II.C.3. Evaluation of Hard-Sphere Phase Shift

Formulae for the hard-sphere phase shift (otherwise known as the potential-scattering phase shift) are given in Table II A.1 for non-Coulomb interactions. What is actually needed in SAMMY is not, however, the phase shifts φ themselves but rather cos(2φ) and sin(2φ). Since evaluation of φ requires the inverse tangent function, results for cos(2φ) and sin(2φ) are more readily generated with fewer computer round-off errors by using trigonometric relationships to generate formulae for cos(2φ) and sin(2φ) directly.

For all l, it is clear from Table II A.1 that φ may be written in the form

$$\varphi = \rho - X \quad , \tag{II C3.1}$$

where

$$X = \tan^{-1} f \tag{II C3.2}$$

and f is a different function of ρ for each value of l. From Eq. (II C3.1), using elementary trigonometric relationships, we find

$$\cos\varphi \;=\; \cos\rho\;\cos X \;+\; \sin\rho\;\sin X \tag{II C3.3}$$

and

$$\sin\varphi \;=-\cos\rho\;\sin X \;+\; \sin\rho\;\cos X \quad . \tag{II C3.4}$$

Thus, $\cos\left(2\,\varphi\right)$ becomes

$$\begin{aligned}\cos\left(2\,\varphi\right) \;&=\; 2\cos^2\varphi - 1 = 2\cos^2\rho\;\;\cos^2 X\;\left(1+\tan\rho\;\tan X\right)^2 - 1 \\ &= 2\;\frac{\cos^2\rho}{1+f^2}\;\left(1+f\;\tan\rho\right)^2 - 1 \quad .\end{aligned} \tag{II C3.5}$$

Similarly, $\sin\left(2\,\varphi\right)$ can be written

$$\begin{aligned}\sin\left(2\varphi\right) \;&=\; 2\cos\varphi\sin\varphi \;=\; 2\cos^2\rho\;\cos^2 X\left(1+\tan\rho\tan X\right)\left(-\tan X+\tan\rho\right) \\ &=\; 2\,\frac{\cos^2\rho}{1+f^2}\left(1+f\;\tan\rho\right)\left(-f+\tan\rho\right) \quad .\end{aligned} \tag{II C3.6}$$

Equations (II C3.5) and (II C3.6) are the form used in SAMMY to evaluate the hard-sphere phase shift terms for non-Coulomb situations.