Analytical equations of the scattering lines

The plane of the detector is entirely defined through the angle α and the distance d from the sample to the detector; any rotation of the setup around the beam's axis is irrelevant for our present purpose. The X-rays scattered at a given angle θ define a cone, the intersection of which with the plane of the detector is -by definition- a conic section. For $\theta < \pi/2-\alpha$, or $\theta > \pi/2-\alpha$, the intersection of the cone with the detector's plane is an ellipse or a hyperbola, respectively.

We derive here the analytical equation of the scattering lines on the detector using the concept of Dandelin spheres, which are tangent to both the cone and the intersecting plane. In the case relevant to ellipses, there are two such spheres the points of contact of which with the plane are the foci. In the case relevant to a hyperbola, there is a single Dandelin sphere which touches the plane at the hyperbola's focus point.

1. Ellipses: $\theta < \pi/2 - \alpha$

The situation relevant to $\theta < \pi/2 - \alpha$ is illustrated in Figure 1, in which some symbols are defined. The Dandelin's sphere the closest to the sample enables to calculate the upper focus of the ellipse. From trigonometry, one has $R_1/l' = \sin(\theta)$ and $R_1/l'' = \cos(\alpha)$, from which one finds that

$$\frac{R_1}{d} = \frac{\sin(\theta)}{\cos(\alpha) + \sin(\theta)} \qquad \text{Eq. 1}$$

where we have used the fact that $l = l' + l''$ is related to d through $d/l = \cos(\alpha)$. Using $f_+ = R_1 \tan(\alpha)$, one obtains

$$\frac{f_+}{d} = \tan(\alpha)\frac{\sin(\theta)}{\cos(\alpha)+\sin(\theta)} \qquad \text{Eq. 2}$$

which is the distance from the beam to the upper focus of the ellipse corresponding to angle *θ*.

To estimate the upper vertex of the ellipse v_+, it is useful to define the angles γ_1 and β_1 as in Figure 2. With these angles, one has $v_+ = f_+ + R_1 \tan(\beta_1)$. Using $\alpha + \beta_1 + \gamma_1 = \pi/2$ and $\beta_1 = \theta + \gamma_1$, one gets $\beta_1 = \pi/4 + 1/2\ (\theta\text{-}\alpha)$, which finally leads to

$$\frac{v_+}{d} = \left[\tan(\alpha) + \frac{1+\tan((\theta-\alpha)/2)}{1-\tan((\theta-\alpha)/2)}\right]\frac{\sin(\theta)}{\cos(\alpha)+\sin(\theta)} \qquad \text{Eq. 3}$$

where we have used Equations 1 and 2. One can check that the latter equation reduces to $u_+/d = \tan(\theta)$ for $\alpha = 0$.

The lower focus of the ellipse is calculated based on an equivalent calculation, starting with the second Dandelin sphere. The ratio of the two radii is $R_2/R_1 = (m + l' + l'')/l'$, and $m = R_2/\cos(\alpha)$. Using the relations already mentioned for *l*' and *l*'', one finally finds

$$\frac{R_2}{R_1} = \frac{\cos(\alpha)+\sin(\theta)}{\cos(\alpha)-\sin(\theta)} \qquad \text{Eq. 4}$$

From Figure 1, $f_+/f_- = R_1/R_2$. One therefore finds from Equations 2 and 3 that

$$\frac{f_-}{d} = \tan(\alpha)\frac{\sin(\theta)}{\cos(\alpha)-\sin(\theta)} \qquad \text{Eq. 5}$$

Such a simple relation does not apply for v_-/v_+. From Figure 2b, one finds $\beta_2 = \pi/4 - (\alpha + \theta)/2$; a similar reasoning as for Equation 3 leads to

$$\frac{v_-}{d} = \left[\tan(\alpha) + \frac{1-\tan((\theta+\alpha)/2)}{1+\tan((\theta+\alpha)/2)}\right]\frac{\sin(\theta)}{\cos(\alpha)-\sin(\theta)} \qquad \text{Eq. 6}$$

One can also check that the latter equation reduces to $v_-/d = \tan(\theta)$ for $\alpha = 0$.

The center of the ellipse y_0, its semi-major axis a, and its semi-minor axis b are given by

$$
\begin{aligned}
Y_0 &= \frac{1}{2}(f_+ - f_-) \\
a &= \frac{1}{2}(v_+ + v_-) \\
b &= \frac{1}{2}\sqrt{(v_+ + v_-)^2 - (f_+ + f_-)^2}
\end{aligned}
\qquad \text{Eq. 7}
$$

which enables to write the equation of the ellipse corresponding to a given angle θ as

$$
\frac{(Y - Y_0)^2}{a^2} + \frac{X^2}{b^2} = 1 \qquad \text{Eq. 8}
$$

Ellipses corresponding to a detector at angle $\alpha = 30°$ and 60° are shown in Figure 3, taken every 5° of θ.

2 Hyperbolas: $\theta > \pi/2 - \alpha$

In the case where $\theta > \pi/2 - \alpha$, the intersection of the scattering cone with the detector plane is no longer an ellipse but a hyperbola. In this case, there is a single Dandelin sphere to consider, as illustrated in Figure 4. The touching point between the sphere and the plane is the focus of the hyperbole; one finds that Equation 2 still applies i.e.

$$
\frac{f}{d} = \tan(\alpha)\frac{\sin(\theta)}{\cos(\alpha) + \sin(\theta)} \qquad \text{Eq. 9}
$$

and the vertex of the hyperbole is found to be equal to

$$
\frac{v}{d} = \tan(\alpha) + \tan(\theta - \alpha) \qquad \text{Eq. 10}
$$

The position of the directrix is given by

$$\frac{\delta}{d} = \frac{\sin(\theta)}{\sin(\alpha)\cos(\alpha)} \frac{1+\sin(\theta)\cos(\alpha)}{\sin(\theta)+\cos(\alpha)} \qquad \text{Eq. 11}$$

Using these values, the eccentricity of the hyperbola is found to be

$$\varepsilon = \frac{v-f}{\delta - v} \qquad \text{Eq. 12}$$

And its Cartesian equation of the hyperbola is

$$\frac{(Y-Y_0)^2}{a^2} - \frac{X^2}{b^2} = 1 \qquad \text{Eq. 13}$$

with

$$\begin{aligned} Y_0 &= f + a\varepsilon \\ a &= \frac{\varepsilon}{\varepsilon^2 - 1}(\delta - f) \\ b &= \frac{\varepsilon}{\sqrt{\varepsilon^2 - 1}}(\delta - f) \end{aligned} \qquad \text{Eq. 14}$$

Hyperbolas are added in blue to Figure 3, corresponding to cones taken every 5° of θ, for $\alpha = 30$ and $\alpha = 60°$.

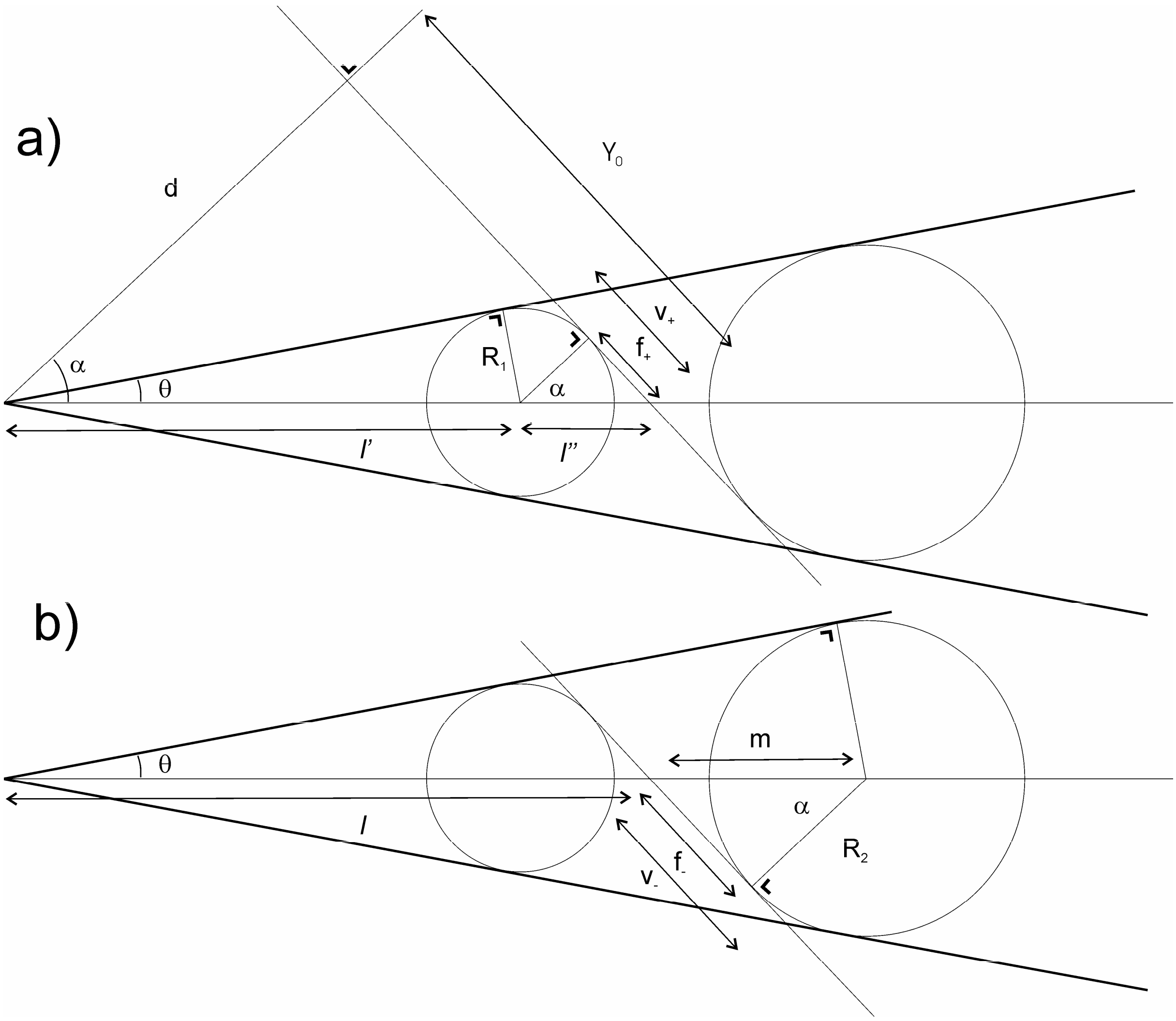

Figure 1. Two Dandelin spheres relevant to the case of ellipses, and definition of some symbols.

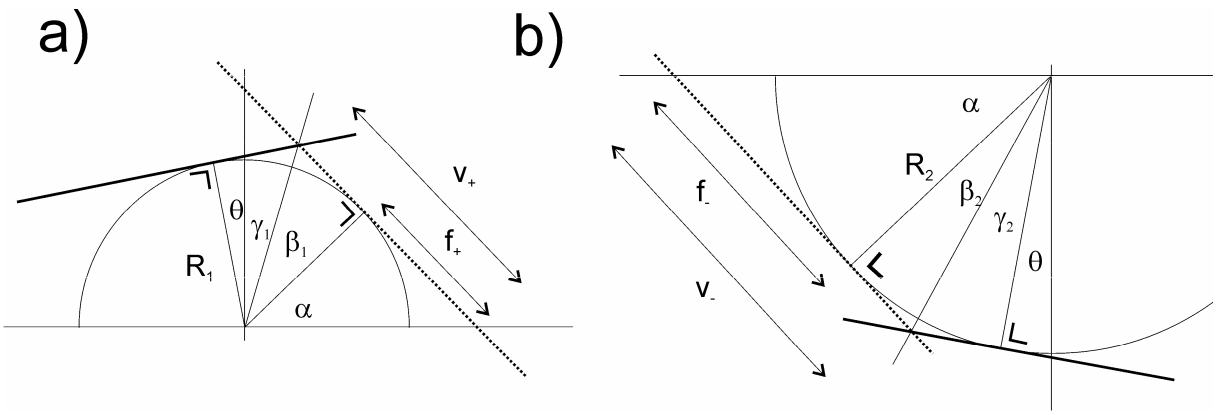

Figure 2. Definition of angles relevant to an ellipse's Dandelin spheres. The overall picture is that of Figure 1.

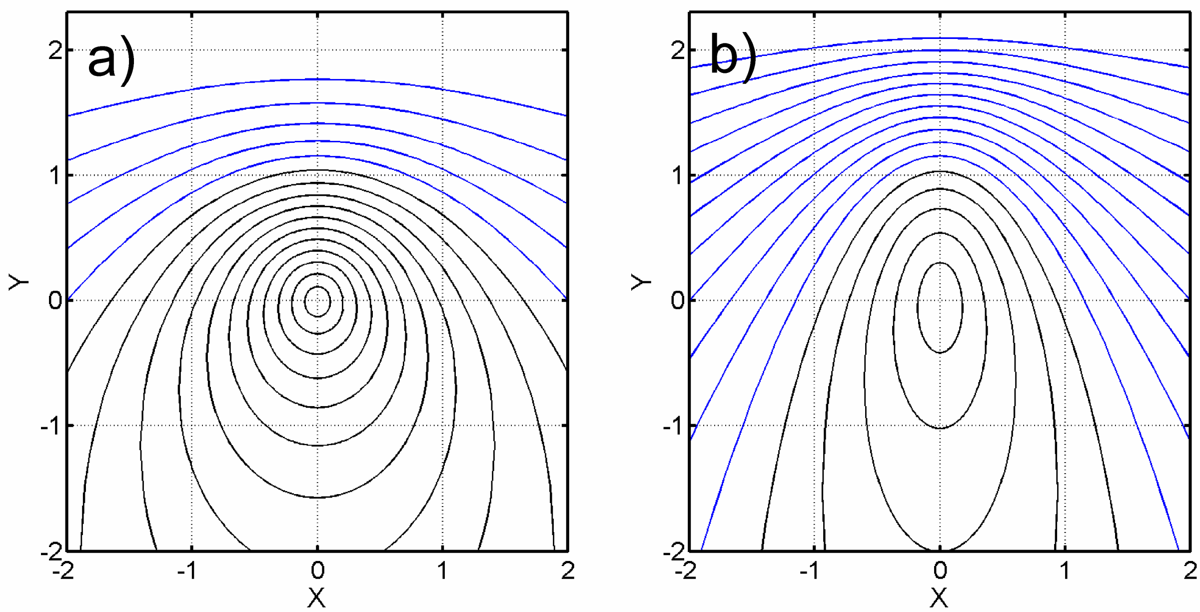

Figure 3. Iso-θ lines, taken every 5° of θ for α = 30 (a) and α = 60° (b). The ellipses are in black and the hyperbolas in blue. The unit of distance in the Figure is the distance from sample to detector.

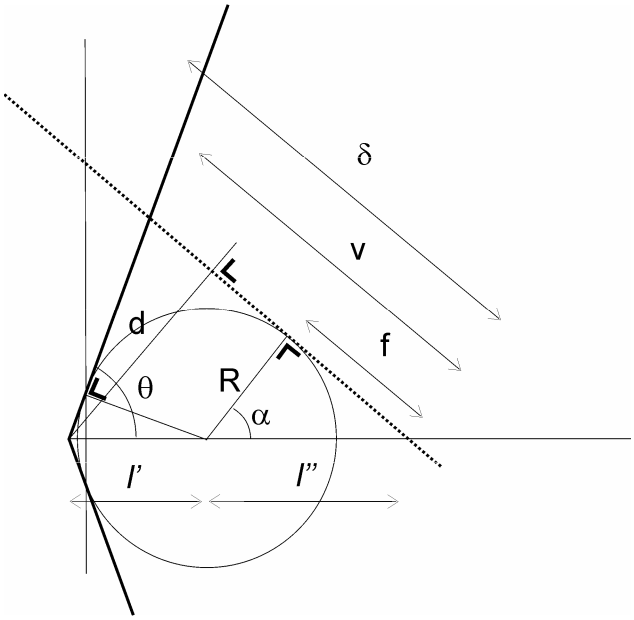

Figure 4. Single Dandelin sphere of a hyperbola, and definition of some symbols.