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ANALYSIS OF NEUTRON DATA IN THE RESONANCE REGION VIA THE COMPUTER CODE SAMMY*

N. M. LARSON

Oak Ridge National Laboratory, Oak Ridge, Tenn. 37831 USA

Abstract Procedures for analysis of resonance neutron cross-section data have been implemented in a state-of-the-art computer code SAMMY,¹⁻³ developed at the Oak Ridge Electron Linear Accelerator (ORELA) at Oak Ridge National Laboratory. A unique feature of SAMMY is the use of Bayes' equations to determine "best" values of parameters, which permits sequential analysis of data sets (or subsets) while giving the same results as would be given by a simultaneous analysis. Another important feature is the inclusion of data-reduction parameters in the fitting procedure. Other features of SAMMY are also described.

INTRODUCTION

In 1979 the need for a multilevel R-matrix code incorporating both (1) the best features of the code MULTI⁴ and (2) the use of Bayes' method was recognized at ORELA. The resulting code, SAMMY,¹⁻³ has evolved continuously over the intervening years in an effort to meet the requirements for analysis of ORELA (and other) data. Four SAMMY analyses are reported at this conference;⁵⁻⁸ a list of publications of other SAMMY analyses is available from the author. In this paper we concentrate on describing options available in SAMMY, rather than on discussing results of specific analyses.

BAYES' METHOD

The major distinguishing feature of SAMMY is its use of Bayes' method rather than least squares to update parameter values and to determine the covariance matrix for those parameters. Bayes' method may be viewed as a *generalized* least-squares technique, for which prior information is incorporated into the equations.

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(Equations and deviations thereof are presented in the SAMMY users' manuals.¹⁻³) As a result, SAMMY has several advantages over codes using least-squares techniques: (1) Inclusion of data covariances is straightforward. (2) If a varied parameter is irrelevant to the data being analyzed, both its value and its uncertainty will be unchanged by the analysis. With least-squares techniques, the value of such a parameter is often subject to unreasonable changes. (3) Results from one analysis may be communicated to a subsequent analysis by using the output parameter values and covariance matrix from the first analysis as input to the second. Output parameter values from the second analysis then produce a valid fit for *both* data sets. (4) As a consequence of item (3), a series of *sequential* analyses of data subsets may be used to obtain results effectively equivalent to those obtained from a single *simultaneous* analysis of the combined data sets. The overall fit for analysis of a data set will lie within experimental uncertainties whether the data set was analyzed in one piece or in several smaller pieces.

DATA-REDUCTION PARAMETERS

A recent innovation in SAMMY is the ability to include data-reduction parameters as well as theory parameters in the fitting procedure. Seven parameters (sample thickness, normalization, and five parameters for energy-dependent backgrounds) are treated explicitly, in the sense that users need merely specify values and uncertainties and set flags to indicate which parameters are to be varied.

In addition to treating some parameters explicitly, SAMMY has available a general scheme to vary any data-reduction parameter. Partial derivatives of the reduced data with respect to the data-reduction parameters are fed into SAMMY along with the data and the statistical uncertainties. (For a method whereby these partial derivatives may be generated, see ref. 9.) SAMMY's fitting procedure (Bayes' method) then updates values and uncertainties for both kinds of parameters. This ability to include data-reduction parameters as part of the fitting procedure allows the correct treatment of data uncertainties, even for very large data sets. The alternative is to treat the data covariance matrix in its full form (off-diagonal), which requires that all correlated data be analyzed simultaneously. This is impractical for very large data sets such as those generated at ORELA.

OTHER FEATURES OF SAMMY

The Reich-Moore approximation to multilevel R-matrix theory is used to generate theoretical cross sections in SAMMY; alternatively, multilevel Breit-Wigner may be used. Contributions from resonances outside the energy region being analyzed may be parameterized either as "dummy" resonances or via a logarithmic function. Virtually any parameter of the R-matrix or external R-function may be varied.

COMPUTER CODE SAMMY

Broadening of both cross sections and partial derivatives is accomplished by numerically folding a Doppler- and/or resolution-broadening function with the theoretical cross section or derivative. The Doppler broadening function is a Gaussian of width proportional to $\sqrt{ET_{eff}}$. Resolution broadening appropriate for a white source is included as a Gaussian function, an exponential function, or a convolution of the two. A more general parameterization of resolution broadening will soon be incorporated, allowing the user to more accurately mimic actual experimental conditions. Broadening parameters may be varied as part of the fitting procedure.

Data types which may be analyzed with SAMMY include transmission, total cross section, elastic and/or inelastic scattering, fission, capture, or absorption cross sections. (Multiple-scattering corrections for capture are not yet incorporated into SAMMY but are planned for the near future.) SAMMY permits analysis of several types of data simultaneously, though such analyses are needed only when data sets are correlated.

Input to SAMMY, though necessarily somewhat complex, was designed to be user-friendly. Where possible, descriptive alphanumeric phrases are used rather than numerical flags whose meanings are more easily misinterpreted. SAMMY tests all input for internal inconsistencies and other obvious errors; in most cases SAMMY will inform the user what error needs correcting.

SAMMY is written in FORTRAN, with few machine-dependent constructions. Dynamic allocation of array storage and the use of temporary files permit SAMMY to run large jobs on relatively small computers. Versions of SAMMY have been adapted for DEC PDP-10, VAX, and IBM computers. Thorough documentation is available, both via extensive comment cards in the FORTRAN and via the users' guide.¹⁻³

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