Astrophysics needs and tools: Overview of AZURE

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

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May 9th-10th 2013

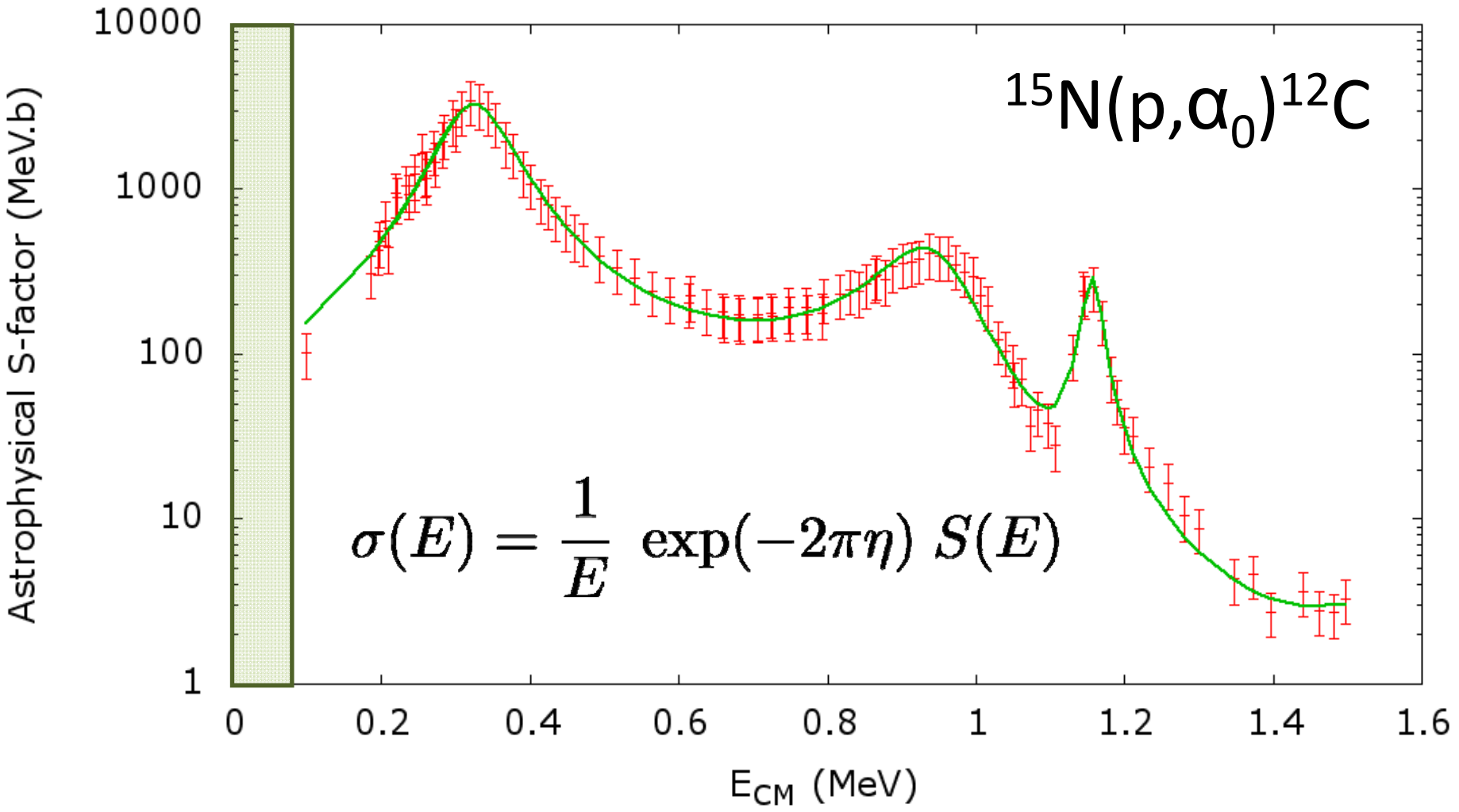
Overview

- 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

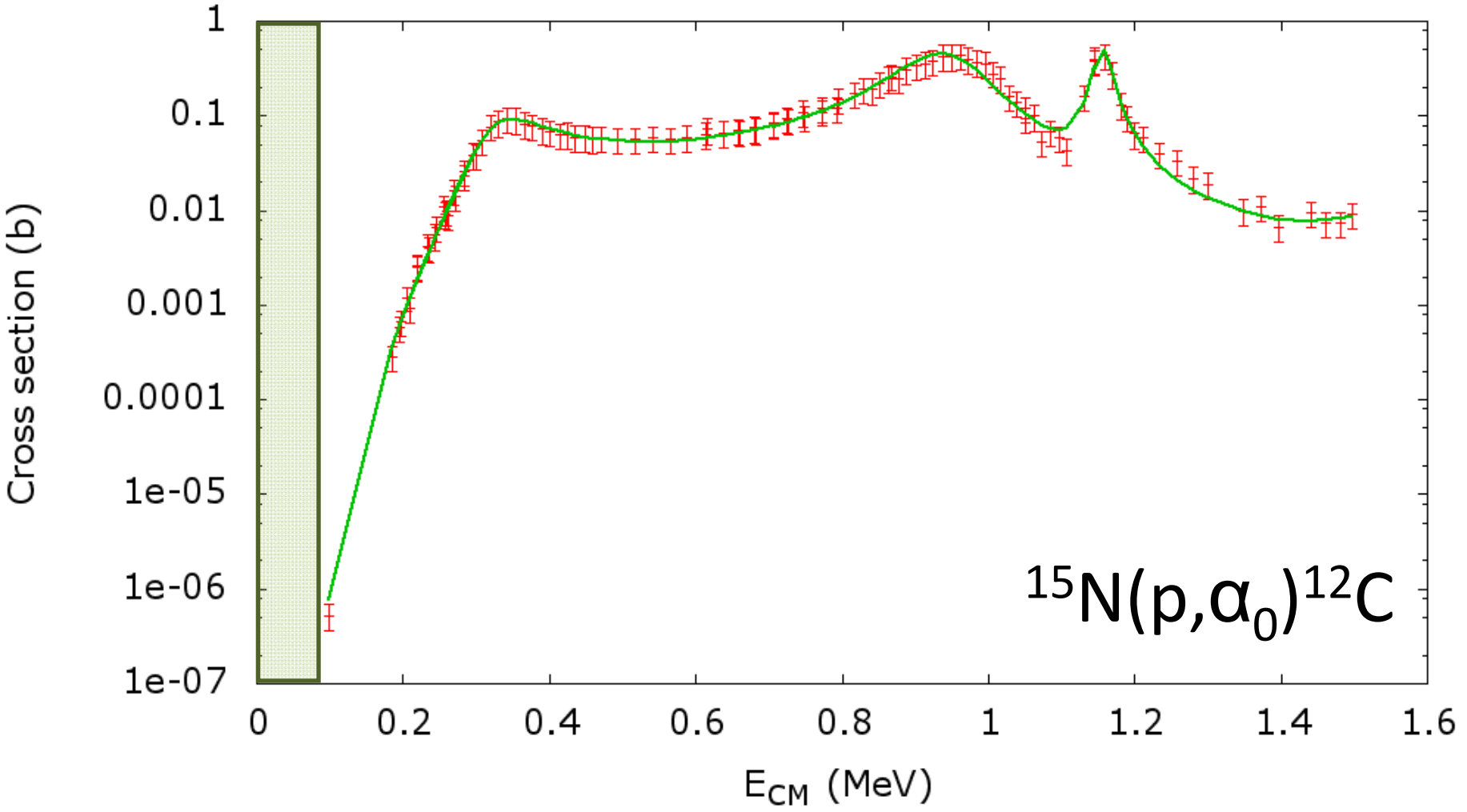
Introduction

Nuclear Astrophysics, R-matrix and AZURE

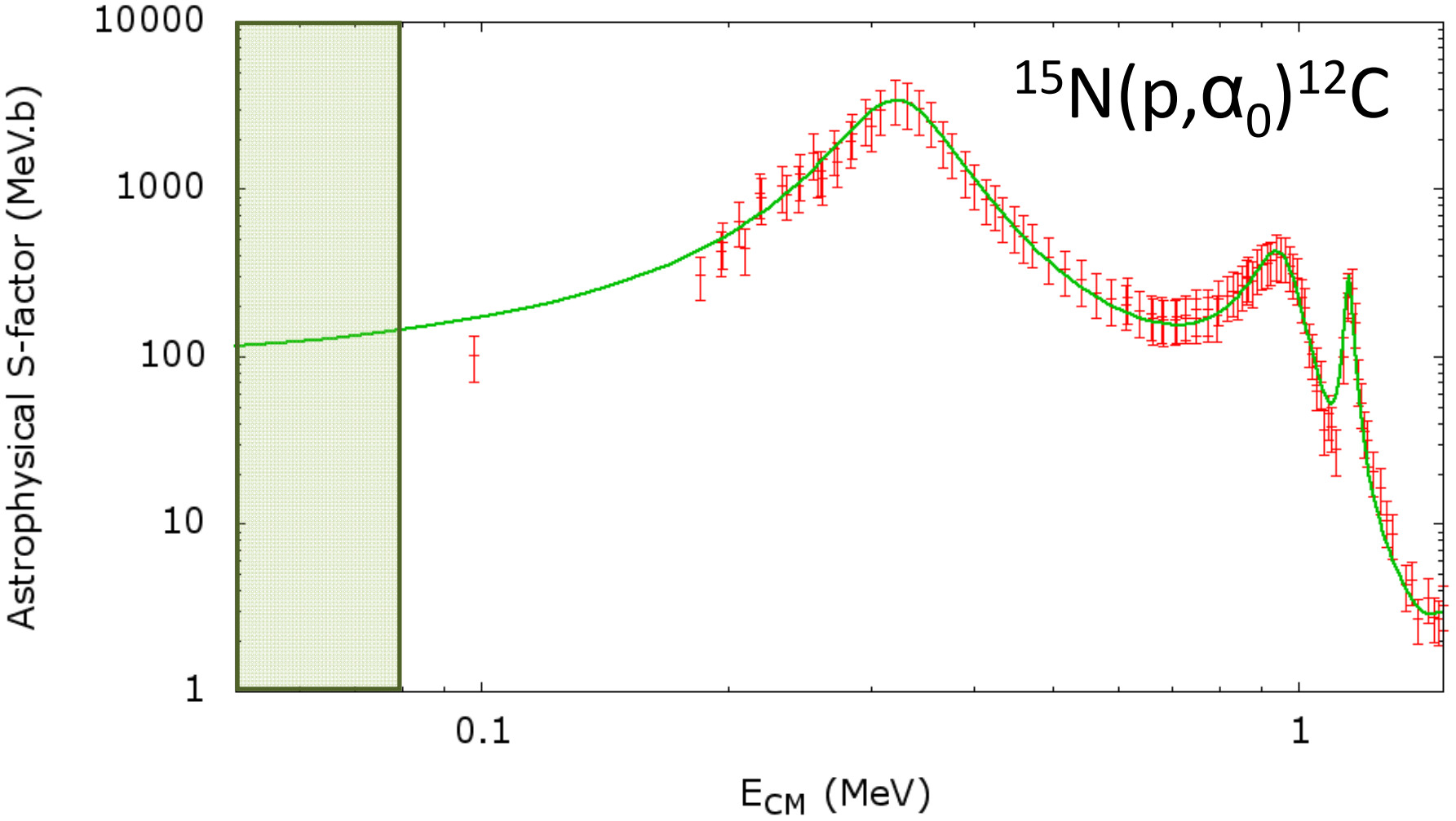
Into the Gamow window...



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

Lane and Thomas, Rev. Mod. Phys. 30, 257 (1958)

R. E. Azuma *et al.*, Phys. Rev. C 81, 041805 (2010)

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

Lane and Thomas, page 265-266, Rev. Mod. Phys. 30, 257 (1958)

Channel spin and angular momentum

$$I_1 = \text{Angular momentum of particle 1}$$

$$I_2 = \text{Angular momentum of particle 2}$$

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

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

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

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

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

Lane and Thomas, page 265-266, Rev. Mod. Phys. 30, 257 (1958)

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?

Lane and Thomas, page 276, Rev. Mod. Phys. 30, 257 (1958)

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

$$\Gamma^o_{\lambda c} = \frac{2P_c\tilde{\gamma}^2_{\lambda c}}{1+\sum_k \tilde{\gamma}^2_{\lambda k}\left(\frac{dS_k}{dE}\right)_{\tilde{E}_\lambda}}$$

Formal

Observed

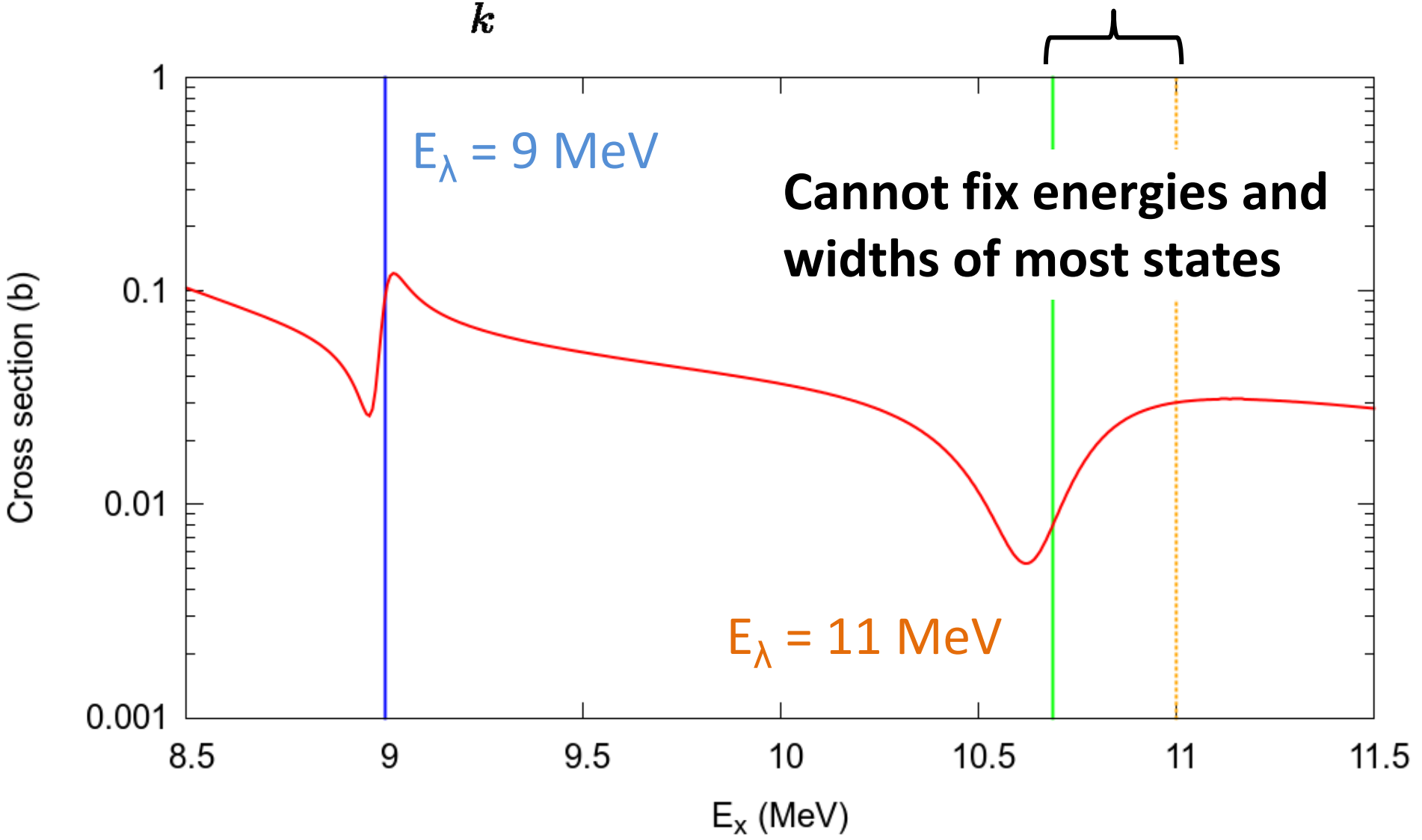
$$\tilde{\gamma}^2_{\lambda c} = \frac{\Gamma^o_{\lambda c}}{P_c}\left[2-\sum_k \frac{\Gamma^o_{\lambda k}}{P_k}\left(\frac{dS_k}{dE}\right)_{\tilde{E}_\lambda}\right]^{-1}$$

"On-resonance" parameters

Lane and Thomas, page 327, Rev. Mod. Phys. 30, 257 (1958)

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

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



Brune parametrization

- Brune's alternative parameterization

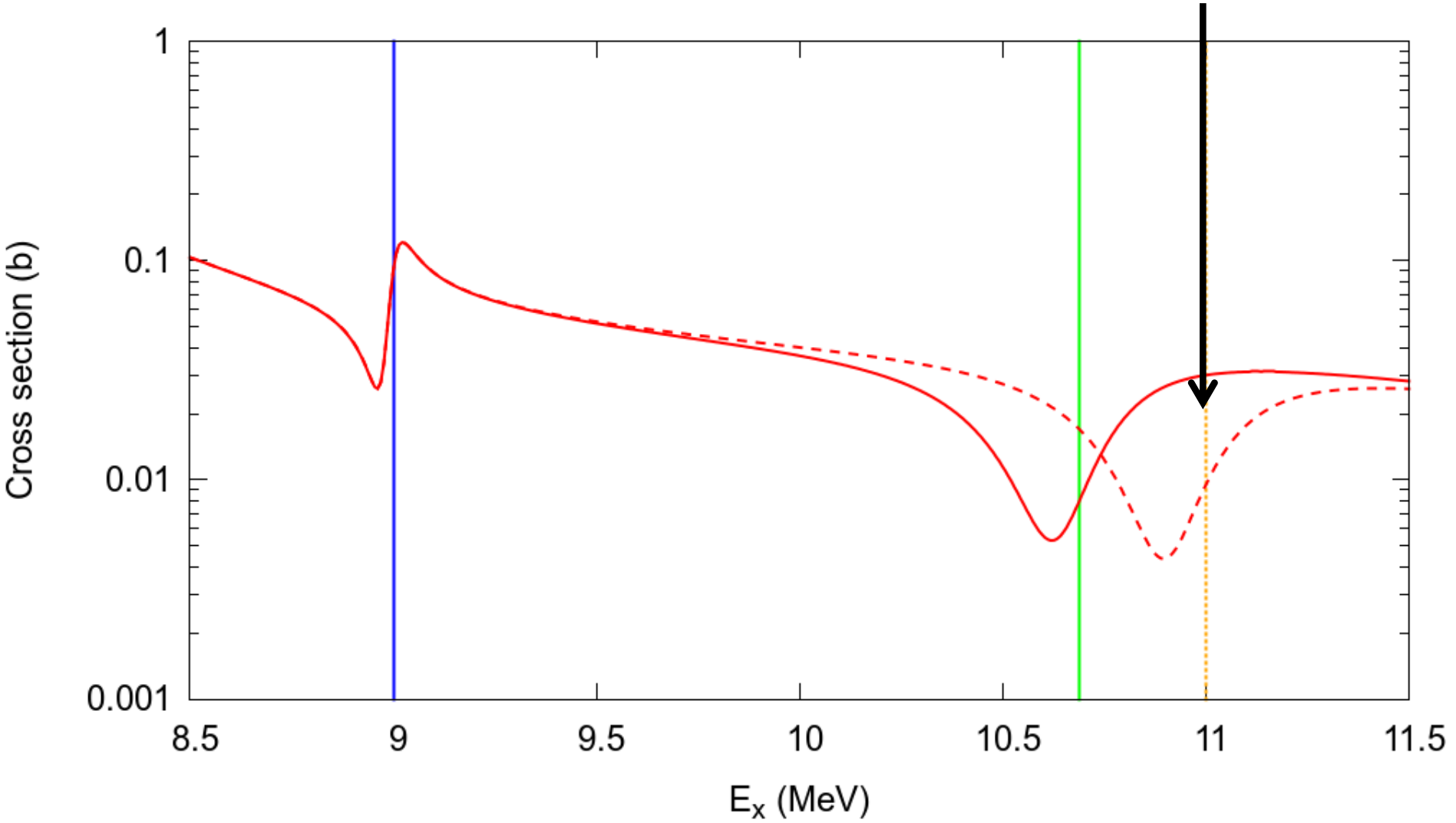
$$\{\tilde{E}_\lambda, \tilde{\gamma}_{\lambda c}\} \rightarrow \{E_\lambda, \gamma_{\lambda c}, B_c\}$$

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

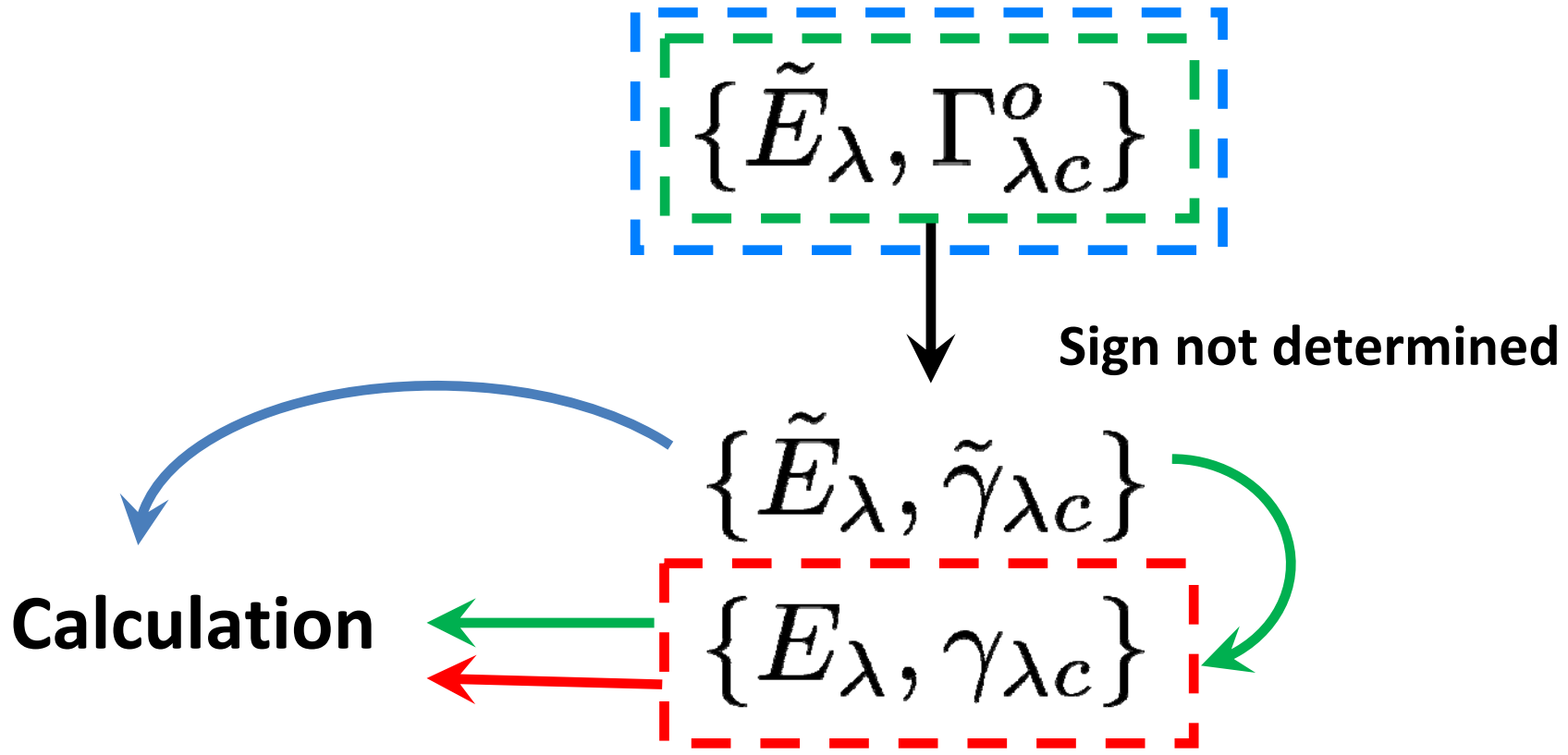
Carl Brune, Phys. Rev. C 66, 044611 (2002)

Decouvemont and Baye, page 28/29, Rep. Prog. Phys 73, 036301 (2010)

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

Lane and Thomas, page 270, 274, 283, Rev. Mod. Phys. 30, 257 (1958)

Fred Barker, Aust. J. Phys. 25, 341 (1972)

Hard-sphere phase shift

- For elastic scattering, must include all hard sphere contributions

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

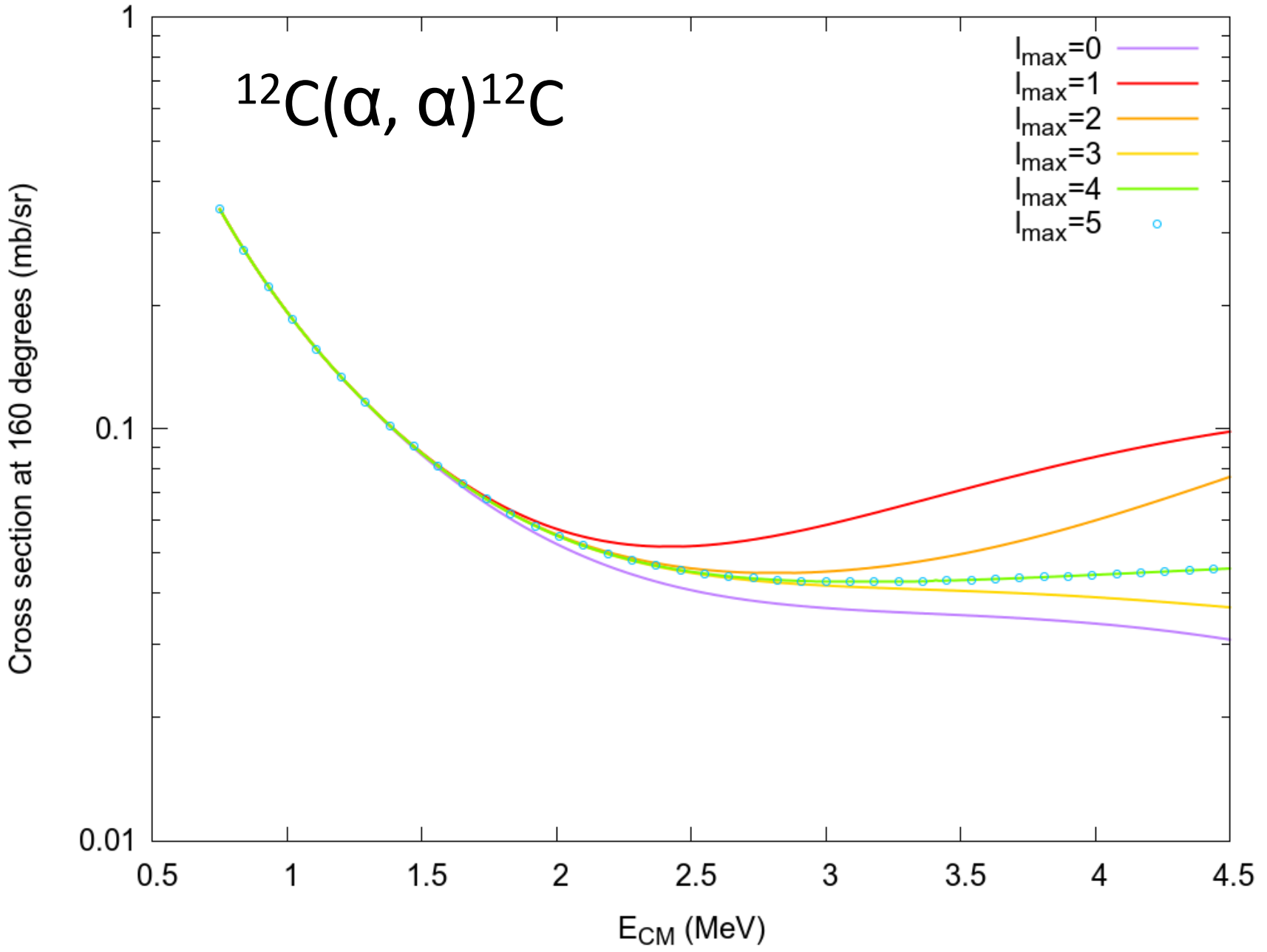
$$\Omega_c^+ = \exp[i(\omega_c - \phi_c^+)]$$

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

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

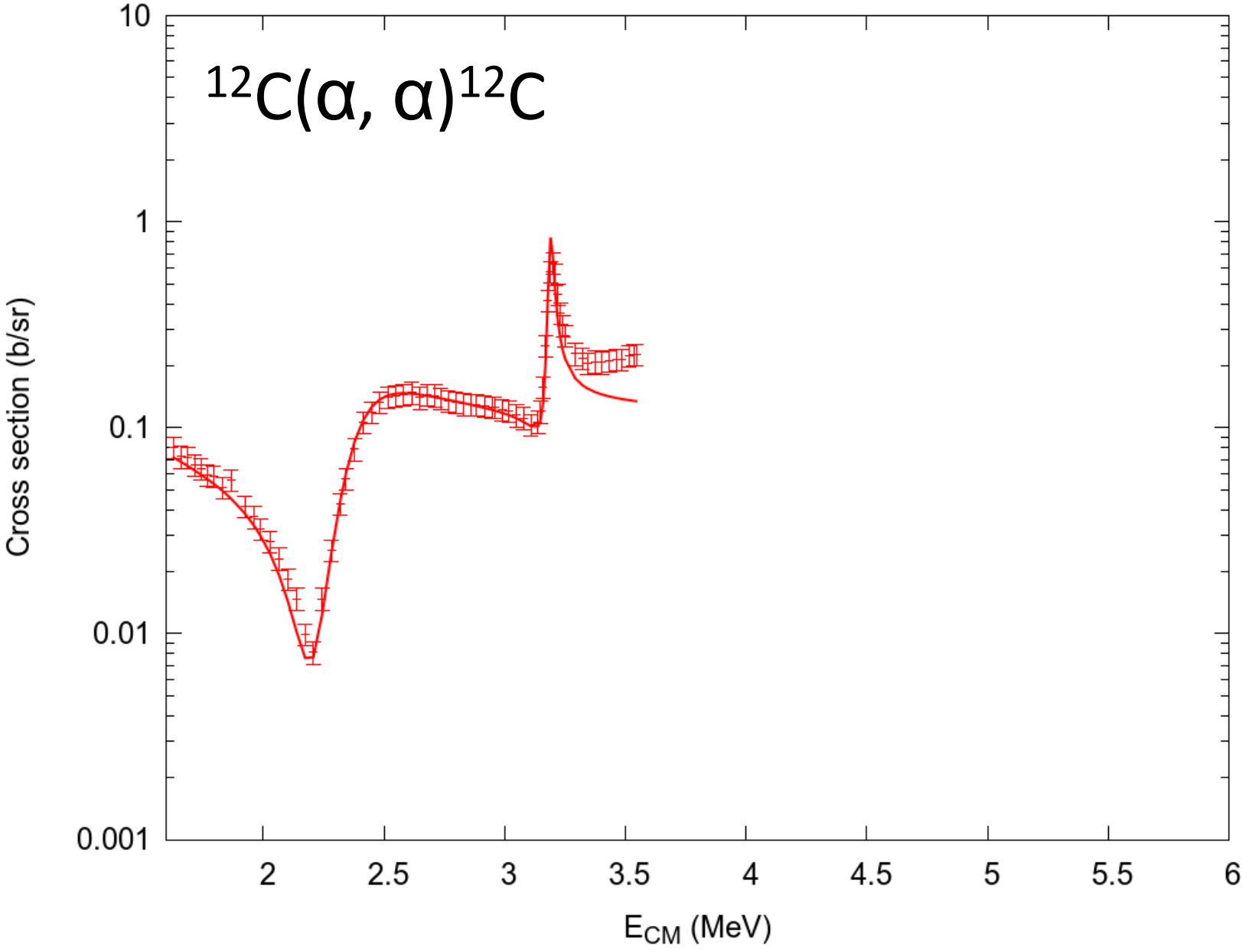
Ruiz *et al.*, PRC 71, 025802 (2005)

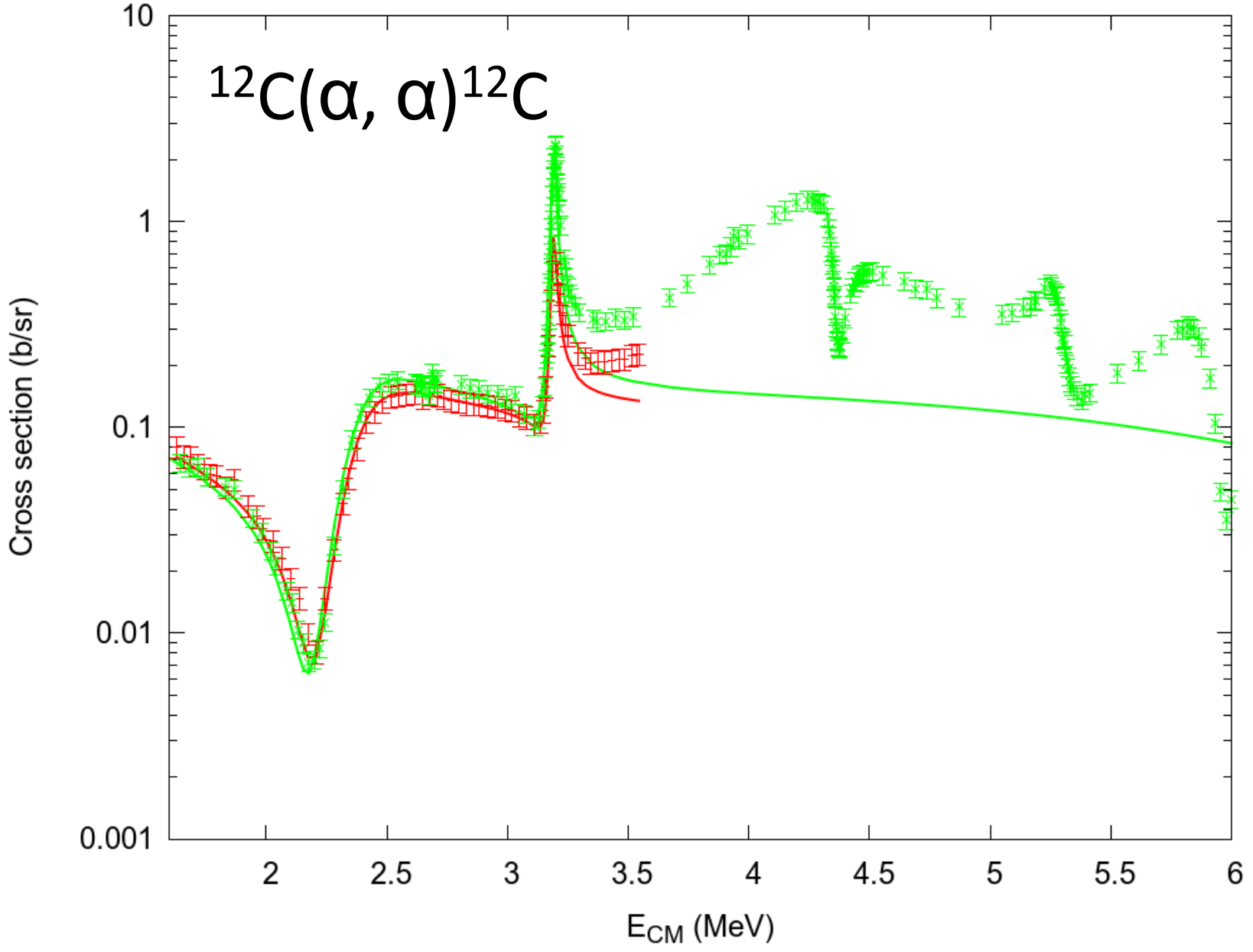
Lane and Thomas, page 271 and 289, Rev. Mod. Phys. 30, 257 (1958)


$^{12}C(\alpha, \alpha)^{12}C$
l_{max}=0
l_{max}=1
l_{max}=2
l_{max}=3
l_{max}=4
l_{max}=5
Cross section at 160 degrees (mb/sr)
1
0.1
0.01
0.5
1
1.5
2
2.5
3
3.5
4
4.5
E_{CM} (MeV)

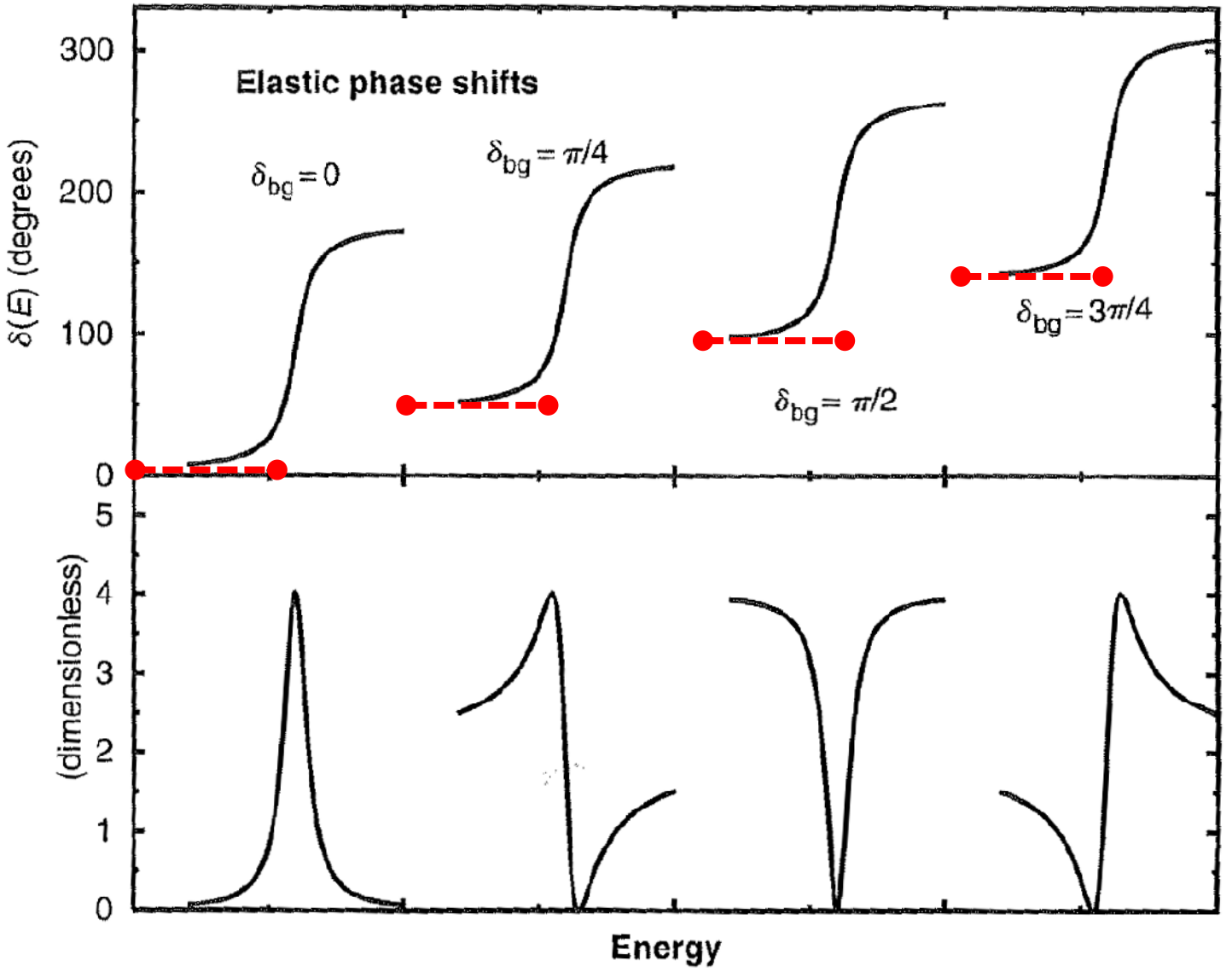
Background resonances

- 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

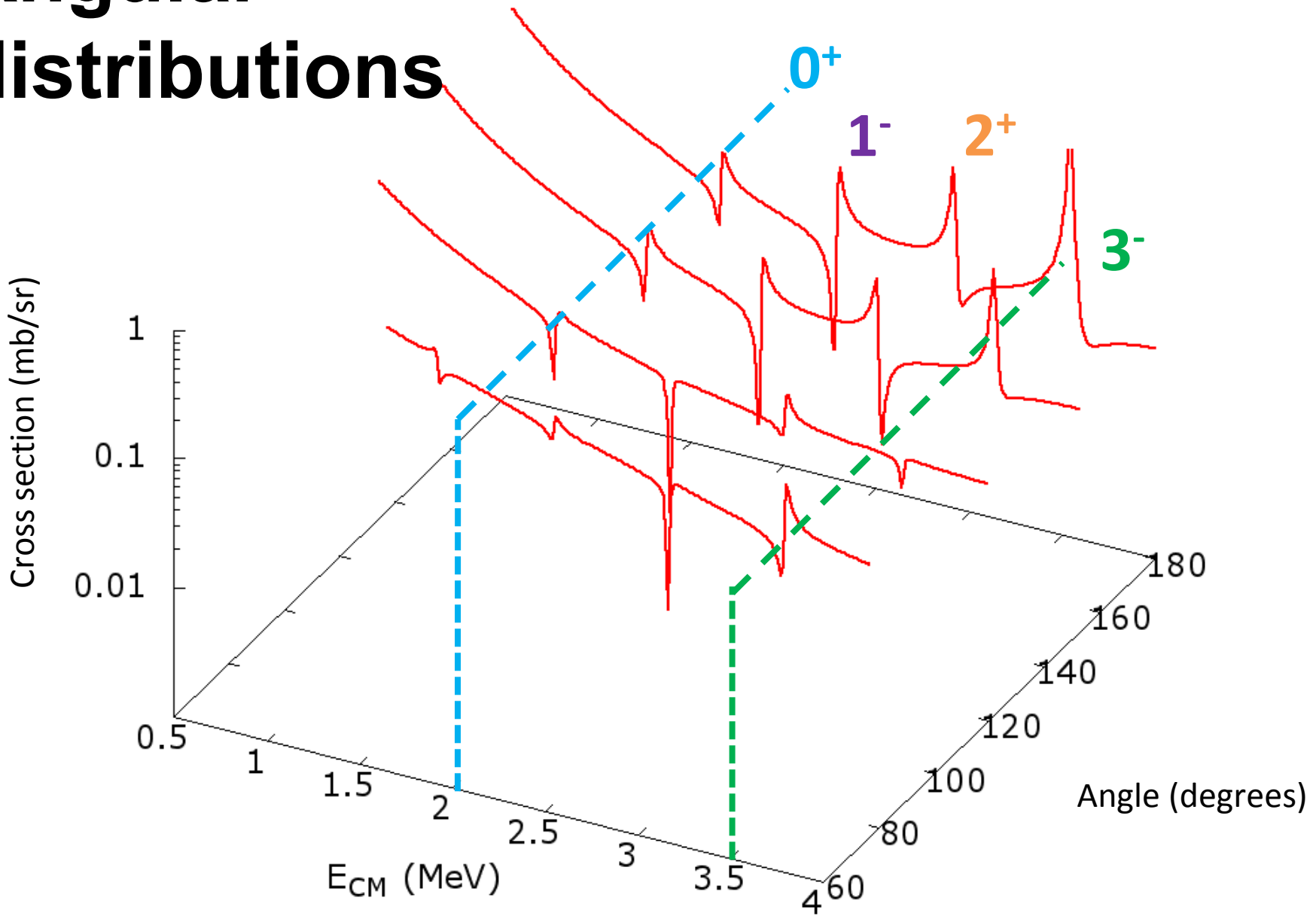

$^{12}C(\alpha, \alpha)^{12}C$
Cross section (b/sr)
10
1
0.1
0.01
0.001
2
2.5
3
3.5
4
4.5
5
5.5
6
E_{CM} (MeV)


$^{12}C(\alpha, \alpha)^{12}C$
Cross section (b/sr)
10
1
0.1
0.01
0.001
2
2.5
3
3.5
4
4.5
5
5.5
6
E_{CM} (MeV)

Resonance shapes



Angular distributions



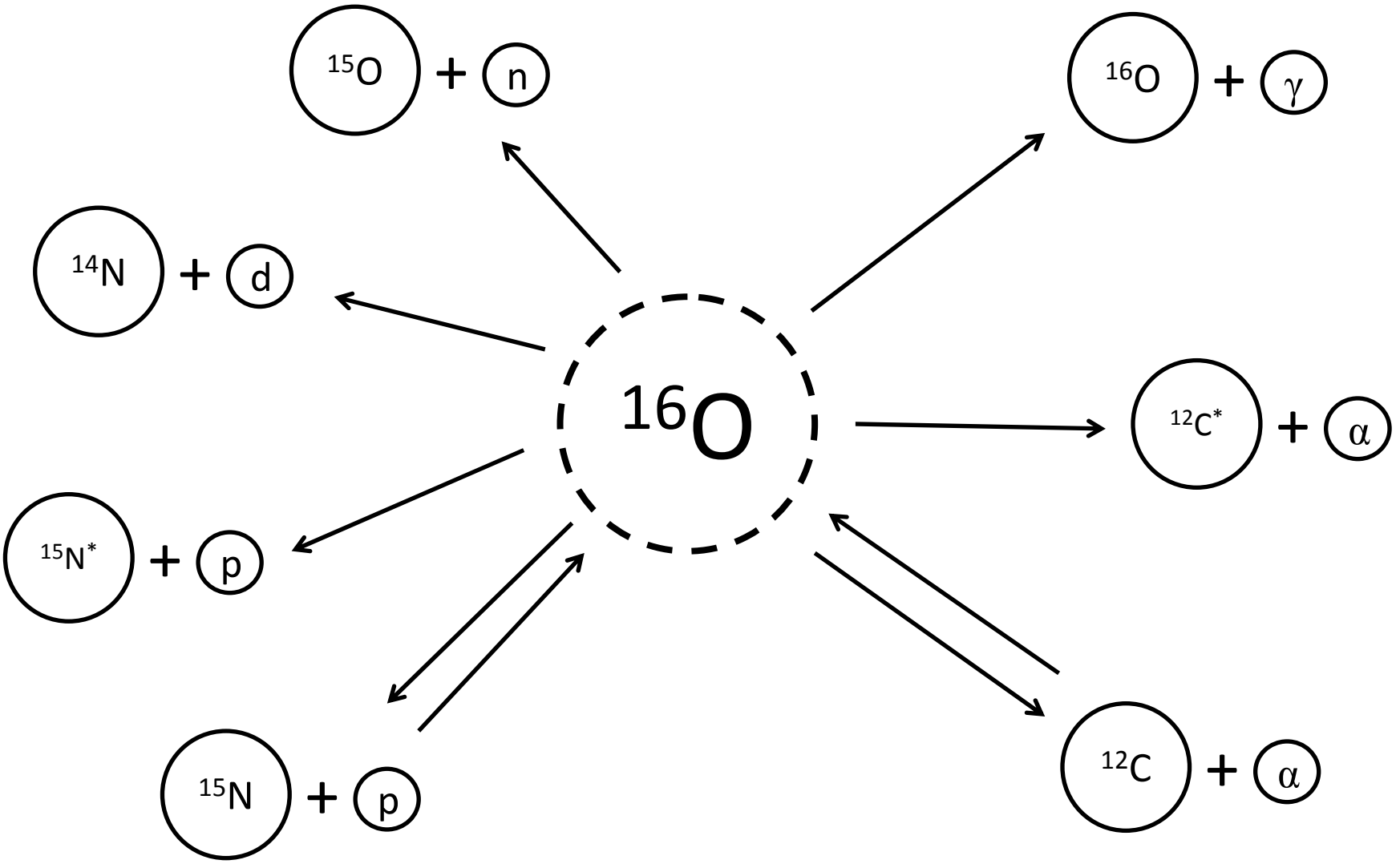
Using AZURE2

Practicalities and Examples

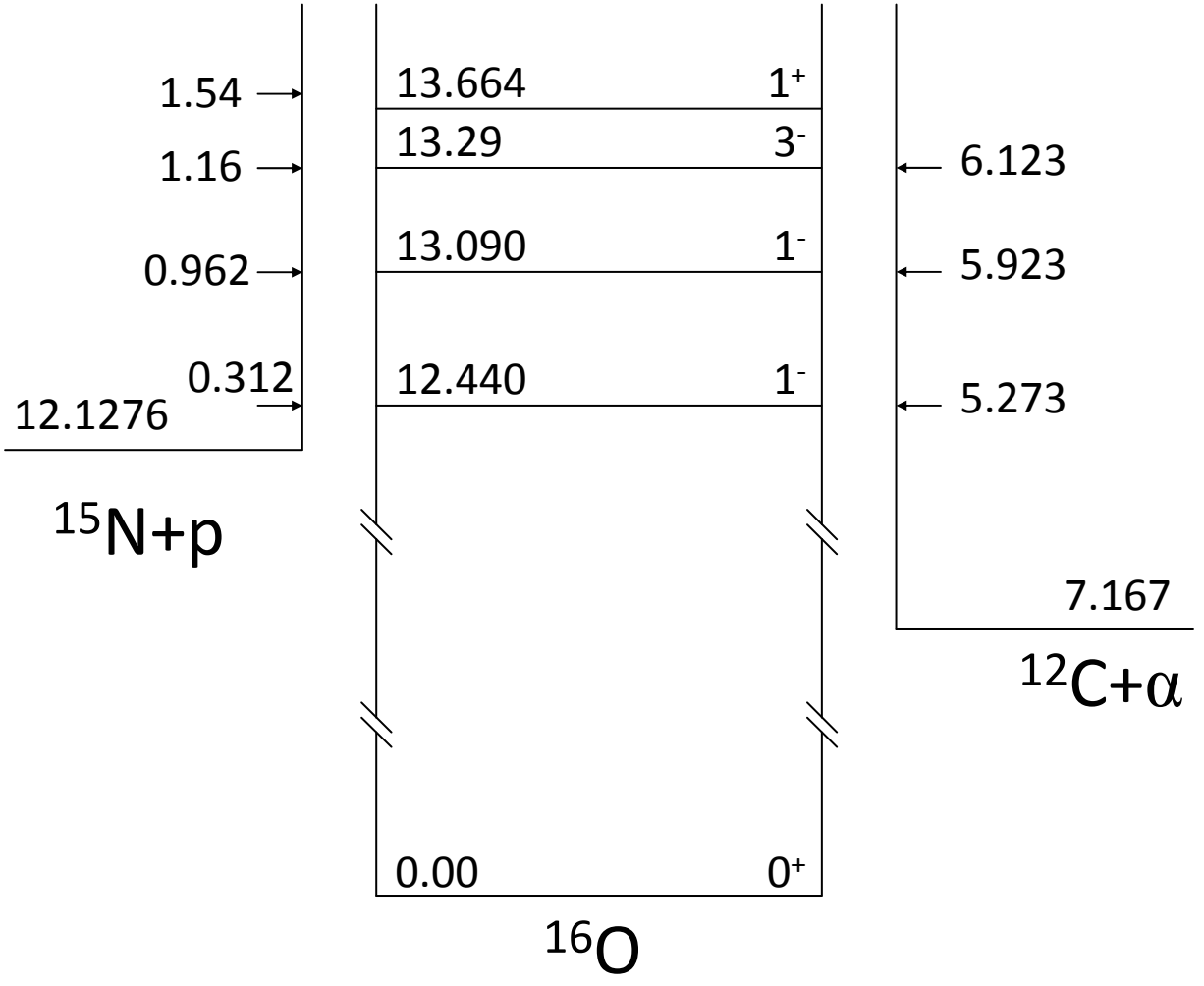
AZURE C++ code overview

- 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)

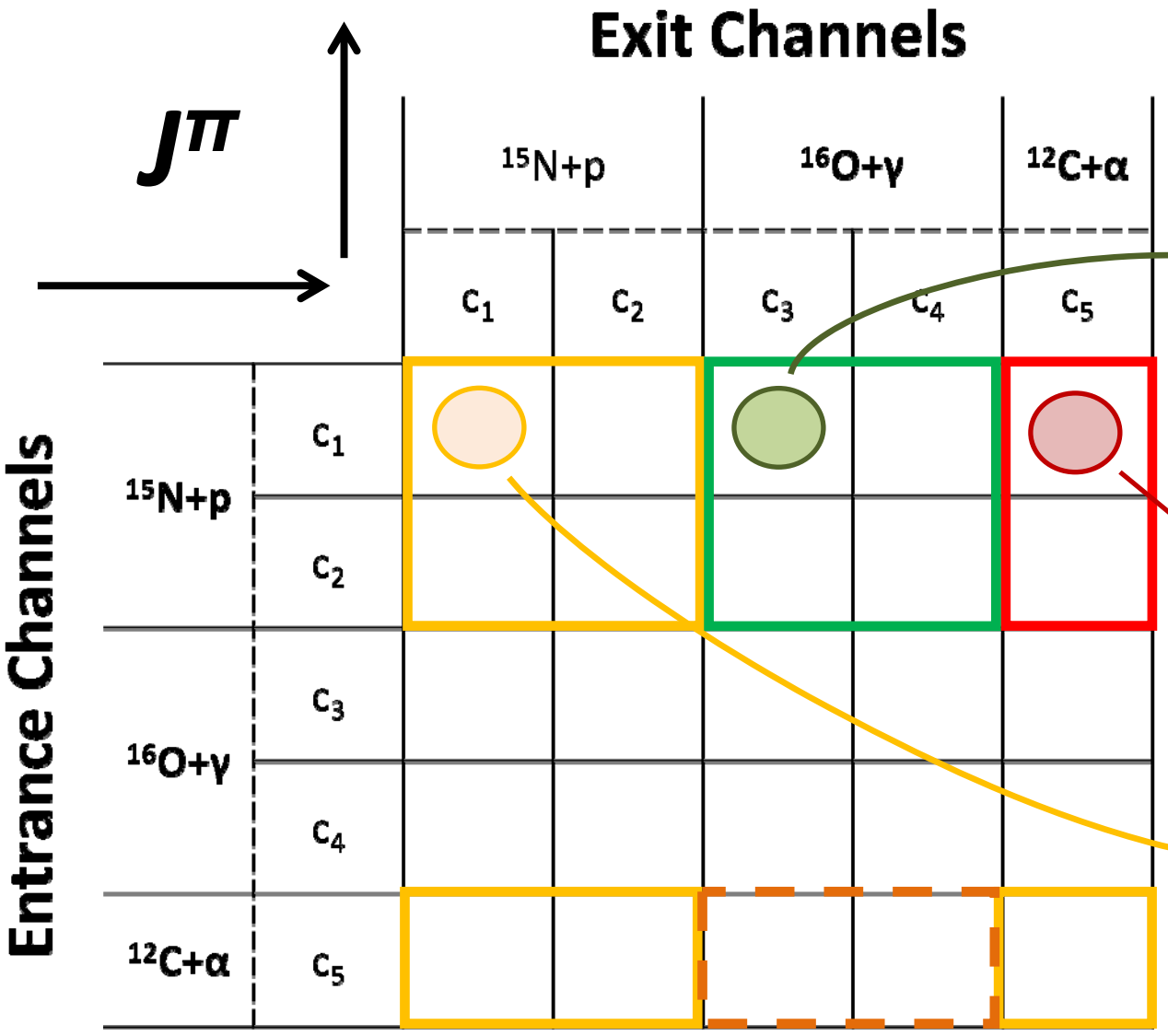
Example: ^{16}O compound reactions



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



^{16}O R-matrix: ^{15}N(p,γ)^{16}O

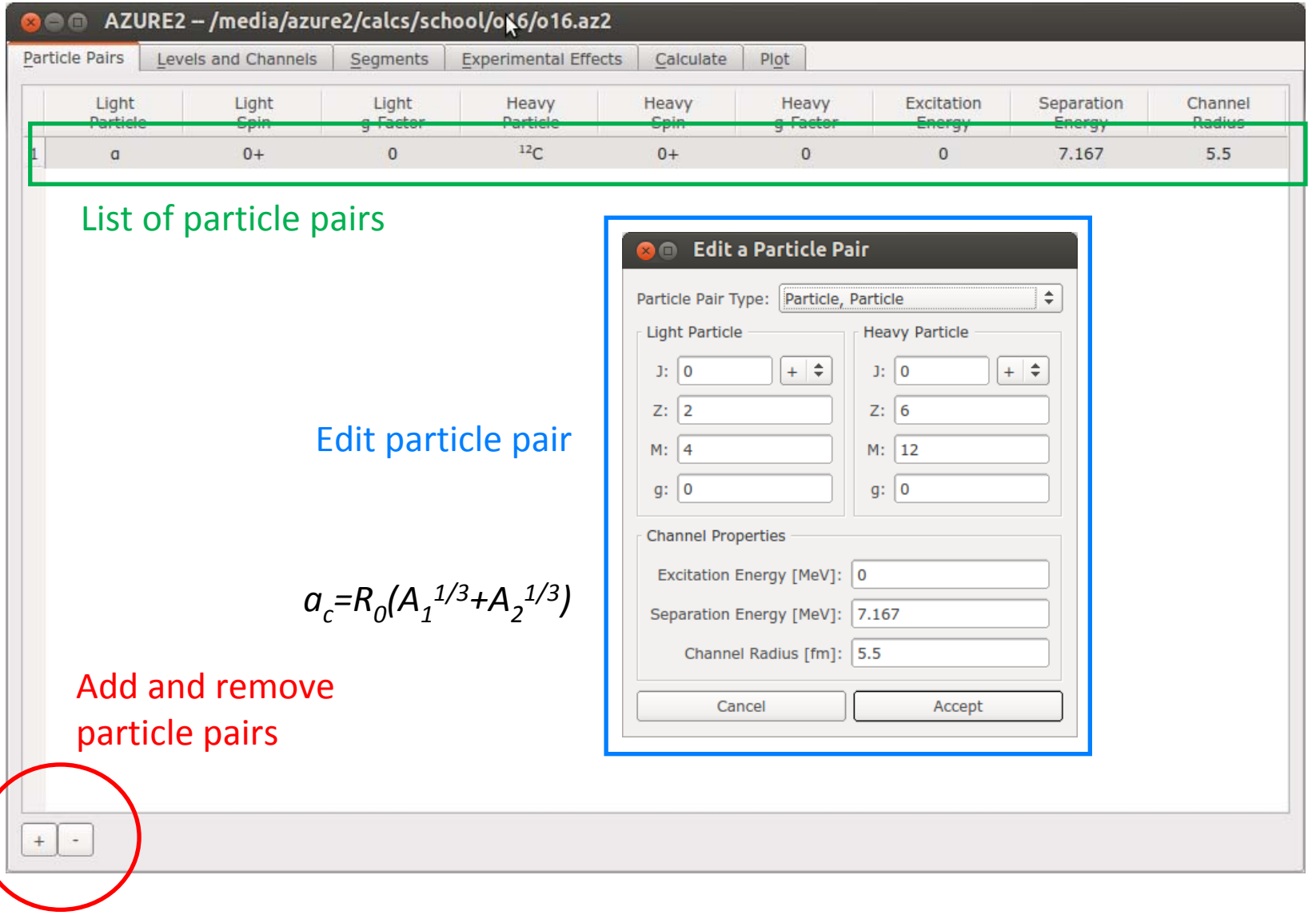


$$R_{c_3 c_1} = \sum_\lambda \frac{\gamma_{\lambda c_3}\gamma_{\lambda c_1}}{E_\lambda - E}$$

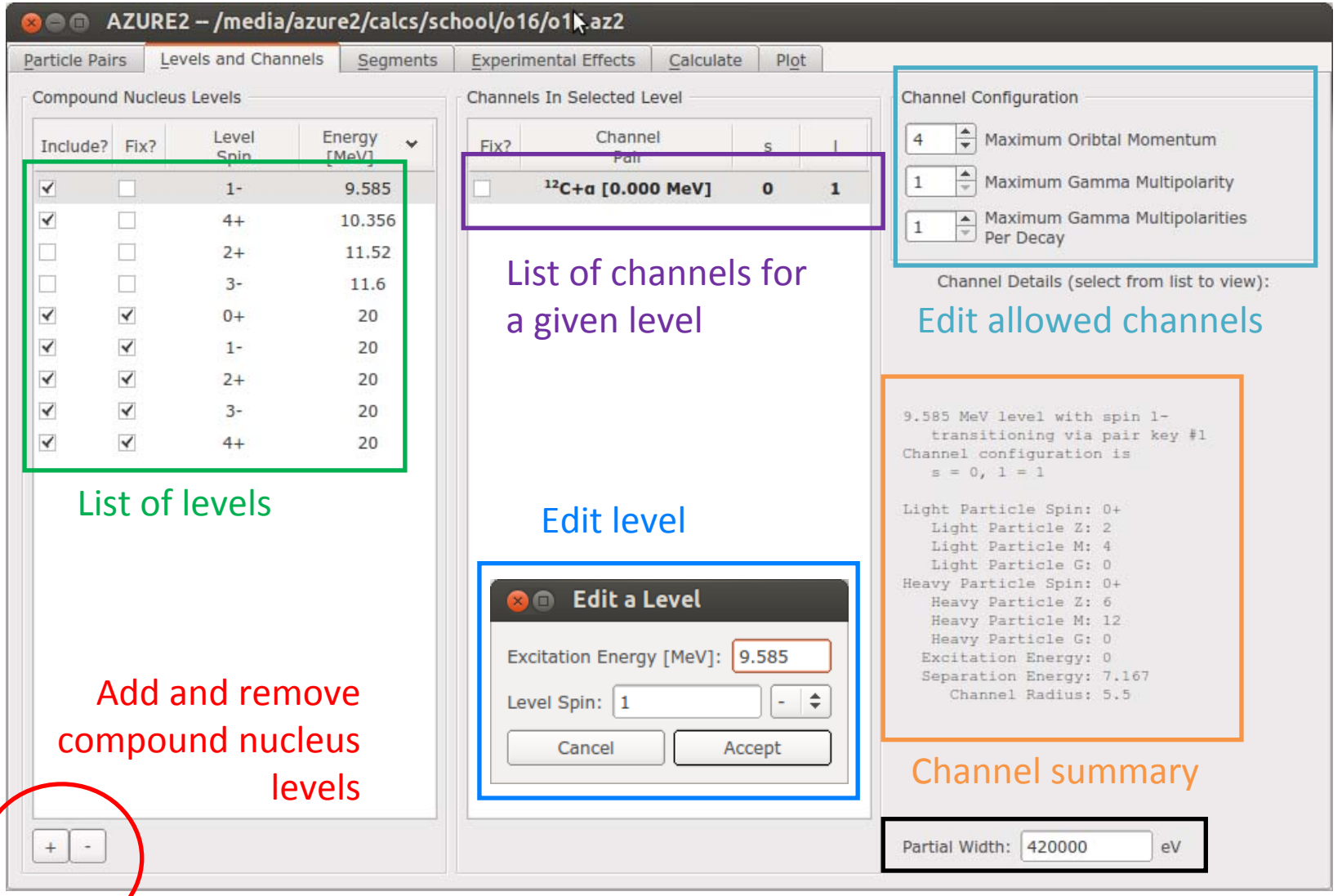
$$R_{c_5 c_1} = \sum_\lambda \frac{\gamma_{\lambda c_5}\gamma_{\lambda c_1}}{E_\lambda - E}$$

$$R_{c_1 c_1} = \sum_\lambda \frac{\gamma_{\lambda c_1}\gamma_{\lambda c_1}}{E_\lambda - E}$$

AZURE add particle pair



AZURE Levels and Channels



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

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

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

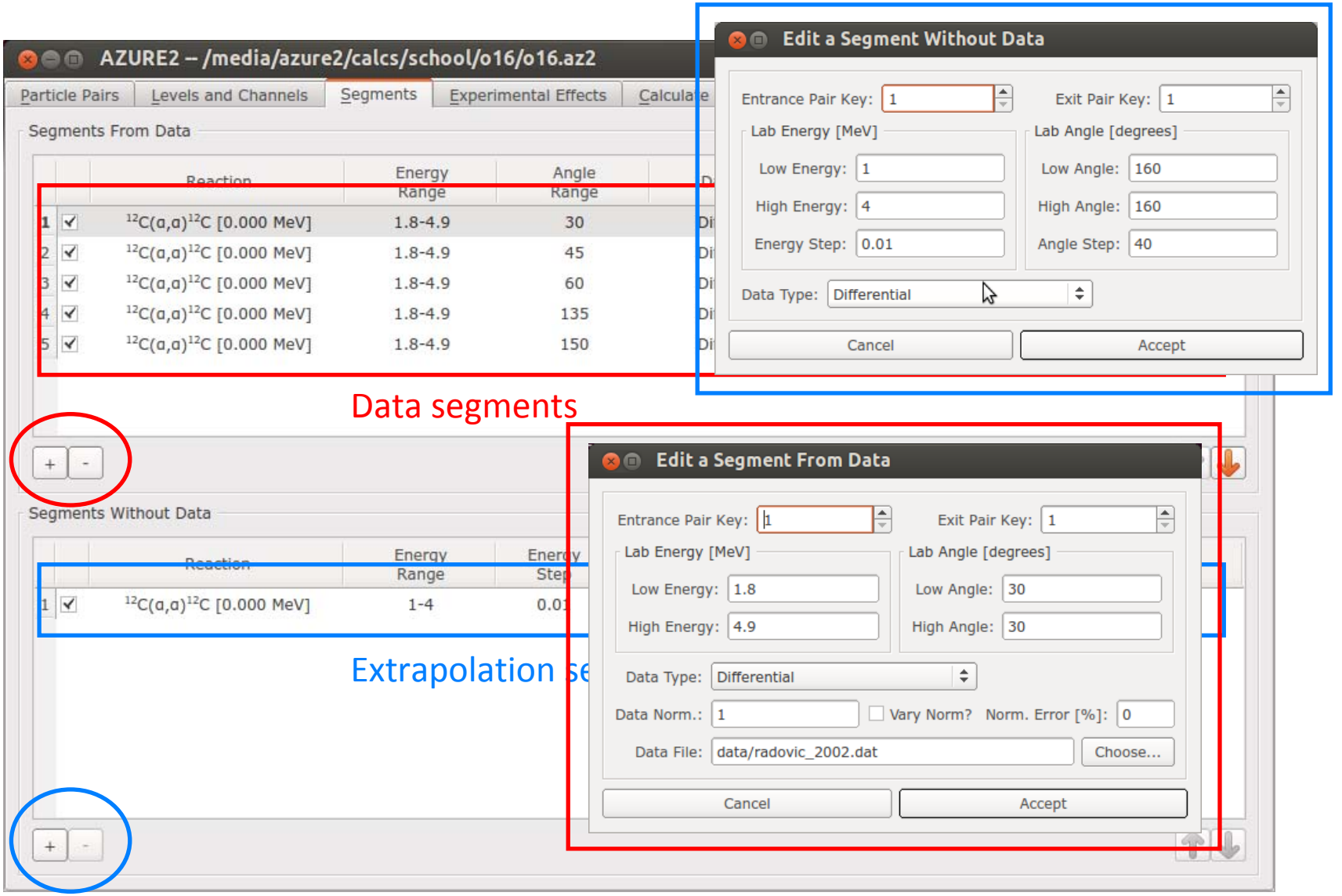
$$I_2 = 0 \qquad \pi_2 = 1$$

$$\therefore s = 0$$

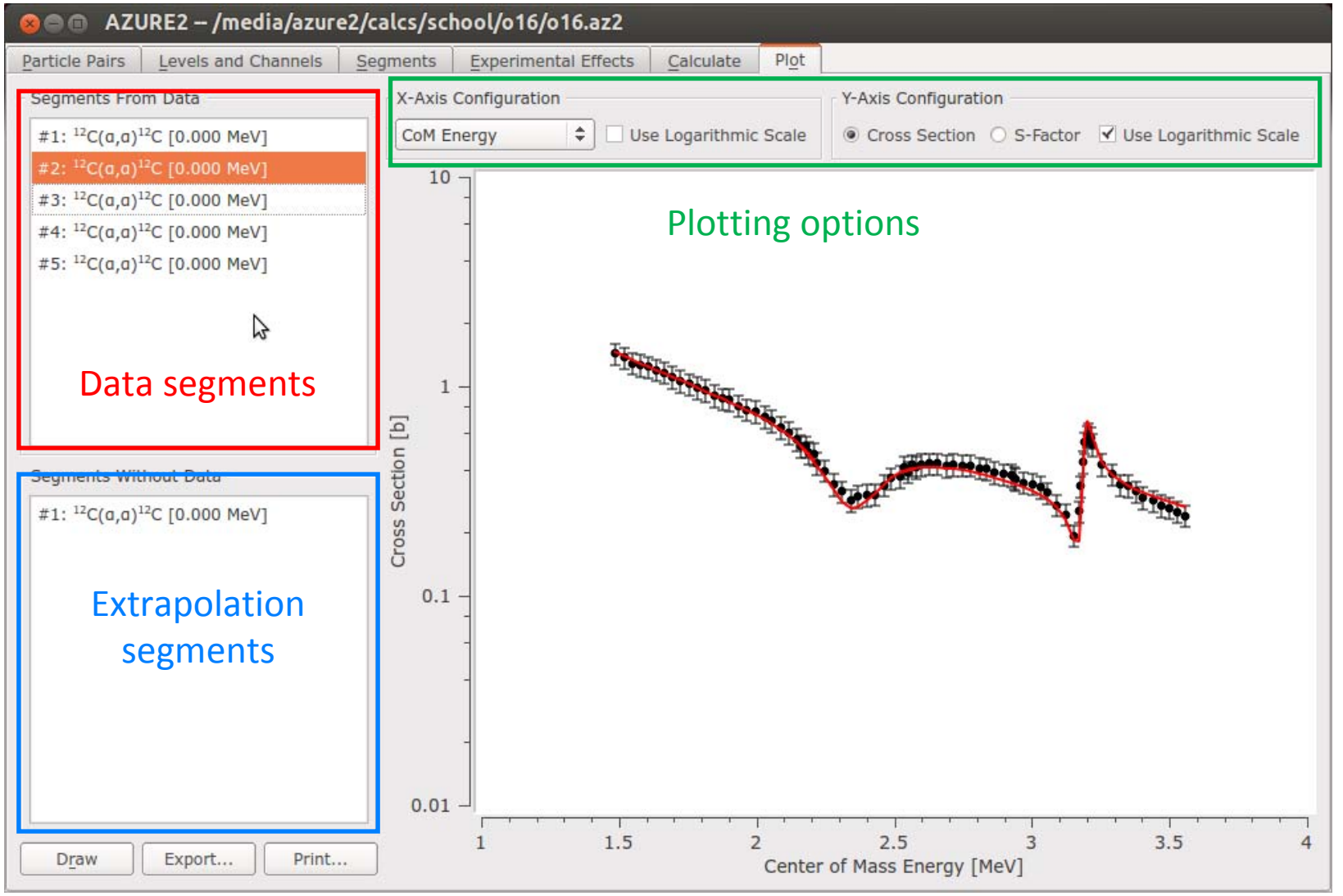
$$\text{and } J = \ell \qquad \pi = \pi_1 \pi_2 (-1)^\ell = (-1)^\ell$$

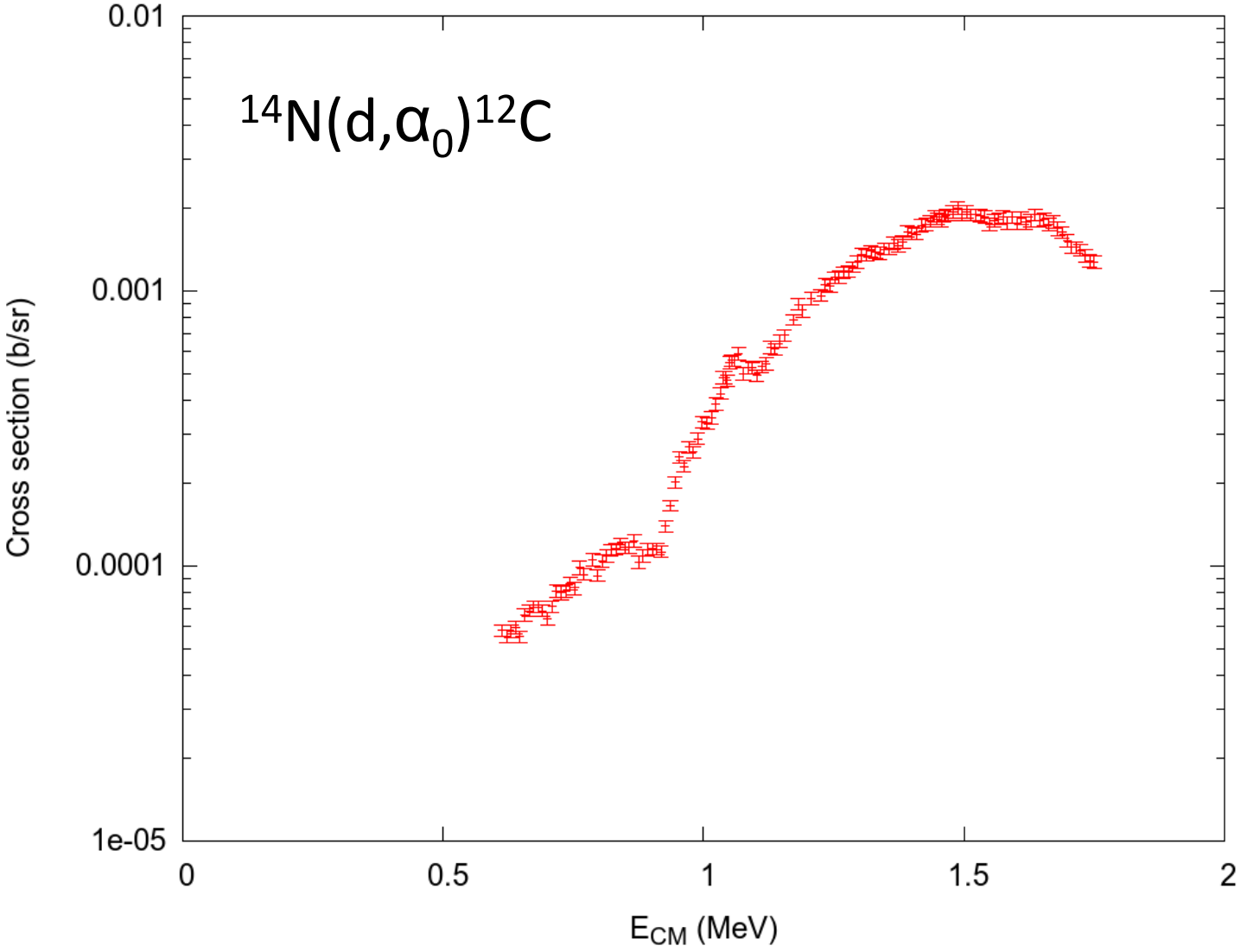
- One channel per *J*, only natural parity states allowed $\pi=(-1)^J$
- In general, many channels allowed per resonance

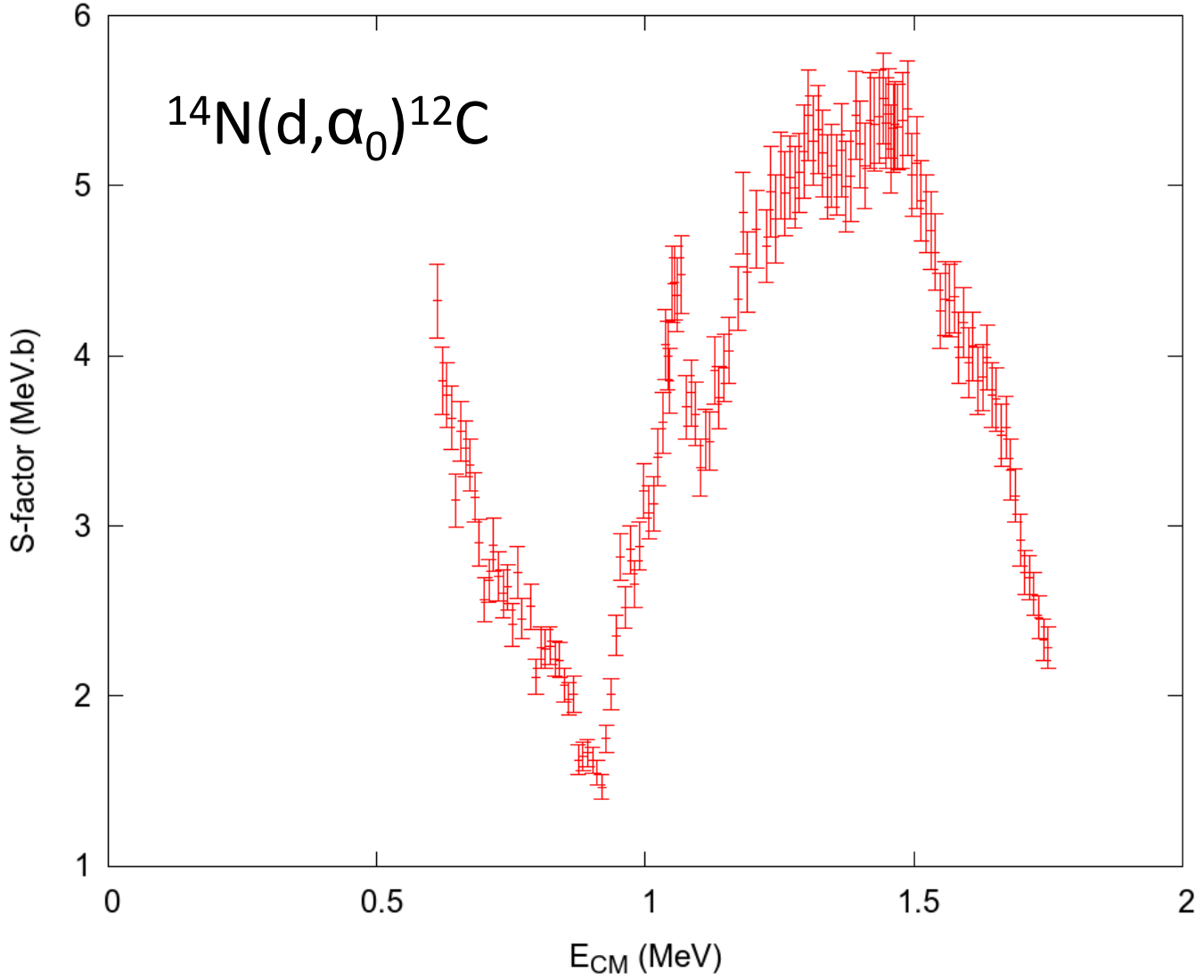
Data and extrapolation segments



Plotting


AZURE2 – /media/azure2/calcs/school/o16/o16.az2
Particle Pairs
Levels and Channels
Segments
Experimental Effects
Calculate
Plot
Segments From Data
#1: 12C(a,a)12C [0.000 MeV]
#2: 12C(a,a)12C [0.000 MeV]
#3: 12C(a,a)12C [0.000 MeV]
#4: 12C(a,a)12C [0.000 MeV]
#5: 12C(a,a)12C [0.000 MeV]
Data segments
Segments Without Data
#1: 12C(a,a)12C [0.000 MeV]
Extrapolation segments
Draw
Export...
Print...
X-Axis Configuration
CoM Energy
Use Logarithmic Scale
Y-Axis Configuration
Cross Section
S-Factor
Use Logarithmic Scale
Plotting options
Cross Section [b]
10
1
0.1
0.01
1
1.5
2
2.5
3
3.5
4
Center of Mass Energy [MeV]


$^{14}N(d,\alpha_0)^{12}C$
Cross section (b/sr)
0.01
0.001
0.0001
1e-05
0
0.5
1
1.5
2
E_{CM} (MeV)


$^{14}N(d,\alpha_0)^{12}C$
S-factor (MeV.b)
E_{CM} (MeV)
6
5
4
3
2
1
0
0.5
1
1.5
2

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 $^{12}C+\alpha$ (^{16}O)
- Further examples: $^{13}C+p$ (^{14}N), $^{21}Na+p$ (^{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

R. E. Azuma *et al.*, Phys. Rev. C 81, 041805 (2010)