II.D.1.b. Derivatives with respect to resonance parameters

From Eq. (II B1.1), the derivatives of the real and imaginary part of R with respect to the resonance u-parameter associated with the resonance energy are

$$\frac{\partial \mathrm{Re}\left[R_{\mu\nu}\right]}{\partial\sqrt{E_\lambda}} = \left[2\,\gamma_{\lambda\mu}\gamma_{\lambda\nu}\sqrt{E_\lambda}\right]\left[\left\{-\left(E_\lambda - E\right)^2 + \left(\overline{\gamma}_{\lambda\gamma}^2\right)^2\right\}/d_\lambda^2\right] \qquad \text{(II D1 b.1)}$$

and

$$\frac{\partial \mathrm{Im}\left[R_{\mu\nu}\right]}{\partial\sqrt{E_\lambda}} = \left[-4\,\gamma_{\lambda\mu}\gamma_{\lambda\nu}\sqrt{E_\lambda}\right]\left[\left\{\left(E_\lambda - E\right)\overline{\gamma}_{\lambda\gamma}^2\right\}/d_\lambda^2\right] \quad . \qquad \text{(II D1 b.2)}$$

The derivatives of R with respect to the u-parameter associated with the eliminated capture width can be written as

$$\frac{\partial \mathrm{Re}\left[R_{\mu\nu}\right]}{\partial\overline{\gamma}_{\lambda\gamma}} = \left[-4\,\gamma_{\lambda\mu}\gamma_{\lambda\nu}\overline{\gamma}_{\lambda\gamma}\right]\left[\left\{\left(E_\lambda - E\right)\overline{\gamma}_{\lambda\gamma}^2\right\}/d_\lambda^2\right] \qquad \text{(II D1 b.3)}$$

and

$$\frac{\partial \mathrm{Im}\left[R_{\mu\nu}\right]}{\partial\overline{\gamma}_{\lambda\gamma}} = \left[2\,\gamma_{\lambda\mu}\gamma_{\lambda\nu}\overline{\gamma}_{\lambda\gamma}\right]\left[\left\{\left(E_\lambda - E\right)^2 - \left(\overline{\gamma}_{\lambda\gamma}^2\right)^2\right\}/d_\lambda^2\right] \quad . \qquad \text{(II D1 b.4)}$$

The derivatives for the particle widths are

$$\frac{\partial \mathrm{Re}\left[R_{\mu\nu}\right]}{\partial\gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}\left(1+\delta_{\mu\nu}\right)\right]\left[\left(E_\lambda - E\right)/d_\lambda\right] \qquad \text{(II D1 b.5)}$$

and

$$\frac{\partial \mathrm{Im}\left[R_{\mu\nu}\right]}{\partial\gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}\left(1+\delta_{\mu\nu}\right)\right]\left[\overline{\gamma}_{\lambda\gamma}^2/d_\lambda\right] \quad . \qquad \text{(II D1 b.6)}$$

In the expressions above, the denominator term d is defined as

$$d_\lambda = \left(E_\lambda - E\right)^2 + \overline{\gamma}_{\lambda\gamma}^{\,4} \quad . \qquad \text{(II D1 b.7)}$$

In each of these equations, the first square bracket contains an energy-independent factor; in the code SAMMY, this factor (times 2) is evaluated outside the energy loop in subroutine BABB and is stored as BR($\mu\nu$,i) for the derivative of the real part of $R_{\mu\nu}$ with respect to the i^{th} parameter, and BI($\mu\nu$,i) for the derivative of the imaginary part of $R_{\mu\nu}$. The quantity in the second square bracket is energy dependent but channel independent. Therefore, it must be generated for each energy and is temporarily stored as UPR(i) and UPI(i) in subroutine ABPART.

One legacy from early versions of SAMMY should be explained in some detail.

To avoid problems arising from the computer's limited precision, and to minimize computing time, partial derivatives for non-*s*-wave ($l > 0$) resonances are truncated to zero far away from the resonance. The working definition of "far away" is 20 times the sum of the partial widths for that resonance, plus 3 times the sum of the Doppler- and resolution-broadening widths, that is, far beyond the region where a resonance should produce any noticeable effect. Specifically, the derivative of the cross section at energy E is set to zero for resonance level λ, if

$$\left|E - E_\lambda\right| > 20\left[\sum\nolimits_c \Gamma_{\lambda c} + \overline{\Gamma}_{\lambda\gamma}\right] + 3\left(D + r\right) \qquad \text{(II D1 b.8)}$$

for resonances with $l > 0$, where D represents the Doppler and r the resolution width. Moreover, the contribution to the imaginary part of R is set to zero whenever the distance from level λ is greater than 100 times that specified in Eq. (II D1 b.8). (The contribution to the *real* part of R is never assumed to be negligible.)

For s-wave resonances ($l = 0$), the user has the option of setting derivatives equal to zero beyond a certain distance, where the distance is twice that specified for non-*s*-waves. To invoke this option, include the command

```
USE S-WAVE CUTOFF
```

in the INPut file. CAUTION: Though the cross-section segment in SAMMY may run slightly faster with the cutoff option invoked, results will not be as accurate. Use of this option is not encouraged.

With the advent of modern computer systems, use of the non-*s*-wave cutoff feature is no longer a necessity. Furthermore, use of this cutoff may lead to problems; in particular, inaccuracies have been noted in the calculation of uncertainties on multigroup averages.

The command

```
USE NO CUTOFFS FOR Derivatives or cross sections
```

can be used to eliminate the non-*s*-wave cutoff. It is recommended that, prior to completion of an analysis, the SAMMY user compare results obtained with and without the cutoff, to determine whether results are sufficiently accurate with the cutoff invoked.