

Astrophysics needs and tools: Overview of AZURE

Nuclear Cross Sections Analysis and R-matrix tools Mini-school

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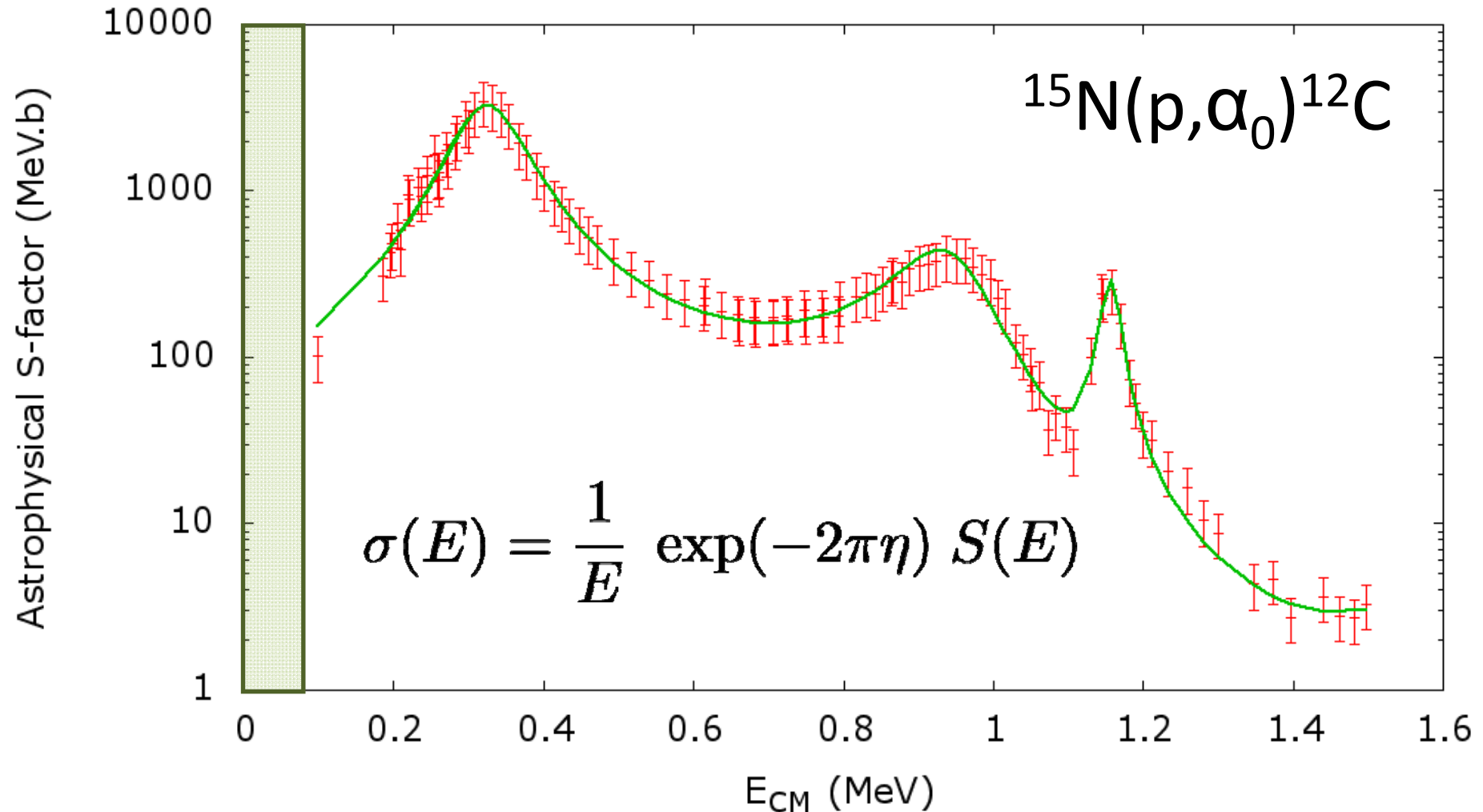
Overview

- Introduction
 - Why do we need the R-matrix in nuclear astrophysics?
- R-matrix with AZURE
 - Definitions
 - Input parameters
 - Background poles
 - Hard-sphere phase shifts
- Using AZURE2
 - Compound nucleus
 - Levels and Channels
 - Data
 - Calculations and fitting
- Final thoughts

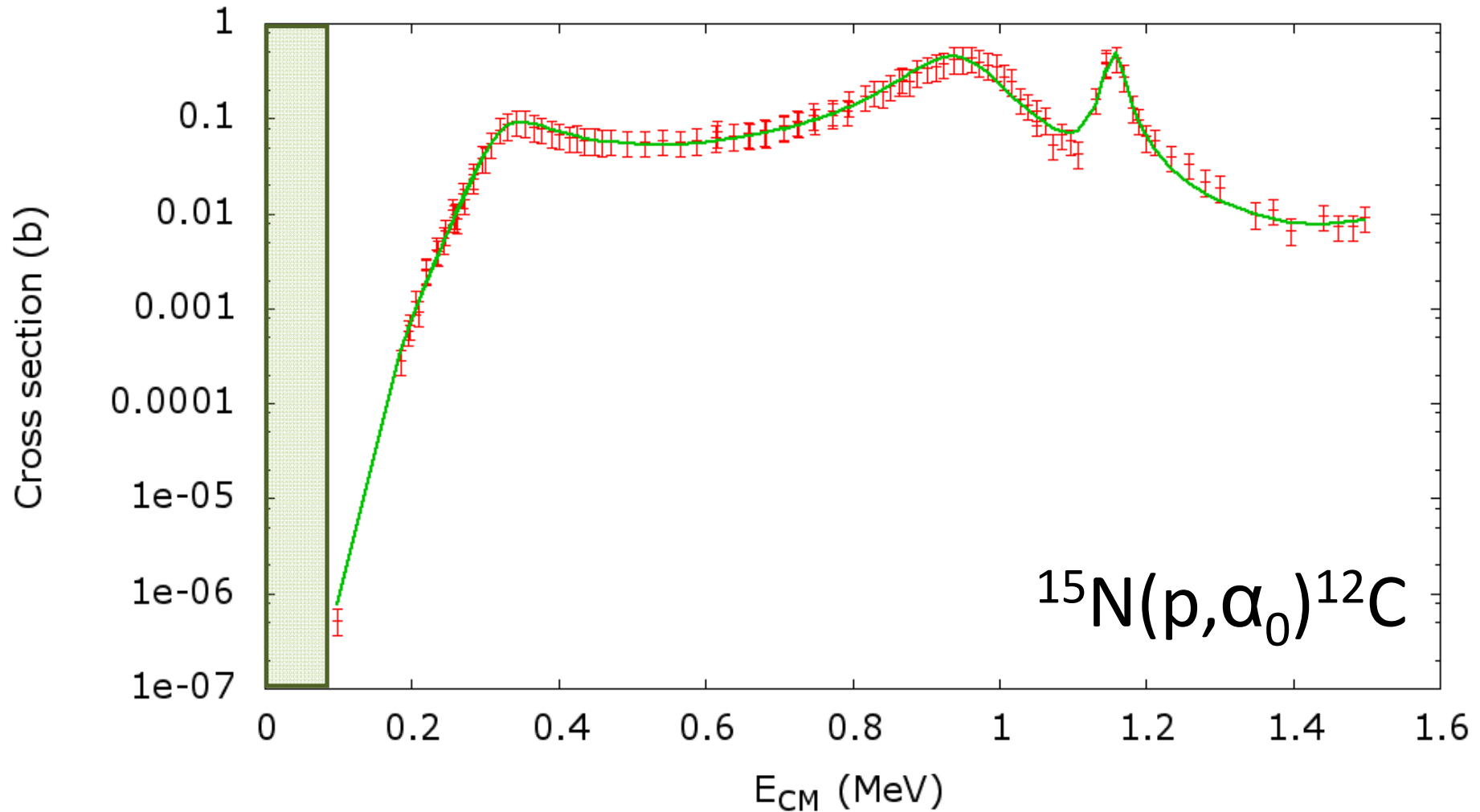
Introduction

Nuclear Astrophysics, R-matrix and
AZURE

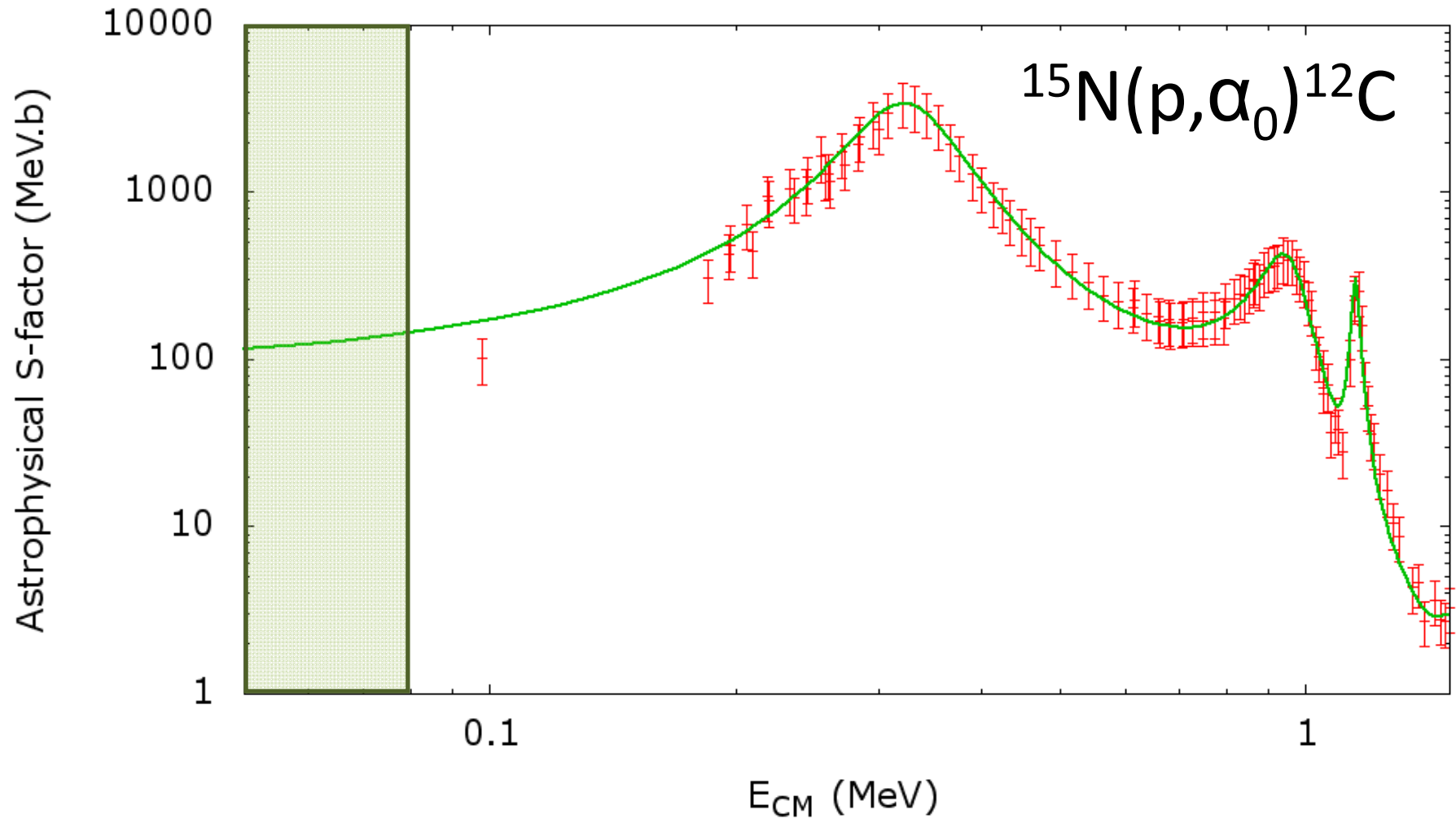
Into the Gamow window...



Into the Gamow window...???



Into the Gamow window...



Low energy cross sections

- **We (usually) cannot measure the cross section...**
- **What determines the low-energy cross section?**
 - Tails of higher lying states?
 - Sub-threshold resonances?
 - Non-compound nuclear processes?
 - Unobserved resonances in the Gamow window?
- **What would help constrain this most?**
 - Direct measurements at higher energies?
 - Resonance widths? (From a different reaction?)
 - ANC measurements from transfer?
 - Lifetime measurements for sub-threshold states? New direct measurements of related channels?
 - New low energy direct measurements.....?

Materials analysis

- **Scattering and reactions...**
 - Backward angle scattering cross sections
 - Reaction and capture cross sections
 - Wide variety of light-ion reactions on light-nuclei
 - Need to know at any energy and angle
- **What do we need?**
 - Which reactions are most important?
 - Understanding historic data sets? Verification experiments?
 - What nuclear data (energies and spin-parities) is available? Is this sufficient?
 - New scattering and reactions measurements?
 - Which angles and energies are most useful?

AZURE: what can it do?

- **R-matrix calculations**
 - Treat all scattering and reaction channels simultaneously
 - Fit resonance parameters to data
 - Extrapolate into the energy range of interest
- **Easy of use**
 - Makes using data from a variety of sources easy
 - Fast enough to practically work with many channels

R-matrix with AZURE

Definitions and parameter
transformations

Definitions

- α = Particle pair
- s = channel spin
- ℓ = relative angular momentum
- $c = \alpha s \ell$ = channel, a particular particle pair with channel spin s and angular momentum ℓ
- λ = compound nucleus state
- $\gamma_{\lambda c}$ = reduced width amplitude
- a = R-matrix radius, marks the division between internal and external regions

Channel spin and angular momentum

I_1 = Angular momentum of particle 1

I_2 = Angular momentum of particle 2

$$\vec{s} = \vec{I}_1 + \vec{I}_2$$

$$s = |I_1 - I_2| \dots I_1 + I_2$$

$$\vec{J} = \vec{s} + \vec{\ell}$$

$$J = |s - \ell| \dots s + \ell$$

where $\pi = \pi_1 \pi_2 (-1)^\ell$ is parity of resonance

Breit-Wigner resonance

- What do we mean by a resonance width?

$$\sigma_{cc'}^{BW}(E) = \frac{\pi\omega}{k_c^2} \frac{\Gamma_c^o \Gamma_{c'}^o}{(E_R - E)^2 + (\Gamma^o/2)^2}$$

$$\Gamma^o = \sum_k \Gamma_k^o$$

$$\tau = \hbar/\Gamma^o$$

- Lifetime $10^{-16} - 10^{-21}$ seconds

What are the parameters in R-matrix?

- Level energies and reduced width amplitudes

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

$$\gamma_{\lambda c} = \left(\frac{\hbar^2}{2\mu_c a_c} \right)^{1/2} \int dS \varphi_c^* X_{\lambda JM}$$

$$H X_{\lambda JM} = E_{\lambda J} X_{\lambda JM}$$

- Arbitrary boundary condition B_c and radius a_c
- How can we relate to Breit-Wigner-type parameters?

R-matrix single resonance (via A-matrix)

$$\sigma_{cc'}(E) = \frac{\pi\omega}{k_c^2} \frac{\Gamma_{\lambda c}\Gamma_{\lambda c'}}{(E_\lambda + \Delta_\lambda - E)^2 + (\Gamma_\lambda/2)^2}$$

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

$$\Delta_\lambda = - \sum_k \gamma_{\lambda k}^2 [S_k(E) - B_k]$$

$$\Gamma_\lambda = \sum_k \Gamma_{\lambda k}$$

$$\omega \equiv g_J = \frac{2J + 1}{(2I_1 + 1)(2I_2 + 1)}$$

Lane and Thomas, page 327, [Rev. Mod. Phys. 30, 257 \(1958\)](#)

Carl Brune <http://arxiv.org/abs/nucl-th/0502087>

Decouvemont and Baye, [Rep. Prog. Phys 73, 036301 \(2010\)](#)

Observed and formal parameters

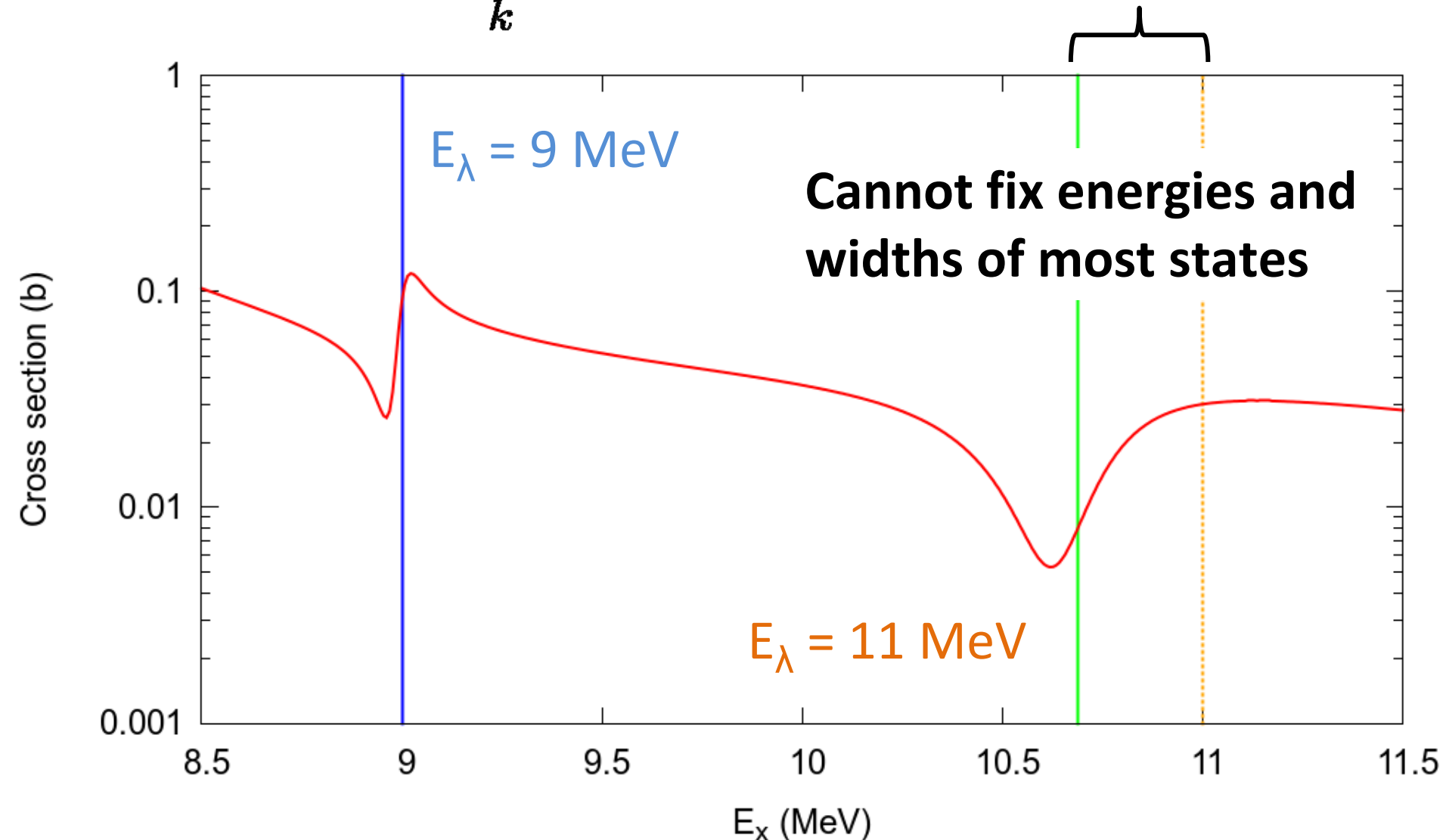
- Choose $B_k = S(E_\lambda)$, then Taylor expand $S(E)$ to define one relationship between physical (BW) and formal (R-matrix) parameters

$$\text{Observed } \Gamma_{\lambda c}^o = \frac{2P_c \tilde{\gamma}_{\lambda c}^2 \text{ Formal}}{1 + \sum_k \tilde{\gamma}_{\lambda k}^2 \left(\frac{dS_k}{dE} \right) \tilde{E}_\lambda}$$

$$\tilde{\gamma}_{\lambda c}^2 = \frac{\Gamma_{\lambda c}^o}{P_c} \left[2 - \sum_k \frac{\Gamma_{\lambda k}^o}{P_k} \left(\frac{dS_k}{dE} \right) \tilde{E}_\lambda \right]^{-1}$$

“On-resonance” parameters

$$\Delta_\lambda = - \sum_k \tilde{\gamma}_{\lambda k}^2 [S_k(E) - B_k] \approx -0.31 \text{ MeV}$$



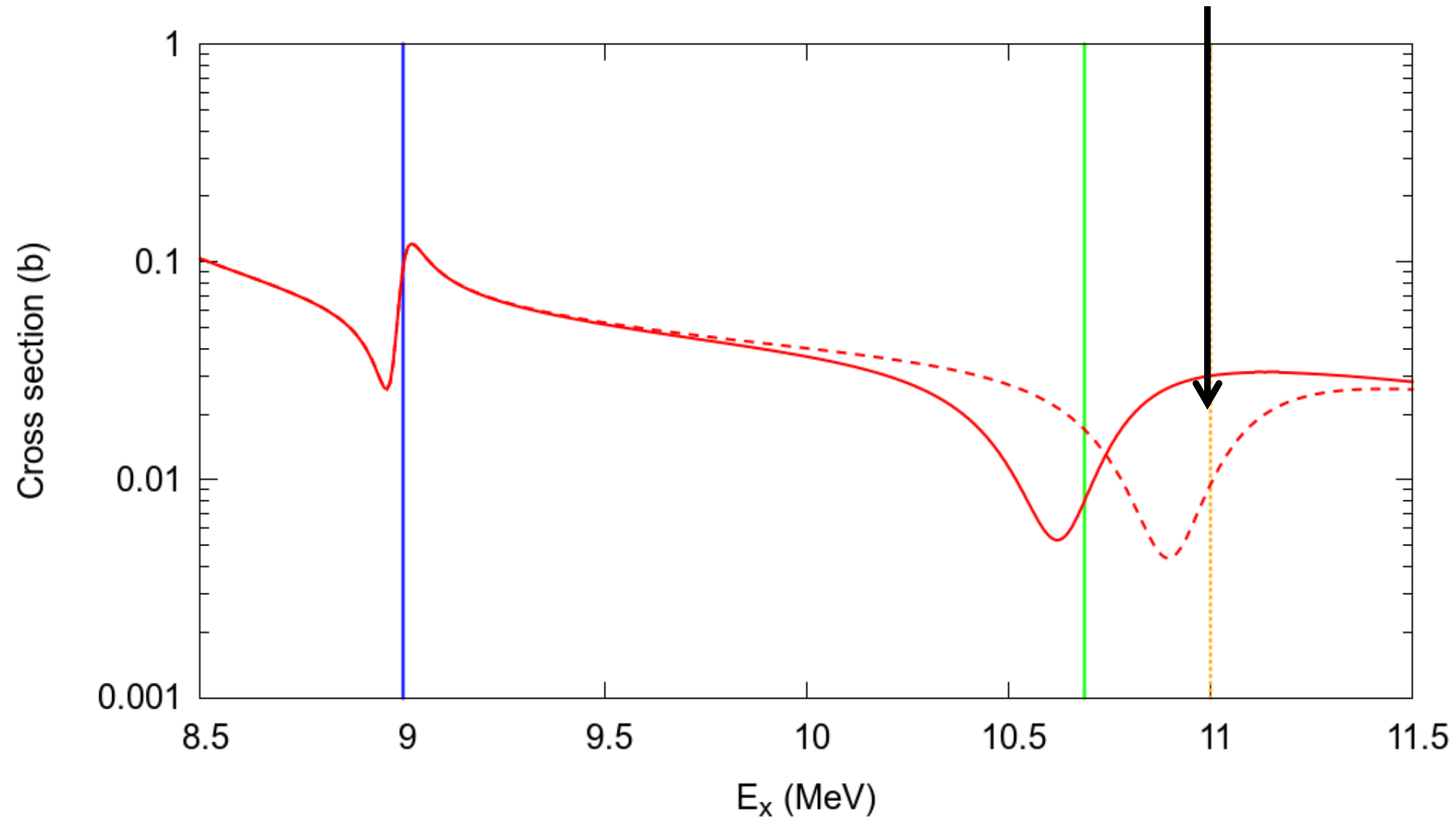
Brune parametrization

- Brune's alternative parameterization

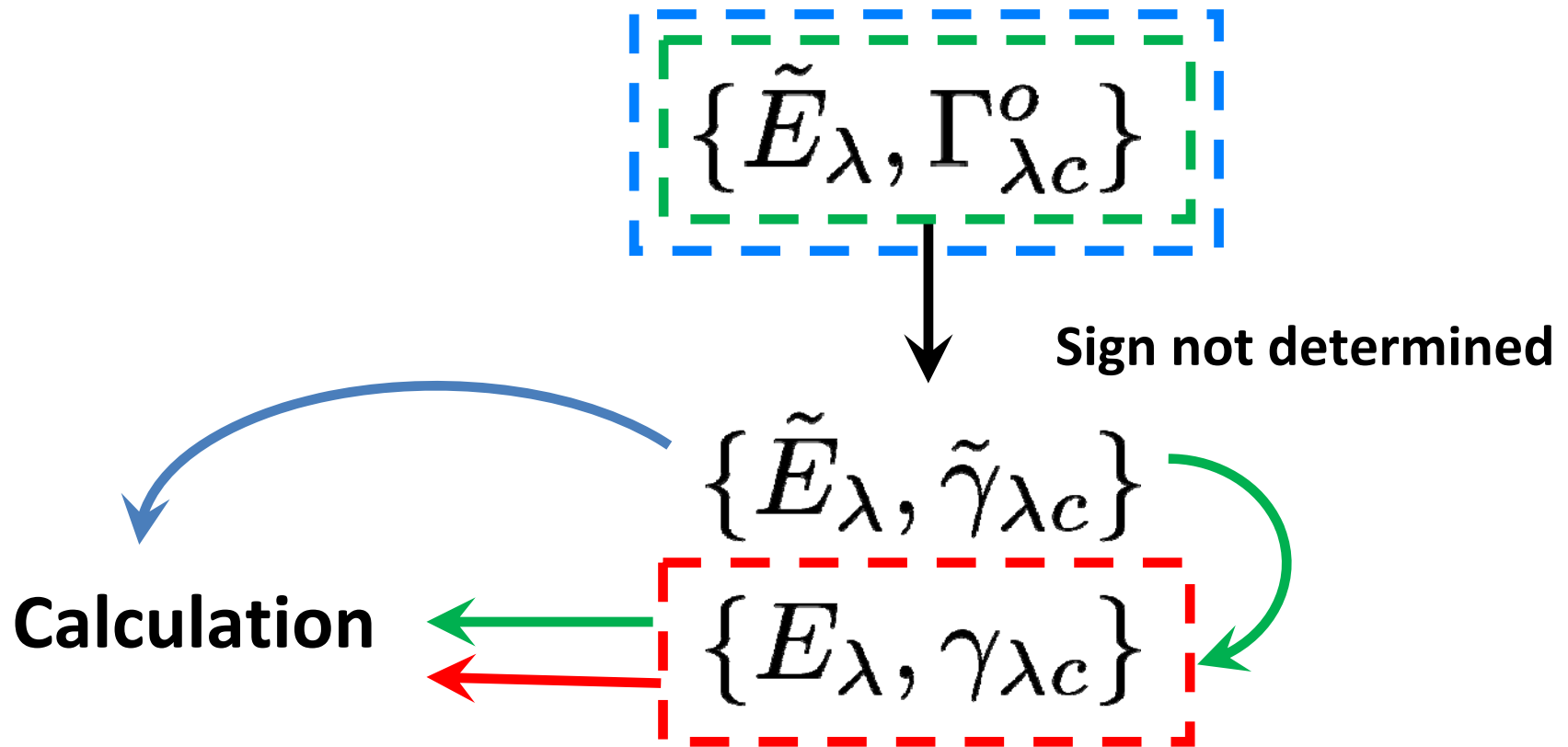
$$\{\tilde{E}_\lambda, \tilde{\gamma}_{\lambda c}\} \rightarrow \{E_\lambda, \gamma_{\lambda c}, B_c\}$$

- Inputting $\uparrow$ far easier
- Also write cross section in terms of alternative parameters – no boundary condition
- In fitting, can now genuinely fix energies and widths

Brune parametrization allows you to input on-resonance energies and widths for ALL states



AZURE Parameter Input



Where a boundary condition required it is always set to the shift function at energy of the lowest level for each spin-parity

AZURE Parmameter Output

- **AZURE Parameter Output:**
 - If using formal widths as parameters, Barker transformation used to iteratively adjust the boundary condition until at resonance energy
 - If using Brune form for cross section, no transformation required

Hard-sphere phase shift

- For elastic scattering, must include all hard sphere contributions

$$U = \Omega \left[1 + \mathfrak{B}^{\frac{1}{2}} \frac{R}{1 - RL^0} \mathfrak{B}^{\frac{1}{2}} w \right] \Omega$$



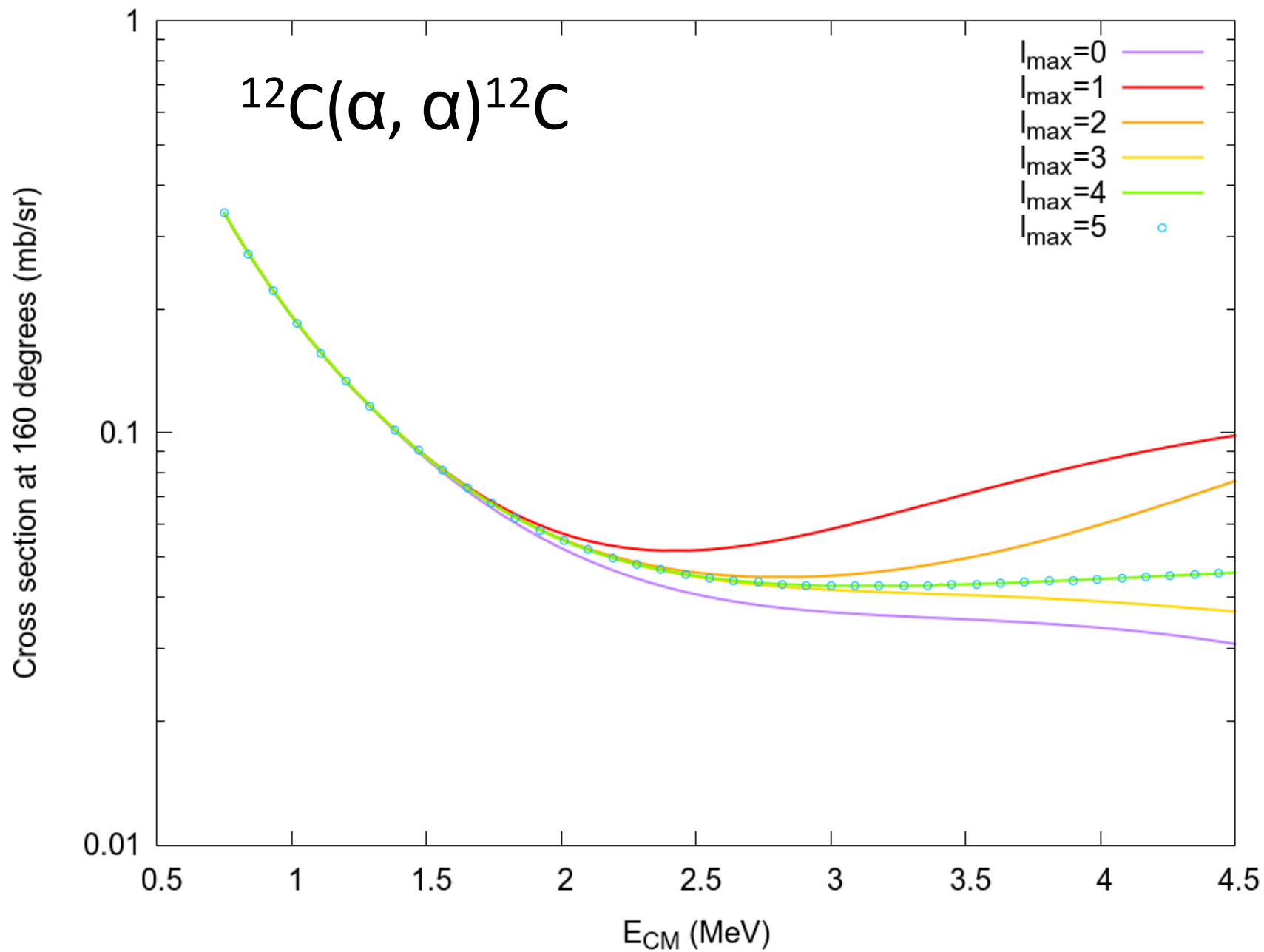
$$\Omega_c^+ = \exp[i(\omega_c - \phi_c^+)]$$

$$\phi_c^+ = \tan^{-1}(F_c/G_c)$$

L. V. Namjoshi *et al.*, PRC 13, 915 (1976)

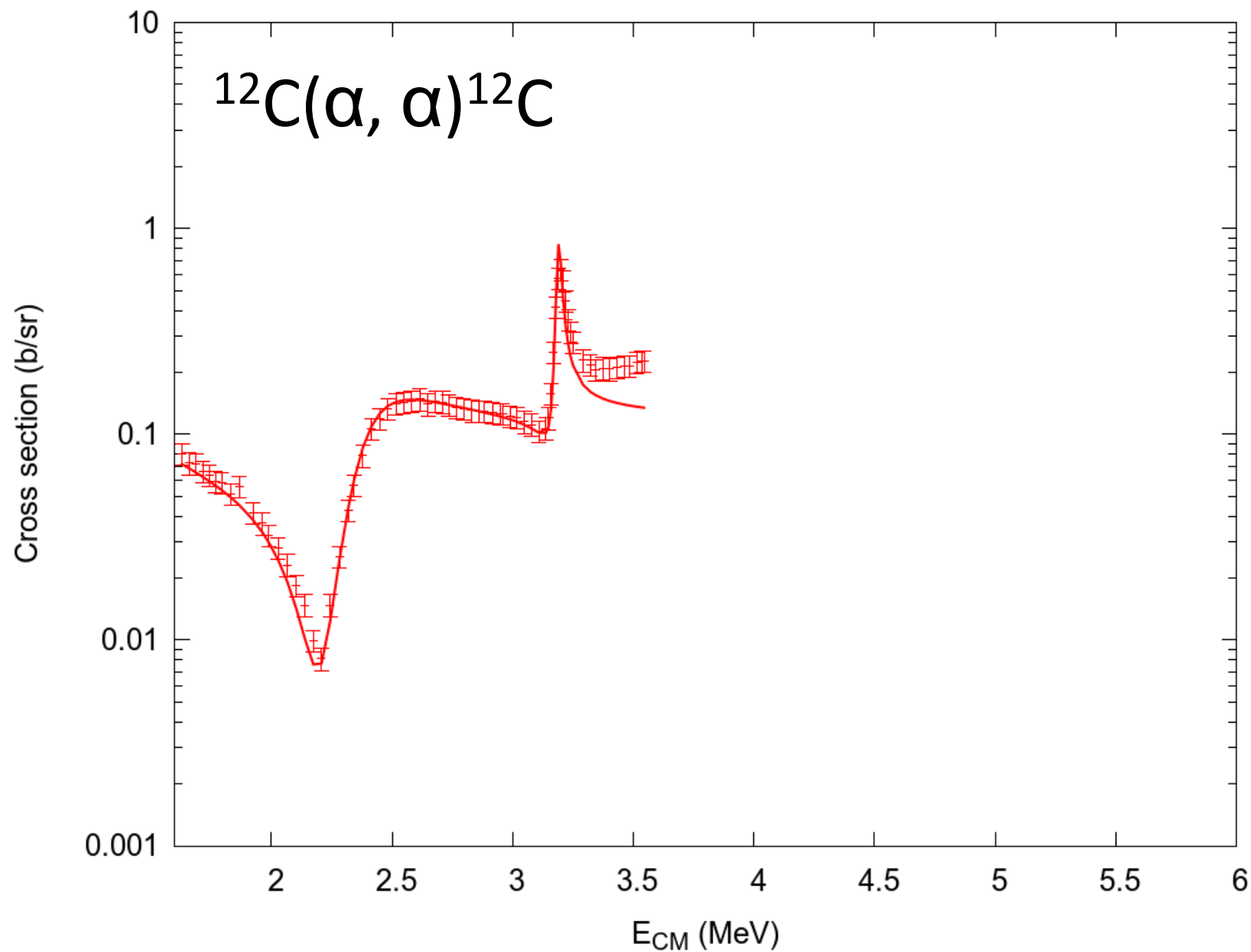
Ruiz *et al.*, PRC 71, 025802 (2005)

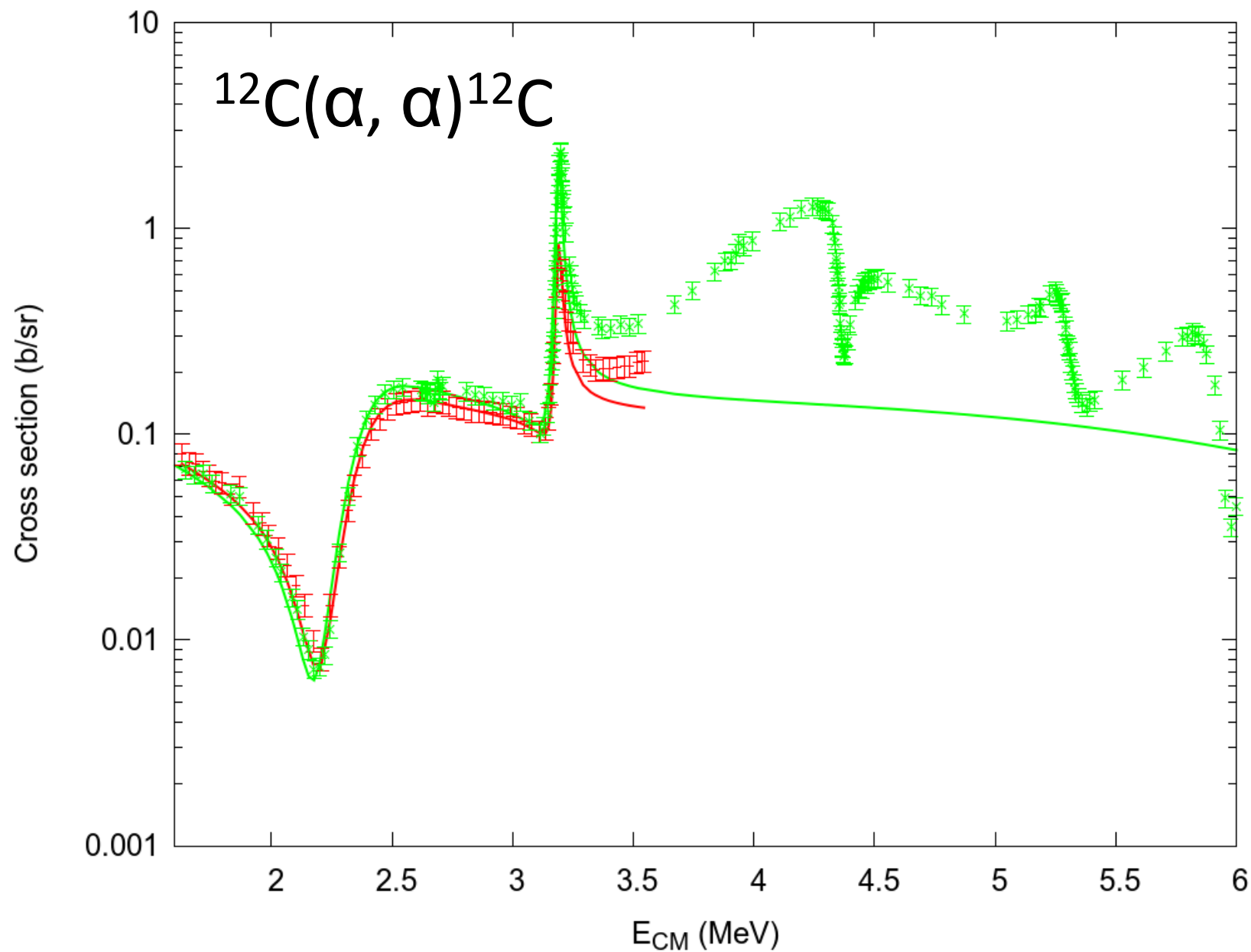
Lane and Thomas, page 271 and 289, [Rev. Mod. Phys. 30, 257 \(1958\)](#)



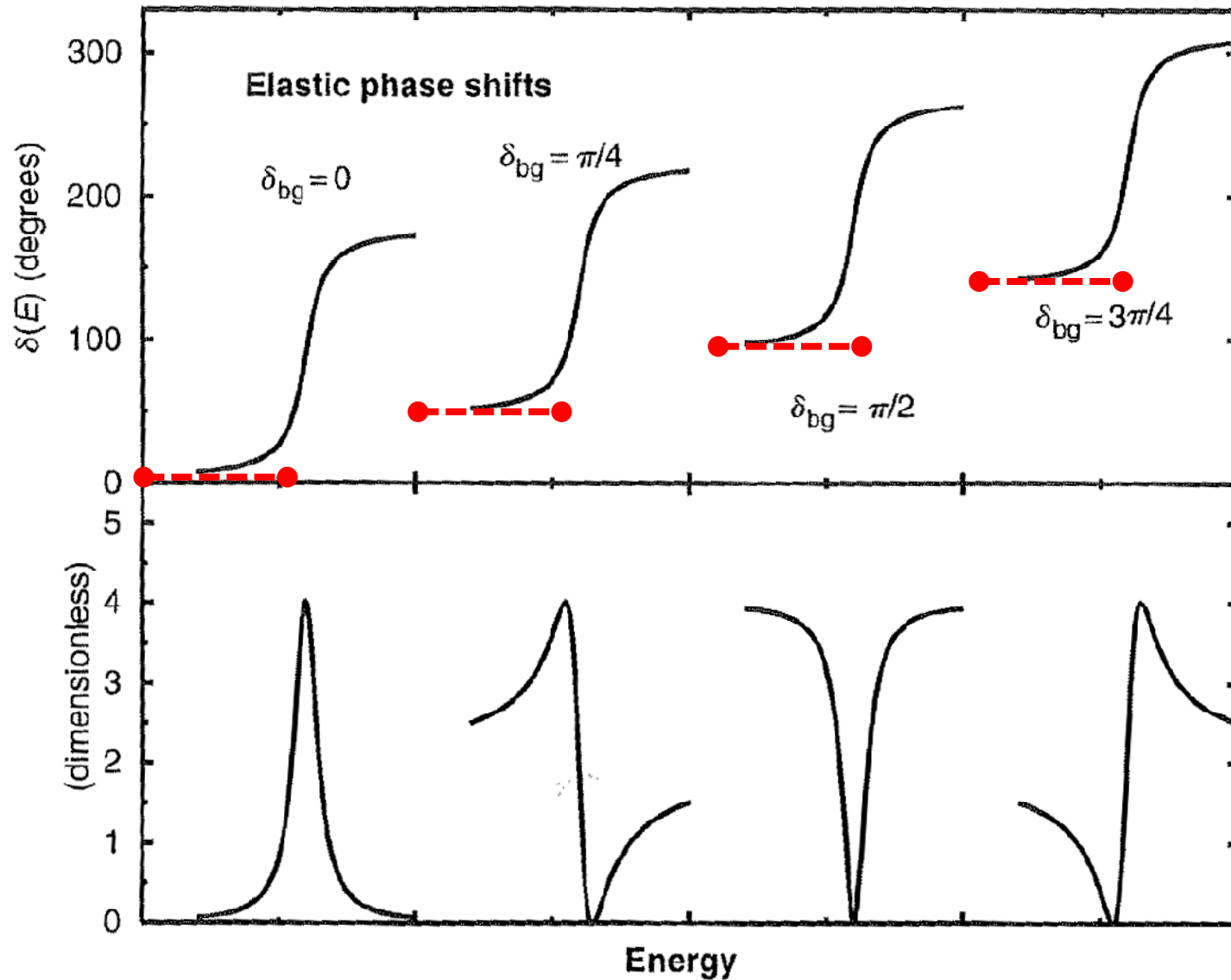
Background resonances

- Infinite expansion, infinite number of levels
- In principle, one pole for each J^π
- Simulate non-resonant contributions...
 - Higher lying resonances excluded in the fit
 - Non-compound nucleus (direct) mechanisms
 - Corrections to hard-sphere phase shift in scattering
- For reaction channels, usually only a few J^π are important

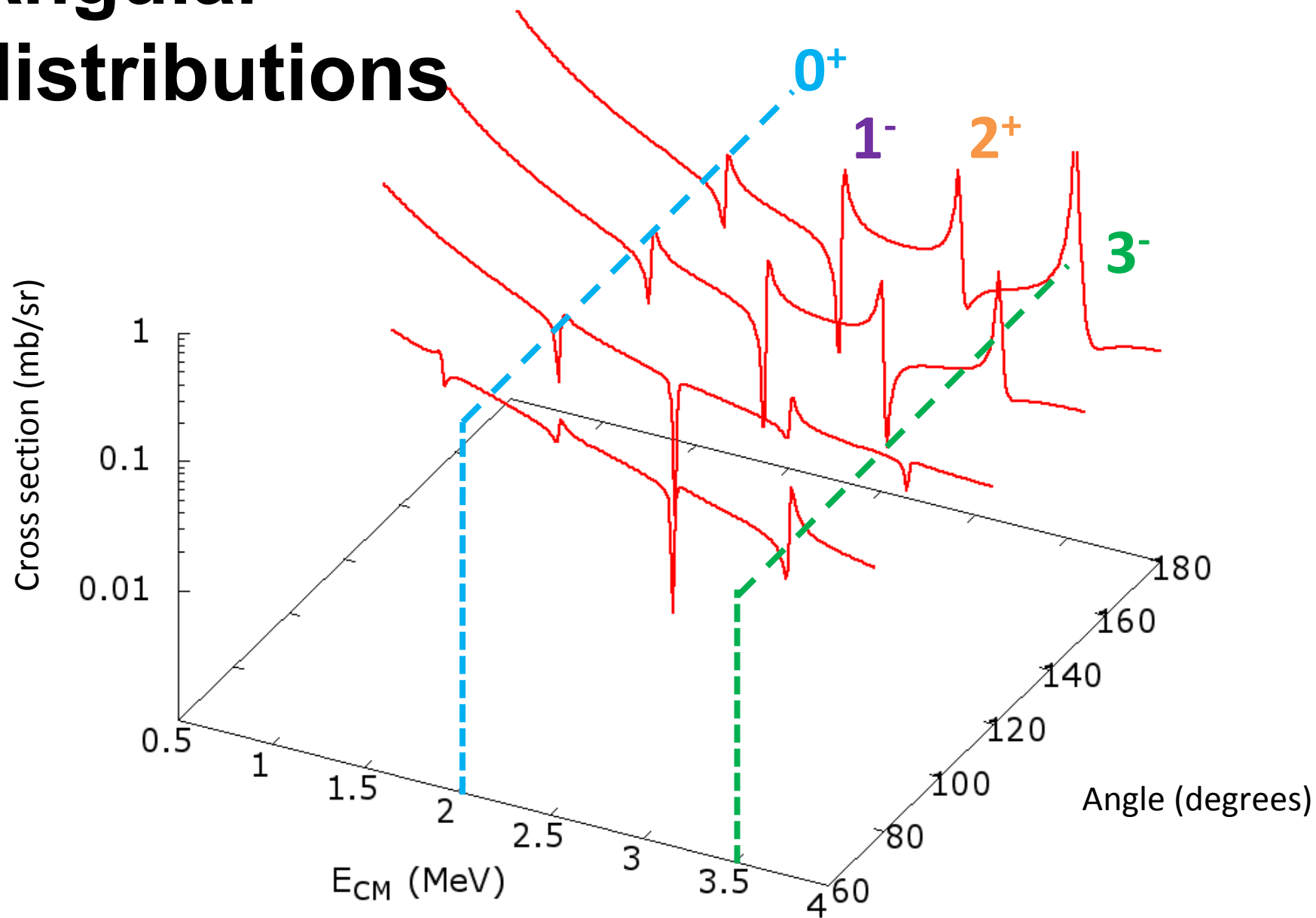




Resonance shapes



Angular distributions



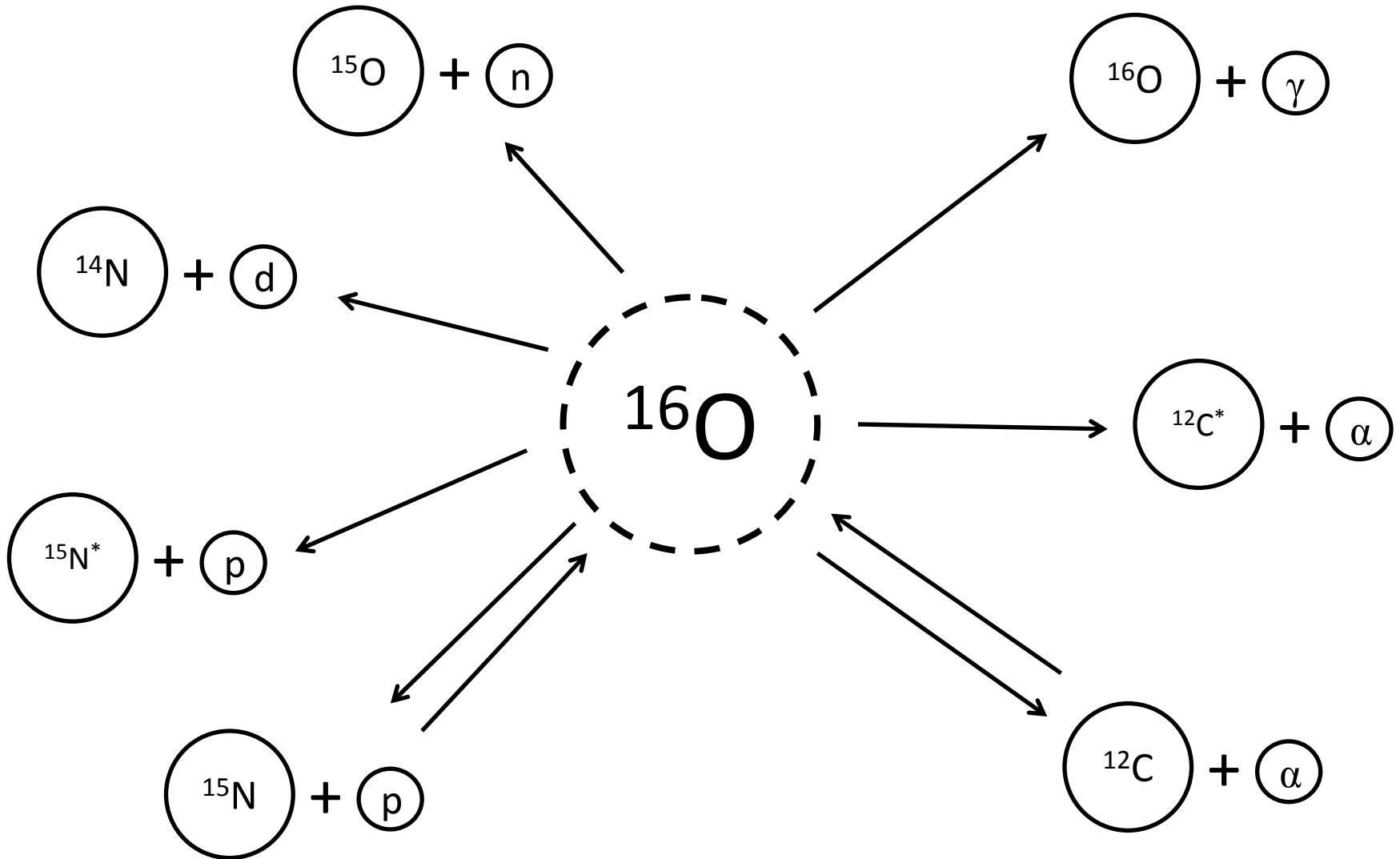
Using AZURE2

Practicalities and Examples

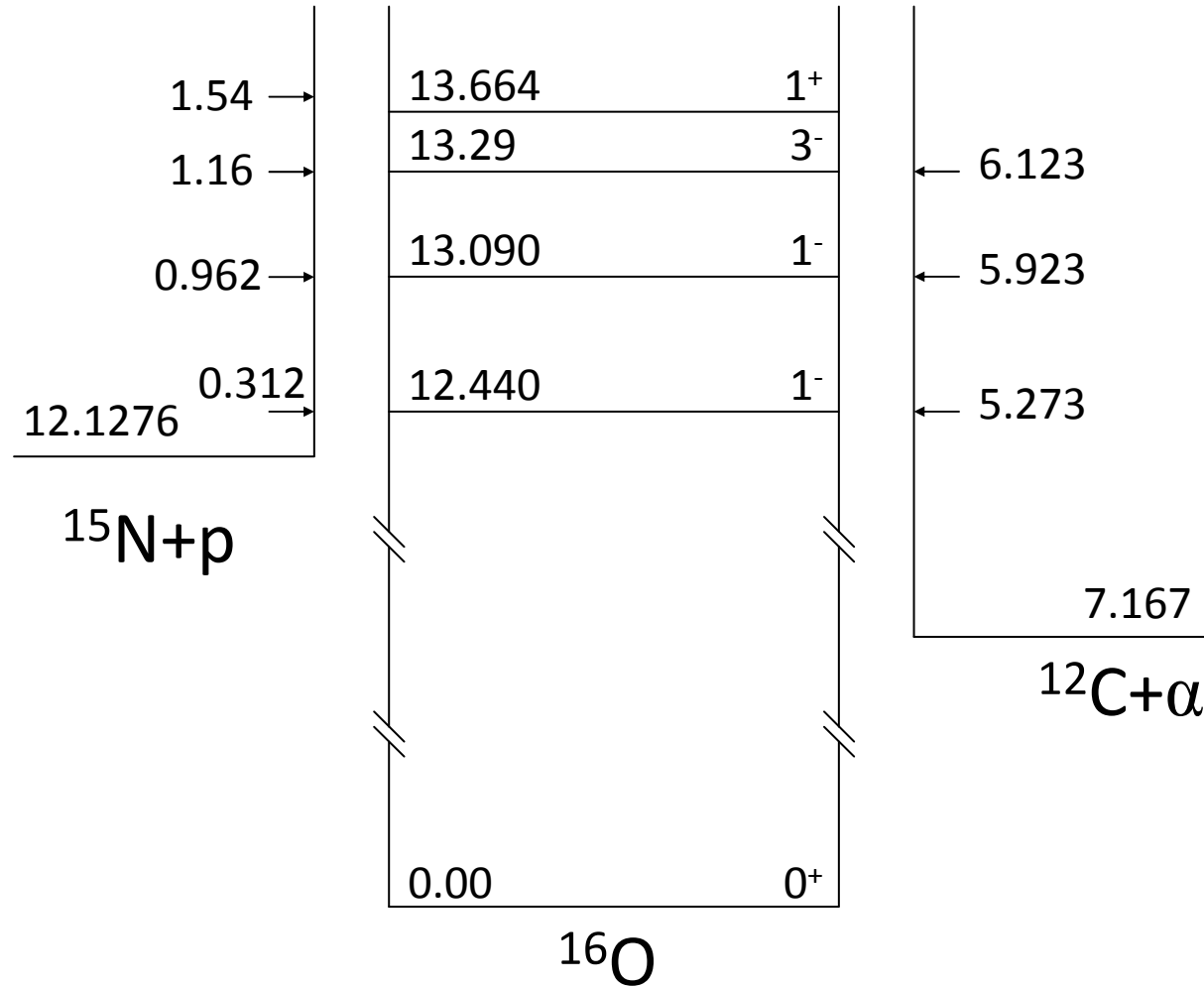
AZURE C++ code overview

- Written exclusively in C++
- Uses GNU Scientific Library and Minuit2
- Parallel using OpenMP (single node)
- All capture and reaction channels simultaneously
- Make extrapolations based on fitted resonance parameters
- Graphical user interface built using Qt and QWT (for plotting)

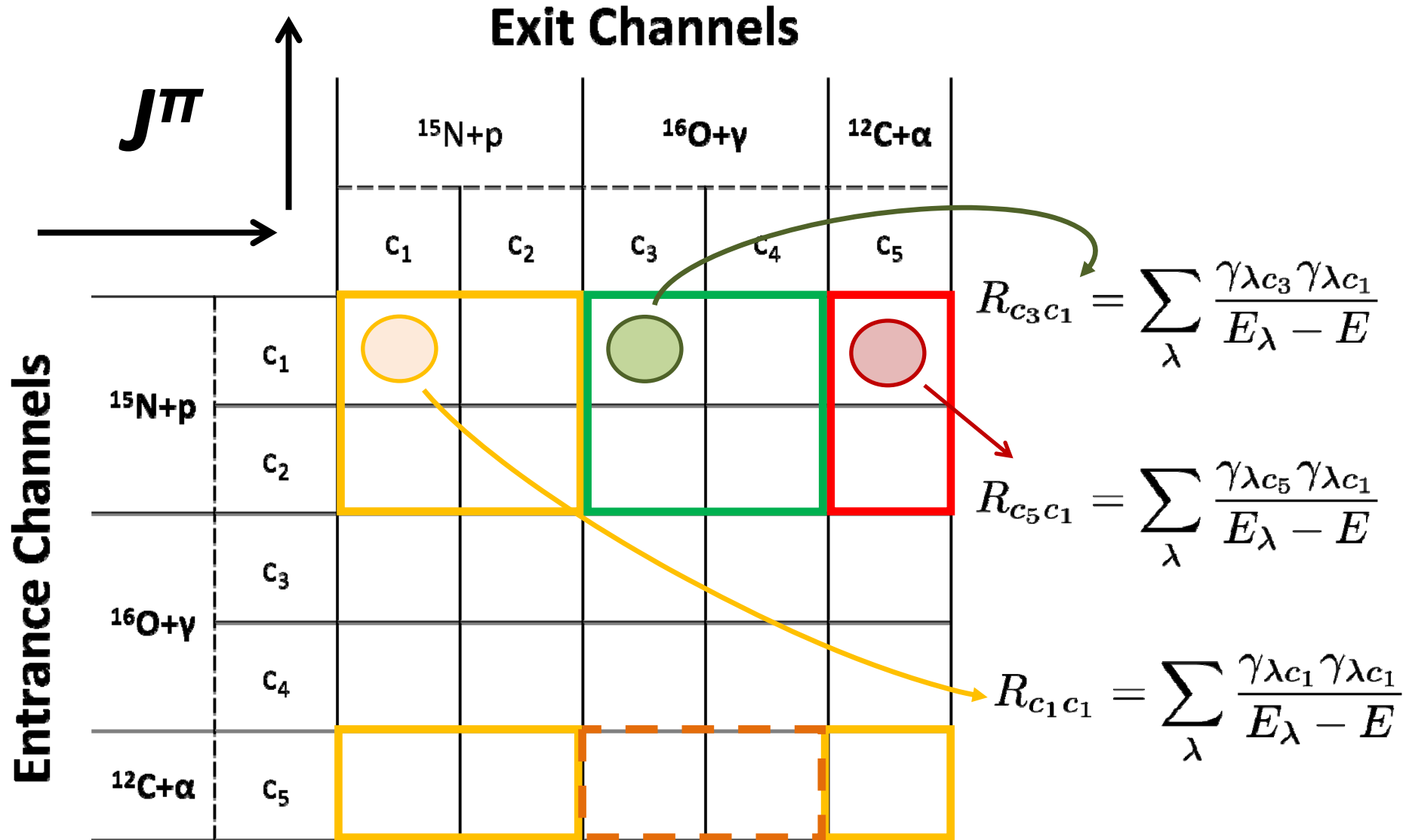
Example: ^{16}O compound reactions



^{16}O thresholds: $^{15}\text{N}(p,\alpha)^{12}\text{C}$



^{16}O R-matrix: $^{15}\text{N}(p,\gamma)^{16}\text{O}$



AZURE add particle pair

AZURE2 – /media/azure2/calcs/school/o16/o16.az2

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	α	0+	0	^{12}C	0+	0	0	7.167	5.5

List of particle pairs

Edit particle pair

$$a_c = R_0(A_1^{1/3} + A_2^{1/3})$$

Add and remove particle pairs

+

-

Edit a Particle Pair

Particle Pair Type: Particle, Particle

Light Particle

J: 0 + -

Z: 2

M: 4

g: 0

Heavy Particle

J: 0 + -

Z: 6

M: 12

g: 0

Channel Properties

Excitation Energy [MeV]: 0

Separation Energy [MeV]: 7.167

Channel Radius [fm]: 5.5

Cancel Accept

AZURE Levels and Channels

The screenshot displays the AZURE2 software interface with the following components and annotations:

- Compound Nucleus Levels:** A table listing levels with columns for 'Include?', 'Fix?', 'Level Spin', and 'Energy [MeV]'.

Include?	Fix?	Level Spin	Energy [MeV]
☒	☐	1-	9.585
☒	☐	4+	10.356
☐	☐	2+	11.52
☐	☐	3-	11.6
☒	☒	0+	20
☒	☒	1-	20
☒	☒	2+	20
☒	☒	3-	20
☒	☒	4+	20
- Channels In Selected Level:** A table showing channels for the selected level.

Fix?	Channel Pair	s	l
☐	$^{12}\text{C} + \alpha$ [0.000 MeV]	0	1
- Channel Configuration:** Settings for the selected channel.
 - Maximum Orbital Momentum: 4
 - Maximum Gamma Multipolarity: 1
 - Maximum Gamma Multipolarities Per Decay: 1
- Channel Details (select from list to view):** Information for the selected channel.

9.585 MeV level with spin 1-
transitioning via pair key #1
Channel configuration is
s = 0, l = 1

Light Particle Spin: 0+
Light Particle Z: 2
Light Particle M: 4
Light Particle G: 0
Heavy Particle Spin: 0+
Heavy Particle Z: 6
Heavy Particle M: 12
Heavy Particle G: 0
Excitation Energy: 0
Separation Energy: 7.167
Channel Radius: 5.5
- Edit a Level:** A dialog box for editing level properties.

Excitation Energy [MeV]: 9.585
Level Spin: 1
- Partial Width:** A field at the bottom right set to 420000 eV.

Annotations:

- List of levels:** Points to the 'Compound Nucleus Levels' table.
- Add and remove compound nucleus levels:** Points to the '+' and '-' buttons at the bottom left.
- List of channels for a given level:** Points to the 'Channels In Selected Level' table.
- Edit level:** Points to the 'Edit a Level' dialog box.
- Edit allowed channels:** Points to the 'Channel Configuration' section.
- Channel summary:** Points to the 'Channel Details' section.
- Edit channel width:** Points to the 'Partial Width' field.

Channels for $^{12}\text{C}+\alpha$

- Calculated automatically by AZURE2
- For $^{12}\text{C}+\alpha$ things are simple:

$$I_1 = 0 \qquad \pi_1 = 1$$

$$I_2 = 0 \qquad \pi_2 = 1$$

$$\therefore s = 0$$

$$\text{and } J = \ell \qquad \pi = \pi_1 \pi_2 (-1)^\ell = (-1)^\ell$$

- One channel per J , only natural parity states allowed $\pi = (-1)^J$
- In general, many channels allowed per resonance

Data and extrapolation segments

The screenshot displays the AZURE2 software interface with the 'Segments' tab selected. The main window is divided into two sections: 'Segments From Data' and 'Segments Without Data'. The 'Segments From Data' section contains a table with five rows of data segments, all for the reaction $^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$ [0.000 MeV] with an energy range of 1.8-4.9 MeV. The angles are 30, 45, 60, 135, and 150 degrees. The 'Segments Without Data' section contains a table with one row of an extrapolation segment for the same reaction and energy range, with an energy step of 0.01 MeV. Two dialog boxes are open: 'Edit a Segment Without Data' and 'Edit a Segment From Data'. The 'Edit a Segment Without Data' dialog shows fields for Entrance Pair Key (1), Exit Pair Key (1), Lab Energy [MeV] (Low: 1, High: 4, Step: 0.01), Lab Angle [degrees] (Low: 160, High: 160, Step: 40), and Data Type (Differential). The 'Edit a Segment From Data' dialog shows fields for Entrance Pair Key (1), Exit Pair Key (1), Lab Energy [MeV] (Low: 1.8, High: 4.9), Lab Angle [degrees] (Low: 30, High: 30), Data Type (Differential), Data Norm. (1), Vary Norm? (unchecked), Norm. Error [%] (0), and Data File (data/radovic_2002.dat). Red and blue annotations highlight specific areas: a red box around the 'Segments From Data' table, a blue box around the 'Segments Without Data' table, a red circle around the '+' and '-' buttons in the 'Segments From Data' section, and a blue circle around the '+' and '-' buttons in the 'Segments Without Data' section.

Data segments

	Reaction	Energy Range	Angle
1	$^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$ [0.000 MeV]	1.8-4.9	30
2	$^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$ [0.000 MeV]	1.8-4.9	45
3	$^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$ [0.000 MeV]	1.8-4.9	60
4	$^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$ [0.000 MeV]	1.8-4.9	135
5	$^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$ [0.000 MeV]	1.8-4.9	150

Extrapolation segments

	Reaction	Energy Range	Energy Step
1	$^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$ [0.000 MeV]	1-4	0.01

Edit a Segment Without Data

Entrance Pair Key: 1 Exit Pair Key: 1

Lab Energy [MeV]

Low Energy: 1 High Energy: 4 Energy Step: 0.01

Lab Angle [degrees]

Low Angle: 160 High Angle: 160 Angle Step: 40

Data Type: Differential

Cancel Accept

Edit a Segment From Data

Entrance Pair Key: 1 Exit Pair Key: 1

Lab Energy [MeV]

Low Energy: 1.8 High Energy: 4.9

Lab Angle [degrees]

Low Angle: 30 High Angle: 30

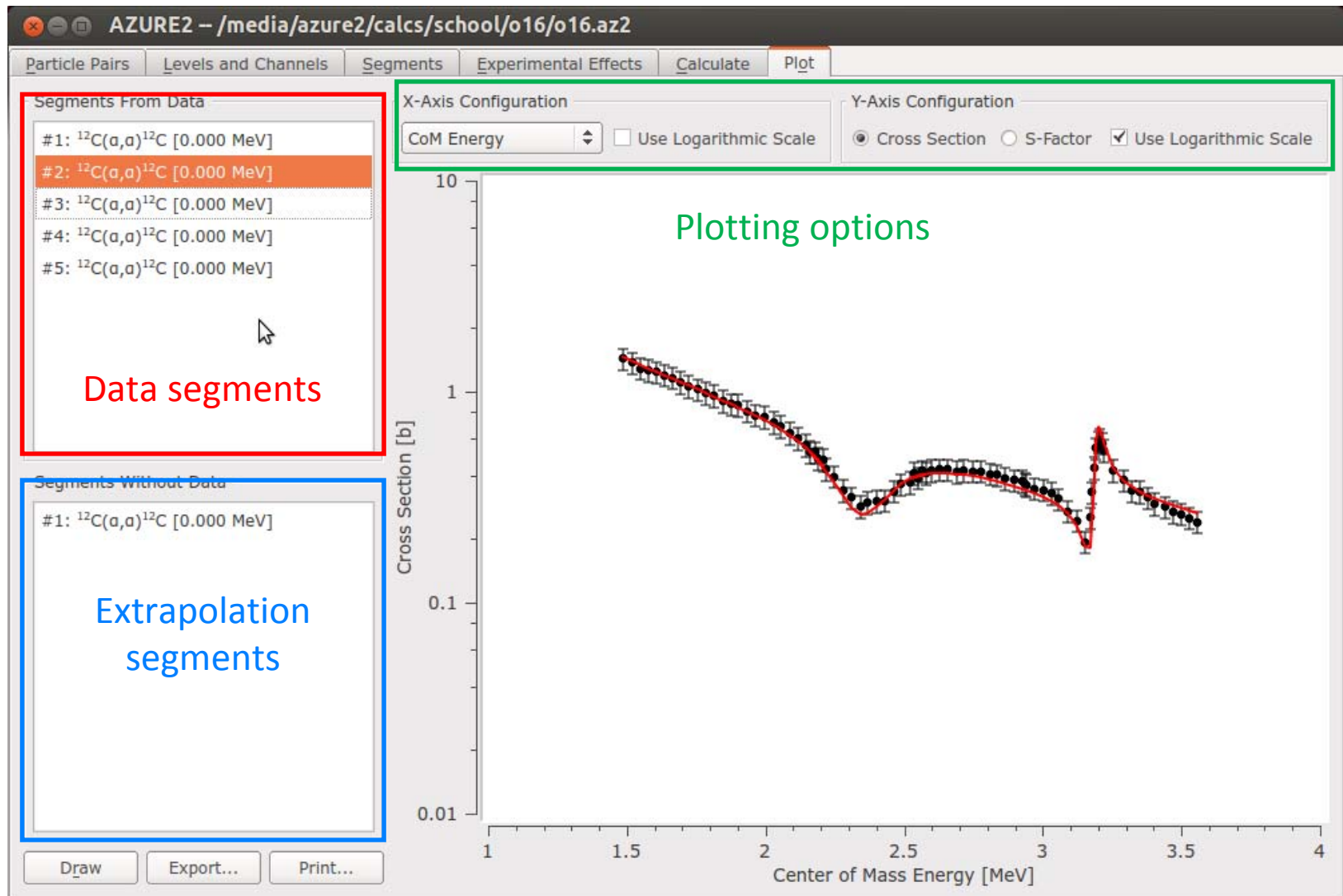
Data Type: Differential

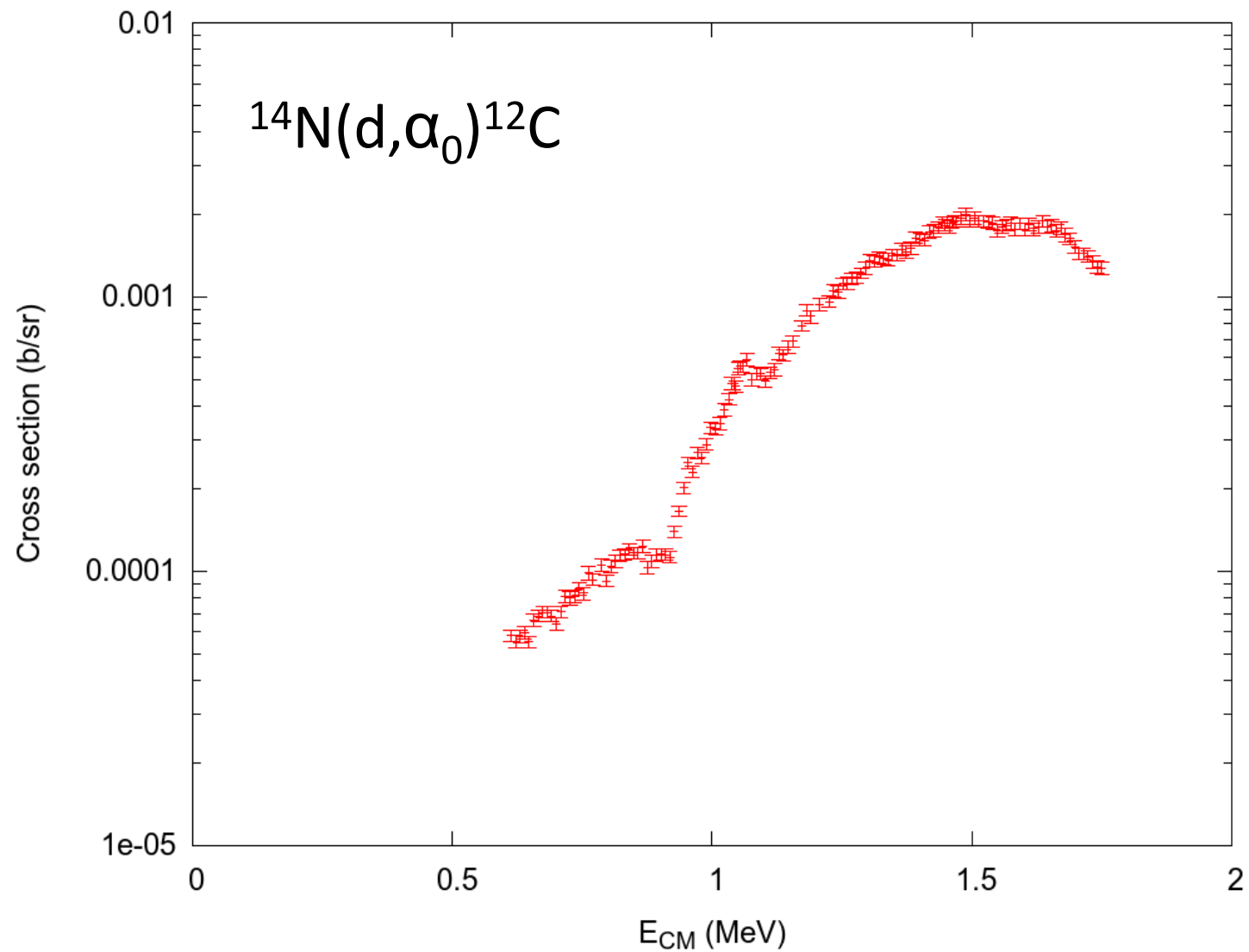
Data Norm.: 1 Vary Norm? Norm. Error [%]: 0

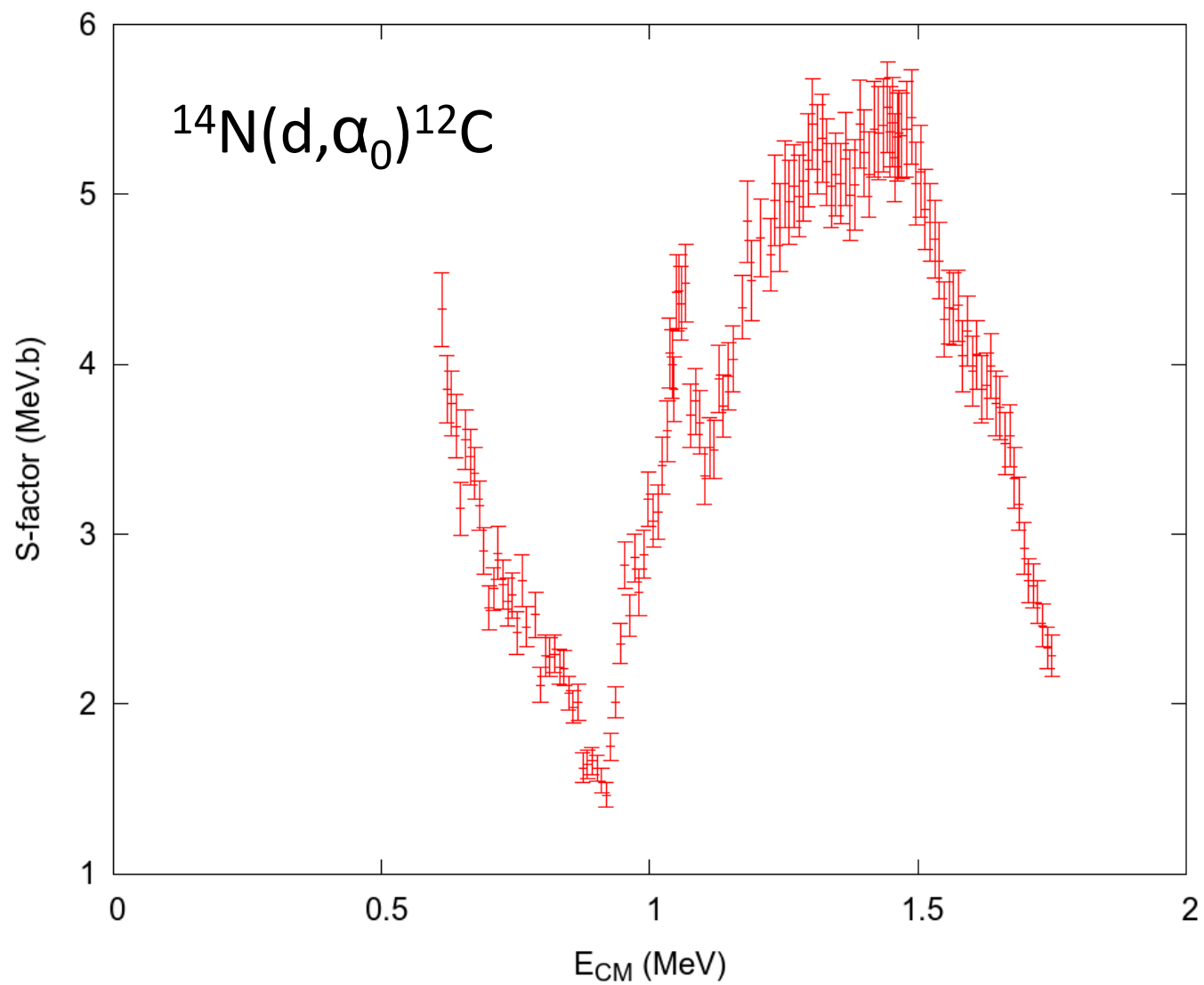
Data File: data/radovic_2002.dat Choose...

Cancel Accept

Plotting







Final thoughts...

Things I haven't mentioned...

- **Capture reactions**
 - External part of capture amplitude can be included
 - Explicitly add the final state as a level, set the ANC as you would a width
- **Experimental effects**
 - Beam convolution – Gaussian distribution of incident energies
 - Target integration – thickness of target
 - Added on per segment basis (different experiments, different targets)
- **Reaction rate calculations**
 - Based on an R-matrix calculation, calculate an astrophysical reaction rate
 - Computationally intensive (quite slow...)
- **Check files**
 - Useful for checking against other codes
 - Can find boundary conditions, penetrabilities etc.,

Afternoon session

- Detailed worked example $^{12}\text{C} + \alpha$ (^{16}O)
- Further examples: $^{13}\text{C} + \text{p}$ (^{14}N), $^{21}\text{Na} + \text{p}$ (^{22}Mg)
- If you have your own problems; great!
 - Data must be laboratory system with light particle incident on heavy target
 - For angle-integrated data, dummy angle must be included
 - Kinematics cheat sheet
 - Ask for further info on getting going...

Masses and Structure

- [US National Nuclear Data Centre](#)
 - Resonance energies, J^π and widths/branches
- [TUNL Nuclear Data Project](#)
 - Energy level of light nuclei ($A < 20$)
 - Energies, widths, reaction specific
- [Berkeley Table of Atomic Masses](#)
 - (Occasionally offline...)
- [Atomic Mass Data Centre](#)
- [Chart of the Nuclides](#)

Reactions

- [EXFOR: Experimental Nuclear Reaction Data](#)
 - Vast resonance of reactions data
 - Varying format (CM/LAB etc.), MUST check against original paper
- [IBANDL: Ion Beam Analysis Nuclear Data Library](#)
- [AZURE](#) website
 - Register to download codes
 - E-mail (James deBoer) for beta of C++ code

Credits...

- Developed at the Joint Institute for Nuclear Astrophysics at University of Notre Dame
- FORTRAN 77 version (2002 ish – present)
 - R. E. Azuma, E. Uberseder, E. C. Simpson, C. R. Brune, H. Costantini, R. J. de Boer, J. Gorres, M. Heil, P. J. LeBlanc, C. Ugalde and M. Wiescher
- C++ version (in development) “AZURE2”
 - Ethan Uberseder, Dick Azuma, James deBoer