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ICTP 40th Anniversary

SMR.1555 - 30

**Workshop on
Nuclear Reaction Data and Nuclear Reactors:
Physics, Design and Safety**

16 February - 12 March 2004

Further on SAMMY (II)

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These are preliminary lecture notes, intended only for distribution to participants

SAMMY Workshop

Workshop on Nuclear Reaction Data and Nuclear
Reactors: Physics, Design and Safety

(16 February - 12 March 2004)

Dr. Nancy M. Larson
Oak Ridge National Laboratory

Part 4.1a, comment on Reich Moore

Reich-Moore Approximation to Multilevel Multi-Channel R-Matrix Theory

F. H. Fröhner, “Evaluation and Analysis of Nuclear Resonance Data,” JEFF Report 18 (2000), page 60:

“Experience has shown that with this approximation [Reich Moore] all resonance cross section data can be described in detail, in the windows as well as in the peaks, even the weirdest multilevel interference patterns ... It works equally well for light, medium-mass and heavy nuclei, fissile and nonfissile.”

When does Reich-Moore *not* work ?

- For direct effects

(R-matrix is a description of *compound* nucleus effects.)

– for example $^{37}\text{Cl}(n,?)$

- “R-Matrix Evaluation of Cl Neutron Cross Sections up to 1.2 MeV”

Sayer, Guber, Leal, Larson, and Rauscher, ORNL/TM-2003/50, March 2003

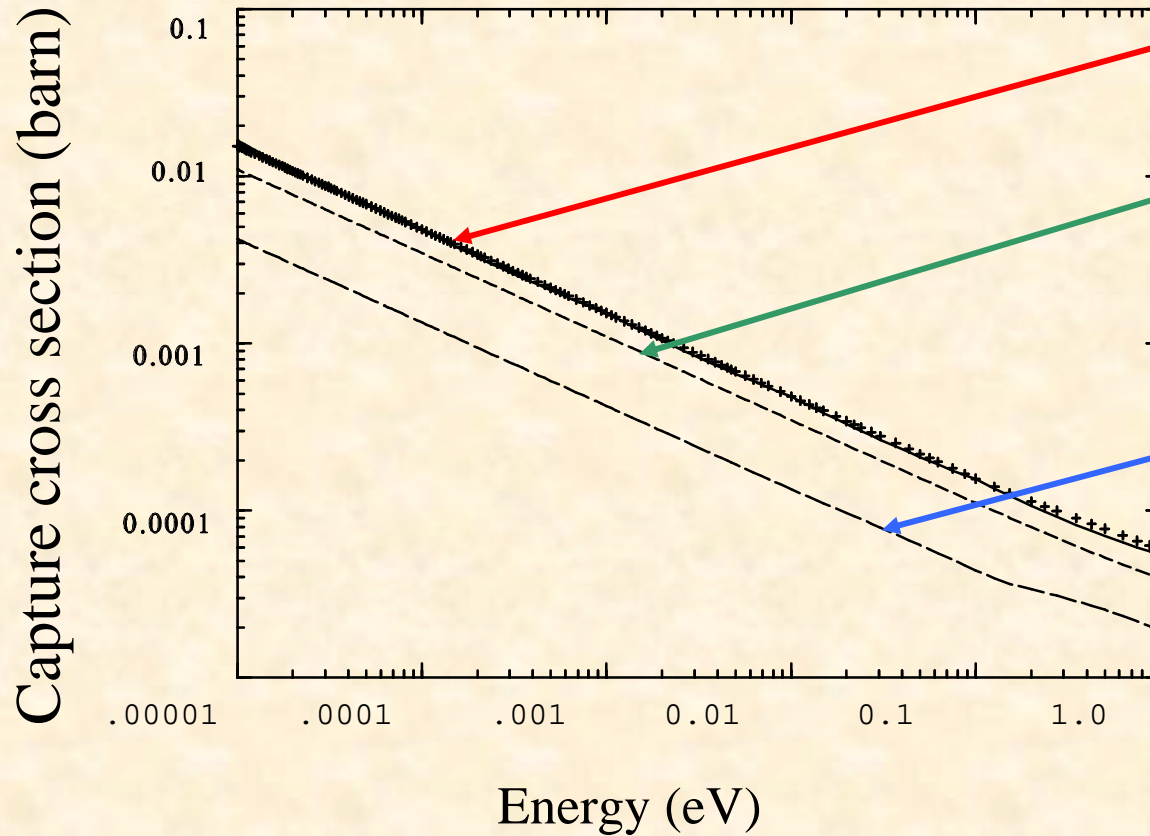
- Direct effects must be added explicitly

- New options are now available in SAMMY for fitting the magnitude of direct capture component

Example: ^{19}F

- **Model calculations by Goran Arbanas, ORNL**
- **Analysis by Luiz Leal, ORNL**
 - **Multiplier initially at 1.0, fitted to 0.547**

^{19}F , continued



+ = data

dash = R-matrix contribution

long dash = direct component

solid line = sum of the two components

When does Reich-Moore *not* work ?

(continued)

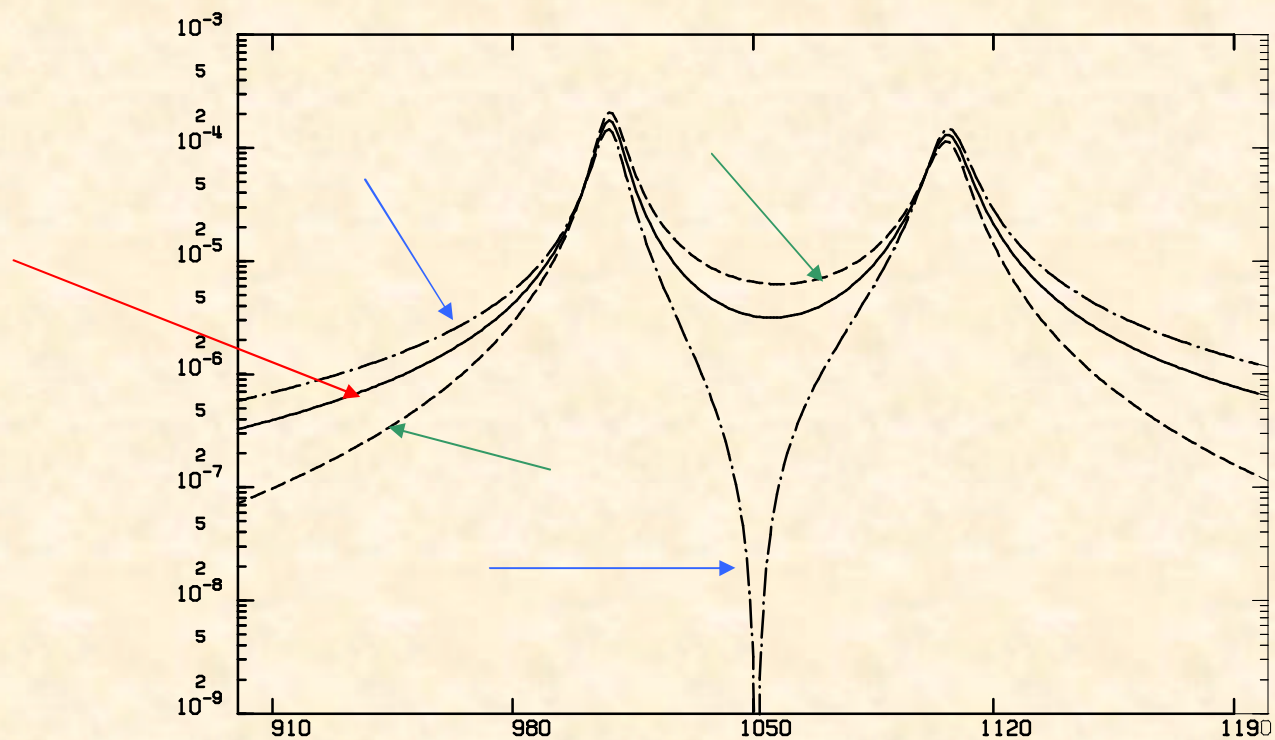
- **When trying to describe interference effects in reactions like**

- $^{12}\text{C}(\alpha,?)$
- $^{15}\text{N}(\text{p},?)$
- $^{21}\text{Ne}(\text{p},?)$
- $^{22}\text{Ne}(\text{n},?)$

when there is level-level interference in the capture channel
because capture is treated “on average” in Reich-Moore approximation

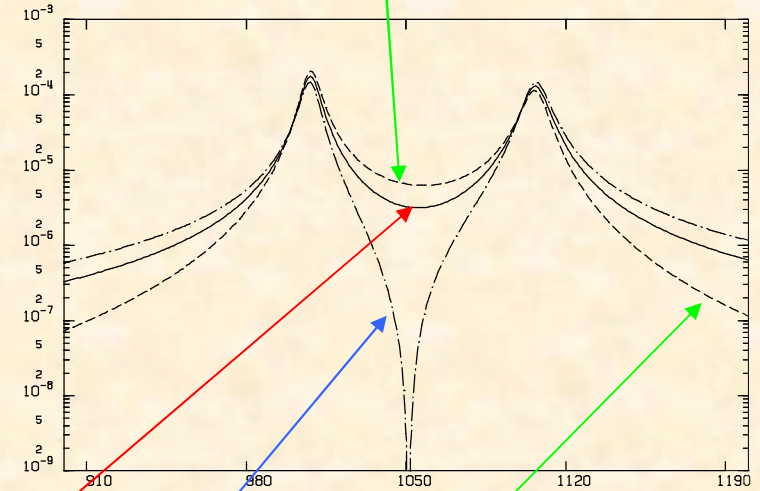
- re Michael Heil, Karlsruhe

- Artificial example is shown on next slide



- Solid line = Reich Moore
- Dot-dash = full R-matrix # 1
- Dash = full R-matrix # 2

Note: can use Reich-Moore to approximate the full R-matrix



	Energy (MeV)	G_2 (eV)	G_n (eV)	G_{react} (eV)
Reich Moore	1.0	1.0	10 000	
	1.1	1.1	11 000	
fake full R-matrix # 1	1.0	10^{-8}	10 000	1.0
	1.1	10^{-8}	11 000	1.1
fake full R-matrix # 2	1.0	10^{-8}	10 000	1.0
	1.1	10^{-8}	11 000	-1.1

**Comparisons with true
R-matrix codes have
shown that this works
well**

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Part 4.1b. Spin group assignments

Problem

- **How to define appropriate spin groups when “starting from scratch”?**
- **Program SAMQUA can help you generate spin groups and channel information in SAMMY-INPut-file format**
 - **SAMQUA is distributed with SAMMY code**
 - **written by Olivier Bouland, Richard Babut, and Nancy Larson**
 - **“SAMQUA - A Program for Generating All Possible Combinations of Quantum Numbers Leading to the Same Compound Nucleus State in the Framework of the R-matrix Code SAMMY,” Olivier Bouland, Richard Babut (Laboratoire d'Etudes de Physique, CEA/Cadarache, France), and Nancy M. Larson; JEFDOC 929 OECD/NEA Publications and ENDF-363 (October 2003).**
- **Nevertheless you should learn how to do this yourself in order to understand what’s going on!**

Notation

- Incident channels:
 - incident particle: spin i and parity p
 - target particle: spin I and parity ?
 - possible channel spins are $|I - i| = s = I + I$
 - orbital angular momentum is l
- Exit channels:
 - first particle: spin i' and parity p'
 - target particle: spin I' and parity ?
 - possible channel spins are $|I' - i'| = s' = I' + I'$
 - orbital angular momentum is l'
- For each l and l' ,
 - figure possible J -parity values for incident channels
 - figure possible J -parity values for exit channels
- Channels with same J -parity are in same spin group

Example: spin groups for $^{14}\text{N}(a,n)^{17}\text{F}$

$$a: \quad i p = 0 +$$

$$^{14}\text{N}: \quad I ? = 1 +$$

$$n: \quad i p = 1/2 +$$

$$^{17}\text{F}: \quad I ? = 5/2 +$$

Step 1: tabulate all possible channels (for a given max l), perhaps on a spread sheet

	i	I	s	l	J
1	0+	1+	1+	0+	1+
2				1-	0-
3					1-
4					2-
5				2+	1+
6					2+
7					3+
8	1/2+	5/2+	2+	0+	2+
9				1-	1-
10					2-
11					3-
12				2+	0+
13					1+
14					2+
15					3+
16					4+
17			3+	0+	3+
18				1-	2-
19					3-
20					4-
21				2+	1+
22					2+
23					3+
24					4+
25					5+

Entrance channels

Exit channels

Example, continued

Step 2: fill in the blanks on the spread sheet

	<i>i</i>	<i>I</i>	<i>s</i>	<i>l</i>	<i>J</i>
1	0+	1+	1+	0+	1+
2	0+	1+	1+	1-	0-
3	0+	1+	1+	1-	1-
4	0+	1+	1+	1-	2-
5	0+	1+	1+	2+	1+
6	0+	1+	1+	2+	2+
7	0+	1+	1+	2+	3+
8	1/2+	5/2+	2+	0+	2+
9	1/2+	5/2+	2+	1-	1-
10	1/2+	5/2+	2+	1-	2-
11	1/2+	5/2+	2+	1-	3-
12	1/2+	5/2+	2+	2+	0+
13	1/2+	5/2+	2+	2+	1+
14	1/2+	5/2+	2+	2+	2+
15	1/2+	5/2+	2+	2+	3+
16	1/2+	5/2+	2+	2+	4+
17	1/2+	5/2+	3+	0+	3+
18	1/2+	5/2+	3+	1-	2-
19	1/2+	5/2+	3+	1-	3-
20	1/2+	5/2+	3+	1-	4-
21	1/2+	5/2+	3+	2+	1+
22	1/2+	5/2+	3+	2+	2+
23	1/2+	5/2+	3+	2+	3+
24	1/2+	5/2+	3+	2+	4+
25	1/2+	5/2+	3+	2+	5+

Example, continued

Step 3: Reorder by $J p$; assign spin-group numbers and channel numbers

Question: Why are some states not assigned to a spin group?

$$a: \quad i p = 0 +$$

$$^{14}\text{N}: \quad I ? = 1 +$$

$$n: \quad i p = 1/2 +$$

$$^{17}\text{F}: \quad I ? = 5/2 +$$

	i	I	s	l	J	sg#	ch#
2	0+	1+	1+	1-	0-	1	1
12	1/2+	5/2+	2+	2+	0+		
3	0+	1+	1+	1-	1-	2	1
9	1/2+	5/2+	2+	1-	1-	2	2
1	0+	1+	1+	0+	1+	3	1
5	0+	1+	1+	2+	1+	3	2
13	1/2+	5/2+	2+	2+	1+	3	3
21	1/2+	5/2+	3+	2+	1+	3	4
4	0+	1+	1+	1-	2-	4	1
10	1/2+	5/2+	2+	1-	2-	4	2
18	1/2+	5/2+	3+	1-	2-	4	3
6	0+	1+	1+	2+	2+	5	1
8	1/2+	5/2+	2+	0+	2+	5	2
14	1/2+	5/2+	2+	2+	2+	5	3
22	1/2+	5/2+	3+	2+	2+	5	4
11	1/2+	5/2+	2+	1-	3-		
19	1/2+	5/2+	3+	1-	3-		
7	0+	1+	1+	2+	3+	6	1
15	1/2+	5/2+	2+	2+	3+	6	2
17	1/2+	5/2+	3+	0+	3+	6	3
23	1/2+	5/2+	3+	2+	3+	6	4
20	1/2+	5/2+	3+	1-	4-		
16	1/2+	5/2+	2+	2+	4+		
24	1/2+	5/2+	3+	2+	4+		
25	1/2+	5/2+	3+	2+	5+		

Example, continued

Step 4: Construct the SAMMY INPut file

Legend:

a = spin group number
b = how many entrance channels
c = how many exit channels
d = channel number
e = 1 if penetrabilities are non-unity
f = 1 if shift factor is non-zero

p J = parity, spin
z = charge for smaller particle
Z = charge for larger particle
L = orbital angular momentum
s = channel spin

a	d	z	e	Z	f	pJ	L	s
1			1		0	-0.0		
	1	2	1	7	0		1	+1.0
2			1		1	-1.0		
	1	2	1	7	0		1	+1.0
	2		1		0		1	+2.0
3			2		2	+1.0		
	1	2	1	7	0		0	+1.0
	2	2	1	7	0		2	+1.0
	3		1		0		2	+2.0
	4		1		0		2	+3.0
4			1		2	-2.0		
	1	2	1	7	0		1	+1.0
	2		1		0		1	+2.0
	3		1		0		1	+3.0
5			1		3	+2.0		
	1	2	1	7	0		2	+1.0
	2		1		0		0	+2.0
	3		1		0		2	+2.0
	4		1		0		2	+3.0
6			1		3	+3.0		
	1	2	1	7	0		2	+1.0
	2		1		0		0	+3.0
	3		1		0		2	+2.0
	4		1		0		2	+3.0

Exercises for the student

- **Assume you need higher l values for the $\alpha + {}^{14}\text{N}$ case described above. Generate the spin group information in this situation.**
- **What are the appropriate spin groups and channels for $n + {}^{16}\text{O}$, assuming your measurements go above the (n,α) threshold?**
- **Extend to include inelastic channels.**

New format options for INPut file

- **Problem:** formats for INPut file are becoming unwieldy due to options not originally available
 - outgoing channel particles have different masses and quantum numbers from incident channel particles
 - charge must be specified
 - threshold and radii must be given
- **Solution:** reorganize and simplify
 - specify the two particles (charge, spin, mass, threshold) independent of spin group definition; provide a label to pair
 - channel definition gives l and s plus pair-label

Example: t100a.inp – the “old” version

```
170(alpha,n)20Ne fit (R. BABUT 03-13-2001) vs BAIR data (Phys. Rev. C 7,4,1973)
O17      16.99913    2000000.0 5500000.0      2  100
```

```
csisrs
```

```
spin of incident particle is +0.0
```

```
use new spin group format
```

```
cm coulomb excitation energies
```

```
cm non coulomb excitation energies
```

```
broadening is not wanted
```

```
5.00000  1.000
```

```
REACTION CROSS SECTION
```

```
2.5
```

```
1      1      1 -0.5  1.000  2.5      170
      1  2  1  8  0      3  2.5      0.0
      2      1      0      1  0.5      0.0      -588708.  3.8003.800  19.992436  1.0086649
2      1      1  0.5  1.000  2.5      170
      1  2  1  8  0      2  2.5      0.0
      2      1      0      0  0.5      0.0      -588708.  3.8003.800  19.992436  1.0086649
3      2      1 -1.5  1.000  2.5      170
      1  2  1  8  0      1  2.5      0.0
      2  2  1  8  0      3  2.5      0.0
      3      1      0      1  0.5      0.0      -588708.  3.8003.800  19.992436  1.0086649
4      2      1  1.5  1.000  2.5      170
      1  2  1  8  0      2  2.5      0.0
```

```
...
```

```

...
  2  2  1  8  0    4  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  3    1    0    2  0.5    0.0    -588708.  3.8003.800  19.992436  1.0086649
  5    3    1 -2.5  1.000  2.5    170
  1  2  1  8  0    1  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  2  2  1  8  0    3  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  3  2  1  8  0    5  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  4    1    0    3  0.5    0.0    -588708.  3.8003.800  19.992436  1.0086649
  6    3    1  2.5  1.000  2.5    170
  1  2  1  8  0    0  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  2  2  1  8  0    2  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  3  2  1  8  0    4  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  4    1    0    2  0.5    0.0    -588708.  3.8003.800  19.992436  1.0086649
  7    3    1 -3.5  1.000  2.5    170
  1  2  1  8  0    1  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  2  2  1  8  0    3  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  3  2  1  8  0    5  2.5    0.0          0  5.00  5.00  16.99913  4.0026
  4    1    0    3  0.5    0.0    -588708.  3.8003.800  19.992436  1.0086649

```

... [incomplete]

t100b.inp - the "new" version

17O(alpha,n)20Ne fit (R. BABUT 03-13-2001) vs BAIR data (Phys. Rev. C 7,4,1973)
 O17 16.99913 2000000.0 5500000.0 2 100

csisrs

spin of incident particle is +0.0
 cm coulomb excitation energies
 cm non coulomb excitation energies
 broadening is not wanted
 particle-pair definitions are given

Comments (between lines)

 a = default for incident, b = def for target

u = Lpent (1 or 0), v = Ishift (0 or 1)

name	a	b	z	Zuv	i	I	m	M Threshold	Reff	Rtru
------	---	---	---	-----	---	---	---	-------------	------	------

alf+17O		2	810	0.0	2.5	4.0026000	16.999130		5.0000000	5.0000000
n+20Ne	n	0	1010	0.5	0.0	1.	19.992436	-588708.0	3.8000000	3.8000000

5.00000 1.000
 REACTION CROSS SECTION

1	1	1	-0.5	1.000	2.5	170
1	alf+17O	3	2.5			
2	n+20Ne	1	0.5			
2	1	1	0.5	1.000	2.5	170
1	alf+17O	2	2.5			
2	n+20Ne	0	0.5			
3	2	1	-1.5	1.000	2.5	170

Information about the two particle pair sets

Spin groups then refer to particle-pair information

```

...
1  alf+17O      1  2.5
   2  alf+17O      3  2.5
   3  n+20Ne      1  0.5
4   2      1  1.5  1.000  2.5      170
   1  alf+17O      2  2.5
   2  alf+17O      4  2.5
   3  n+20Ne      2  0.5
5   3      1 -2.5  1.000  2.5      170
   1  alf+17O      1  2.5
   2  alf+17O      3  2.5
   3  alf+17O      5  2.5
   4  n+20Ne      3  0.5
6   3      1  2.5  1.000  2.5      170
   1  alf+17O      0  2.5
   2  alf+17O      2  2.5
   3  alf+17O      4  2.5
   4  n+20Ne      2  0.5
7   3      1 -3.5  1.000  2.5      170
   1  alf+17O      1  2.5
   2  alf+17O      3  2.5
   3  alf+17O      5  2.5
   4  n+20Ne      3  0.5

```

[... incomplete]

t100by.inp – the “newest” version

17O(alpha,n)20Ne fit (R. BABUT 03-13-2001) vs BAIR data (Phys. Rev. C 7,4,1973)
O17 16.99913 2000000.0 5500000.0 2 100

csisrs

cm coulomb excitation energies

cm non coulomb excitation energies

broadening is not wanted

key-word particle-pair definitions are given

Name = alf+17O

Pa = alpha Pb=170 Zb=8 Sb=2.5 Mb=16.999130

Mass a = 4.0026000000

Name = n+20Ne

pa=n particle b = 20Ne Zb=10 Mass b = 19.992436

Q=588708.0

Key word
particle
pair
definitions

5.00000 1.000
REACTION CROSS SECTION
1 1 1 -0.5 1.000
1 alf+17O 3 2.5
2 n+20Ne 1 0.5
2 1 1 0.5 1.000
1 alf+17O 2 2.5
2 n+20Ne 0 0.5
3 2 1 -1.5 1.000
1 alf+17O 1 2.5
2 alf+17O 3 2.5
3 n+20Ne 1 0.5 ...

...
4 2 1 1.5 1.000
1 alf+17O 2 2.5
2 alf+17O 4 2.5
3 n+20Ne 2 0.5
5 3 1 -2.5 1.000
1 alf+17O 1 2.5
2 alf+17O 3 2.5
3 alf+17O 5 2.5
4 n+20Ne 3 0.5
...
6 3 1 2.5 1.000
1 alf+17O 0 2.5
2 alf+17O 2 2.5
3 alf+17O 4 2.5
4 n+20Ne 2 0.5
7 3 1 -3.5 1.000
1 alf+17O 1 2.5
2 alf+17O 3 2.5
3 alf+17O 5 2.5
4 n+20Ne 3 0.5
[... incomplete]

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Part 4.2, Experimental Conditions

2. Mathematical description of experimental effects

What experimental effects?

Includes all the complexity from being part of the real world:

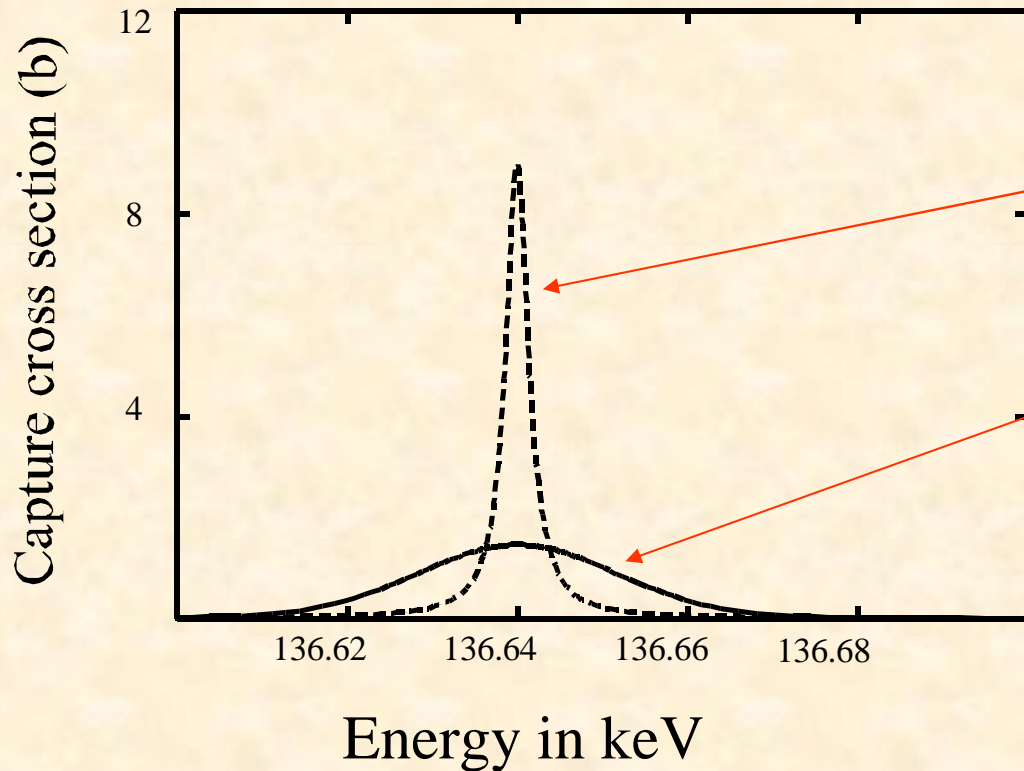
- Many neutrons, not just one
- Many nuclei (sample is finite size)
- Many kinds of nuclei (isotopes, chemical compounds, impurities)
- Nucleus is moving (finite temperature)
- Time is not exact
- Distance is not exact
- Neutron-producing target is finite size
- Detector is finite size
- etcetera

Doppler broadening

Doppler broadening is average over thermal motion of particles in sample.

- **The nuclei in the sample are not sitting still, but are in random thermal motion.**
 - In macroscopic terms, the temperature is not absolute zero.
- **Two options to describe the sample nuclei:**
 - 1. **Crystal lattice model (the sample behaves like a solid).**
 - 2. **Free gas model (the sample behaves a gas).**
- **Option 2 works in most physical situations, even for very heavy nuclei (e.g. lead, uranium).**
 - **The energy of the neutron is so large with respect to the vibrational mode of the Bragg structure, that solid-state effects are unimportant.**

Doppler broadening, continued



Capture cross section for ^{58}Ni without Doppler broadening (dashed curve) and with Doppler broadening at 300 K (solid curve)

Doppler broadening, continued

- **Historically**, codes used *high-energy Gaussian approximation* (HEGA) to the free gas model (FGM) because of its convenient analytical properties:
 - HEGA + Breit-Wigner => psi, chi functions
- **Today**, one should use FGM, never HEGA.
 - There is no penalty for doing so (FGM runs as fast as HEGA)
 - FGM is more accurate, works at all energies
- **Re: “Doppler Broadening Revisited”**
 - N. M. Larson, M. C. Moxon, L. C. Leal, and H. Derrien, ORNL/TM-13525, Oak Ridge National Laboratory, Oak Ridge, TN (1998)

Free gas model (FGM)

- Derivation of equations for FGM of Doppler broadening is available

- Ask for handout (4x2a.pdf)

- Resulting equations:

Not the usual way this is written, but this is the best way to program FGM.

$$\bar{S}\left(\frac{mv^2}{2}\right) = \frac{1}{v^2 u \sqrt{p}} \int_{-\infty}^{\infty} dw w^2 s(w) \exp\left(-\frac{(v-w)^2}{u^2}\right)$$

$$u = \sqrt{\frac{2kT}{M}}$$

$$s(w) = S\left(m(w)^2/2\right) \text{ for } w \geq 0$$

$$= -S\left(m(-w)^2/2\right) \text{ for } w < 0$$

Doppler broadening in SAMMY

[Section numbers refer to SAMMY users' guide]

- via SAMMY's "free gas model" (FGM), **Section IV.B.1**
 - integrations performed numerically using appropriate velocity-grid
 - "velocity" = square root of energy
 - relatively accurate and relatively efficient for all energies, even where there is structure

- via Leal-Hwang (LH), **Section IV.B.2**
 - exact free gas model
 - is solution of partial differential equation having same form as one-dimensional time-dependent heat equation
 - efficient where cross section is smooth

Doppler broadening in SAMMY, cont.

- **via Gaussian (HEGA), Section IV.B.3**
 - high energy approximation
 - integrations performed numerically using energy-grid appropriate for resonance structure
 - use is discouraged !
- **Crystal-lattice model (CLM), Section IV.B.4**
 - may be important for some low-energy cross sections
 - now available in SAMMY
 - based on Dmitri Naberejnev's DOPUSH model
 - Based on Bob MacFarlane's implementation in NJOY
 - integrations performed numerically using velocity-grid appropriate for resonance structure

Doppler broadening in SAMMY, cont.

- Which to use?

- **FGM** → usually

- Requires virtually no more time than HEGA

- LH → only with very smooth cross section

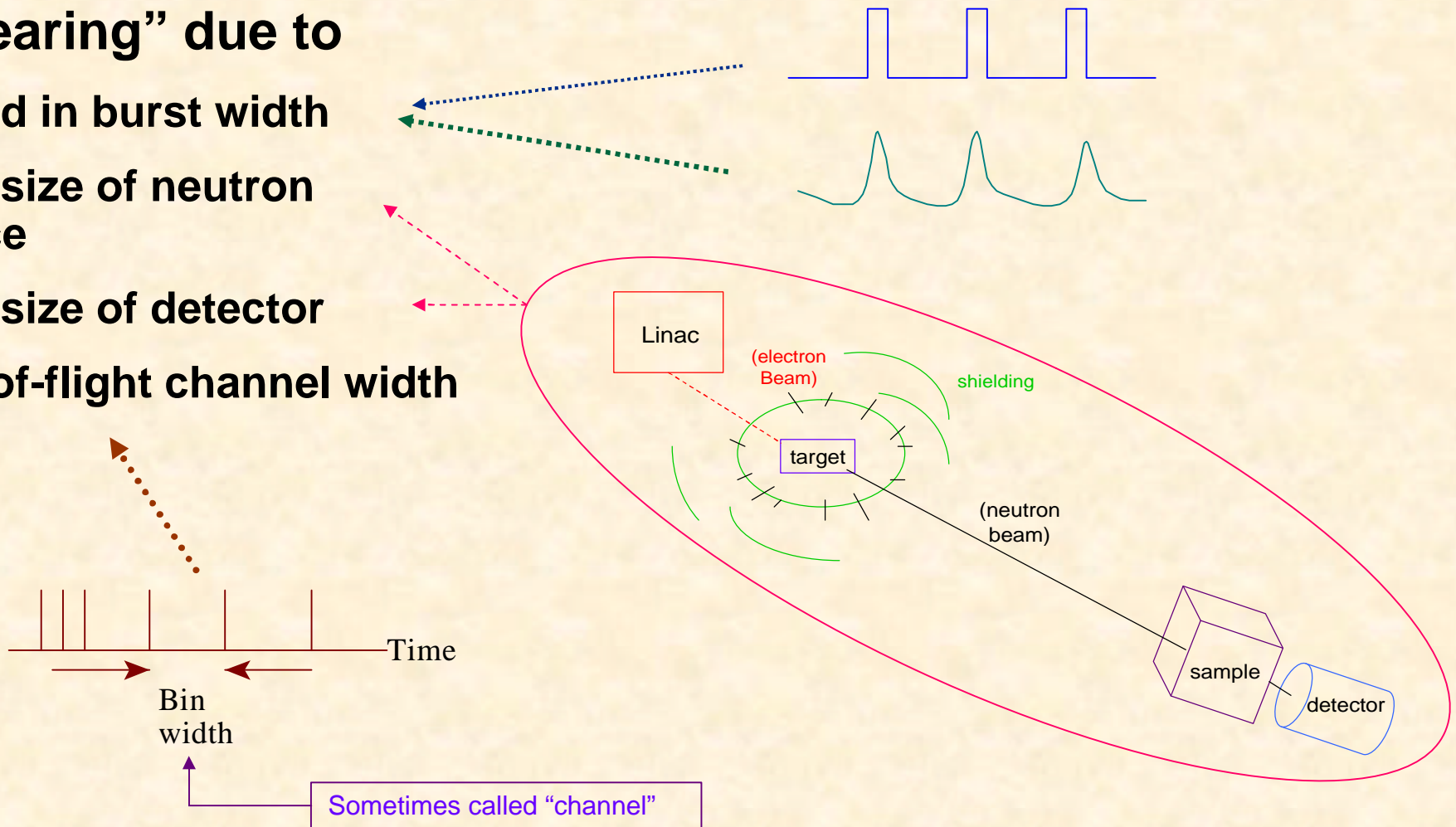
- HEGA → never!

- **CLM** → when solid-state effects are important

- Computer runs take much longer than with FGM

Resolution broadening

- is “smearing” due to
 - spread in burst width
 - finite size of neutron source
 - finite size of detector
 - time-of-flight channel width
 - etc



Resolution broadening, cont.

- Mathematically, this smearing can be described by a resolution-broadening function of the form $R(E,E')$,

$$\bar{s}(E) = \int dE' R(E,E') s(E')$$

written as a function of energy, but could be length or time

- where generally $R(E,E')$ depends only on the energy difference $E - E'$.
- There is no “standard” resolution broadening function.
- SAMMY contains five or six distinct methods. Values for almost all parameters can be fitted to data.

Need to fit the particular machine and the particular experiment.

Analyst picks the general form, SAMMY helps choose parameter values.

Resolution Broadening in SAMMY

- Quick-&-easy version (Gaussian plus exponential tail) (**RSL**)
- Oak Ridge resolution function (**ORR**)
- RPI resolution function (also useful for Geel data) (**RPI**)
- Energy-average from E to E - ? (**DEX**)
- User-Defined Resolution function (**UDR**)
 - [implemented but not fully functional]
- Combinations **RSL** + **DEX** + one of {**ORR**, **RPI**, **UDR**}

Resolution, in more detail

[Section numbers refer to SAMMY users' guide R6]

- **Gaussian and/or exponential (Section IV.C.1)**
 - convolution of Gaussian approximation for three components (path length, burst width, channel width)
 - integrations performed numerically using energy-grid appropriate for resonance structure

the original version, maybe the best one to start with on a new analysis

Resolution, continued

- **Oak Ridge Resolution Function (ORR) (IV.C.2)**
 - analytic convolution (where possible) of four components, with realistic descriptions for all four
 - designed for use with ORELA data
- **RPI Resolution Function (Section IV.C.3)**
 - ditto, designed for use with data from Linac at Rensselaer Polytechnic Institute
 - extension should be useful for data from Geel facility

**“realistic”
resolution
functions**

Resolution, continued

- **Energy-average from E-DE to E (DEX) (IV.C.4)**
 - available in M6-Beta & M6 release of SAMMY code
 - useful for charged-particle work

- **Numerical description (UDR) (IV.C.5)**
 - preliminary version available in M6-Beta & M6 release of SAMMY code, but not yet thoroughly tested and debugged

- **Combination of two or three types types**
 - Gaussian plus DEX plus one of {ORR, RPI, UDR}

Resolution functions, continued

- **Details for all of the resolution functions are available elsewhere**
 - in the users' manual
 - in file 4x2b.pdf

SAMMY's integration method for Doppler and resolution broadening

See Section IV.A of SAMMY users' manual

Wanted: to evaluate integrals of the form

$$\langle f(E_i) \rangle = \int_{E_{min}}^{E_{max}} dE' B(E_i, E') f(E')$$

where

- $\{E_i\}$ is a predetermined set of grid points on which we wish to know the broadened values $\langle f(E) \rangle$
- $f(E')$ are the unbroadened theoretical values (for cross section, transmission, etc.)
- $B(E, E')$ is the Doppler- or resolution-broadening function
- $E_{min} = 0$ and $E_{max} = 8$, but in practice smaller range is used

Integration, continued

“auxiliary grid”

Solution: choose points $\{E_j'\}$ and associated weights $\{W_j\}$ such that

$$\int_a^b dE' B(E_i, E') f(E') \approx \sum_j B(E_i, E_j') f(E_j') W_j$$

where the approximation is exact if $B(E_i, E') f(E')$ is a polynomial of some specified degree

Integration, continued

- **Choice of auxiliary grid is somewhat arbitrary**
- **SAMMY's choice (see Section IV.A in SAMMY users' manual):**
 - start with experimental grid
 - add extra points between each point in grid (optional)
 - add points to the extremities (i.e. outside data range) so can broaden the end-points
 - add enough points to adequately describe each resonance
 - test the resulting grid to be sure spacings do not vary too wildly among neighboring points; make adjustments if needed

Integration, continued

- **Most integrations in SAMMY use the four-point progressive interpolation method of Mintz and Jordan**
 - [M. D. Mintz and D. P. Jordan, *A 'Progressive' Interpolation Scheme for Hand and Digital Computer Analysis of Tabulated Data*, Lawrence Livermore Laboratory Report UCRL-7681 (1964)]
 - For details, see the SAMMY users' guide

Integration, continued

- **Important !**

- The user (*not* the author) is responsible for being sure that the auxiliary grid is sufficiently dense!

- **WHY must the grid be dense?**

- Unbroadened cross sections would not be well-defined on a sparse grid. Hence the integrations would not be accurate.

- **WHY doesn't SAMMY check this? Other codes do (e.g., NJOY).**

- Large amounts of computation time are required for checks.
- SAMMY runs are repeated over and over (with slight modifications each time). (NJOY runs are not repeated like this.)

Integration, continued

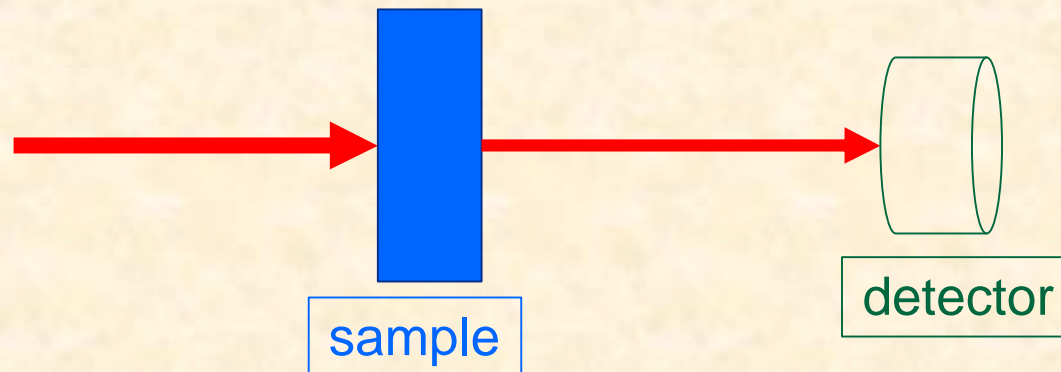
- **How can the user check this?**
 - There are user-controlled options for increasing the density of points in the auxiliary grid. Use them!
 - See card 2 of the INPut file, Table VIA.1 in users' manual.
 - Compare Doppler- and resolution-broadened results from dense vs. sparse grids.
 - Early in your analysis, use the sparsest grid that gives reasonable results.
 - Near the end of your work, perhaps you would want to use a denser grid to ensure greater accuracy.

Finite size of sample

- **In transmission measurements**
 - Corrections are relatively simple here
- **In capture or fission measurements**
 - Corrections can be extremely complicated here

Finite size: transmission experiment

- **Transmission is probably the easiest experiment**
 - Send a beam through a sample



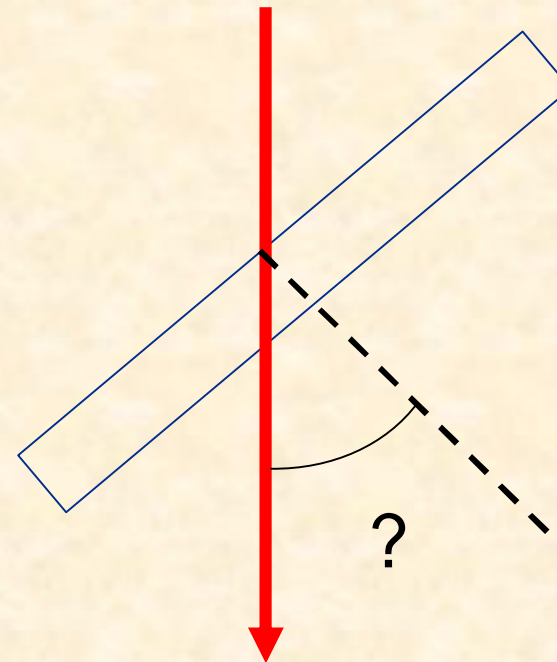
- Measure what comes out the other side (the transmission T)
- Result is directly related to the total cross section s and the sample thickness n

$$T = e^{-nS}$$

Finite size: T (continued)

- **Sample oriented at angle to beam? Correct by modifying the apparent value of n**

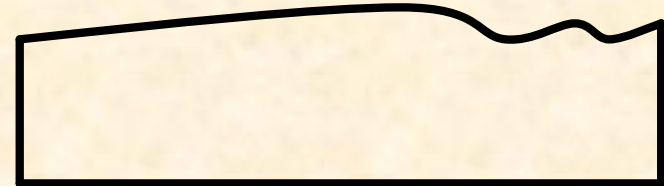
$$n_{\text{apparent}} = n / \cos (?)$$



Finite size: T (continued)

- **Non-uniform thickness n ? Correct by treating n as variable.**

- (Pictures are grossly exaggerated!)

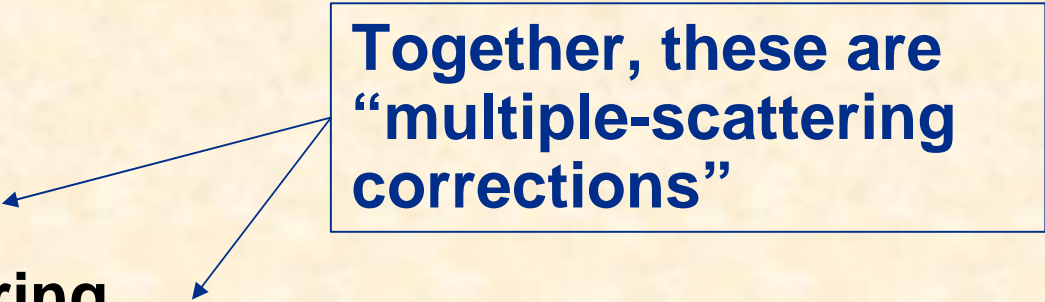


Finite size: capture or fission

- **Three effects:**

- **Self-shielding**
- **Single-scattering**
- **Double-plus scattering**

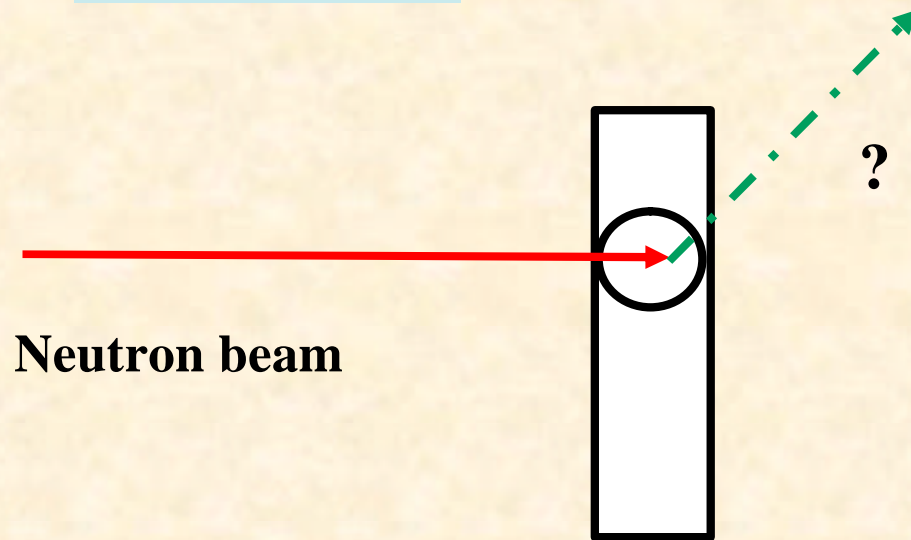
Together, these are
“multiple-scattering
corrections”

A blue-bordered box containing the text "Together, these are 'multiple-scattering corrections'". Two blue arrows originate from the bottom-left corner of the box, pointing to the text "Single-scattering" and "Double-plus scattering" in the list above.

We'll discuss capture only;
remember that results apply
to fission as well.

Multiple Scattering Corrections

Thin sample



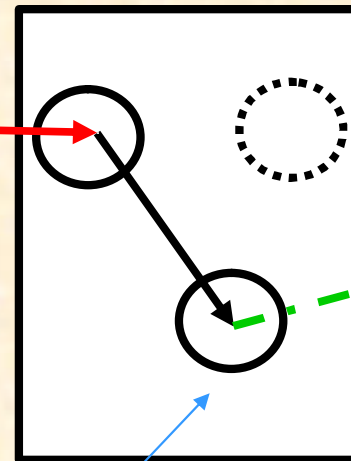
Neutron beam

This is a completely unrealistic situation. Real samples are much thicker.

Single scattering corrections

Thicker sample

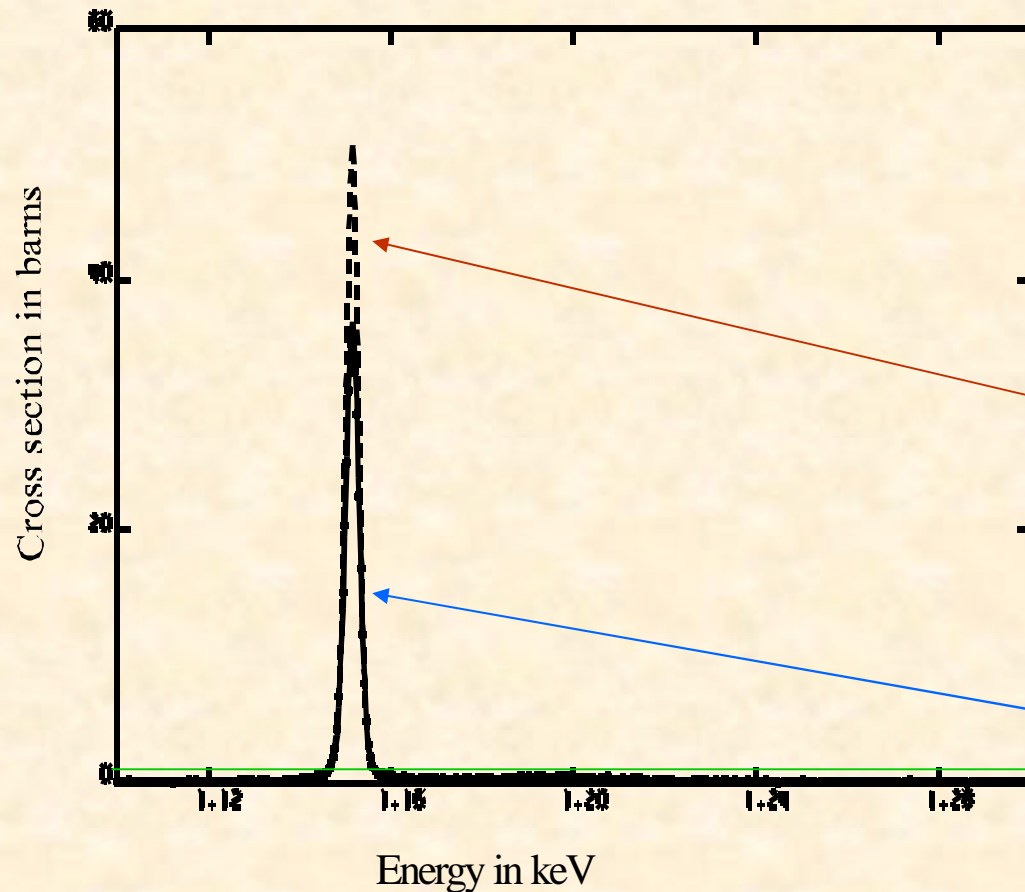
Neutron beam



Self-shielding
Exact, Easy

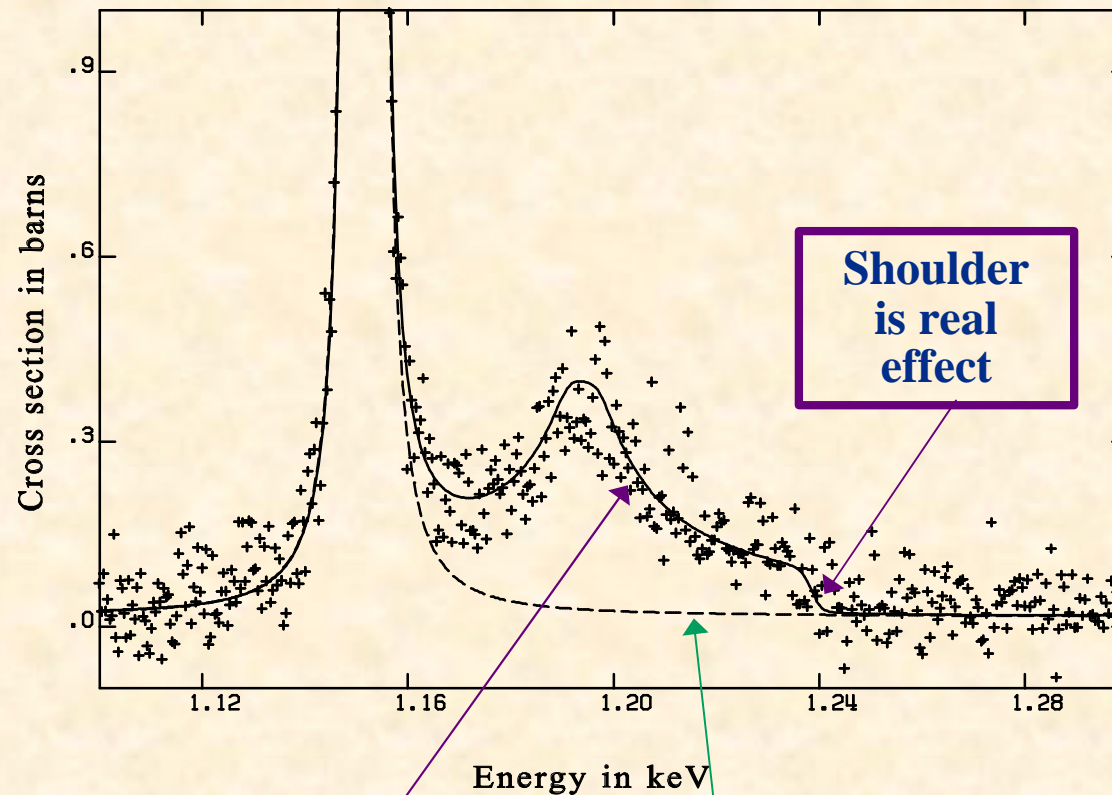
Single-scattering followed by capture

- exact for simplified geometry
- complicated mathematics
- complicated coding
- (simplifies if target is infinite slab)



The 1.15-keV ^{56}Fe resonance in natural iron capture data of R. Spencer et al. Dashed curve is SAMMY calculation without self-shielding or single-scattering correction; solid curve includes those corrections.

Let's look at this on a different scale...



The 1.15-keV ^{56}Fe resonance in natural iron capture data of R. Spencer et al. Dashed curve is SAMMY calculation without self-shielding or single-scattering correction; solid curve includes those corrections.

Single scattering, cont.

- **May be even more important when single-scattering peak does *not* show**
 - Heavier nuclei (smaller energy shift)
 - Wider resonances
 - Neighboring resonances
- **Could distort shape and/or position of resonances**

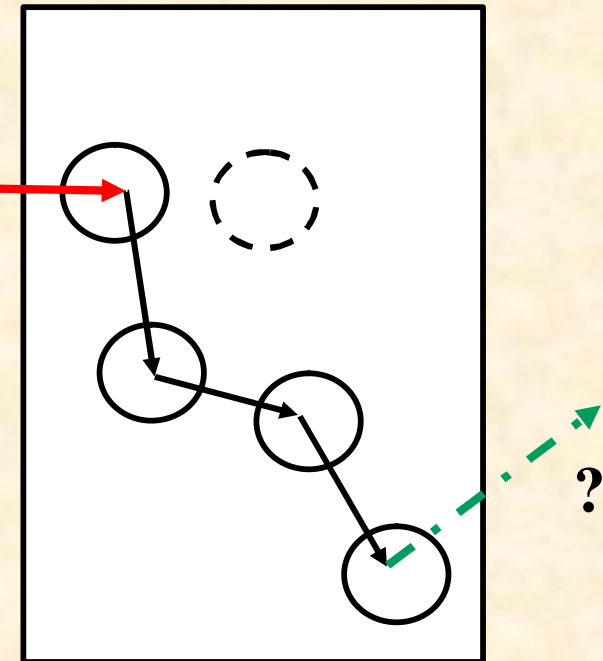
More-than-one scattering

**Thicker sample yet,
multiple scattering**

**double-plus scattering
followed by capture**

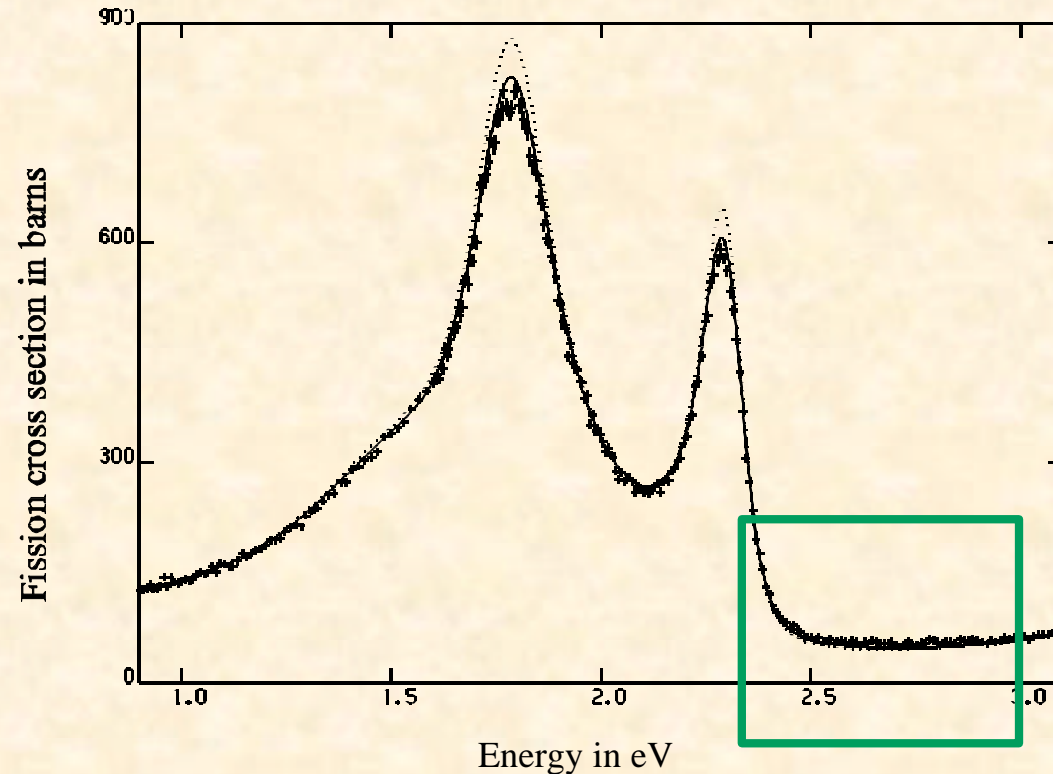
- requires six-fold embedded integrations for each scatter
- treat only in gross approximation

Neutron beam

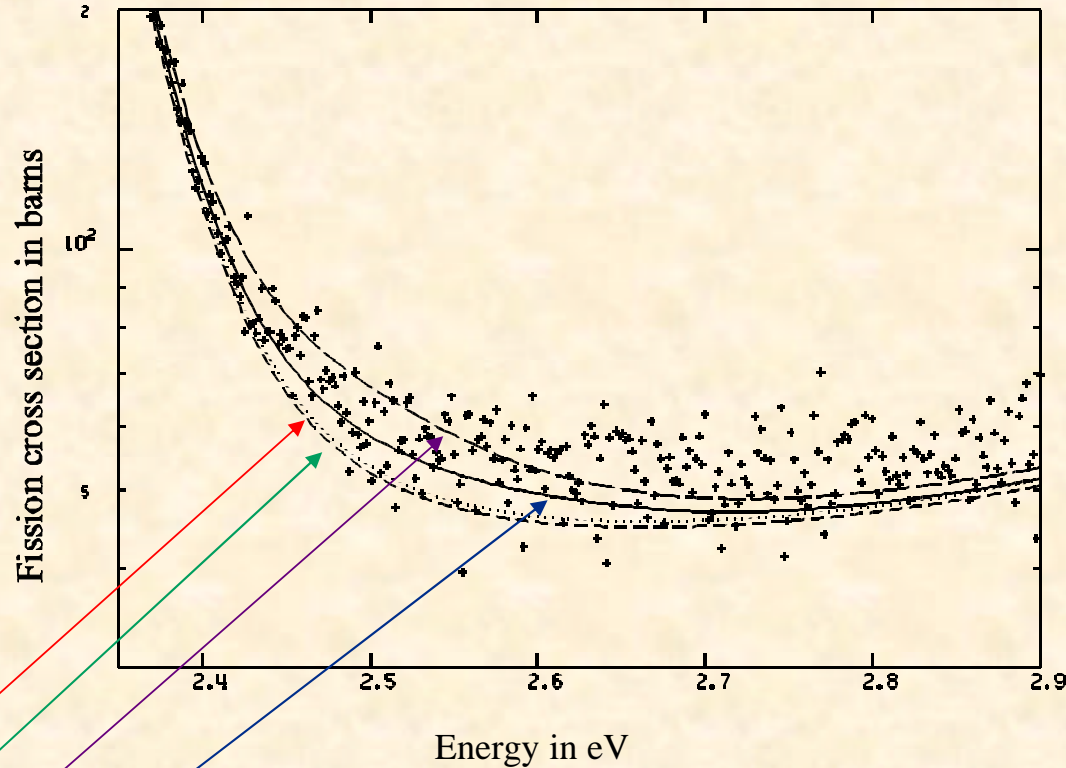


Ideas for SAMMY's treatment were borrowed from Mick Moxon, and developed independently

Fission cross section for ^{233}U

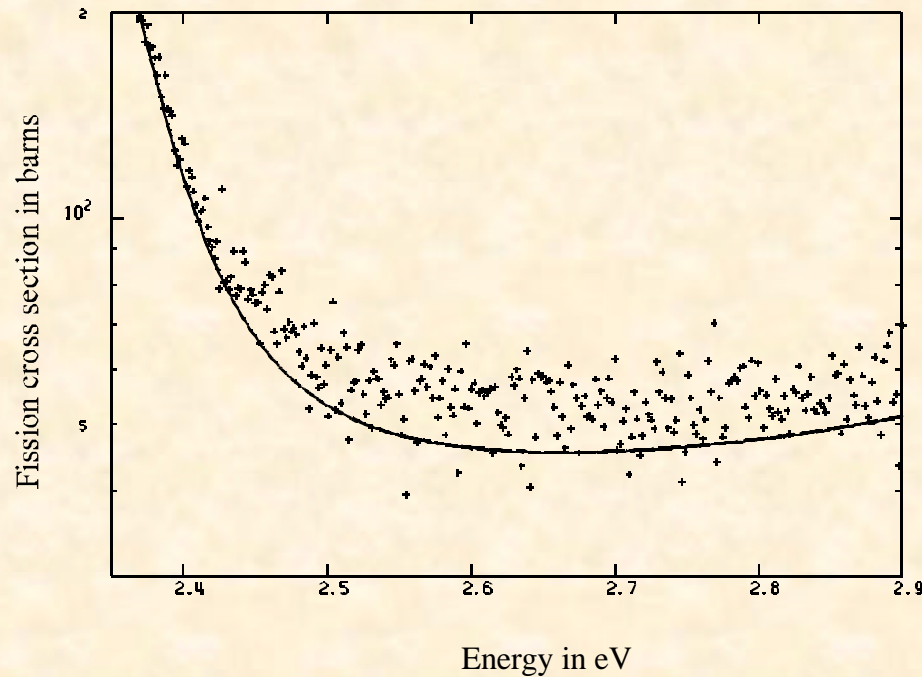


- ++ Measurement of Klaus Guber et al. at ORELA (data averaged by 5)**
- __ Preliminary SAMMY analysis of Herve Derrien**
- ... Using same resonance parameters without finite-size corrections**



- ++ + **ORELA measurement**
- **No finite-size corrections to calculated cross section**
- **With self-shielding but no multiple-scattering**
- - - **With multiple-scattering corrections but infinite-slab for single**
- — **With full multiple-scattering including edge-effects correction**

Same as previous slide, but with no Aluminum in the sample



**Fission chamber used $^{233}\text{U}_3\text{O}_8$ clad onto aluminum plates...
~100 times as much Al as U.**

All the scattering was due to Al !

Caution!

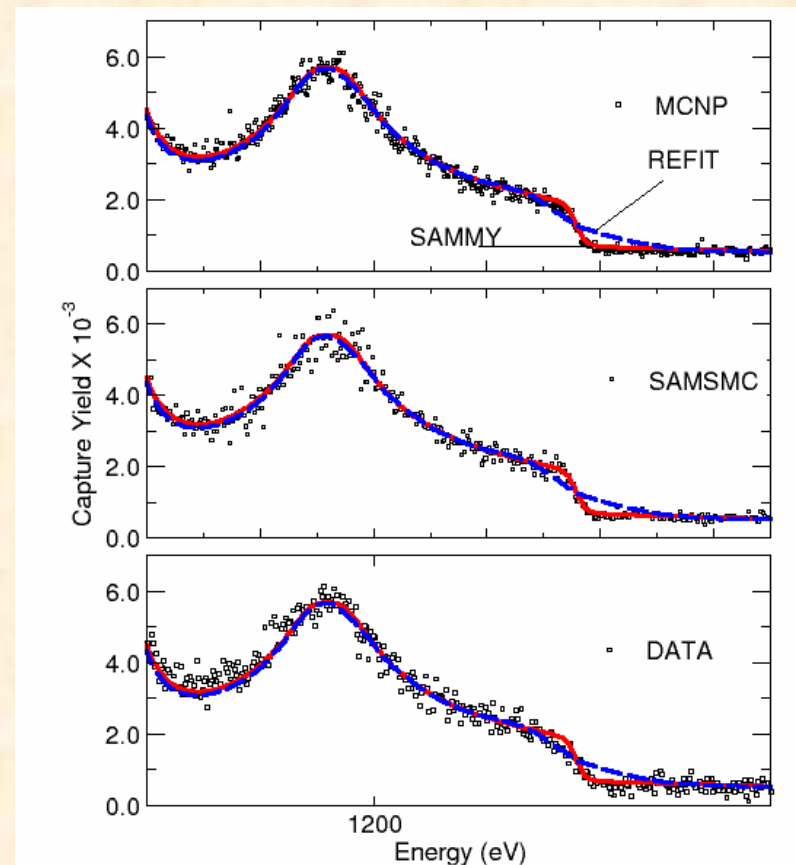
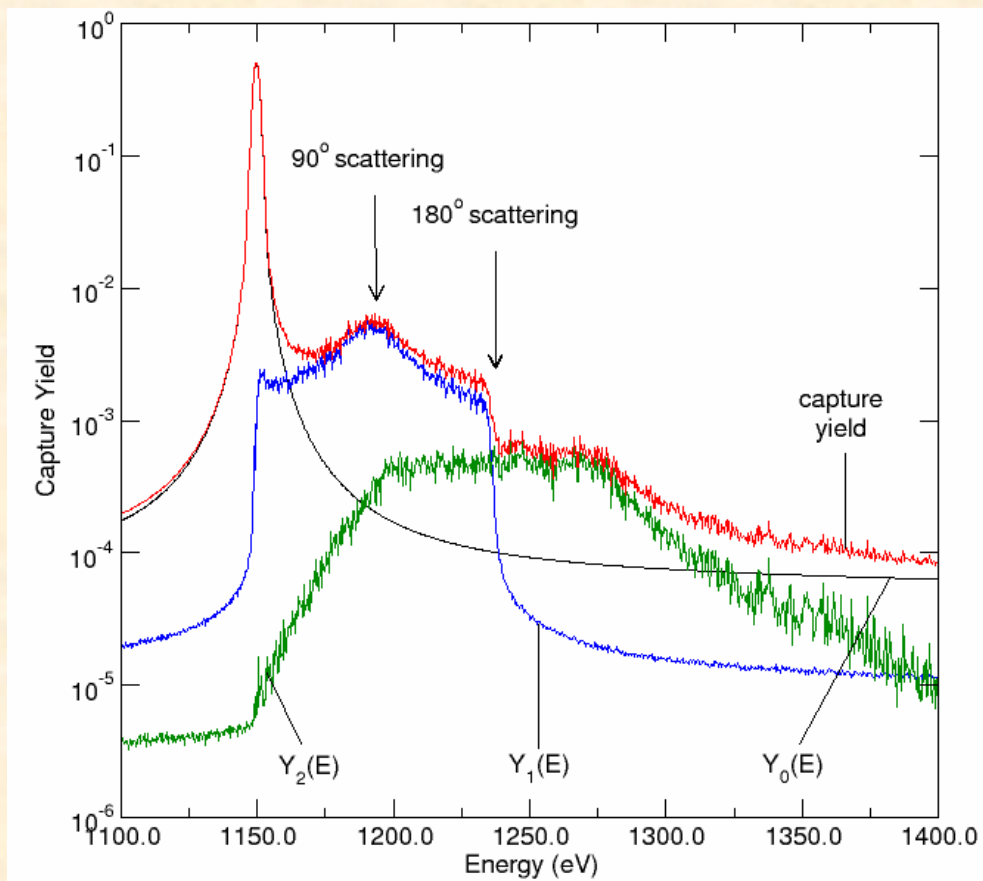
- When using more than one nuclide and requiring multiple-scattering corrections, *be sure* to define the isotopes/nuclides in the PARAmeter file. It is not sufficient to give abundances only in the INPut file.
- Release M5 and subsequent of SAMMY is dummy-proofed against this,
 - previous releases will merrily calculate garbage.

Equations for multiple-scattering corrections

- **Are in the SAMMY users' guide**
- **Are also in the pdf file 4x2c.pdf**
 - **Equations and description for self-shielding**
 - **Equations and description of single-scattering correction**
 - **Infinite slab approximation**
 - **Including edge-effects (non-infinite slab)**
 - **Equations and description of double-plus scattering correction**
 - **More examples**

One more picture re multiple scattering

^{56}Fe 1.3 mm



Figures from PhD thesis of Gilles Noguere, comparing Monte-Carlo to SAMMY to REFIT

Also see this paper...

**“Validation of Multiple-Scattering Corrections in the
Analysis Code SAMMY”**

N. M. Larson and K. N. Volev

*International Conference on the New Frontiers of Nuclear
Technology : Reactor Physics, Safety and High-Performance
Computing (Physor 2002)*

October 2002 in Seoul, South Korea

Published on CD rom

**End of multiple-scattering corrections
End of finite-size corrections**

Normalization and background

Section IV.E.3.a in R6 of SAMMY Users' Manual

- “Corrected” theoretical value T (for cross section, transmission, etc.) is given by

$$T(E) = a T_u(E) + b(E)$$

where T_u = uncorrected theoretical value

a = normalization

$b(E)$ = background

Norm & background, cont.

In SAMMY, there are three methods of specifying backgrounds:

1. Use any or all of the following (but only one of each):

$$b_1(E) = B_a$$

$$b_2(E) = B_b / \nu E$$

$$b_3(E) = B_c \nu E$$

$$b_4(E) = B_d e^{-B_f / \nu E}$$

Norm & background, cont.

2. Use as many of these as needed

$$b_1(E) = A$$

$$b_2(E) = A e^{-Bt}$$

$$b_3(E) = A t^B$$

$$b_4(E) = e^{A + Bt + C / \ln(t)}$$

where time t is derived from the energy

and L is the flight-path length $t = \sqrt{mL^2 / 2E}$

Norm & background, cont.

3. The user can provide a point-wise description of the background.

This option has been available from the beginning, but has not been used extensively. It therefore comes with no guarantees.

- **(One other option: add direct capture cross section as energy-dependent point-wise cross section)**

More than one type of nuclide in sample

- **Examples:**
 - Multiple isotopes
 - Chemical compounds (e.g. oxides)
 - Contaminants
- **What do *you* do about these? Specify each nuclide independently...**
 - Spin and parity, charge, etc. (in INPut file)
 - Spin groups (in INPut file)
 - Mass and abundance (in PARAmeter file)
 - Resonances (in PARAmeter file)

More than one nuclide, continued

- **What does SAMMY do about these?**
 - Includes appropriate angular momentum algebra for each nuclide
 - Includes proper kinematics for each nuclide
 - Doppler broadening is [now] done properly for each nuclide (mass-dependent)
 - Multiple-scattering corrections etc. are calculated using all nuclides
- **Details are given in the computer exercises (see Exercise ex012)**

Concluding comments regarding corrections for experimental conditions

- **Virtually all parameters may be varied (fitted)**
 - **Uncertainties are therefore reflected in final results**
- **On the drawing board:**
 - **Uncertainties due to non-varied parameters will be incorporated into the fitting procedure**
 - **More input options will be made available**
 - **UDR Resolution function will be improved**
 - ...

End of experimental effects