathcal{O}_{\alpha s l v m}^{+} = (i^l Y_m^{(l)}) \frac{O_{\alpha l}^{+}}{v_\alpha^{\frac{1}{2}} r_\alpha} \psi_{\alpha s v}.$$

The condition of continuity for the wavefunction at the boundaries gives:

$$Ce^{-\alpha L/2} = B\sin(-kL/2) \quad \text{so} \quad C=-D$$
$$De^{-\alpha L/2} = B\sin(kL/2)$$

The condition of continuity for the derivative of the wavefunction gives:

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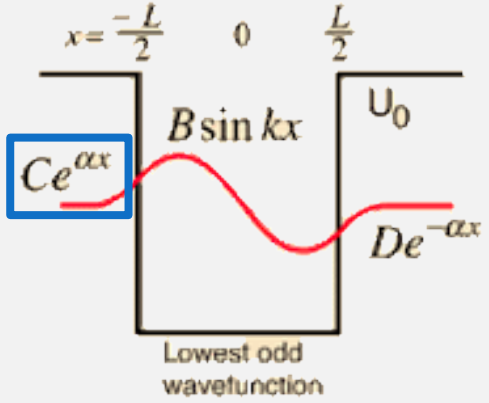

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Remember a square well potential? The solution to the wave functions outside the box is an exponential function, which is just another special function

INTERNAL WAVE FUNCTIONS

- We make very few assumptions about the internal wave functions
  - They satisfy the wave equation

$$H\Psi_{JM} = E\Psi_{JM},$$

  - They can be expanded in mutually orthogonal eigenfunctions (level wave functions)

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

  - We will end up associating this λ index with a level in the compound nucleus
  - We don't know $X_{\lambda JM}$ and will never actually define them further

FUNCTIONS AT THE CHANNEL SURFACE $R_C = A_C$

external functions (more definitions)

$$L_c \equiv (\rho_c O_c'/O_c)_{r_c=a_c} = S_c + iP_c, \tag{4.4}$$

the real and imaginary parts of which are, according to (2.13b), (2.12), and (2.17), respectively,

Shift function

$$S_c^+ = [\rho_c(F_cF_c' + G_cG_c')/(F_c^2 + G_c^2)]_{r_c=a_c},$$
$$S_c^- = (\rho_c W_c'/W_c)_{r_c=a_c}; \tag{4.4a}$$

Coulomb Penetrability function

$$P_c^+ = [\rho_c/(F_c^2 + G_c^2)]_{r_c=a_c},$$
$$P_c^- = \text{zero}. \tag{4.4b}$$

In the case of the positive-energy channels, the ratio

$$\Omega_c^+ = (I_c/O_c)_{r_c=a_c} \tag{4.5}$$

is a unit-modulus complex number which is expressible as

$$\Omega_c^+ \equiv \Omega_{cl}^+ = \exp i(\omega_c - \phi_c^+), \tag{4.5a}$$

where

Hard sphere phase shifts

$$\phi_c^+ \equiv \phi_{cl}^+ = \tan^{-1}(F_c/G_c). \tag{4.5b}$$

MATCHING WAVE FUNCTIONS AT THE BOUNDARY SURFACE

- We match the wave functions and their derivatives at the boundary surface

By taking the logarithmic derivative at the channel surface

$$\Psi_{JM}=\sum_{\lambda} A_{\lambda J}X_{\lambda JM}, \qquad HX_{\lambda JM}=E_{\lambda J}X_{\lambda JM}.$$

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

Convolution of the surface wave function (external) and the internal wave function, which we can't solve!

- To solve for $\gamma_{\lambda c}$ analytically we would have to know the form of the internal wave functions $X_{\lambda JM}$
- Instead, the $\gamma_{\lambda c}$ and E_λ become parameters that are obtained by fitting to data. They are just numbers after all (reduced width amplitudes and pole energies).
- There is a $\gamma_{\lambda c}$ for each possible decay channel for each level, which can lead to quite a lot of fit parameters depending on our specific problem
- The $\gamma_{\lambda c}$ are the **reduced width amplitudes**
- The $\gamma_{\lambda c}^2$ are the **reduced widths**

ASIDE: REDUCED WIDTH AMPLITUDE

How much do the two particles fusing together look like an internal state?

- Kind of like a spectroscopic factor $\gamma_{\lambda c} \equiv (\hbar^2/2M_c a_c)^{\frac{1}{2}} \int \varphi_c^* X_{\lambda J M} dS,$
- Wigner limit: $\gamma_W^2 = 3\hbar^2/2\mu a^2$
- **Normalized reduced width** $\theta_{\lambda c}^2 = \gamma_{\lambda c}^2/\gamma_{W,c}^2 \approx 1$

GREEN'S THEOREM

Green's theorem, single channel

$$\left(u_2\frac{du_1}{dr}-u_1\frac{du_2}{dr}\right)_{r=a}+\frac{2M}{\hbar^2}(E_1-E_2)\int_0^a u_1u_2dr=0,$$

Boundary condition

$$(du_\lambda/dr)_{r=a}=0.$$

The Green's function that relates the value of the wave function to its derivative on the surface.

$$G(r,a)=\frac{\hbar^2}{2Ma}\sum_\lambda\frac{u_\lambda(r)u_\lambda(a)}{E_\lambda-E}$$

The R-function

$$R=G(a,a)=\sum_\lambda \gamma_\lambda^2/(E_\lambda-E),$$

This R-matrix is essentially the result of these boundary conditions

RELATION TO THE COLLION FUNCTION

A general solution Ψ_l may always be expressed in the external region as a linear combination of the linearly independent $\mathcal{I}_l$ and $\mathcal{O}_l$ waves of (2.19):

$$\Psi_l \sim \mathcal{I}_l - U_l \mathcal{O}_l. \qquad (1.12)$$

The coefficient U_l is thus the amplitude of the unit-flux outgoing wave $\mathcal{O}_l$ which is associated with a unit-flux incoming wave $\mathcal{I}_l$; it is called the *collision* or *scattering function*.

- Matching the internal and external wave functions at the surface

$$U_l = \frac{I_l}{O_l} \cdot \frac{1 - L_l^* R_l}{1 - L_l R_l},$$

- The collision matrix can also be expressed as a phase shift

$$U_l = \exp(2i\delta_l),$$

where

$$\delta_l = \tan^{-1}[R_l P_l / (1 - R_l S_l)] - \phi_l + \omega_l,$$

Nuclear phase shift

CONNECTION WITH GENERAL REACTION THEORY OR THE COLLISION MATRIX (U)

Generalized to the multichannel case,
The R-matrix

$$R_{c'c}=\sum_{\lambda}\gamma_{\lambda c'}\gamma_{\lambda c}/(E_{\lambda}-E).$$

Connection to the collision matrix

$$\mathbf{U}^{J}=\boldsymbol{\varrho}^{\frac{1}{2}}\mathbf{O}^{-1}(1-\mathbf{R}^{J}\mathbf{L}^{0})^{-1}(1-\mathbf{R}^{J}\mathfrak{L}^{0})\mathbf{I}\boldsymbol{\varrho}^{-\frac{1}{2}}$$

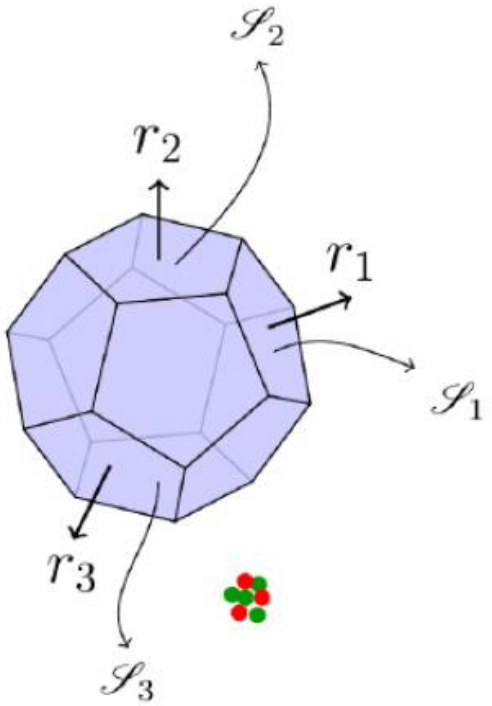
All these other matrices besides R can be calculated from special functions

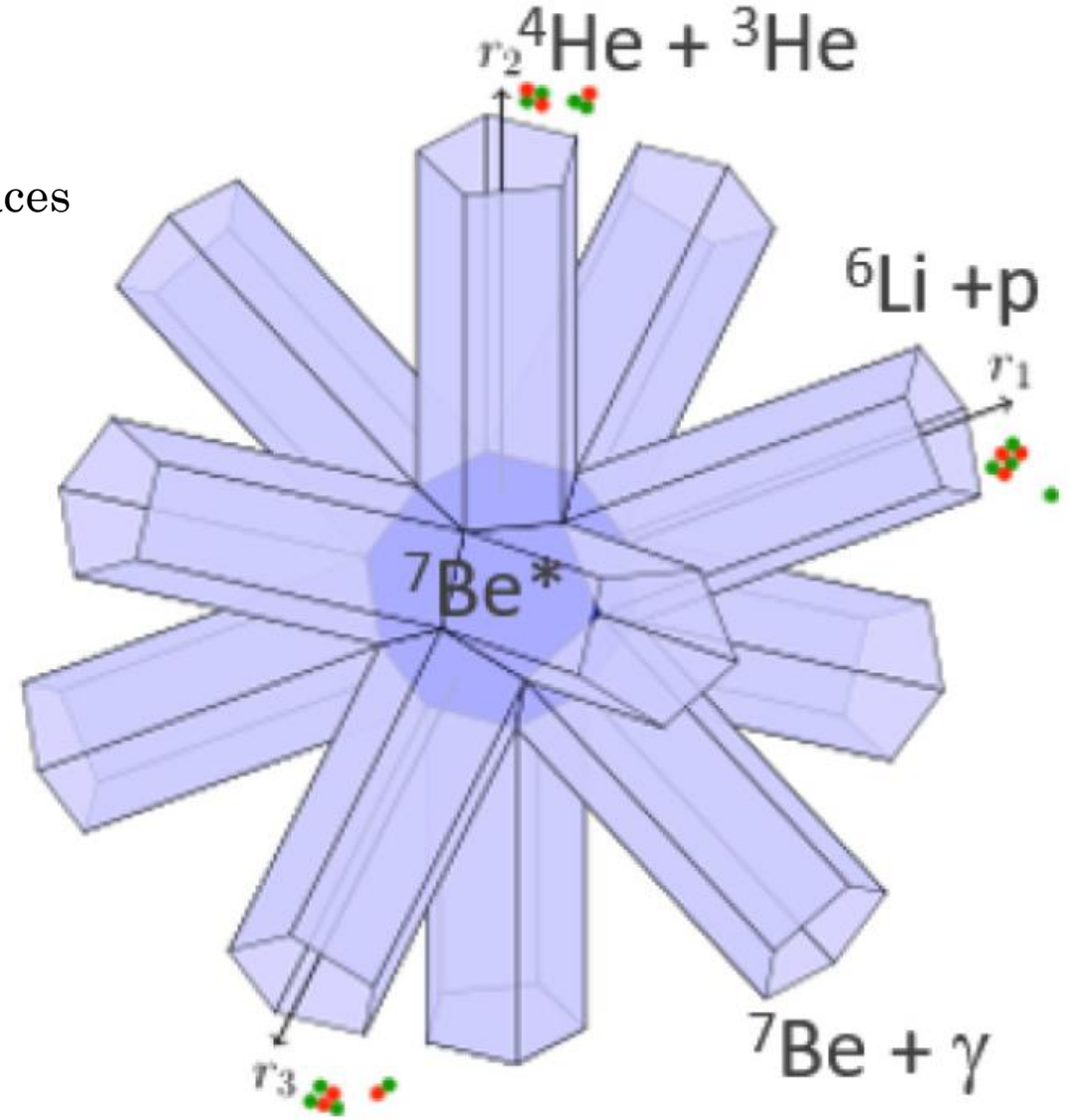
Transition Matrix (T-matrix)

$$T_{\alpha's'l',\alpha sl}{}^{J}=e^{2i\omega_{\alpha'l'}}\delta_{\alpha's'l',\alpha sl}-U_{\alpha's'l',\alpha sl}{}^{J}.$$

- The mathematics is similar to that of wave guides in E&M

Channel Surfaces





De Saint Jean *et al.* (2021)

THERE ARE A LOT OF DIFFERENT METHODS TO DERIVE THIS

Nuclear Physics **4** (1957) 503—528; © *North-Holland Publishing Co., Amsterdam*

THE BLOCK OPERATOR

UNE FORMULATION UNIFIÉE DE LA THÉORIE DES RÉACTIONS NUCLÉAIRES

CLAUDE BLOCH

Centre d'Études Nucléaires de Saclay, Gif-sur-Yvette (S. & O.)

Reçu le 13 avril 1957

Abstract: The determination of the scattering matrix in the theory of nuclear reactions is essentially equivalent to the construction of the Green function for the Schrödinger equation in the internal region of the configuration space with proper boundary conditions at the nuclear surface. This Green function can be expressed as the inverse of an operator involving the sum of the Hamiltonian and of a "boundary value operator" which is different from zero only on the nuclear surface where it has a singularity of the same kind as a Dirac function. A general operator expression for the scattering matrix is derived. This expression can be transformed into a matrix expression by introducing an arbitrary basis of orthonormal functions in the internal region. The Wigner-Eisenbud and the Peierls-Kapur formulations are obtained by an appropriate choice of the internal functions. When a large number of resonances contribute to the cross-section, the expansion of the scattering matrix in terms of resonances of the compound system is not useful, and a more appropriate starting point can be obtained from a perturbation expansion of the scattering matrix which is easily derived from the general operator expression. A simple statistical assumption is proposed in order to determine the dominant terms in such an expansion. It leads to the optical model for the elastic scattering and to the direct interactions for the inelastic scattering.

- Descouvemont and Baye (2010)

$$\mathcal{L}(B) = \frac{\hbar^2}{2\mu}\delta(r-a)\left(\frac{\mathrm{d}}{\mathrm{d}r} - \frac{B}{r}\right)$$

- B is the boundary parameter (an arbitrary constant)
- Inhomogeneous Block-Schrödinger equation

$$(H_l + \mathcal{L}(B) - E)u_l^{\mathrm{int}} = \mathcal{L}(B)u_l^{\mathrm{ext}}$$

$$u_l^{\mathrm{int}}(a) = u_l^{\mathrm{ext}}(a) \qquad u_l^{\mathrm{int}'}(a) = u_l^{\mathrm{ext}'}(a)$$

$$(H_l + \mathcal{L}(B) - E)G_l(r,r') = \delta(r-r')$$

$$u_l^{\mathrm{int}}(r) = \int_0^a G_l(r,r')\mathcal{L}(B)u_l^{\mathrm{ext}}(r')\,\mathrm{d}r'$$

Green's function solution

Single channel case

$$R_l(E) = \frac{\hbar^2}{2\mu a}G_l(a,a) \qquad R_l(E,B) = \sum_{n=1}^{N}\frac{\gamma_{nl}^2}{E_{nl}-E}$$

MAIN TAKE-AWAYS

- The cross section is derived in terms of a partial wave expansion $$W(\theta) = \sum_k a_k P_k(\cos(\theta))$$
- The solution is a series of poles: $$R_{cc'} = \sum_{\lambda=1}^{\infty} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E}$$
- The square is proportional to observables like the cross section $$\sigma \propto |R_{cc'}|^2$$
- We have a much more physically constrained fit function than the Briet-Wigner approximation

TRUNCATION OF MANY THINGS

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

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

- Drastic truncations are often made, how can this approach still work?

λ = level index

- 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

THE (UNPOLARIZED) DIFFERENTIAL) CROSS SECTION

$$(2s+1)\frac{k_\alpha^{\,2}}{\pi} d\sigma_{\alpha s,\,\alpha' s'} d\Omega_{\alpha'} = (2s+1)\left|C_{\alpha'}(\theta_{\alpha'})\right|^2 \delta_{\alpha' s',\,\alpha s}$$

$$+ \sum_{\substack{J_1 J_2 M_1 M_2 \\ l_1 l_2 l_1' l_2' \\ \nu\nu' m_1' m_2'}} (2l_1+1)^{\frac{1}{2}}(2l_2+1)^{\frac{1}{2}}(sl_1\nu 0 \,|\, J_1 M_1)$$

$$\times (sl_2\nu 0 \,|\, J_2 M_2)(s' l_1' \nu' m_1' \,|\, J_1 M_1)(s' l_2' \nu' m_2' \,|\, J_2 M_2)$$

$$\times (T_{\alpha' s' l_1',\,\alpha s l_1}{}^{J_1} Y_{m_1'}{}^{(l_1')}(\Omega_{\alpha'}))$$

$$\times (T_{\alpha' s' l_2',\,\alpha s l_2}{}^{J_2} Y_{m_2'}{}^{(l_2')}(\Omega_{\alpha'}))^*$$

$$+ \sum_{\substack{JMll' \\ m'\nu\nu'}} (2l+1)^{\frac{1}{2}}(sl\nu 0 \,|\, JM)(s' l' \nu' m' \,|\, JM)$$

$$\times \delta_{\alpha' s' \nu',\,\alpha s \nu} 2\,\mathrm{Re}\left[i T_{\alpha' s' l',\,\alpha s l}{}^{J} Y_{m'}{}^{(l')}(\Omega_{\alpha'}) C_{\alpha'}(\theta_{\alpha'})\right].$$

Coulomb term

Resonance term

Interference term

ADSIDE: WOLFENSTEIN TRACE FORMALISM

- General formalism to calculate any observable
- Lincoln Wolfenstein
  - MS**W** effect
  - Neutrino oscillations in matter
- Polarization observables give us constraints on each element of the T-matrix, but they are hard to measure experimentally

Complete transition (T) matrix

Talk by Mark Paris (LANL)

- Wolfenstein formalism

$$\left\langle O_f \right\rangle = \frac{1}{\mathrm{Tr}(\rho_f)} \mathrm{Tr}(\rho_f O_f) = \frac{1}{\mathrm{Tr}(\rho_f)} \mathrm{Tr}(M \rho_i M^\dagger O_f),$$

$$\rho = a a^\dagger, \text{ and } a_f = M a_i.$$

$$\text{Using the expansion } \rho_i = \frac{1}{\mathrm{Tr}(\mathbb{1}_i)} \sum_i \left\langle O_i \right\rangle O_i,$$

$$\text{and defining } \mathrm{Tr}(\rho_f) = \sigma_0(\theta) \text{ gives finally}$$

$$\sigma_0(\theta) \left\langle O_f \right\rangle = \frac{1}{\mathrm{Tr}(\mathbb{1}_i)} \sum_i \left\langle O_i \right\rangle \mathrm{Tr}(M O_i M^\dagger O_f), \qquad \begin{cases} O_i = O_1 \otimes O_2 \\ O_f = O_3 \otimes O_4 \end{cases}$$

$$M_{fi} = \frac{4\pi}{k_i} \left\langle \phi^{\mu'}_{s'} \middle| \hat{T} \middle| \phi^{\mu}_{s} \right\rangle = \frac{4\pi}{k_i} \sum_{JMl'l} \left\langle \phi^{\mu'}_{s'} \middle| \mathcal{Y}^M_{Js'l'} \right\rangle T^J_{s'l',sl} \left\langle \mathcal{Y}^M_{Jsl} \middle| \phi^{\mu}_{s} \right\rangle.$$

Lincoln Wolfenstein
1923-2015

https://www-nds.iaea.org/index-meeting-crp/CM-R-matrix-2016/docs/Paris_2016.pdf

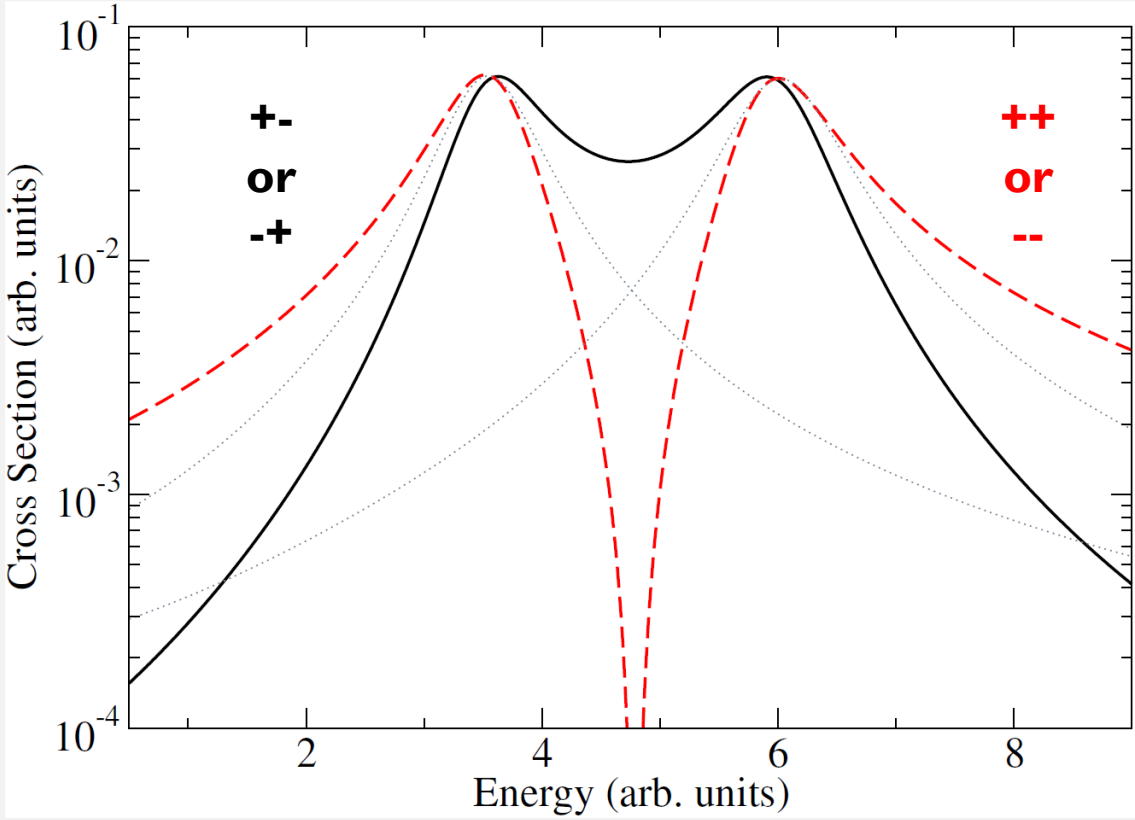
WHY THE BOTHER?

- Reduced width amplitudes are real, but can be positive or negative in sign

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

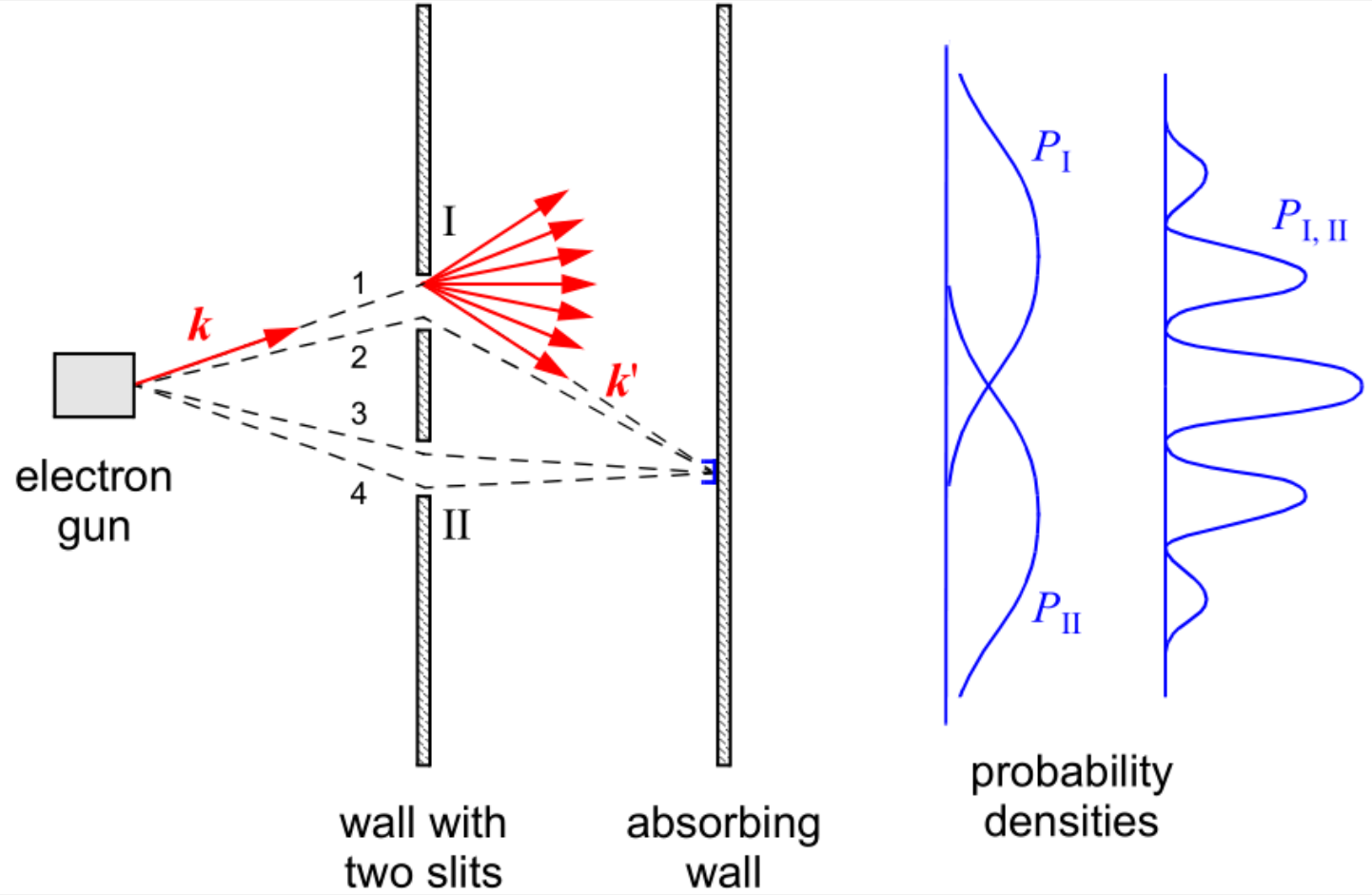
$$R_{cc'} = \sum_{\lambda=1}^{2} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E} = \frac{\gamma_{1c}\gamma_{1c'}}{E_1 - E} + \frac{\gamma_{2c}\gamma_{2c'}}{E_2 - E}$$

$$\sigma \propto |R_{cc'}|^2$$



THE CLASSIC EXAMPLE: THE DOUBLE SLIT EXPERIMENT

- Classically, the two signals would just add together (incoherently)
- In the quantum world, (indistinguishable) things add together coherently

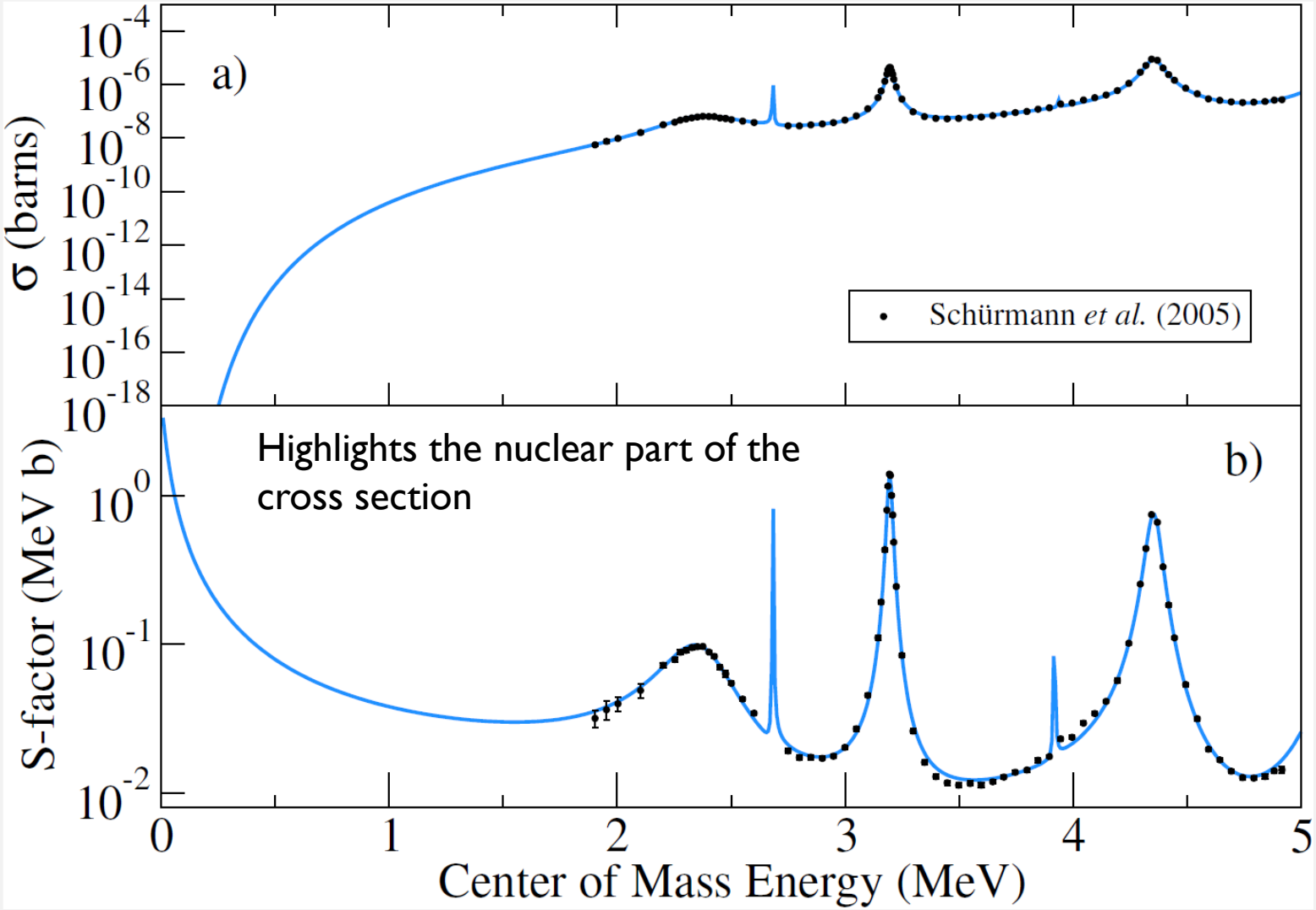


ASTROPHYSICAL S-FACTOR

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

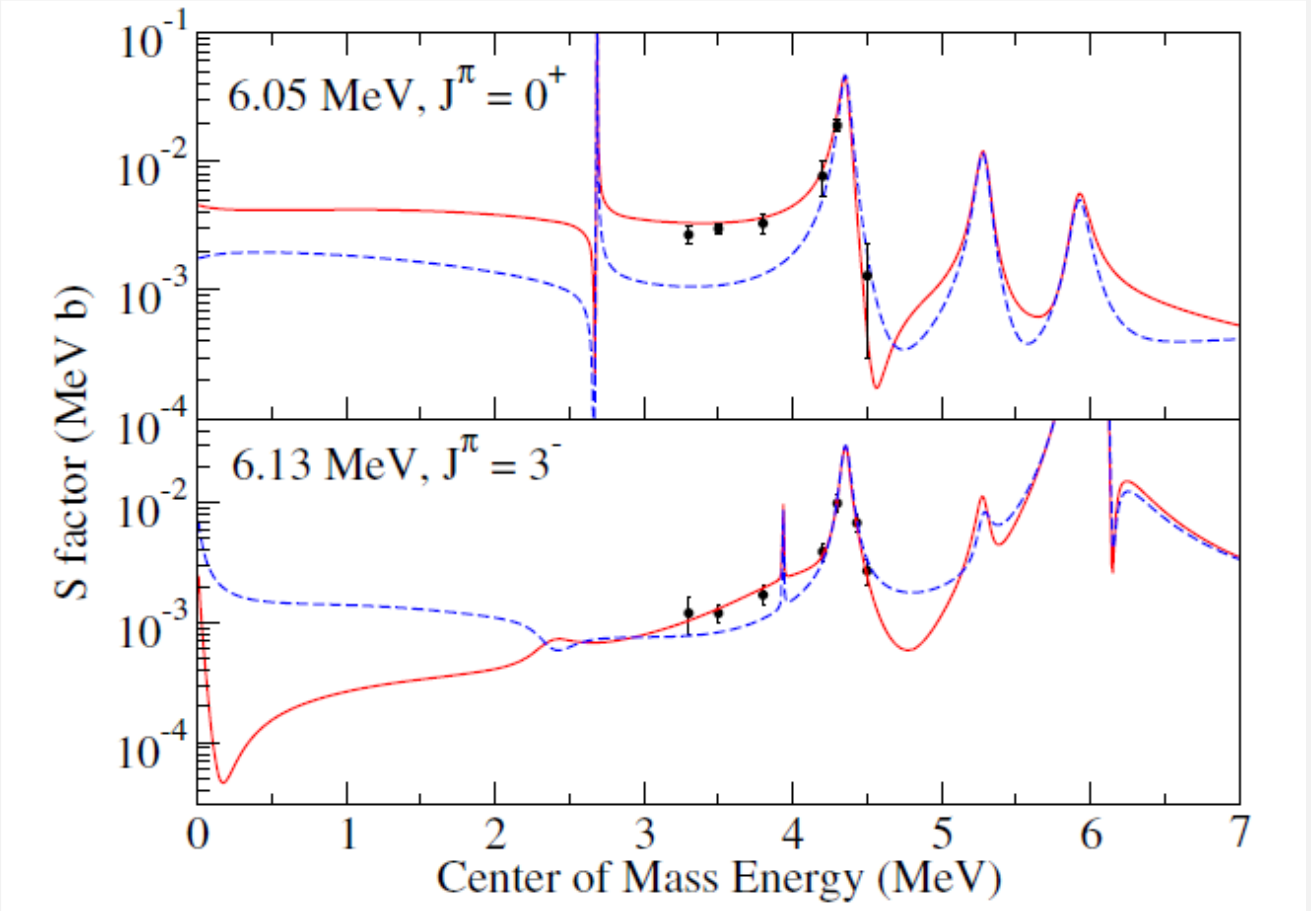
$$\eta = \sqrt{\frac{\mu}{2E}}\frac{Z_1 Z_2 e^2}{\hbar^2}$$

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

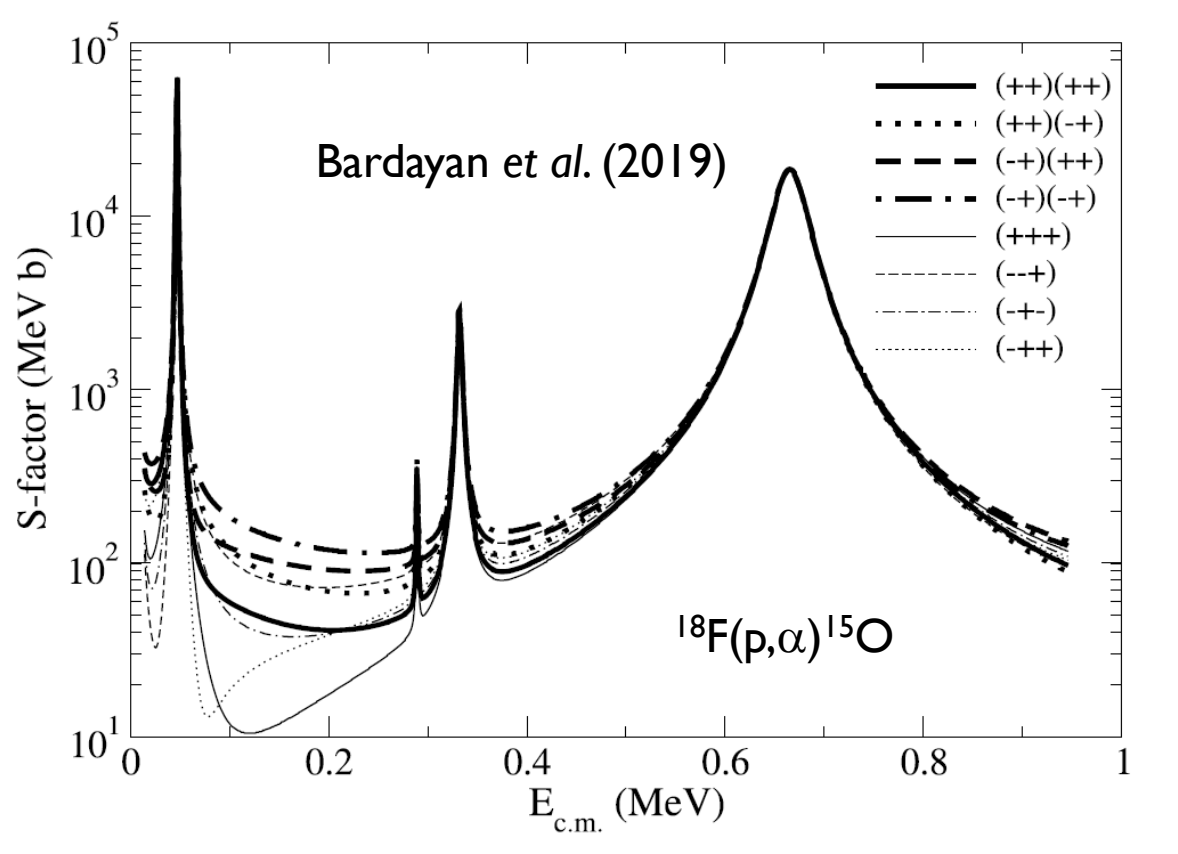


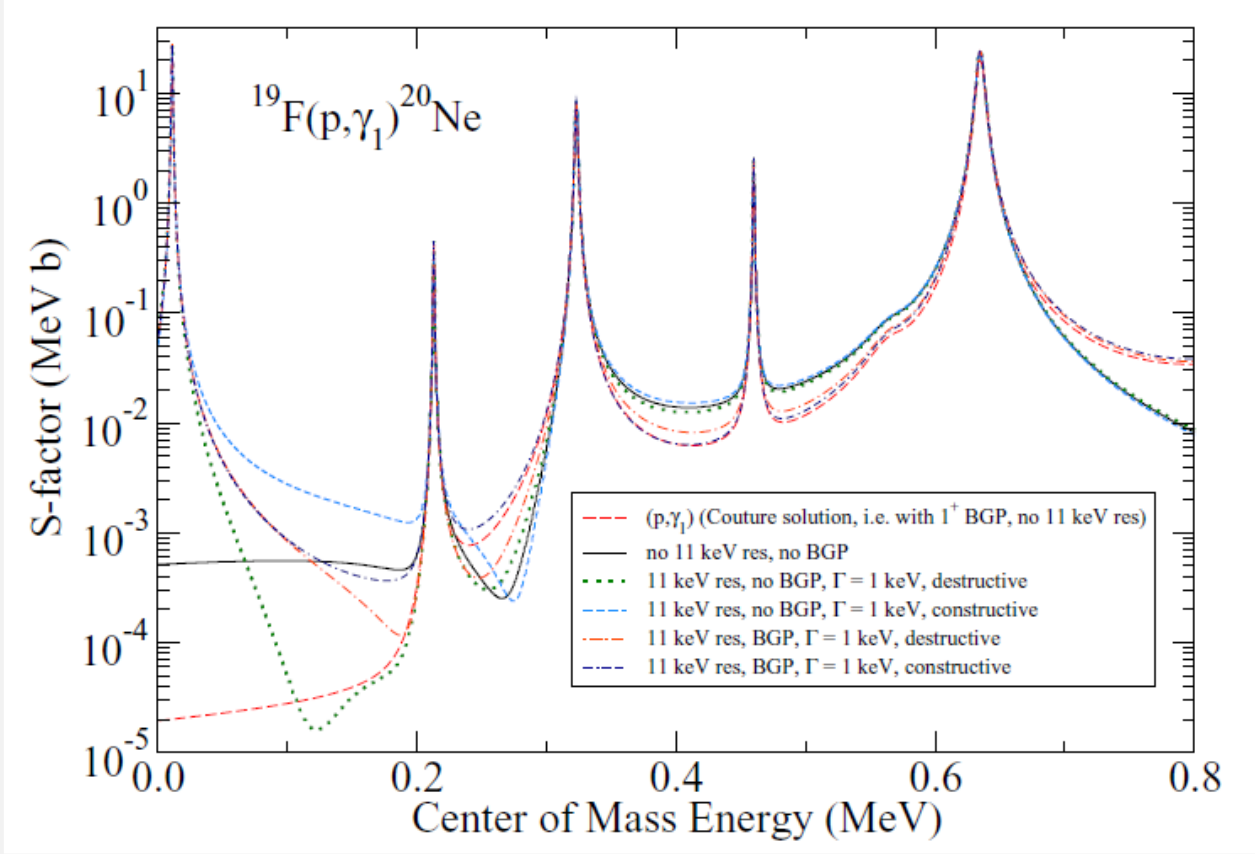
INTERFERENCE

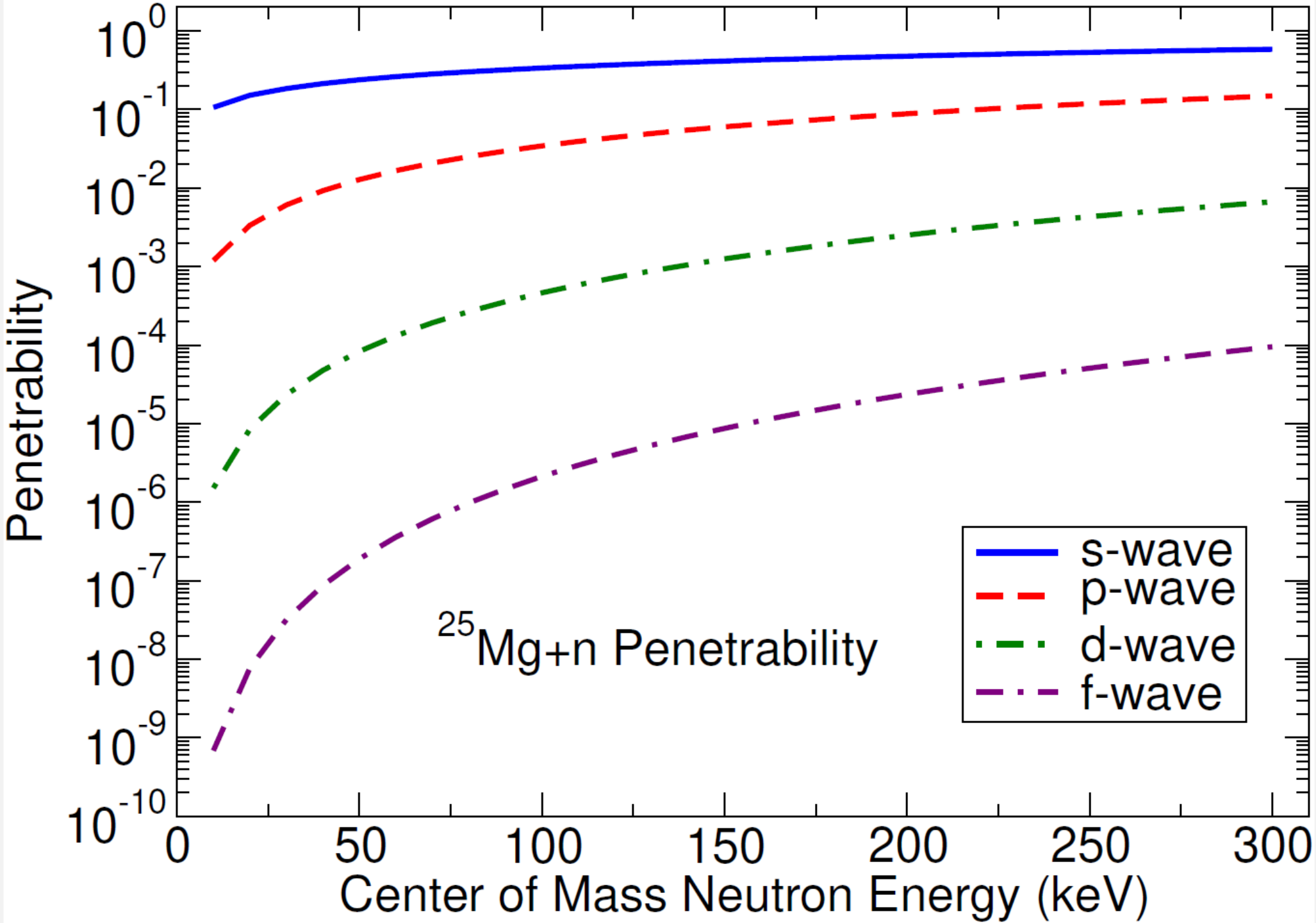
- Included in the SHAPE of the cross section, is the correct modeling of the interference between resonances, which is very important for EXTRAPOLATING the cross section to low energy



MULTI-RESONANCE INTERFERENCE






Penetrability
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
0
50
100
150
200
250
300
Center of Mass Neutron Energy (keV)
^{25}Mg+n Penetrability
s-wave
p-wave
d-wave
f-wave

l = 0,
1
2
3

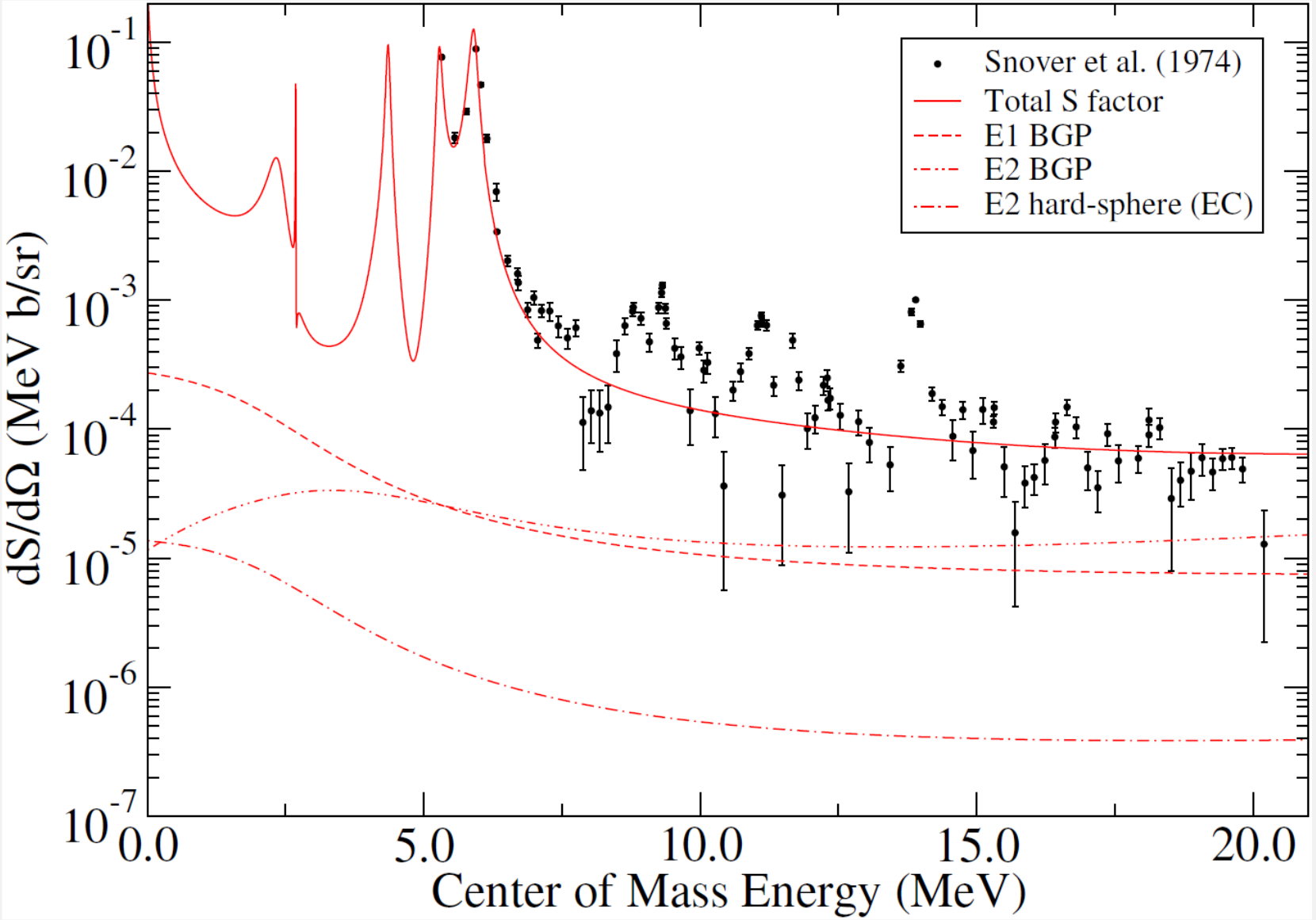
BACKGROUND POLES (BGP)

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

- Since there is a different R-matrix for each J^π, one should consider at least one BGP for each
- Can represent two (or maybe even more distinct physical things)
  - A real level at an energy just higher than the data
  - The sum of all levels at higher energy
  - The "potential" contribution to the cross section (non-resonant)
- In practice you want your data to extend to an energy range where the cross section is weaker at higher energy

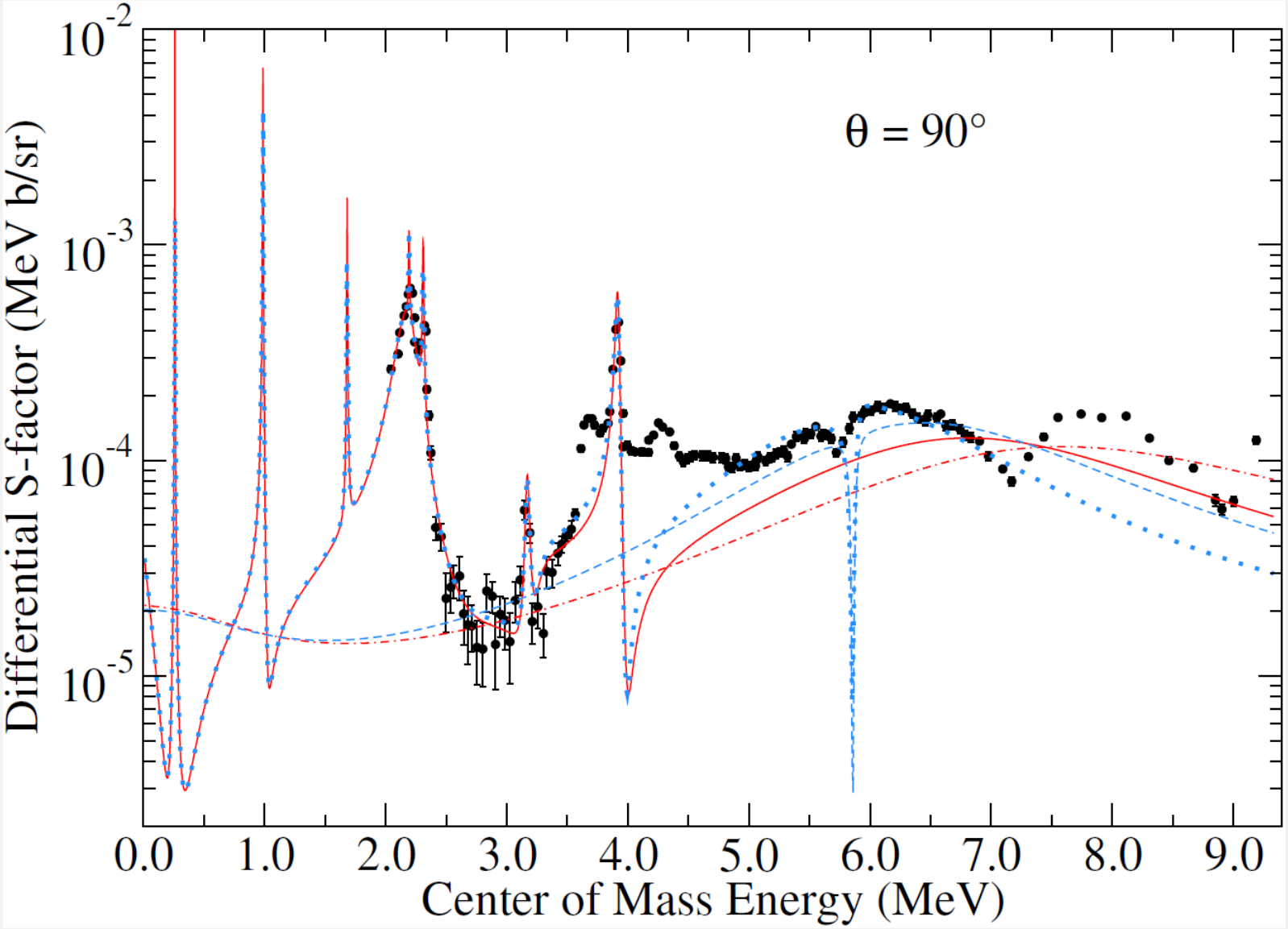
BGPS CONTINUED

- 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



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



Transformations from *R*-matrix to observable parameters

Following Thomas (1951), it is instructive to make a one level approximation to the level matrix $\boldsymbol{A}$. This leads (ignoring the hard-sphere contribution if $c = c'$) to

$$|T_{cc'}|^2 = \frac{\Gamma_{\lambda c}\Gamma_{\lambda c'}}{(E_\lambda - E + \Delta_\lambda)^2 + \frac{1}{4}\left(\sum_{c''}\Gamma_{\lambda c''}\right)^2}, \qquad (38)$$

where $\Gamma_{\lambda c} = 2P_c\gamma_{\lambda c}^2$ is the formal partial width for channel c and Δ_λ is the energy-dependent level shift:

$$\Delta_\lambda = -\sum_c \gamma_{\lambda c}^2[S_c(E) - B_c]. \qquad (39)$$

Special conditions

“on-resonance” condition

$$B_c = S_c(E_\lambda),$$

Observable condition

$$\Delta_\lambda \approx (\tilde{E}_\lambda - E) \sum_c \tilde{\gamma}_{\lambda c}^2 \frac{dS_c}{dE}(\tilde{E}_\lambda)$$

$\tilde{E}_\lambda$ Observable energy

$\tilde{\Gamma}_{\lambda c}$ Observable width

$$|T_{cc'}|^2 = \frac{\tilde{\Gamma}_{\lambda c}\tilde{\Gamma}_{\lambda c'}}{(\tilde{E}_\lambda - E)^2 + \frac{1}{4}\left(\sum_{c''} \tilde{\Gamma}_{\lambda c''}\right)^2},$$

Careful to note!

$$\tilde{\Gamma}_{\lambda c} = \frac{2P_c\tilde{\gamma}_c^2}{1+\sum_{c'}\tilde{\gamma}_{\lambda c'}^2\frac{dS_{c'}}{dE}(\tilde{E}_\lambda)}.$$

observable

$$\Gamma_{\lambda c} = 2P_c\gamma_{\lambda c}^2$$

formal

BRUNE PARAMETERIZATION

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
(Receved 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

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

PRIMARY γ-RAY TRANSITIONS

- Often implemented using perturbation theory
  - Works in cases where the electromagnetic part of the interaction is small compared to the hadronic part
  - **Alternative approaches include Reich-Moore and relativistic wave functions**
- Can include a direct capture model
  - **External Capture**

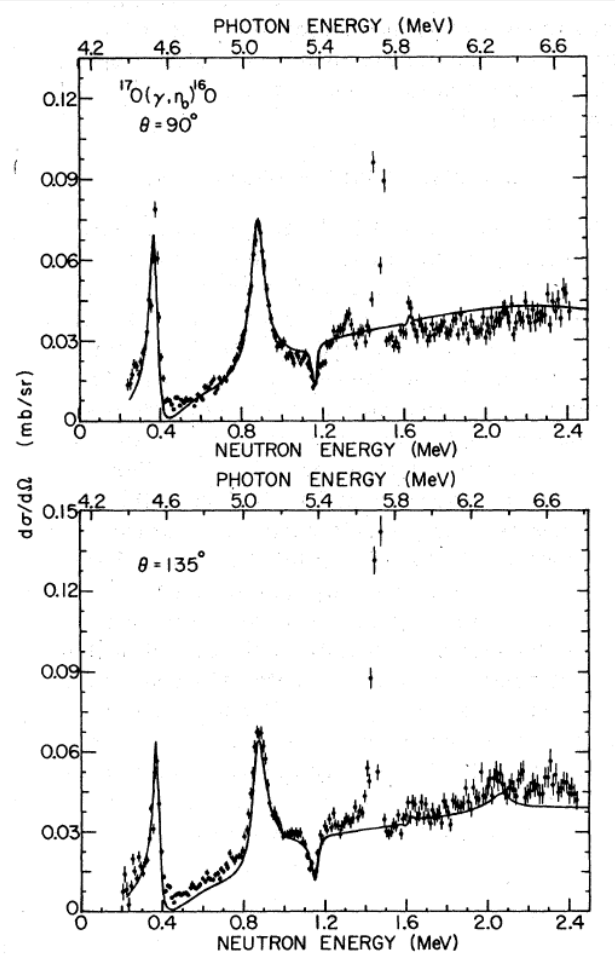
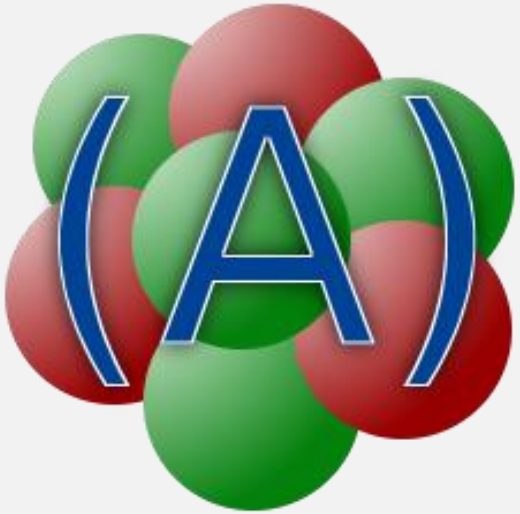


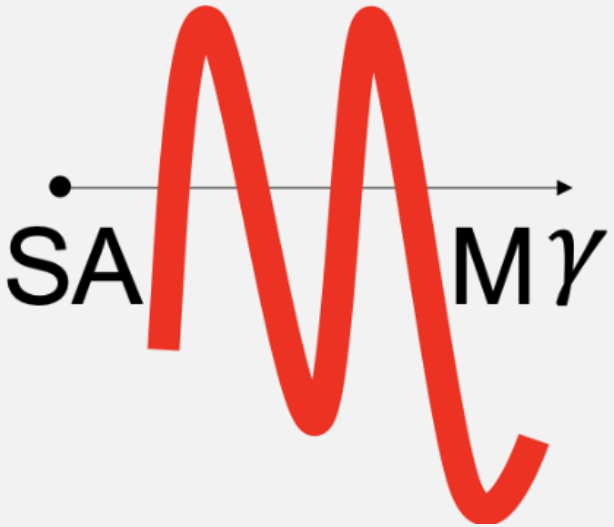
FIG. 5. Final R-matrix analysis of the observations of the $^{17}O(\gamma,n_0)^{16}O$ reaction. The parameters used in this analysis, Tables III and IV, also describe the $^{16}O(n,n)^{16}O$ reaction. The interference minimum at 5.38 MeV is not as deep as that given by the simple hard-sphere model.

- First used by Holt *et al.* (1978) to fit $^{17}O(n,\gamma)^{16}O$ data
- Used by Barker and Kajino (1991) to fit $^{12}C(\alpha,\gamma)^{16}O$
- Used by Angulo and Descouvemont (2001) to fit $^{14}N(p,\gamma)^{15}O$
- Detailed description in deBoer *et al.* (2017) by Carl Brune
- **Mathematic implementation is rather cumbersome**

WHY R-MATRIX?

- Assumption: the data is correct
- **Maximum flexibility** → can most accurately reproduce experimental data
- **Maximum flexibility** → easiest to mess up / most influenced by incorrect data
- Track record is pretty good
- It's been used for a long time, a lot of the details of the formalism have been derived and are accessible in the literature
- **Computer codes are available and accessible**



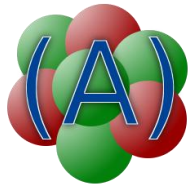


LECTURE 2: PHENOMENOLOGICAL APPLICATION OF R-MATRIX

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

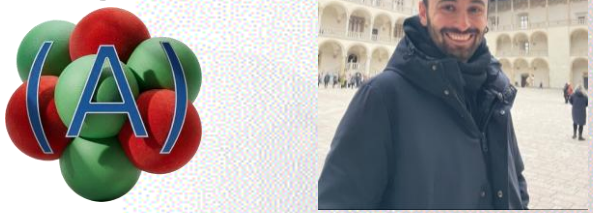
- Originally developed by R.E. Azuma under the Joint Institute for Nuclear Astrophysics (JINA), published 2010

- 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/



WHAT ARE AZURE2'S MAIN CAPABILITIES?

- Designed originally for charged particle reactions and for extrapolations to low energy
  - $^{12}C(\alpha,\gamma)^{16}O$ was the benchmark reaction
- Radiative capture
- Simultaneous multiple exit and entrance channel fits (AZURE2)
- Lots of active development
  - Neutron resolution / experimental routines
  - Thick-target yields
  - Improved Coulomb functions / error handling
  - Secondary gamma-ray angular distributions after particle emission

File Configure Documentation

Particle Pairs | Levels and Channels | Segments | Experimental Effects | Calculate | Plot

	Light Particle	Light Spin	Light g-Factor	Heavy Particle	Heavy Spin	Heavy g-Factor	Excitation Energy	Separation Energy	Channel Radius
1	*p*	1/2+	0	^{17}O	5/2+	0	0	5.60646	4.46
2	γ	1+	0	^{18}F	3+	0	0.9372	0	0
3	γ	1+	0	^{18}F	1+	0	1.70081	0	0
4	γ	1+	0	^{18}F	2-	0	2.10061	0	0
5	γ	1+	0	^{18}F	2+	0	2.52335	0	0
6	γ	1+	0	^{18}F	3-	0	3.79149	0	0
7	γ	1+	0	^{18}F	2+	0	3.83917	0	0
8	γ	1+	0	^{18}F	3+	0	4.1159	0	0
9	α	0+	0	^{14}N	1+	0	0	4.41463	5.44
10	γ	1+	0	^{18}F	1+	0	0	0	0
11	γ	1+	0	^{18}F	5+	0	1.12136	0	0
12	γ	1+	0	^{18}F	2+	0	3.06184	0	0
13	γ	1+	0	^{18}F	3+	0	3.3582	0	0
14	γ	1+	0	^{18}F	4+	0	4.652	0	0
15	γ	1+	0	^{18}F	2+	0	4.9636	0	0
16	γ	1+	0	^{18}F	1-	0	3.1339	0	0
17	γ	1+	0	^{18}F	0+	0	1.04155	0	0
18	γ	1+	0	^{18}F	1+	0	4.36015	0	0

+ -

Graphical user interface (Qt)

WHAT FIT PARAMETERS DOES AZURE2 USE?

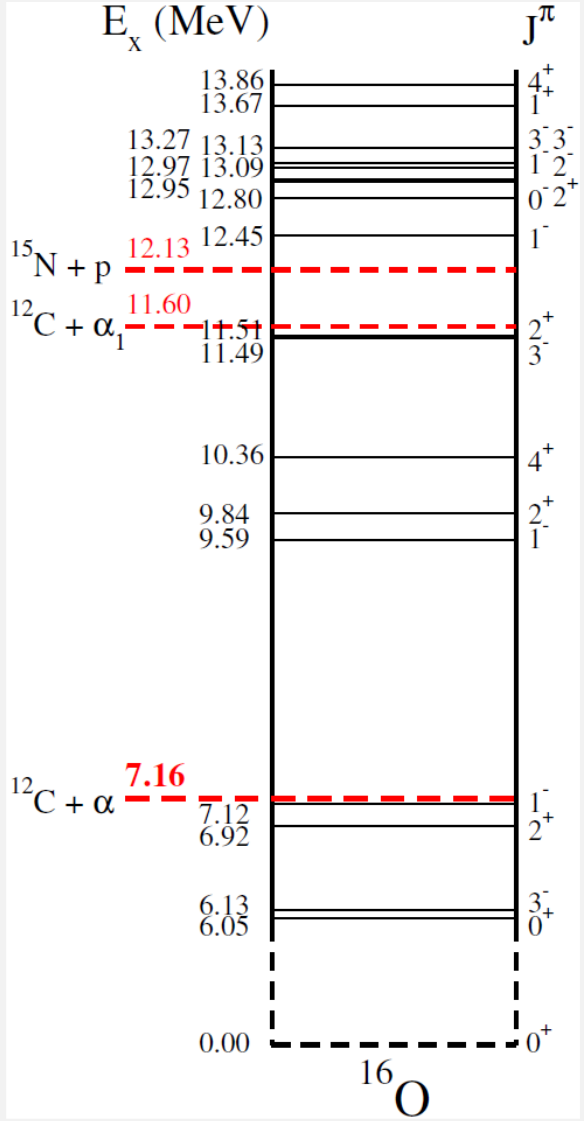
- We use the alternative parameterization of Brune (2002) to replace formal R-matrix parameters (pole energies, reduced widths) with observable level parameters (Level energies, partial widths, asymptotic normalization coefficients)
- This alternative parameterization was a real improvement in accessibility for the R-matrix technique, because the formal parameters have no intuitive meaning, so they are more difficult to work with.
- Also, by using observable parameters it means that there are no large databases where parameter values are already cataloged that can be used as initial starting values for a fit.

E_{level} (keV)	XREF	Jπ	$T_{1/2}$
0.0	A DE GHIJKLM	1/2-	9.965 m *4* % ε = 100
2364.9 *6*	DEFGHI K	1/2+	31.7 keV *8* % IT = 0.00158 *13* % p = 100
3502 *2*	A DEFGHIJK	3/2-	62 keV *4* % IT = 0.0011 % p = 100
3547 *4*	D FGHI K	5/2+	47 keV 7 % p = 100 % IT < 4.3E-6

We can use the parameters listed in compilations like NNDC directly.

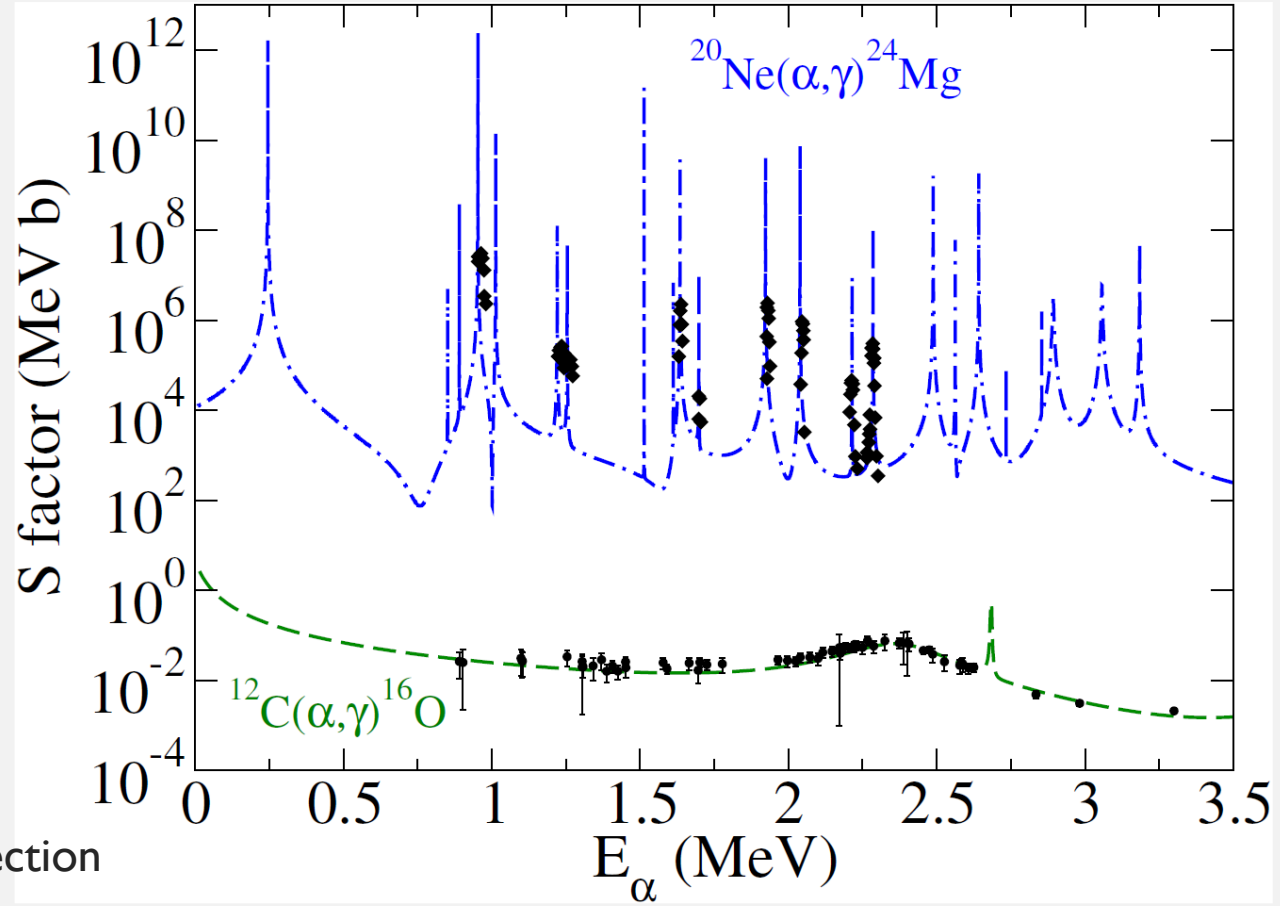
THE IMPORTANCE OF ADDITIONAL CONSTRAINTS

- The phenomenological R-matrix theory only 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, e.g. few data with poorly understood level structure, then you need to be very careful about your claims (uncertainties)
  - "More careful" usually equals "Many more calculations to test different assumptions".
- The inclusion of additional information from nuclear structure / theory helps a lot, if it is available.



WHAT KIND OF REACTIONS ARE APPLICABLE FOR *R*-MATRIX?

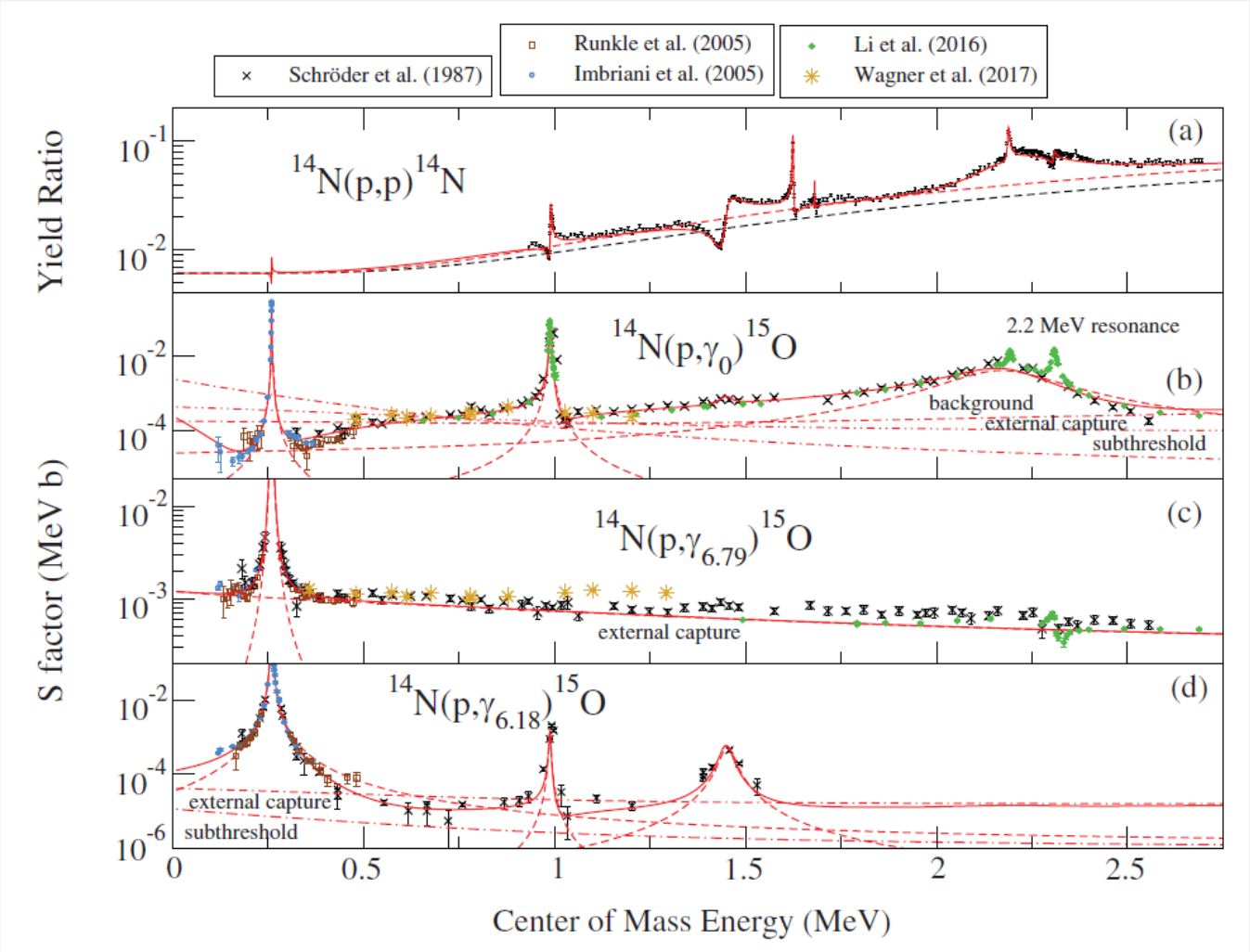
- Usually Compound Nucleus
  - Two step reactions (a+A → C* → b+B)
    - No three body yet…
  - Usually nucleon – nucleon reactions
    - But can also be extended to capture (a+A → C* + γ)
    - And even (C* + β → b+B)
- Usually low energy
  - Low angular momentum dominates
- Usually low level density
  - Practical limitations
- Useful when broad resonances are present in the cross section



RADIATIVE CAPTURE

- We very often need to analyze radiative capture data
- Because this is an E&M interaction, it is not a viable channel for standard R-matrix
- 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)
  - Asymptotic Normalization Coefficient (ANC) gives the magnitude of the direct capture
  - **See the many works by Akram Mukhamedzhanov**

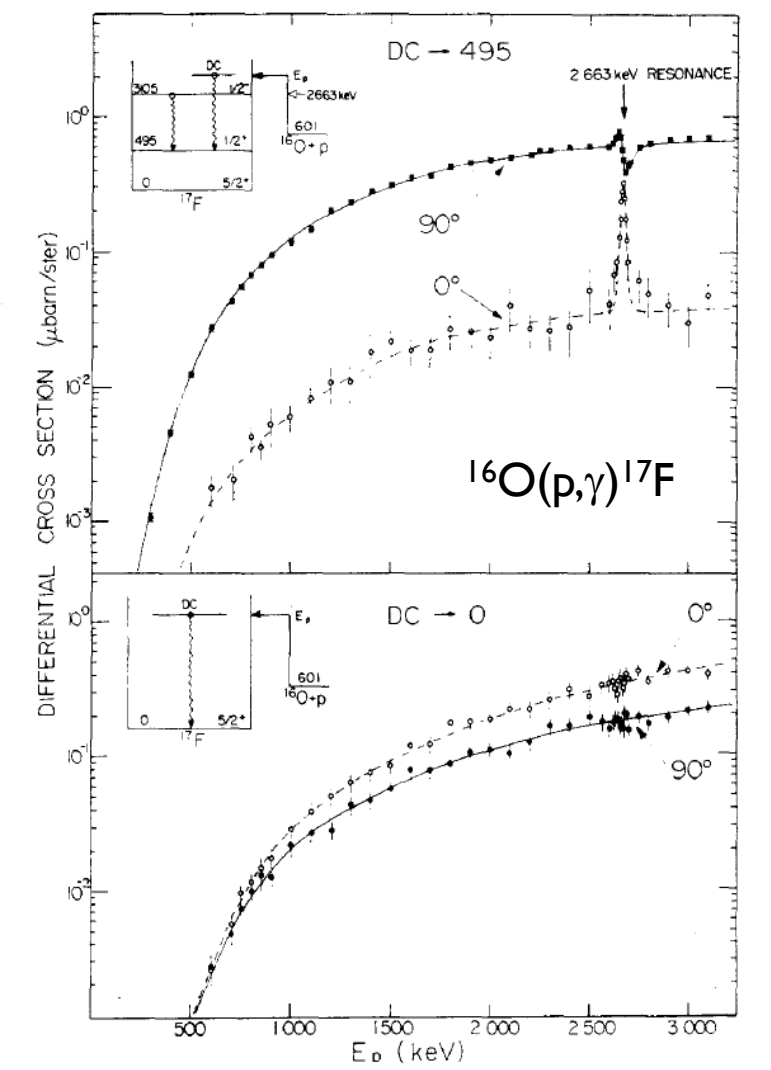
$$C_{\lambda c} = \frac{(2m_a a_c)^{1/2}}{\hbar W_c(a_c)} \frac{\gamma_{\lambda c}}{[1+\sum_{c'}\gamma_{\lambda c'}^2 (dS_{c'}/dE)(E_\lambda)]^{1/2}},$$

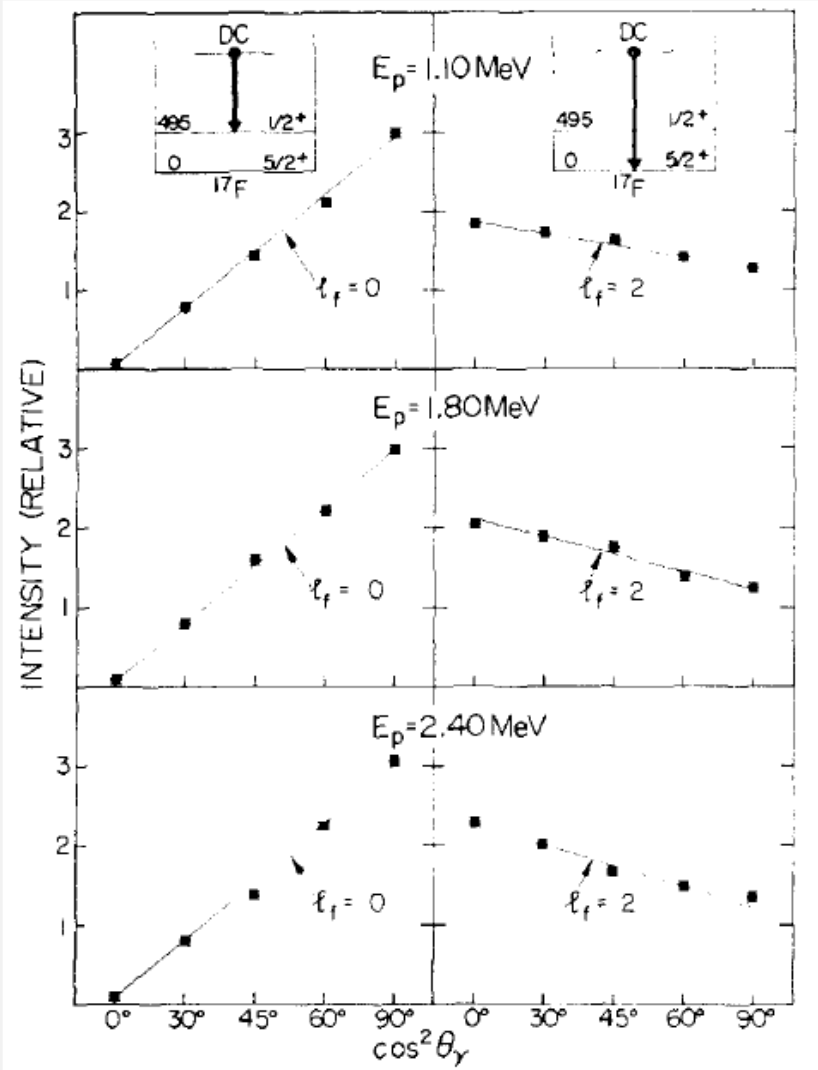


Acharya *et al.* (2025), Solar Fusion III

RADIATIVE DIRECT OR COMPOUND CAPTURE?

- Coulomb penetrability energy dependance



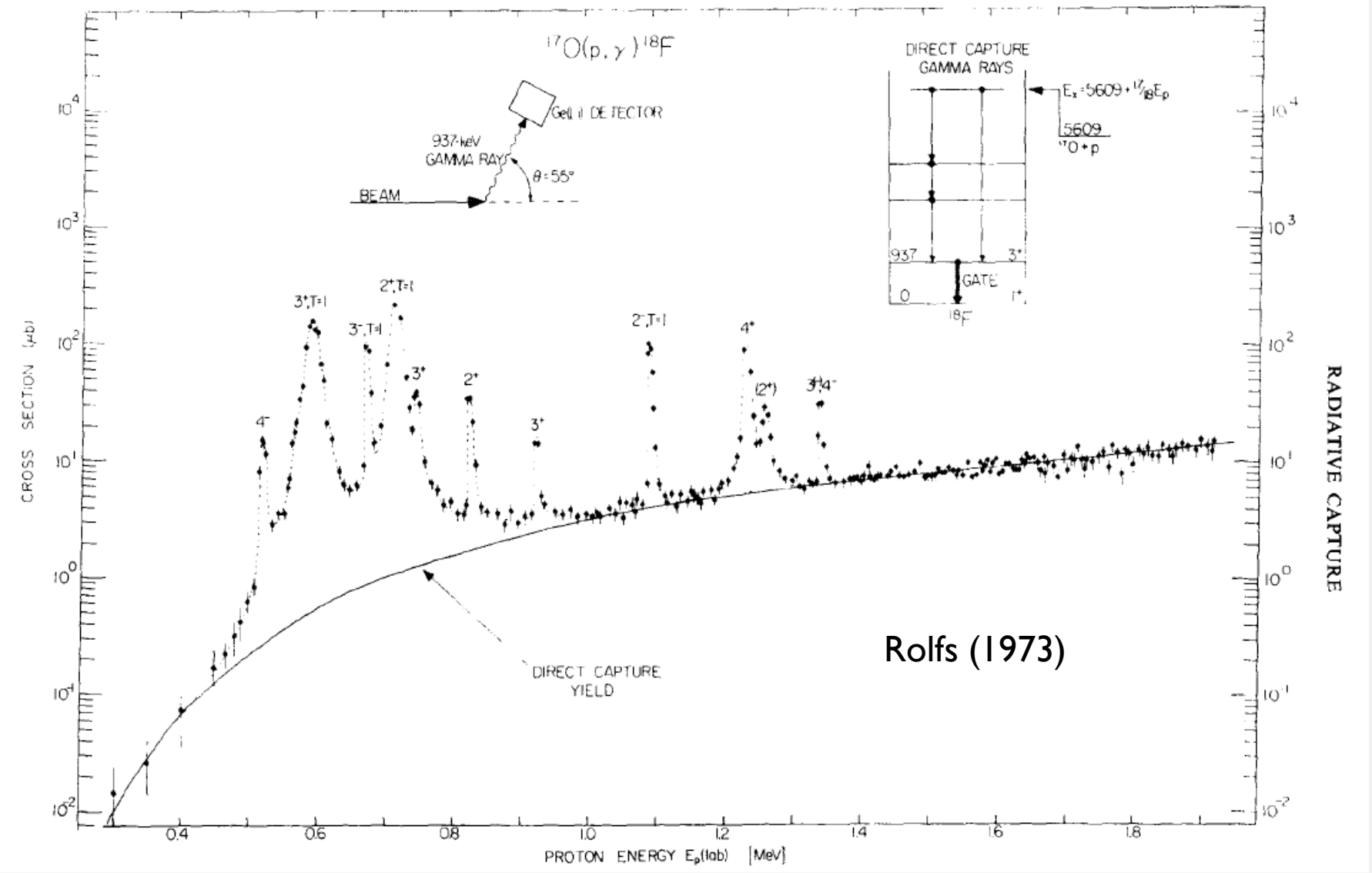


Rolfs (1973), DC model

- Characteristic angular distributions

$$W(\vartheta) = \sin^2\vartheta$$

A COMMON CASE: NARROW RESONANCE SUPERIMPOSED ON A DC BACKGROUND



Rolfs (1973)

The ANC connection

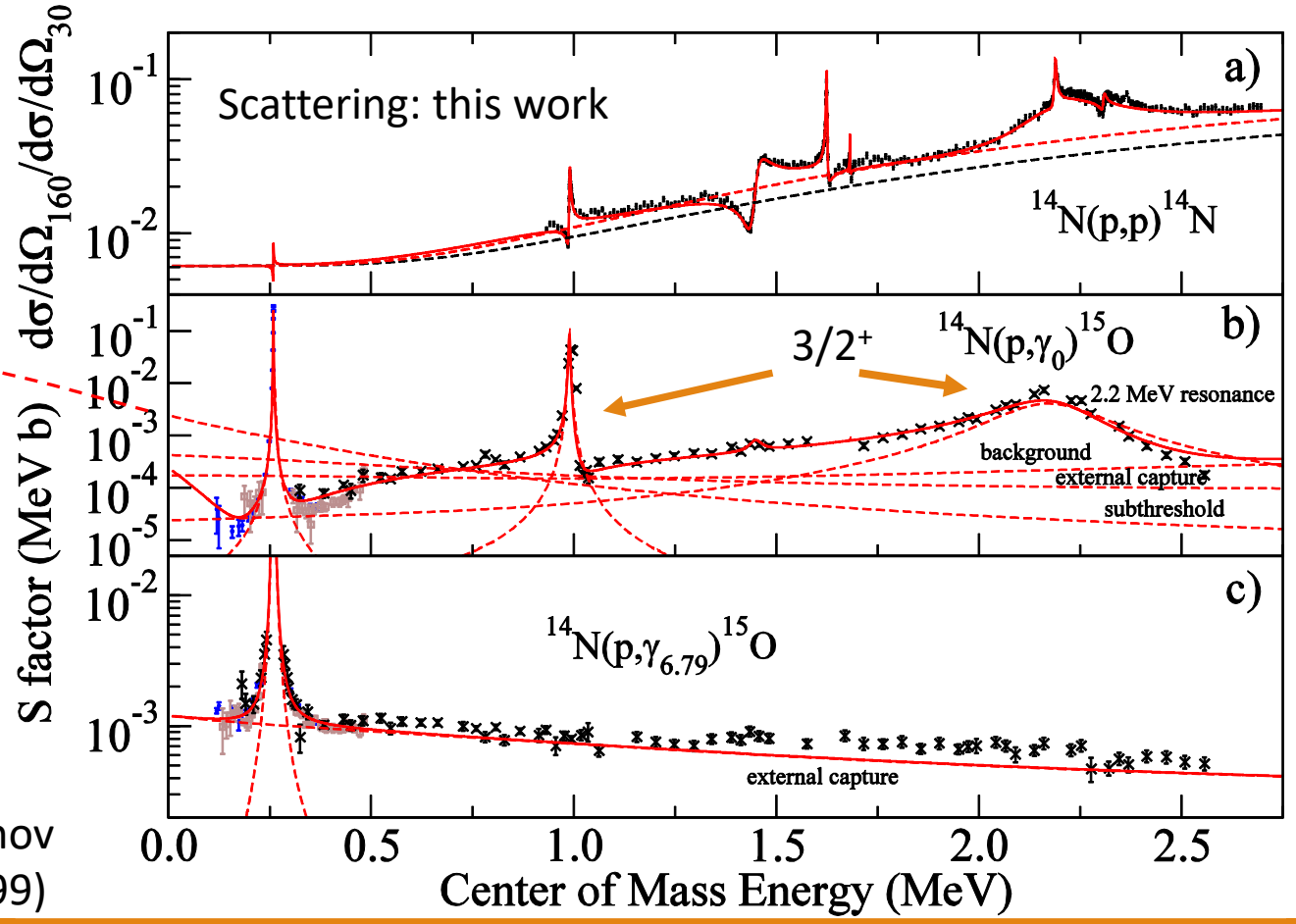
Subthreshold
Width **ANC$_p$**

E_R = -0.51 MeV
$J^\pi = 3/2^+$

Subthreshold
Width **ANC$_p$**
Height $\Gamma_{\gamma 0}$

Strength of the
Direct Capture
ANC$_p$

Mukhamedzhanov
and Tribble (1999)



R-matrix Contributions to the cross section

- Resonances (Γ_p, Γ_γ, E)
- Subthreshold states (ANCs, γ-decays)
- Direct Capture (ANCs)

Capture: Imbriani et al. (2005), Runkle et al. (2005), Schroeder et al. (1987)

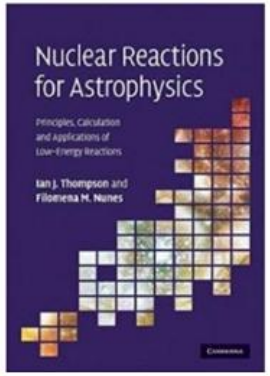
ASIDE: ANCS CAN BE OBTAINED FROM TRANSFER DATA THROUGH POTENTIAL MODEL ANALYSIS

COMPUTER CODES

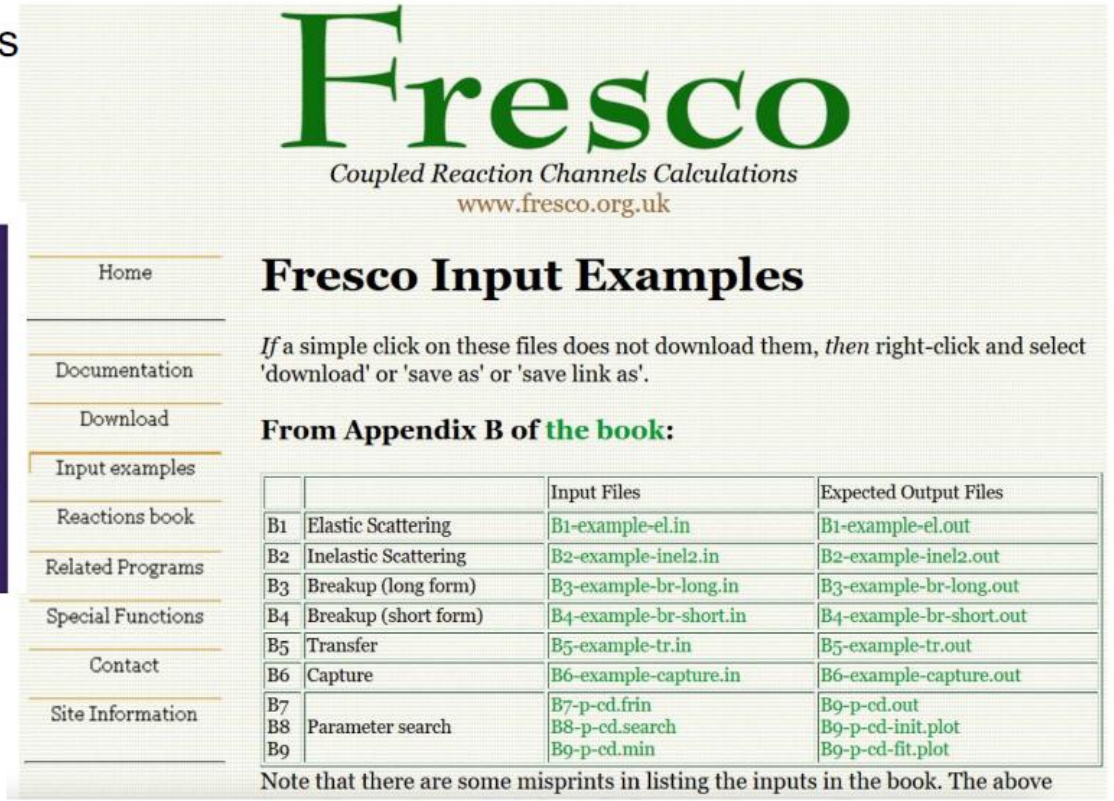
TECHNISCHE UNIVERSITÄT DARMSTADT

FRESCO developped by I. Thompson, Surrey, is an open source software for transfer and (in)elastic reactions

- DWBA, CCBA, CRC
- Non relativistic
- Widely used in the community
- Details in book:
- www.fresco.org.uk



Other codes exist and are accessible: DWUCK (old), ECIS (Dirac equations, relativistic) for DWBA.



Fresco

Coupled Reaction Channels Calculations

www.fresco.org.uk

Home | Documentation | Download | Input examples | Reactions book | Related Programs | Special Functions | Contact | Site Information

Fresco Input Examples

If a simple click on these files does not download them, *then* right-click and select 'download' or 'save as' or 'save link as'.

From Appendix B of the book:

		Input Files	Expected Output Files
B1	Elastic Scattering	B1-example-el.in	B1-example-el.out
B2	Inelastic Scattering	B2-example-inel2.in	B2-example-inel2.out
B3	Breakup (long form)	B3-example-br-long.in	B3-example-br-long.out
B4	Breakup (short form)	B4-example-br-short.in	B4-example-br-short.out
B5	Transfer	B5-example-tr.in	B5-example-tr.out
B6	Capture	B6-example-capture.in	B6-example-capture.out
B7 B8 B9	Parameter search	B7-p-cd.frin B8-p-cd.search B9-p-cd.min	B9-p-cd.out B9-p-cd-init.plot B9-p-cd-fit.plot

Note that there are some misprints in listing the inputs in the book. The above

ASIDE: FITTING TRANSFER DATA WITH R-MATRIX

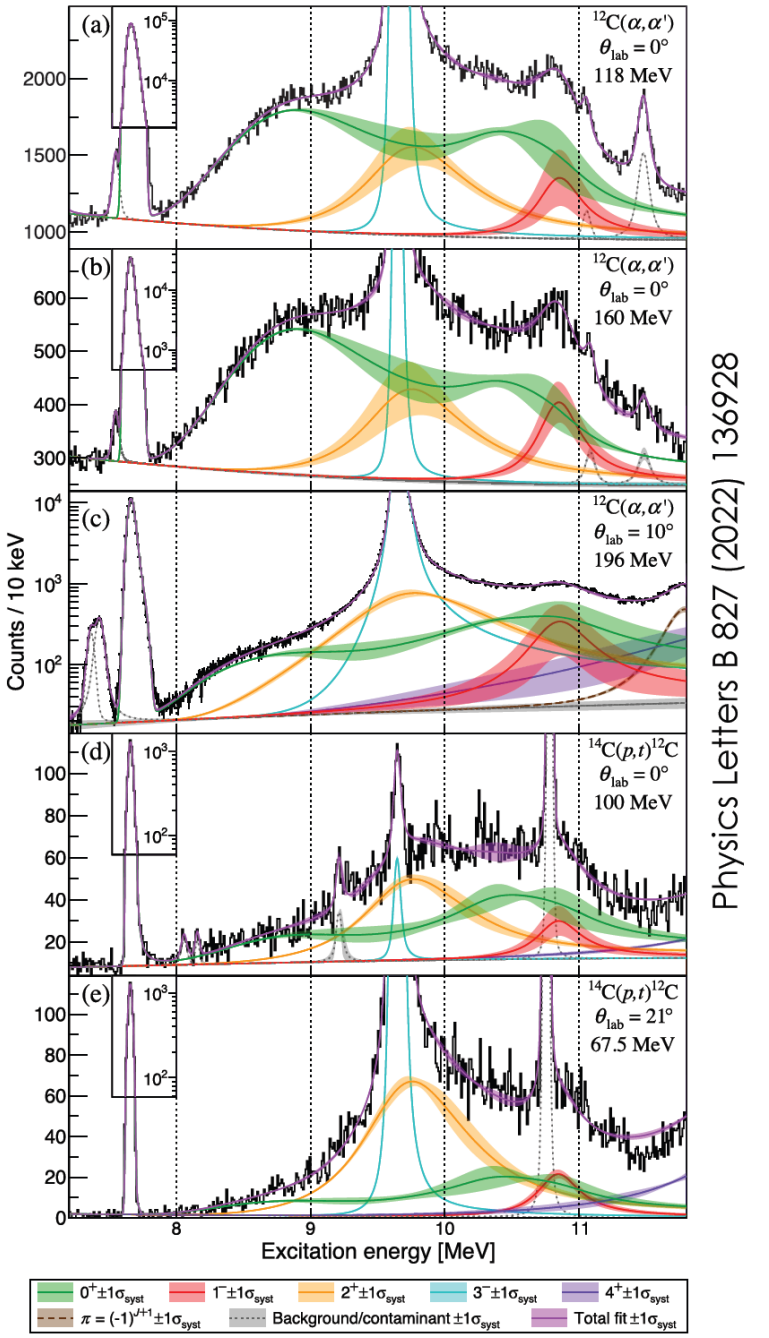
- Transfer spectra can be fit with R-matrix theory
  - and some would argue that it really should be because interference can be important
- Can be implemented using a perturbative approach, where the feeding amplitudes are treated as free parameters and are essentially the same as the reduced widths
- Kevin C.W. Li at University of Oslo is doing a lot of work in this area

$$N_{ab,c}(E) = P_c \left| \sum_{\lambda,\mu}^{N} G^{\frac{1}{2}}_{\lambda ab} \gamma_{\mu c} A_{\lambda\mu} \right|^2$$

For 1 level:

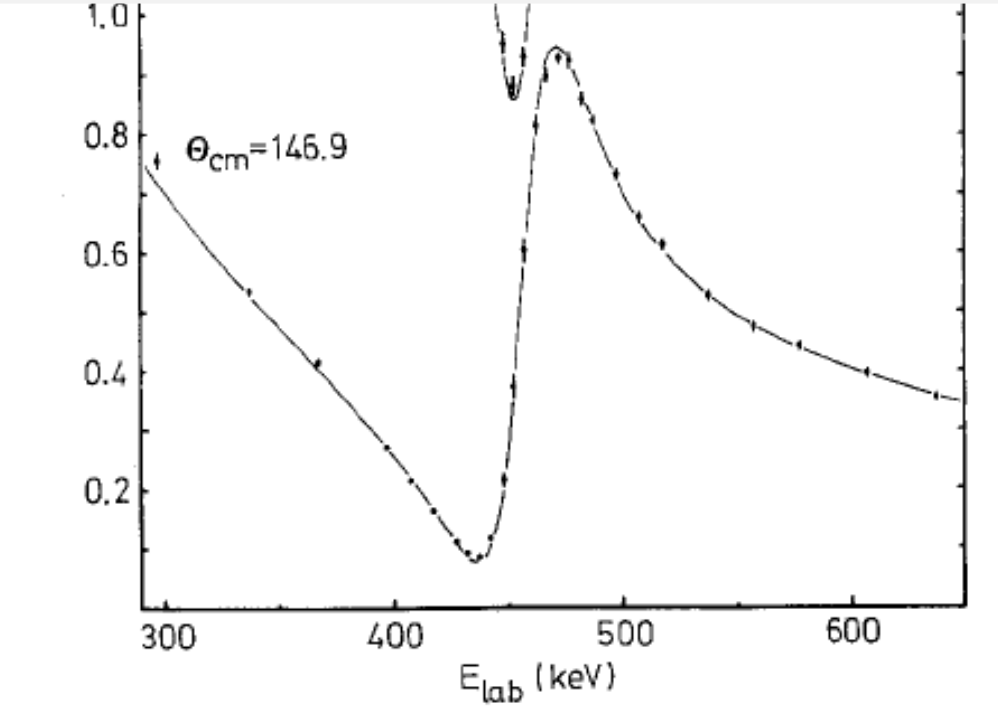
$$N_{ab,c}(E) = \frac{G_{ab}\,\Gamma_c}{(E - E_r - \Delta)^2 + \frac{1}{4}\Gamma^2},$$

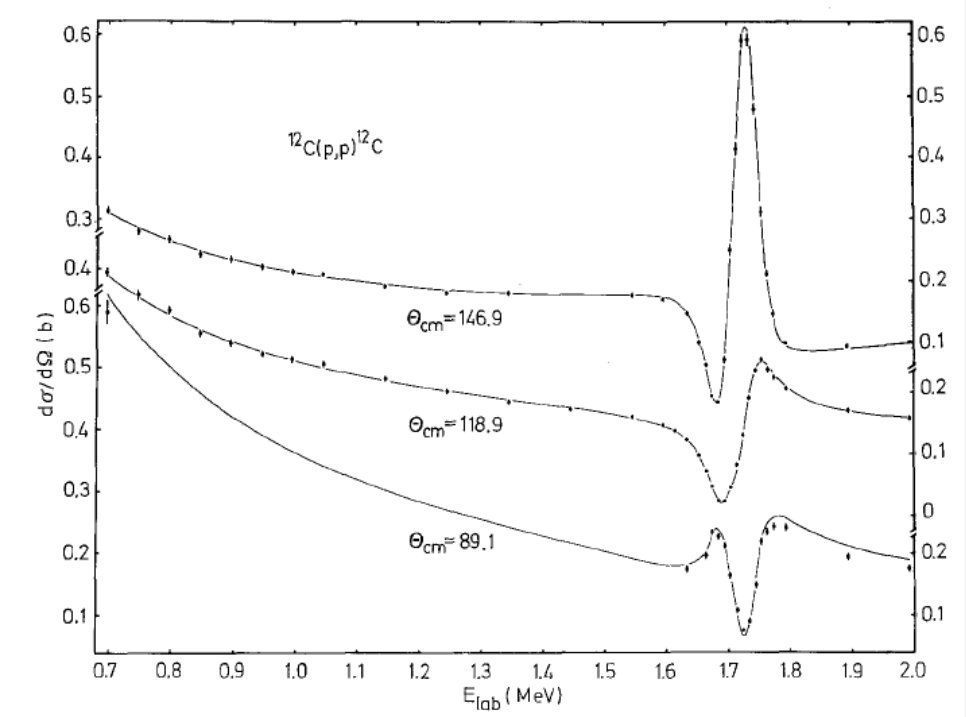
$G^{1/2}_{\lambda ab}$: feeding amplitude, should be related to the scattering amplitude



Physics Letters B 827 (2022) 136928

A PHENOMENOLOGICAL R-MATRIX ANALYSIS EXAMPLE: $^{12}C(p,p)^{12}C$ AND $^{12}C(p,\gamma)^{13}N$

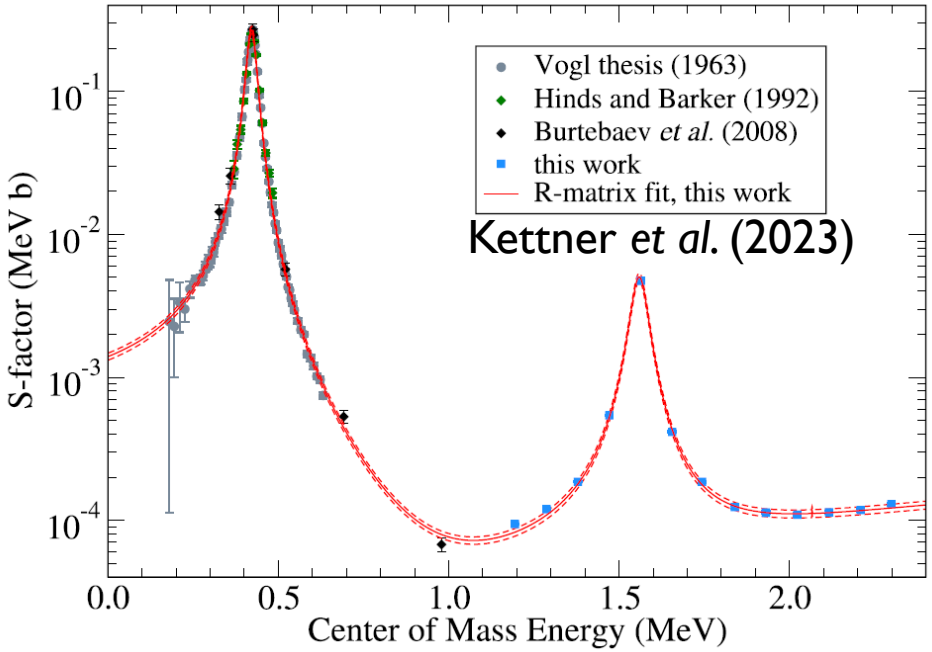


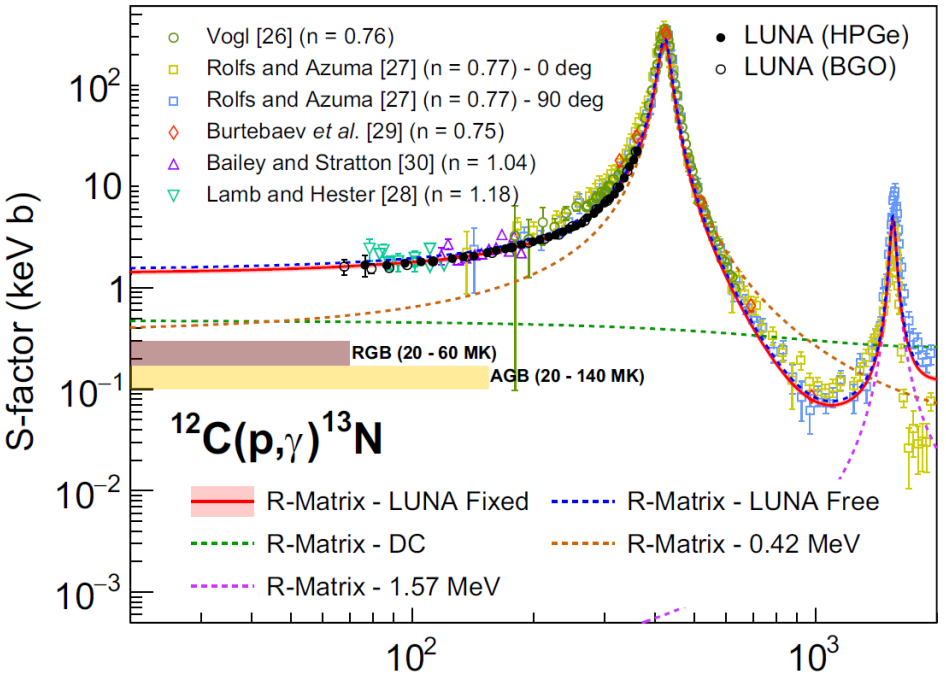


- E_{lab} of resonances are about 450 keV and 1.73 MeV
- $E_{c.m.} = E_{lab} \times M_H / (M_H + M_L) = E_{lab} \times 12 / (12+ 1.007276) = 415$ keV and 1.60 MeV
- $E_x = E_{c.m.} + S_i = E_{c.m.} + 1.9435$ MeV = 2.3585 or 3.5435 MeV

DATA FOR $^{12}C(p,\gamma)$

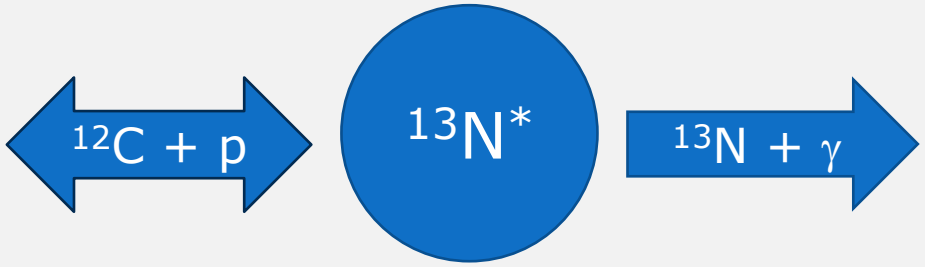
- Resonances observed at a similar energy in radiative capture studies
- New measurements from LUNA, Notre Dame, Felsenkeller and ATOMKI
- A very nice collection of updated cross sections, that are more consistent with each other, span a wide energy range and have more precise uncertainty quantification





Skowronski *et al.* (2023)

LEVEL STRUCTURE OF ^{13}N REVIEW



- **An ideal case for R-matrix**
- Low level density
- Isolated set of levels near threshold
- Resonances are broad enough to easily measure but not too broad so that their shape can't be easily discerned

E_{level} (keV)	XREF	Jπ	$T_{1/2}$
0.0	A DE GHIJKLM	1/2-	9.965 m *4* % ε = 100
2364.9 *6*	DEFGHI K	1/2+	31.7 keV *8* % IT = 0.00158 *13* % p = 100
3502 *2*	A DEFGHIJK	3/2-	62 keV *4* % IT = 0.0011 % p = 100
3547 *4*	D FGHI K	5/2+	47 keV *7* % p = 100 % IT < 4.3E-6
6364 *9*	CD FGH KL	5/2+	11 keV % p = 100
6886 *8*	CD FGH K	3/2+	115 keV *5* % p = 100
7155 *5*	CD FGH K	7/2+	9.0 keV *5* % p = 100
7376 *9*	A CD FGHIJKL	5/2-	75 keV *5* % p = 100
7900	FG	3/2+	≈ 1500 keV % p = 100
8918 *11*	A D FG IJ L	1/2-	230 keV % p = 100
9000	C GH J	9/2+	280 keV *30*
9476 *8*	A CD FGH J	3/2-	30 keV % p = 100
1025E+1 *15*	E	(1/2+)	≈ 280 keV % IT = ? % p = ?
10360	A CD FGH	5/2-	30 keV % p = 100

Sp = 1.9435 MeV

Almost 3 MeV gap

NNDC.BNL.GOV

LOW ENERGY LEVEL STRUCTURE OF ^{13}N FROM NNDC

XREFs ☑ J^{π} ☑ $T_{1/2}$/Decay ☑ E(γ) ☑ I(γ) ☑ M(γ) ☑ Final Levels ☑

E(level) (keV)	XREF	J^{π}(level)	$T_{1/2}$(level)	E(γ) (keV)	I(γ)	M(γ)	Final Levels
0.0	ABCD F LMNOPQ UVWXYZabcdefghijklmnopqrstuvwxyz01234	1/2-	9.9584 m *36* % ε = 100				
2367.8 *8*	LM OP S UV XY b def jkl rstu x z0 23	1/2+	34.5 keV *3*	≈2367.7	100	[E1]	0.0 1/2-
3500.4 *8*	A CDE LMNOP S UV XYZ f h jklm rst v x z012	3/2-	55.0 keV *6*	1135.6 3500.3	8.4 100	[E1] [M1+E2]	2367.8 1/2+ 0.0 1/2-
3544.5 *5*	E LM O S UV XYZab def h jk r t 0 2	5/2+	49.0 keV *5*				

- Now that we have a better idea of what excitation energies we have we can try to identify the corresponding resonances (Ex = 2.3585 or 3.5435 MeV)
- We could see two resonances but there are actually three levels around the energies we are looking for!
- The first one is well separated so our estimated level at 2.3585 MeV must correspond to the one at 2.3678 MeV in the table. We can also see that the width is reasonable, some 10's of keV that we could also estimate from the cross section curve

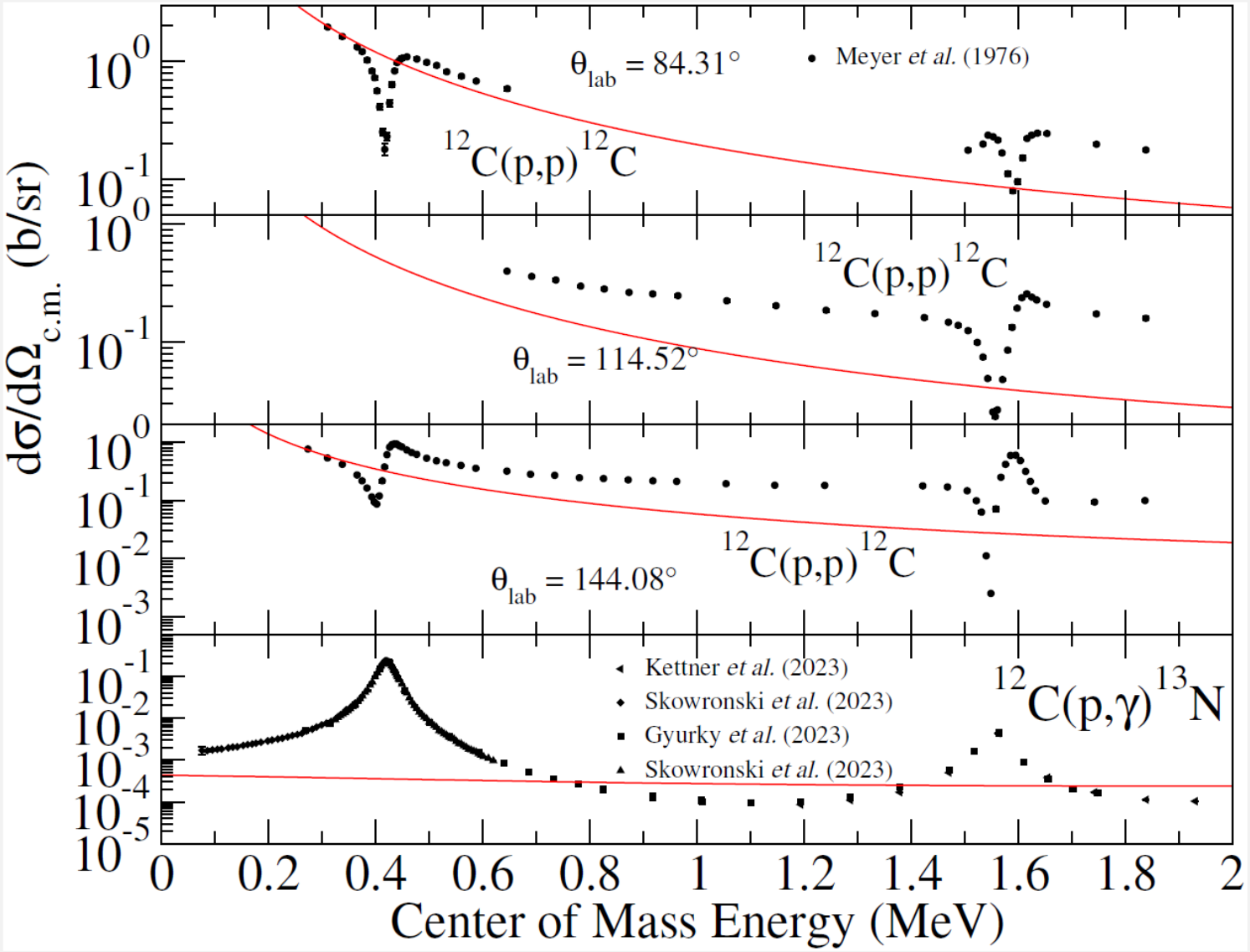
LOW ENERGY LEVEL STRUCTURE OF ^{13}N FROM NNDC

XREFs ☑ | J^{π} ☑ | $T_{1/2}$/Decay ☑ | E(γ) ☑ | I(γ) ☑ | M(γ) ☑ | Final Levels ☑

E(level) (keV)	XREF	J^{π}(level)	$T_{1/2}$(level)	E(γ) (keV)	I(γ)	M(γ)	Final Levels
0.0	ABCD F LMNOPQ UVWXYZabcdefghijklmnopqrstuvwxyz01234	1/2-	9.9584 m *36* % ε = 100				
2367.8 *8*	LM OP S UV XY b def jkl rstu x z0 23	1/2+	34.5 keV *3*	≈2367.7	100	[E1]	0.0 1/2-
3500.4 *8*	A CDE LMNOP S UV XYZ f h jklm rst v x z012	3/2-	55.0 keV *6*	1135.6 3500.3	8.4 100	[E1] [M1+E2]	2367.8 1/2+ 0.0 1/2-
3544.5 *5*	E LM O S UV XYZab def h jk r t 0 2	5/2+	49.0 keV *5*				

- We guessed that our other level was at about 3.5435 MeV
- The table gives two levels at 3.5004 and 3.5445 MeV.
- The second one seems to be closer to the energy we guessed, but both have widths that seem to be comparable and similar to the width we might guess (again some 10's of keV roughly)
- We'll put both into our calculation and see what happens

INDIVIDUAL CONTRIBUTIONS: COULOMB SCATTERING AND RADIATIVE DIRECT CAPTURE

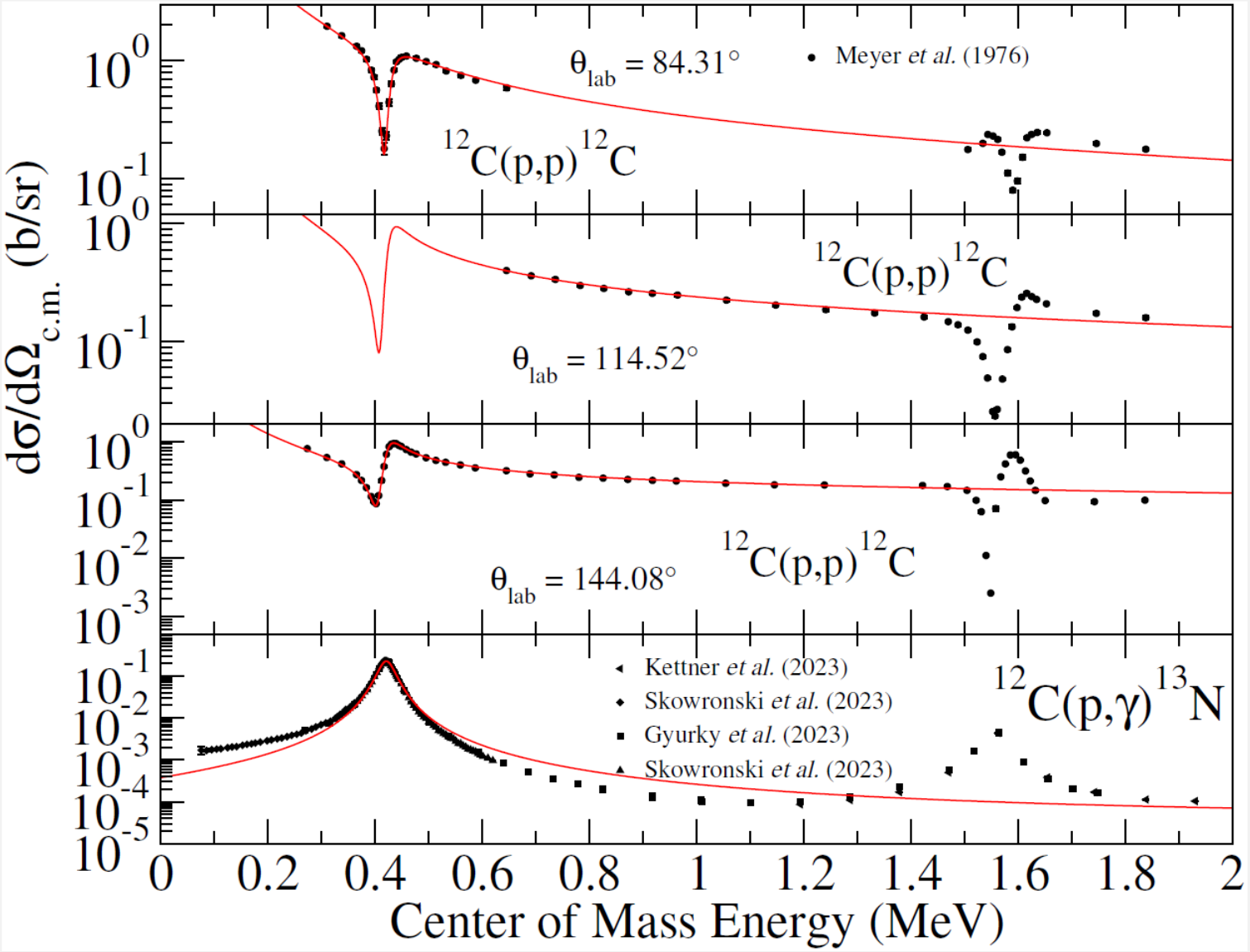


E_{level} (keV)	XREF	Jπ	$T_{1/2}$
0.0	A DE GHIJKLM	1/2-	9.965 m *4* % ε = 100
2364.9 *6*	DEFGHI K	1/2+	31.7 keV *8* % IT = 0.00158 *13* % p = 100
3502 *2*	A DEFGHIJK	3/2-	62 keV *4* % IT = 0.0011 % p = 100
3547 *4*	D FGHI K	5/2+	47 keV *7* % p = 100 % IT < 4.3E-6
6364 *9*	CD FGH KL	5/2+	11 keV % p = 100
6886 *8*	CD FGH K	3/2+	115 keV *5* % p = 100

Level parameters:

- Ground state proton ANC = 1.65 $fm^{-1/2}$
- Where does it come from?
  - Fits to this data
  - Proton transfer measurements (direct reaction studies)

INDIVIDUAL CONTRIBUTIONS: LOWEST ENERGY PROTON-UNBOUND LEVEL

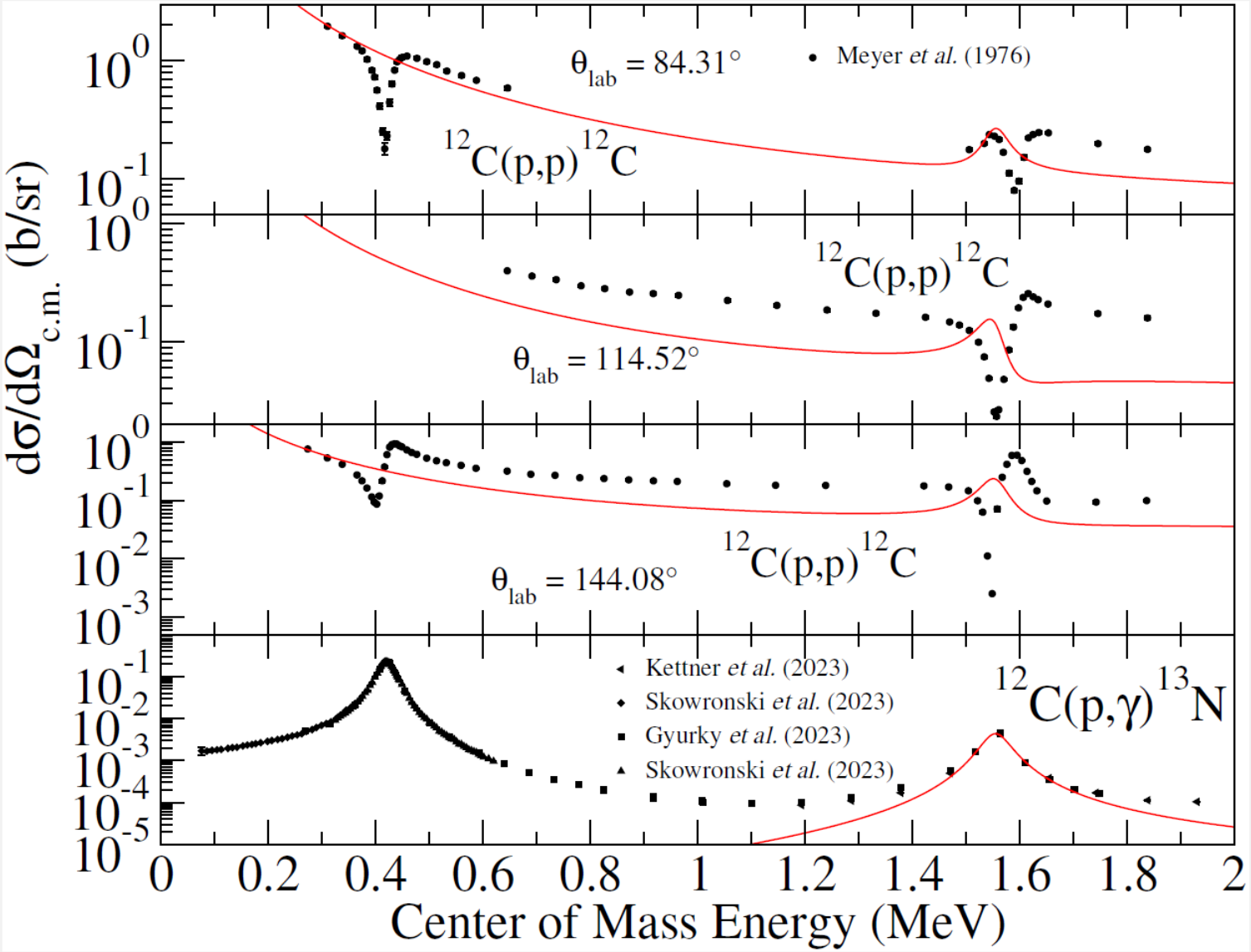


E_{level} (keV)	XREF	Jπ	$T_{1/2}$
0.0	A DE GHIJKLM	1/2-	9.965 m *4* % ε = 100
2364.9 *6*	DEFGHI K	1/2+	31.7 keV *8* % IT = 0.00158 *13* % p = 100
3502 *2*	A DEFGHIJK	3/2-	62 keV *4* % IT = 0.0011 % p = 100
3547 *4*	D FGHI K	5/2+	47 keV *7* % p = 100 % IT < 4.3E-6
6364 *9*	CD FGH KL	5/2+	11 keV % p = 100
6886 *8*	CD FGH K	3/2+	115 keV *5* % p = 100

Level parameters:

- First excited state J^{π}, E, proton width, γ-width
- Where do they come from?
  - Fits to this data
  - Many other measurements

INDIVIDUAL CONTRIBUTIONS: SECOND EXCITED STATE

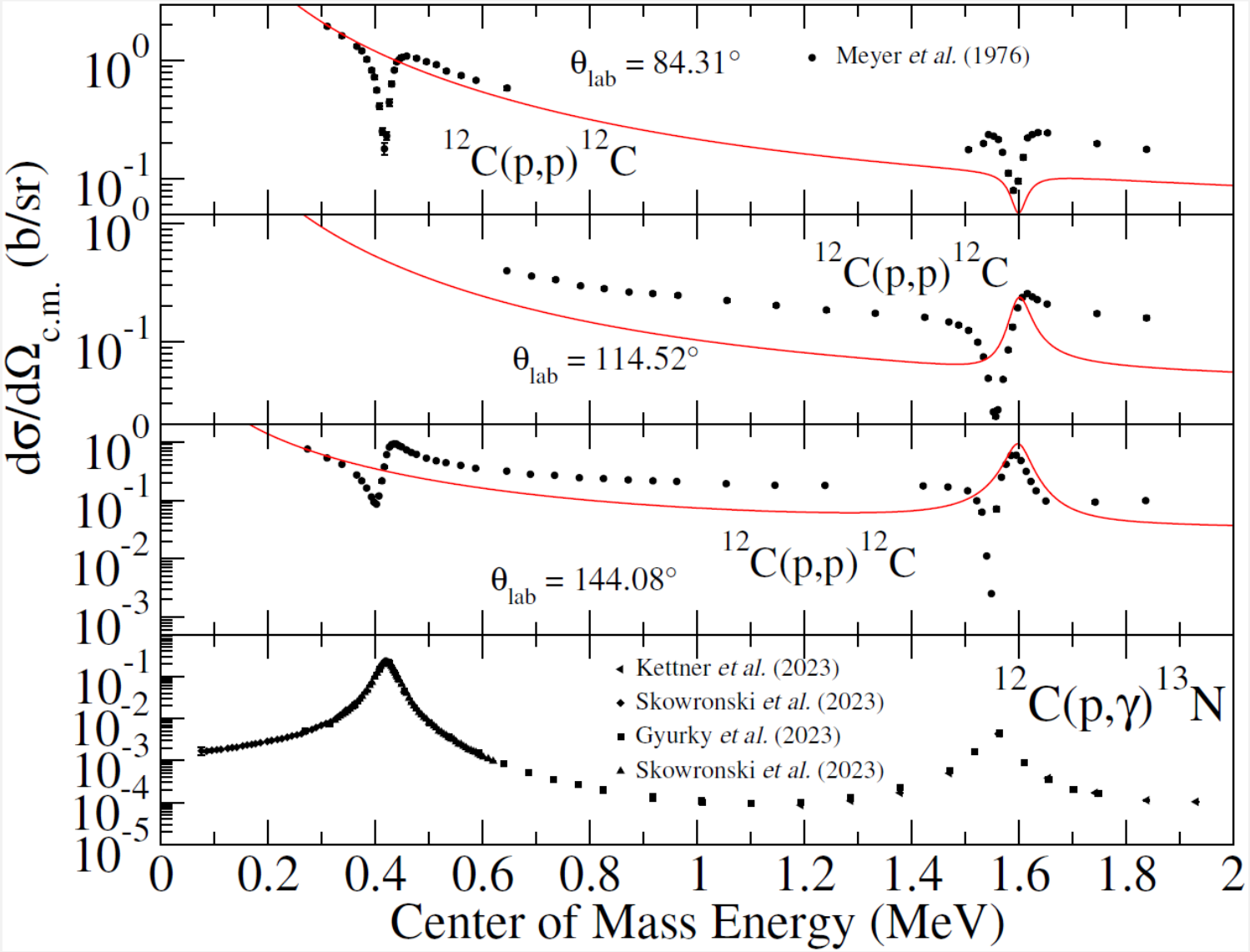


E_{level} (keV)	XREF	Jπ	$T_{1/2}$
0.0	A DE GHIJKLM	1/2-	9.965 m *4* % ε = 100
2364.9 *6*	DEFGHI K	1/2+	31.7 keV *8* % IT = 0.00158 *13* % p = 100
3502 *2*	A DEFGHIJK	3/2-	62 keV *4* % IT = 0.0011 % p = 100
3547 *4*	D FGHI K	5/2+	47 keV *7* % p = 100 % IT < 4.3E-6
6364 *9*	CD FGH KL	5/2+	11 keV % p = 100
6886 *8*	CD FGH K	3/2+	115 keV *5* % p = 100

Level parameters:

- First excited state J^{π}, E, proton width, γ-width
- Where do they come from?
  - Fits to this data
  - Many other measurements

INDIVIDUAL CONTRIBUTIONS: THIRD EXCITED STATE

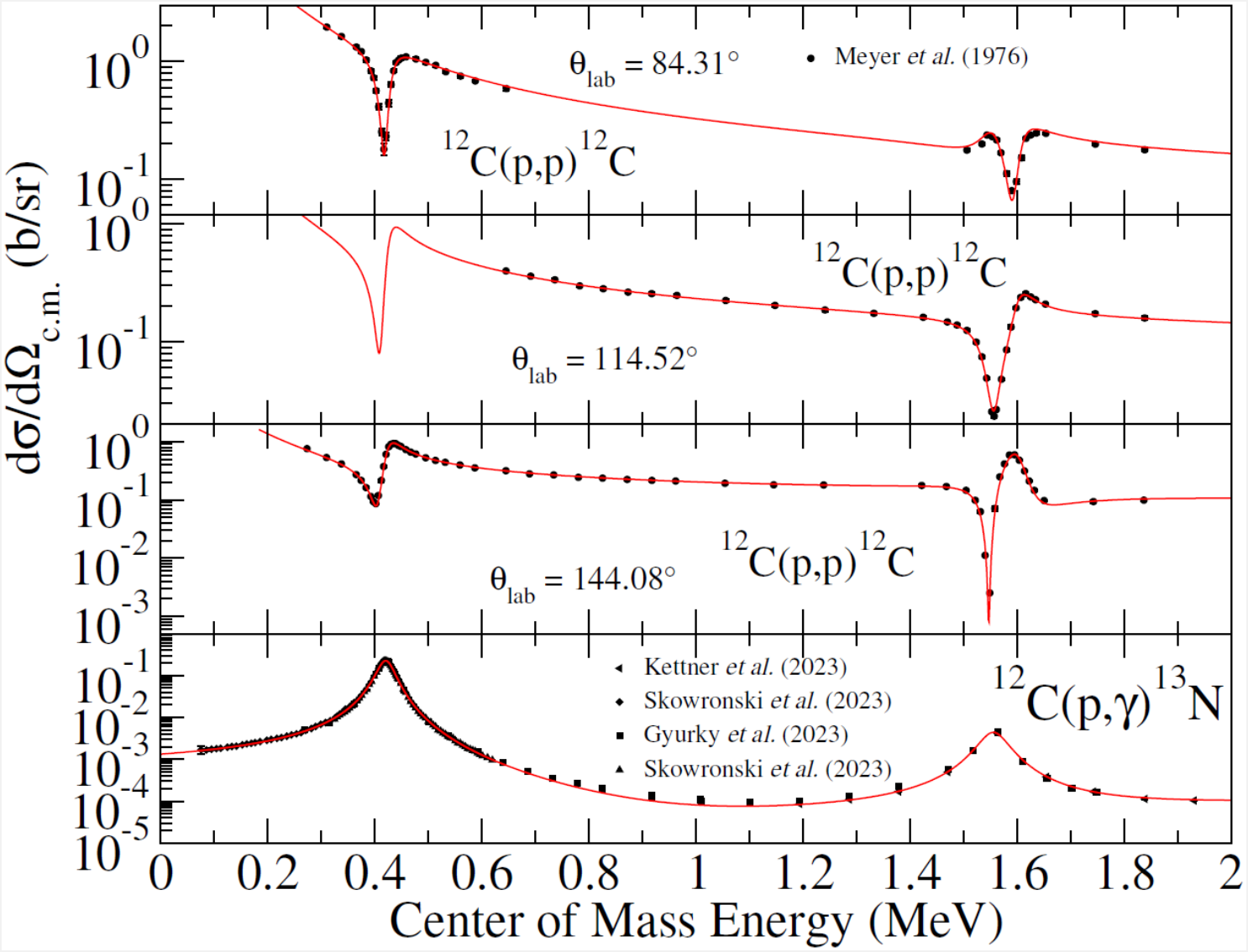


E_{level} (keV)	XREF	Jπ	$T_{1/2}$
0.0	A DE GHIJKLM	1/2-	9.965 m *4* % ε = 100
2364.9 *6*	DEFGHI K	1/2+	31.7 keV *8* % IT = 0.00158 *13* % p = 100
3502 *2*	A DEFGHIJK	3/2-	62 keV *4* % IT = 0.0011 % p = 100
3547 *4*	D FGHI K	5/2+	47 keV *7* % p = 100 % IT < 4.3E-6
6364 *9*	CD FGH KL	5/2+	11 keV % p = 100
6886 *8*	CD FGH K	3/2+	115 keV *5* % p = 100

Level parameters:

- First excited state J^{π}, E, proton width, γ-width
- Where do they come from?
  - Fits to this data
  - Many other measurements

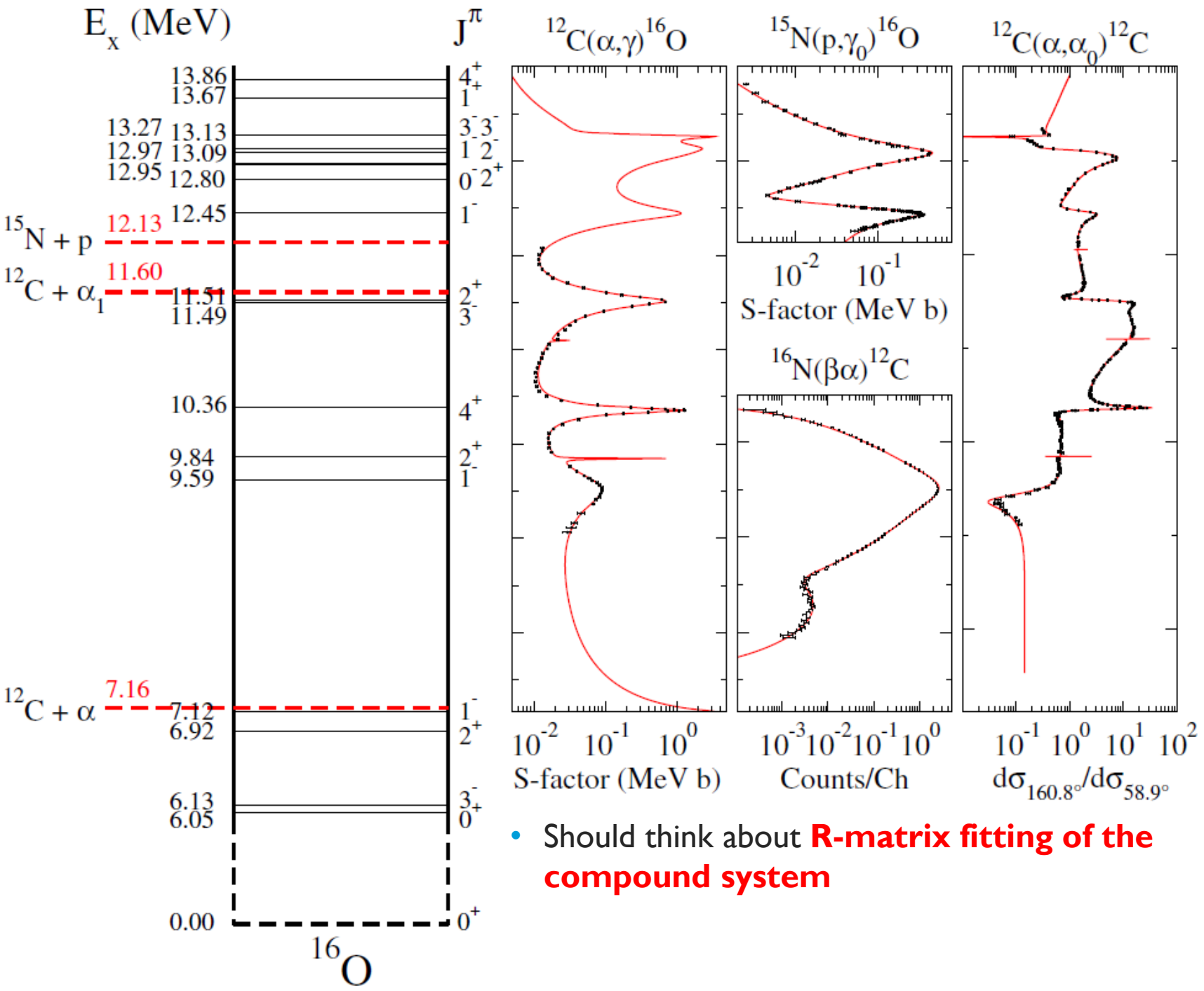
INDIVIDUAL CONTRIBUTIONS: ALL CONTRIBUTIONS



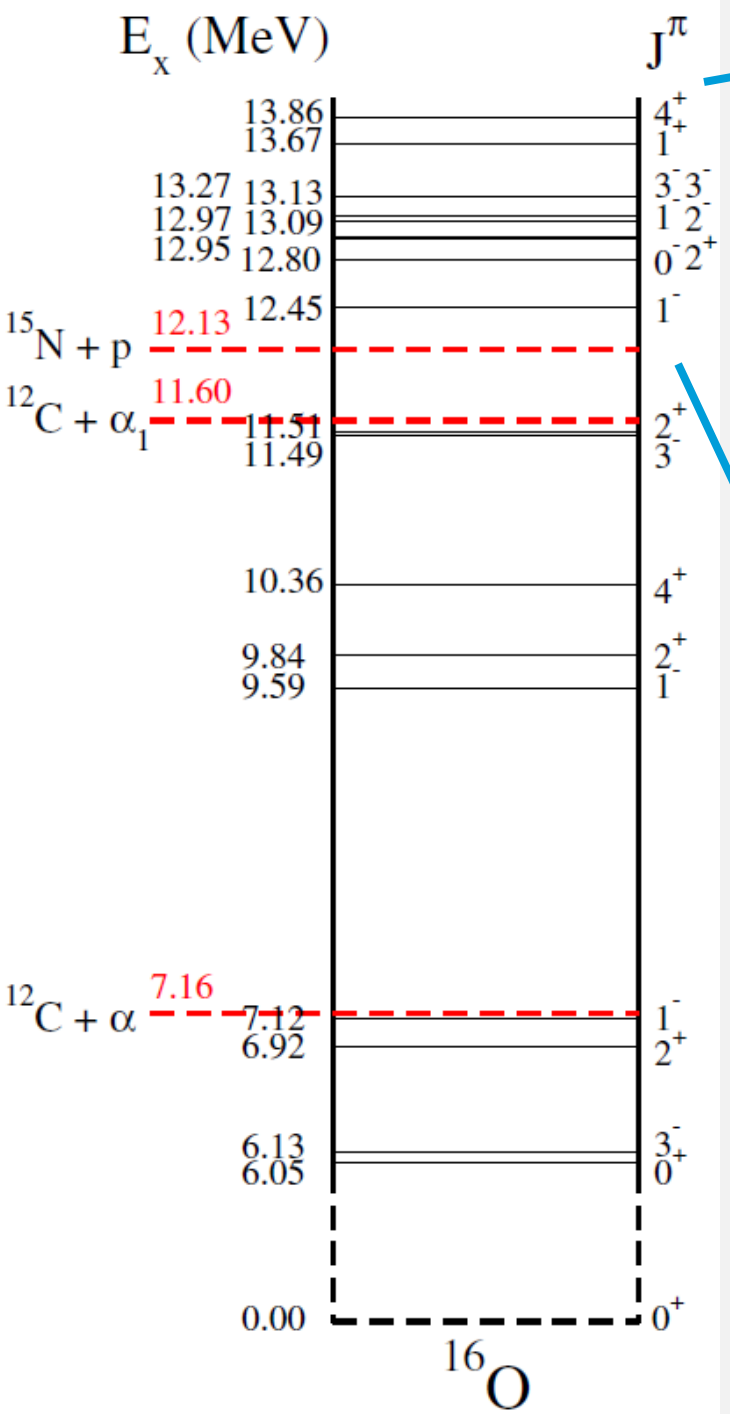
E_{level} (keV)	XREF	Jπ	$T_{1/2}$
0.0	A DE GHIJKLM	1/2-	9.965 m *4* % ε = 100
2364.9 *6*	DEFGHI K	1/2+	31.7 keV *8* % IT = 0.00158 *13* % p = 100
3502 *2*	A DEFGHIJK	3/2-	62 keV *4* % IT = 0.0011 % p = 100
3547 *4*	D FGHI K	5/2+	47 keV *7* % p = 100 % IT < 4.3E-6
6364 *9*	CD FGH KL	5/2+	11 keV % p = 100
6886 *8*	CD FGH K	3/2+	115 keV *5* % p = 100

Level parameters:

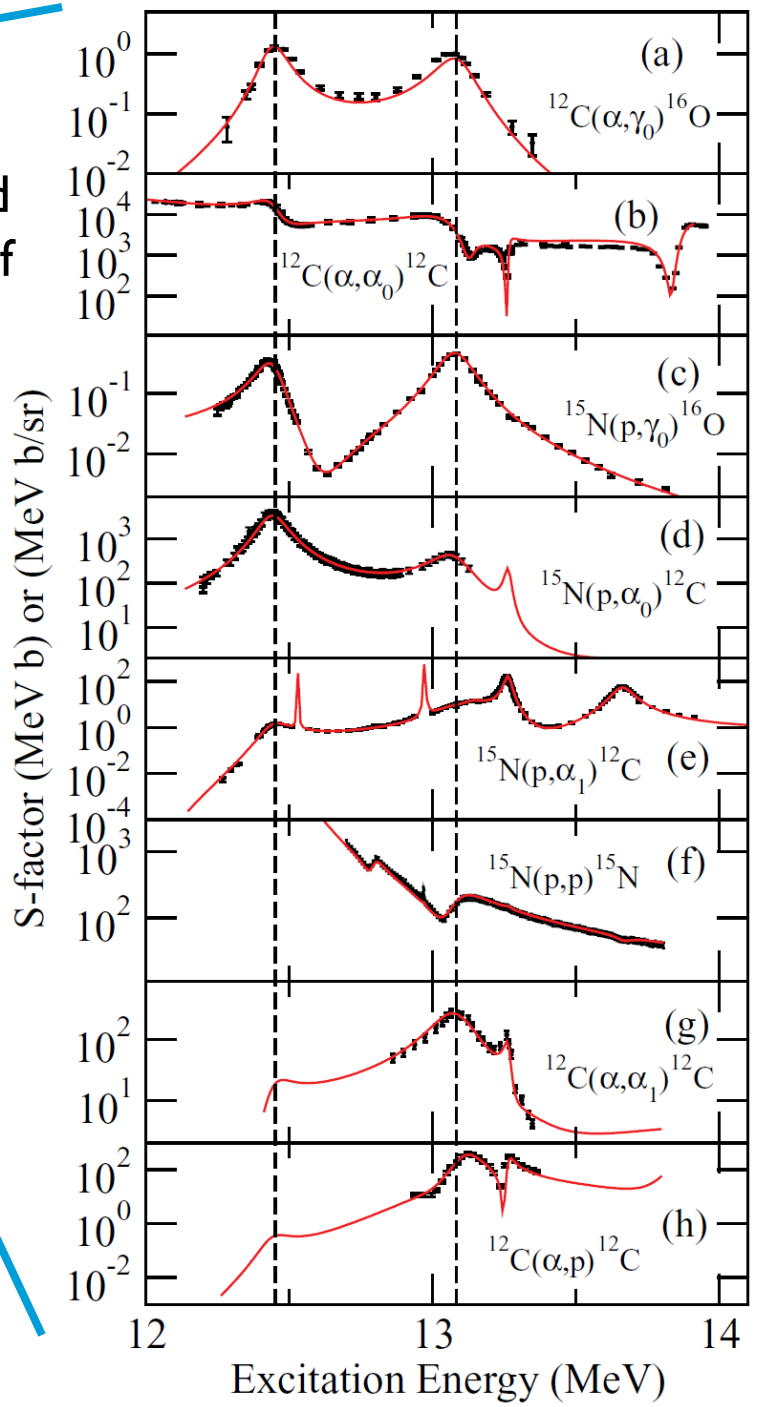
- First excited state J^{π}, E, proton width, γ-width, ANC
- Note that to extract accurate values for each of the level parameters from this data, this fit is about the minimum amount of complexity



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



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



WE HAVE OUR MODEL, BUT NOW WE MUST MATCH IT TO DATA

- Problem: We don't really measure cross sections in the laboratory, **we measure experimental yields**

$$F(E_0) = \int_{E_0-\Delta}^{E_0} \int_{E=-\infty}^{+\infty} \frac{\sigma(E')}{\epsilon(E')} g(E - E_0) dE' dE \tag{5}$$

where $\sigma(E')$ is the cross section devoid of experimental effects. The function $g(E' - E)$ is the *spreading* function that represents the energy distribution of the beam particles and the function $\epsilon(E')$ is the stopping cross section that represents the energy distribution resulting from beam particle scattering within the target. The function $F(E_0)$ is the final simulated spectrum where E_0 is the mean beam energy.

- Convolution functions need to be evaluated, this often drastically increases computation times

EXPERIMENTAL RESOLUTION

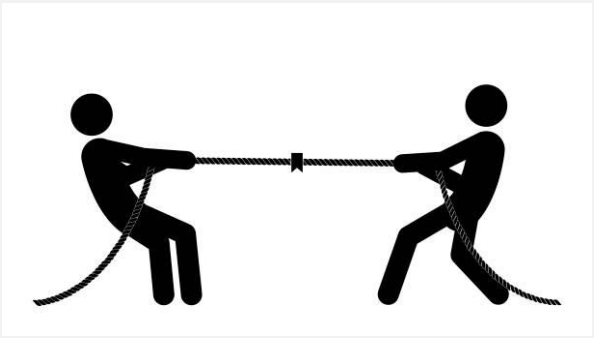
- We are often limited in our experimental resolution by practical constraints
- Target thickness vs resolution

Thin target yield approximation

$$A = \sigma N_b N_t \varepsilon$$

σ = cross section
N_b = number of beam particles
N_t = number of target atoms
ε = detection efficiency
A = counts you see in your detector

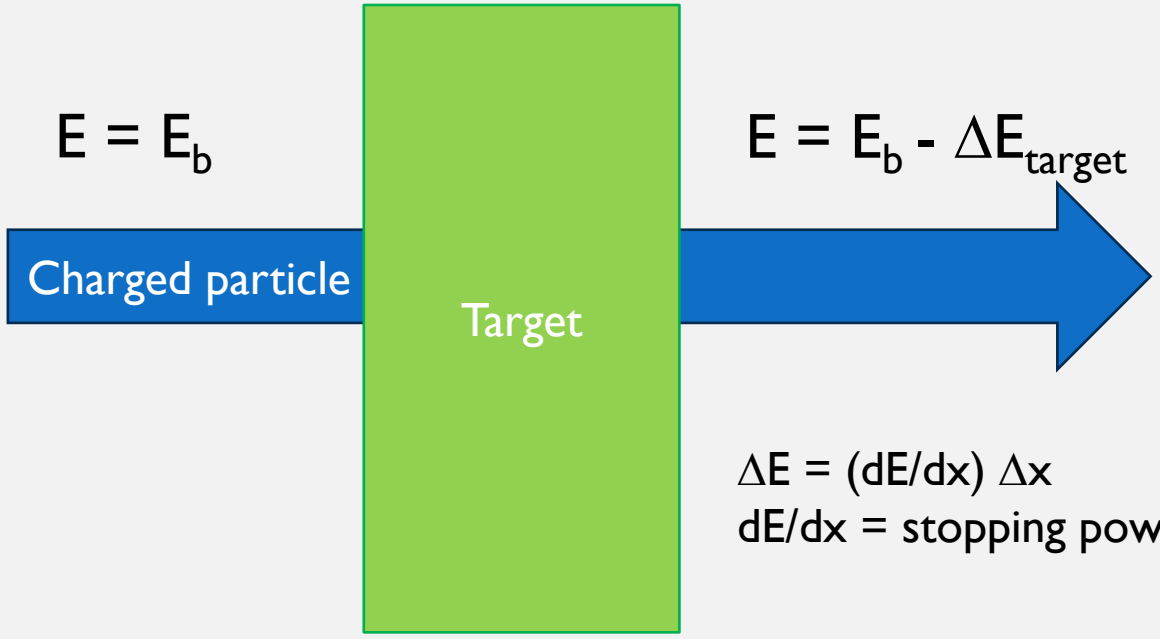
An infinitely **thin** target is needed for perfect resolution



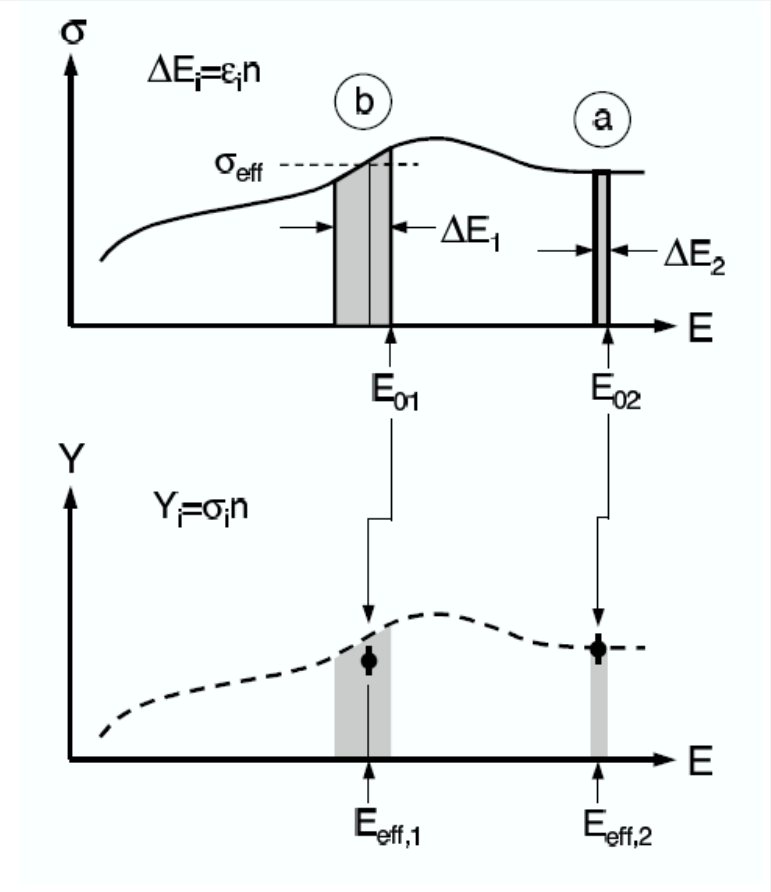
An infinitely **thick** target is needed to maximize the count rate in your detector

BEAM ENERGY LOSS THROUGH A TARGET

- Your particle beam (protons, α particles, etc.) loose energy as they pass through your target due, primarily, with collisions with electrons
  - Atomic stopping powers (are tabulated, difficult to model)



Iliadis' book



CONVOLUTION OF THEORY WITH EXPERIMENTAL RESOLUTION

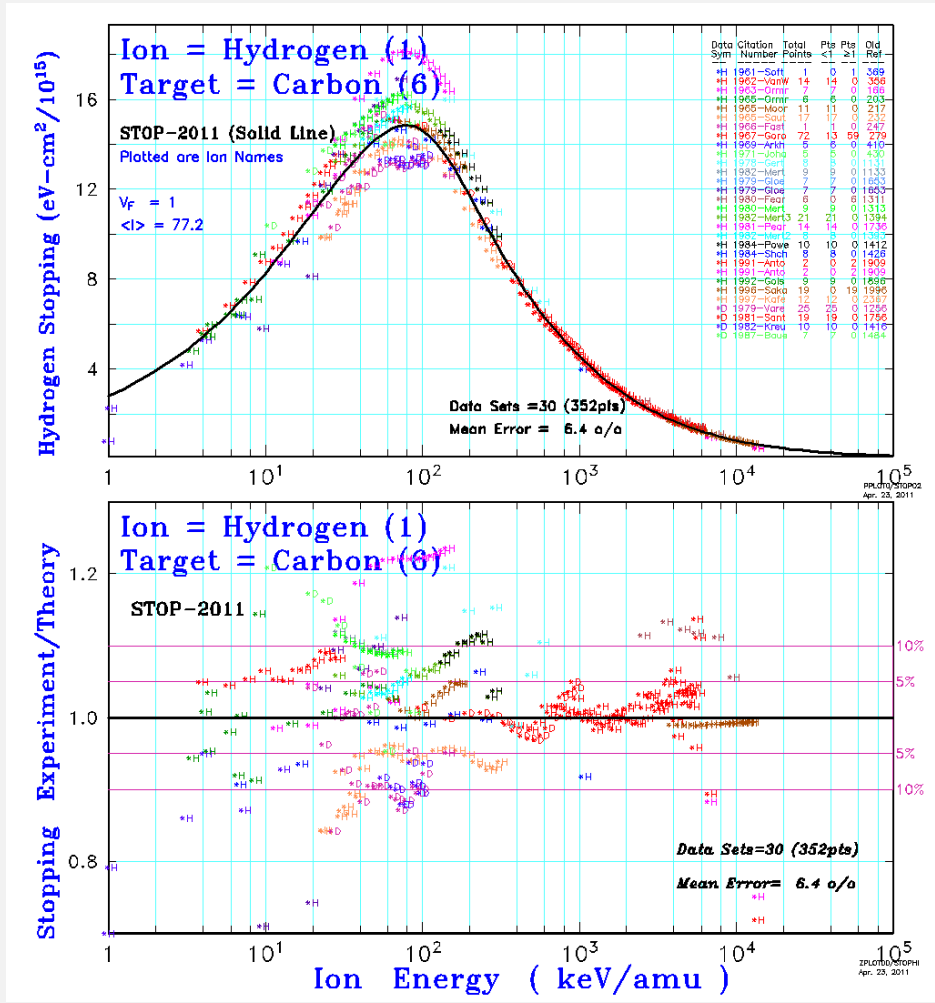
- We need to apply these resolution effects to the theory calculation to accurately compare with the data
- Convolution integral

$$F(E_0) = \int_{E_0-\Delta}^{E_0} \int_{E=-\infty}^{+\infty} \frac{\sigma(E')}{\epsilon(E')} g(E - E_0) dE' dE$$

$g(E' - E)$ is the spreading function

$\epsilon(E')$ is the stopping power

Protons stopping in carbon, srim.org



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}N+n measurements from the literature
- Computationally expensive! ☹

Example: TOF resolution function

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

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

ToF resolution approximation

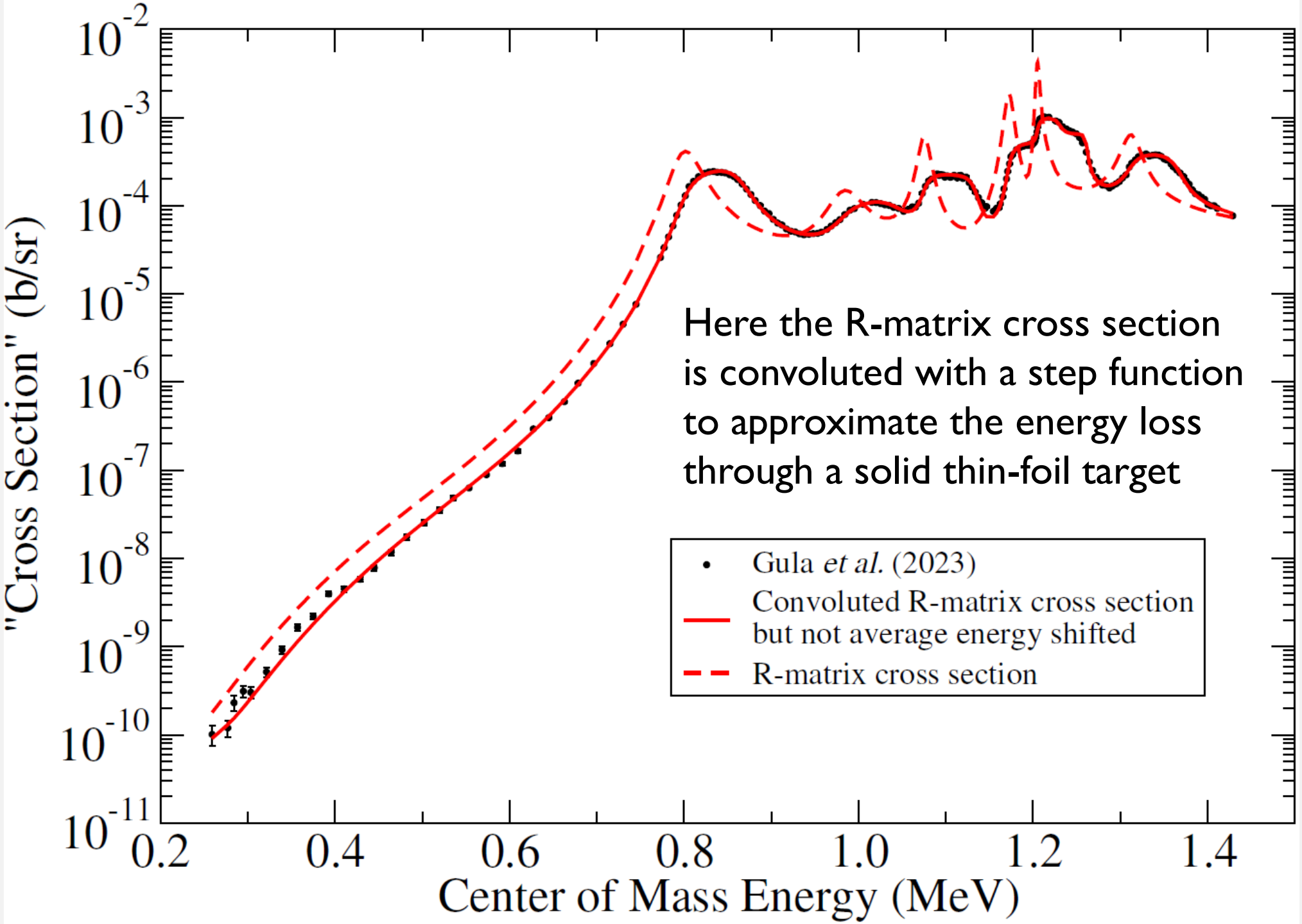
$$\sigma_b(E-\varepsilon) = 2(E-\varepsilon)\left(\left(\frac{dL}{L}\right)^2 + \left(\frac{dt}{L}\right)^2 \left(\frac{2c^2}{m_n c^2}\right)(E-\varepsilon)\right)^{1/2}$$

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

Charged particle energy loss plus straggling

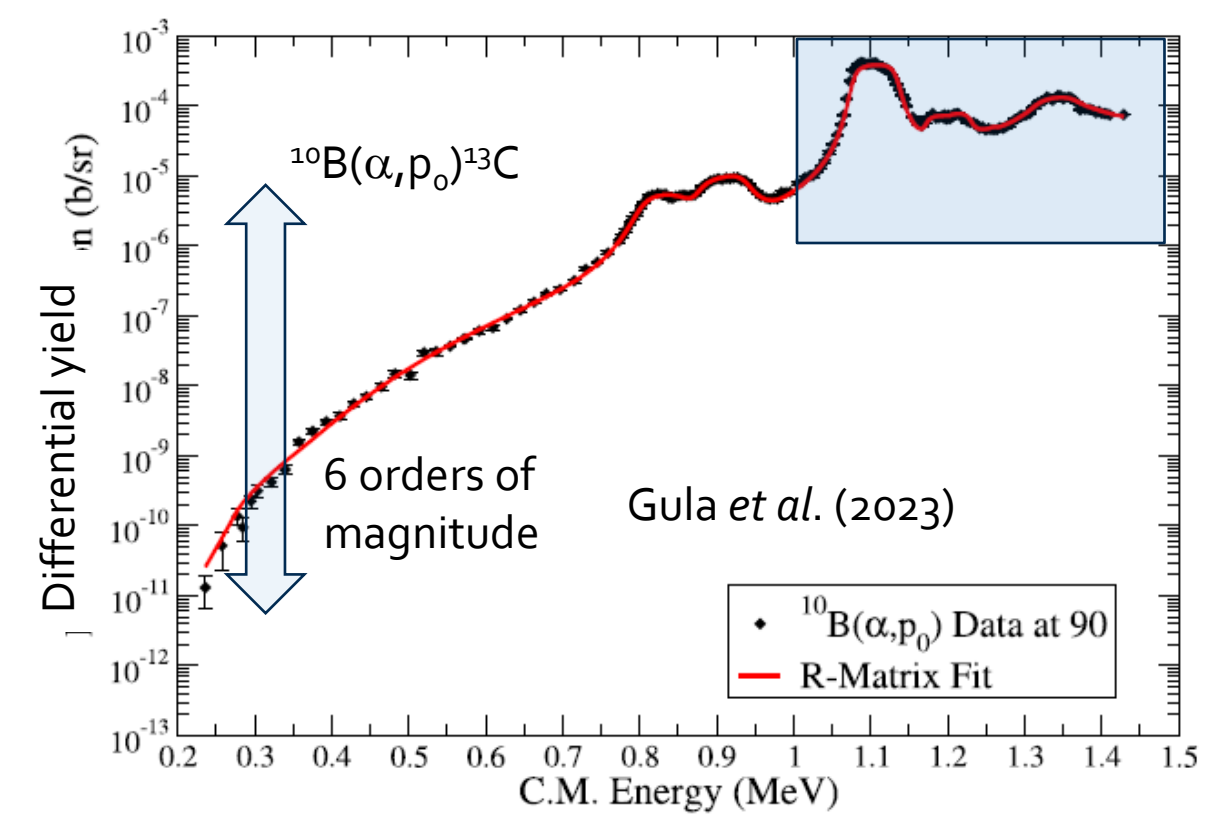
$$\sigma_{str}(E) = \alpha_{str}\sqrt{E_0 - E}$$

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


"Cross Section" (b/sr)
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
10^-8
10^-9
10^-10
10^-11
0.2
0.4
0.6
0.8
1.0
1.2
1.4
Center of Mass Energy (MeV)
Here the R-matrix cross section is convoluted with a step function to approximate the energy loss through a solid thin-foil target
Gula et al. (2023)
Convoluted R-matrix cross section but not average energy shifted
R-matrix cross section

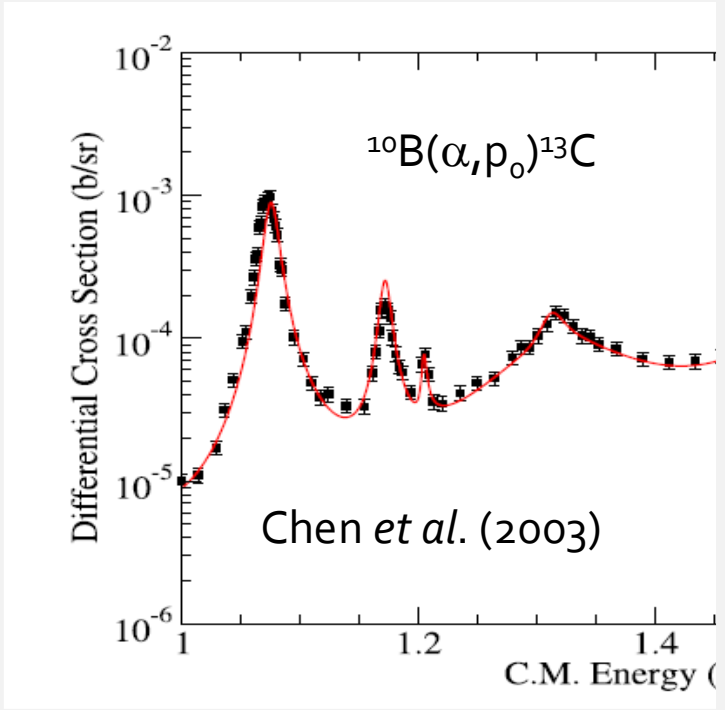
RESOLUTION DUE TO TARGET THICKNESS

Thick target, 50 µg/cm²



Significant resolution distortion

Thin target, 0.035 µg/cm²



Negligible resolution distortion

STRAGGLING

1.05 MeV resonance in $^{13}C(\alpha,n)^{16}O$
10.2(10) ug/cm^2

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

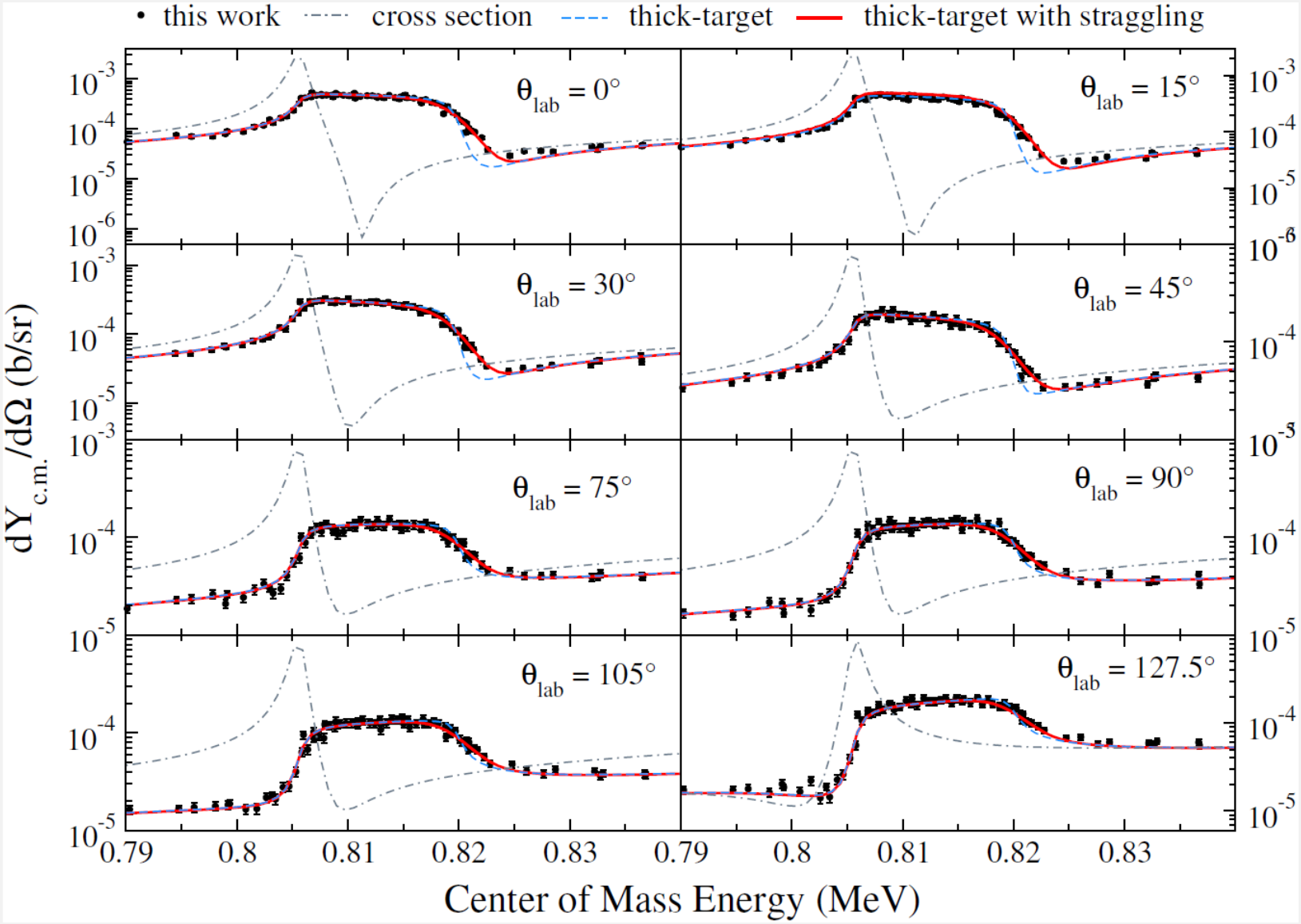
Step function for energy loss

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

Gaussian part for straggling

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

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

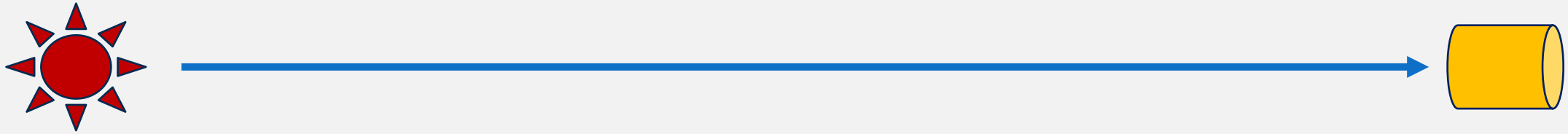


NEUTRON TIME OF FLIGHT

Source
Beam buncher (dt)

Time of flight distance (dL)

Detector thickness (dL)



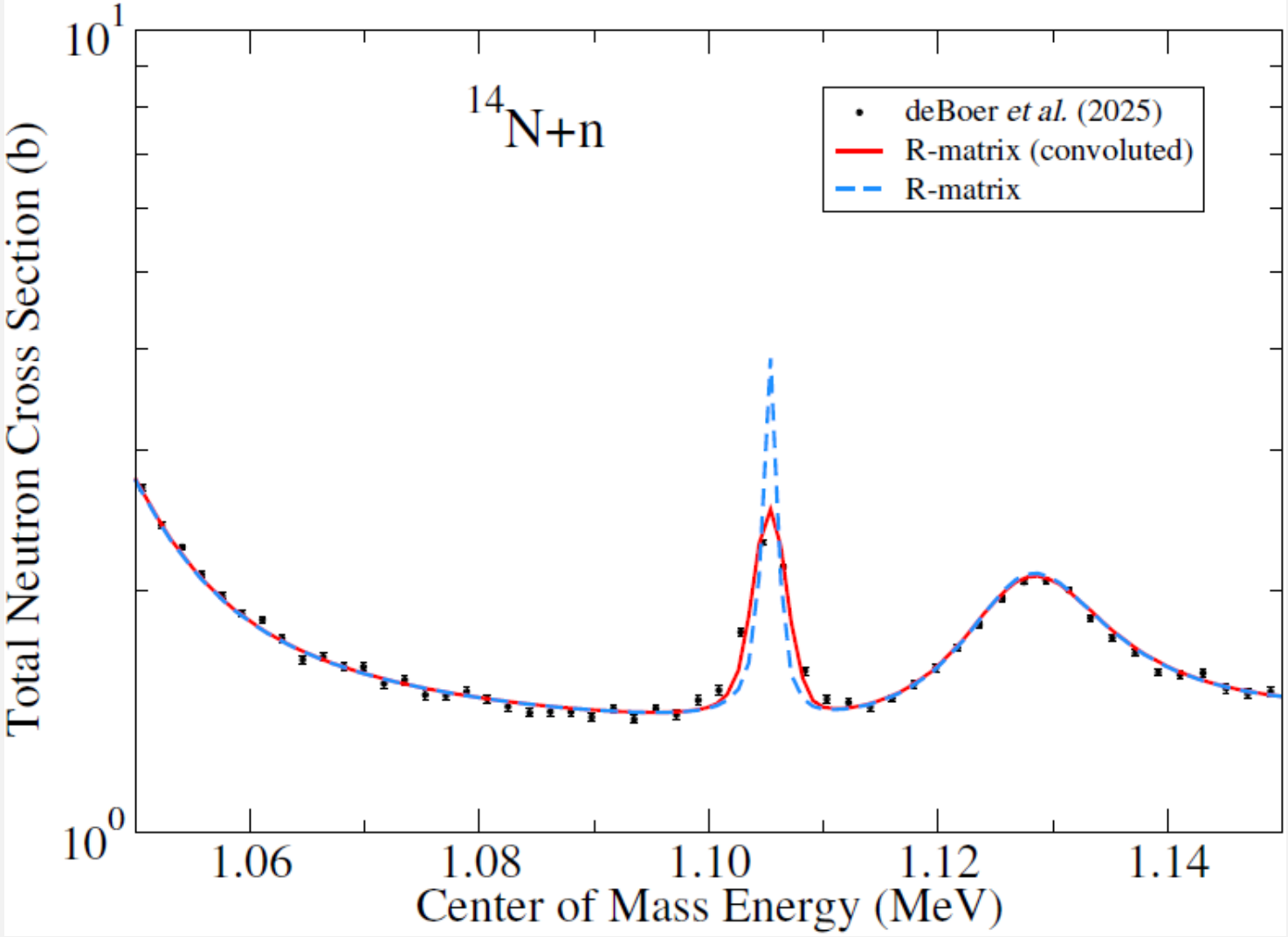
$$Y(E) = \int_{-\infty}^{\infty} f(\varepsilon) \cdot g(E-\varepsilon) d\varepsilon$$

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

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

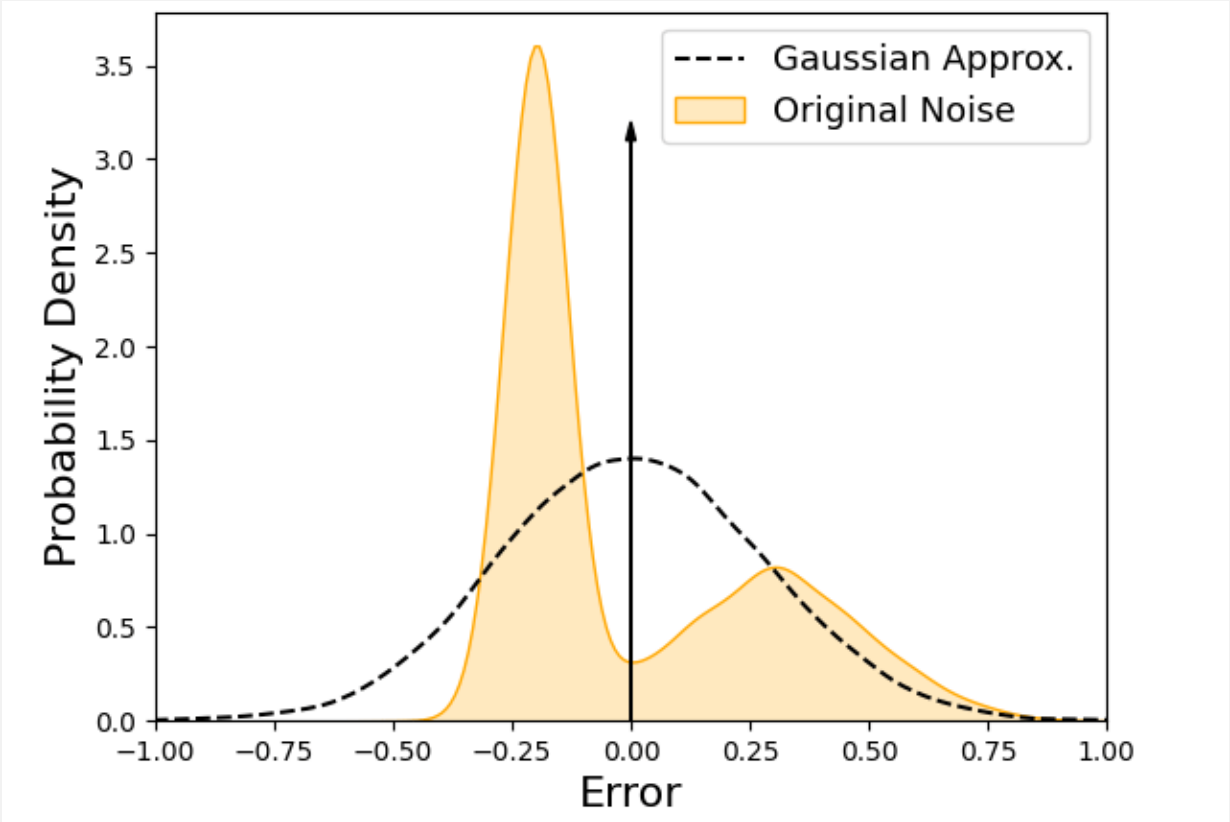
NEUTRON TIME OF FLIGHT

- See the SAMMY user manual for example

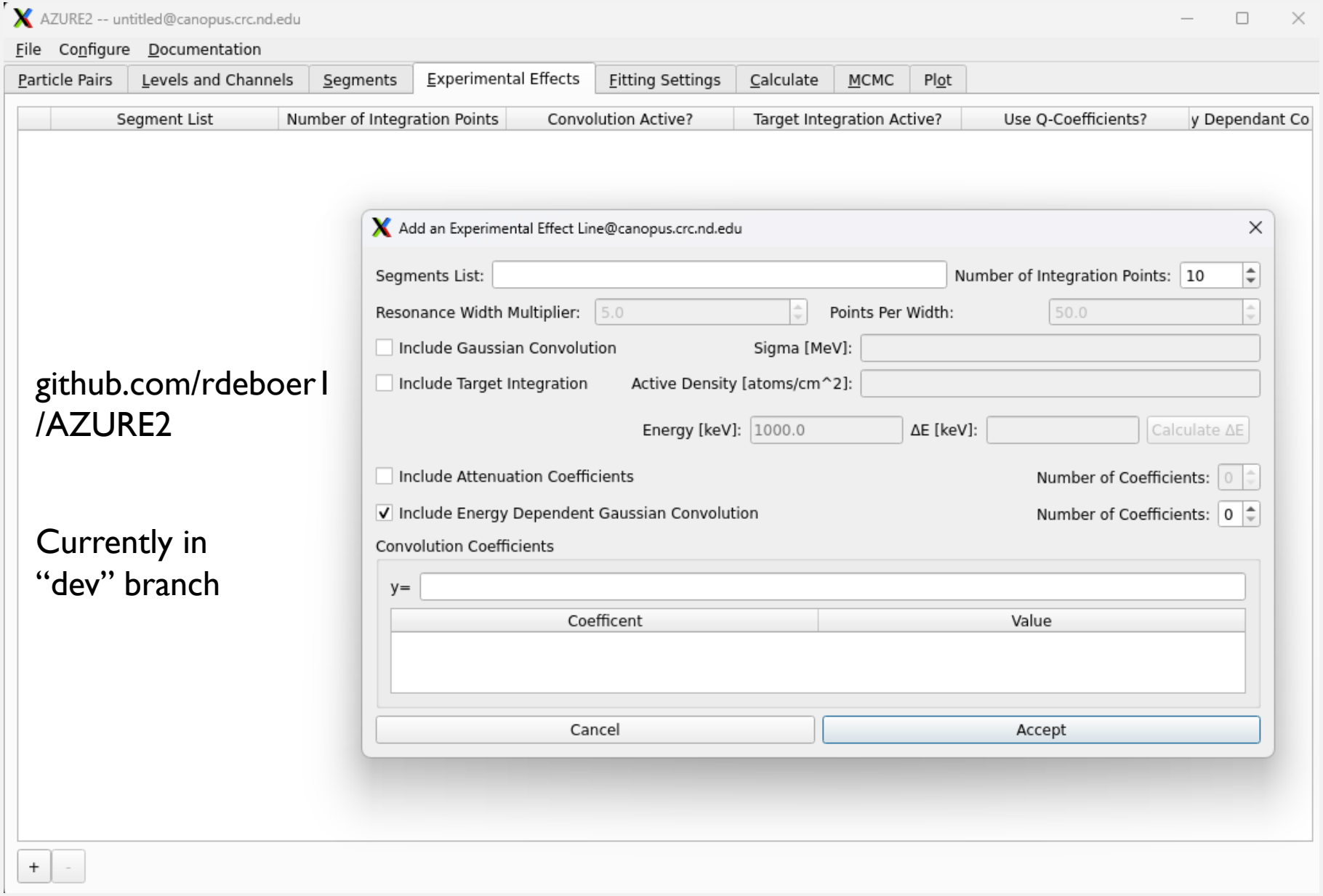


IN PRACTICE…

- In practice, we usually assign a Gaussian PDF in cases where we don't know the underlying PDF. We need to make some kind of estimate.
- Central limit theorem states that if you have several different uncertainty contributions, when you combine them, the final distribution will tend towards a Gaussian distribution.
- We're always trying to improve, that's science
  - We strive to develop new measurements where the uncertainties become reduced and can be better characterized.



ADDITIONAL RESOLUTION OPTIONS IN AZURE2



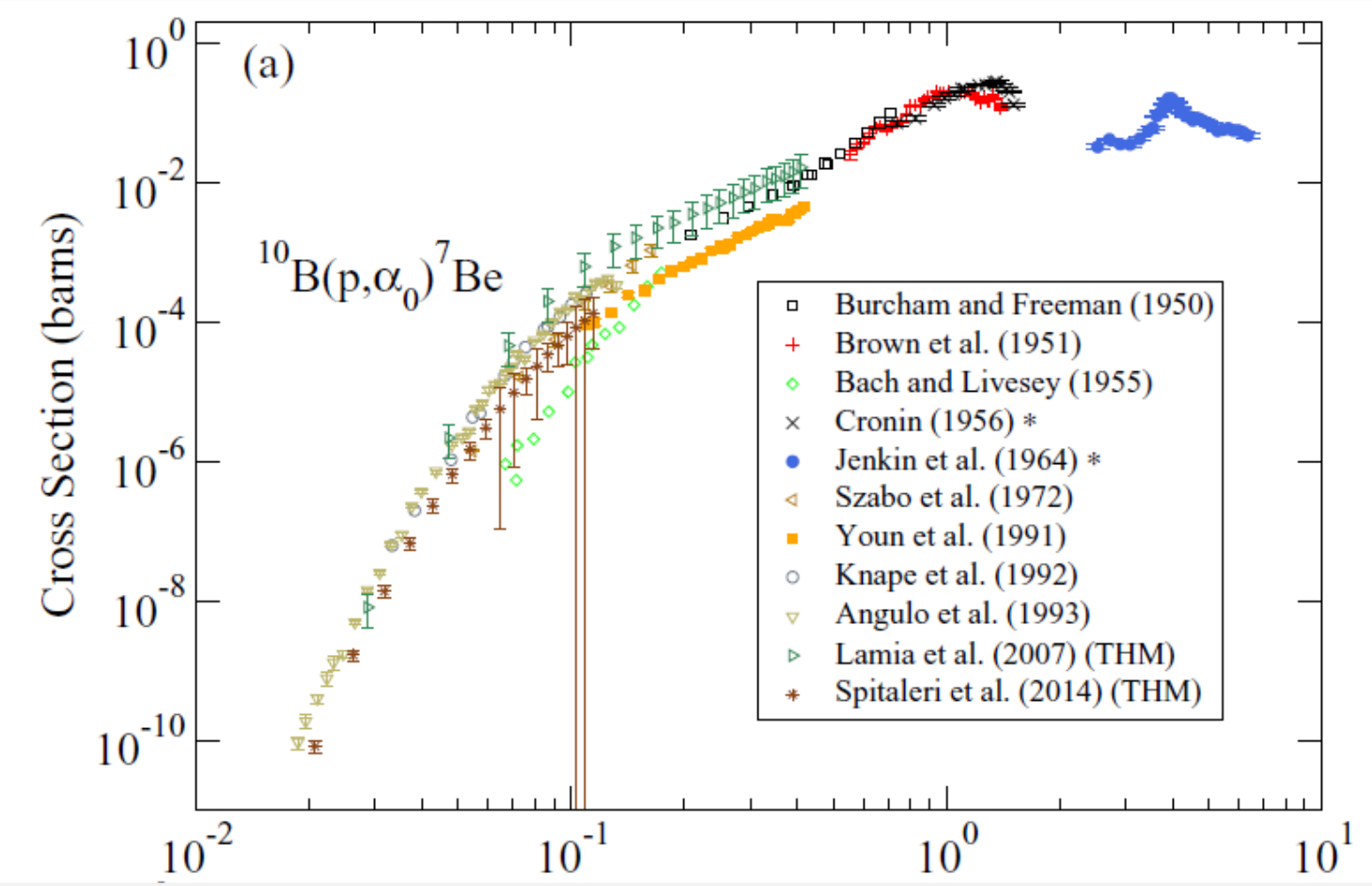
github.com/rdeboer1/AZURE2

Currently in "dev" branch

Jakub Skowronski

FITTING MULTIPLE DATA SETS SIMULTANEOUSLY

- Traditionally, we try to divide our uncertainties into these two groups of independent (point-to-point) or common mode
- However, many times uncertainties are some mixture and we need to approximate
  - New Bayesian methods can help to remove these approximations
- We usually fit using a χ^2 function to quantify how well our theory matches the experimental data
- We need to be careful when we have several data sets



MULTIPLE DATA SET χ^2

$$\chi^2 = \sum_i \left(\sum_j \frac{(f(x_{i,j}) - n_i y_{i,j})^2}{(n_i \sigma_{i,j})^2} + \frac{((1-n_i)/n_i)^2}{\delta^2_{exp,i}} \right)$$

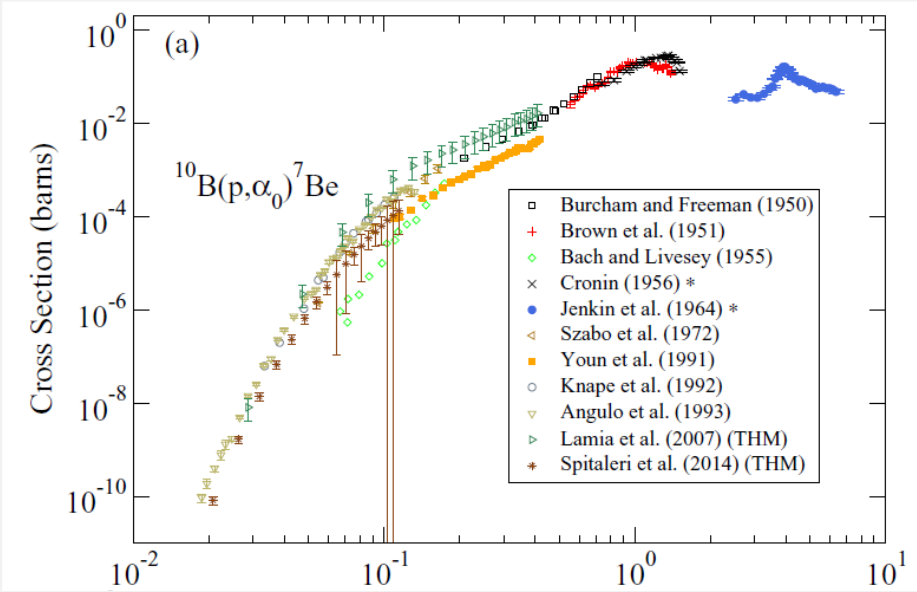
$f(x_{i,j})$ is the theoretical function (e.g. an R-matrix calculation)

$y_{i,j}$ is an experimental data point

$\sigma_{i,j}$ is the point-to-point uncertainty on a data point (usually statistics)

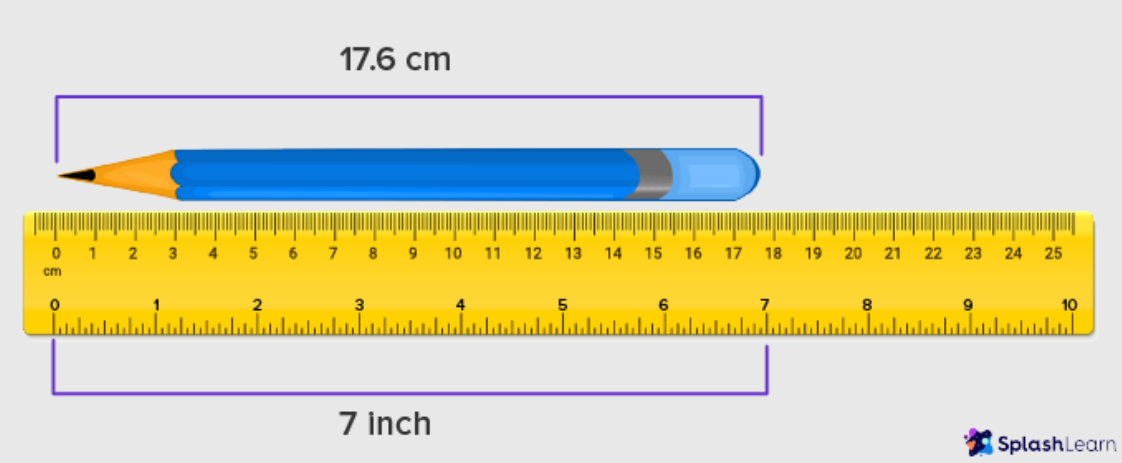
n_i is a normalization factor for each data set and its uncertainties

$\delta^2_{exp,i}$ is the square of the common mode uncertainty in each data set



COMMON SYSTEMATIC UNCERTAINTIES

- Especially for the common mode uncertainties, we don't really know much about them, so we take the assumption that if we average over many measurements, we'll approach the true value and get a smaller overall common mode uncertainty
- We must be careful though, because some uncertainties are common even to different measurements!
  - We can't "double count" uncertainties or it will artificially reduce our combined uncertainty. This can be very tricky sometimes and can be easy to overlook.



Example, we can measure the length of something many times with a ruler, but we can never do better than the common mode uncertainty, i.e. the smallest increment of the ruler.

$$\bar{x} = \frac{X}{N} = \frac{\sum_i x_i}{N}$$

$$\Delta\bar{x} = \frac{\Delta X}{N} = \frac{\sqrt{\sum_i (\Delta x_i)^2}}{N}$$

BAYESIAN UNCERTAINTY ESTIMATION

- There are several practical advantages
  - Communicate additional information to your goodness of fit tests that you wouldn't be able to do using a strictly frequentist approach
  - Since it is a fundamental part of Bayesian analysis, definition of priors is straight-forward
    - They can be given any probability distribution (probability density function, PDF) that the user likes
- Bayesian uncertainty estimation is usually implemented using **Markov Chain Monte Carlo** (MCMC), a method of intelligently sampling the parameter space
  - **This method is also straight-forward**, but it can be computationally taxing
  - These methods are widely used and are implemented in freely available and rigorously tested computational routines (Python, C++, R, etc.)



WHAT ARE THE INPUTS TO A BAYESIAN UNCERTAINTY ANALYSIS?

- Experimental data (also for frequentist)
- (log) Likelihood function (also for frequentist)
- **Priors**
  - Initial constraints on fit parameters
  - Type of probability distribution and specific constraints on it
  - Common PDF examples: Uniform, Normal (Gussian), Lognormal, asymmetric Gaussian

$$-\ln \mathcal{L} = \frac{1}{2} \sum_{i,j} \frac{[\, f(x_{i,j}) - n_i\, y_{i,j}\,]^2}{(n_i\, \sigma_{i,j})^2} + \frac{1}{2} \sum_{i} \frac{(n_i - 1)^2}{\delta^2_{\text{syst.},i}},$$

Parameter	Distribution
$E_{\text{ex}}(1^-, 0)$	$N(8.04, 0.02)$
$C_n(1^-, 0)$	$U(0.0001, 0.1)$
$\Gamma_\alpha(1^-, 0)$	$N(2000, 700)$
$C_n(2^+, 0)$	$U(0, 10)$
$C_\alpha(2^+, 0)$	$U(-4000, 4000)$
$E_{\text{ex}}(2^+, 1)$	$N(8.22, 0.01)$
$\Gamma_n(2^+, 1)$	$N(200, 100)$
$\Gamma_\alpha(2^+, 1)$	$N(-1700, 100)$
$E_{\text{ex}}(3^-, 0)$	$N(8.29, 0.006)$
$\Gamma_n(3^-, 0)$	$N(-5600, 700)$
$\Gamma_\alpha(3^-, 0)$	$N(-2900, 200)$
n_{WAG}	$U(0.1, 50)$
n_{SCH}	$U(0.1, 50)$
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n_{WEI}	$U(0.1, 50)$
TT_{BAI}	$U(3.8 \times 10^{+17}, 2 \times 10^{+17})$
TT_{WEI}	$U(3 \times 10^{+17}, 5 \times 10^{+17})$
ES_{WEI}	$U(-0.2, 0.4)$

Bayesian uncertainty analysis using MCMC in AZURE2

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

BAND
Bayesian Analysis of Nuclear Dynamics

NSF, CSSI program

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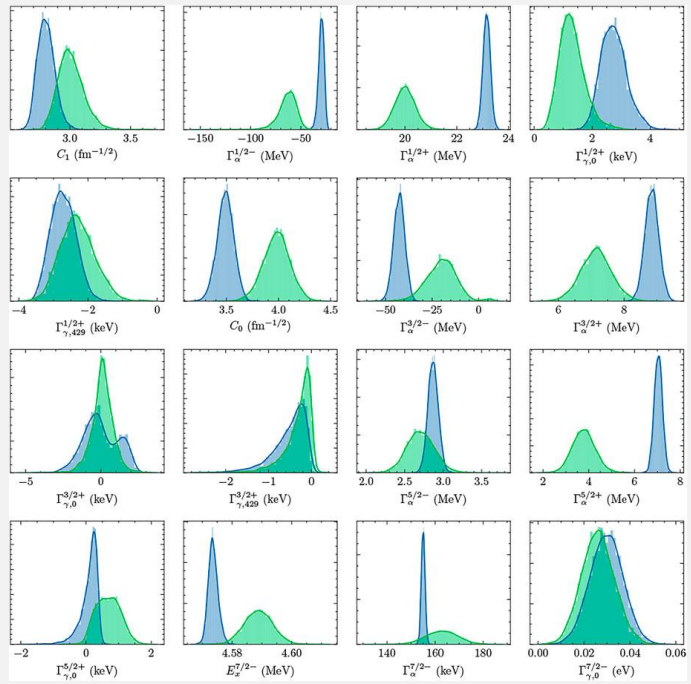
Performing Bayesian Analyses With AZURE2 Using BRICK: An Application to the ^{7}Be System

Daniel Odell[1]* Carl R. Brune[1] Daniel R. Phillips[1] Richard James deBoer[2] Som Nath Paneru[1,3]

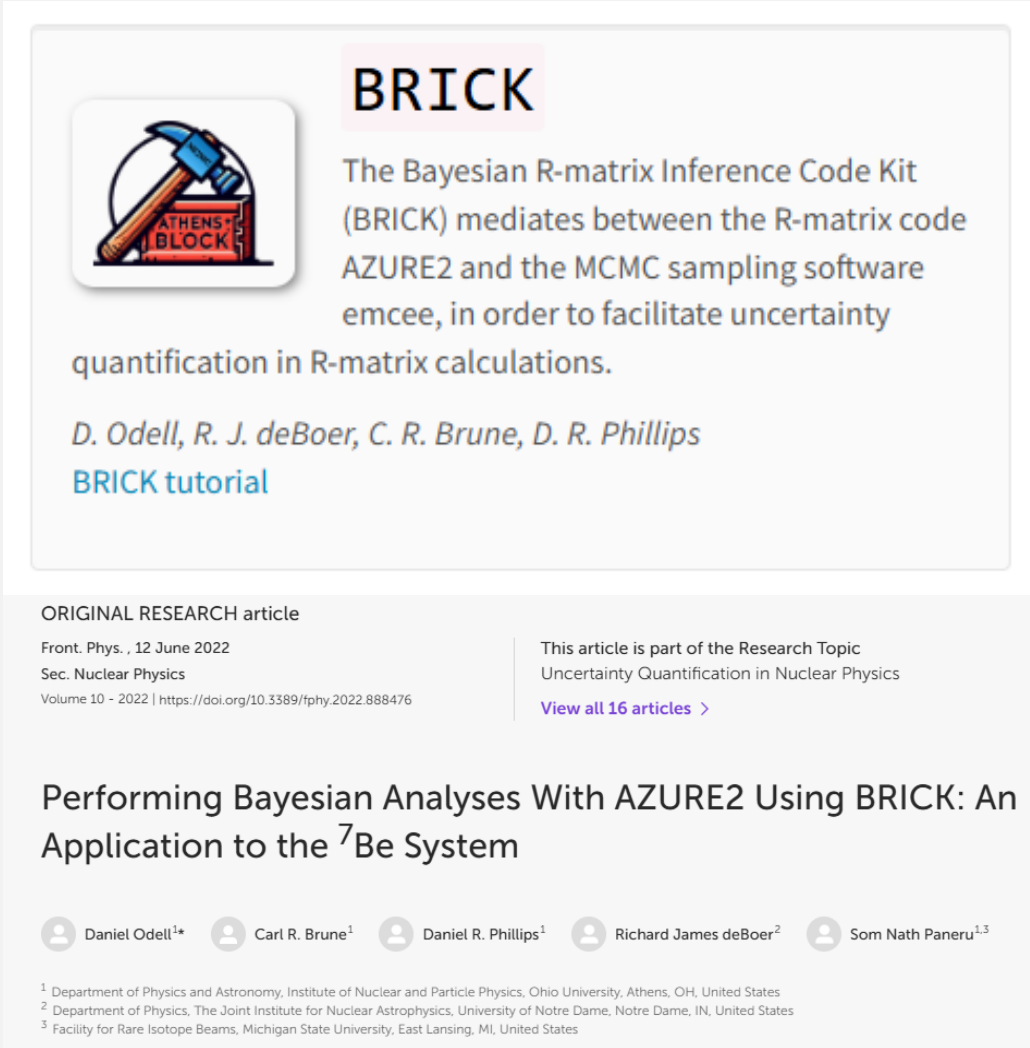
[1] Department of Physics and Astronomy, Institute of Nuclear and Particle Physics, Ohio University, Athens, OH, United States
[2] Department of Physics, The Joint Institute for Nuclear Astrophysics, University of Notre Dame, Notre Dame, IN, United States
[3] Facility for Rare Isotope Beams, Michigan State University, East Lansing, MI, United States



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



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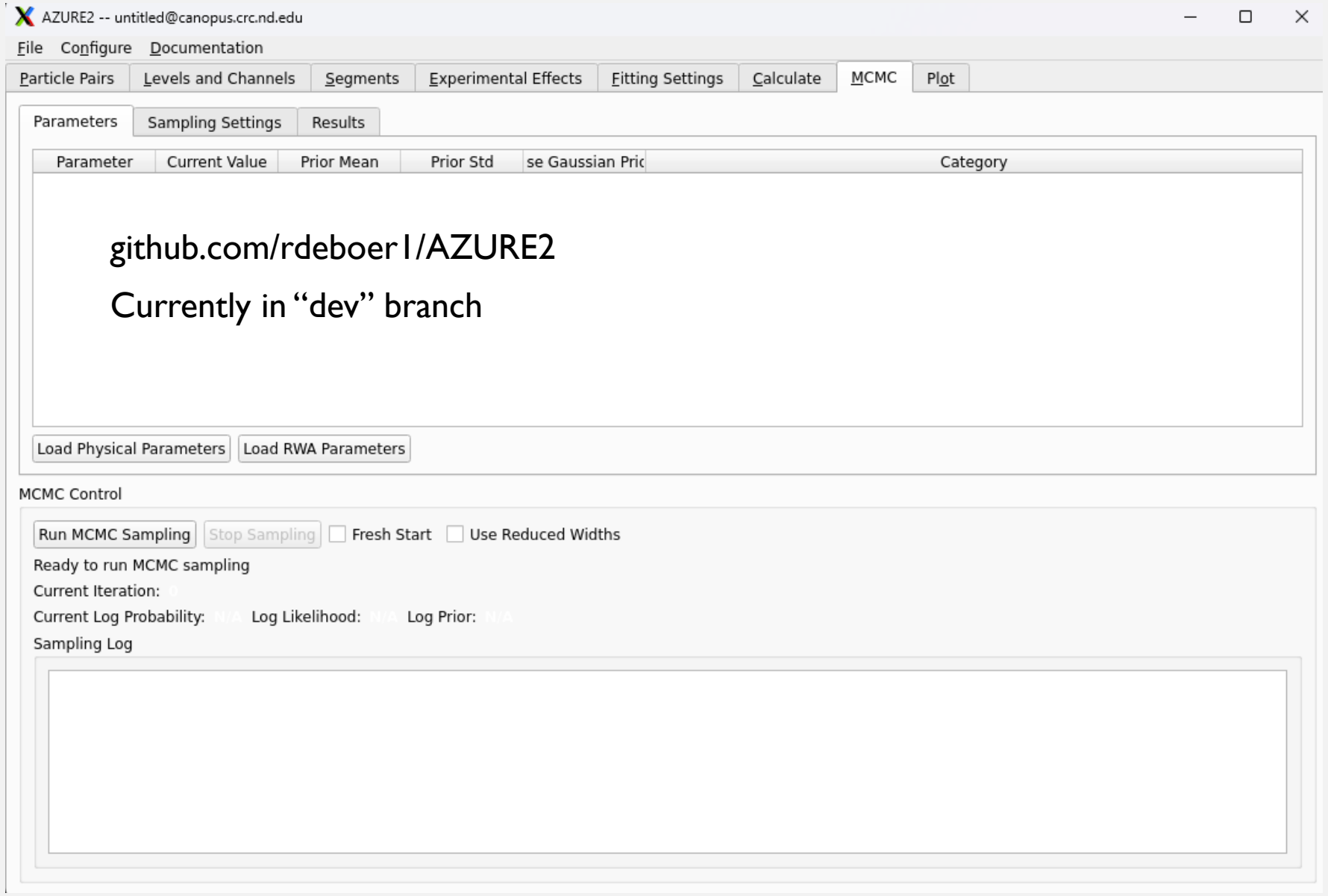
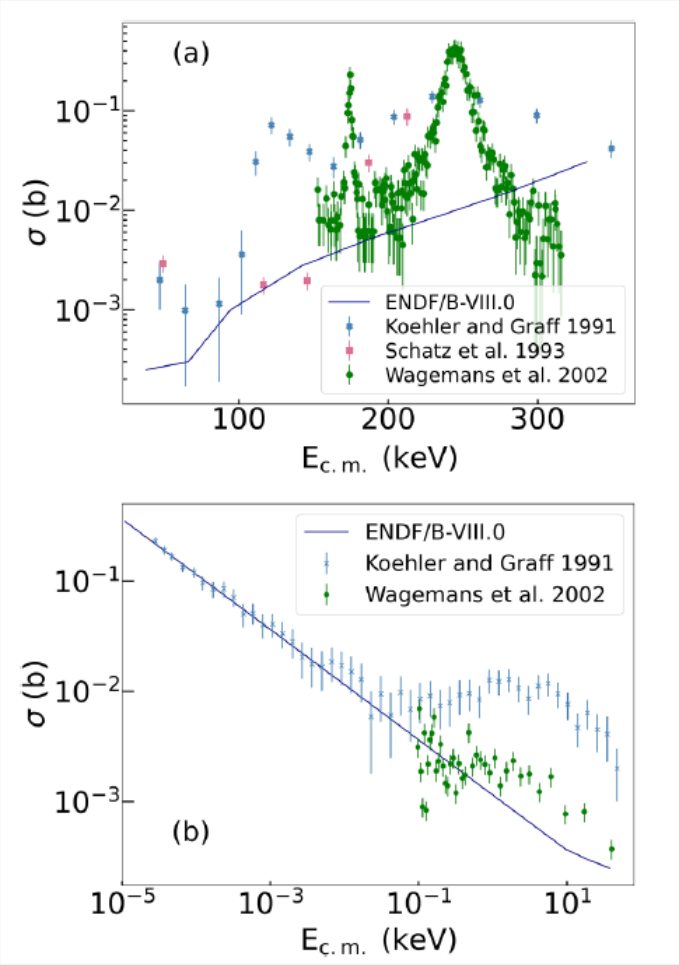
WORKING ON NATIVE MCMC IN AZURE2

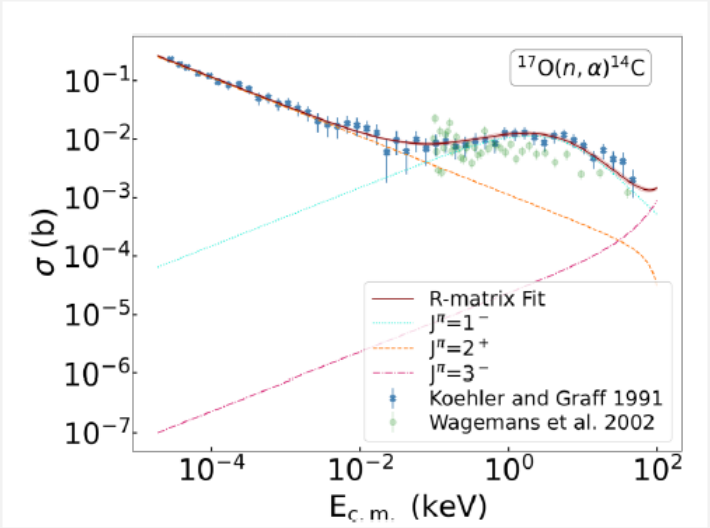


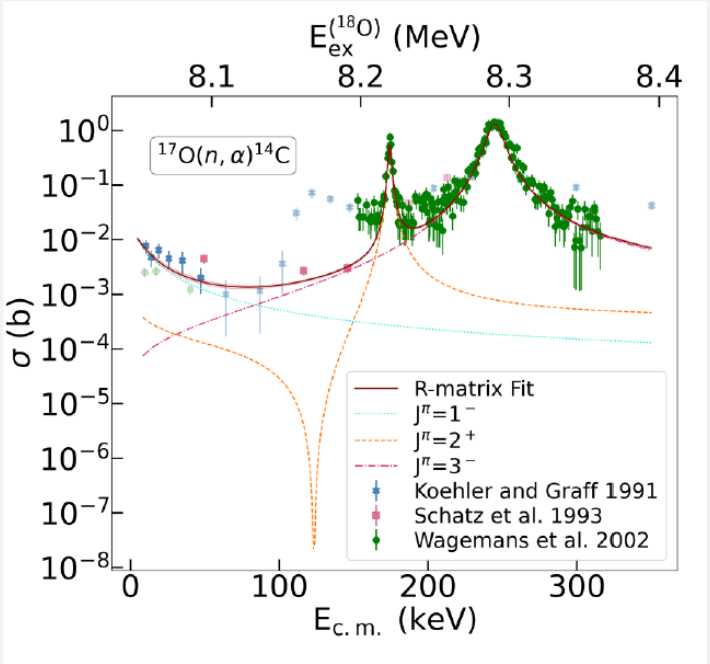
Jakub Skowronski

Make decisions about the quality of prior data sets
(This is where it can get subjective)

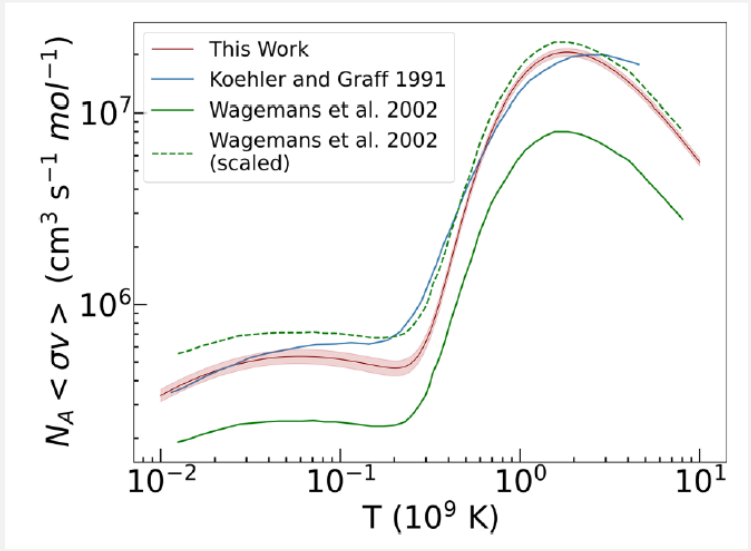


Get best fit to data





Perform uncertainty analysis



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TT_{WEI}	$U(3 \times 10^{+17}, 5 \times 10^{+17})$
ES_{WEI}	$U(-0.2, 0.4)$

Priors

Parameter	Posterior median ± C.I.
$E_{ex}(1^-, 0)$	$8.03885\ (+4.4 \times 10^{-4}, -4.6 \times 10^{-4})$
$C_n(1^-, 0)$	$4.92 \times 10^{-3}\ (+6.5 \times 10^{-4}, -5.6 \times 10^{-4})$
$\Gamma_\alpha(1^-, 0)$	$2040\ (+220, -220)$
$C_n(2^+, 0)$	$0.47\ (+0.17, -0.10)$
$C_\alpha(2^+, 0)$	$-1440\ (+400, -450)$
$E_{ex}(2^+, 1)$	$8.218552\ (+9.4 \times 10^{-5}, -9.5 \times 10^{-5})$
$\Gamma_n(2^+, 1)$	$219\ (+17, -16)$
$\Gamma_\alpha(2^+, 1)$	$-1925\ (+75, -75)$
$E_{ex}(3^-, 0)$	$8.28921\ (+2.0 \times 10^{-4}, -2.1 \times 10^{-4})$
$\Gamma_n(3^-, 0)$	$-8400\ (+330, -330)$
$\Gamma_\alpha(3^-, 0)$	$-3250\ (+130, -130)$
n_{WAG}	$2.87\ (+0.13, -0.13)$
n_{SCH}	$1.29\ (+0.21, -0.16)$
n_{KOE}	$1.007\ (+2.9 \times 10^{-2}, -2.8 \times 10^{-2})$
n_{BAI}	$1.234\ (+7.1 \times 10^{-2}, -6.4 \times 10^{-2})$
n_{WEI}	$0.9231\ (+8.1 \times 10^{-3}, -7.7 \times 10^{-3})$
TT_{BAI}	$4.68 \times 10^{+17}\ (+2.4 \times 10^{+16}, -2.5 \times 10^{+16})$
TT_{WEI}	$6.26 \times 10^{+17}\ (+2.9 \times 10^{+16}, -3.0 \times 10^{+16})$
ES_{WEI}	$2.43 \times 10^{-3}\ (+3.8 \times 10^{-4}, -4.1 \times 10^{-4})$

Posteriors

Correlation matrix for fit parameters

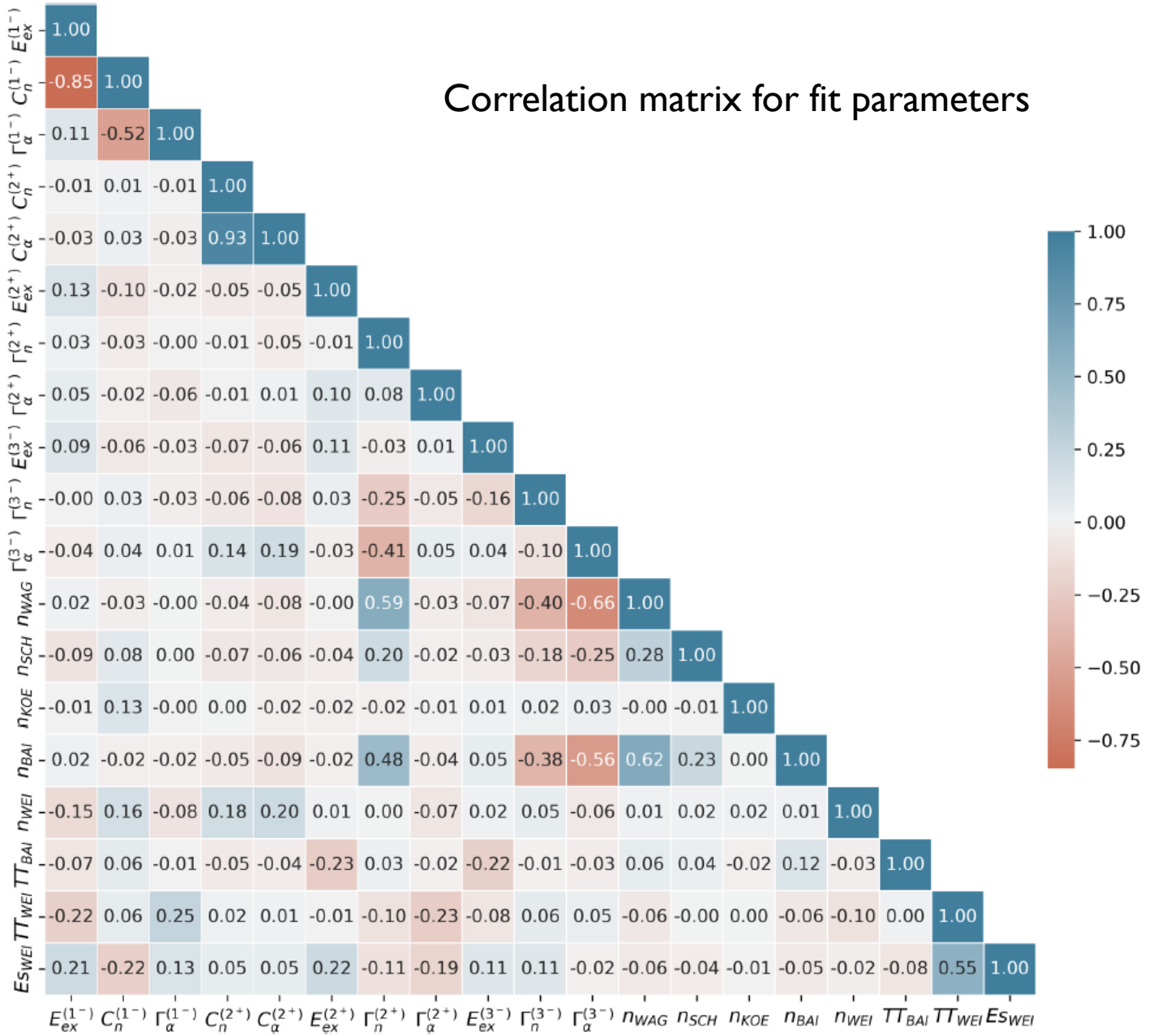
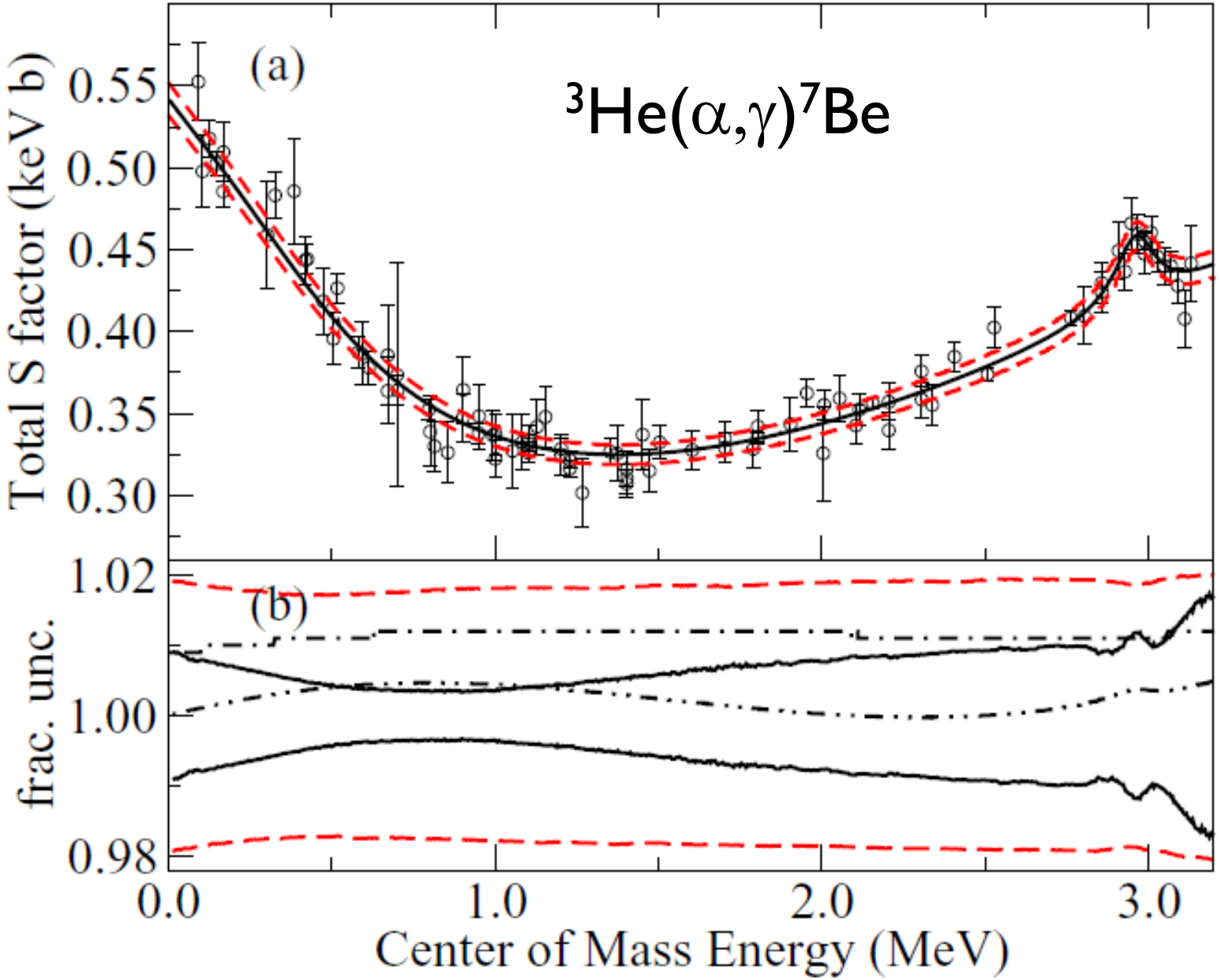


FIG. 7. Covariance matrix for the *R*-matrix fit parameters.

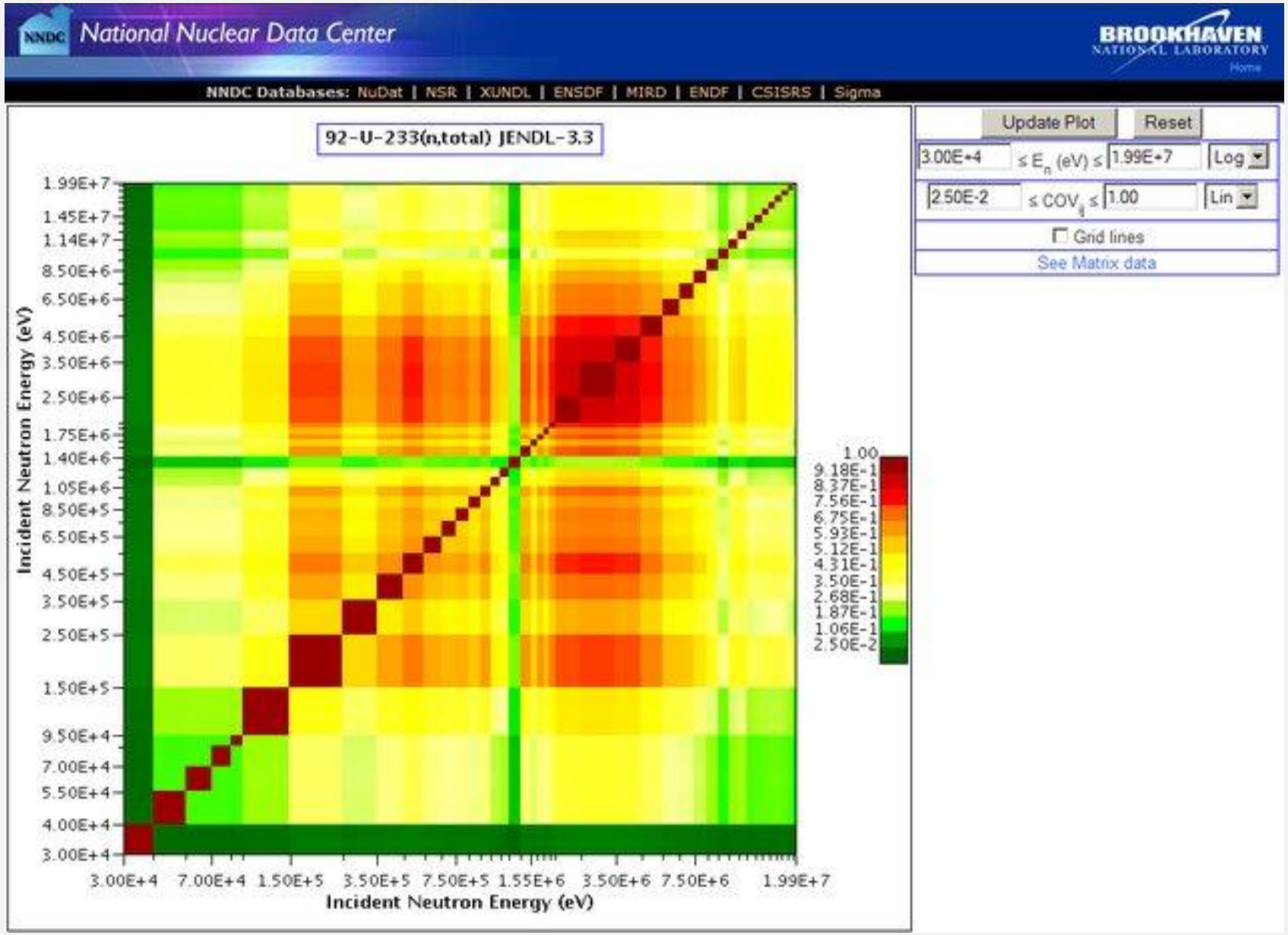
SYSTEMATIC UNCERTAINTIES DOMINATE

- **In many case, the systematic and model uncertainties dominate over the statistical uncertainties**
- This is not a good situation from an uncertainty perspective because while the statistical uncertainties are very well defined, the systematic ones are not
- "Never measure anything too well."
  - This is kind of a joke, but in a way it is true. As you reduce other uncertainties that previously dominated, you then often must worry about new sources of uncertainty that were previously negligible
  - But that is also scientific progress!



DATA COVARIANCE MATRIX

- A more detailed and accurate way of cataloging uncertainties for nuclear data
- Harder to implement?



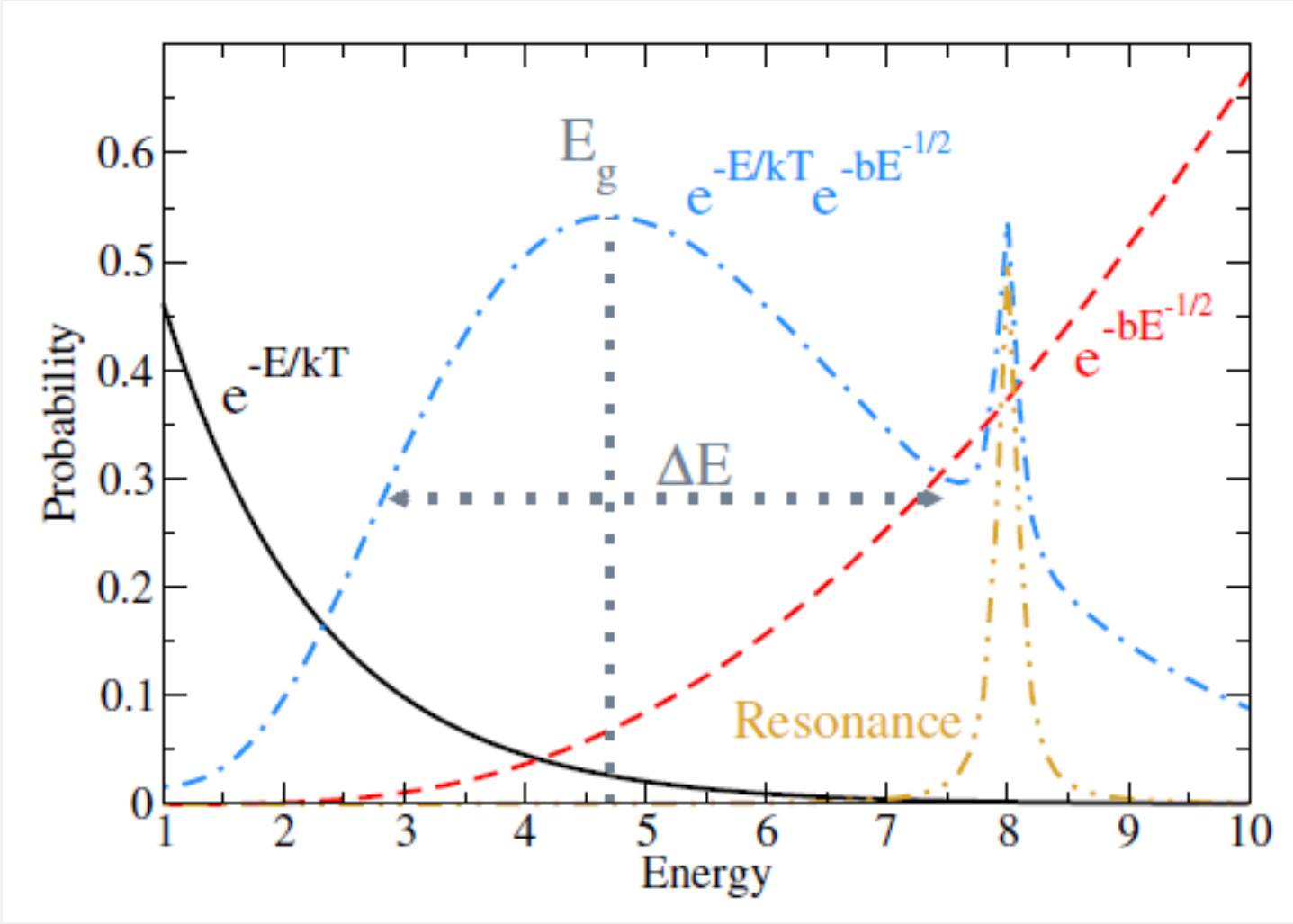
GAMOW ENERGY

- The energy of interest is the convolution of the Maxwell-Boltzmann velocity distribution of particles in the stellar environment and the penetrability of the reaction

$$E_G = 0.122(Z_1^2 Z_2^2 \mu T_9^2)^{1/3}$$

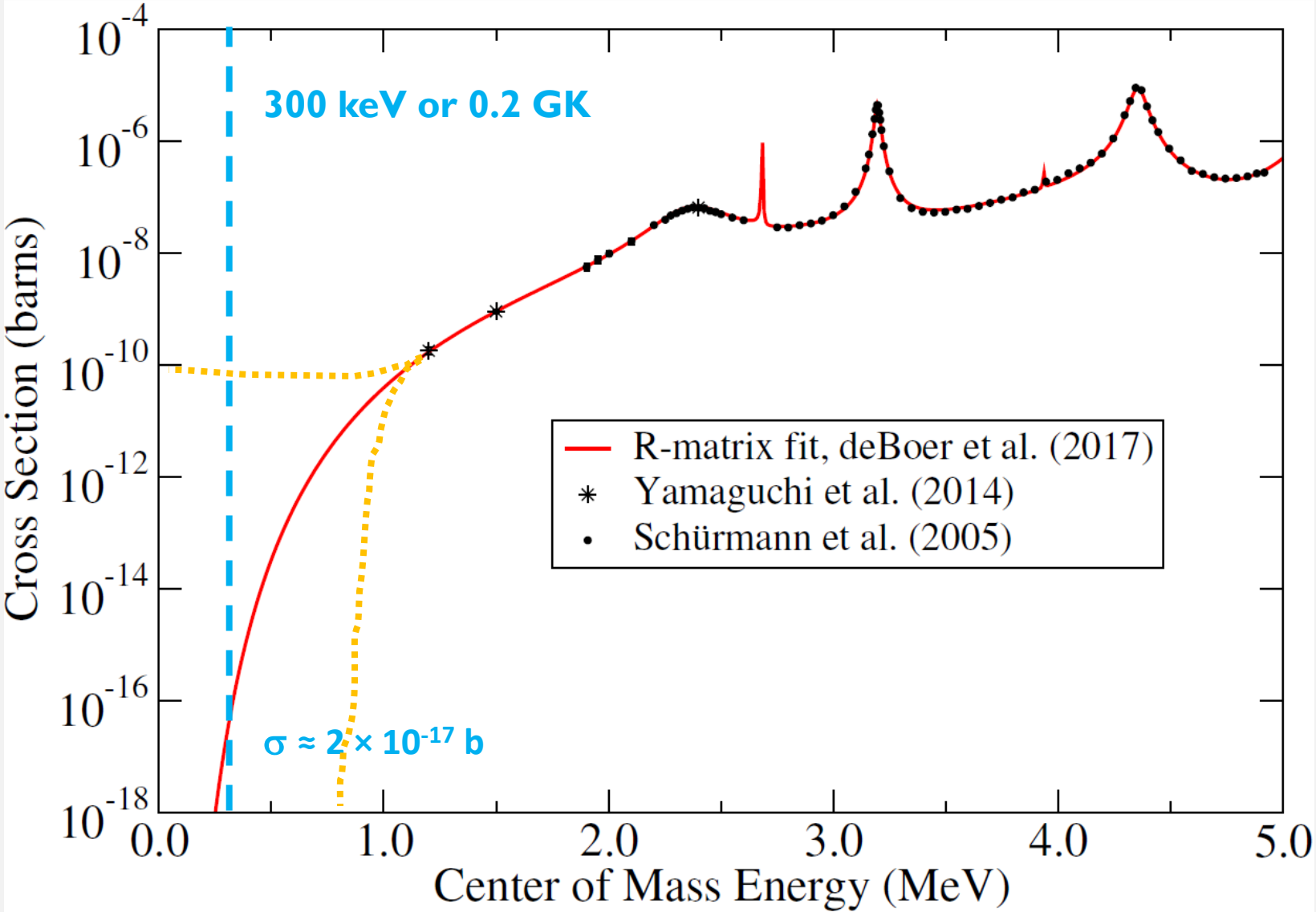
$$\Delta E = 0.236(Z_1^2 Z_2^2 \mu T_9^5)^{1/6}$$

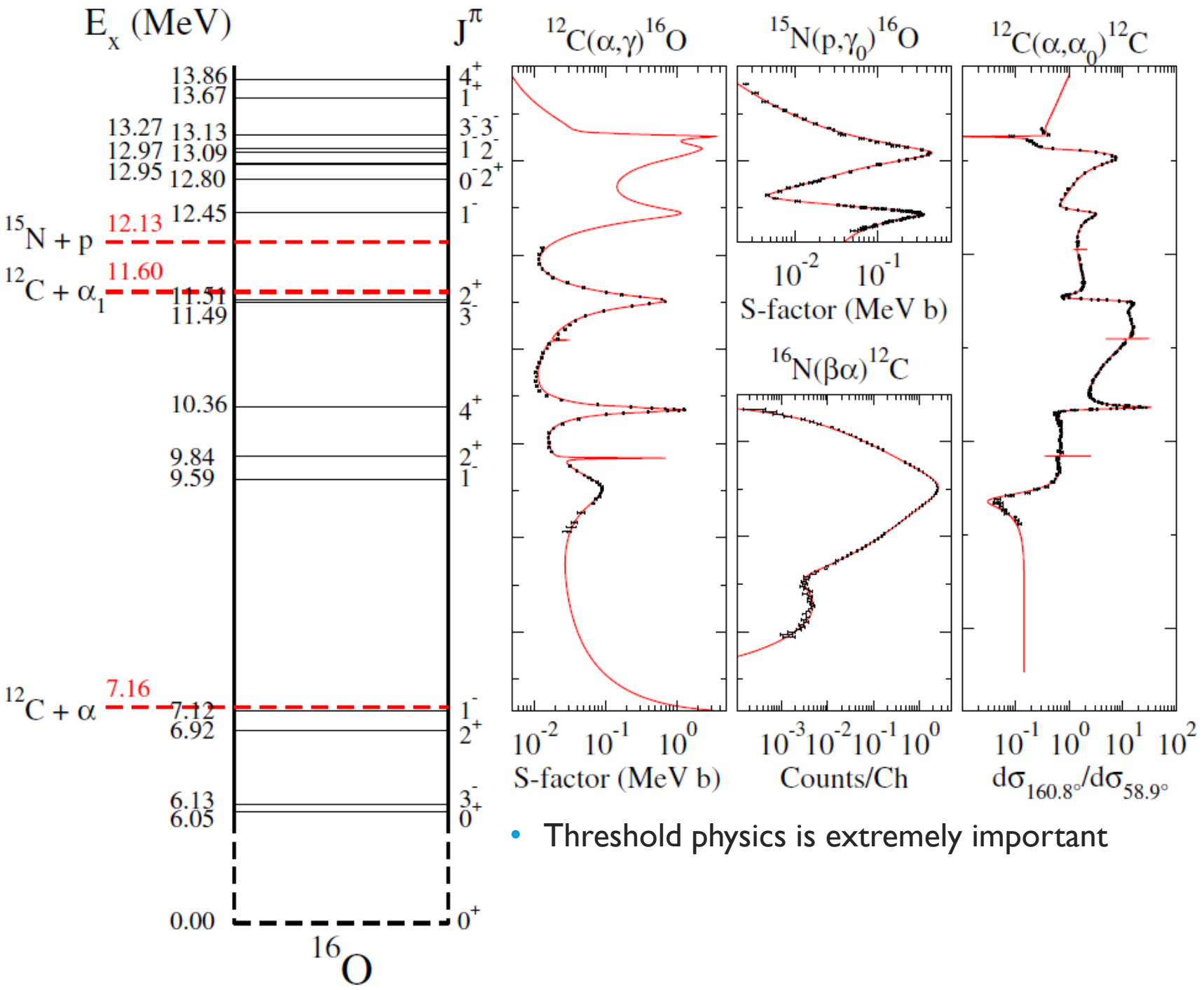
- where Z_1 and Z_2 are the number of protons in the interacting particles, u is the reduced mass and T_9 is the temperature in GK.
- **Formulation is a rough approximation!**



EXAMPLE: $^{12}C(\alpha,\gamma)^{16}O$ EXTRAPOLATION TO LOW ENERGY

- In nuclear astrophysics, the temperatures in a star correspond to very low energies in the cross section
- For charged particle induced reactions, this means that the cross section is so small that it is very challenging to measure it
- For this reason, we need to measure the cross section at higher energy and the extrapolate to the energies of interest
- This extrapolation requires nuclear theory to constrain it

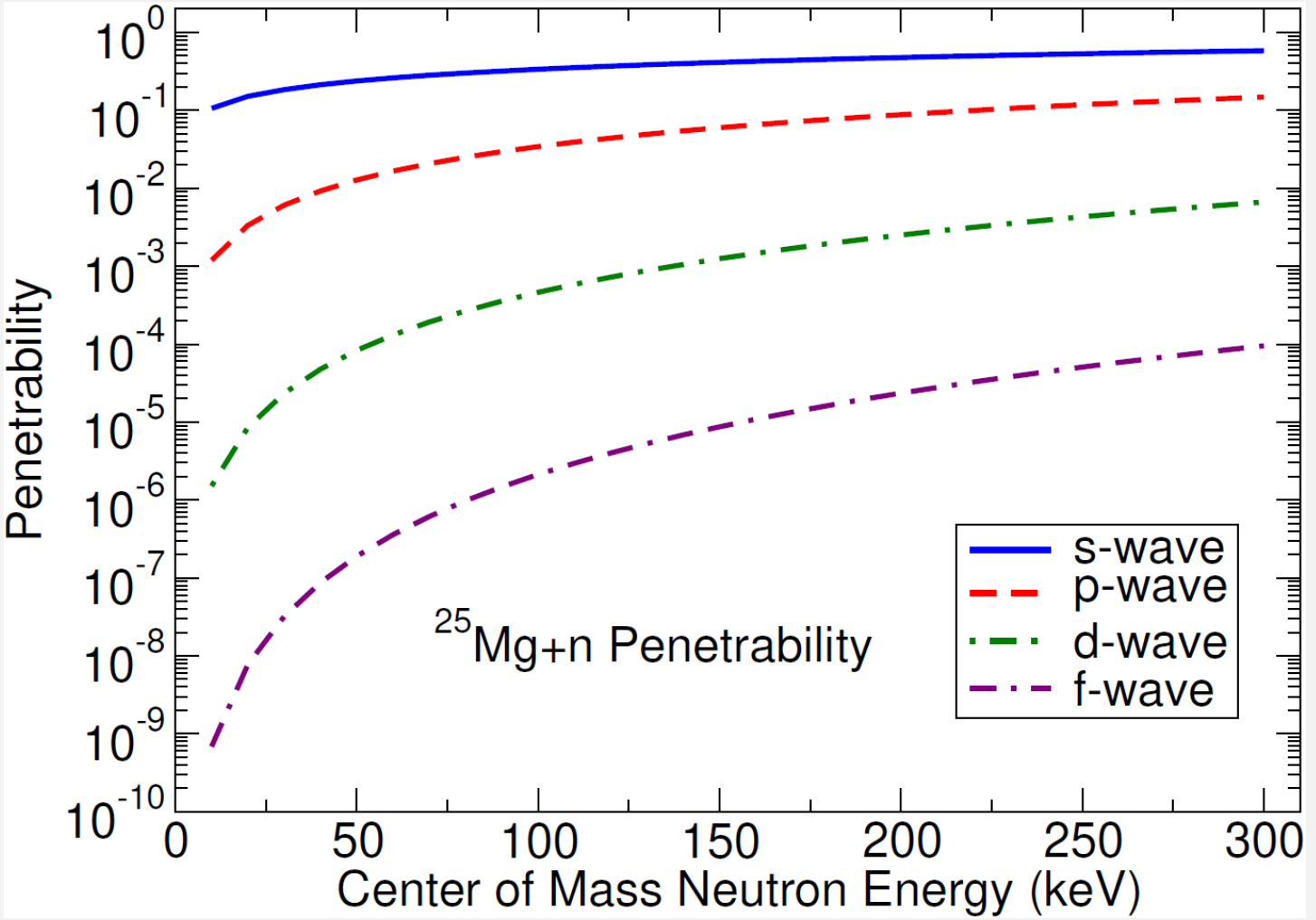




- Threshold physics is extremely important

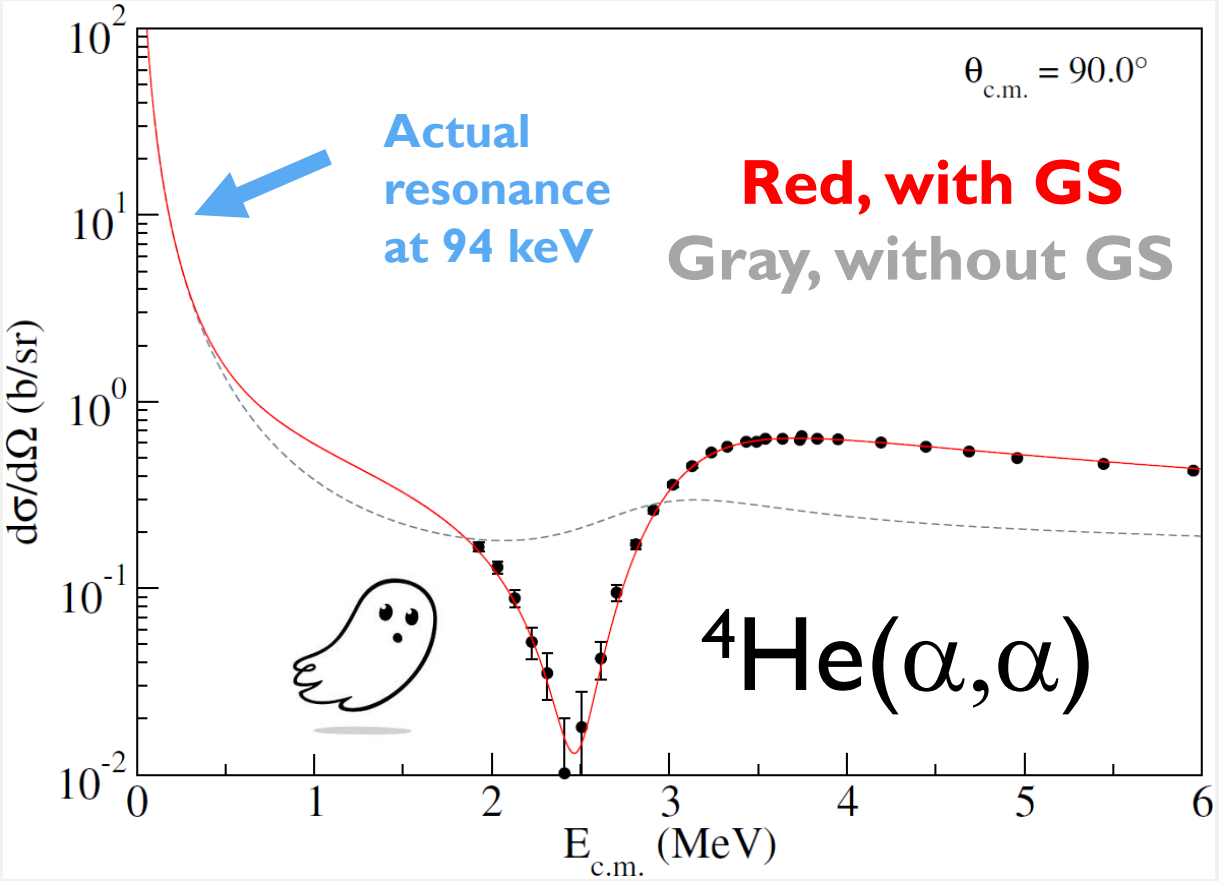
PENETRABILITY

- **Penetrability distorts the cross section near thresholds**
- Results in "strange looking" cross sections
  - Ghost resonances
- Resonances that require higher partial waves to form are suppressed near thresholds
- The effective level density decreases

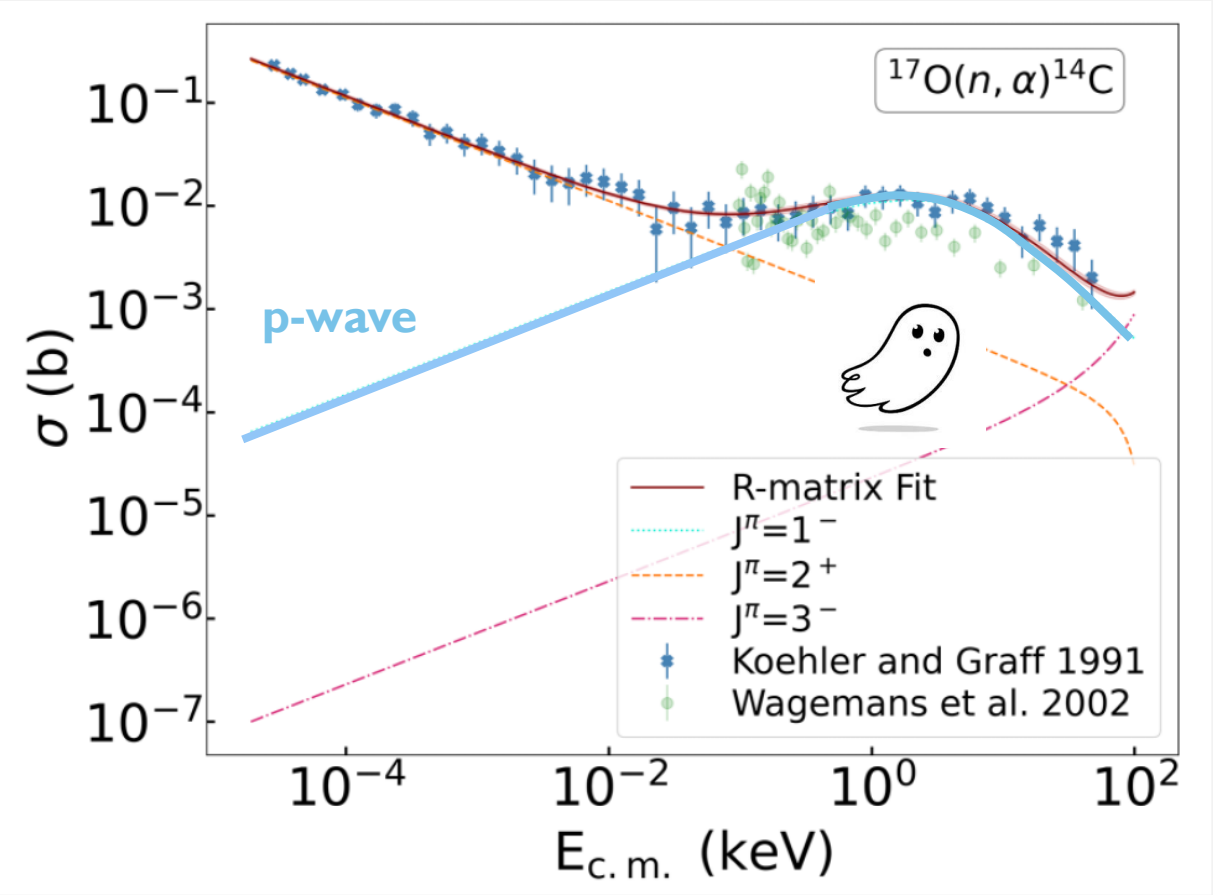


GHOST RESONANCES

0^+ ground state in ^{8}Be

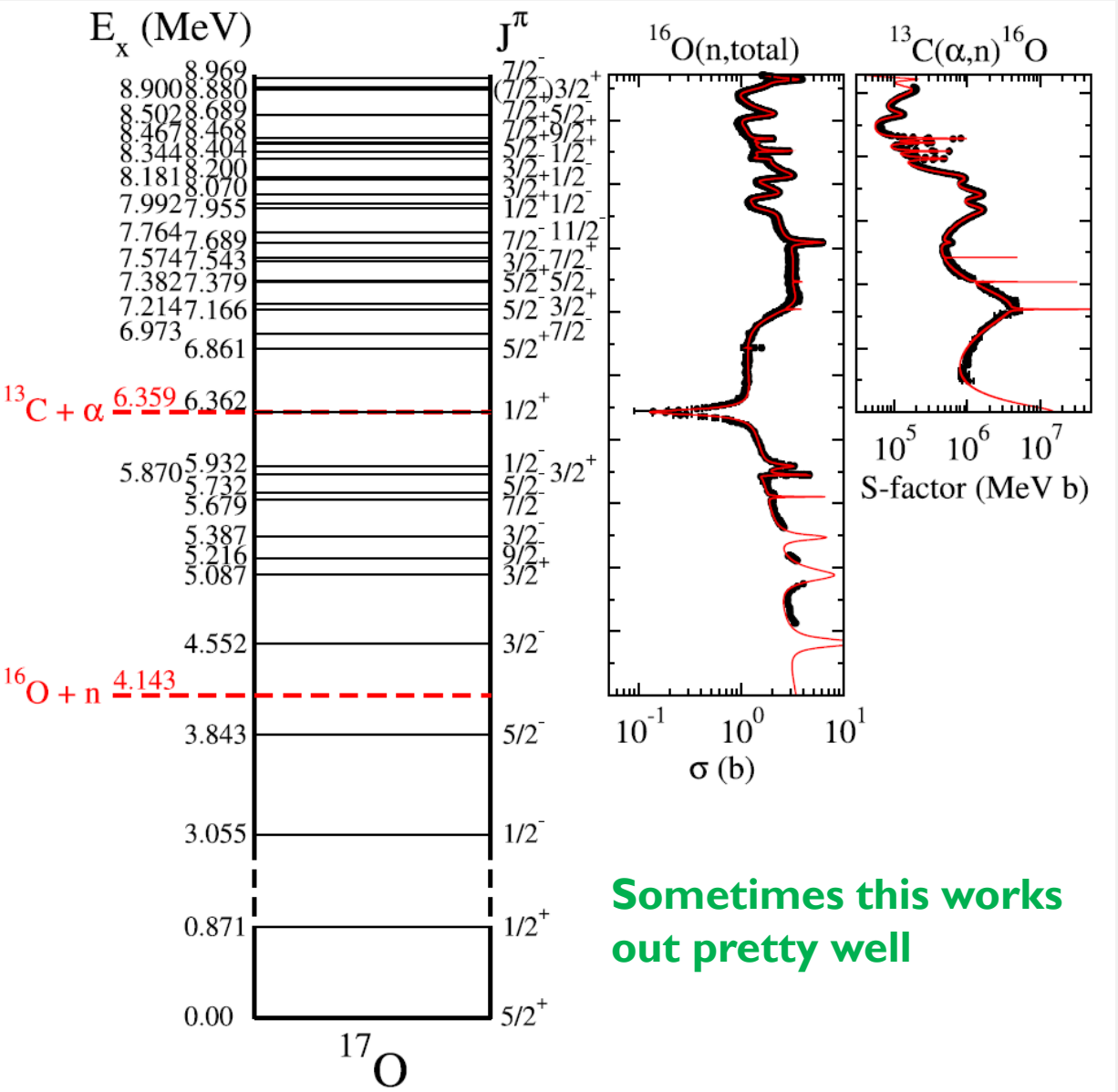


1^- bound state at -5 keV in ^{18}O

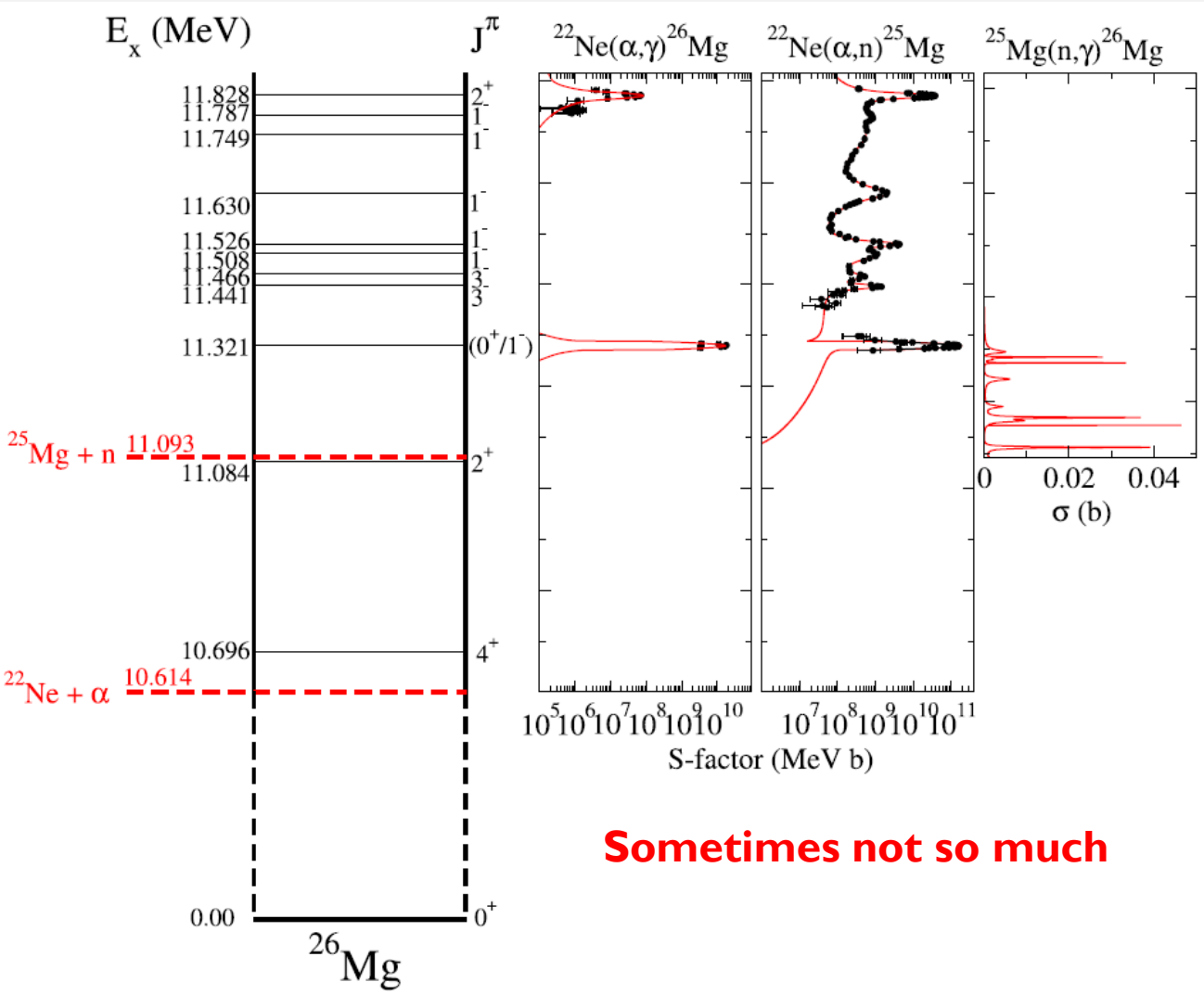


Oliva *et al.* (2024)

NEUTRON PRODUCING REACTIONS CAN BE HIGHLY CONSTRAINED THROUGH TOTAL NEUTRON CROSS SECTIONS



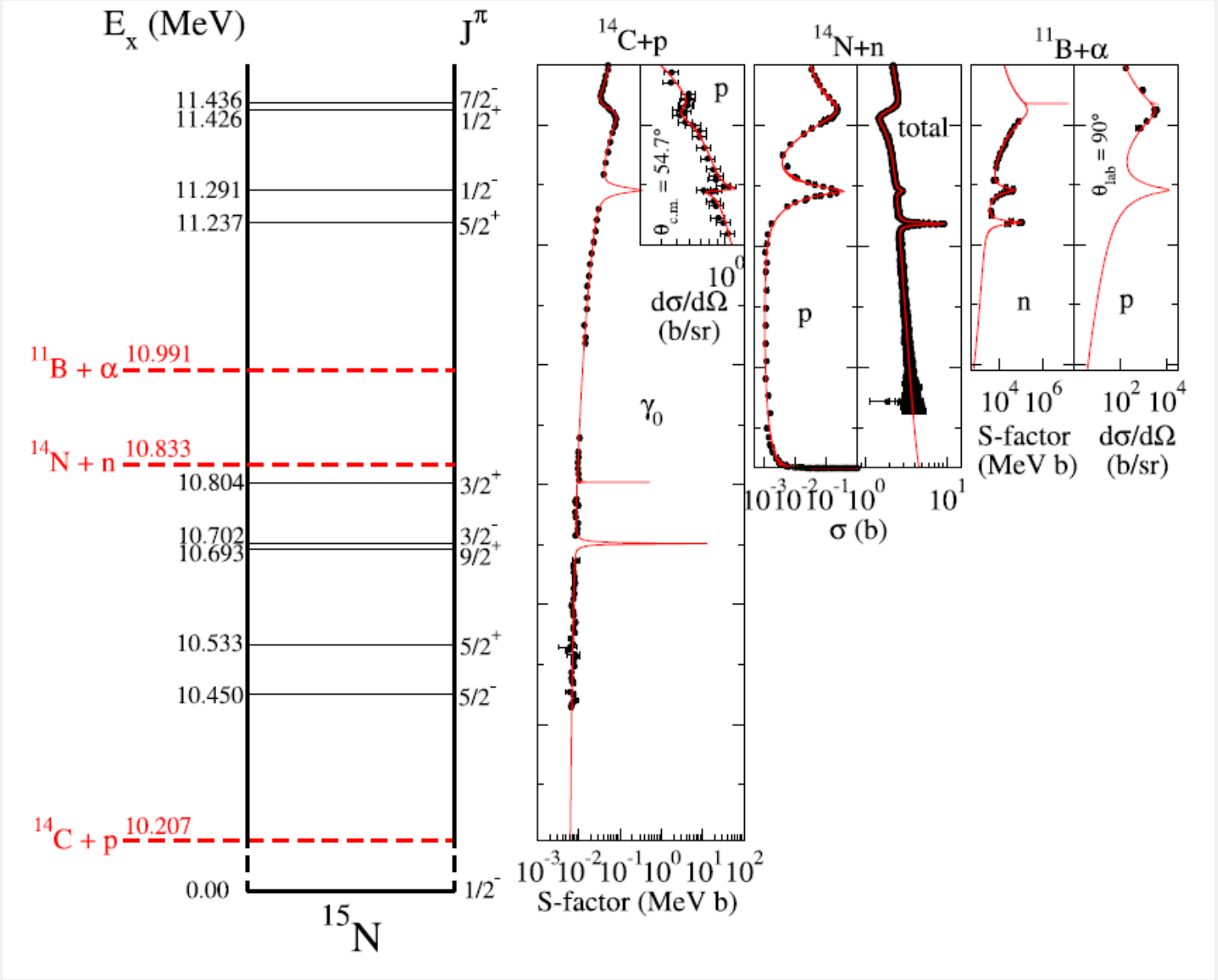
Sometimes this works out pretty well



Sometimes not so much

MULTICHANNEL FITTING

- More work
  - More data, more level structure
  - More computation time
- More confidence
  - More checks on physics consistency
  - More checks on data consistency
- Phenomenological fitting
  - You get out what you put in (effort + data + level information)



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
- Uncertainty Quantification (UQ)
- Artificial Intelligence (AI)
  - Assisted analysis workflow
- Experimental Design

NUCLEAR DATA EVALUATION

ENDF/B-VIII.0: The 8^{th} Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data

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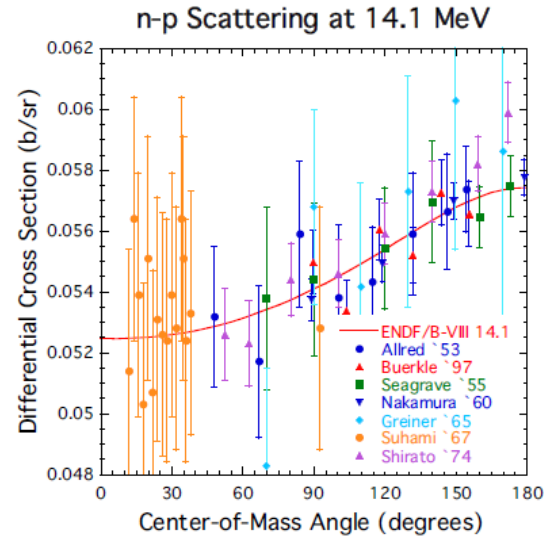

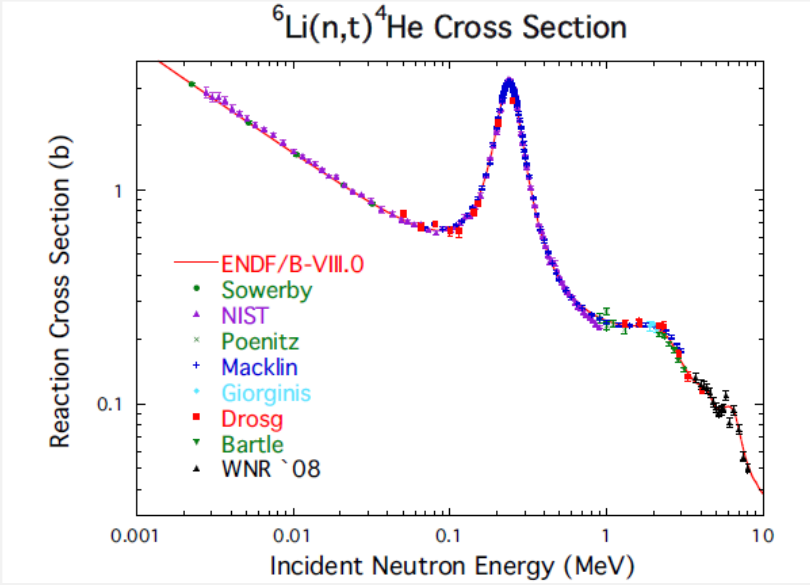

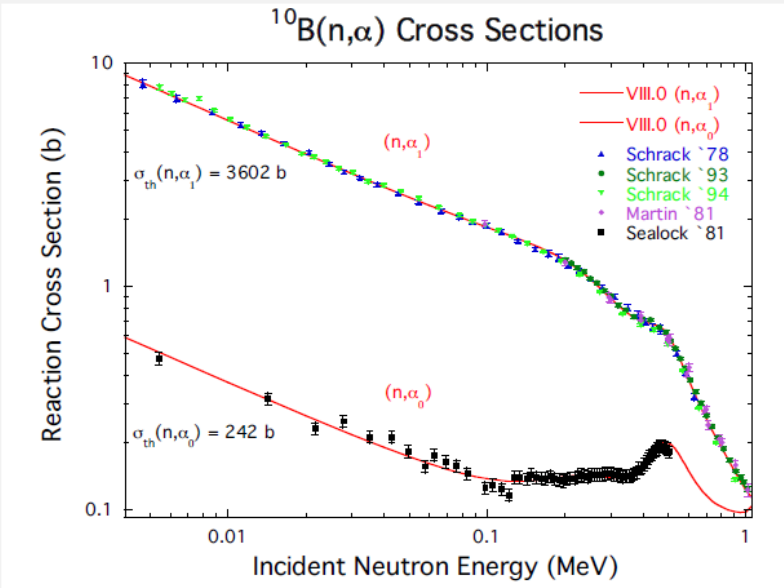

SOME SUGGESTED REFERENCES

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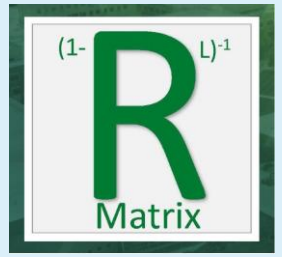
R-MATRIX SCHOOL **2027**



- A series of three R-matrix schools organized by **Marco Pigni** (ORNL), Carl Brune (OU) and myself (UND)
- Will likely take place in July of 2027
- Hosted by the University of Notre Dame, may take place elsewhere
- 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**

This work is supported by the Office of Science, Nuclear Physics within the U.S. Department of Energy funding opportunity DE-FOA-0003238.

U.S. DEPARTMENT of ENERGY

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