The Application of R-Matrix Analysis to Experimental Data

1 - Resonance Properties

Alex Murphy & David Mountford

THE UNIVERSITY OF EDINBURGH

Contents

- The R-Matrix Formalism
- Context: The $^{18}F(p,\alpha)^{15}O$ Reaction
- (Doing an…) R-Matrix analysis
- Comparison of R-Matrix Codes
- Conclusions

R-Matrix

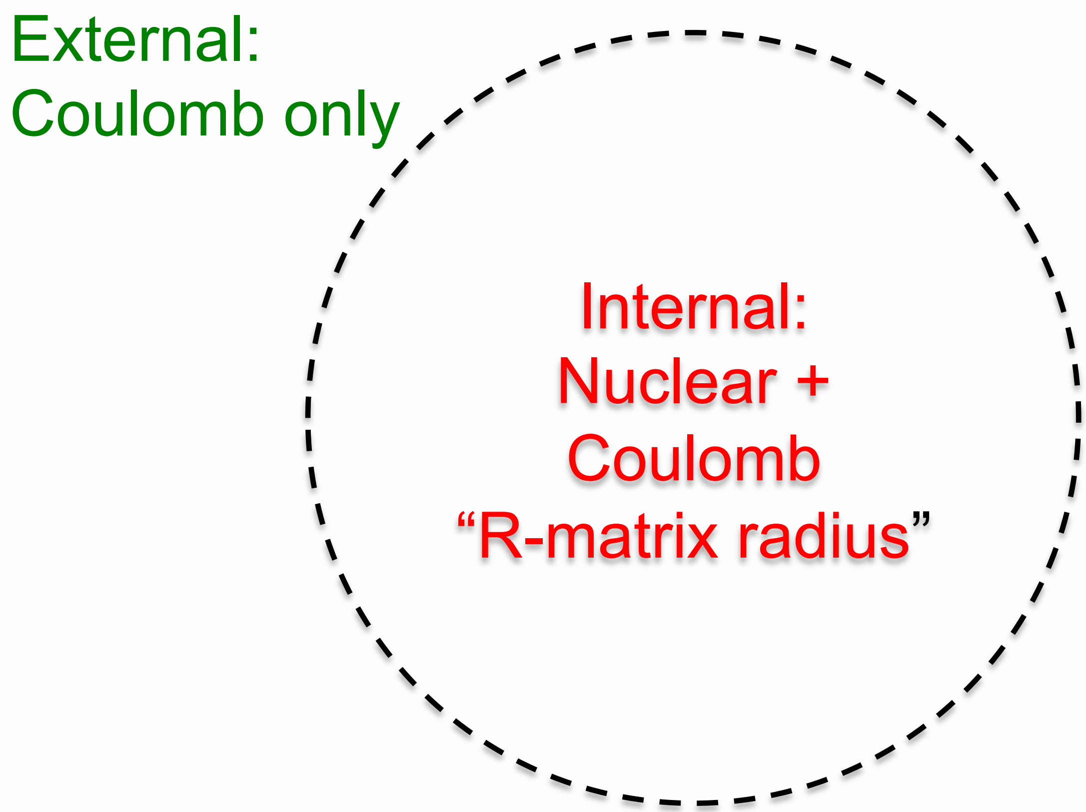
The experimentalist's hope

…but it's never quite that easy…

Some Theory…

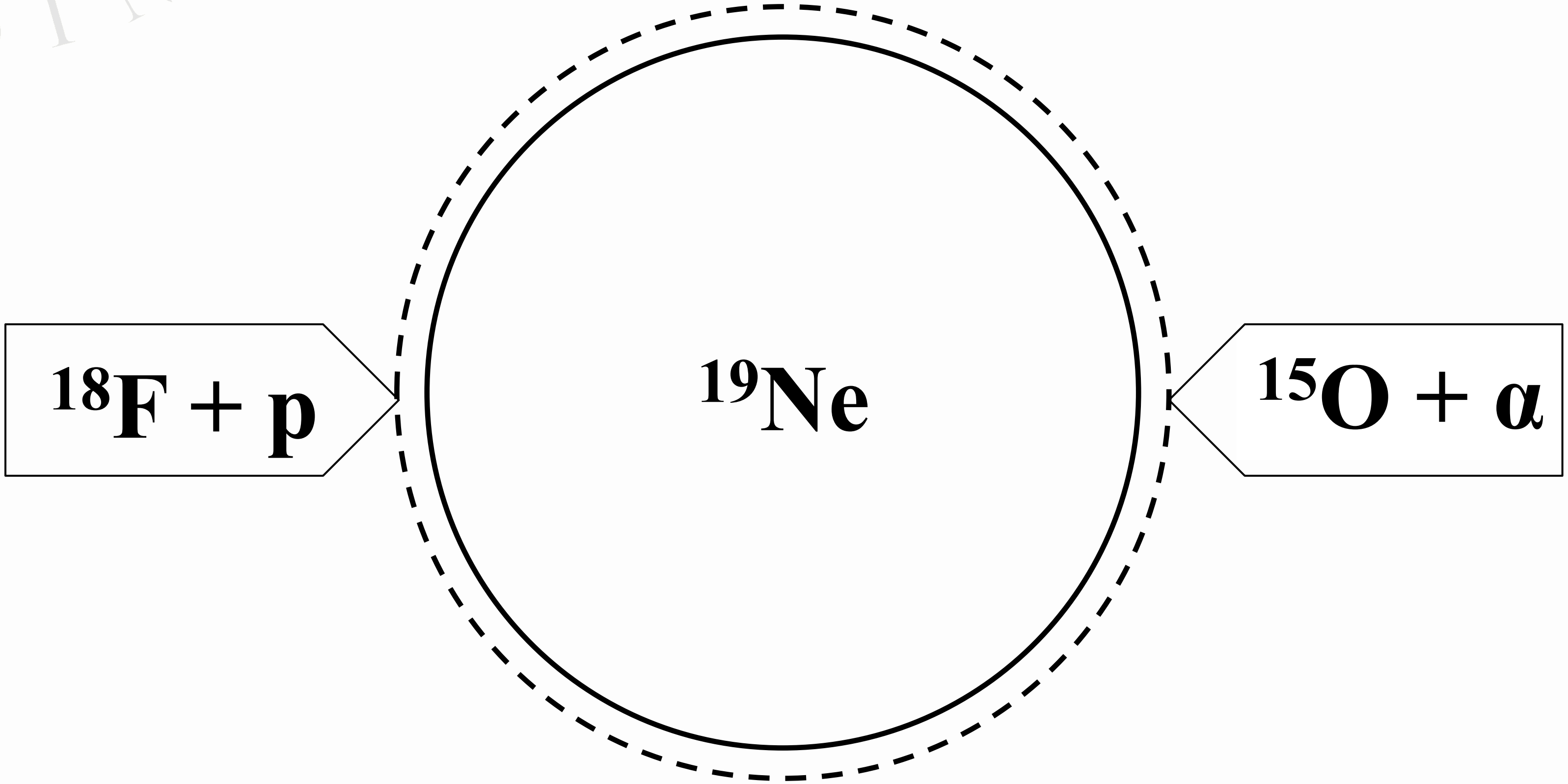
The R-Matrix Formalism

- “Bible”: Lane and Thomas, Rev. Mod. Phys. 30, 257 (1958)[1]
- Basics: split system into internal and external regions:



The R-Matrix Formalism

- R-Matrix radius ~ nuclear radius, slightly larger
- Various incoming "channels"



The R-Matrix Formalism

- Internal Region:
  - Wavefunction not well understood, cannot obtain cross section…
    - Radial and spherical contributions
    - Set of orthonormal basis functions

$$\Psi = \sum_c \psi_c \phi_c = \sum_\lambda C_\lambda \chi_\lambda$$

- Calculating coefficients and solving Schrodinger equation:

$$\phi_c \left(\frac{\hbar^2}{2\mu_c r_c} \right)^{1/2} = \sum_\lambda (E_\lambda - E)^{-1} \sum_{c'} \left(\frac{\hbar^2}{2\mu_{c'} r_{c'}} \right)^{1/2} \gamma_{\lambda c} \gamma_{\lambda c'} \left[\rho_{c'} \phi'_{c'} - \phi_{c'} b_{c'} \right]$$

- Purely radial
- All spherical dependence absorbed by γ
- Extract "R-matrix":

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

The R-Matrix Formalism

- External Region:
  - Purely Coulomb potential
  - Radial wavefunction is well understood combination of well known Coulomb functions:

$$\phi_c = \frac{1}{\sqrt{v_c}}\left(A_c I_c - \sum_{c'} U_{cc'} A_{c'} O_c\right)$$

$$I_c = \left(G_c - iF_c\right)e^{i\omega_c}$$

$$O_c = \left(G_c + iF_c\right)e^{-i\omega_c}$$

- $U_{cc'}$ = scattering matrix
- Substitution into internal wavefunction gives scattering matrix in terms of R-matrix:

$$U = \rho^{1/2} O^{-1}\left(1 - RL\right)^{-1}\left(1 - RL^*\right) I \rho^{-1/2}$$

The R-Matrix Formalism

- To cross section:
  - One U for every J^π group

$$\frac{d\sigma}{d\Omega} \propto \left| U_J U_{J'}^* \right|$$

- U ~ $e^{2i\delta}$, δ = total phase shift:

$$\frac{d\sigma}{d\Omega} \propto \cos\left(2\left(\delta_J - \delta_{J'}\right)\right)$$

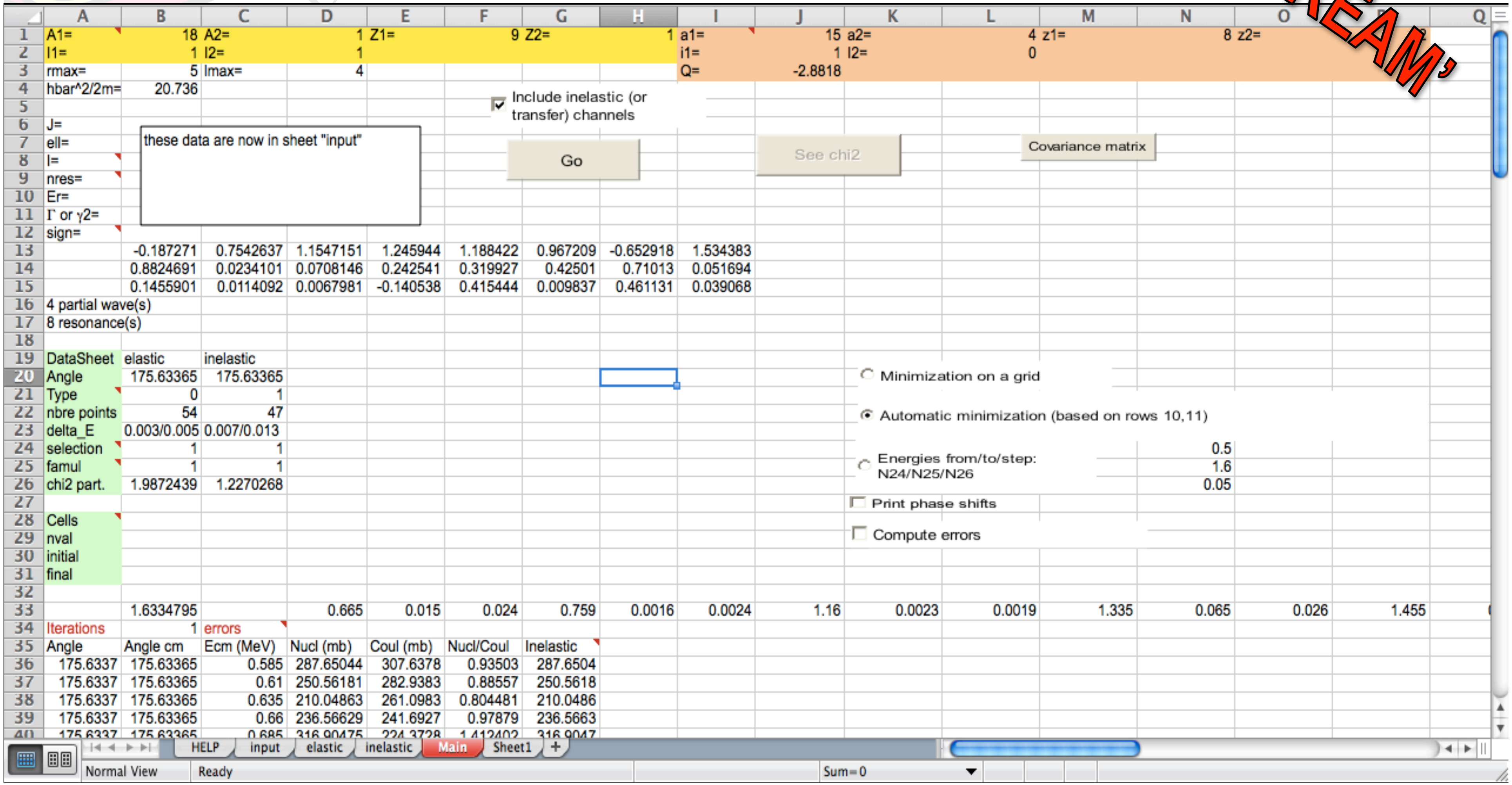
- δ = phase of U
- Cross section calculated either directly from U or from phase shifts

R-Matrix Implementation

'Still 'Living the DREAM'

- Simplified multi channel code (P. Descouvement):

$$\frac{d\sigma}{d\Omega} \propto \cos\left(2\left(\delta_J - \delta_{J'}\right)\right)$$



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	A1=	18	A2=	1	Z1=	9	Z2=	1	a1=	15	a2=	4	z1=	8	z2=	
2	I1=	1	I2=	1					i1=	1	I2=	0				
3	rmax=	5	lmax=	4					Q=	-2.8818						
4	hbar^2/2m=	20.736														
5																
6	J=															
7	ell=															
8	l=															
9	nres=															
10	Er=															
11	Γ or γ2=															
12	sign=															
13		-0.187271	0.7542637	1.1547151	1.245944	1.188422	0.967209	-0.652918	1.534383							
14		0.8824691	0.0234101	0.0708146	0.242541	0.319927	0.42501	0.71013	0.051694							
15		0.1455901	0.0114092	0.0067981	-0.140538	0.415444	0.009837	0.461131	0.039068							
16	4 partial wave(s)															
17	8 resonance(s)															
18																
19	DataSheet	elastic	inelastic													
20	Angle	175.63365	175.63365													
21	Type	0	1													
22	nbre points	54	47													
23	delta_E	0.003/0.005	0.007/0.013													
24	selection	1	1											0.5		
25	famul	1	1											1.6		
26	chi2 part.	1.9872439	1.2270268											0.05		
27																
28	Cells															
29	nval															
30	initial															
31	final															
32																
33		1.6334795		0.665	0.015	0.024	0.759	0.0016	0.0024	1.16	0.0023	0.0019	1.335	0.065	0.026	1.455
34	Iterations	1	errors													
35	Angle	Angle cm	Ecm (MeV)	Nucl (mb)	Coul (mb)	Nucl/Coul	Inelastic									
36	175.6337	175.63365	0.585	287.65044	307.6378	0.93503	287.6504									
37	175.6337	175.63365	0.61	250.56181	282.9383	0.88557	250.5618									
38	175.6337	175.63365	0.635	210.04863	261.0983	0.804481	210.0486									
39	175.6337	175.63365	0.66	236.56629	241.6927	0.97879	236.5663									
40	175.6337	175.63365	0.685	316.90475	224.3728	1.412402	316.9047									

these data are now in sheet "input"

Include inelastic (or transfer) channels

Go

See chi2

Covariance matrix

Minimization on a grid

Automatic minimization (based on rows 10,11)

Energies from/to/step: N24/N25/N26

Print phase shifts

Compute errors

HELP | input | elastic | inelastic | Main | Sheet1

Normal View | Ready | Sum=0

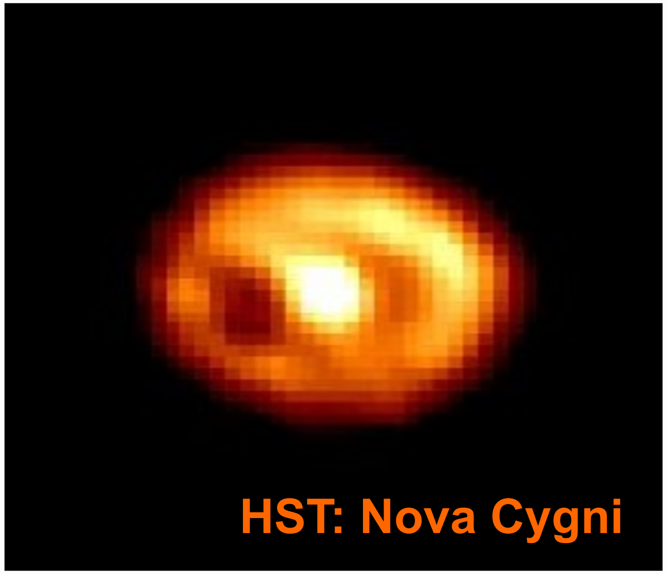
Experimental Work

$^{18}F(p,\alpha)^{15}O$

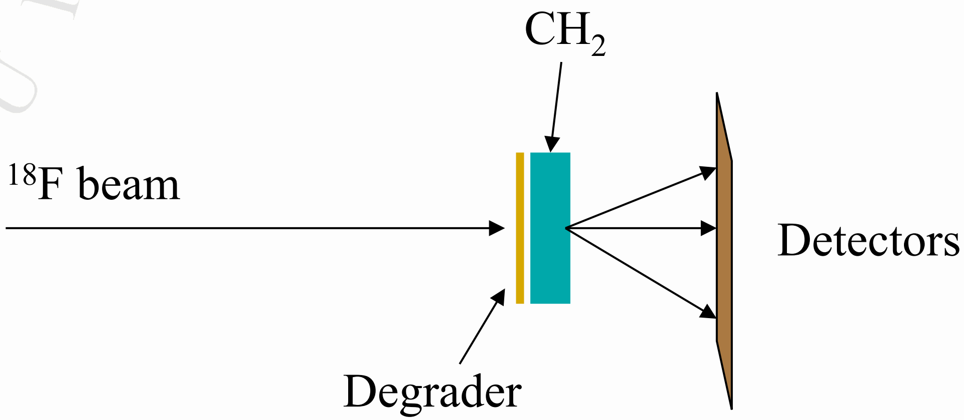
Motivation

- ^{18}F is the dominant gamma-ray emitter in novae
- Abundance strongly dependent on rate of this reaction
- Reaction proceeds through poorly known resonances in ^{19}Ne
- Theoretical expectation of additional states

Need to find and characterise states in ^{19}Ne



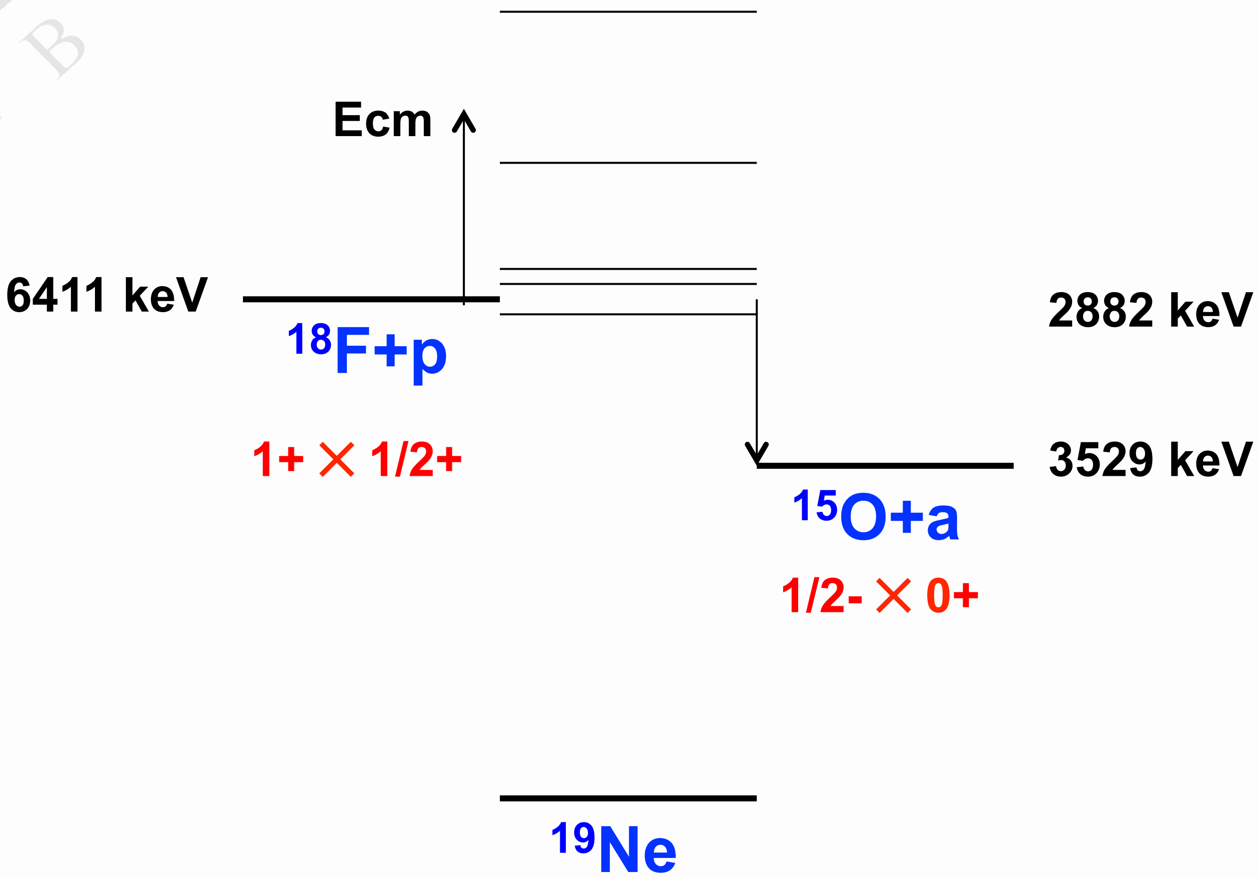
Generic Set Up



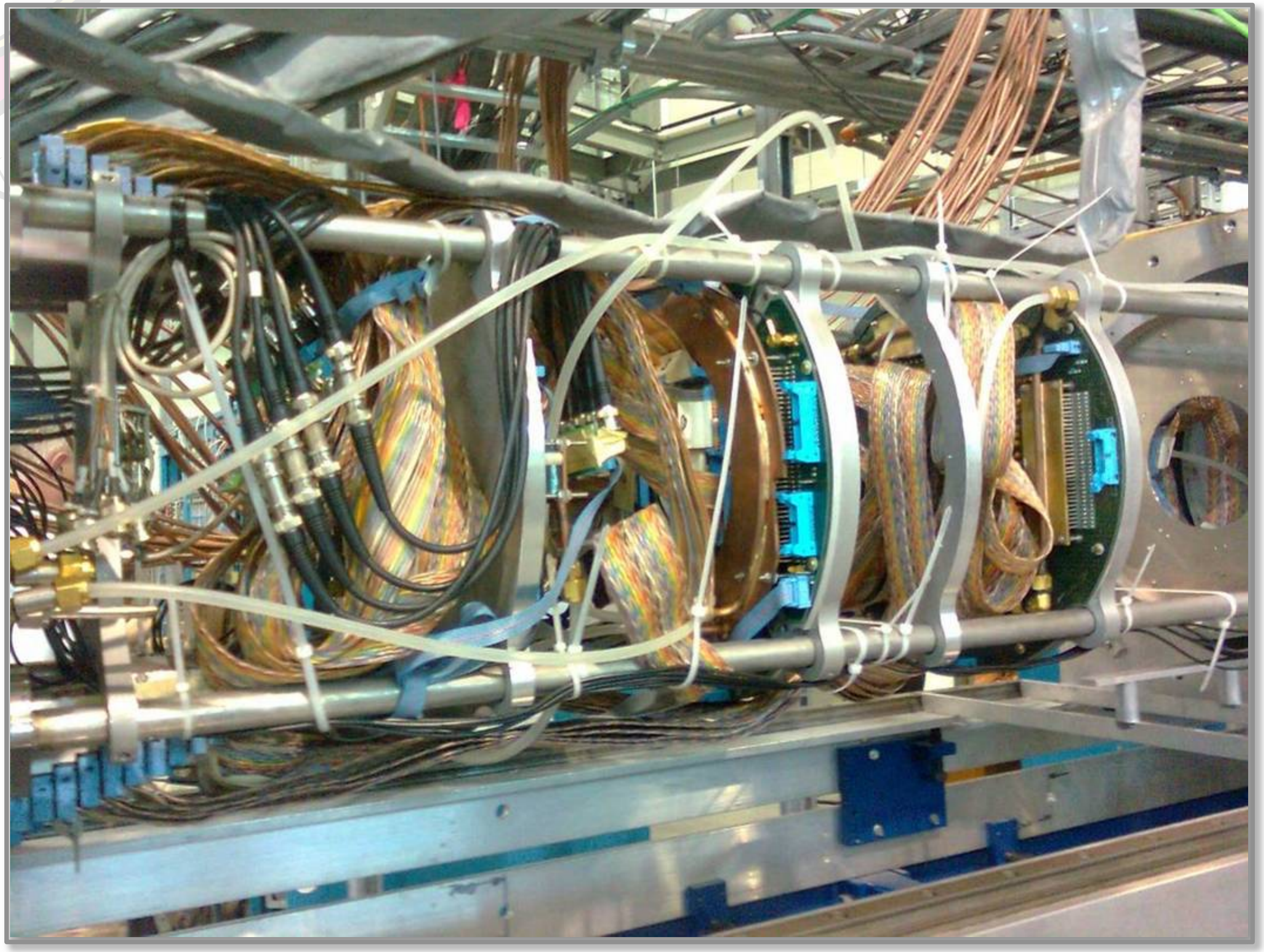
- Pure, intense ^{18}F beam
- 'Thick' CH_2 target
- ^{18}F stopped in target
- Adjust beam energy &target thickness for desired *Ecm* coverage
- Protons and alpha particles detected downstream in DSSDs

Simultaneous excitations functions of $^{18}F(p,p)^{18}F$ & $^{18}F(p,\alpha)^{15}O$

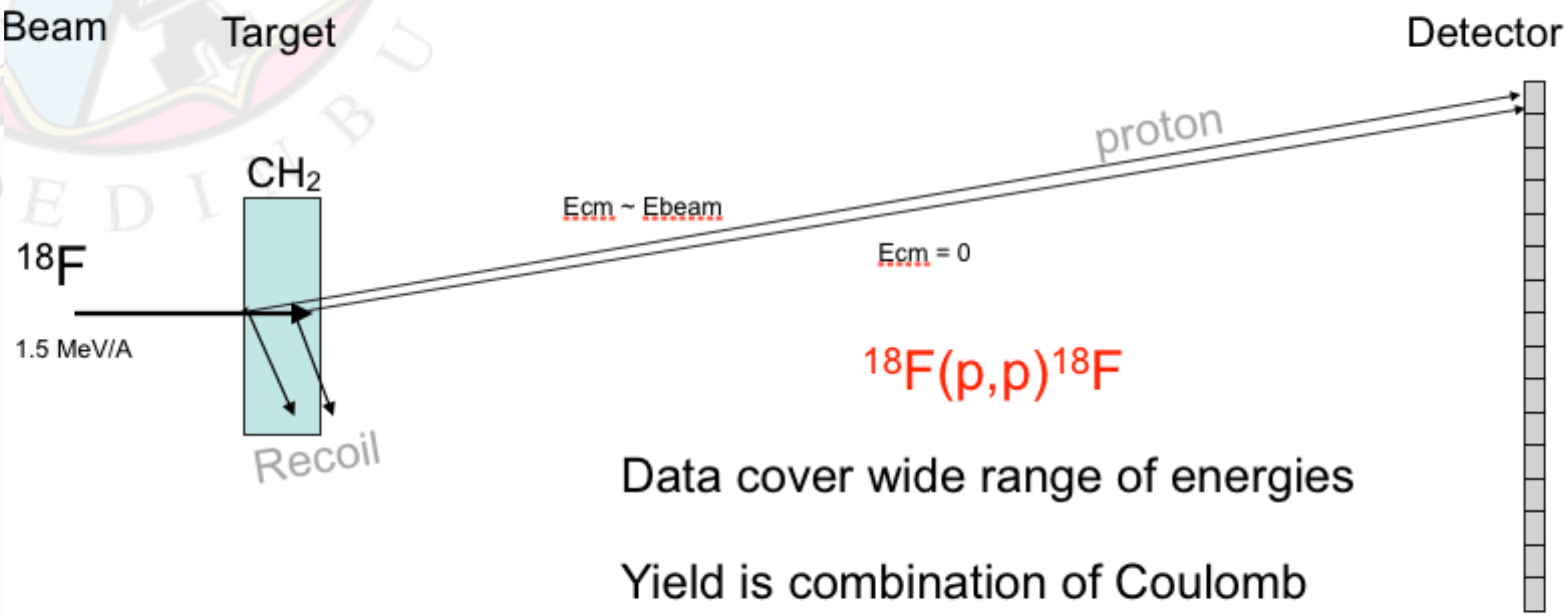
Physics



Actual Set Up



Thick Target Technique



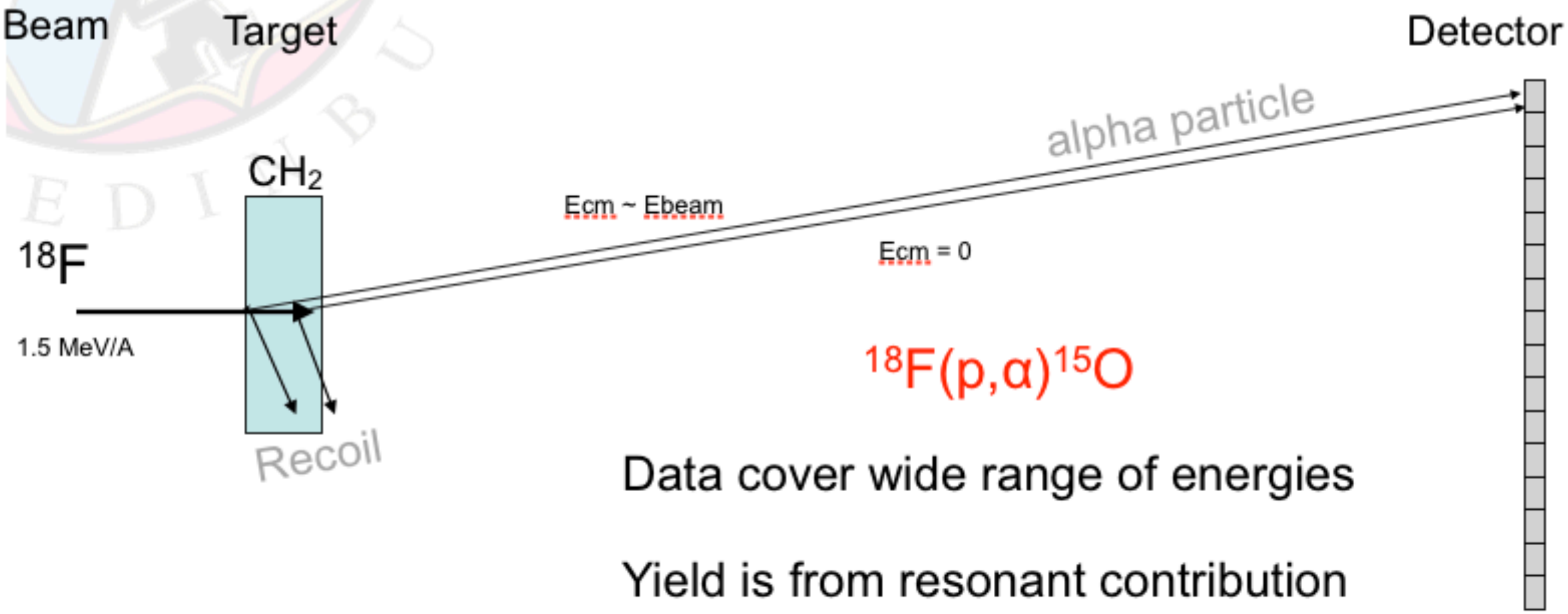
$^{18}F(p,p)^{18}F$

Data cover wide range of energies

Yield is combination of Coulomb scattering and resonant contribution

Detailed shape of excitation function contains required nuclear information

Thick Target Technique



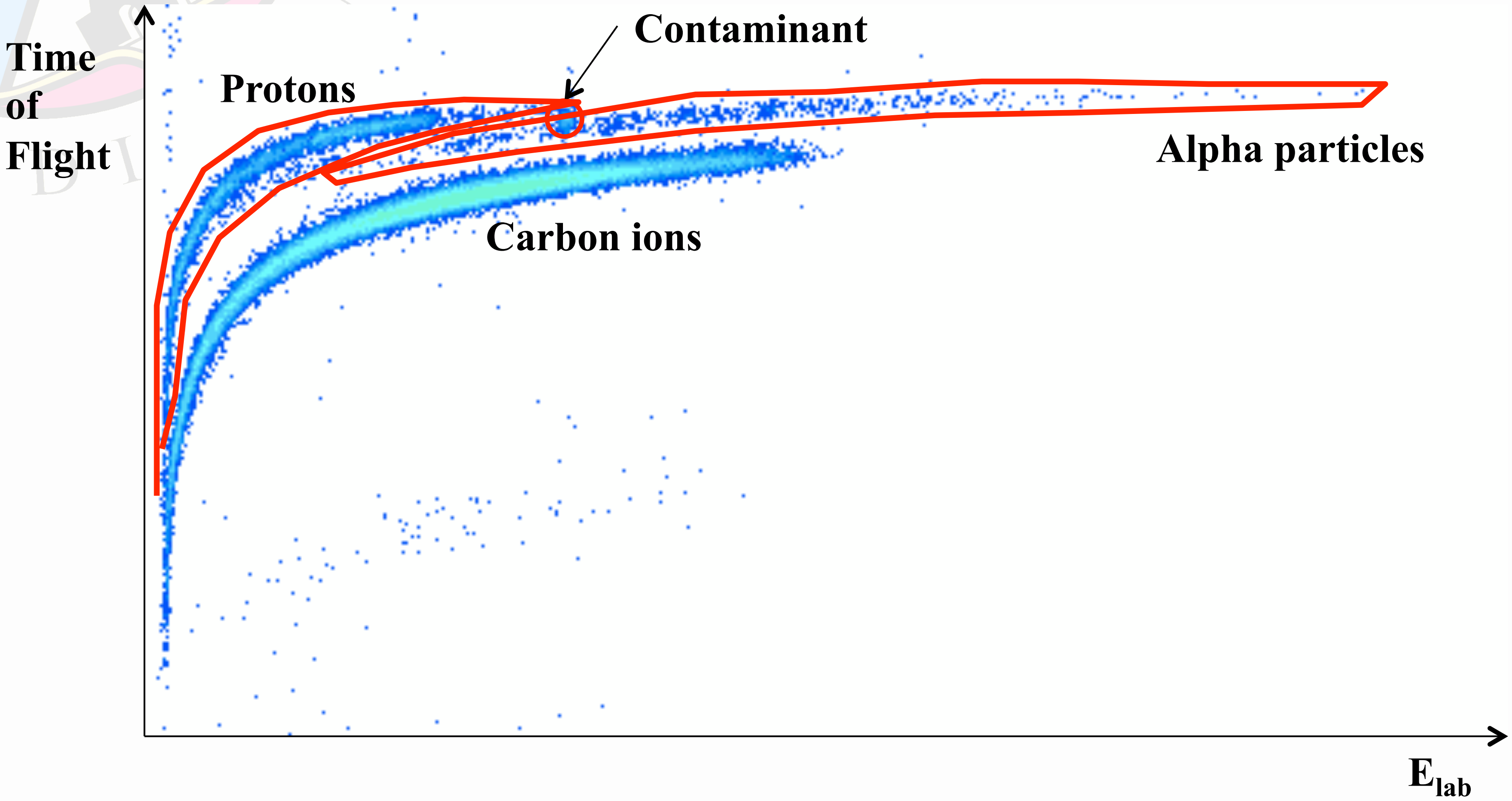
$^{18}F(p,\alpha)^{15}O$

Data cover wide range of energies

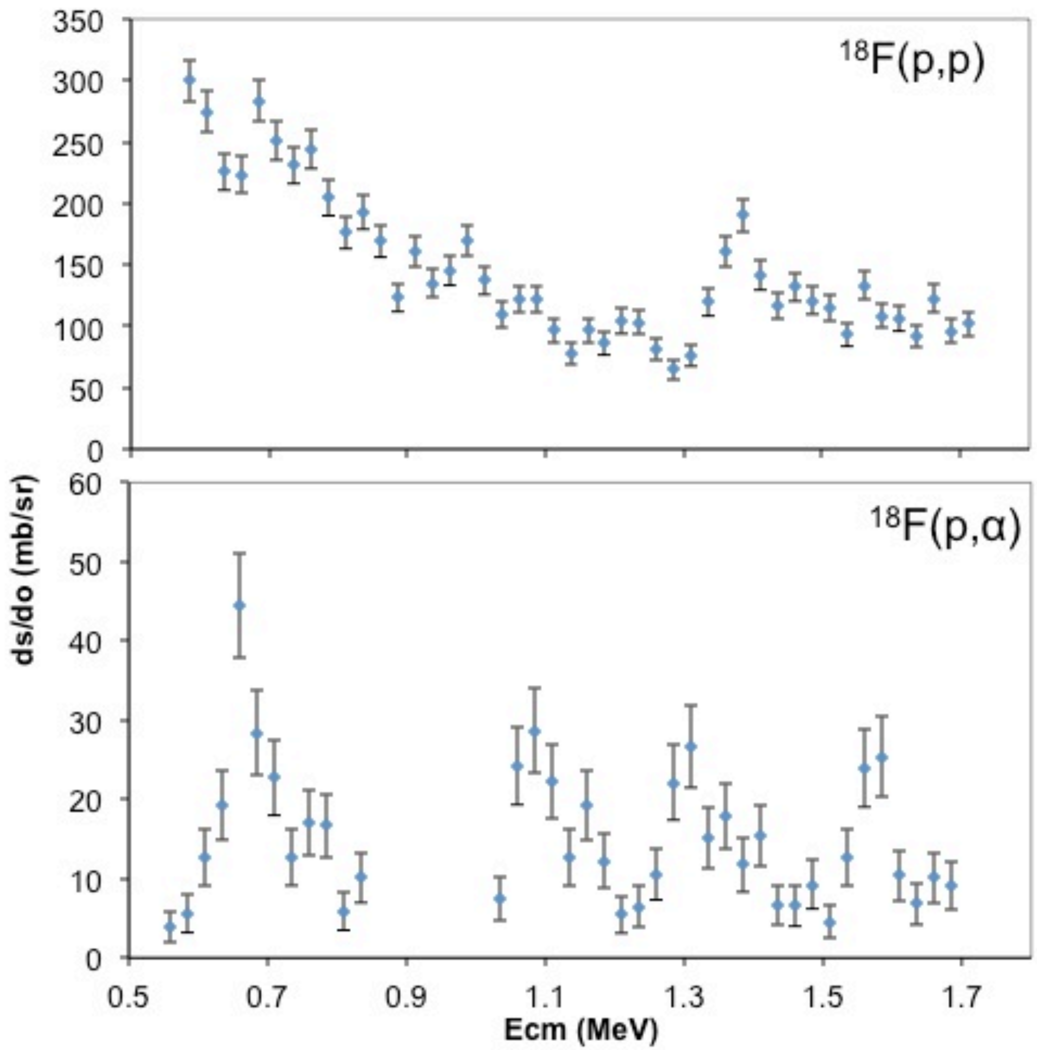
Yield is from resonant contribution only

Shape is simpler

Experimental Data



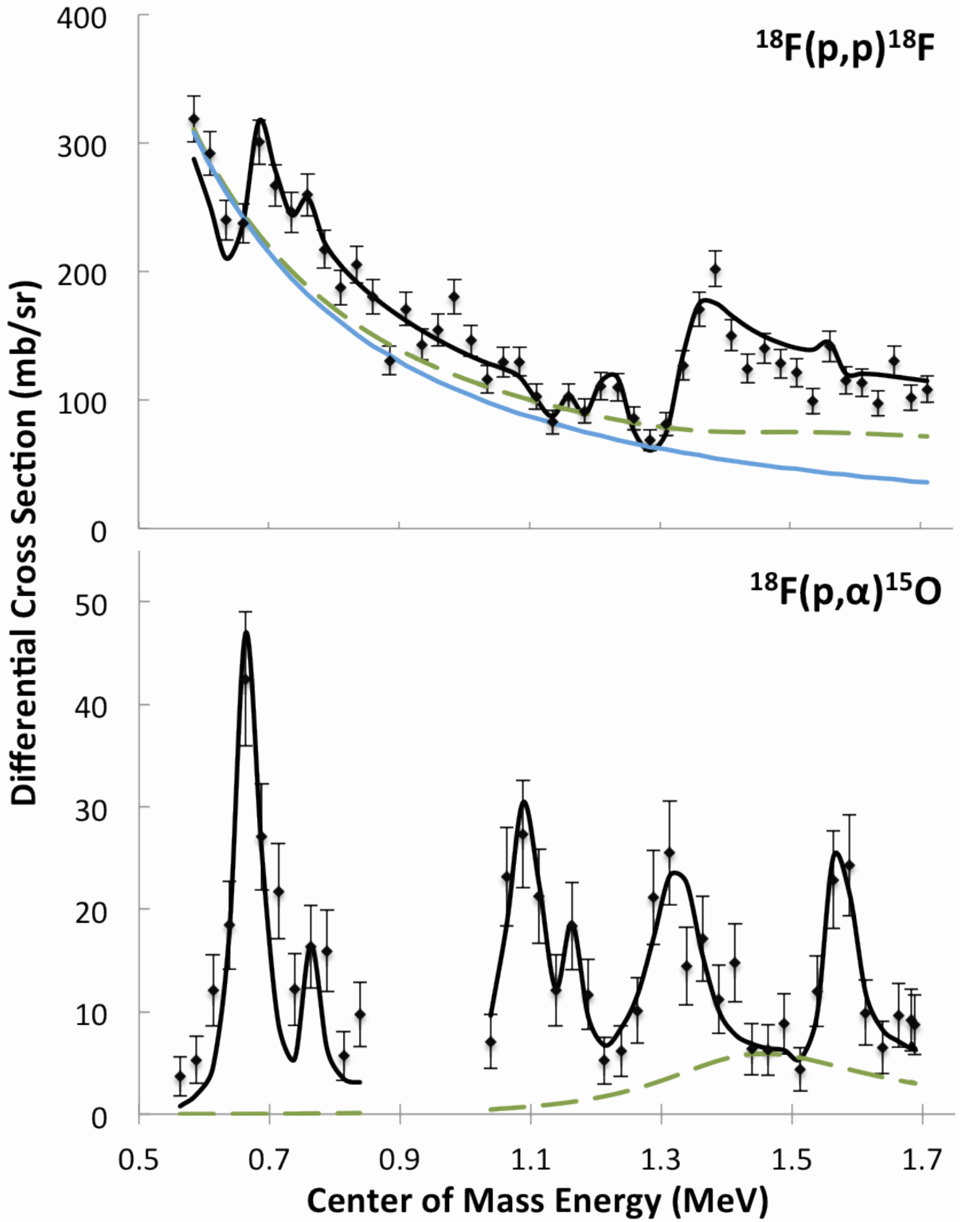
Experimental Data



Results

	Ecm (MeV)	Jπ	Γp(keV)	Γα(keV)	Int
A	0.665	3/2+	15	24	+
B	0.759(20)	3/2+	1.6(5)	2.4(6)	
C	1.096(11)	5/2+	3(1)	54(12)	
D	1.160(34)	3/2+	2.3(6)	1.9(6)	
E	1.219(22)	3/2-	21(3)	0.1(1)	
F	1.335(6)	3/2+	65(8)	26(4)	-
G	1.455(38)	1/2+	55(12)	347(92)	
H	1.571(13)	5/2+	1.7(4)	12(3)	

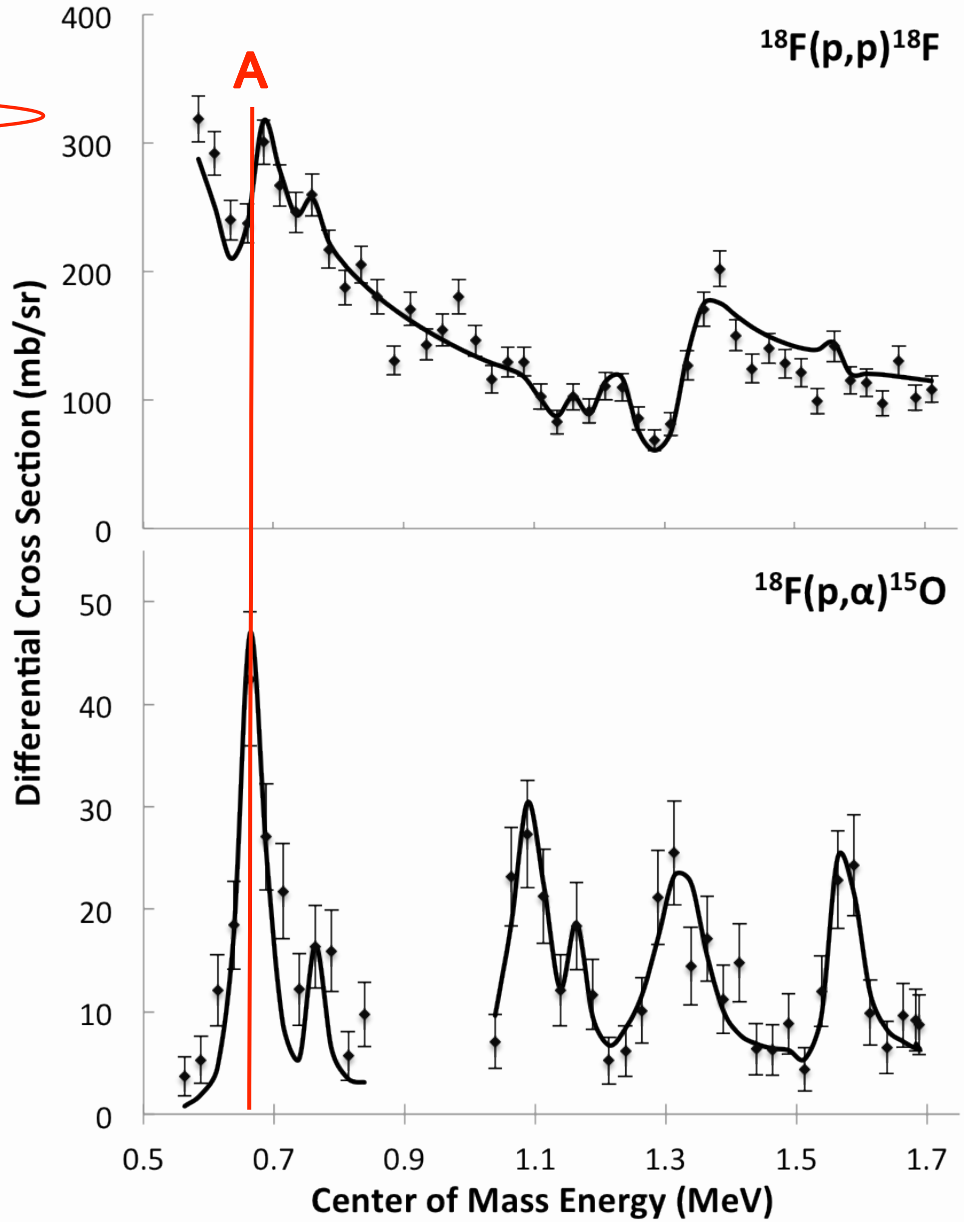
- Results of R Matrix analysis carried out using DREAM code from P. Descouvemont
- Mountford *et al.*, Phys. Rev. C **85**, 022801(R) (2012)



Preliminary Results (A)

	Ecm (MeV)	J^{π}	Γp(keV)	Γα(keV)	Int
A	0.665	3/2+	15	24	+
B	0.759(20)	3/2+	1.6(5)	2.4(6)	
C	1.096(11)	5/2+	3(1)	54(12)	
D	1.160(34)	3/2+	2.3(6)	1.9(6)	
E	1.219(22)	3/2-	21(3)	0.1(1)	
F	1.335(6)	3/2+	65(8)	26(4)	-
G	1.455(38)	1/2+	55(12)	347(92)	
H	1.571(13)	5/2+	1.7(4)	12(3)	

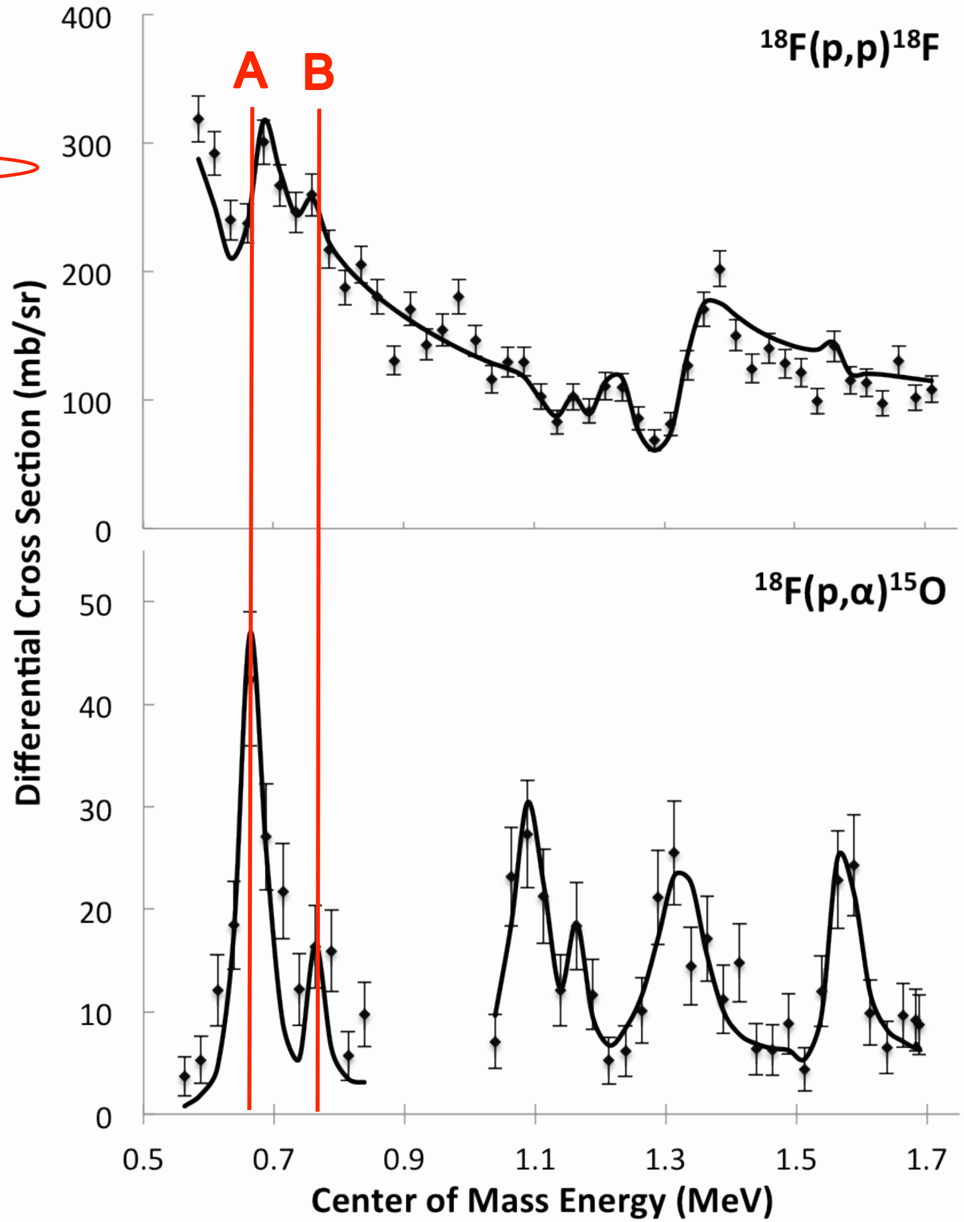
- Well known '665keV' state
- Cross sections scaled to this state



Preliminary Results (B)

	Ecm (MeV)	J^{π}	Γp(keV)	Γα(keV)	Int
A	0.665	3/2+	15	24	+
B	0.759(20)	3/2+	1.6(5)	2.4(6)	
C	1.096(11)	5/2+	3(1)	54(12)	
D	1.160(34)	3/2+	2.3(6)	1.9(6)	
E	1.219(22)	3/2-	21(3)	0.1(1)	
F	1.335(6)	3/2+	65(8)	26(4)	-
G	1.455(38)	1/2+	55(12)	347(92)	
H	1.571(13)	5/2+	1.7(4)	12(3)	

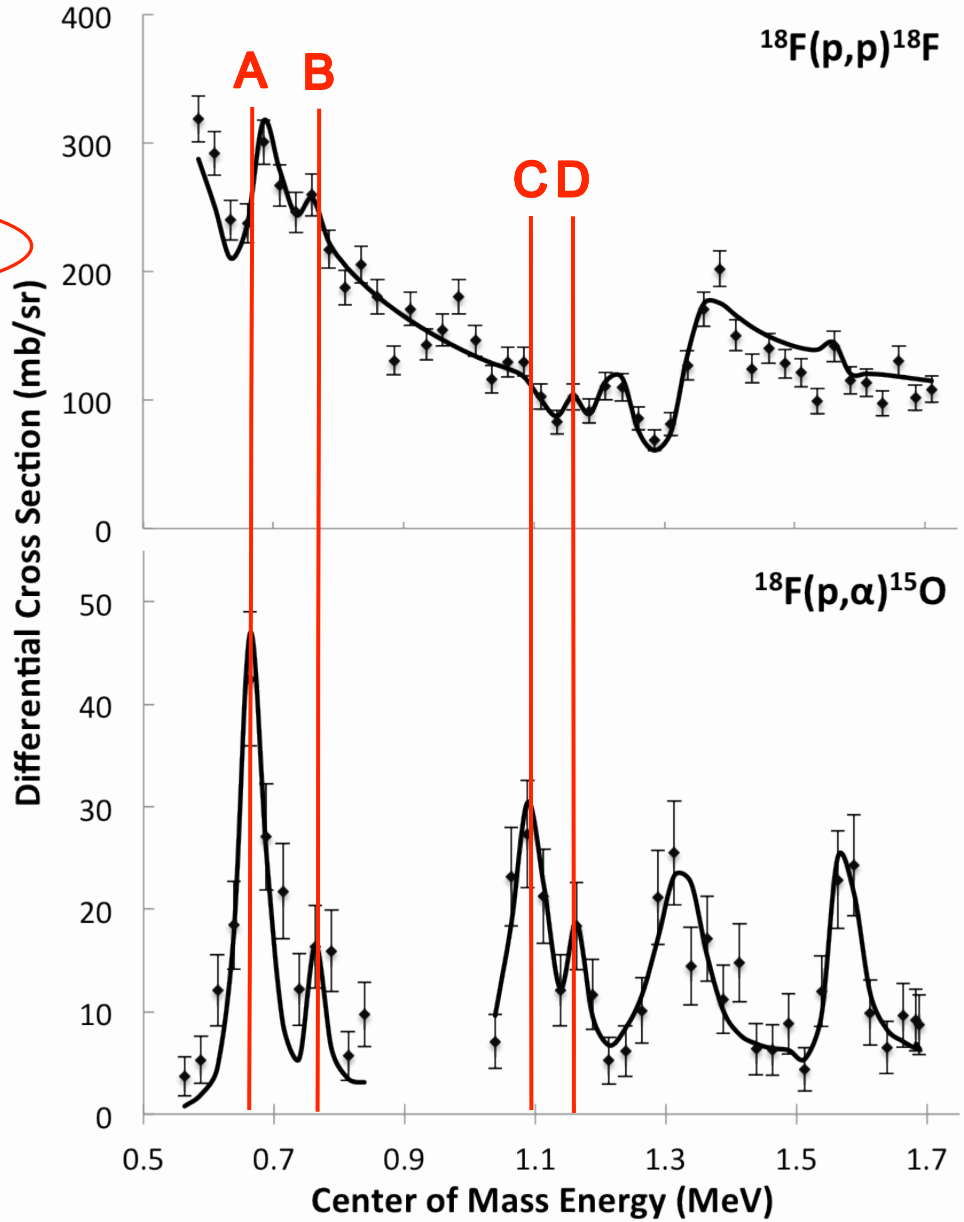
- Reported by Nesaraja/ Dalouzy
- Significantly weaker than Dalouzy
- Consistent in strength with Nesaraja



Preliminary Results (C & D)

	Ecm (MeV)	J^π	Γp(keV)	Γα(keV)	Int
A	0.665	3/2+	15	24	+
B	0.759(20)	3/2+	1.6(5)	2.4(6)	
C	1.096(11)	5/2+	3(1)	54(12)	
D	1.160(34)	3/2+	2.3(6)	1.9(6)	
E	1.219(22)	3/2-	21(3)	0.1(1)	
F	1.335(6)	3/2+	65(8)	26(4)	-
G	1.455(38)	1/2+	55(12)	347(92)	
H	1.571(13)	5/2+	1.7(4)	12(3)	

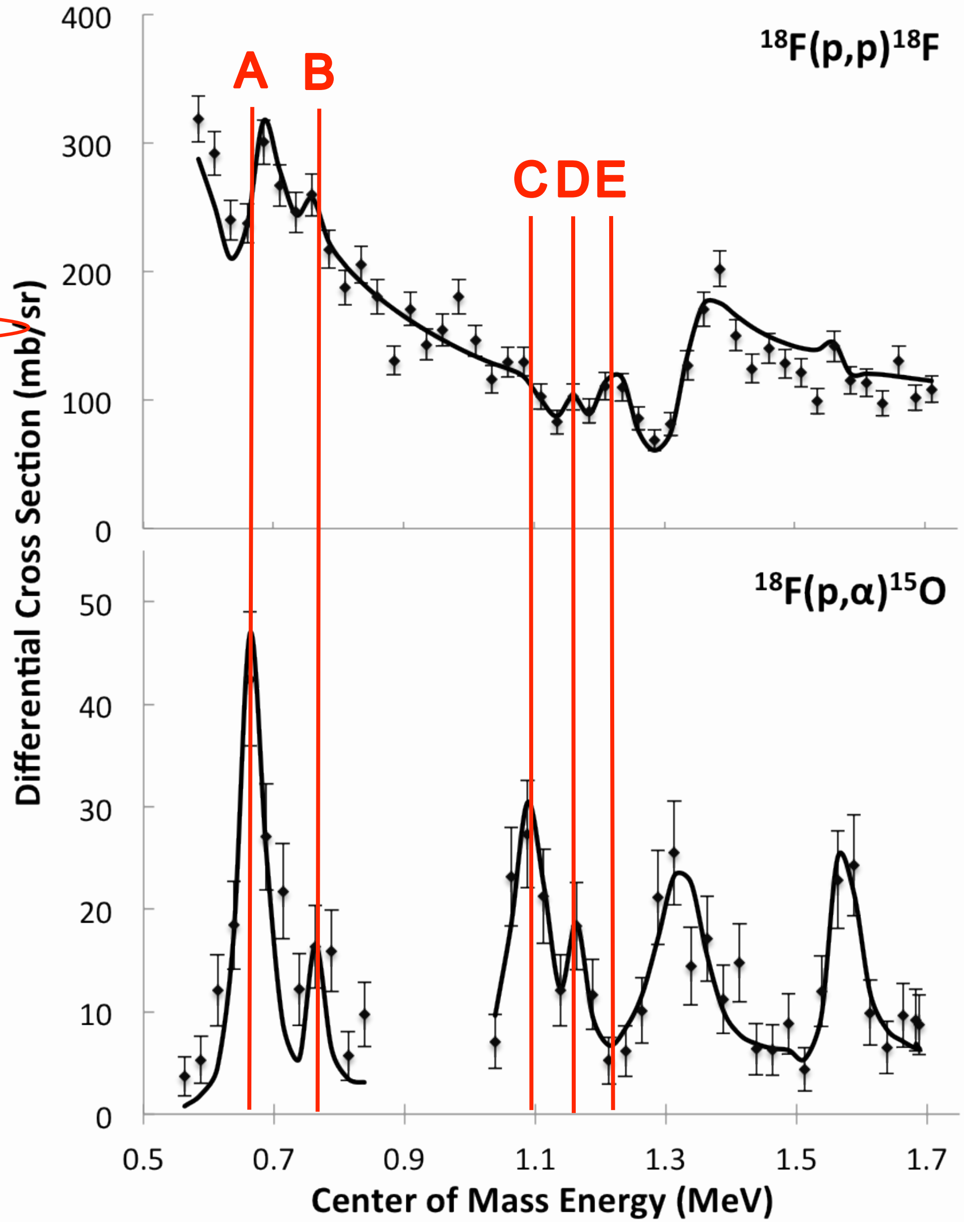
- C reported by Murphy – narrower but current result relatively consistent
- C and D reported by Dalouzy/Nesaraja at different strengths
- C in good agreement in energy



Preliminary Results (E)

	Ecm (MeV)	Jπ	Γp(keV)	Γα(keV)	Int
A	0.665	3/2+	15	24	+
B	0.759(20)	3/2+	1.6(5)	2.4(6)	
C	1.096(11)	5/2+	3(1)	54(12)	
D	1.160(34)	3/2+	2.3(6)	1.9(6)	
E	1.219(22)	3/2-	21(3)	0.1(1)	
F	1.335(6)	3/2+	65(8)	26(4)	-
G	1.455(38)	1/2+	55(12)	347(92)	
H	1.571(13)	5/2+	1.7(4)	12(3)	

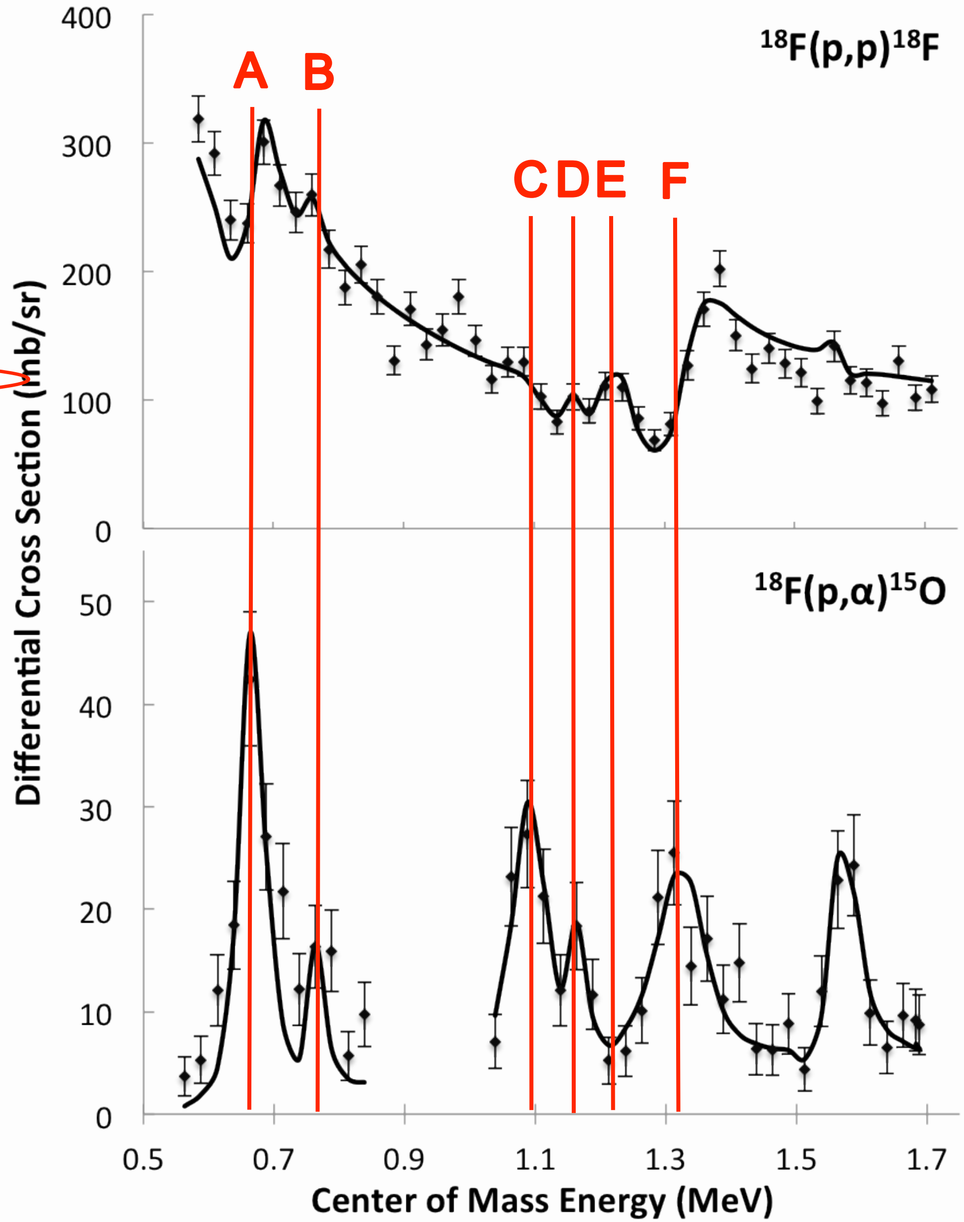
- Previously reported by Nesaraja and Murphy
- Agreement in spin with Murphy
- No agreement in strength
- Required to fit bottom of state F



Preliminary Results (F)

	Ecm (MeV)	J^{π}	Γp(keV)	Γα(keV)	Int
A	0.665	3/2+	15	24	+
B	0.759(20)	3/2+	1.6(5)	2.4(6)	
C	1.096(11)	5/2+	3(1)	54(12)	
D	1.160(34)	3/2+	2.3(6)	1.9(6)	
E	1.219(22)	3/2-	21(3)	0.1(1)	
F	1.335(6)	3/2+	65(8)	26(4)	-
G	1.455(38)	1/2+	55(12)	347(92)	
H	1.571(13)	5/2+	1.7(4)	12(3)	

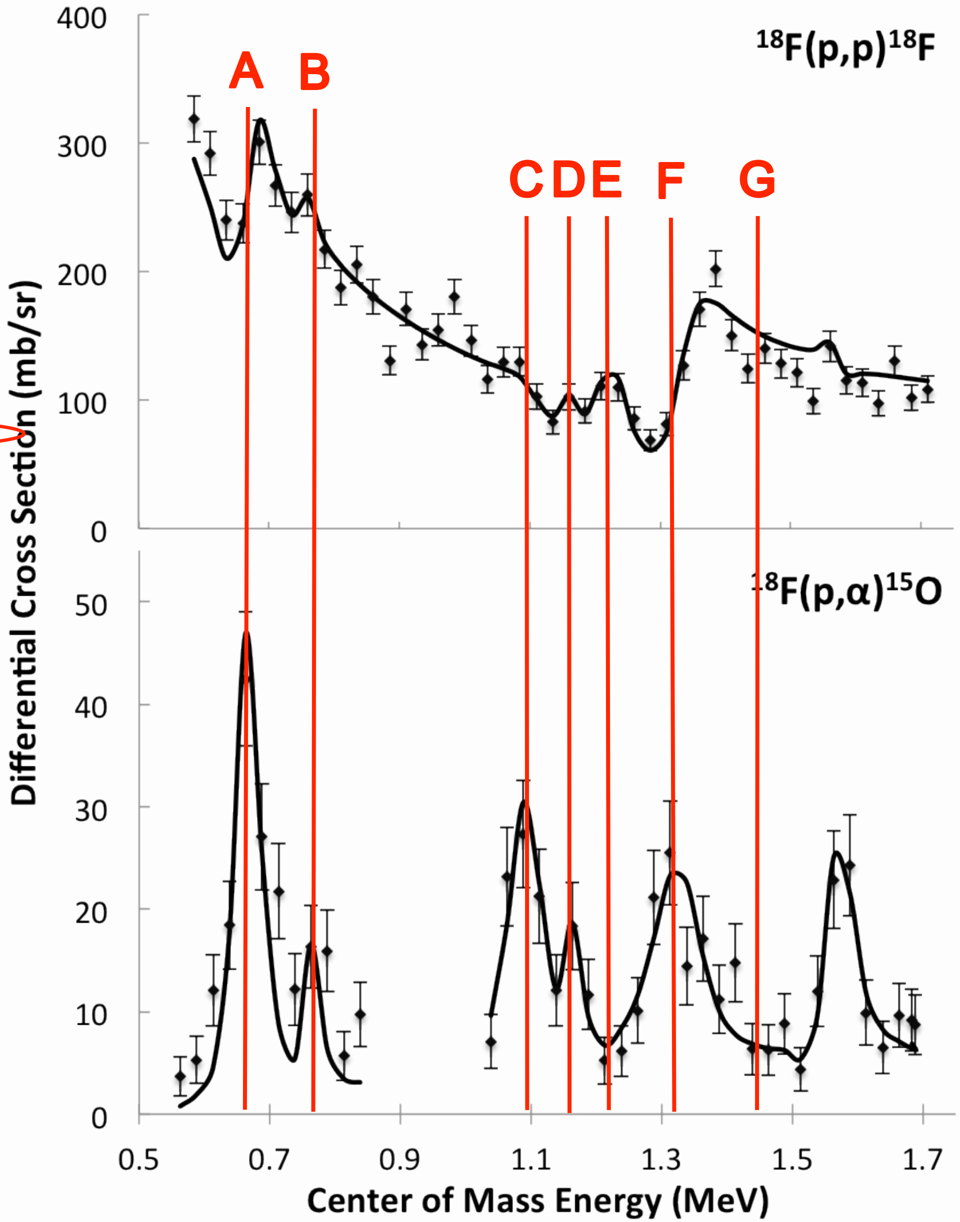
- Observed by Murphy with less strength
- New strength due to strong correlation with state G



Preliminary Results (G)

	Ecm (MeV)	J^π	Γp(keV)	Γα(keV)	Int
A	0.665	3/2+	15	24	+
B	0.759(20)	3/2+	1.6(5)	2.4(6)	
C	1.096(11)	5/2+	3(1)	54(12)	
D	1.160(34)	3/2+	2.3(6)	1.9(6)	
E	1.219(22)	3/2-	21(3)	0.1(1)	
F	1.335(6)	3/2+	65(8)	26(4)	-
G	1.455(38)	1/2+	55(12)	347(92)	
H	1.571(13)	5/2+	1.7(4)	12(3)	

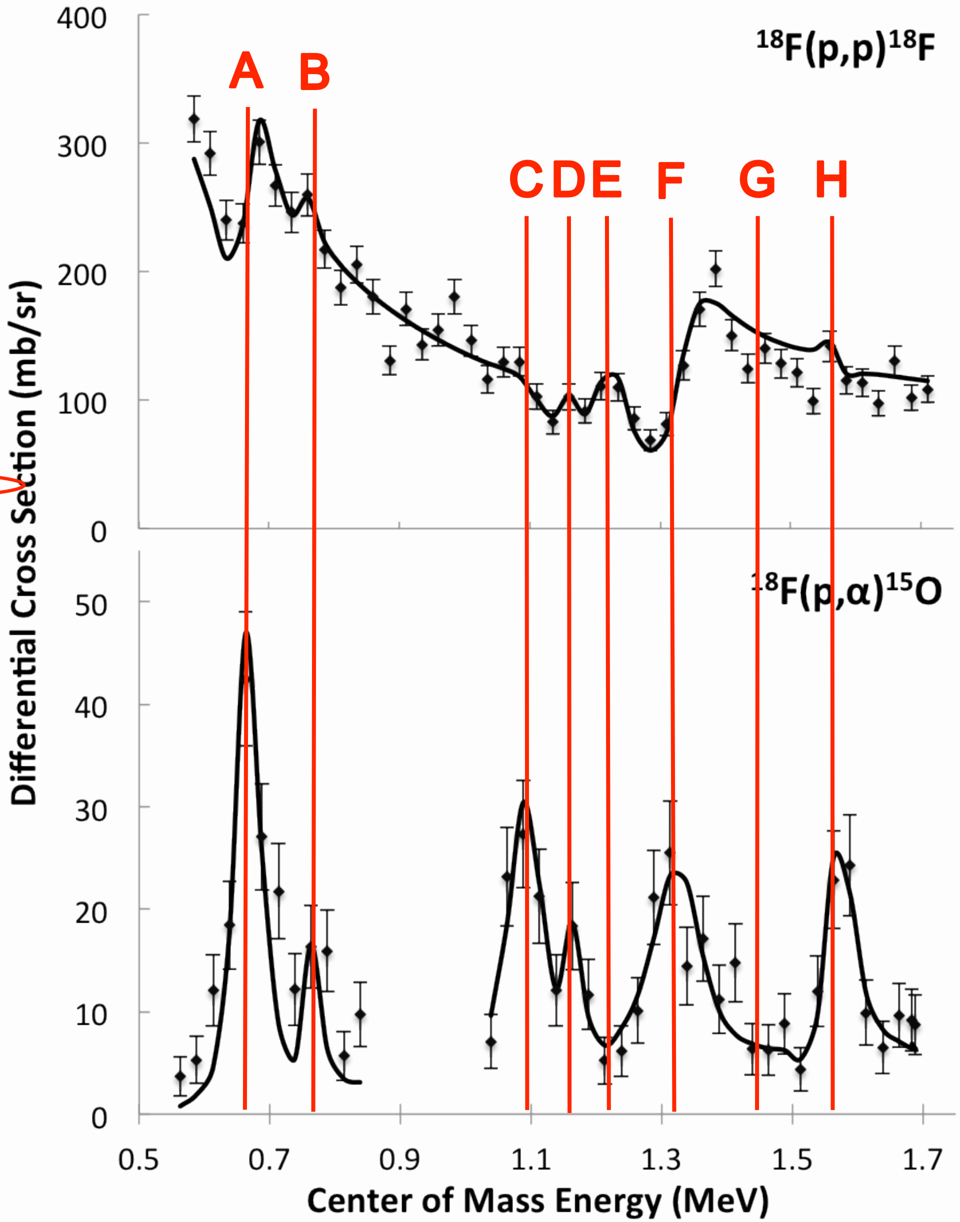
- Descouvemont state?
- Stay tuned…



Preliminary Results (H)

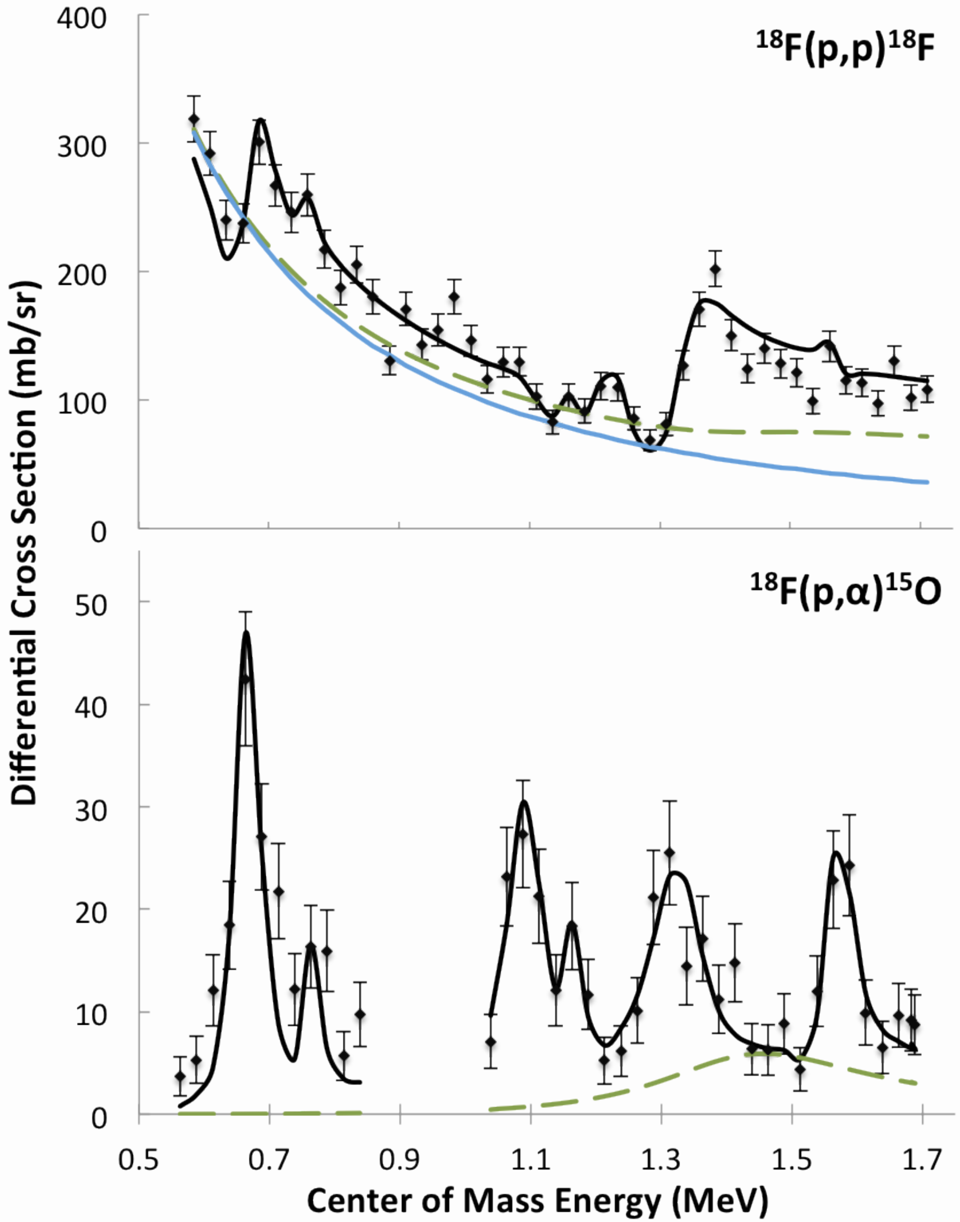
	Ecm (MeV)	Jπ	Γp(keV)	Γα(keV)	Int
A	0.665	3/2+	15	24	+
B	0.759(20)	3/2+	1.6(5)	2.4(6)	
C	1.096(11)	5/2+	3(1)	54(12)	
D	1.160(34)	3/2+	2.3(6)	1.9(6)	
E	1.219(22)	3/2-	21(3)	0.1(1)	
F	1.335(6)	3/2+	65(8)	26(4)	-
G	1.455(38)	1/2+	55(12)	347(92)	
H	1.571(13)	5/2+	1.7(4)	12(3)	

- Observed by Dalouzy (alternative π) and Murphy (alternative J)
- Dalouzy J unambiguous but π inferred
- Current data strongly favours $J^{\pi}=5/2^{+}$ at consistent strengths



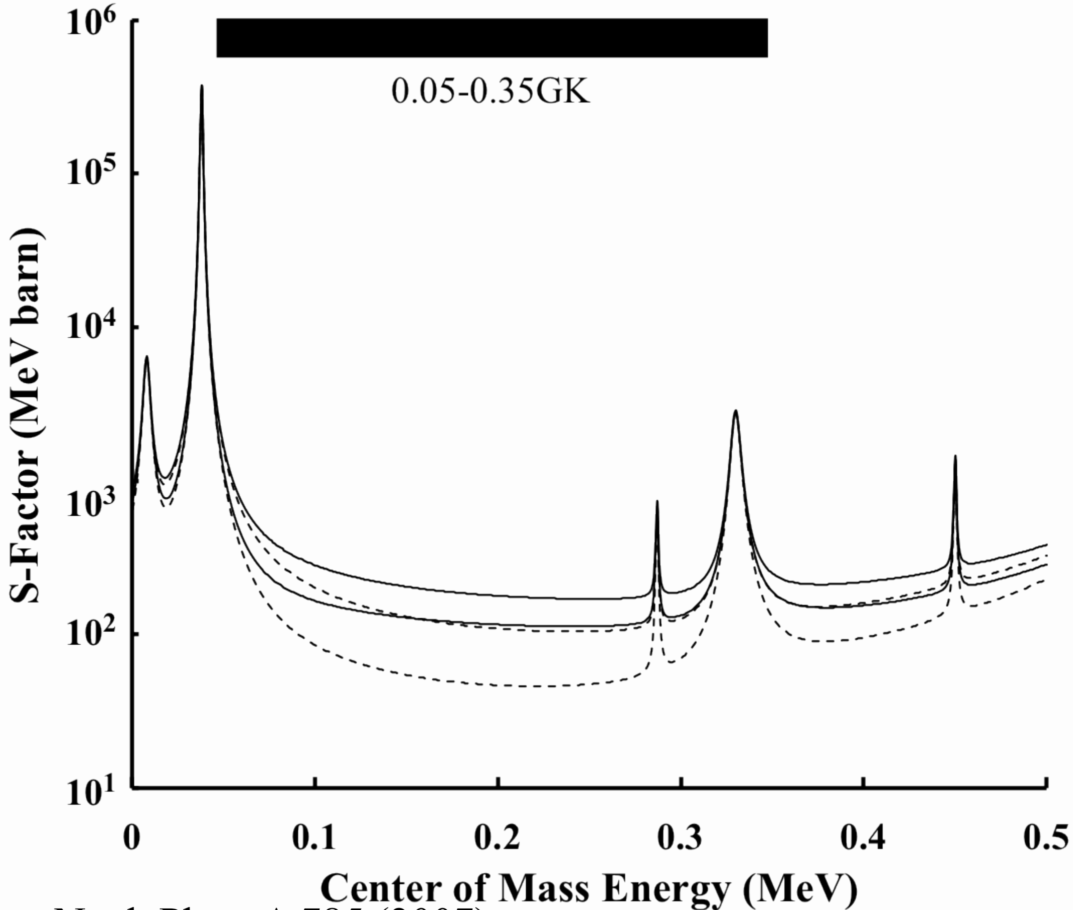
Dufour/Descouvemont State??

- Candidate state observed at E_{CM}=1.455MeV (G)
- More than a factor of 2 *narrower* than predicted in proton channel
- More than a factor of 2 *broader* than predicted in alpha channel
- But consistent in total width (402(93)keV) with Dalouzy (292(107)keV
- Broad state **is required** to fit to data



Impact: Enhanced S-Factor

- Low energy and sub-threshold parameters as in [3]
- Enhanced by prediction of [2]

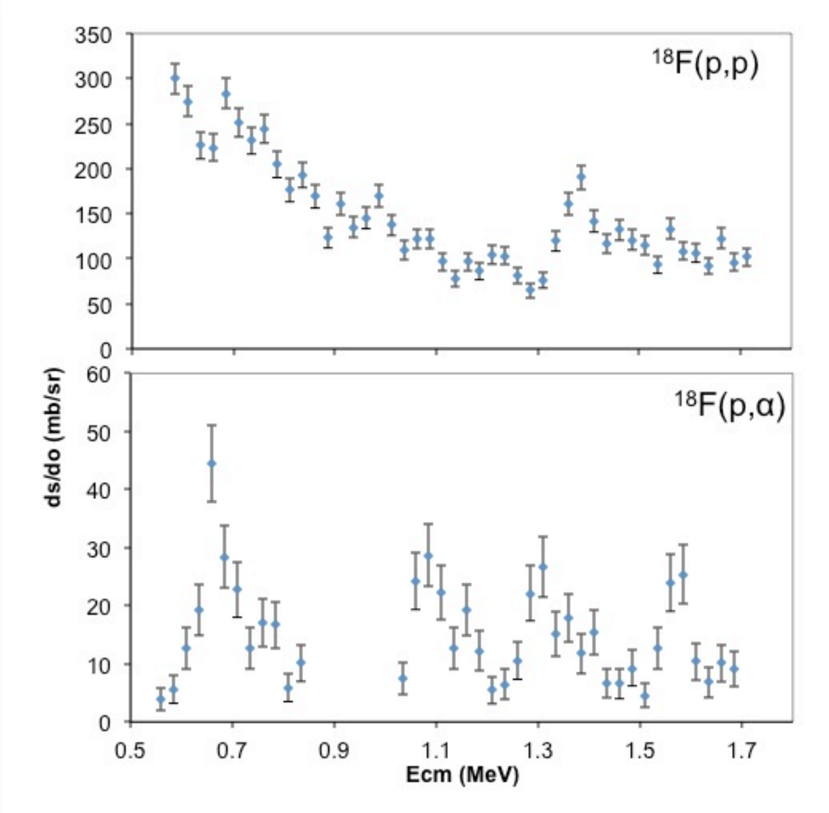


[2] Dufour/Descouvement, Nucl. Phys. A 785 (2007)
[3] Iliadis *et al.*, Nucl. Phys. A 841, 251 (2010)

A bit more about the fitting…

Problems

- Many parameter fit
- 10 x statistics in (p,p) channel compared to (p,α)
- Changing energy resolution



Solutions…

Energy Resolution

- Monte Carlo to estimate energy resolution
- dE(E) in (some) R-Matrix code

Complexity

- Iterative analysis
  - Literature values
  - Trial and error (by eye adjustments)
  - Fitting single resonances
  - Fitting multiple resonances
  - Fitting multiple channels
  - Fitting entire data set

Statistics

- Play God
  - Initially adjust error bars to change weightings
  - Make active use of error matrix (covariance)

Include additional contributions to final error bars!

Co-variance

TABLE II. Covariance matrix for all parameters allowed to vary in the fitting process.

B			C			D			E			F			G			H			Par.	
$E_{c.m.}$	Γ_p	Γ_α	$E_{c.m.}$	Γ_p	Γ_α	$E_{c.m.}$	Γ_p	Γ_α	$E_{c.m.}$	Γ_p	Γ_α	$E_{c.m.}$	Γ_p	Γ_α	$E_{c.m.}$	Γ_p	Γ_α	$E_{c.m.}$	Γ_p	Γ_α		
1	−0.51	0.99	0	0	0	0	0	0	0	0	0	0	0.02	0.02	−0.01	0.01	0	0	0	0	$E_{c.m.}$	B
	1	−0.51	0.01	0.03	0	0	0	0	−0.01	0.07	−0.02	0	−0.08	0.01	0	−0.03	0.04	0	0	0	Γ_p	
		1	0	0.01	0.01	0	0	0.01	0	0.01	0.01	−0.02	0.03	0.03	−0.02	0.01	0.02	0	0	0	Γ_α	
			1	0.14	0.03	0.05	0.02	0.05	−0.02	0.01	0.50	−0.01	0.01	0.04	0.12	−0.14	0.02	−0.01	−0.02	−0.01	$E_{c.m.}$	C
				1	−0.27	0.08	−0.02	0.07	−0.09	−0.05	−0.11	0.02	0.01	0.07	−0.27	0.21	0.25	0.09	0.05	0.11	Γ_p	
					1	0.02	0.13	0.07	−0.01	−0.02	−0.05	−0.02	0.06	0.07	0.10	0.21	−0.25	0.12	0.11	0.22	Γ_α	
						1	−0.78	0.99	−0.02	0.02	0.10	−0.03	0.08	0.08	−0.07	0.05	0.01	0	0	0	$E_{c.m.}$	D
							1	−0.71	−0.04	0.15	0.07	−0.01	−0.04	0.02	0.02	−0.05	0.05	0	0	−0.01	Γ_p	
								1	−0.01	0.02	0.17	−0.08	0.13	0.12	−0.07	0.03	0.03	0	−0.01	−0.01	Γ_α	
									1	−0.11	0.11	−0.02	0.04	0.04	−0.13	0.03	0.10	0	0.01	0	$E_{c.m.}$	E
										1	−0.29	0.01	−0.42	0.07	−0.13	0.03	0.06	0	0	−0.01	Γ_p	
											1	−0.08	0.24	0.18	0.02	−0.46	0.27	−0.13	−0.20	−0.34	Γ_α	
												1	−0.50	0.17	0.04	0.08	−0.22	0	0	0	$E_{c.m.}$	F
													1	−0.02	−0.23	0.18	−0.08	−0.01	0.02	0.02	Γ_p	
														1	−0.56	0.33	−0.08	−0.01	0.03	0.01	Γ_α	
															1	−0.33	0	−0.33	0.22	0.19	$E_{c.m.}$	G
																1	−0.69	−0.19	0.53	0.60	Γ_p	
																	1	0.03	−0.41	−0.51	Γ_α	
																		1	−0.63	−0.39	$E_{c.m.}$	H
																			1	0.93	Γ_p	
																				1	Γ_α	

Alternative R-Matrix Implementation: AZURE

- Generally available code from JINA
- No limit to number of channels

$$\frac{d\sigma}{d\Omega} \propto \left| U_J U_{J'}^{*} \right|$$

PHYSICAL REVIEW C **81**, 045805 (2010)

AZURE: An *R*-matrix code for nuclear astrophysics

R. E. Azuma,[1,2] E. Uberseder,[2,*] E. C. Simpson,[2,3] C. R. Brune,[4] H. Costantini,[2,5] R. J. de Boer,[2] J. Görres,[2] M. Heil,[6] P. J. LeBlanc,[2] C. Ugalde,[2,†] and M. Wiescher[2]

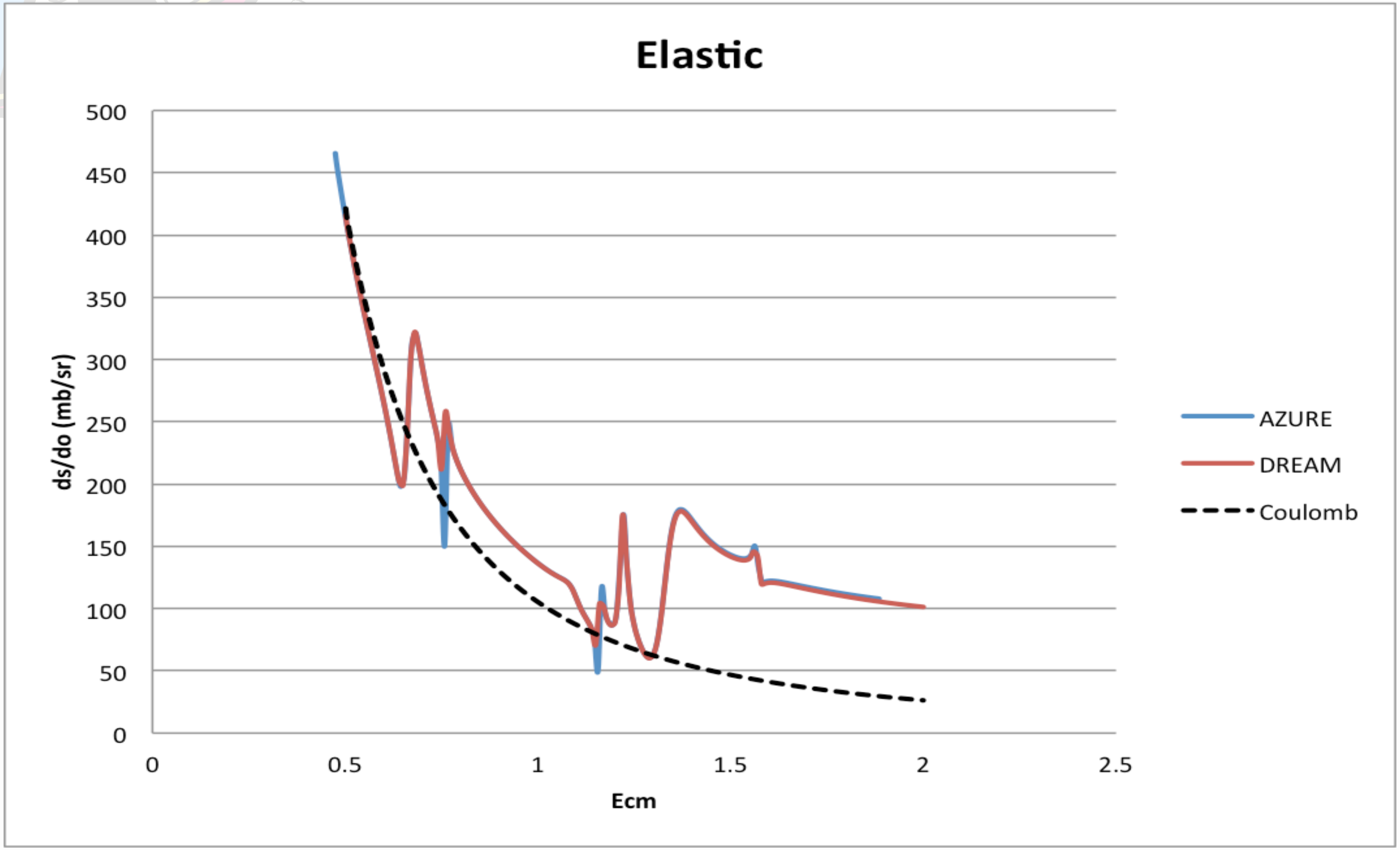
[1]*Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada*
[2]*University of Notre Dame, Department of Physics, Notre Dame, Indiana 46556, USA*
[3]*Department of Physics, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford, Surrey GU2 7XH, United Kingdom*
[4]*Department of Physics and Astronomy, Ohio University, Ohio 45701, USA*
[5]*Istituto Nazionale Fisica Nucleare (INFN), Genova, Italy*
[6]*GSI Darmstadt, Planckstr. 1, 64291 Darmstadt, Germany*
(Received 11 January 2010; published 26 April 2010)

The paper describes a multilevel, multichannel *R*-matrix code, AZURE, for applications in nuclear astrophysics. The code allows simultaneous analysis and extrapolation of low-energy particle scattering, capture, and reaction cross sections of relevance to stellar hydrogen, helium, and carbon burning. The paper presents a summary of *R*-matrix theory, code description, and a number of applications to demonstrate the applicability and versatility of AZURE.

DOI: 10.1103/PhysRevC.81.045805 PACS number(s): 26.20.Cd, 25.40.Lw, 24.10.−i

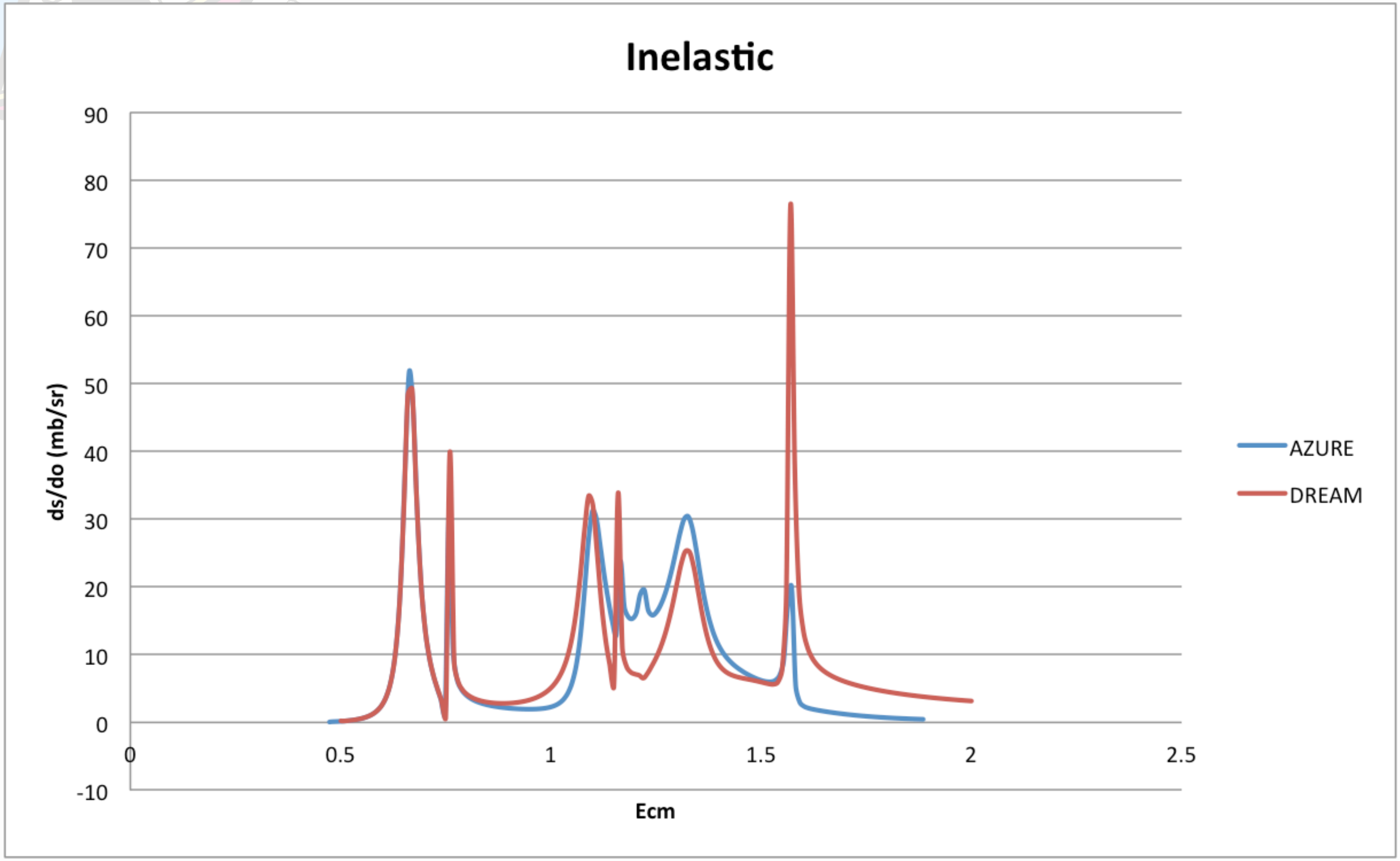
R-Matrix Comparison

- Same parameters in each code:



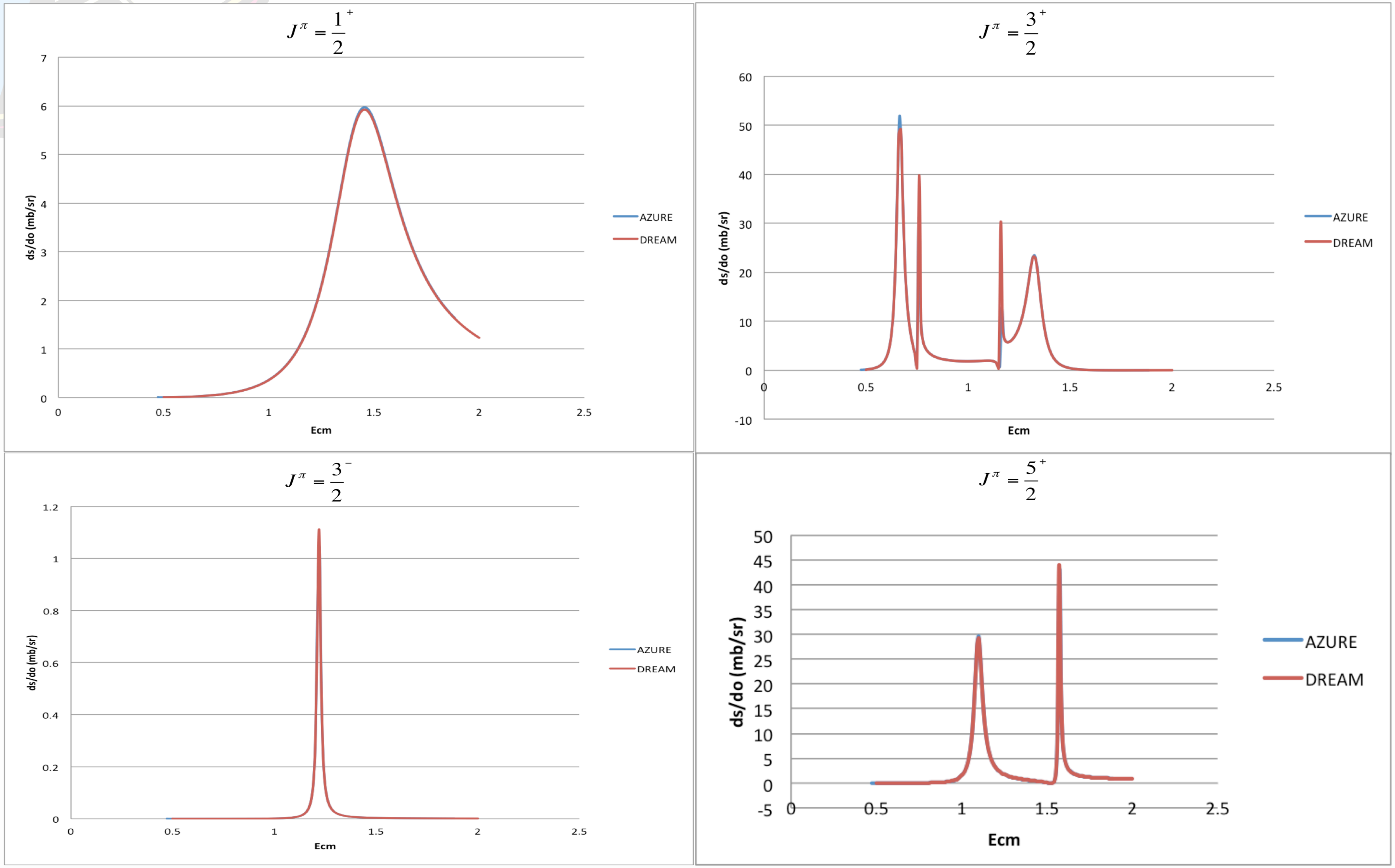
R-Matrix Comparison

- Same parameters in each code:



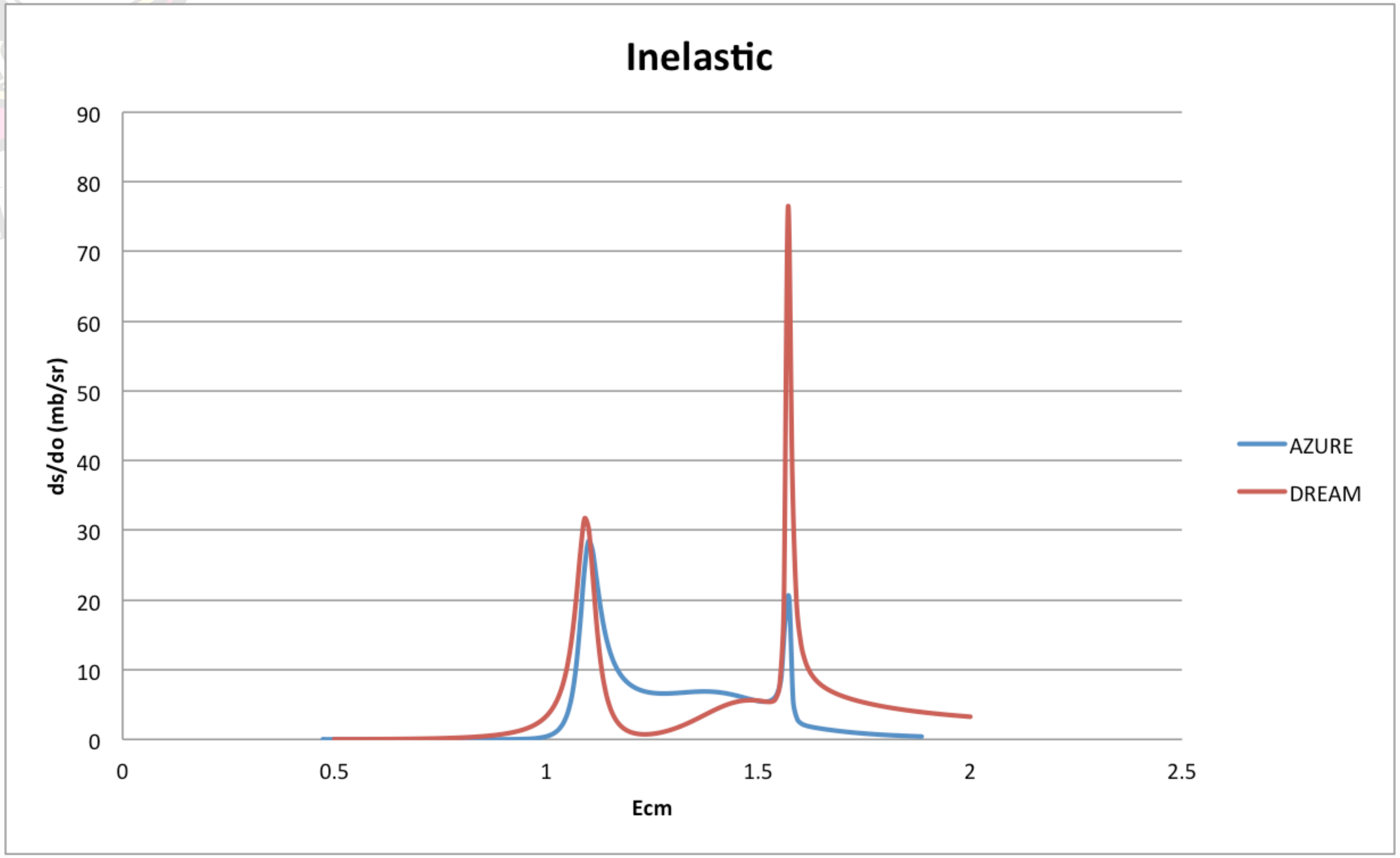
R-Matrix Comparison

- Individual J^{π} groups:



R-Matrix Comparison

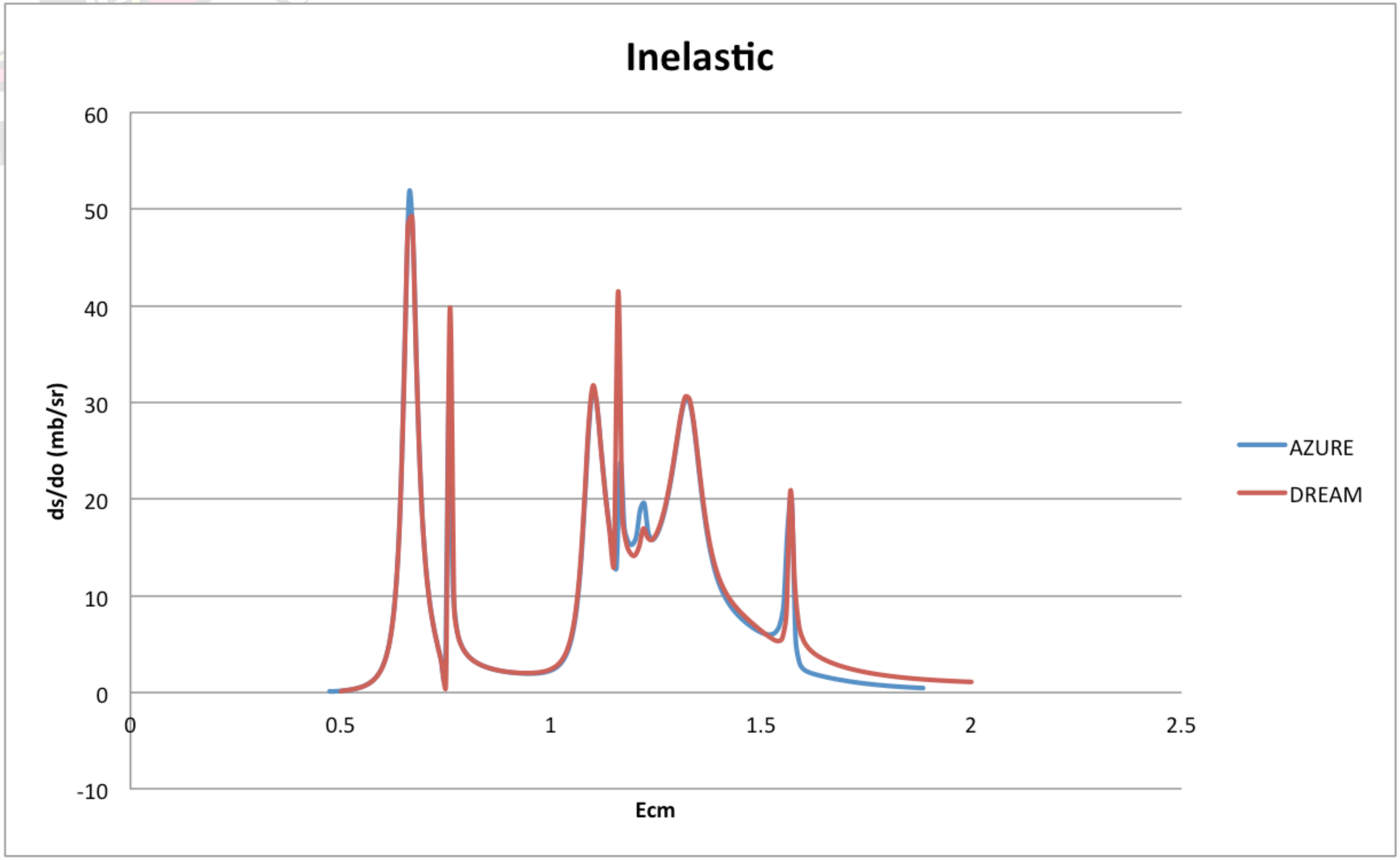
- Combining $1/2^+$ and $5/2^+$:



- Opposite interference between groups
- Discrepancy is not in angular coupling coefficients

R-Matrix Comparison

- Discrepancy arises in use of arctan to calculate δ's, alternative interference:



R-Matrix Comparison

Mountford et al [6] E_{CM} (MeV)	J^π	Γ_p (keV)	Γ_α (keV)	AZURE Results E_{CM} (MeV)	Γ_p (keV)	Γ_α (keV)
0.665	$\frac{3}{2}^+$	15.2	23.8	0.665	15.2	23.8
0.759(20)	$\frac{3}{2}^+$	1.6(5)	2.4(6)	0.755(77)	1.7(17)	3.3(33)
1.096(11)	$\frac{5}{2}^+$	3(1)	54(12)	1.097(29)	3.3(20)	71(45)
1.160(34)	$\frac{3}{2}^+$	2.3(6)	1.9(6)	1.149(14)	2.5(25)	2.1(21)
1.219(22)	$\frac{3}{2}^-$	21(3)	0.1(1)	1.211(17)	27(17)	0.2(2)
1.335(6)	$\frac{3}{2}^+$	65(8)	26(4)	1.339(23)	65(13)	31(27)
1.455(38)	$\frac{1}{2}^+$	55(12)	347(92)	1.498(176)	44(23)	313(147)
1.571(13)	$\frac{5}{2}^+$	1.7(4)	12(3)	1.569(30)	1.7(12)	8(6)

Conclusions

- R-matrix formalism extremely useful for extracting resonance parameters for astrophysical reactions

- New data obtained in study of astrophysically important $^{18}F(p,\alpha)^{15}O$ reaction

- Analysis, aided by R-Matrix calculations, finds candidate for newly proposed s-wave state

Enhanced rate of ^{18}F destruction → less ^{18}F → detectability distance reduced

Collaborators

D. J. Mountford, T. Davinson, P. J. Woods (University of Edinburgh),
A. Laird, J. R. Brown (University of York), N. de Sereville (Orsay),
C. Angulo (Tractebel Engineering), N. L. Achouri (LPC Caen),
F. de Oliveira, P. Ujic, O. Kamalou (GANIL), S. T. Pittman (ORNL),
P.Descouvemont (Universite Libre de Bruxelles),
M. Wiescher, E. Uberseder and R. J. deBoer (University of Notre Dame)

Thank You