II.D.1.e. Derivatives with respect to *p*-parameters

As described in Section II.B.1, internally SAMMY operates in terms of the *u*-parameters, these being the parameters whose values are to be fitted via Bayes' equations (see Section IV). The *u*-parameters are related, but not necessarily equal, to the parameters whose values are given in the INPut and/or PARameter files, which are denoted as *p*-parameter.

When only the SAMMY code is used for calculations, there is no confusion arising from switching between *u*- and *p*-parameters. The transformation from *u*- to *p*-parameters also poses no difficulties in communicating parameter *values* between SAMMY and other codes (e.g., via ENDF files). However, in communicating uncertainty, covariance, or sensitivity (partial derivative) information, care must be taken to ensure that transformations are properly made.

In particular, the transformations involving the resonance energy and the partial widths must be calculated carefully.* The *p*-parameter for a particle width Γ, for example, is related to the corresponding *u*-parameter γ via the transformation [see Eq. (II B1.7)]

$$u_{\Gamma_{\lambda c}} = \gamma_{\lambda c} = \pm \sqrt{\frac{\Gamma_{\lambda c}}{2P_l\left(\left|E_\lambda - \Xi_c\right|\right)}} \quad , \tag{II D1 e.1}$$

where P in this equation is the penetrability (with the appropriate angular momentum l for this channel) evaluated at E_λ, the energy of the resonance.

From Eqs. (II A.8) and (II A.9), P has the form

$$P_l = P_l(\rho) \qquad \text{with} \qquad \rho = \beta\, a_c \sqrt{\left(\left|E_\lambda - \Xi\right|\right)} \quad , \tag{II D1 e.2}$$

in which β is a mass factor given explicitly in Eq. (II A.9), a_c is the channel radius, and Ξ represents the threshold energy. The ± sign in Eq. (II D1 e.1) is as given in the PARameter file (Table VI B.2). E_λ is another *p*-parameter, for which the corresponding *u*-parameter is

$$u_{E_\lambda} = \begin{cases} \sqrt{E_\lambda} & \text{for } E_\lambda > 0 \\ -\sqrt{-E_\lambda} & \text{for } E_\lambda < 0 \quad , \end{cases} \tag{II D1 e.3}$$

from Eq. (II B1.6).

In the following discussion, most subscripts are omitted, for simplicity's sake. Equations for negative-energy resonances are indicated within square brackets.

* In early versions of SAMMY, these transformations were done incorrectly. These mistakes have been corrected in release R7 of this manual and in sammy-7.0.0 and subsequent releases of the code.

Consider a function f of the two u-parameters γ and u (which we take to be the u-parameter associated with the resonance energy). This function might be the cross section, or some other function such as transmission or average cross section. The equations of transformation to the two p-parameters Γ and E_λ are given above. The derivatives of f with respect to the p-parameters are therefore

$$\frac{\partial f}{\partial \Gamma} = \frac{\partial \gamma}{\partial \Gamma}\frac{\partial f}{\partial \gamma} + \frac{\partial u}{\partial \Gamma}\frac{\partial f}{\partial u} \tag{II D1 e.4}$$

and

$$\frac{\partial f}{\partial E_\lambda} = \frac{\partial \gamma}{\partial E_\lambda}\frac{\partial f}{\partial \gamma} + \frac{\partial u}{\partial E_\lambda}\frac{\partial f}{\partial u} \quad . \tag{II D1 e.5}$$

The partial derivatives of the u-parameters with respect to the p-parameter Γ can readily be found from Eqs. (II D1 e.1) and (II D1 e.3) as

$$\frac{\partial \gamma}{\partial \Gamma} = \pm \frac{1}{\sqrt{2P}}\frac{1}{2}\Gamma^{-1/2} = \pm\frac{1}{2}\sqrt{\frac{\Gamma}{2P}}\frac{1}{\Gamma} = \frac{\gamma}{2\Gamma} \quad , \tag{II D1 e.6}$$

and

$$\frac{\partial u}{\partial \Gamma} = 0 \quad . \tag{II D1 e.7}$$

The derivative of u with respect to E_λ is relatively straight forward:

$$\begin{gathered} \frac{\partial u}{\partial E_\lambda} = \frac{1}{2}E_\lambda^{-1/2} = \frac{1}{2u} = \frac{u}{2E_\lambda} \\ \left[\frac{\partial u}{\partial E_\lambda} = \frac{1}{2}\left(-E_\lambda\right)^{-1/2} = -\frac{1}{2u} = \frac{u}{2E_\lambda} \quad \text{if } E_\lambda < 0\right]. \end{gathered} \tag{II D1 e.8}$$

The derivative of γ with respect to E_λ is somewhat more complicated, having the form

$$\frac{\partial \gamma}{\partial E_\lambda} = \pm\sqrt{\frac{\Gamma}{2}}\left(-\frac{1}{2}\right)P^{-3/2}\frac{dP}{d\rho}\frac{\partial \rho}{\partial E_\lambda} = \mp\frac{1}{2}\sqrt{\frac{\Gamma}{2P}}\frac{P'}{P}\frac{\partial \rho}{\partial E_\lambda} = -\frac{\gamma P'}{2P}\frac{\partial \rho}{\partial E_\lambda} \quad , \tag{II D1 e.9}$$

in which we have defined P' to be $dP/d\rho$. From Eq. (II D1 e.2), for $E_\lambda > \Xi$, it follows that

$$\frac{\partial \gamma}{\partial E_\lambda} = -\frac{\gamma P'}{2P}\frac{\beta a}{2\sqrt{\left(E_\lambda - \Xi\right)}} = -\frac{\gamma P'}{4P}\frac{\rho}{\left(E_\lambda - \Xi\right)} \quad . \tag{II D1 e.10}$$

Similarly, for $E_\lambda < \Xi$, we find

$$\frac{\partial\gamma}{\partial E_\lambda} = -\frac{\gamma P'}{2P}\frac{\partial}{\partial E_\lambda}\,\beta a\sqrt{-\left(E_\lambda-\Xi\right)} = -\frac{\gamma P'}{2P}\frac{\beta a\left(-1\right)}{2\sqrt{-\left(E_\lambda-\Xi\right)}}$$
$$= +\frac{\gamma P'}{4P}\frac{\beta a\sqrt{-\left(E_\lambda-\Xi\right)}}{-\left(E_\lambda-\Xi\right)} = -\frac{\gamma P'}{4P}\frac{\rho}{\left(E_\lambda-\Xi\right)} \quad . \tag{II D1 e.11}$$

Equations (II D1 e.4) and (II D1 e.5) can therefore be rewritten as

$$\frac{\partial f}{\partial\Gamma} = \frac{\gamma}{2\Gamma}\frac{\partial f}{\partial\gamma} + 0 \tag{II D1 e.12}$$

and

$$\frac{\partial f}{\partial E_\lambda} = -\frac{\gamma P'}{4P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{\partial f}{\partial\gamma} + \frac{u}{2E_\lambda}\frac{\partial f}{\partial u} \quad . \tag{II D1 e.13}$$

Similarly, if the function f is defined in terms of p-parameters, the derivatives of f with respect to the u-parameters are given by

$$\frac{\partial f}{\partial\gamma} = \frac{\partial\Gamma}{\partial\gamma}\frac{\partial f}{\partial\Gamma} + \frac{\partial E_\lambda}{\partial\gamma}\frac{\partial f}{\partial E_\lambda} \tag{II D1 e.14}$$

and

$$\frac{\partial f}{\partial u} = \frac{\partial\Gamma}{\partial u}\frac{\partial f}{\partial\Gamma} + \frac{\partial E_\lambda}{\partial u}\frac{\partial f}{\partial E_\lambda} \quad . \tag{II D1 e.15}$$

That is, the inverse transformation (from p-space to u-space) requires the use of the partial derivatives of p-parameters with respect to the u-parameters. These derivatives have the form

$$\frac{\partial\Gamma}{\partial\gamma} = \pm 2P\,2\gamma = \pm 4P\gamma = \frac{2\Gamma}{\gamma} \quad , \tag{II D1 e.16}$$

$$\frac{\partial E_\lambda}{\partial\gamma} = 0 \quad , \tag{II D1 e.17}$$

and

$$\frac{\partial E_\lambda}{\partial u} = 2u = \frac{2E_\lambda}{u} \qquad \left[\ \frac{\partial E_\lambda}{\partial u} = -2u = \frac{2E_\lambda}{u} \ \text{ if } E_\lambda < 0\right] \quad . \tag{II D1 e.18}$$

The partial derivative of Γ with respect to u requires special care to evaluate correctly. For $u^2 = E_\lambda > \Xi$, this derivative has the form

$$\begin{aligned} \frac{\partial \Gamma}{\partial u} &= 2\frac{\partial P}{\partial u}\gamma^2 = \frac{2P\gamma^2}{P}\frac{dP}{d\rho}\frac{\partial \rho}{\partial u} = \Gamma\frac{P'}{P}\frac{\partial}{\partial u}\left(\beta a\sqrt{\left(u^2-\Xi\right)}\right) \\ &= \Gamma\frac{P'}{P}\frac{\beta a 2u}{2\sqrt{\left(u^2-\Xi\right)}} = \Gamma\frac{P'}{P}\frac{\beta a\sqrt{\left(u^2-\Xi\right)}\,u}{\left(E_\lambda-\Xi\right)} = \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u}\ . \end{aligned} \qquad \text{(II D1 e.19)}$$

If $0 < E_\lambda = u^2 < \Xi$, this partial derivative takes the form

$$\begin{aligned} \frac{\partial \Gamma}{\partial u} &= 2\frac{\partial P}{\partial u}\gamma^2 = \frac{2P\gamma^2}{P}\frac{dP}{d\rho}\frac{\partial \rho}{\partial u} = \Gamma\frac{P'}{P}\frac{\partial}{\partial u}\left(\beta a\sqrt{-\left(u^2-\Xi\right)}\right) \\ &= \Gamma\frac{P'}{P}\frac{\beta a\left(-2u\right)}{2\sqrt{-\left(u^2-\Xi\right)}} = \Gamma\frac{P'}{P}\frac{\beta a\sqrt{-\left(u^2-\Xi\right)}\left(-u\right)}{-\left(u^2-\Xi\right)} \\ &= \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u}\ . \end{aligned} \qquad \text{(II D1 e.20)}$$

[Finally, if $0 > E_\lambda = -u^2$, then

$$\begin{aligned} \frac{\partial \Gamma}{\partial u} &= 2\frac{\partial P}{\partial u}\gamma^2 = \frac{2P\gamma^2}{P}\frac{dP}{d\rho}\frac{\partial \rho}{\partial u} = \Gamma\frac{P'}{P}\frac{\partial}{\partial u}\left(\beta a\sqrt{-\left(-u^2-\Xi\right)}\right) \\ &= \Gamma\frac{P'}{P}\frac{\beta a\left(2u\right)}{2\sqrt{\left(u^2+\Xi\right)}} = \Gamma\frac{P'}{P}\frac{\beta a\,u\sqrt{\left(u^2+\Xi\right)}}{\left(-\right)\left(-u^2-\Xi\right)} \\ &= \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u}\ , \end{aligned} \qquad \text{(II D1 e.21)}$$

in a form which is compatible with the other versions.]

Substituting Eqs. (II D1 e.16) through (II D1 e.19) into Eqs. (II D1 e.14) and (II D1 e.15) gives

$$\frac{\partial f}{\partial \gamma} = \frac{2\Gamma}{\gamma}\frac{\partial f}{\partial \Gamma} + 0 \qquad \text{(II D1 e.22)}$$

and

$$\frac{\partial f}{\partial u} = \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u}\frac{\partial f}{\partial \Gamma} + \frac{2E_\lambda}{u}\frac{\partial f}{\partial E_\lambda}\ . \qquad \text{(II D1 e.23)}$$

Using the formulae in Eqs. (II D1 e.22) and (II D1 e.23), it is possible to demonstrate that the second transformation is the inverse of the first. That is, if one substitutes the expressions for $\partial f / \partial \Gamma$ and $\partial f / \partial E_\lambda$ from Eqs. (II D1 e.22) and (II D1 e.23) into Eqs. (II D1 e.12) and (II D1 e.13), or vice-versa, the resulting equations are identities.

Consider, now, the definition of the covariance matrix associated with a particular set of values. The covariance matrix associated with the *u*-parameters is denoted (as in Section IV) as matrix *M,* where

$$M_{ij} = \langle \delta u_i \, \delta u_j \rangle \quad , \tag{II D1 e.24}$$

in which δu_i represents a small increment in the value of parameter u_i , and the angle brackets represent the "expectation value." Diagonal elements of this matrix are the square of the uncertainties on the parameter values; off-diagonal elements describe the connectedness between different parameters.

To communicate SAMMY results to ENDF files, it is necessary to generate the covariance matrix associated with the *p*-parameters (here this matrix is denoted by *Q*). This matrix is generated by making use of the relationship between a small increment in a *p*-parameter and a small increment in each of the *u*-parameters:

$$\delta p_k = \sum_i \frac{\partial p_k}{\partial u_i} \delta u_i \quad , \tag{II D1 e.25}$$

so that Q becomes

$$Q_{kl} = \langle \delta p_k \, \delta p_l \rangle = \sum_{i,j} \frac{\partial p_k}{\partial u_i} \langle \delta u_i \, \delta u_j \rangle \frac{\partial p_l}{\partial u_j} \quad . \tag{II D1 e.26}$$

The expansion of this covariance matrix for the two-parameter example discussed above will not be given here, but is proposed as an exercise for the student.

Reminder: It is the *p*-parameters (not the *u*-parameters) that are listed in the SAMMY PARameter files (input and output) and in the SAMMY output file (SAMMY.LPT). Likewise, it is the *p*-parameters* which are listed in ENDF File 2.** Therefore, the covariance matrix elements given in ENDF File 32 must correspond to the *Q* matrix defined above; that is, the covariance matrix listed in ENDF File 32 must be the appropriate covariance matrix for the resonance parameters.

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* For the LRF=7 format, an option exists to list the reduced width amplitudes γ rather than the partial widths Γ. In this case, no transformation from *u*- to *p*-parameter space is necessary for the partial widths, but only for the resonance energies.

** Caveat: When a reduced-width amplitude is negative, it is not Γ but $G = -\Gamma$ that is listed in the ENDF file. ENDF covariance matrices are expressed in terms of *G*, not Γ.

When the cross section is calculated as a function of the u-parameters, a small increment in the calculated cross section is given by

$$\delta\sigma = \sum_n \frac{\partial\sigma}{\partial u_n}\delta u_n \quad . \tag{II D1 e.27}$$

Therefore the covariance matrix $\boldsymbol{C_{ij}}$ for the cross section is found from

$$C_{ij} = \left\langle \delta\sigma_i\,\delta\sigma_j \right\rangle = \left\langle \sum_n \left(\frac{\partial\sigma_i}{\partial u_n}\delta u_n \right) \sum_m \left(\frac{\partial\sigma_j}{\partial u_m}\delta u_m \right) \right\rangle$$

$$= \sum_{n,m} \frac{\partial\sigma_i}{\partial u_n} \left\langle \delta u_n\, \delta u_m \right\rangle \frac{\partial\sigma_j}{\partial u_m} \tag{II D1 e.28}$$

$$= \sum_{n,m} \frac{\partial\sigma_i}{\partial u_n} M_{nm} \frac{\partial\sigma_j}{\partial u_m} \quad ,$$

in which M is again defined as the covariance matrix for the u-parameters. In order to print the covariance matrix resonance parameters for the p-parameters into the ENDF formats, it is necessary to transform the parameter covariance matrix from M to Q. That transformation is made by inserting the formulae

$$\frac{\partial\sigma_i}{\partial u_n} = \sum_k \frac{\partial p_k}{\partial u_n} \frac{\partial\sigma_i}{\partial p_k} \tag{II D1 e.29}$$

and

$$\frac{\partial\sigma_j}{\partial u_m} = \sum_l \frac{\partial p_l}{\partial u_m} \frac{\partial\sigma_j}{\partial p_l} \tag{II D1 e.30}$$

into the previous expression, Eq. (II D1 e.28), yielding

$$C_{ij} = \sum_{n,m,k,l} \frac{\partial\sigma_i}{\partial p_k} \frac{\partial p_k}{\partial u_n} M_{nm} \frac{\partial p_l}{\partial u_m} \frac{\partial\sigma_j}{\partial p_l} \tag{II D1 e.31}$$

or

$$C_{ij} = \sum_{k,l} \frac{\partial\sigma_i}{\partial p_k} Q_{kl} \frac{\partial\sigma_j}{\partial p_l} \quad , \tag{II D1 e.32}$$

where Q is given by

$$Q_{kl} = \sum_{n,m} \frac{\partial p_k}{\partial u_n} M_{nm} \frac{\partial p_l}{\partial u_m} \quad . \tag{II D1 e.33}$$

For the case in which only one elastic width contains an energy-dependent penetrability, the p-parameter covariance matrix must be modified for all elements involving a width having energy-dependent penetrability.