II.D.1.a. Derivatives with respect to R-matrix

For resonance and R^{ext} parameters, the derivative of the cross section may be written as

$$\frac{\partial \sigma}{\partial u_i} = \sum_{\substack{c \le d \\ e \le f}} \frac{\partial R_{cd}}{\partial u_i} \frac{\partial W_{ef}}{\partial R_{cd}} \frac{\partial U_{ef}}{\partial W_{ef}} \frac{\partial \sigma}{\partial U_{ef}} \quad , \qquad \text{(II D1 a.1)}$$

where the index J has been suppressed, since it is fixed for a given parameter u. Indices c, d, e, and f denote channels. The restriction $c \le d$ indicates that the sum includes, for example, only terms with indices $c_1 c_2$ and not terms with indices $c_2 c_1$ (for $c_1 \neq c_2$); this restriction results from the symmetry of R and W (or X) with respect to interchange of indices.

Each term in the expression (II D1 a.1) will be evaluated separately, starting with the right-most term. All except $\partial R / \partial u$ are evaluated in this section; $\partial R / \partial u$ is discussed in subsequent sections.

The derivatives of cross section with respect to the real part of U can be expressed as

$$\frac{\partial \sigma}{\partial U^r} = \frac{\partial \sigma}{\partial U}\frac{\partial U}{\partial U^r} + \frac{\partial \sigma}{\partial U^*}\frac{\partial U^*}{\partial U^r} = \frac{\partial \sigma}{\partial U} + \frac{\partial \sigma}{\partial U^*} = 2\,\mathrm{Re}\left[\frac{\partial \sigma}{\partial U}\right] \quad , \qquad \text{(II D1 a.2)}$$

where the asterisk implies complex conjugate, and U and U^* are treated as independent entities. Similarly the derivative with respect to the imaginary part of U is given by

$$\frac{\partial \sigma}{\partial U^i} = \frac{\partial \sigma}{\partial U}\frac{\partial U}{\partial U^i} + \frac{\partial \sigma}{\partial U^*}\frac{\partial U^*}{\partial U^i} = i\frac{\partial \sigma}{\partial U} - i\frac{\partial \sigma}{\partial U^*} = -2\,\mathrm{Im}\left[\frac{\partial \sigma}{\partial U}\right] \quad . \qquad \text{(II D1 a.3)}$$

It follows that the derivative of the cross section with respect to U can be written as

$$\frac{\partial \sigma}{\partial U} = \mathrm{Re}\left[\frac{\partial \sigma}{\partial U}\right] + i\,\mathrm{Im}\left[\frac{\partial \sigma}{\partial U}\right] = \frac{1}{2}\left(\frac{\partial \sigma}{\partial U^r} - i\frac{\partial \sigma}{\partial U^i}\right) \quad . \qquad \text{(II D1 a.4)}$$

Using Eq. (II D1 a.4), values for the partial derivative of σ with respect to U are found from Eqs. (II A.8) to (II A.11), which give

$$\frac{\partial \sigma^{total}}{\partial U_{ef}} = -\frac{\pi g}{k^2}\delta_{ef} \quad , \qquad \text{(II D1 a.5)}$$

$$\frac{\partial \sigma_{\alpha\alpha}}{\partial U_{ef}} = -\frac{\pi g}{k^2}\left(\delta_{ef} - U^*_{ef}\right) \quad , \qquad \text{(II D1 a.6)}$$

$$\frac{\partial \sigma_{\alpha\alpha'}}{\partial U_{ef}} = \frac{\pi g}{k^2} U_{ef}^* \qquad \text{for } \alpha' \neq \alpha, \tag{II D1 a.7}$$

and

$$\frac{\partial \sigma^{capture}}{\partial U_{ef}} = -\frac{\pi g}{k^2} U_{ef}^* \quad . \tag{II D1 a.8}$$

Derivatives of a complex variable (such as U) with respect to another complex variable (such as W) may be generated directly, without separately considering the real and imaginary parts of each variable; this is demonstrated explicitly in Section II.D.3. Here, we make use of this result to evaluate $\partial U / \partial W$ and $\partial W / \partial R$.

Derivatives of U_{ef} with respect to W_{ef} are formed directly from Eq. (II A.4), which may be expressed as

$$U_{ef} = \Omega_e W_{ef} \Omega_f \quad , \tag{II D1 a.9}$$

so that

$$\frac{\partial U_{ef}}{\partial W_{ef}} = \Omega_e \Omega_f \quad . \tag{II D1 a.10}$$

Derivatives of W with respect to R are formed from Eqs. (II B1.3) and (II B1.4), which we rewrite as

$$\begin{aligned} W = I + 2iX &= I + 2i\left(\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1} R\sqrt{P}\right) \\ &= I + 2i\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}\left[R-L^{-1}+L^{-1}\right]\sqrt{P} \\ &= I + 2i\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}\left[R-L^{-1}\right]\sqrt{P} + 2i\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}\left[L^{-1}\right]\sqrt{P} \\ &= I - 2i\sqrt{P}L^{-1}\sqrt{P} + 2i\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1} L^{-1}\sqrt{P} \quad . \end{aligned} \tag{II D1 a.11}$$

Explicitly displaying the indices, Eq. (II D1 a.11) takes the form

$$W_{ef} = I - 2i\delta_{ef} P_e L_f^{-1} + 2i\sqrt{P_e}\, L_e^{-1}\, Y_{ef}\, L_f^{-1}\sqrt{P_f} \quad , \tag{II D1 a.12}$$

where we have set

$$Y_{ef} = \left[\left(L^{-1}-R\right)^{-1}\right]_{ef} \quad . \tag{II D1 a.13}$$

In [NL80, Appendix A] and also in Section II.D.3 of this manual, we show that the derivative of Y with respect to R is given by

$$\frac{\partial Y_{ef}}{\partial R_{cd}} = Y_{ec} Y_{df} + Y_{ed} Y_{cf} \left(1 - \delta_{cd}\right) \quad . \tag{II D1 a.14}$$

Substitution of this expression into the derivative of Eq. (II D1 a.12) gives

$$\frac{\partial W_{ef}}{\partial R_{cd}} = 2i \sqrt{P_e}\, L_e^{-1} \left[Y_{ec} Y_{df} + Y_{ed} Y_{cf} \left(1 - \delta_{cd}\right) \right] L_f^{-1} \sqrt{P_f} \quad . \tag{II D1 a.15}$$

Alternatively, we may write

$$\frac{\partial X_{ef}}{\partial R_{cd}} = \sqrt{P_e}\, L_e^{-1} \left[Y_{ec} Y_{df} + Y_{ed} Y_{cf} \left(1 - \delta_{cd}\right) \right] L_f^{-1} \sqrt{P_f} \quad , \tag{II D1 a.16}$$

which is the more practically useful form in SAMMY.

Derivatives of R with respect to u depend upon which particular u-parameter is being considered. Parameters of the external R-matrix, resonance parameters, and channel radii are described in the next subsections.