VIII. UNRESOLVED RESONANCE REGION

As a first step towards expansion into the unresolved resonance region, Fritz Fröhner's code FITACS [FF89] has been obtained and inserted into SAMMY. FITACS uses Hauser-Feshbach theory with width fluctuations. The adjustable parameters are neutron strength functions, distant-level parameters, average radiation widths (at $E = 0$), and average fission widths (at $E = 0$). The energy dependence of the radiation widths is specified via the giant dipole model, of the fission widths via Hill-Wheeler fission barrier transmission coefficients, and of the mean level spacing for *s*-waves via the Gilbert-Cameron composite formula. Mean spacings for $l > 0$ are given via the Bethe formula. Moldauer's prescription is used for partial cross sections. Details of the theory are presented in Section VIII.A.

Initially (for release M2 of the code), FITACS was incorporated into SAMMY (as segments SAMFFF and SAMACS) in a limited fashion only. Internal changes were made, to be consistent with SAMMY notation and to use dynamic dimensioning of arrays. The M + W version of Bayes' method has replaced the fitting procedure used in FITACS. Calculation of penetrabilities was extended to all l values (FITACS had used only s, p, d, and f-waves). The output included files from which plots can be made. Results were reported in SAMMY.PAR in the same format as is used in the input file (as well as in more human-legible fashion in SAMMY.LPT).

Subsequently, additional modifications, improvements, and new features have been made in the SAMMY URR treatment:

- Partial derivatives with respect to varied parameters are calculated exactly rather than approximately.
- A more efficient integration routine has been written for the Dresner integral, Eq. (VIII A.5).
- It is possible to include (and vary, if desired) a normalization for each data set.
- Elastic cross section data may be fitted.
- There is no limit on the number or type of experimental data sets. Data may be kept in separate files rather than appended to the parameter file.
- The output has been modified to conform more closely to SAMMY conventions.
- An "annotated" PARameter file, including key-word-based input, is the default input option, and the only option available for output. (Files in the original format can still be used for input, but options are limited with that format.)
- Different sets of average resonance parameters can be used in different energy ranges.

- Output can be produced in ENDF/B format, for both File 2 (resonance parameters) and File 32 (covariance matrices). ENDF files cannot be used for input, because the ENDF format requires a more limited theoretical description than does FITACS/SAMMY.

- The fitting procedure can be performed sequentially, in similar fashion as in the resolved resonance region. That is, output PARameter and COVariance files from the fit to one data set may be used as input to another run which fits another data set. [Initially, only simultaneous fitting of all data sets was permitted.]

- "No-Bayes" runs can be made: cross sections will be calculated from the resonance parameters, but no fitting will be done.

Additions being considered for future revisions of the code include the following:

- Multiple nuclides in the sample
- An option to calculate multigroup cross sections and covariances
- An option to include integral quantities in the fit
- Extensions to the theory
- Additional ENDF capability (requiring ENDF format changes)
- A link between the resolved resonance parameters and those for the unresolved region, in order to provide more consistent evaluated cross sections
- Methodologies for retroactive generation of covariance matrices, similar to that used in the resolved resonance region

Input for analysis of data in the unresolved resonance region is described in Section VIII.B. Output is described in Section VIII.C. The relationship between ENDF parameters and SAMMY/URR parameters is discussed in Section VIII.D.

For an example of the use of SAMMY/URR, see [HD00] and test cases 73, 88, 127, 133, 134, 142, and 145.