SAMMY Workshop Part 4.2

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Part 4.2, Experimental Conditions

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

2. Mathematical description of experimental effects

What experimental effects?

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

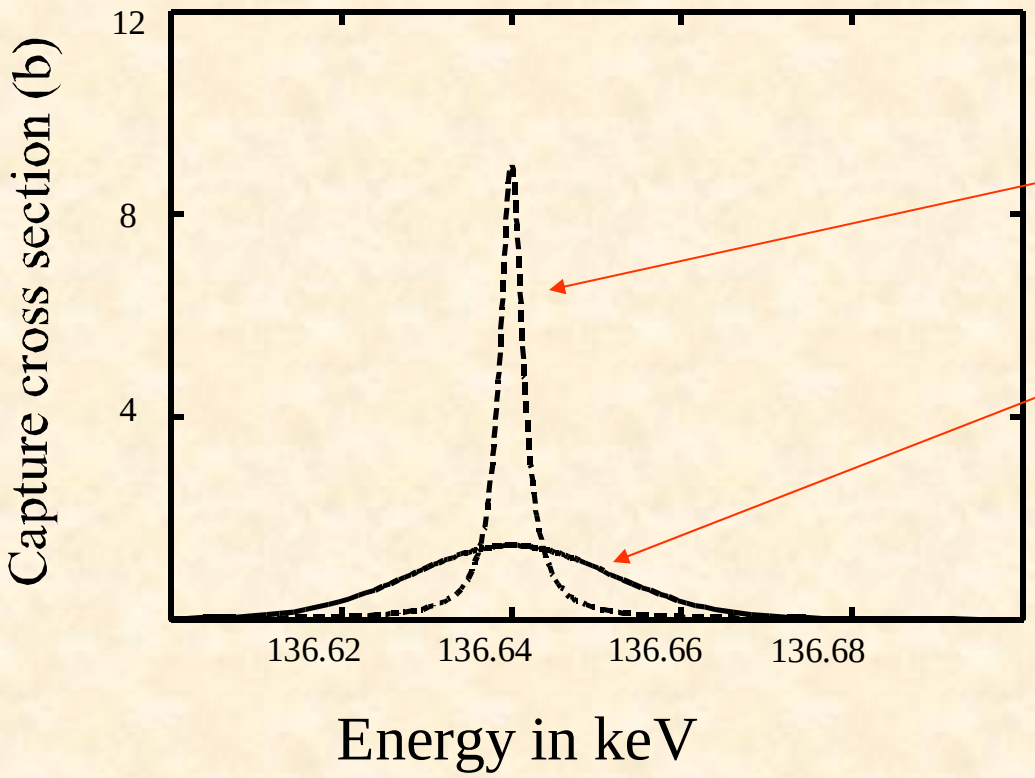
- **Many neutrons, not just one**
- **Many nuclei (sample is finite size)**
- **Many kinds of nuclei (isotopes, chemical compounds, impurities)**
- **Nucleus is moving (finite temperature)**
- **Time is not exact**
- **Distance is not exact**
- **Neutron-producing target is finite size**
- **Detector 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, nevertheless an efficient and reliable way to program FGM.

$$\bar{\sigma}\left(mv^2/2\right) = \frac{1}{v^2 u\sqrt{\pi}} \int_{-\infty}^{\infty} d\,w\;\; w^2 s(w) \exp\left\{-(v-w)^2/u^2\right\}$$

$$u = \sqrt{\frac{2kT}{M}} \qquad s(w) = \begin{cases} \sigma\left(m(\;\;w)^2/2\right) & \text{for } w \geq 0 \\ -\sigma\left(m(-w)^2/2\right) & \text{for } w \leq 0 \end{cases}$$

Doppler broadening in SAMMY

[Section numbers refer to SAMMY users' guide, Revision 7]

(not yet published but coming soon)

- **via SAMMY's "free gas model" (FGM), Section III.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 III.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.

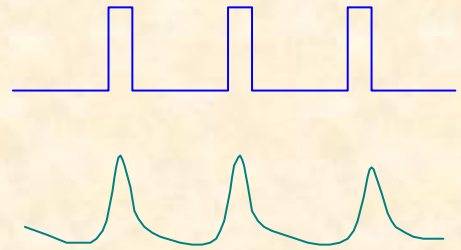
- **via Gaussian (HEGA), Section III.B.3**
  - **high energy approximation**
  - **integrations performed numerically using energy-grid appropriate for resonance structure**
  - **use is discouraged !**
- **Crystal-lattice model (CLM), Section III.B.4**
  - **may be important for some low-energy cross 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**

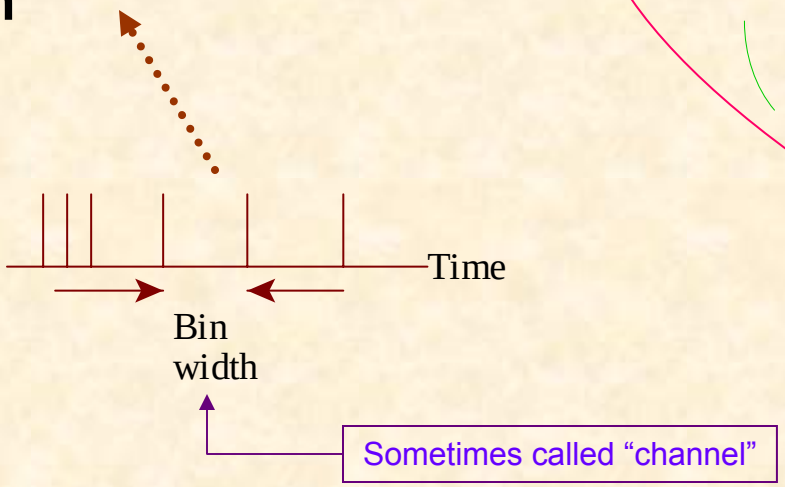
Doppler broadening in SAMMY, cont.

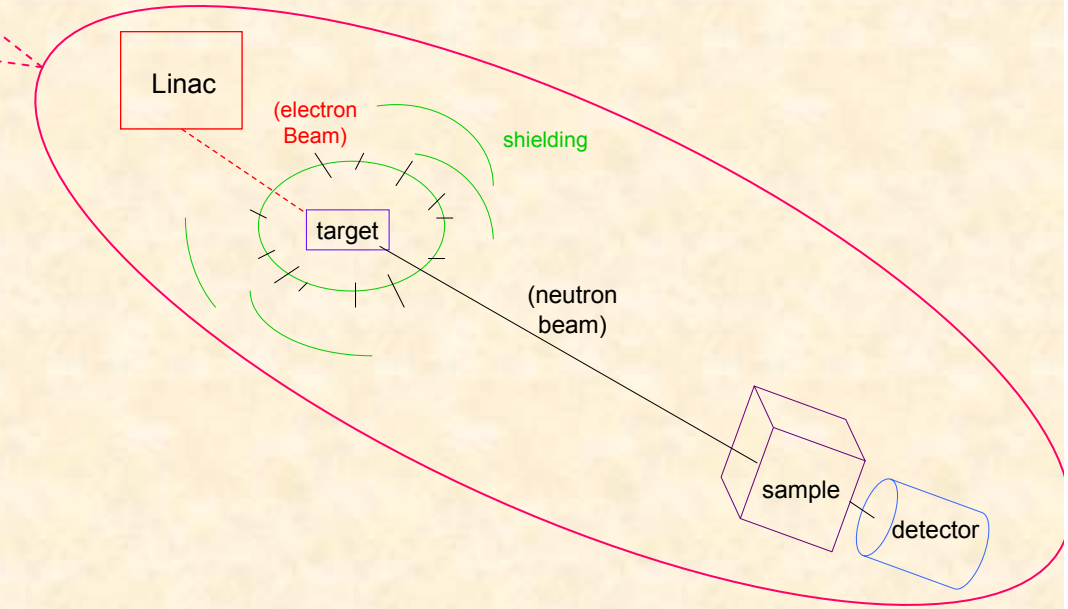
- Which to use?
  - **FGM ➔ usually**
    - **Requires virtually no more time that HEGA**
  - **LH ➔ only with very smooth cross section**
  - **HEGA ➔ never!**
  - **CLM ➔ when solid-state effects are important**
    - **Computer runs take much longer than with FGM**

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 $R(E,E')$,**

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

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.**

Need to fit the particular machine and the particular experiment.

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

- **SAMMY contains five or six distinct methods. Values for almost all parameters can be fitted to data.**

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 - Δ (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 R7]

- **Gaussian and/or exponential (Section III.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) (III.C.2)**
  - **analytic convolution (where possible) of four components, with realistic descriptions for all four**
  - **designed for use with ORELA data**

"realistic" resolution functions

- **RPI Resolution Function (Section III.C.3)**
  - **ditto, designed for use with data from Linac at Rensselaer Polytechnic Institute**
  - **extension should be useful for data from Geel and nTOF facilities**

Resolution, continued

- **Energy-average from E-DE to E (DEX) (III.C.4)**
  - **available in M6-Beta & M6 release of SAMMY code**
  - **useful for charged-particle work**
- **Numerical description (UDR) (III.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 III.A of SAMMY users' manual, R7

Wanted: to evaluate integrals of the form

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

where

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

Integration, continued

"auxiliary grid"

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

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

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 III.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!**

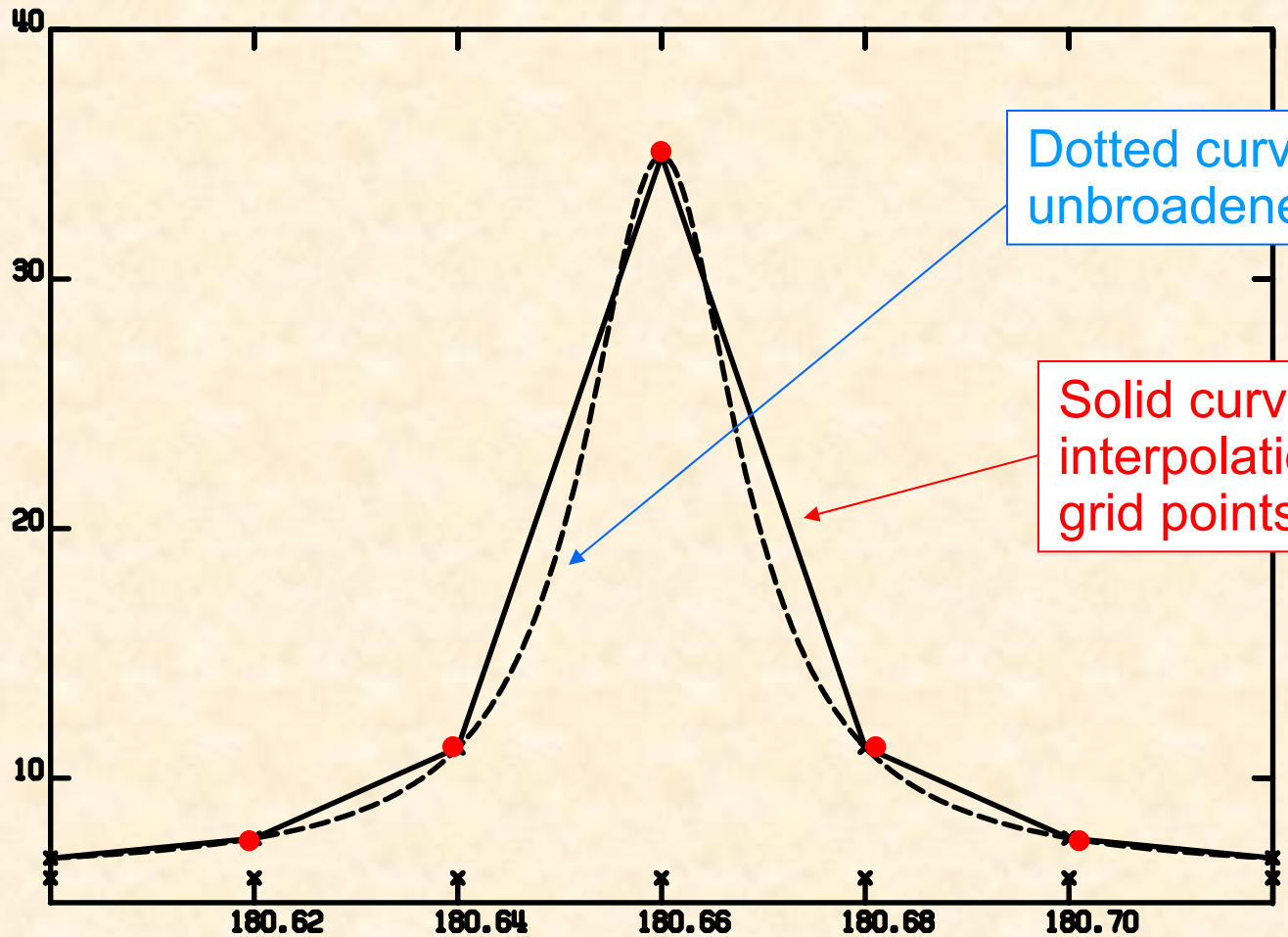
- **WHY must the grid be dense?**
  - **Unbroadened cross sections would not be well-defined on a sparse grid. Hence the integrations would not be accurate.**

- **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.**

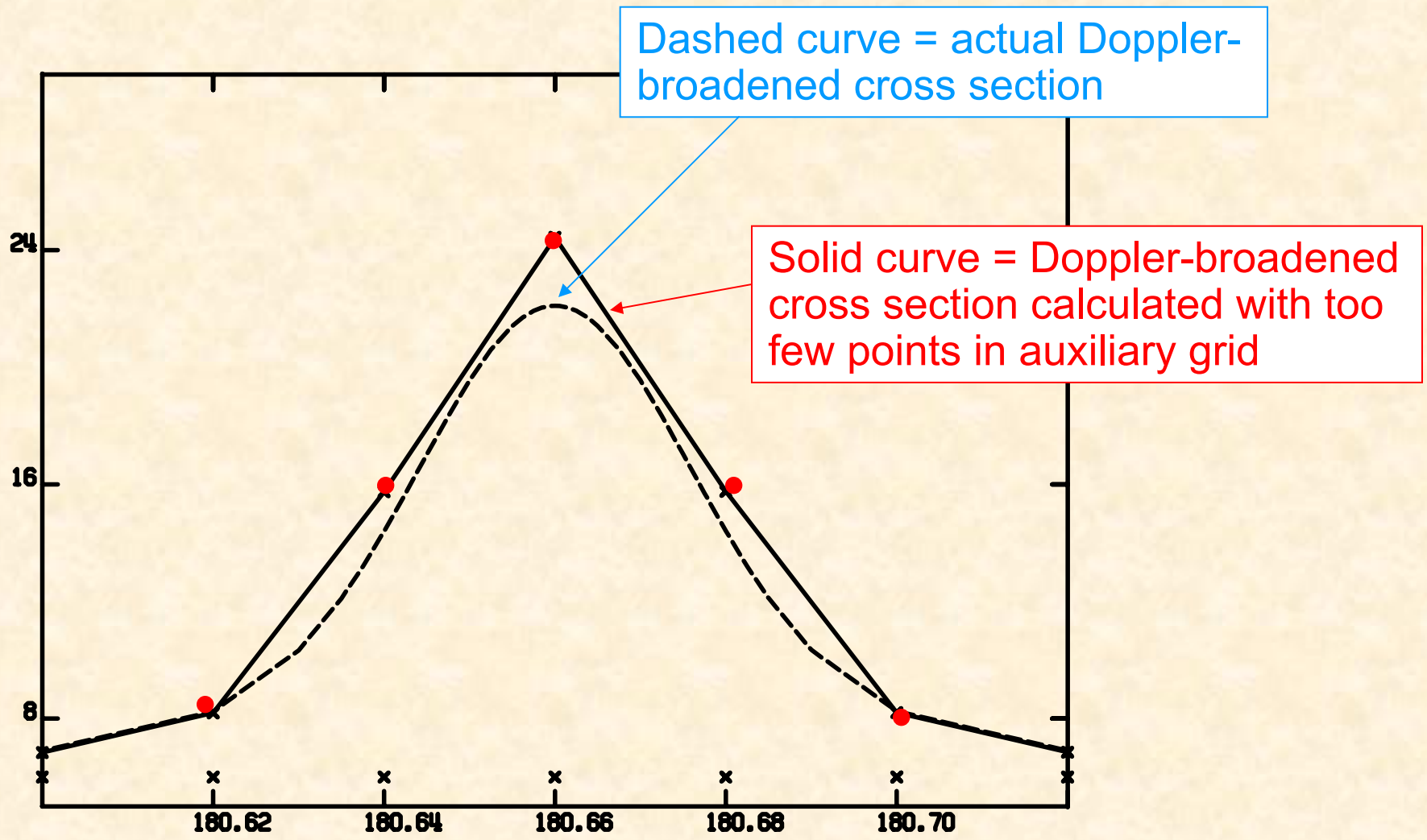
Using too few points to describe unbroadened cross section ...



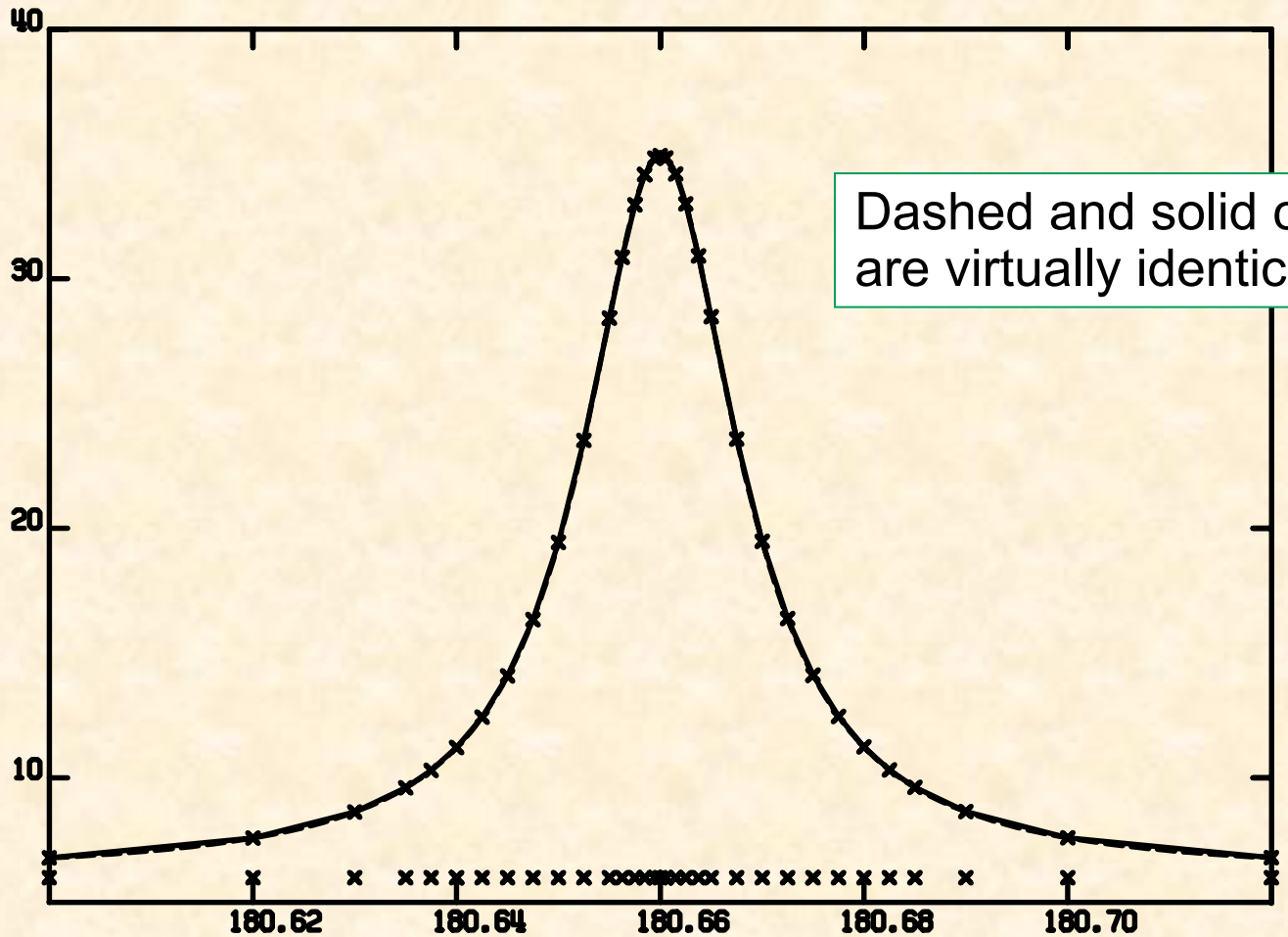
Dotted curve = actual unbroadened cross section

Solid curve = linear interpolation between grid points ●

Too few points, continued

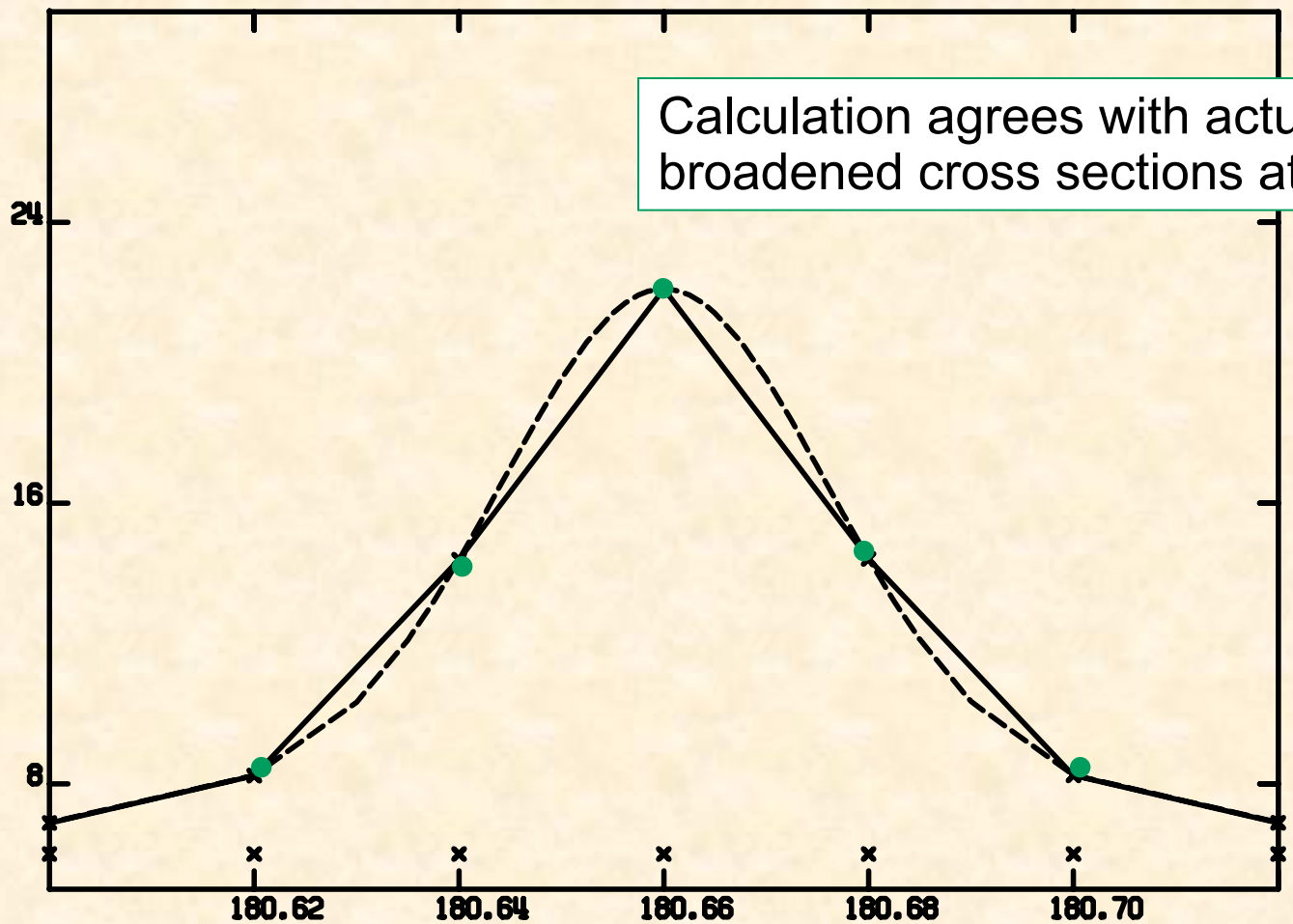


Using an adequate number of points to describe unbroadened cross section ...



Dashed and solid curves are virtually identical.

With an adequate grid, continued



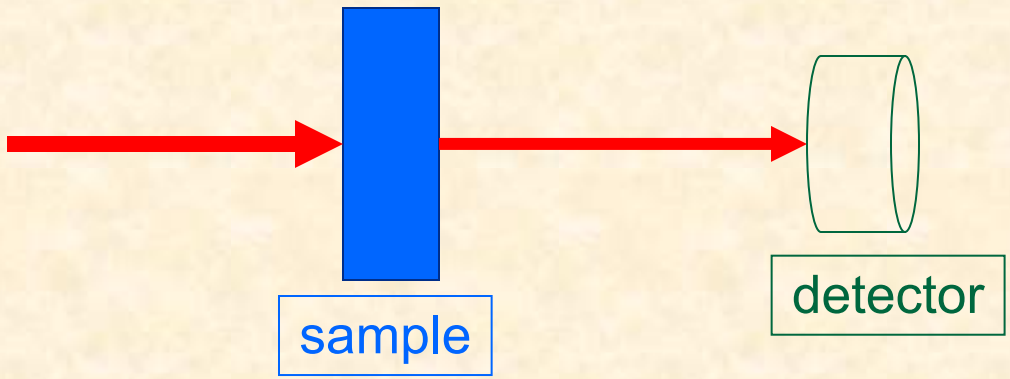
Calculation agrees with actual Doppler-broadened cross sections at the grid points.

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**



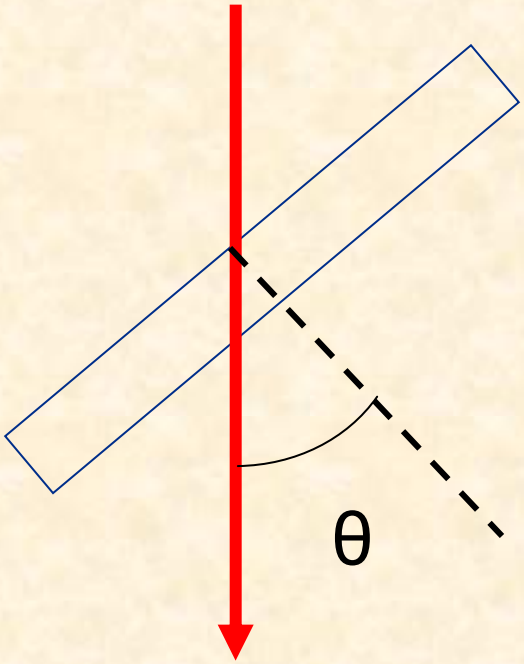
  - **Measure what comes out the other side (the transmission T)**
  - **Result is directly related to the total cross section σ and the sample thickness n**

$$T = e^{-n\sigma}$$

Finite size: T (continued)

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

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



Finite size: T (continued)

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

(Pictures are grossly exaggerated!)

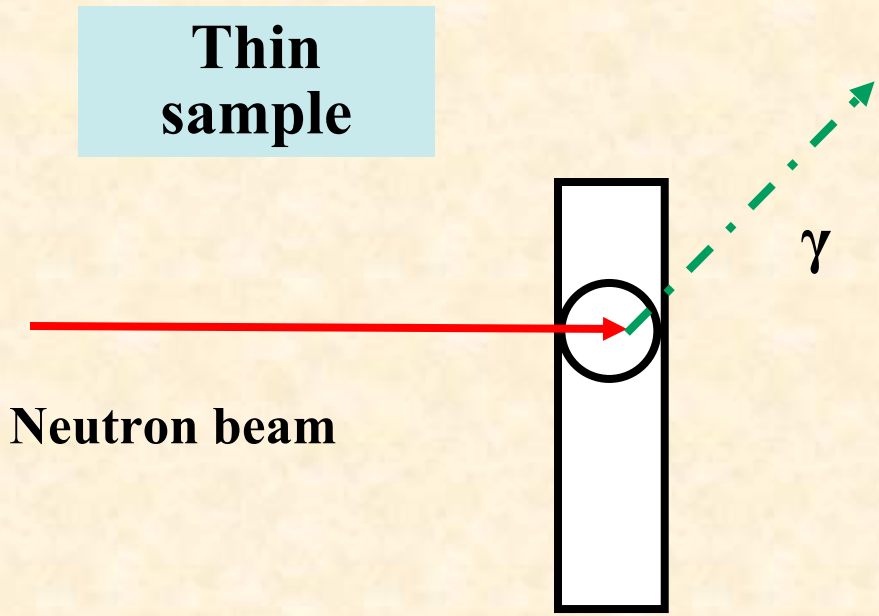
Finite size: capture or fission

- **Three effects:**
  - **Self-shielding**
  - **Single-scattering**
  - **Double-plus scattering**

Together, these are "multiple-scattering corrections"

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

Multiple Scattering Corrections

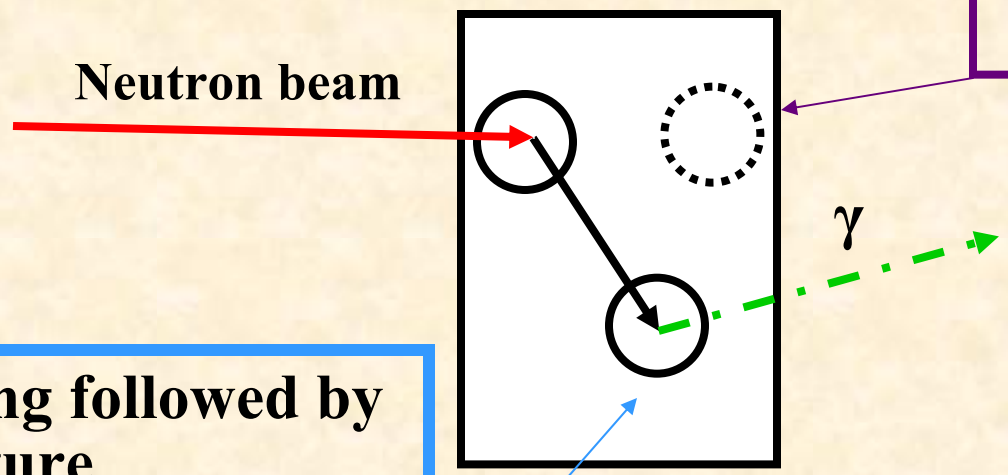


This is a completely unrealistic situation. Real samples are much thicker.

Single scattering corrections

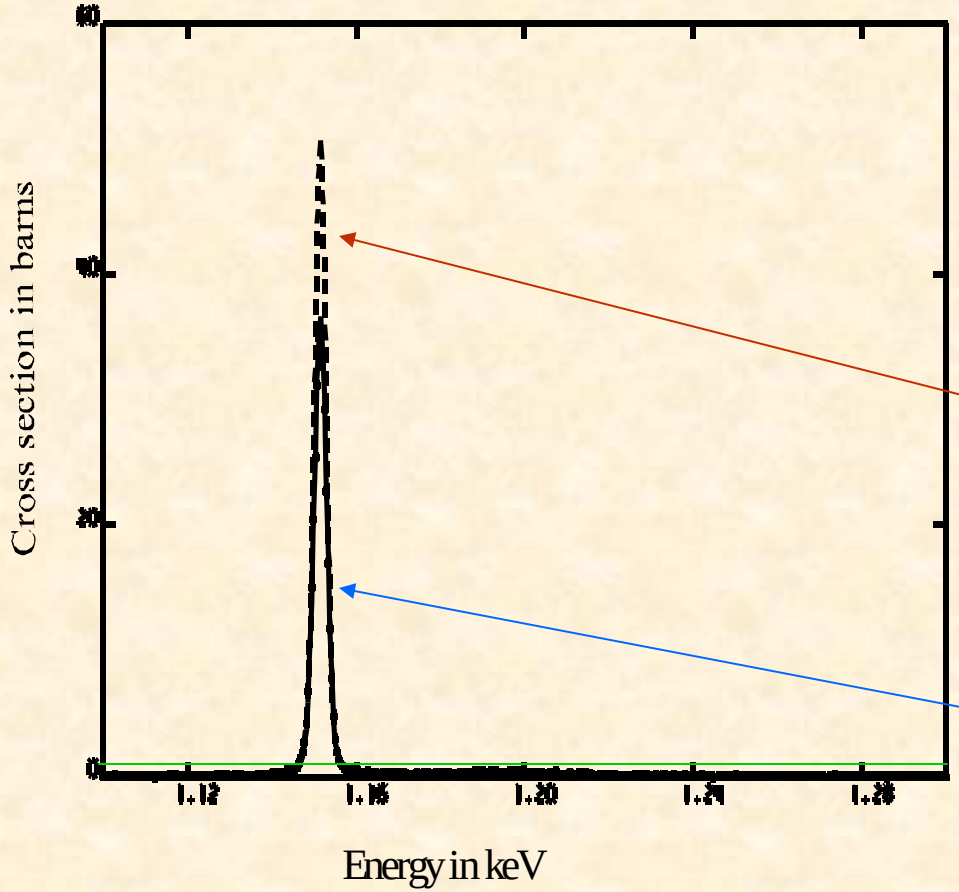
Thicker sample

Self-shielding
Exact, Easy



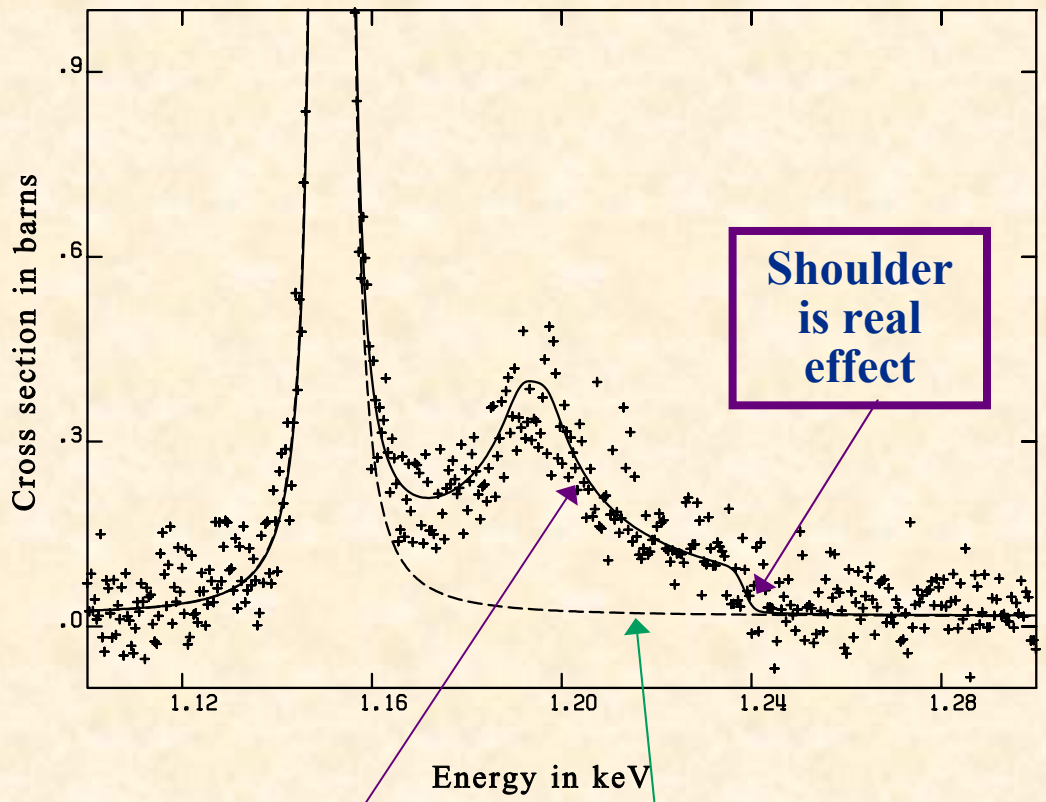
Single-scattering followed by capture

- 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…



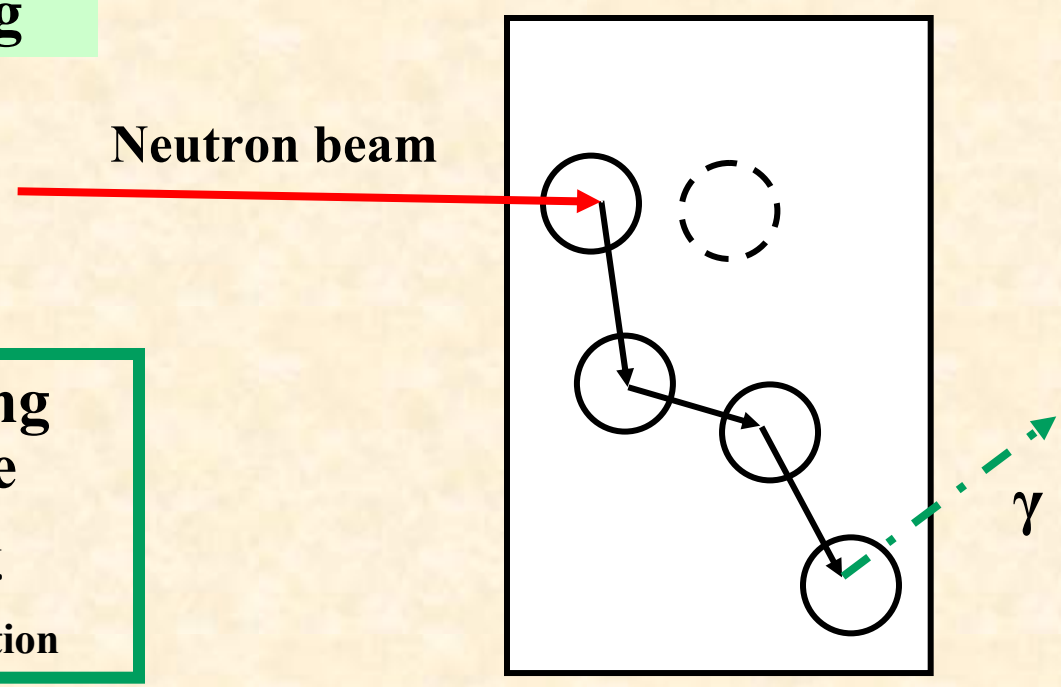
The 1.15-keV ^{56}Fe resonance in natural iron capture data of R. Spencer et al. Dashed curve is SAMMY calculation without self-shielding or single-scattering correction; solid curve includes those corrections.

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

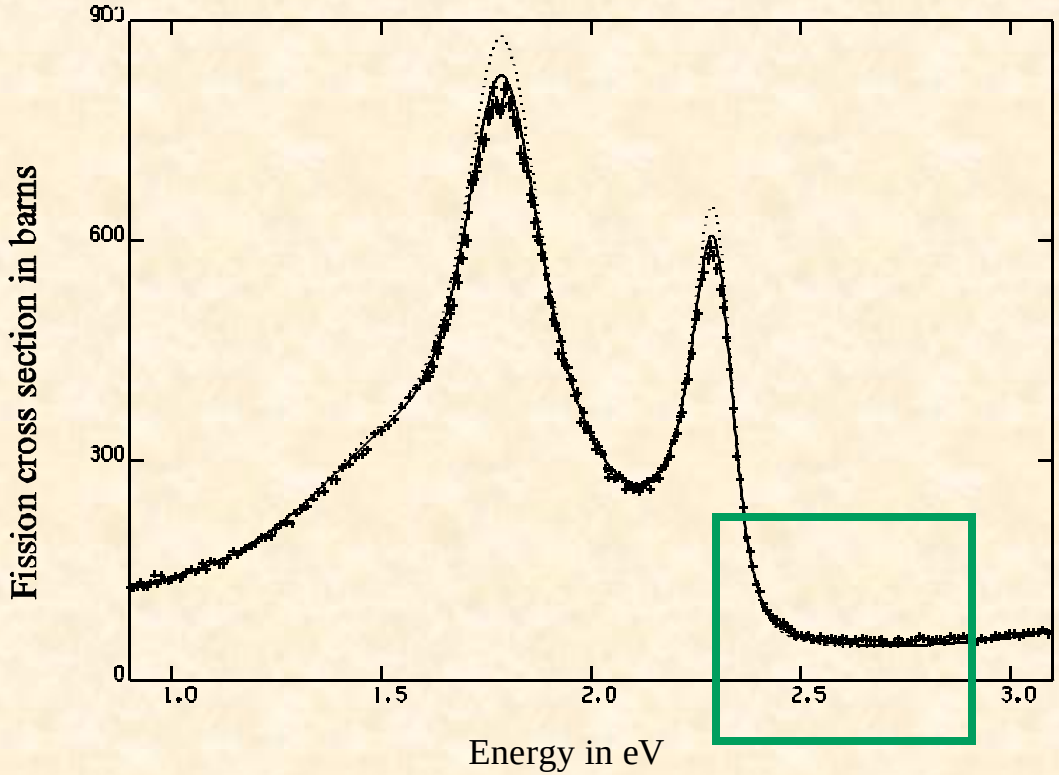


double-plus scattering followed by capture

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

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

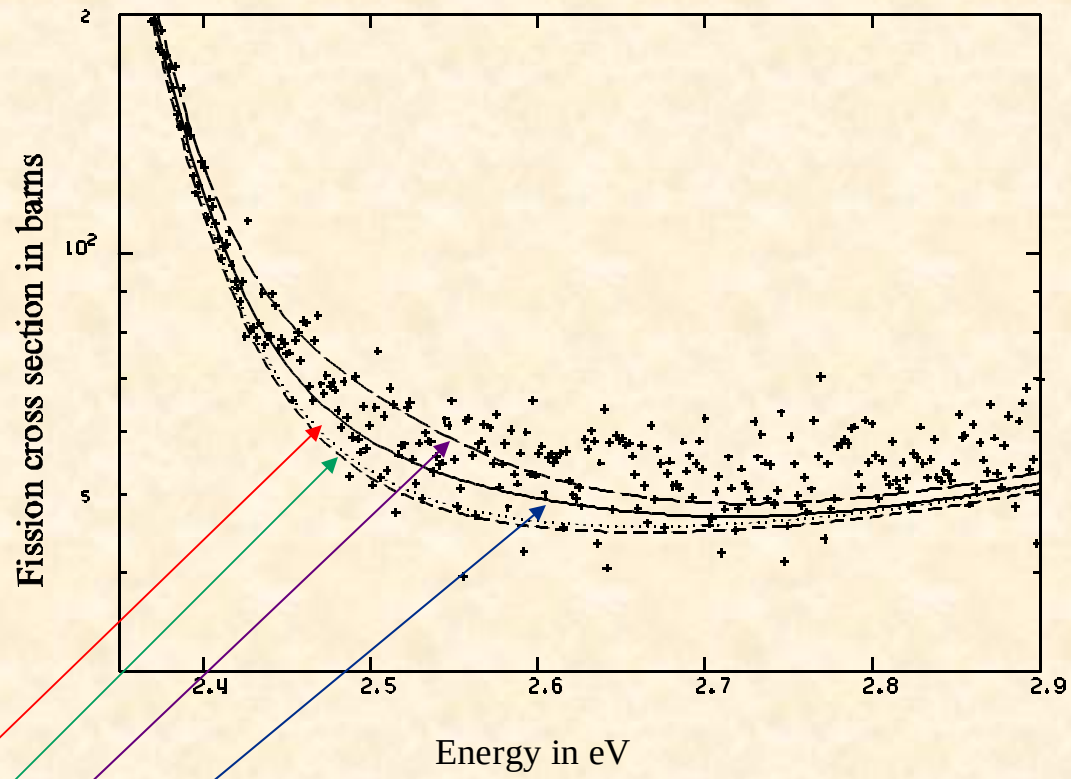
Fission cross section for ^{233}U



++ 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

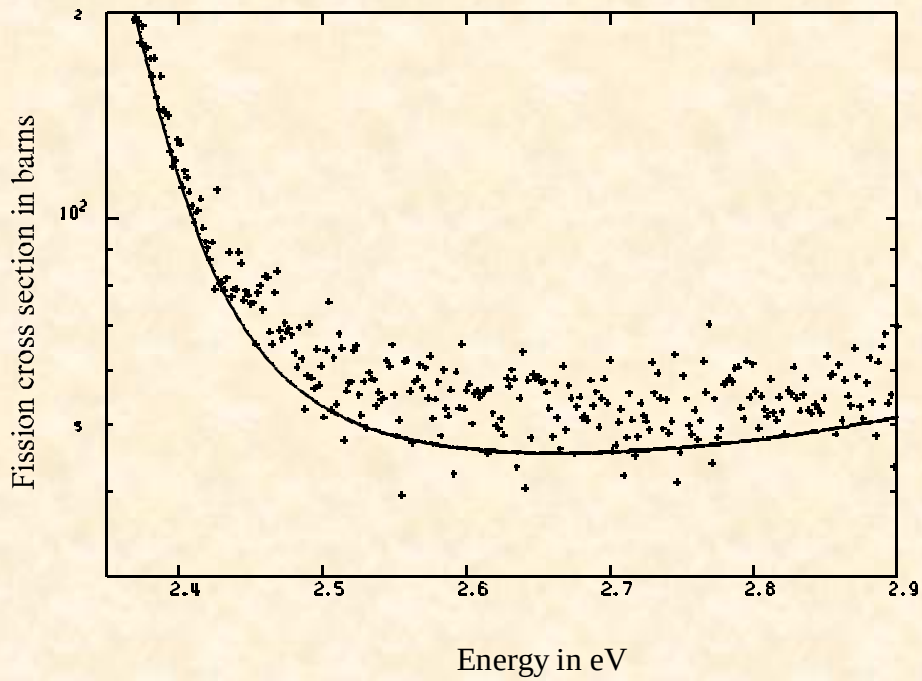
…… No finite-size corrections to calculated cross section

------ 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 $^{233}U_3O_8$ 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 <u>in the PARameter file</u>. It is not sufficient to give abundances only in the INPut file.**

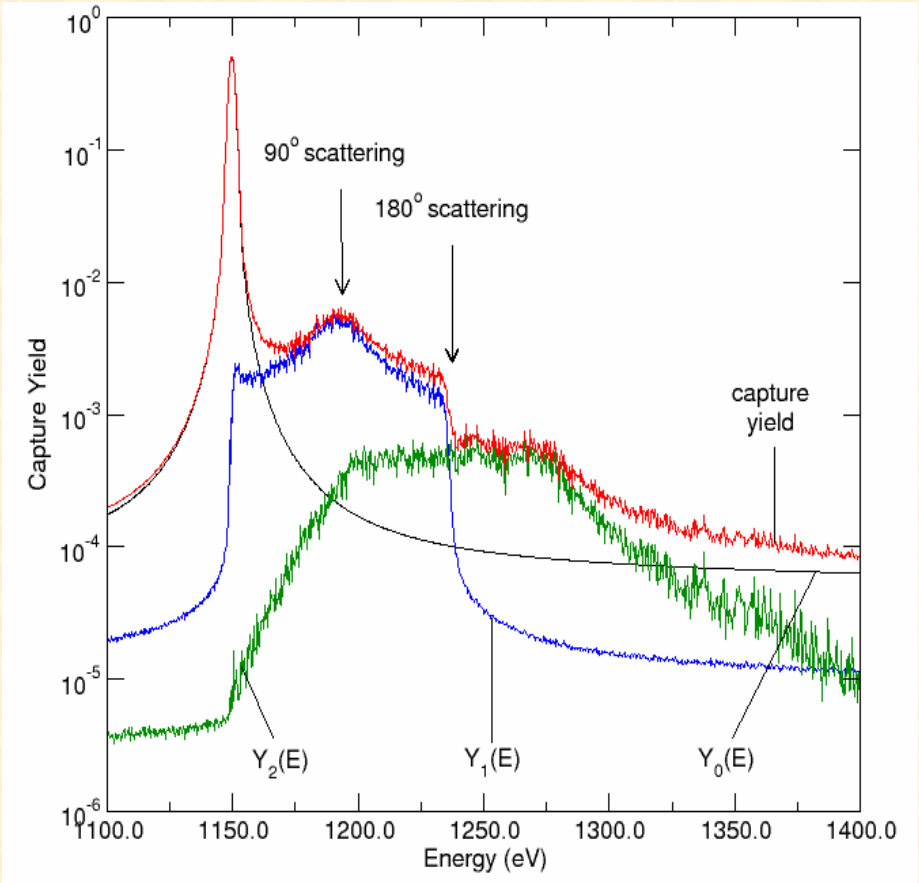
- **Release M5 and subsequent of SAMMY is dummy-proofed against this,**
  - **Previous releases will merrily calculate garbage.**

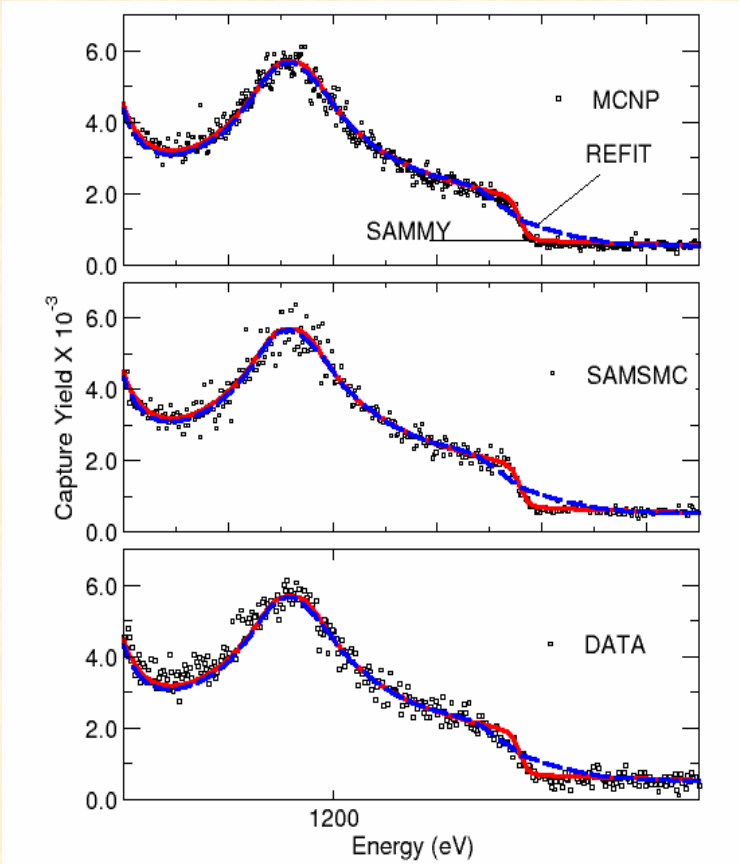
Equations for multiple-scattering corrections

- **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 III.E.3.a in R7 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):**

$$b_1(E) = B_a$$

$$b_2(E) = B_b \ / \sqrt{E}$$

$$b_3(E) = B_c \sqrt{E}$$

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

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 or PAR file)**
  - **Spin groups (in INPut file or PAR 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 broadens for each nuclide (mass-dependent)**
  - **Calculates multiple-scattering corrections etc. 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**
- **Virtually all parameters may be PUP'd**
  - **Values are fixed but uncertainties are propagated through the fitting process**

To be discussed in great detail later

- **On the drawing board:**
  - **More options**
  - **Improvements to UDR Resolution function**
  - **…**

End of experimental effects