Nuclear Data for Science and Technology (1988 MITO), 573- 576, Copyright © 1988 JAERI.

RESONANCE PARAMETER ANALYSIS WITH SAMMY

Nancy M. Larson and Francis G. Perey

Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 37831-6356
United States of America

Abstract: The multilevel R-matrix computer code SAMMY has evolved over the past decade to become an important analysis tool for neutron data. SAMMY uses the Reich-Moore approximation to the multilevel R-matrix and includes an optional logarithmic parameterization of the external R-function. Doppler broadening is simulated either by numerical integration using the Gaussian approximation to the free gas model or by a more rigorous solution of the partial differential equation equivalent to the exact free gas model. Resolution broadening of cross sections and derivatives also has new options that more accurately represent experimental situations. SAMMY treats constant normalization and some types of backgrounds directly and treats other normalizations and/or backgrounds with the introduction of user-generated partial derivatives. The code uses Bayes' method as an efficient alternative to least squares for fitting experimental data. SAMMY allows virtually any parameter to be varied and outputs values, uncertainties, and covariance matrix for all varied parameters. Versions of SAMMY exist for VAX, FPS, and IBM computers.

(resonance parameters, R-matrix formalism)

Introduction

Analysis of neutron resonance cross-section or transmission data requires the use of sophisticated techniques to describe correctly all aspects of the experimental situation. Not only must the cross sections be calculated properly, but also Doppler- and resolution-broadening effects must be incorporated correctly, backgrounds and normalizations must be included as needed, and methods must be designed for simultaneous analysis of different data sets. The computer code SAMMY[1] has evolved over a period of years to meet these needs. SAMMY uses the Reich-Moore formalism for the generation of theoretical cross sections and Bayes' method as the fitting procedure. The 1985 version of SAMMY was described at the Santa Fe Conference;[2] in this paper we emphasize improvements subsequent to that conference.

Generation of Theoretical Cross Sections

Method

The Reich-Moore approximation[3] to multilevel R-matrix[4] is used for calculating the theoretical cross sections. Alternatively, the analyst can choose to use the multilevel Breit Wigner formalism.[5] Effects from resonances outside the energy region being analyzed may be included either by introducing "dummy" resonances or by using a logarithmic parameterization of the external R-function.

For compatibility with ENDF[6] SAMMY now permits the use of one radius for the potential scattering phase shift and another for evaluation of penetrability factor and level shift factor. Because ℓ-dependent radii have been found necessary for structural material analyses, SAMMY now allows the user to specify different radii (or sets of radii) for different spin groups; this option also accommodates the inclusion of several isotopes within one data set.

Parameters Which May Be Varied

For each resonance, the energy, gamma width, neutron width, and fission width(s) may be varied. Any of the seven parameters of the external R-function may be varied, as may any of the radii.

Doppler Broadening

Method

Two methods of simulating Doppler broadening are available in SAMMY.

Original The original method of Doppler broadening uses the Gaussian approximation to the free gas model. The numerical method of integration is based on that of code MULTI,[7] which used a four-point progressive interpolation scheme with the experimental data points used as the basis for the integration mesh. In SAMMY we have recently improved the automatic portion of the technique by judiciously introducing additional integration points to yield correct results in the neighborhood of small resonances. In addition, the user now has the option to add extra integration points between data points, thus increasing the accuracy for sparse data sets.

New The second method uses the exact free gas model. Our numerical solution of the partial differential equation employs a technique developed by Leal and Hwang.[8] Their technique uses an energy grid which is uniformly spaced with respect to $\sqrt{E}$ and thus requires considerable computer time and storage space. However, unlike SAMMY's original method, this method can be used at very low energies.

Parameters Which May Be Varied

The effective temperature may be varied for either of these methods of Doppler broadening.

Resolution Broadening

Method

Four different methods of simulating resolution broadening are available in SAMMY.

Original The first three, borrowed from MULTI, are: (a) Gaussian approximation for the distribution of flight path lengths and/or for the distribution of travel times; (b) exponential approximation; and (c) combination of Gaussian plus exponential. SAMMY now permits the input exponential width to be energy-dependent.

New The fourth method, recently developed and incorporated into SAMMY, is based on ideas discussed in Ref 9. This method uses a more realistic resolution function which is a convolution of functions representing four aspects of resolution broadening: (a) electron burst (square function of travel time); (b) the beam moderator (chi square distribution); (c) the neutron detector (exponential function of travel time, two forms available); and (d) time of flight channel (square function of travel time). Though this method was developed with ORELA data in mind, it is also likely to be useful with data from other white source facilities with proper modifications in the parameter values.

Parameters Which May Be Varied

Original The Gaussian and/or exponential widths may be varied in the original three methods.

New For the new method, any of the parameters may be varied. These include: (a) the electron burst width; (b) the coefficients in the expansion of moderator length as a function of energy; (c) the detector thickness and the distance to first collision; and/or (d) the channel width. Channel widths can differ from one energy region to another.

Data Reduction Parameters

Method

The sample thickness, an overall constant normalization, and four different analytical models for backgrounds are provided internally in SAMMY. The four backgrounds are: (a) constant; (b) linear in time; (c) inversely proportional to time; and (d) decaying exponential in time.

Other data reduction parameters require user-supplied partial derivatives of the (reduced) data with respect to those parameters. Possible types of parameters include: (a) energy-dependent normalization; (b) background proportional to some other cross section; and (c) variation in flux intensity. One method of generating the needed partial derivatives is discussed in Ref 10.

Parameters Which May Be Varied

Sample thickness, constant normalization, and parameters for the analytic background may all be varied. These latter include: (a) the constant background; (b) the coefficient of time; (c) the coefficient of inverse time; and (d) the exponential decay constant and the coefficient of the exponential.

Any of those data reduction parameters for which the user has provided partial derivatives may be varied.

Bayes' Method

The technique chosen for "fitting" theoretical calculations to experimental data in SAMMY is Bayes' method, which is a generalized least squares method for which all prior information is utilized. Our derivation of Bayes' equations is based on Bayes' theorem plus three assumptions involving normality and linearity; both the derivation and the assumptions are described in the SAMMY users' manual.[1]

Advantages

We have found numerous advantages to using Bayes' method rather than a more conventional least squares: (a) The method makes use of all information available to the analyst. (b) The equations retain a memory of earlier results. (c) Results of one analysis may be used as input to another. (d) Use of Bayes' equations ensures that sequential analyses are equivalent to simultaneous analysis. (e) Bayes' equations produce fewer numerical difficulties than least squares. (f) Contrary to least squares, parameters that do not affect the data will not "wander off" during the fitting procedure, but will remain relatively unchanged. (g) Off-diagonal data covariance matrices are automatically incorporated into the equations.

The price paid for these advantages is that starting values of parameters must be within the linear constraints of the theory. Successful users of SAMMY have discovered that the best results are obtained if starting values are obtained by a preliminary fit using limited energy ranges or using a simplified theory such as single-level Breit Wigner.

Implementation

Two forms of Bayes' equations are used in SAMMY: One, which we call the "N+V inversion scheme", involves the inversion of a symmetric matrix whose dimensions are the number of data points. This scheme is used when the number of parameters dominates. The second is called the "I+Q inversion scheme" and involves inversion of a nonsymmetric matrix whose dimensions are the number of varied parameters. This scheme is used when the number of data points dominates.

Data Types

Total cross section, transmission, elastic and/or inelastic scattering, fission cross section, capture cross section (without multiple scattering effects), and/or absorption cross section data may be analyzed in SAMMY. As many as seven data sets (of the same or different types) may be analyzed simultaneously [though they need not be unless data sets are correlated]. Off-diagonal data covariances may be included. Analyses can be made of data from either isotopically pure or natural materials.

The option to exclude specified spin groups from the calculation allows use of the same parameter set (and associated covariance matrix) for analyses of quite different data sets. Thus consistent analyses can be made of transmission data plus spin separated fission data, or of data from natural materials plus isotopic data.

Programming Details

Computer Systems

SAMMY is "up" on at least three types of computers, the VAX, the Floating Point Systems (FPS) Array Processor (AP), and the IBM. SAMMY is written in FORTRAN. On the ORELA VAX 785, the code is compiled using the FORTRAN 77 compiler. On the FPS and IBM, SAMMY compiles with the current version of those computers' FORTRAN compilers. Most coding is not machine-dependent.

SAMMY Segments

SAMMY is divided into two dozen stand-alone programs or "segments". The segments communicate via temporary files. One segment calls another using the RUN subroutine, which is a system program on the VAX and FPS and an assembly-language routine on the IBM.

Other Features of SAMMY

Input

In the input file which the analyst must prepare before running SAMMY, commands are in alphanumeric form, permitting the analyst to see at a glance what a run should be doing. Many input errors will be recognized as such by SAMMY, which then prints an error message and, if the error is severe, aborts execution. The analyst must also provide a parameter file which contains initial values and uncertainties (plus covariances if they are known) for all variable parameters. Finally, a data file contains the experimental information (energies, cross sections or transmissions, and uncertainties).

Output

SAMMY produces several different types of output files. An "LPT" file, intended to be printed and examined by the analyst, contains initial and final values of the parameters and covariance matrix as well as other information generated during the SAMMY run. A binary "COV" file stores the parameter covariance matrix (and considerable other information as well) for possible use as input for a subsequent SAMMY run. An "ODF" or "plot" file contains the information from which plots of data, initial theoretical curves, and final theoretical curves can be made.

In addition to calculating updated parameter values and covariance matrices, SAMMY can provide certain special types of output: (a) Energy-averaged theoretical values and uncertainties for comparison to summed experimental data. (b) An output file of the updated resonance parameters in ENDF/B-VI format.[6] (c) The summed strength function and the corresponding covariance matrix.

Optimization

The user is spared difficulties of adjusting array sizes when using SAMMY, since dynamic allocation of array storage automatically permits the greatest number of data points for the given number of varied parameters. Very large arrays are stored in temporary files, pieces of which are read as needed.

Auxiliary programs

Auxiliary programs are available to be used in conjunction with SAMMY to perform specific tasks.

SAMADD, SAMMIX Manipulation of parameter and/or covariance files, to reorganize which data-related parameters are to be in use and which to be moth-balled temporarily, is performed by the two programs SAMADD and SAMMIX.

SAMEST Because array dimensions are not fixed in advance, but rather are adjusted dynamically as SAMMY runs, it is nontrivial to determine in advance what configuration of parameters and data points will fit into a computer. SAMEST estimates the array storage requirements for the configuration specified by the user.

SAMF2V, SAMV2F Conversion of binary files from the FPS computer system to the VAX is accomplished by SAMF2V, and the reverse by SAMV2F.

SAMCNV The purpose of this program is to read the output binary covariance file and produce an ASCII file which contains the complete covariance matrix for all resonance parameters, including those which were not varied during the runs which produced the SAMMY binary covariance file.

FORODF To produce plots of experimental cross sections (or transmissions), theoretical cross sections from initial and/or adjusted values of the parameters, uncertainties, etc., from the ORELA Data Format (ODF) "plot file" produced by SAMMY, ORELA analysts use the code FORODF.[11] This is a general-purpose plotting code for ODF files and is not specifically a SAMMY-related program.

Examples

Over 25 publications have discussed resonance parameter analyses using SAMMY; a list is available from the authors. A recent SAMMY analysis, which makes uses of many of the new features of SAMMY, is reported at this conference.[12]

Documentation

SAMMY is thoroughly documented: Comment cards are sprinkled liberally throughout the FORTRAN, facilitating understanding and updating of the code. More important from a user's point of view is the existence of an extensive users' manual.[1] The manual contains detailed discussions of each aspect of SAMMY, including definitions of terms and mathematical derivations. Tables show input formats for each input file. A few examples are given in the manual, including both input and output; additional examples are available from the authors.

Future Plans

Multiple-scattering effects and self-shielding for capture experiments have not yet been included in SAMMY, but are being studied for possible future incorporation into the code. Also under consideration is the question of adjusting energy scales so that resonances appearing in different measurements occur at the same energies in each data set.

Acknowledgements

The authors wish to thank SAMMY users G. de Saussure, C. M. Perey, and D. C. Larson for their input to and review of this report and of the poster presentation. The patient assistance of Sue Damewood in typing both this report and the poster pages is gratefully acknowledged.

Research is sponsored by the Office of Energy Research, Nuclear Physics, U.S. Department of Energy, under contract DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

REFERENCES

1. N. M. Larson, *Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations*, ORNL/TM-9179 (1984). See also ORNL/TM-9179/R1 (1985) and ORNL/TM-9179/R2 (to be published in 1988).

2. N. M. Larson, "Analysis of Neutron Data in the Resonance Region via the Computer Code SAMMY, Nuclear Data for Basic and Applied Science," Vol. 2, *Proceedings of the International Conference, Santa Fe, New Mexico*, Gordon and Breach Science Publishers, 1533-1536 (1986).

3. C. W. Reich and M. S. Moore, *Phys. Rev.* **111**, 929 (1958).

4. A. M. Lane and R. G. Thomas, *Rev. Mod. Phys.* **30**, 257 (1958).

5. H. A. Bethe, *Rev. Mod. Phys.* **9**, 69 (1937).

6. "Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF-6," to be published.

7. George F. Auchampaugh, *MULTI, A FORTRAN Code for Least-Squares Shape Fitting of Neutron Cross-Section Data Using the Reich-Moore Multilevel Formalism*, LA-5473-MS, Los Alamos Scientific Laboratory, Los Alamos, NM (1974).

8. Luiz C. Leal and Richard N. Hwang, "A Finite Difference Method for Treating the Doppler Broadening of Neutron Cross Sections," *Transactions of the American Nuclear Society* **55**, 340 (1987).

9. D. C. Larson, N. M. Larson, and J. A. Harvey, *ORELA Flight Path 1: Determinations of its Effective Length vs Energy, Experimental Energies, and Energy Resolution Function and Their Uncertainties*, ORNL/TM-8880, 1984.

10. N. M. Larson, *User's Guide for ALEX: Uncertainty Propagation from Raw Data to Final Results for ORELA Transmission Measurements*, ORNL/TM-8676, ENDF-332, 1984.

11. J. G. Craven, *OPRODF, A DECsystem-10 Data Manipulation for ORELA Data Formatted Files*, ORNL/CSD/TM-45 (May 1978).

12. "R-Matrix Analyses of the ^{235}U and ^{239}Pu Neutron Cross Sections," H. Derrien, G. de Saussure, L. C. Leal, R. B. Perez, and N. M. Larson, paper AA10(072), presented at this conference.