IV.C. CONSTRUCTING THE PARAMETER SET

Several distinct types of parameters may be varied (i.e., "fitted" or "searched on" in least-squares jargon) in SAMMY. Alternatively, these parameters may be treated as PUPs (propagated uncertainty parameters, as described in Section IV.D.2). Input values for all varied parameters are given in the PARameter file, Table VI B.2; input values for PUPs may generally be given in either the PARameter file or the INPut file. The different types of parameters are listed below; the list is not necessarily all-inclusive.

- Resonance energies and widths: that is, the Reich-Moore R-matrix parameters as described in Section II.B.1 (or the Breit-Wigner parameters as discussed in Section II.B.3). Values for energies and widths are provided via card set 1 of Table VI B.2.

- The matching radii (or channel radii) for the different spin groups and/or potential scattering vs. penetrabilities and shift factors. Values for the matching radii are given in card set 7 or card set 7a of Table VI B.2.

- The seven parameters of the external R-function. These are described in Section II.B.1.d; values are input to the code as shown in card set 3 of Table VI B.2.

- Effective temperature for Doppler broadening, as described in Section III.B. Input is in card set 4 of Table VI B.2.

- Resolution-broadening parameters. For the original formulation (Gaussian and/or exponential) of resolution broadening, Section III.C.1, input is in card set 4 of Table VI B.2. For the Oak Ridge Resolution Function of Section III.C.2, input is in card set 9. For the RPI/GELINA/nTOF Resolution Function of Section III.C.3, input is in card set 14.

  [The parameter for the straight-line energy average resolution function, Section III.C.4, is not variable. Until the author is able to do more extensive testing, it is recommended that parameters of the user-defined resolution function, Section III.C.5, also not be considered variable.]

- Normalization and background functions. See Section III.E.3.a for description and card sets 6 and 13 for input details.

- Abundances for the various nuclides. See card set 10 of Table VI B.2.

- Sample thickness *n*. See card set 4 of Table VI B.2.

- Any of the miscellaneous parameters in card set 11 of Table VI B.2.

- Detector efficiencies, card set 15 of Table VI B.2.

For each parameter of each type, the user sets a flag that specifies whether that particular parameter is to be treated as a constant number (flag = 0), varied (flag = 1), or PUP'd (flag = 3). SAMMY counts the number NFPALL of flagged (varied + PUP'd) parameters and sets up an array *U* of dimension NFPALL. The initial values *P* needed in Bayes' equations [see, for example,

Eq. (IV A1.2)] are stored in *U*. These values are not necessarily the same as those input in the PARameter file, but bear some functional relationship to the input form. For example, *U* will equal the reduced width amplitude $\gamma_{\lambda c}$ rather than the channel width $\Gamma_{\lambda c}$ [see Eq. (II A1.3)]. Details concerning conversion to the "*u*-parameters" are given in the sections relevant to the particular parameter.

Input uncertainties and correlations are likewise converted to represent the uncertainties and correlations on the *u*-parameters. Let p_i represent a physical parameter as input in the PARameter file, and let u_i be the related *u*-parameter. Since $u_i = u_i(p_i)$ is a precisely specified functional relationship, we also know $\partial u_i / \partial p_i$. Therefore, assuming u_i is unrelated to other parameters, a small increment in u_i is related to an increment in p_i via $\delta u_i = (\partial u_i / \partial p_i)\delta p_i$. This relationship may then be used to convert from the covariance matrix for *p* to the covariance matrix for *u*; that is,

$$M_{ij} = \langle \delta u_i \, \delta u_j \rangle = \frac{\partial u_i}{\partial p_i} \langle \delta p_i \, \delta p_j \rangle \frac{\partial u_j}{\partial p_j} \quad , \qquad \text{(IV C.1)}$$

where *M* is the covariance matrix needed for Bayes' equations, and $\langle \delta p_i \delta p_j \rangle$ represents the "input" or initial covariance matrix.

In some cases, a *u*-parameter may be related to more than one of the *p*-parameters. This is true, for example, when both the resonance energy and the neutron width are flagged; see Section II.D.1.e for a discussion of the modifications that must be made in this case. The appropriate version of Eq. (IV C.1) for this situation is

$$M_{ij} = \langle \delta u_i \delta u_j \rangle = \sum_{k,l} \frac{\partial u_i}{\partial p_k} \langle \delta p_k \delta p_l \rangle \frac{\partial u_j}{\partial p_l} \quad . \qquad \text{(IV C.2)}$$