IV. THE FITTING PROCEDURE

In order to determine the parameter values that give the "best fit" of theoretical values to experimental measurements, a fitting procedure is needed. The procedure must properly incorporate all uncertainties in the measured data, including both statistical and systematic uncertainties, and should provide appropriate uncertainties and correlations for the resulting set of parameter values.* The fitting procedure must be able to deal with nonlinear systems.

The procedure used in SAMMY is Bayes' method, sometimes denoted "generalized least squares." See Section XI.C for a philosophical discussion of the implications of the use of Bayes' method.

(In the limit of infinite prior uncertainty, under the customary assumptions of normality, Bayes' method reduces to the more familiar least-squares method. SAMMY contains provisions for using the least-squares method rather than the more powerful generalized least squares; see Section IV.E.3 for details.)

Section IV.A is devoted to a formal description of the relevant equations for Bayes' method. Starting from Bayes' theorem [HJ61] and three basic assumptions, formulae are derived for updating parameter values and parameter covariance matrix elements based on information contained in the data currently being analyzed. These formulae, in their several guises, are hereafter referred to as Bayes' equations. The three versions used in the SAMMY code are derived in Section IV.A.1, and the iterative versions thereof (for use with nonlinear systems) in Section IV.A.3. Formulae for chi squared are developed and discussed in Section IV.A.2.

Implementation of each of the three versions of Bayes' equations in SAMMY is described in Section IV.B.

Most input parameters may be fitted in the SAMMY code, though the actual fitted parameter is not always the variable given in the input. For example, though values for the resonance energies are given in the PARameter file, the variable used in the fitting procedure is the square root of the resonance energy. In Section IV.C, parameters that may be varied are listed.

Section IV.D contains a discussion of the Data Covariance Matrix (DCM), its role in Bayes' equations, and SAMMY's various treatments of the DCM. SAMMY has the ability to read, store, and invert a full off-diagonal DCM; however, the reader should be aware that this is a highly inefficient method for treating experimental uncertainties. Instead, when components of the DCM are generated external to SAMMY, those components (rather than the DCM itself) should be used as input to the code via the User-Supplied Implicit DCM option (Section VI.C.3.b has input details for this option). To include the contribution from uncertainties on SAMMY input parameters, the Propagated Uncertainty Parameter (PUP) option is available; see the discussion in Section IV.D.2

* Uncertainties determined by R-matrix codes are often deemed to be too small. It is this author's opinion that the resonance parameter uncertainties are correct, but that the resonance parameter covariance matrix alone is insufficient to describe all the uncertainty in the evaluated cross sections. For further discussion on this topic, the reader is refered to Section IV.E.6.

and the input details in Section VI.C.3.a. In both cases, the full DCM is not calculated; instead, the treatment is via SAMMY's Implicit Data Covariance (IDC) method, described in Section IV.D.3.

Section IV.E contains information about a variety of topics related to covariances. For a discussion of simultaneous (rather than sequential) fitting of several data sets, see Section IV.E.1. In Section IV.E.2, information is found on SAMMY's retroactive covariance method, whereby a parameter covariance matrix can be generated that is approximately correct for a given parameter set. To use an infinite prior parameter covariance matrix (i.e., to use the least-squares equations), see Section IV.E.3. Generating the covariance matrix associated with the theoretical cross section is described in Section IV.E.4. Section IV.E.5 describes SAMMY's method for calculating average values and uncertainties for certain classes of resonance parameters (e.g., the average capture or neutron width for all resonances in a particular spin group). Finally, Section IV.E.6 contains a discussion of the capability of the resonance parameter covariance matrix (RPCM) to produce credible cross section covariance matrices, and describes available methods for altering or augmenting the SAMMY-produced RPCM, in preparation for reporting to ENDF and/or publishing results.