SAMMY Workshop Part 4.2b

Dr. Nancy M. Larson
Oak Ridge National Laboratory

Part 4.2b, Resolution Broadening Formulae

Updated January 2004

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

RESOLUTION BROADENING

Resolution broadening is "smearing" due to

- spread in burst width
- finite size of neutron source
- time-of-flight channel width
- finite size of detector
- etc

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

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

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.

Resolution Broadening in SAMMY

(Section numbers refer to the SAMMY users' manual 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
- Oak Ridge Resolution Function (ORR) (Section IV.C.2)
  - analytic convolution (where possible) of four components, with realistic descriptions for all four
- 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
- Energy-average from E-DE to E (DEX) (Section IV.C.4)
  - available in M6-Beta release of SAMMY code
- 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 Function # 1

Original Gaussian and/or Exponential

(See Section IV.C.1 of the SAMMY users' manual)

Gaussian: combination of three components:

- a square function of (flight-path) length
  - input is the full width of a square distribution in length (i.e. $\sqrt{12}\times$ standard deviation of a Gaussian)

- burst width, a Gaussian in time
  - input is the full width at half max of Gaussian

- channel width, a square function in time
  - input is full width of square function
  - different values may be specified for different energy ranges

Exponential, or Gaussian plus exponential

- provides asymmetric component to the resolution function

Resolution Function # 2

Oak Ridge Resolution Function

(See Section IV.C.2 of the SAMMY users' manual)

A "realistic" resolution function, the convolution of four components:

- electron burst width
- neutron source
- time-of-flight channel width
- detector

Each component is described mathematically as a function of either time t or flight-path-length l, then converted to a function of t using (for fixed E)

$$E = \frac{m}{2} \frac{l^2}{t^2}$$

The "complete" resolution function is the convolution of the four individual pieces:

$$I(t) = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2 \int I_3(t_2-t_3)\,dt_3\; I_4(t_3)$$

Integrations are analytical where possible (to maximize speed and accuracy), numerical where necessary.

Components of the Oak Ridge Resolution Function

1. electron burst width, a square function in time:
   where p is the burst width in nanoseconds

$$I_1(t) = \begin{cases} 1/p & \textit{for } 0 < t < p \\ 0 & \textit{otherwise} \end{cases}$$

2. neutron source, two possibilities:

   2a. *ORELA Water Moderator*

   χ^2 distribution with $2(m+1)$ degrees of freedom, where m is any positive integer:

$$I'_{2a}(l) = \frac{l^m}{m!\ \Lambda^{m+1}} \exp\left(-\frac{l}{\Lambda}\right)$$

   where l = the flight-path-length variable
   and moderation distance Λ is a mean free path.
   Value of Λ varies with energy as $\Lambda = \Lambda_0 + \Lambda_1 \ln(E) + \Lambda_2 (\ln(E))^2$.

2b. tantalum target

$$I'_{2b}(l) = \begin{cases} 0 & for \quad l < x'_1 \\ u'(l) + v'(l) & for \ x'_1 < l < x'_2 \\ u'(l) + w'(l) & for \ x'_2 < l < x'_3 \\ w'(l) & for \ x'_3 < l \end{cases}$$

where the functions $u'(l)$, $v'(l)$, and $w'(l)$ are defined as

$$u'(l) = N' \exp\{-\varepsilon'^2 (l - x'_0)^2\} \qquad for \ x'_1 < l < x'_3$$

$$v'(l) = \frac{N'\alpha' l}{x'_2} \exp\{-\beta'(l - x'_2)\} \qquad for \ x'_1 < l < x'_2$$

and

$$w'(l) = N'\alpha' \exp\{-\beta'(l - x'_2)\} \qquad for \ x'_2 < l$$

3. time-of-flight channel width

$$I_3(t) = \begin{cases} 1/c & \textit{for } 0 < t < c \\ 0 & \textit{otherwise} \end{cases}$$

where channel width c may be different for different energy-regions.

4. detector

4a. *NE110 Detector*

$$I'_{4a}(l) = \begin{cases} \Delta \ \exp(-\lambda\sigma l) & \textit{for } 0 < l < \delta \\ 0 & \textit{otherwise} \end{cases}$$

δ = thickness of the NE110 detector

λ = number of molecules per mm.b of detector
(0.0047 for NE110)

$\sigma(E)$ = total cross section of detector material
($CH_{1.104}$ for NE110)

Δ = normalization factor found from $\int I'_{4a} = 1$:

$$\Delta = \frac{\lambda\sigma}{1 - \exp(-\lambda\sigma\delta)}$$

4b. *Lithium Glass Detector*

$$I_{4b}(t) = \begin{cases} D\,g & for\ 0 < t < d \\ D\ \exp(-f\,(t-d)) & for\ d < t \end{cases}$$

g = constant,
D is chosen to give $\int I'_{4b} = 1$:

$$D = \frac{f}{1 + g\,f\,d}$$

Resolution Function # 3

RPI Resolution Function

(See Section IV.C.3 of the SAMMY users' manual)

Another "realistic" resolution function, convolution of three components, designed for use with data taken at the Gaerttner LINAC at Rensselaer Polytechnic Institute:

- electron burst width
- neutron source + detector
- time-of-flight channel width

Each component is described mathematically as a function of *t*.

The "complete" resolution function is the convolution of the three individual pieces:

$$I(t) = \int I_1(t - t_1)\, dt_1 \int I_2(t_1 - t_2)\, dt_2 \;\; I_3(t_2)$$

Integrations are analytical where possible (to maximize speed and accuracy) and numerical where necessary.

Components of the RPI Resolution Function

1. electron burst width, a Gaussian function in time

$$I_1(t) = \frac{w}{\sqrt{\pi}} e^{-w^2 t^2}$$

$2\sqrt{\ln 2}/w = p$ is full width at half max of the burst

3. time-of-flight channel = square function of time

$$I_3(t) = \begin{cases} 1/c & \text{for } -c/2 < t < c/2 \\ 0 & \text{otherwise} \end{cases}$$

where channel width c may be different for different energy-regions

2. neutron source + detector, chi-squared plus exponentials

$$I_2(t) = A_0 \left\{ \frac{(t+\tau)^2}{2!\ \Lambda^3}\ e^{-(t+\tau)/\Lambda} + A_1 \left[A_2\, e^{-A_3 (t+t_0)} + A_4\, e^{-A_5 (t+t_0)} \right] + \sum_{i=1}^{5} B_{2i-1}\, e^{-B_{2i}(t+t_0)} \right\}$$

where τ, Λ, and A_1 are functions of energy, A_0 is normalization –

$$\Lambda(E) = \Lambda_0 + \Lambda_1 \ln(E) + \Lambda_2 [\ln(E)]^2 + \Lambda_3\, E^{\Lambda_4}$$

$$\tau(E) = \tau_1\, e^{-\tau_2 E} + \tau_3\, e^{-\tau_4 E} + \tau_5 + \tau_6\, E^{\tau_7}$$

$$A_1(E) = a_1\, e^{-a_2 E} + a_3\, e^{-a_4 E} + a_5 + a_6\, E^{a_7}$$

Other quantities in $I_2(t)$ are independent of energy.

The five exponential terms in $I_2(t)$ were added in an attempt to describe the Geel resolution function at all energies.

Resolution Function # 4

Numerical Resolution Function

Preliminary version is in SAMMY M6, but not thoroughly tested

This is another "realistic" resolution function, a convolution of several components, designed for use when other forms are not adequate. The components are:

- electron burst width (Gaussian function of time)
- time-of-flight channel width (square function of time; accordeon = crunch boundaries)
- user-defined numerical function of time at specified energies, with linear interpolation in between
- other user-defined numerical function(s)

The "complete" resolution function is the numerical convolution of the individual pieces:

$$I(t) = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2 \ldots \int I_{n-1}(t_{n-2}-t_{n-1})\,dt_{n-1}\, I_n(t_{n-1})$$

NOTE: What you gain in flexibility you lose in accuracy and computation speed.

To use the UDR resolution function

- add lines to INPut or PARameter file (see draft of page 122v.1 for users' guide)
- create file with udr function, formatted as described in table below
- see test case tr114 for example of how this might work

Format for Numerical User-Defined Resolution Function

Line No.	Col-umn	What	Meaning
1,2,...	any	Descriptive information, as many lines as needed	
3	1-5	----- (at least five hyphens)	end of descriptive information
4	1-?	Energy (eV)	energy at which resolution function will be given
5,6,...	1-?	Time (ns), Function	value of resolution function at the specified time
7	(end with a blank line)		

Repeat lines 4-7 as many times as needed, being sure to have same number of (time, function) values for each energy.

Note:

- Resolution function is assumed to be linear in time between the specified points
- SAMMY interpolates linearly to find resolution function at other energies
- It is probably not necessary to normalize the resolution function
- Use this with caution! It has not yet been thoroughly tested. Let me know about the successes as well as the failures. (Send e-mail to me at LarsonNM@ornl.gov .)