II.D. DERIVATIVES

In order to make use of sophisticated fitting procedures such as Bayes' equations (Section IV of this manual), it is necessary to know the partial derivatives of the theory with respect to the parameters to be fitted (the "varied parameters"). The easiest method for calculating derivatives of cross sections with respect to resonance parameters is to use a numerical difference approximation, of the form

$$\frac{\partial\sigma}{\partial P} \approx \frac{\sigma\left(P+\Delta P\right)-\sigma\left(P\right)}{\Delta P} \quad , \tag{II D.1}$$

or, to avoid problems from the asymmetry of that approximation,

$$\frac{\partial\sigma}{\partial P} \approx \frac{\sigma\left(P+\Delta P\right)-\sigma\left(P-\Delta P\right)}{2\Delta P} \quad . \tag{II D.2}$$

Numerical methods, however, are neither as accurate nor as efficient or rapid as analytic derivatives. For that reason, SAMMY uses analytic derivatives wherever possible. In particular, derivatives of cross sections with respect to resonance parameters are all calculated analytically.

To reiterate: SAMMY does NOT use numerical derivatives of the form (II D.1). When a numerical derivative is absolutely necessary, the form (II D.2) is used. For R-matrix parameters, analytic derivatives are always used. (The only exception to this rule is for charged-particle shift factors and penetrabilities, for which calculations of both the functions and the derivatives require numerical techniques.)

The R-matrix equations are expressed in terms of the reduced-width amplitude γ rather than the partial width Γ. In the SAMMY code, the amplitudes are the parameters to be varied. In general, SAMMY distinguishes between "*u*-parameters" and "*p*-parameters": The *u*-parameter is the variable whose value is sought by the fitting procedure. The *p*-parameter is the parameter whose value is given in the SAMMY input and output files. There is a well-defined relationship between the two, but the relationship is not necessarily one to one. For example, the value for the neutron width specified in the input PARameter file (see Table VI B.2 in Section VI.B) is related to three parameters, any or all of which might be varied:

$$\Gamma_{\lambda n} = 2P_l(\rho)\gamma_{\lambda n}^2 \quad ,$$

$$\rho_\lambda = k_\lambda a_n \quad , \tag{II D.3}$$

and

$$\hbar k_\lambda = \frac{M}{m+M}\sqrt{2mE_\lambda} \quad .$$

Here γ_λ, a_n, and E_λ all may be varied parameters. In the SAMMY input, varied parameters are indicated by a flag, whose value (0, 1, or 3) indicates how that parameter is to be treated. The convention is that a flag on Γ denotes the status of the γ parameter, because the other two (the radius and the energy) are separately flagged.

Throughout this document, when the varied *u*-parameter is different from the flagged *p*-parameter, the equations relating the two are given explicitly. For the R-matrix (in all its various guises), the *u*-parameter associated with the resonance energy is

$$u\left(E_\lambda\right) = \pm\sqrt{\left|E_\lambda\right|} \quad , \tag{II D.4}$$

where the negative sign is chosen if E_λ is negative, and the *u*-parameter associated with the width is

$$u\left(\Gamma_{\lambda c}\right) = \gamma_{\lambda c} \quad . \tag{II D.5}$$

In the following sections, equations are given for the derivatives of the cross section with respect to the R-matrix parameters for the Reich-Moore approximation (Section II.D.1) and for the Breit-Wigner approximations (Section II.D.2). Additional details are in Section II.D.3.