SAMMY Workshop Part 6

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Part 6, Higher-energy regions

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Higher-Energy Regions:

- Unresolved- Resonance Region
- High-Energy Region

Method: beg, borrow, steal from existing codes; incorporate into SAMMY (with the authors' blessings)

Initial modifications are for compatibility only, eventually refine and expand

Equations for Unresolved Resonance Region

SAMMY implementation based on Fritz Fröhner's FITACS program

- Hauser-Feshbach theory gives average total cross section

$$<\sigma_c> = \frac{\pi g_c}{k_c^2} \left(1 - \mathrm{Re} <S_{cc}>\right)$$

- Average scattering matrix $<S>$ is given by

$$<S_{cc}> = e^{-2i\varphi_c} \frac{1 - <R_{cc}> L_c^{0*}}{1 - <R_{cc}> L_c^{0}}$$

- Average R-matrix is

$$<R_{cc}> = R_c^{inf} + i\pi s_c$$

with

φ_c = hard-sphere scattering phase
R_c^{inf} = distant-level parameter
s_c = pole strength, equal to $S_c \sqrt{E} / 2 k_c a$
S_c = strength function
a = R-matrix matching radius

- Moldauer's prescription gives (non-elastic) partial cross sections in terms of "transmission coefficients" T_x

$$<\sigma_{ab}> = \frac{2\pi g_a}{k_a^2} \frac{T_a T_b}{T} \int_0^{inf} dt\ e^{-t T_\gamma / T} \prod_{c \notin \gamma} \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}}$$

where

a	=	incident channel	b	=	exit channel
ν_c	=	degrees of freedom (multiplicity)			
T_c	=	transmission coefficient	γ	=	photon channels
T	=	sum over all channels, $T = \sum_c T_c$			

- Transmission coefficient for neutron channels is

$$T_c = 1 - |<S_{cc}>|^2 = \frac{4\pi P_c s_c}{1 - <R_{cc}> L_c}$$

- Transmission coefficient for photon channel for spin J is

$$T_\gamma = 2\pi <\Gamma_\gamma> / D_J$$

- Transmission coefficient for fission channel for spin J is

$$T_f = 2\pi <\Gamma_f> / D_J$$

where D_J is the mean level spacing.

- Bethe formula gives J-dependence of the mean level spacing

$$\left(D_J(E)\right)^{-1} = \left(d(E)\right)^{-1} \left\{ \exp\left[\frac{-J^2}{2\left(\sigma(E)\right)^2}\right] - \exp\left[-\frac{(J+1)^2}{2\left(\sigma(E)\right)^2}\right] \right\}$$

where
d is independent of J
σ is the spin cutoff whose value is determined by the code.

- Gilbert-Cameron composite formula is used for energy dependence of the mean level spacing :

  - At low energy ($E_x \leq E_0$) use the constant-temperature formula

$$D^{-1} \propto C_3 \frac{\exp\left(C_2\sqrt{E_0 - PE}\right)}{(E_0 - PE)^{3/2}} \exp\left[\frac{E_x - E_0}{2}\left(\frac{C_2}{\sqrt{E_0 - PE}} - \frac{3}{E_0 - PE}\right)\right]$$

where E_x = excitation energy of compound nucleus

E_0 = matching energy , is given by the constant-temperature formula

PE = pairing energy

C_2 and C_3 = constants

  - At higher energies ($E_x \geq E_0$), use the Fermi-Gas formula

$$D^{-1} \propto C_3 \frac{\exp\left(C_2\sqrt{E_x - PE}\right)}{(E_x - PE)^{3/2}}$$

- Radiation widths $<\Gamma_\gamma>$ depend only on parity π and on E.
  Energy dependence calculated with giant dipole resonance model.

- Fission widths $<\Gamma_f>$ vary with spin as well as parity and E. Energy dependence calculated with the Hill-Wheeler fission barrier transmission coefficients.

$$<\Gamma_f(E)> = <\Gamma_f(0)> \frac{1 + \exp\left(E_{HW} / W_{HW}\right)}{1 + \exp\left(-(E - E_{HW}) / W_{HW}\right)}$$

where

E_{HW} = Hill-Wheeler threshold energy

W_{HW} = Hill-Wheeler threshold width

Assumptions for derivation of Moldauer's prescription

- Single-level Breit-Wigner is an adequate description of the cross section (i.e., resonances are well separated).

- Neutron widths obey the Porter-Thomas distribution (chi-squared with one degree of freedom); averages are therefore weighted with this distribution.

- The average of products can be written as the product of averages.

- Channels with the same transmission coefficients may be combined by introducing multiplicities.

Input for Unresolved-Resonance Region

Files needed:

- INPut file with three lines; the optional fourth line may be used only for Version M5 or later, not M2 or M2a.

  Card Set 1: This line is title only.

  Card Set 2: Nuclide name, atomic weight, energy range

  Card Set 3: UNRESOLVED RESONANCE REGION

  (optional): EXPERIMENTAL DATA ARE IN SEPARATE FILES

- ACS file (same as Fröhner's original FITACS file); see table for details (page 6-9).

- DATa files (for version M5 or later); see table for details.

Input for ACS file for treatment of the unresolved resonance region

Line No.	Description
1 - 4	First four lines are alphanumeric title
5	Number of iterations, fitting tolerance (essentially, delta chi-squared). Note that integers are to be specified as real numbers. All formats are F10
6	Mass in amu, radius in Fermi (or use default), neutron binding energy in MeV, pairing energy *PE* in MeV. Again, formats are F10
7,8,...	Center-of-mass excitation energy, spin, and parity for the *n*th target level (beginning with ground state)
9	(Blank)
10	Strength function S_c, uncertainty, distant-level parameter R_c^{inf}, uncertainty, radiation width $<\Gamma_\gamma>$ in eV, uncertainty, mean level spacing D in eV for $l = 0$
11	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 1$
12	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 2$
13, 14, ...	As above, for higher l values as needed
15	(Blank)
16, ...	Average fission width $<\Gamma_f>$ (eV), degree of freedom ν_f for fission width distribution, Hill-Wheeler threshold energy E_{HW}, HW threshold width W_{HW}, , uncertainty on the average fission width
17	(Blank)
(Cards 18-21 may appear in separate files, for Version M5 or later, if the phrase EXPERIMENTAL DATA ARE IN SEPARATE FILES appears in the INPut file.)	
18	Type of cross-section data (TOTAl, CAPTure, FISSion, or INELastic)
19	Uncertainties are RELAtive or ABSOlute
20, ...	Energy, cross section, uncertainty (Note: if RELAtive then need specify only for first data point, rest are assumed to be the same)
21	(Blank)
22, ...	Repeat 18 to 21 as many times as needed, in any order
(The following cards are relevant only for version M5 or later, not for M2 or M2a.)	
23	The single word "NORMALIZATION" in all capital letters or all lower case
24	Type of cross section, normalization parameters $a, \Delta a, b, \Delta b, c, \Delta c$, where the normalization for this data set is given by $norm = a + b E^c$
25, etc.	Repeat once for each data set. Note that normalizations must appear in the same order in which the data sets appear. SAMMY will check to be sure the data types are consistent

Changes made for SAMMY-M2

- Internal changes to be consistent with SAMMY notation and to use dynamic dimensioning
- Bayes' method for fitting procedure (prototype for eventual "restructured" SAMMY fitting module)
- Extension to all *l* - values
- Output includes "odf" files (plotting files)
- Results are reported in same format as input ACS file, in SAMMY.PAR (as well as in more legible fashion in SAMMY.LPT)

More recent changes (available in future releases):

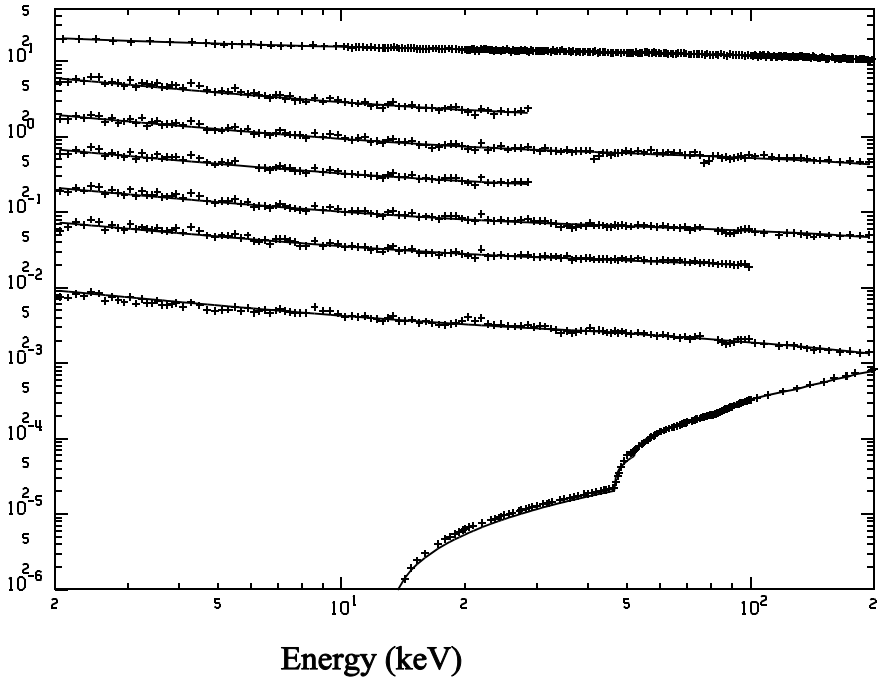
- As many data sets as desired (original code permitted at most one of each type)
- Separate file for each data set
- Energy-dependent normalization for each data set; normalization parameters can be varied
- Refinement (debugging) of partial derivatives for more accurate fitting
- More efficient quadrature scheme for Dresner integral

Needed Yet:

- Use results of resolved-resonance region analysis as input for analysis of unresolved region
- Experience!
- Generalize the theory as needed

Example: ^{235}U

(from current work of Herve Derrien; please note that results are preliminary and are not to be distributed)



SAMURR fit of ^{235}U experimental data in the energy range 2 keV to 200 keV. Crosses represent the experimental data (or evaluated data); solid lines are the cross sections calculated from average resonance parameters and nuclear parameters. The upper curve is the total cross section of Harvey (ORNL). The other curves represent (from upper to lower):

- Blons (Saclay) fission cross section (not modified)
- Migneco (Geel) fission cross section (divided by 3)
- Wagemans (Geel) fission cross section (didided by 9)
- Weston (ORNL) fission cross section (divided by 27)
- Perez (ORNL) fission cross section (divided by 81)
- Capture cross section inferred from Weston fission and experimental values of alpha (divided by 243)
- Inelastic cross section from ENDF/B-VI (divided by 1000)

Experimental fission data are average values from the original values found in the EXFOR file, using the same energy grid in the averaging code. The following parameters were varied:

- neutron strength function of angular momentum $l = 0, 1, 2$
- average fission widths
- average capture widths
- effective radius
- normalization coefficient for each set of fitted data

The normalization coefficients allow us to obtain a consistent set of data, which means that the same set of nuclear and average resonance parameters could represent all data in the experimental data base (after corrections for the remaining experimental effects).

Published results –

"Neutron Total Cross Sections of ^{235}U from Transmission Measurements in the Energy Range 2 keV to 300 keV and Statistical Model Analysis of the Data," H. Derrien, J. A. Harvey, N. M. Larson, L. C. Leal, and R.Q. Wright, ORNL/TM-2000/129, May 2000.

TNG

- Was written by Peter Fu of ORNL
- Is a multi-step Hauser-Feshbach model code for calculating neutron-induced reaction cross sections
- Contains a pre-equilibrium model formulated to be consistent with the Hauser-Feshbach part for conservation of angular momentum
- Has been in continuous development and used for ENDF/B data evaluations for nearly 30 years at ORNL
- Is being generalized for proton- and alpha-induced reaction cross sections