R-matrix Analysis (II)

TALENT Course 6

Theory for exploring nuclear reaction experiments

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R-matrix Analysis (II)

- Tutorial so far:
  - Setup the particle pairs
  - Added states to compound nucleus
  - Identified spins and parities of states
  - Fit the widths and energies to experimental data
- Background resonances
- Fitting with MINUIT - examples
- Sensitivity to R-matrix radius parameter
- Error analysis with MINUIT

$0^+, 0^-, 1^+, 1^-,$
$2^+, 2^- \ldots$
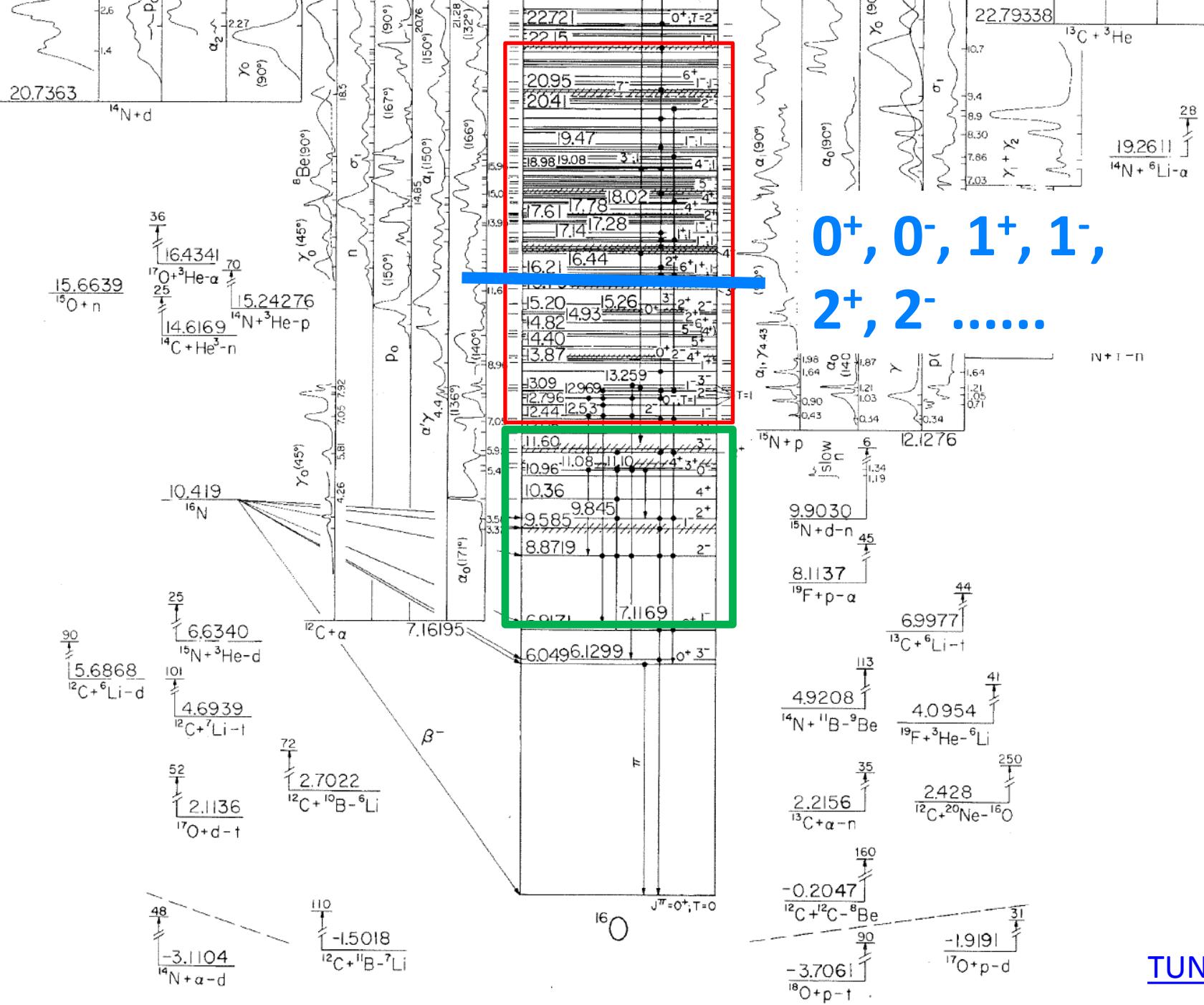
TUNL

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
  - (Weak) Non-compound nucleus (direct) mechanisms
  - Corrections to hard-sphere phase shift in scattering

- For reaction channels, usually only a few J^π are important

- For scattering, all J^π may be required

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

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

$S_{\alpha 1}(^{16}O)$

$S_p(^{16}O)$

Cross section (b/sr)

Probable background from a specific resonance

E_{CM} (MeV)

E_x=8.67 MeV

E_x=13.17 MeV
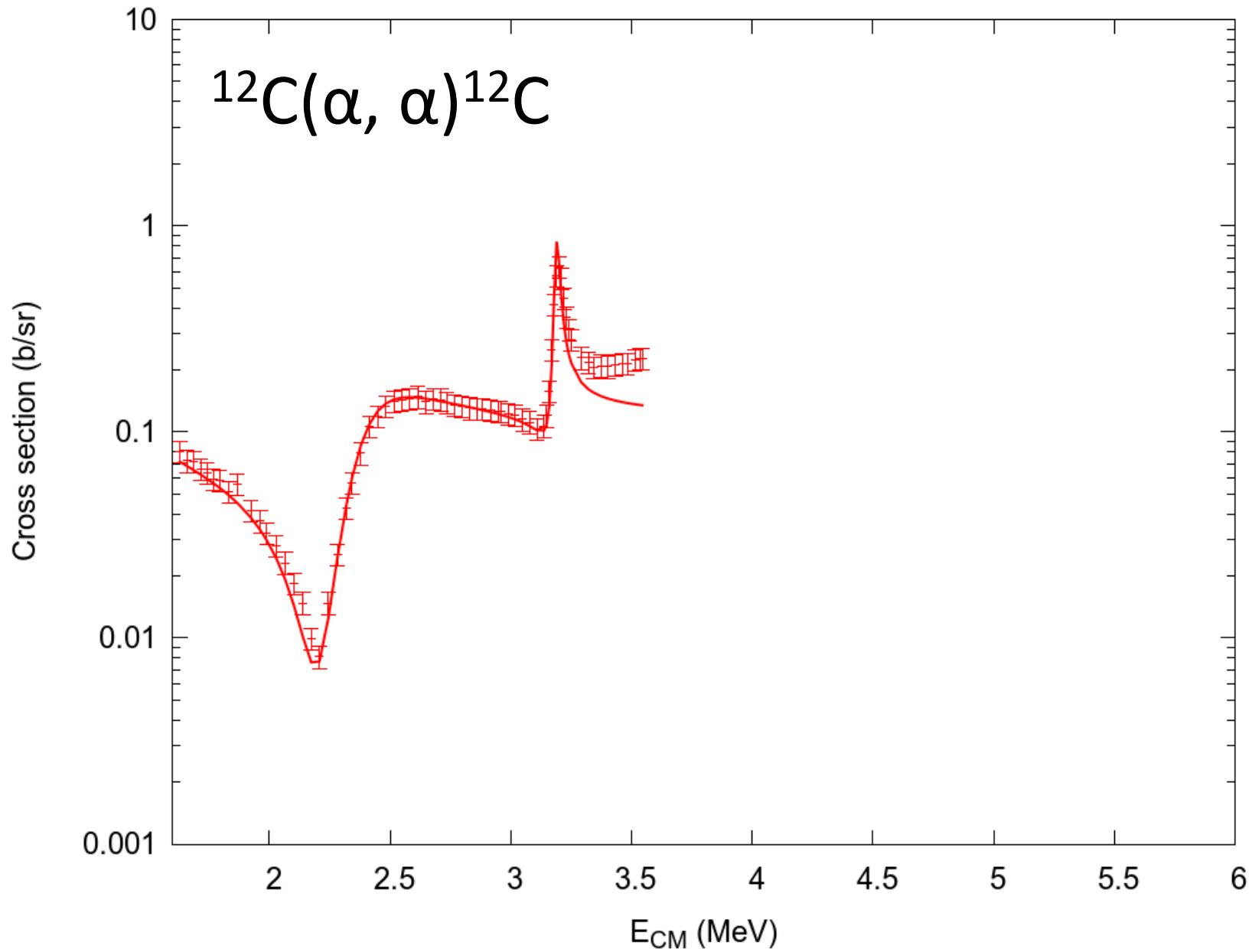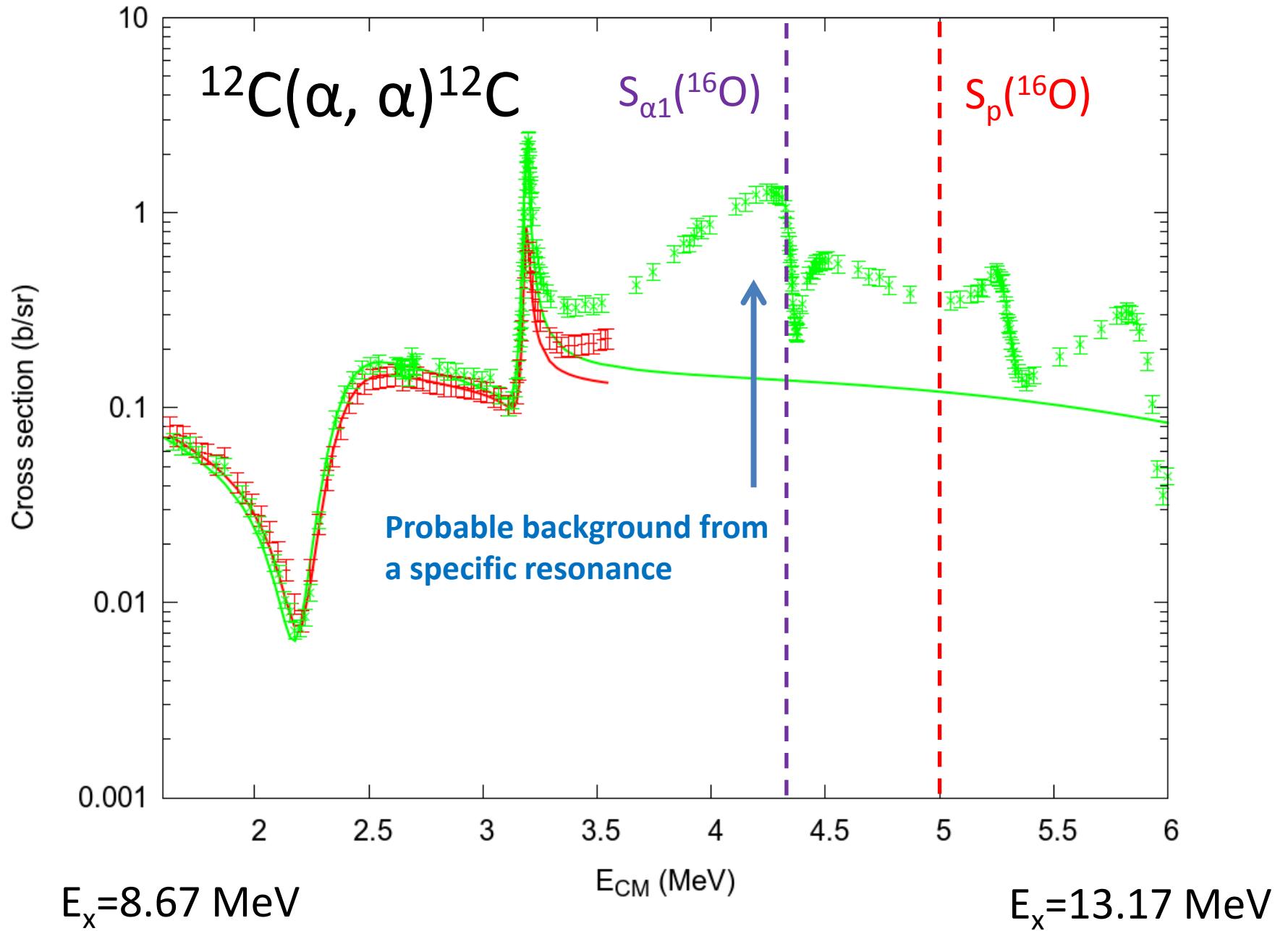
| E_{level} (keV)	XREF	$J\pi$	$T_{1/2}$	E_γ (keV)	I_γ	γ mult.	Final level	
9585 *11*	A E IJ LMNO	1−	420 keV *20* % IT = 6.7E-6 *10* % α = 100	2688 *11* 9582 *11*	12 *4* 100 *16*	[E1] [E1]	6917.1 0.0	2+ 0+
9844.5 *5*	A C E HIJKLMNO Q	2+	0.62 keV *10* % IT = 0.0016 *3* % α = 100	2927.1 *8* 3794.6 *12* 9841.2 *5*	34 *7* 30 *7* 100 *7*	[M1] [E2] [E2]	6917.1 6049.4 0.0	2+ 0+ 0+
10356 *3*	A C E I KLMNO Q	4+	26 keV *3* % IT = 2.4E-4 *4* % α = 100	3439 *3* 4225 *3* 10352 *3*	100 *10* <1.6 9E-5 *3*	[E2] [E1] [E4]	6917.1 6129.89 0.0	2+ 3− 0+
10957 *1*	E HI LM Q	0−	5.5 fs *35*	3839.6 *10*	100	[M1]	7116.85	1−
11080 *3*	E HI Q	3+	< 12 keV					
11096.7 *16*	A C E KLMNO	4+	0.28 keV *5* % IT = 0.0020 *6* % α = 100	4179.0 *17* 4966.0 *16*	81 *20* 100 *42*	[E2] [E1]	6917.1 6129.89	2+ 3−
11260?	A I	(0+)	2500 keV % α = 100					
11520 *4*	A C E KLMNO	2+	71 keV *3* % IT = 9.4E-5 *3* % α = 100	4402 *4* 4602 *4* 5470 *5* 11516 *4*	≤0.9 4.4 *11* 4.6 *8* 100.0 *13*	[E1] [M1] [E2] [E2]	7116.85 6917.1 6049.4 0.0	1− 2+ 0+ 0+
11600 *20*	A	3−	800 keV *100* % α = 100					
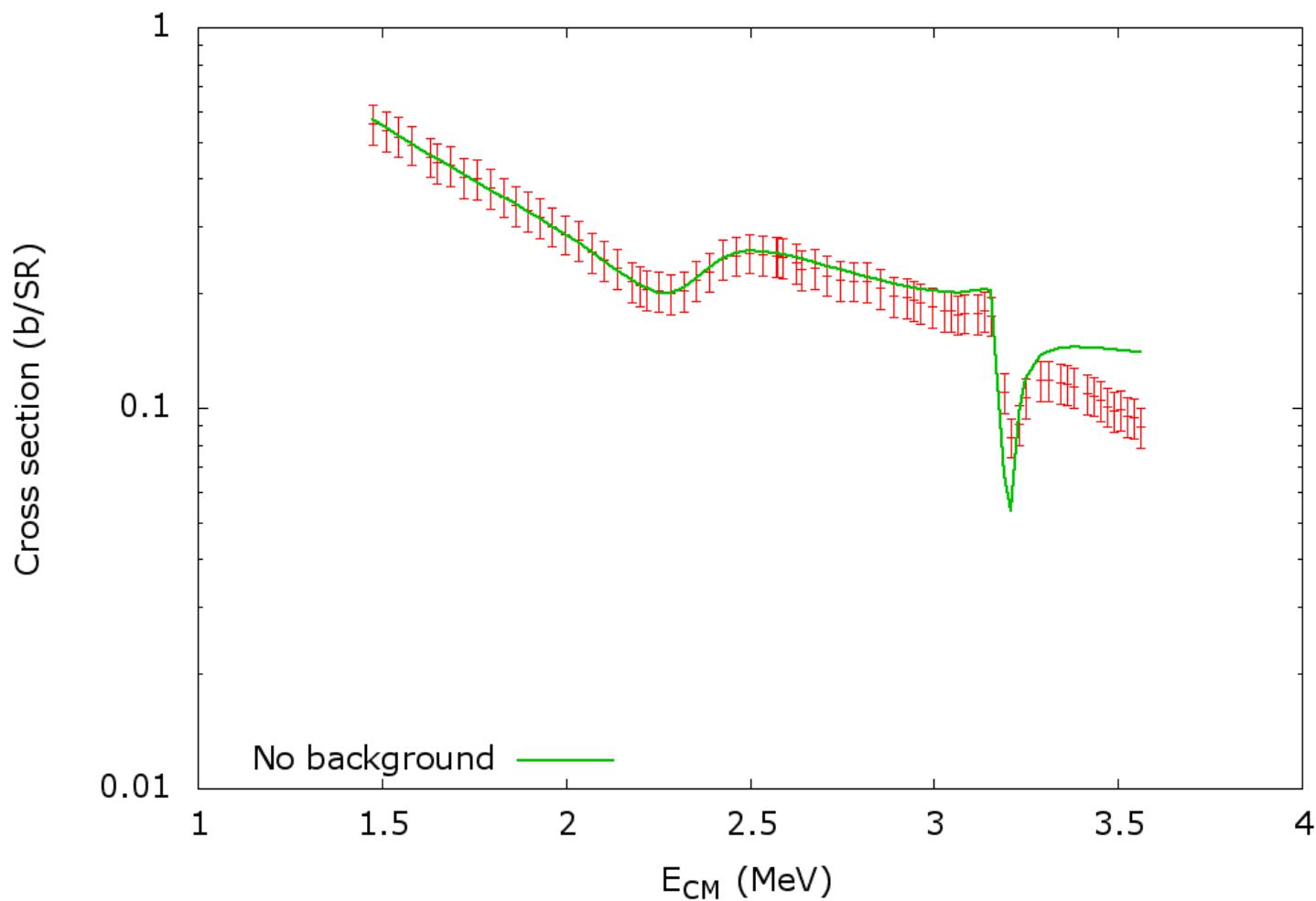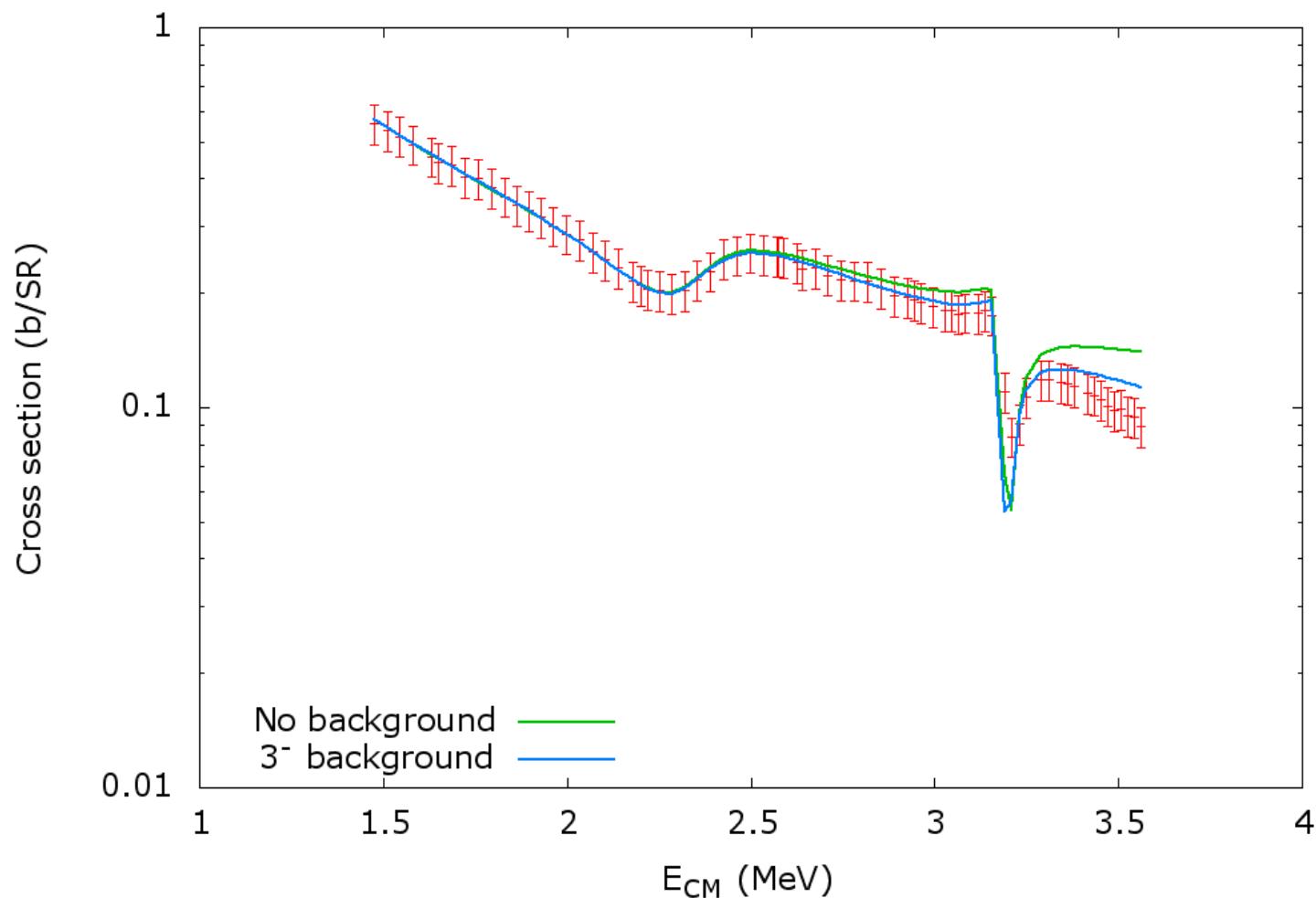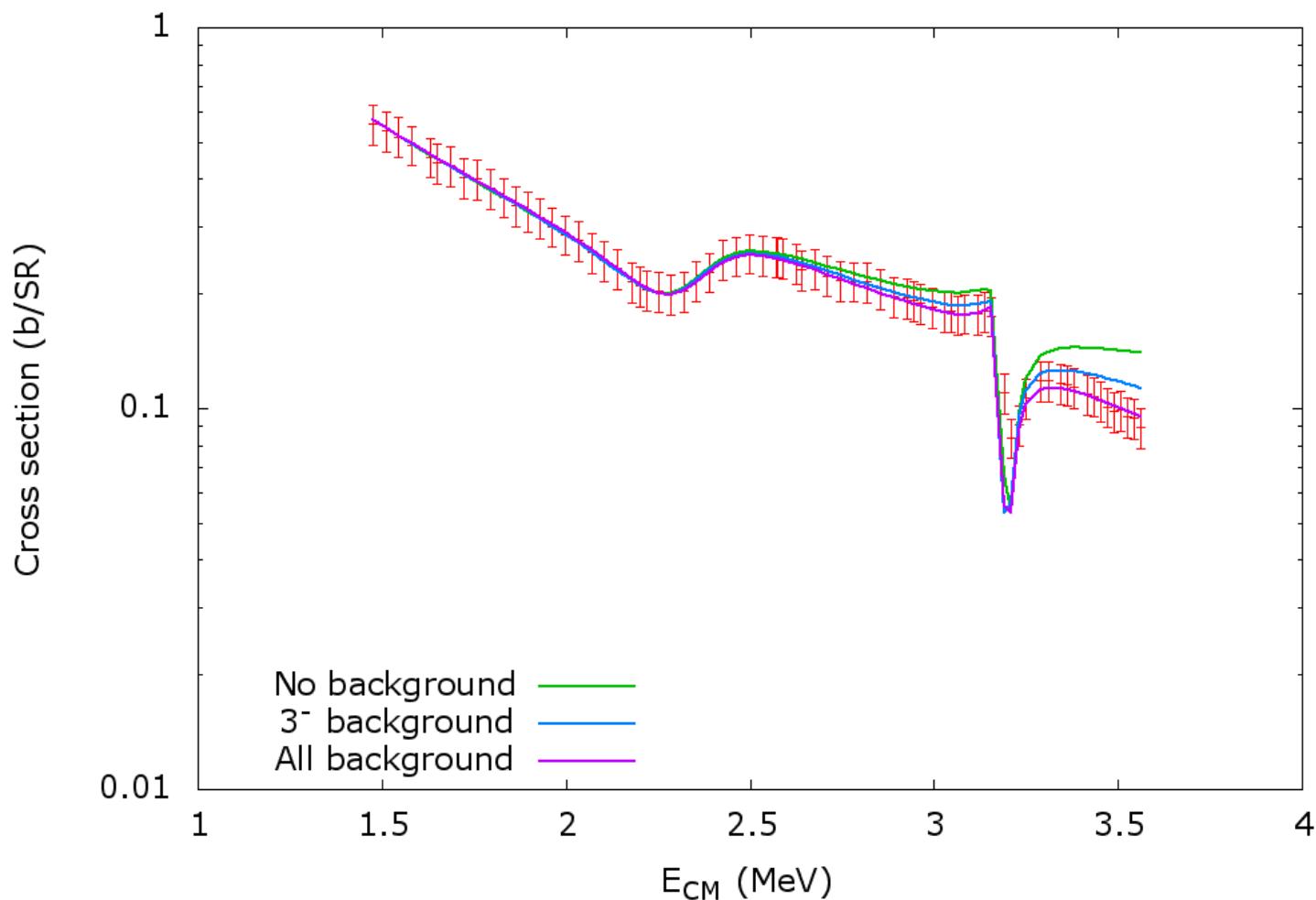
Sensitivity to R-matrix radius

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Radius	E (MeV)	Γ (keV)	E (MeV)	Γ (keV)
5.0	9.5803	415	10.3563	31.7
5.5	9.5764	392	10.3569	30.4
6.0	9.5659	376	10.3567	29.8
NNDC	9.585	420±20	10.356	26±3

$a = 1.5 \, (2^{1/3} + 12^{1/3}) = 5.32$
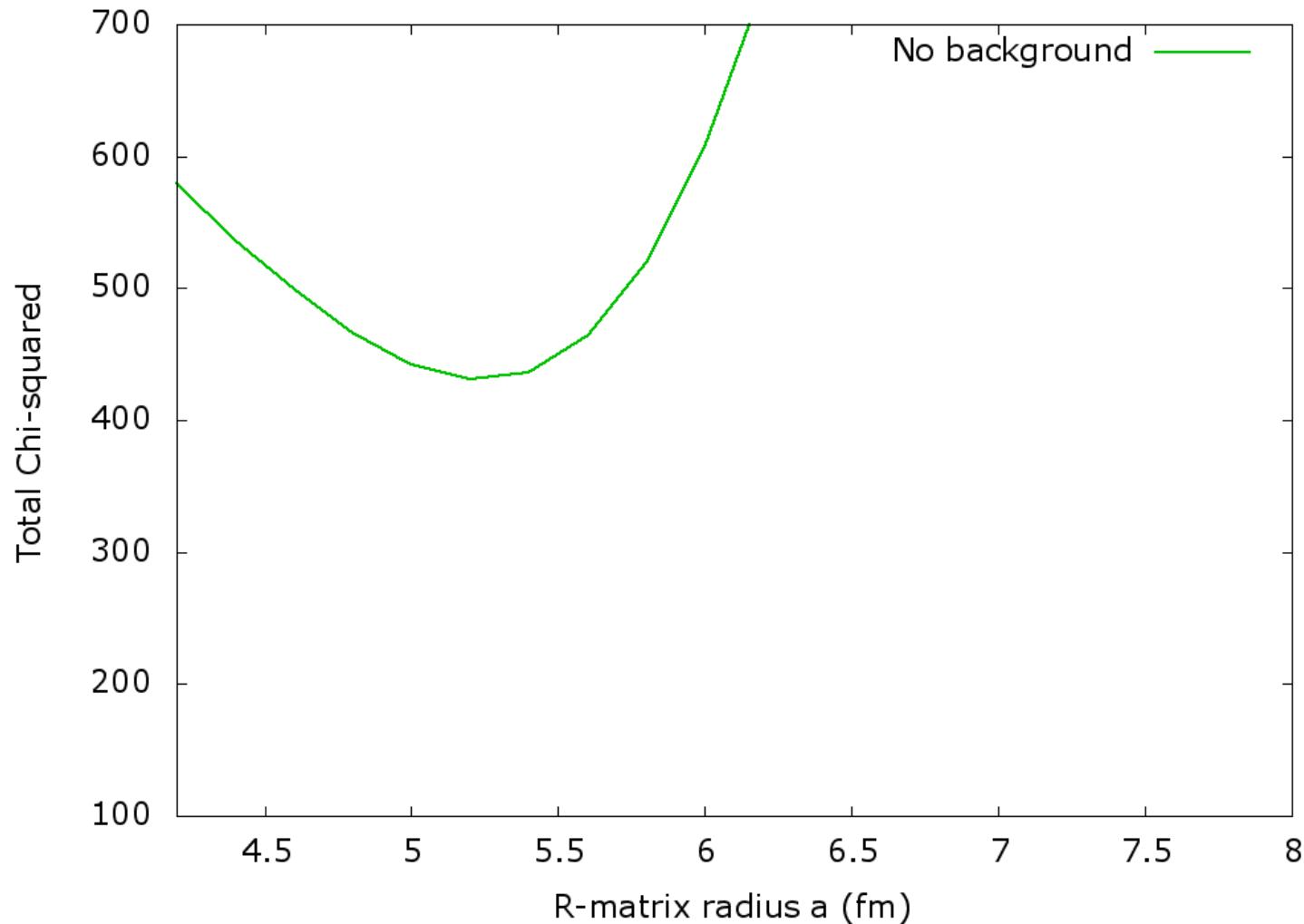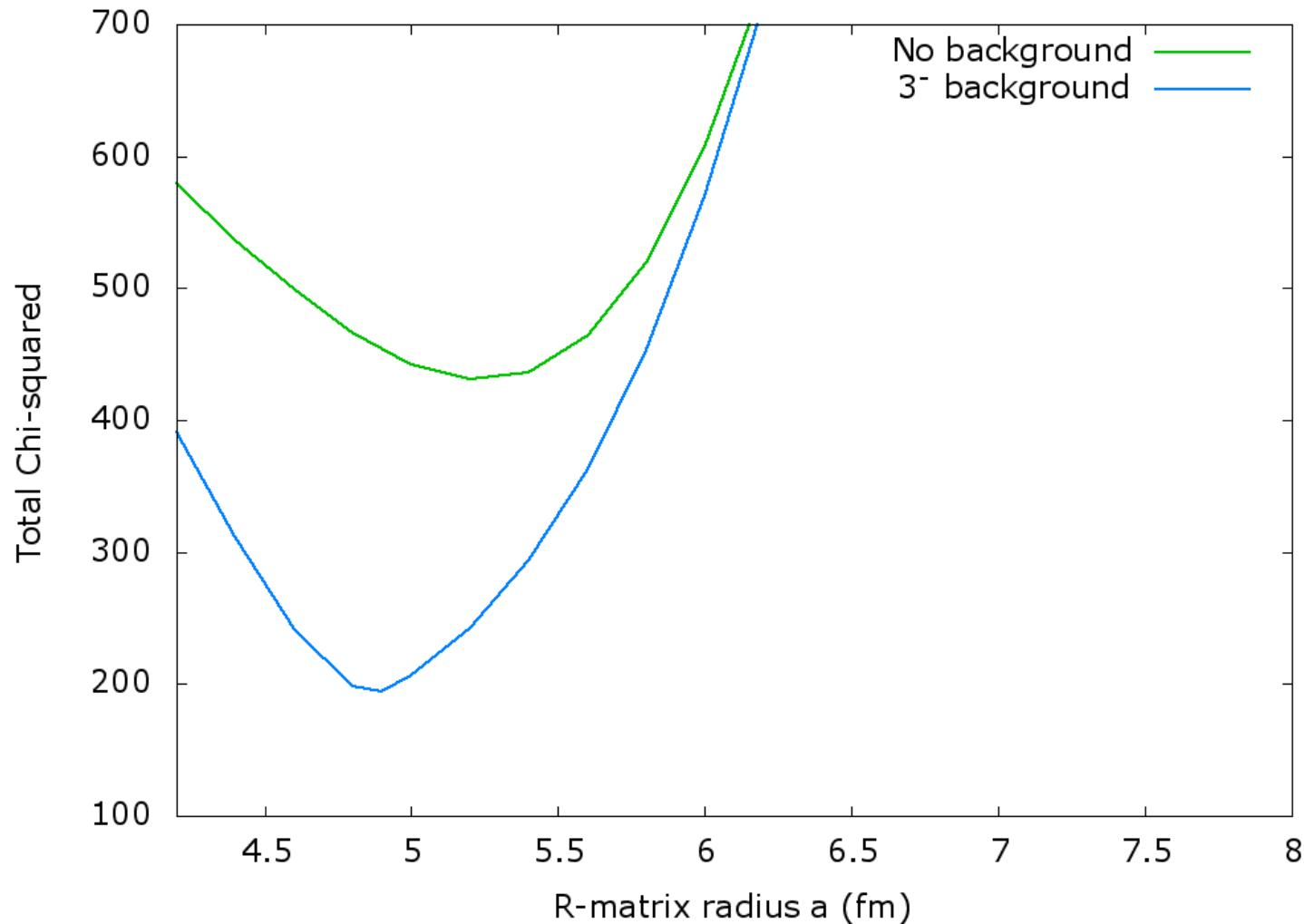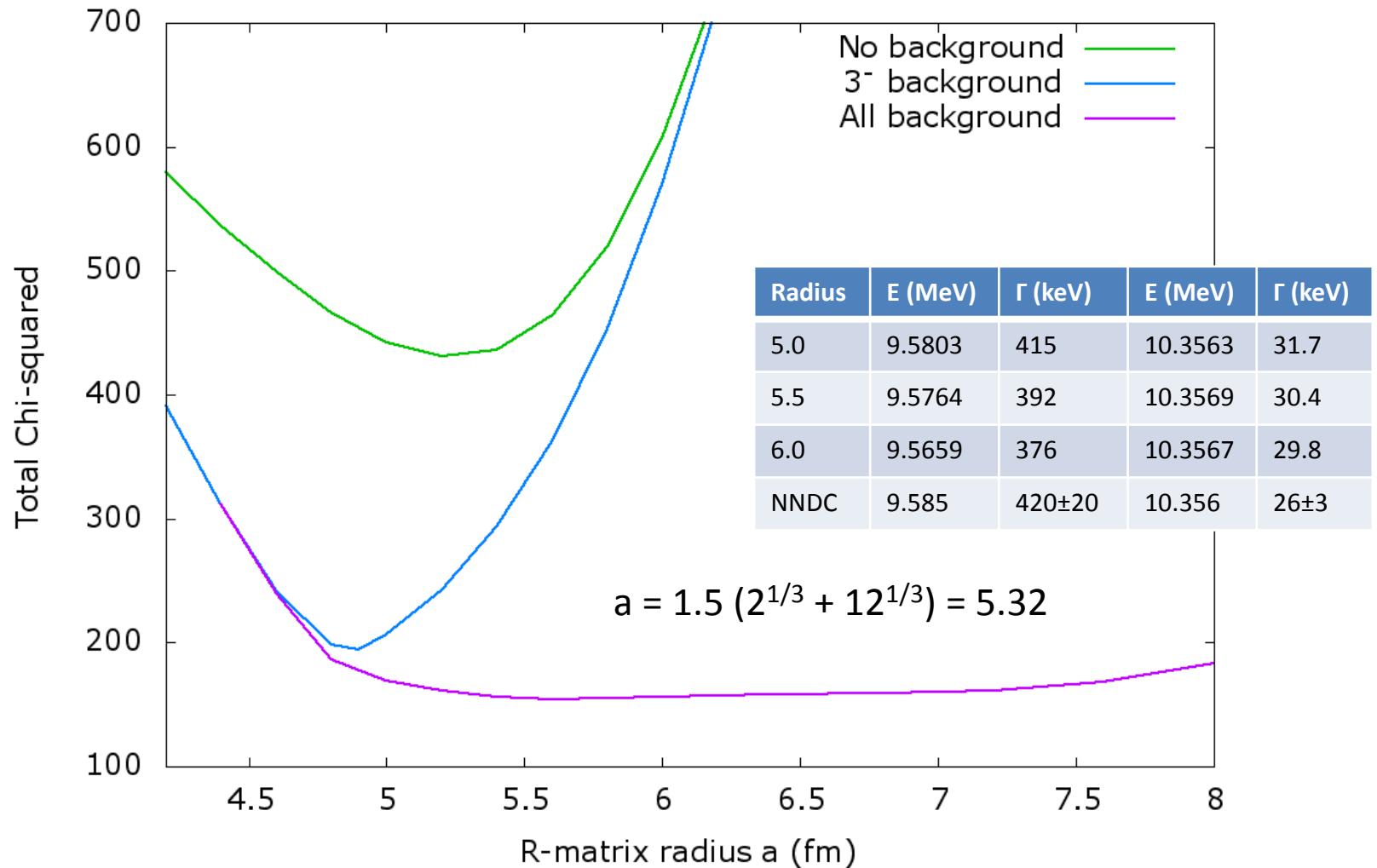
Fitting in R-matrix

- Chi-squared minimization using MINUIT2

$$\chi^2 = \sum_{i=1}^{N} \frac{(\sigma_{th} - \sigma_{exp})^2}{\Delta\sigma_{exp}^2}$$

MINUIT2 Fitting

- You are far smarter than the fitting routine!
- MINUIT is very effective at optimizing the parameters if the starting set is good...
- ... But it doesn't understand the spectrum and the physical significance of parameters
- The essential elements must be all in place - energies, widths and interferences must be approximately correct
- Start simple and build up the calculation
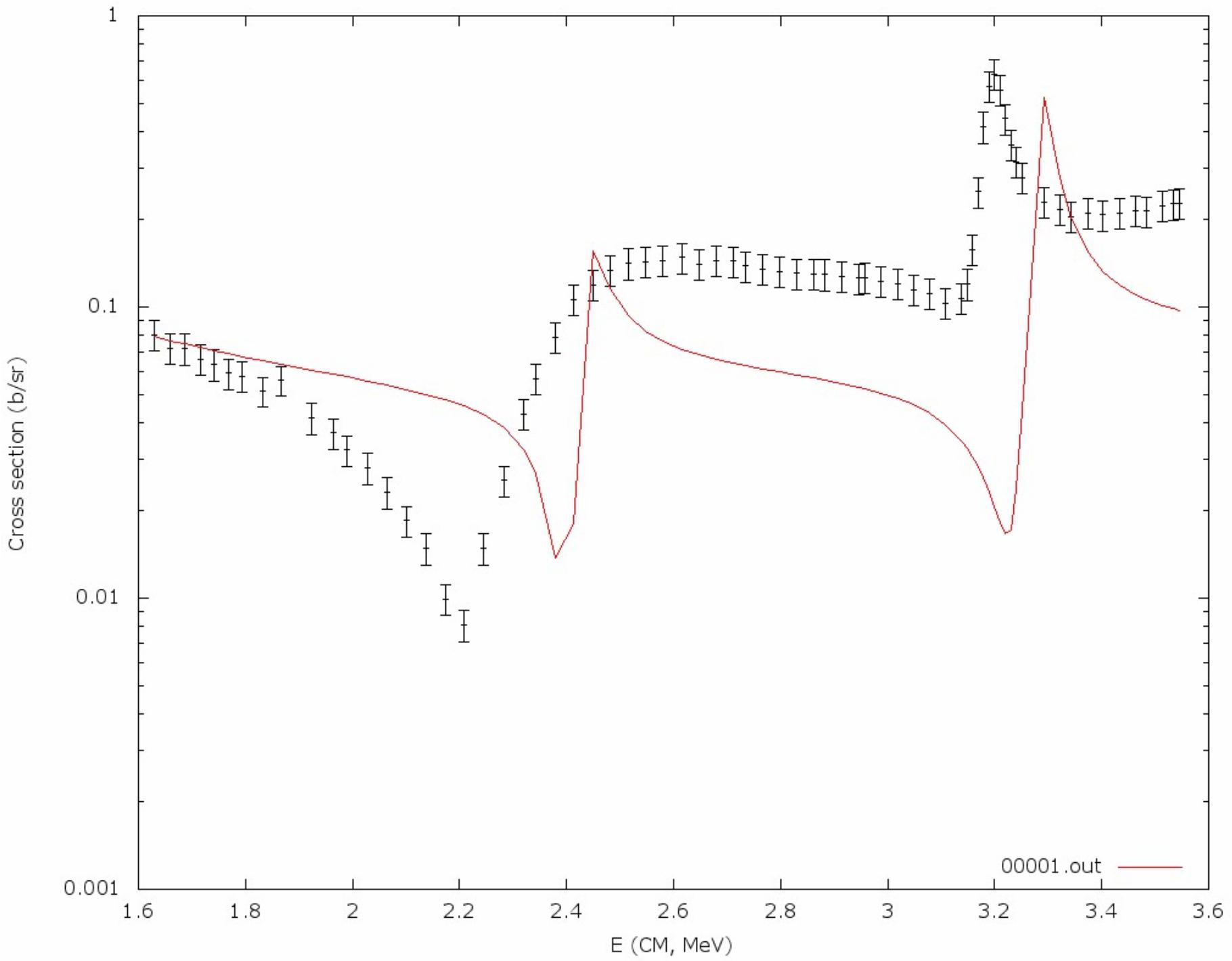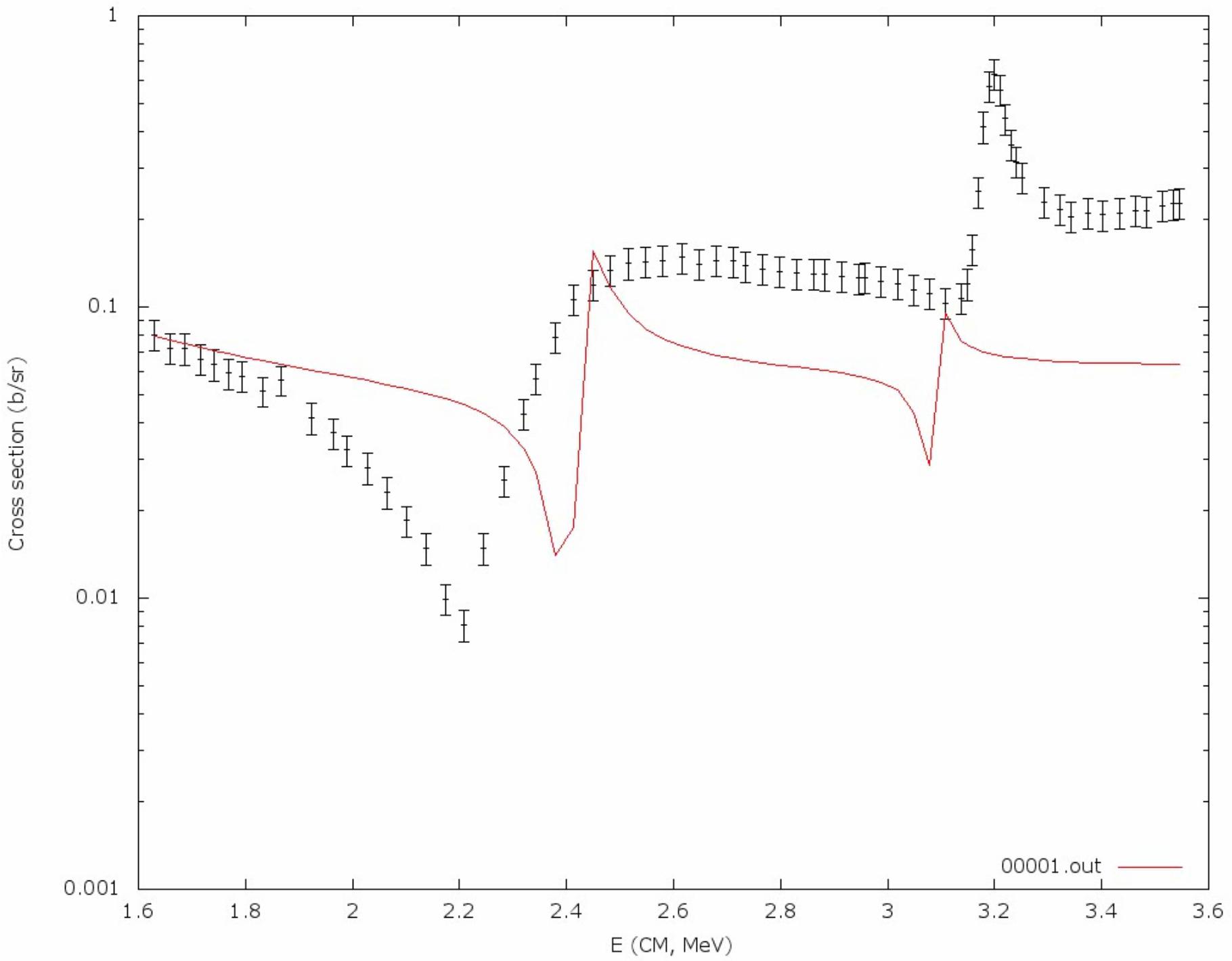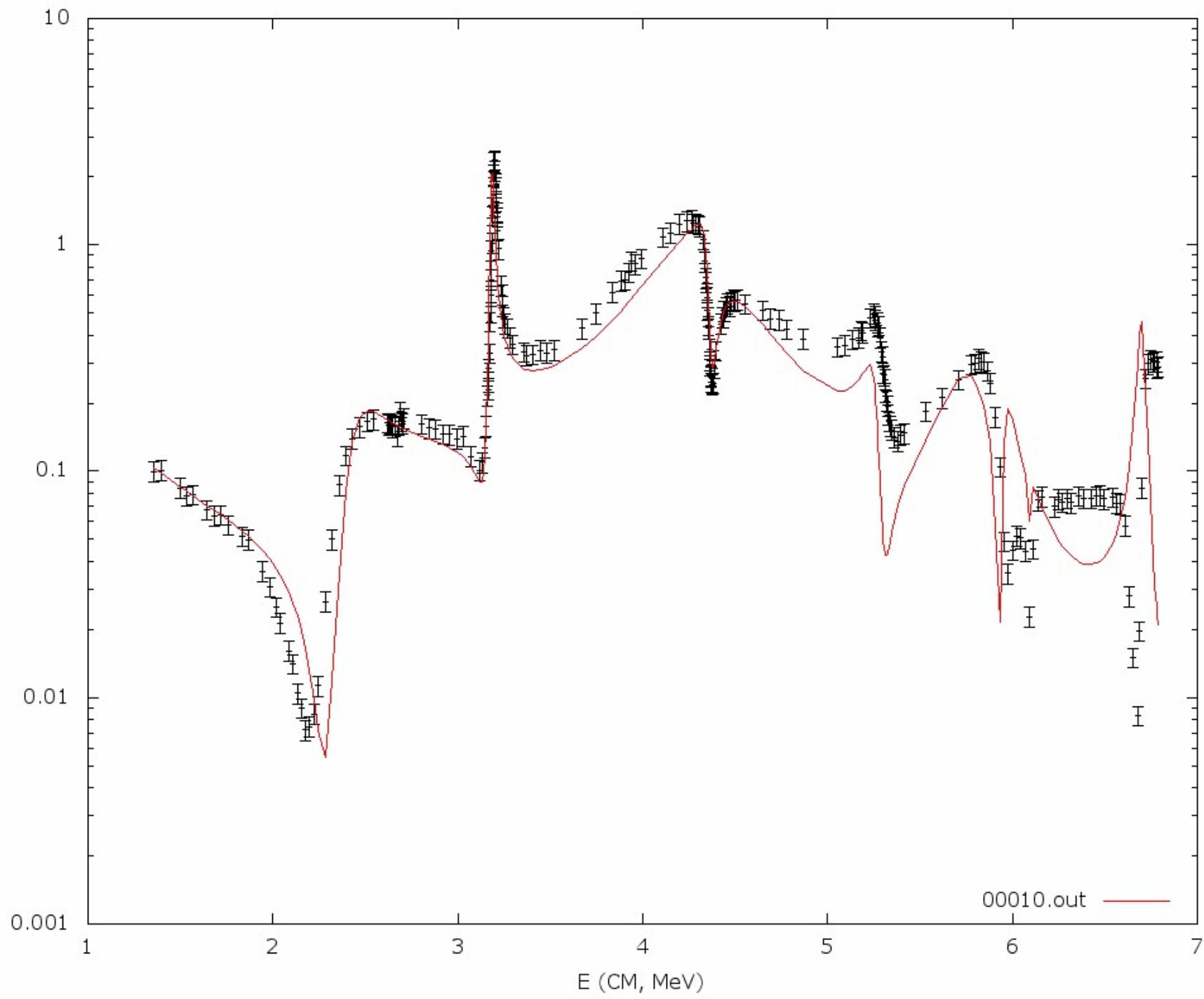
Parameter errors

- After the fit we have an optimal set of **P** parameters **{p⁰}**

- Taylor expand the chi-squared about the fitted parameters:

$$\chi^2(\{p\}) \approx \chi^2(\{p^0\}) + \frac{1}{2} \sum_{m,n=1}^{P} H_{nm}(p_m - p_m^0)(p_n - p_n^0)$$

$$H_{nm} = \frac{\partial^2}{\partial p_n \partial p_m} \chi^2(\{p\})$$

See e.g. F. James, *Statistical Methods in Experimental Physics*
and Filomena's Lectures from last week

Parameter errors and correlations

- One sigma variation in the probability is given by:

$$\chi^2(\{p\}) = \chi^2(\{p^0\}) + 1$$

$$\therefore \frac{1}{2} \sum_{m,n=1}^{P} H_{mn}(p_m - p_m^0)(p_n - p_n^0) = 1$$

- This defines multi-dimensional ellipses in parameters space around the minimum

- Parameter correlations defined as:

$$\rho_{ij} = \frac{V_{ij}}{\Delta_i \Delta_j}$$

$$\text{where} \quad \boldsymbol{V} = 2\boldsymbol{H}^{-1}$$

See e.g. F. James, *Statistical Methods in Experimental Physics*
and Filomena's Lectures from last week

Parameter correlation matrix

MINOS Error analysis: output/covariance_matrix.out

Parameter List

```
    j=1_la=1_energy (  0)           9.585402e+00 Fitted by Minuit        9.585 1⁻
 j=1_la=1_ch=1_rwa (  1)           7.826643e-01 Fitted by Minuit
    j=2_la=1_energy (  2)           1.500000e+01 Fixed                    15.000 3⁻
 j=2_la=1_ch=1_rwa (  3)           3.922930e+03 Fitted by Minuit
    j=3_la=1_energy (  4)           1.035718e+01 Fitted by Minuit        10.353 4⁺
 j=3_la=1_ch=1_rwa (  5)           4.609894e-01 Fitted by Minuit
```

Correlation Matrix

	0	1	3	4	5
0	1.000000	0.496720	-0.000224	0.087533	-0.135543
1	0.496720	1.000000	-0.000294	0.136914	-0.217443
3	-0.000224	-0.000294	1.000000	-0.000075	-0.000354
4	0.087533	0.136914	-0.000075	1.000000	-0.092854
5	-0.135543	-0.217443	-0.000354	-0.092854	1.000000

Other capabilities...

- **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 (slow...)

Summary

Phenomenological R-matrix fitting provides one method to understand the structure of nuclei at low excitations.

It provides a means to calculate low-energy scattering and reaction cross sections for nuclear astrophysics, materials analysis and other applications.

R-matrix calculations should begin as simply as possible, identifying the strongest states, before adding weaker contributions. Fitting using MINUIT should only be done once the key elements are established.

In principle the R-matrix fits should be weakly dependent on the R-matrix radius parameter, but this should be checked.