II.D.1.c. Derivatives with respect to channel radius

Derivatives with respect to channel radius a require modification of the procedure outlined in Section II.D.1.b, since phase shifts φ and penetrabilities P also depend on channel radius (sometimes called "matching radius"). All dependence on a is via ρ, where

$$\rho = k\, a \quad , \tag{II D1 c.1}$$

and momentum $\hbar k$ in the center-of-mass reference frame is described in Section II.C.2; k is the wave number in units of inverse length. The derivative of the cross section with respect to the radius can be written

$$\frac{\partial \sigma}{\partial a} = \frac{\partial \sigma}{\partial \rho}\frac{\partial \rho}{\partial a} = k\frac{\partial \sigma}{\partial \rho} \quad . \tag{II D1 c.2}$$

Our problem therefore reduces to finding $\partial\sigma / \partial\rho$.

The derivative of the cross section with respect to ρ may be formed from Eq. (II A.1):

$$\begin{aligned} \frac{\partial \sigma_{cc'}}{\partial \rho} &= \frac{\pi}{k_c^2} g_c \left[\left(\delta_{cc'} - U_{cc'}\right) \frac{\partial U^*_{cc'}}{\partial \rho} + \left(\delta_{cc'} - U^{J*}_{cc'}\right) \frac{\partial U_{cc'}}{\partial \rho} \right] \\ &= \frac{2\pi}{k_c^2} g_c \left[\delta_{cc'} \frac{\partial \operatorname{Re}\left(U_{cc'}\right)}{\partial \rho} - \operatorname{Re}\left(U^{J*}_{cc'} \frac{\partial U_{cc'}}{\partial \rho} \right) \right] \quad . \end{aligned} \tag{II D1 c.3}$$

From the definitions of Ω and φ, Eqs. (II A.4) and (II A.5), the partial of U with respect to ρ may be written as

$$\frac{\partial U_{cc'}}{\partial \rho} = -i \frac{\partial \varphi_c}{\partial \rho} U_{cc'} + \Omega_c \frac{\partial W_{cc'}}{\partial \rho} \Omega_{c'} - i\, U_{cc'} \frac{\partial \varphi_{c'}}{\partial \rho} \quad . \tag{II D1 c.4}$$

Equation (II D1 c.3) can therefore be written as

$$\begin{aligned} \frac{\partial \sigma_{cc'}}{\partial \rho} = \frac{2\pi}{k_c^2} g_c \; \Bigg\{ & \delta_{cc'} \operatorname{Re}\left(-2i \frac{\partial \varphi_c}{\partial \rho} U_{cc} + \Omega_c^2 \frac{\partial W_{cc}}{\partial \rho} \right) \\ & - \operatorname{Re}\left(U^*_{cc'} \left[-i \left(\frac{\partial \varphi_c}{\partial \rho} + \frac{\partial \varphi_{c'}}{\partial \rho} \right) U^J_{cc'} + \Omega_c \frac{W_{cc'}}{\partial \rho} \Omega_{c'} \right] \right) \Bigg\} \quad , \end{aligned} \tag{II D1 c.5}$$

or

$$\frac{\partial \sigma_{cc'}}{\partial \rho} = \frac{2\pi}{k_c^2} g_c \left\{ \delta_{cc'} \operatorname{Re}\left(-2i \frac{\partial \varphi_c}{\partial \rho} U^J_{cc} + \Omega_c^2 \frac{\partial W_{cc}}{\partial \rho} \right) \right.$$
$$\left. - \operatorname{Re}\left(\Omega_c^* W_{cc'}^* \Omega_{c'}^* \left[-i \left(\frac{\partial \varphi_c}{\partial \rho} + \frac{\partial \varphi_{c'}}{\partial \rho} \right) \Omega_c W_{cc'} \Omega_{c'} + \Omega_c \frac{W_{cc'}}{\partial \rho} \Omega_{c'} \right] \right) \right\} \quad . \tag{II D1 c.6}$$

Because $\Omega_c \, \Omega^*_c = 1$, this simplifies to the form

$$\frac{\partial \sigma_{cc'}}{\partial \rho} = \frac{2\pi}{k_c^2} g_c \ \operatorname{Re}\left\{ \delta_{cc'} \Omega_c^2 \left(-2i \frac{\partial \varphi_c}{\partial \rho} W_{cc} + \frac{\partial W_{cc}}{\partial \rho} \right) \right.$$
$$\left. - \left(W_{cc'}^* \left[-i \left(\frac{\partial \varphi_c}{\partial \rho} + \frac{\partial \varphi_{c'}}{\partial \rho} \right) W_{cc'} + \frac{\partial W_{cc'}}{\partial \rho} \right] \right) \right\} \quad . \tag{II D1 c.7}$$

Derivatives of hard-sphere phase shifts φ are formed by direct differentiation of the formulae in Table II A.1 for non-Coulomb and of the equations in Section II.C.4 for Coulomb.

The derivatives of W are found in similar fashion to the derivatives with respect to resonance parameters, beginning with Eq. (II D1 a.11):

$$\begin{aligned} \frac{\partial W_{cc'}}{\partial \rho} = & -2i\,\delta_{cc'}\, L_c^{-1} \frac{\partial P_c}{\partial \rho} + 2i\delta_{cc'}\, P_c\, L_c^{-2} \left(\frac{\partial S_c}{\partial \rho} + i \frac{\partial P_c}{\partial \rho} \right) \\ & + 2i \frac{\partial P_c}{\partial \rho} \frac{1}{2\sqrt{P_c}} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \sqrt{P_{c'}} \\ & + 2i \sqrt{P_c} \left(-L_c^{-2} \right) \left(\frac{\partial S_c}{\partial \rho} + i \frac{\partial P_c}{\partial \rho} \right) \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \sqrt{P_{c'}} \\ & + 2i \sqrt{P_c}\, L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} \left(\frac{\partial S_{c'}}{\partial \rho} + i \frac{\partial P_{c'}}{\partial \rho} \right) \left(L_{c'}^{-2} \right) \sqrt{P_{c'}} \\ & + 2i \sqrt{P_c} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \frac{\partial P_{c'}}{\partial \rho} \frac{1}{2\sqrt{P_{c'}}} \\ & + 2i \sum_{c''} \sqrt{P_c} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc''} L_{c''}^{-1} \left(\frac{\partial S_{c''}}{\partial \rho} + i \frac{\partial P_{c''}}{\partial \rho} \right) \\ & \qquad \times L_{c''}^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{c''c'} L_{c'}^{-1} \sqrt{P_{c'}} \quad . \end{aligned} \tag{II D1 c.8}$$

This expression can be greatly simplified by setting

$$\vartheta_{cc'} = \sqrt{P_c} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \sqrt{P_{c'}} - P_c L_c^{-1} \delta_{cc'} \quad , \tag{II D1 c.9}$$

which gives

$$\begin{aligned} \frac{\partial W_{cc'}^J}{\partial \rho} = &+ i \frac{\partial P_c}{\partial \rho} \frac{1}{P_c} \vartheta_{cc'} + i \, \vartheta_{cc'} \frac{1}{P_{c'}} \frac{\partial P_{c'}}{\partial \rho} \\ &+ 2i \sum_{c''} \vartheta_{cc''} P_{c''}^{-1} \left(\frac{\partial S_{c''}}{\partial \rho} + i \frac{\partial P_{c''}}{\partial \rho} \right) \vartheta_{c''c'} \quad . \end{aligned} \tag{II D1 c.10}$$

Derivatives of penetrabilities P_c and shift factors S_c are found by direct differentiation of the formulae in Table II A.1 for non-Coulomb and Section II.C.4 for Coulomb. Derivatives of the cross sections with respect to ρ are then found by substituting results from Eq. (II D1 c.10) into Eq. (II D1 c.7).