“Self shielding” corrections for slab samples in thin containers

We consider a solid slab sample within a container. Two measurements are performed, (i) on the sample in its container and (ii) on the empty container. The corresponding measured intensities are as follows:

$$I_{sc}^{m} = I_s f_{s,sc} + I_c f_{c,sc}$$
$$I_{c}^{m} = I_c f_{c,c}$$

where

I_s “True” sample intensity

I_c “True” container intensity

I_{sc}^{m} Measured intensity for sample in container

I_{c}^{m} Measured intensity for empty container

$f_{c,sc}$ Self-shielding of scattering by the container when measuring sample in container

$f_{s,sc}$ Self-shielding of scattering by the sample when measuring sample in container

$f_{c,c}$ Self-shielding of scattering by the container when measuring empty container

Note that all intensities are functions of the scattering angle.

The “true” sample intensity is obtained from the following expression

$$I_s = \left(I_{sc}^{m} - I_{c}^{m} \cdot \frac{f_{c,sc}}{f_{c,c}} \right) \cdot \frac{1}{f_{s,sc}} = \left(I_{sc}^{m} - I_{c}^{m} \cdot \mathrm{SAF} \right) \cdot \frac{1}{\mathrm{SSF}}$$

where the so-called “sample attenuation factor” $\mathrm{SAF} \equiv f_{c,sc} / f_{c,c}$ and the “self-shielding factor” $\mathrm{SSF} \equiv f_{s,sc}$. General expressions for these quantities are available [1], but here we will use simplified expressions appropriate to the case of a weakly scattering container, i.e. a container with thin walls and small cross sections.

The factor SSF

We consider a solid slab sample of thickness t, uniformly illuminated by a beam that makes an angle ψ_0 with respect to the normal to the slab (see figures 1 and 2), where $-\frac{\pi}{2} \le \psi_0 \le \frac{\pi}{2}$. Its macroscopic scattering, absorption and total removal cross sections are Σ_S, Σ_A and $\Sigma_T = \Sigma_S + \Sigma_A$ respectively. Its transmission $T = \exp\left[-\Sigma_T t \sec\psi_o\right]$.

Reflection case

The probability of single scattering into the infinitesimal solid angle $\delta\Omega$ when $\pi/2 < |\psi| < \pi$ (see figure 1), followed by escape, is

$$S_1(\psi_o,\psi)\delta\Omega = \int_0^t \exp\left[-\Sigma_T d_0^s - \Sigma_T d_1^s\right]\cdot\left(\delta\Sigma_S^{(2\theta)}dy\right) = \int_0^t \exp\left[-\Sigma_T y\sec\psi_o + \Sigma_T y\sec\psi\right]\cdot\left(\delta\Sigma_S^{(2\theta)}dy\right) \Rightarrow$$

$$\Rightarrow \frac{\left\{1-\exp\left[-\Sigma_T t\left(\sec\psi_o - \sec\psi\right)\right]\right\}}{\Sigma_T\left(\sec\psi_o - \sec\psi\right)}\cdot\delta\Sigma_S^{(2\theta)}$$

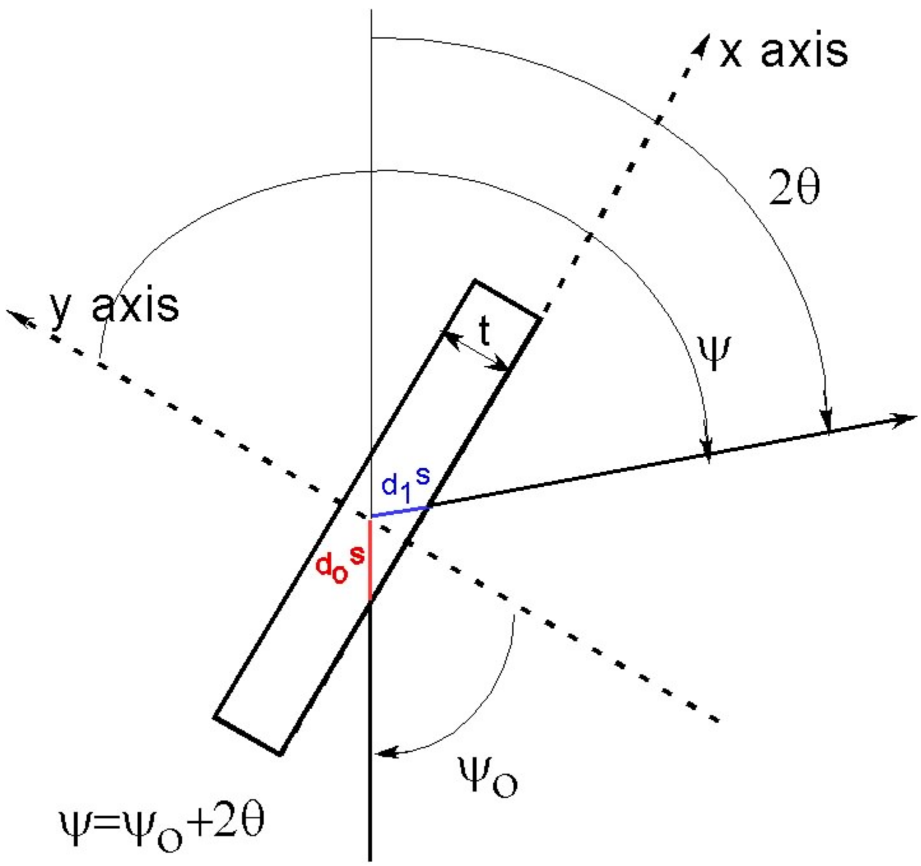


Figure 1 Reflection case.

where $\delta\Sigma_S^{(2\theta)}$ is the corresponding differential scattering cross section, d_o^s is the distance traveled through the sample before scattering, and d_1^s is the distance traveled through the sample after scattering (see figure 1).

Transmission case

The probability of single scattering into the infinitesimal solid angle $\delta\Omega$ when $|\psi| < \pi/2$ (see figure 2), followed by escape, is

$$S_1(\psi_o,\psi)\delta\Omega = \int_0^t \exp\left[-\Sigma_T d_0^s - \Sigma_T d_1^s\right]\cdot\left(\delta\Sigma_S^{(2\theta)}dy\right) = \int_0^t \exp\left[-\Sigma_T y\sec\psi_o - \Sigma_T\left(t-y\right)\sec\psi)\right]\cdot\left(\delta\Sigma_S^{(2\theta)}dy\right) \Rightarrow$$

$$S_1(\psi_o,\psi)\delta\Omega = \delta\Sigma_S^{(2\theta)}\cdot\int_0^t \exp\left[\left(-\Sigma_T\sec\psi_o + \Sigma_T\sec\psi\right)y - \Sigma_T t\sec\psi\right]\cdot dy \Rightarrow$$

$$S_1(\psi_o,\psi)\delta\Omega = \delta\Sigma_S^{(2\theta)}\cdot\exp\left[-\Sigma_T t\sec\psi\right]\cdot\frac{\left\{1-\exp\left[-\Sigma_T t\left(\sec\psi_o - \sec\psi\right)\right]\right\}}{\Sigma_T\left(\sec\psi_o - \sec\psi\right)}$$
$$= \delta\Sigma_S^{(2\theta)}\frac{\left\{\exp\left(-\Sigma_T t\sec\psi\right) - \exp\left(-\Sigma_T t\sec\psi_0\right)\right\}}{\left(\Sigma_T\sec\psi_o - \Sigma_T\sec\psi\right)}$$

When $\psi = \psi_0$ or when $\psi = -\psi_0$ the probability of single scattering reduces to

$$S_1(\psi_o,\psi)\delta\Omega = \delta\Sigma_S^{(2\theta)}\cdot\exp\left[-\Sigma_T t\sec\psi_0\right] = \delta\Sigma_S^{(2\theta)}T\,.$$

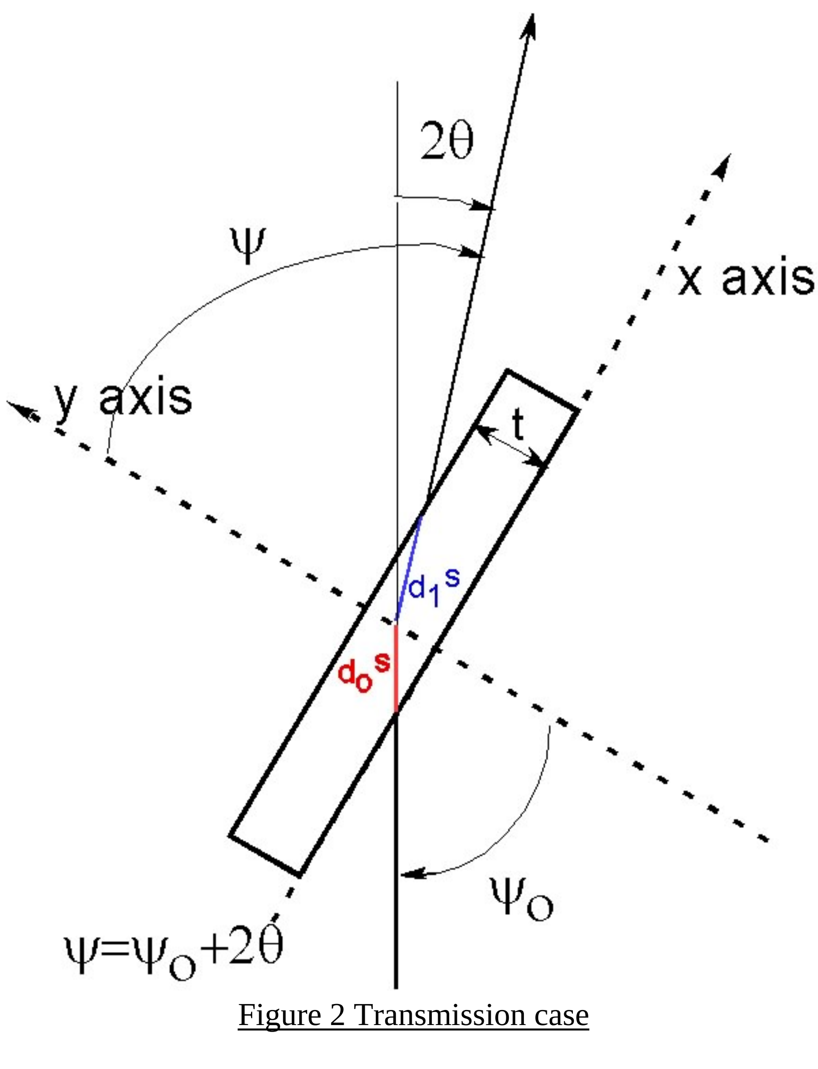


Figure 2 Transmission case

Writing $\zeta = \Sigma_T t$, the SSF is as follows:

$$\mathrm{SSF} \equiv f_{s,sc}(\psi_0,\psi) = \frac{S_1(\psi_0,\psi)}{\delta\Sigma_S^{(\psi)} t} = \left\{ \begin{array}{ll} |\psi| \le \dfrac{\pi}{2} & \dfrac{\exp[-\zeta\sec\psi] - \exp[-\zeta\sec\psi_0]}{\zeta(\sec\psi_0 - \sec\psi)} \\ \dfrac{\pi}{2} < |\psi| < \pi & \dfrac{1-\exp[-\zeta(\sec\psi_0 - \sec\psi)]}{\zeta(\sec\psi_0 - \sec\psi)} \end{array} \right\}$$

Note that $\mathrm{SSF}(\psi) = \mathrm{SSF}(-\psi)$ for all values of ψ since $\sec(\psi) = \sec(-\psi)$.

Writing $\psi = 2\theta + \psi_o$ we obtain

$$\mathrm{SSF} = \left\{ \begin{array}{ll} -\dfrac{\pi}{2} - \psi_o < 2\theta < \dfrac{\pi}{2} - \psi_o & \dfrac{\exp[-\zeta\sec(2\theta+\psi_o)] - \exp[-\zeta\sec\psi_0]}{\zeta(\sec\psi_0 - \sec(2\theta+\psi_o))} \\ -\pi \le 2\theta \le -\dfrac{\pi}{2} - \psi_o ; \dfrac{\pi}{2} - \psi_o \le 2\theta \le \pi & \dfrac{1-\exp[-\zeta(\sec\psi_0 - \sec(2\theta+\psi_o))]}{\zeta(\sec\psi_0 - \sec(2\theta+\psi_o))} \end{array} \right\}$$

The factor SAF

For a weakly scattering container in slab geometry the SAF may be written as follows:

$$\mathrm{SAF} = \frac{1}{2t_c} \int_c \exp\left[-\Sigma_T d_0^s - \Sigma_T d_1^s\right] \cdot dy$$

where t_c is the thickness of one of the walls and the integral is performed for all points within the container on a line parallel to the y axis (figure 3). Figure 3 represent the terms in the expressions for both the reflection and transmission cases. Writing $\zeta = \Sigma_T t$, the SAF reads as follows:

$$\mathrm{SAF} = \left\{ \begin{array}{ll} |\psi| \le \dfrac{\pi}{2} & \dfrac{1}{2}\left\{\exp(-\zeta\sec\psi_o) + \exp(-\zeta\sec\psi)\right\} \\ \dfrac{\pi}{2} < |\psi| < \pi & \dfrac{1}{2}\left\{1 + \exp(\zeta[\sec\psi - \sec\psi_o])\right\} \end{array} \right.$$

Note that $\mathrm{SAF}(\psi) = \mathrm{SAF}(-\psi)$ for all values of ψ since $\sec(\psi) = \sec(-\psi)$.

Writing $\psi = 2\theta + \psi_o$ we obtain

$$\mathrm{SAF} = \left\{ \begin{array}{ll} -\dfrac{\pi}{2} - \psi_o \le 2\theta \le \dfrac{\pi}{2} - \psi_o & \dfrac{1}{2}\left\{\exp[-\zeta\sec\psi_o] + \exp[-\zeta\sec(2\theta+\psi_o)]\right\} \\ -\pi \le 2\theta \le -\dfrac{\pi}{2} - \psi_o ; \dfrac{\pi}{2} - \psi_o \le 2\theta \le \pi & \dfrac{1}{2}\left\{1 + \exp[\zeta\sec(2\theta+\psi_o) - \zeta\sec\psi_o]\right\} \end{array} \right.$$

[1] See, e.g., J.R.D. Copley, D.L. Price and J. M. Rowe, “A system of programs for the reduction of data from a time-of-flight spectrometer”, Nucl. Instr. Meth., 107 (1973) 501-507, ibid., 114 (1974) 411 (erratum).

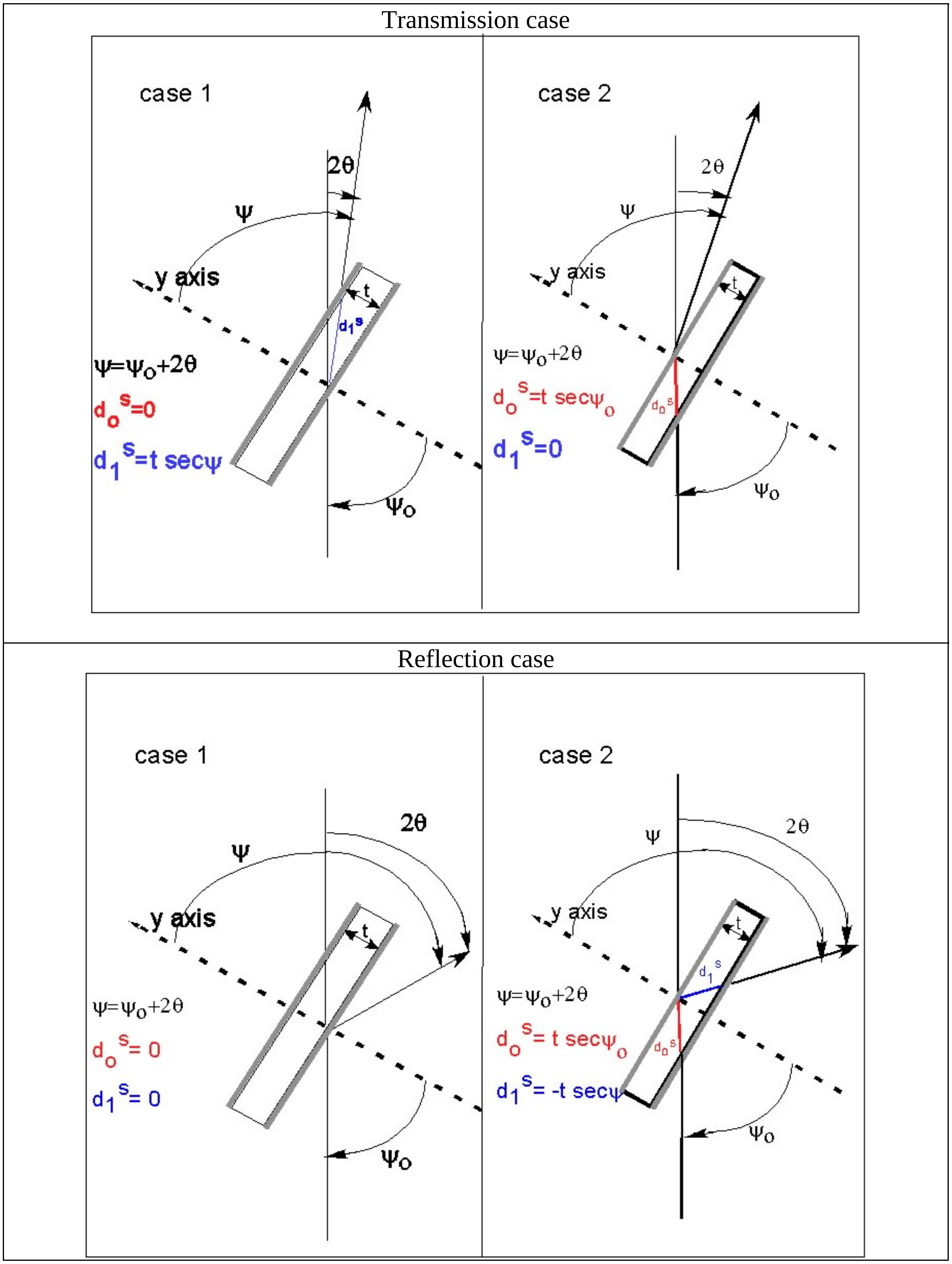


Figure 3 Self Attenuation Factor: Transmission and reflection cases

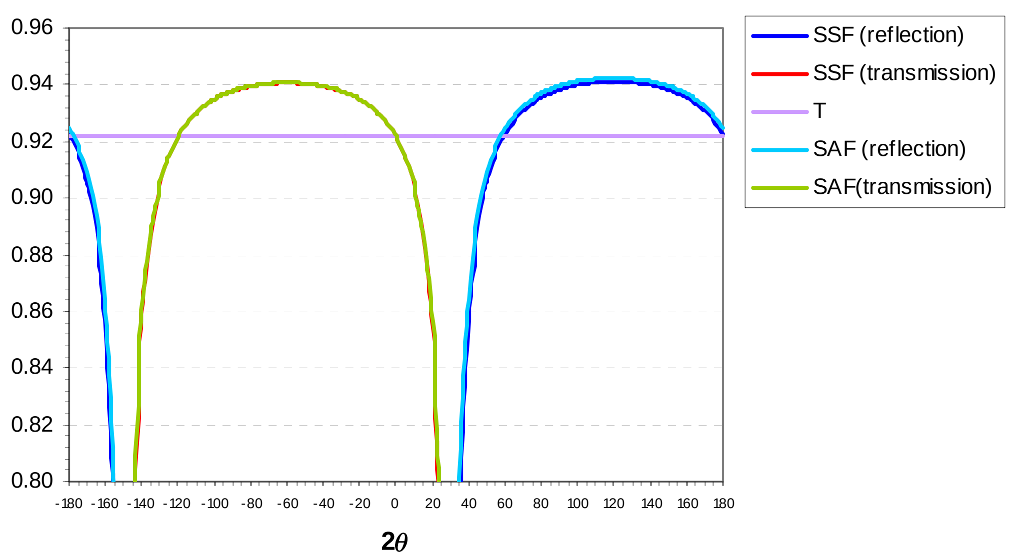
An example

This example is taken from recent measurements by Li Liu (MIT). For these experiments $\psi_o = 60^o$, and ζ was determined from a transmission measurement in normal incidence, i.e. with $\psi_o = 0^o$. The measured transmission was 96% so $\zeta = -\ell n(0.96)$.

$$\mathrm{SSF}(2\theta) = \begin{cases} -150^o \le 2\theta \le 30^o & \dfrac{\exp\left[-\zeta \sec\left(2\theta + 60^o\right)\right] - \exp\left[-\zeta \sec 60^o\right]}{\zeta\left(\sec 60^o - \sec\left(2\theta + 60^o\right)\right)} \\ -180^o \le 2\theta \le -150^o; 30^o \le 2\theta \le 180^o & \dfrac{1 - \exp\left[-\zeta\left(\sec 60^o - \sec\left(2\theta + 60^o\right)\right)\right]}{\zeta\left(\sec 60^o - \sec\left(2\theta + 60^o\right)\right)} \end{cases}$$

$$\mathrm{SAF}(2\theta) = \begin{cases} -150^o \le 2\theta \le 30^o & \dfrac{1}{2}\left\{\exp\left[-\zeta \sec\left(2\theta + 60^o\right)\right] + \exp\left[-\zeta \sec 60^o\right]\right\} \\ -180^o \le 2\theta \le -150^o; 30^o \le 2\theta \le 180^o & \dfrac{1}{2}\left\{1 + \exp\left[-\zeta\left(\sec 60^o - \sec\left(2\theta + 60^o\right)\right)\right]\right\} \end{cases}$$

The plot below shows calculated SSFs and SAFs, and the transmission T for $\psi_o = 60^o$.



Appendix: Exact and approximate relationships

1. We have already noted that $\boxed{\mathrm{SAF}(\psi)=\mathrm{SAF}(-\psi)}$ and $\boxed{\mathrm{SSF}(\psi)=\mathrm{SSF}(-\psi)}$.

2. The following expressions are valid for all values of ζ:

$$\mathrm{SSF}=\begin{cases} |\psi|\le\dfrac{\pi}{2} & \dfrac{\exp[-\zeta\sec\psi]-\exp[-\zeta\sec\psi_0]}{\zeta(\sec\psi_0-\sec\psi)} \\ \dfrac{\pi}{2}<|\psi|<\pi & \dfrac{1-\exp[-\zeta(\sec\psi_0-\sec\psi)]}{\zeta(\sec\psi_0-\sec\psi)} \end{cases}$$

$$\mathrm{SAF}=\begin{cases} |\psi|\le\dfrac{\pi}{2} & \dfrac{1}{2}\{\exp(-\zeta\sec\psi_o)+\exp(-\zeta\sec\psi)\} \\ \dfrac{\pi}{2}<|\psi|<\pi & \dfrac{1}{2}\{1+\exp(\zeta[\sec\psi-\sec\psi_o])\} \end{cases}$$

Inspecting these expressions we find that for all ψ,

$\boxed{\mathrm{SAF}(\psi)=\exp(-\zeta\sec\psi)\cdot\mathrm{SAF}(\psi+\pi)}$ and $\boxed{\mathrm{SSF}(\psi)=\exp(-\zeta\sec\psi)\cdot\mathrm{SSF}(\psi+\pi)}$.

3. In the limit of weak scattering by the sample, $\zeta\ll1$. Writing $a=\zeta\sec\psi_0$ and $b=\zeta\sec\psi$ and expanding the exponentials we obtain

$$\mathrm{SSF}=\begin{cases} |\psi|\le\dfrac{\pi}{2} & \dfrac{\exp[-b]-\exp[-a]}{a-b}=\dfrac{1-b+\frac{1}{2}b^2-\frac{1}{6}b^3-1+a-\frac{1}{2}a^2+\frac{1}{6}a^3+\ldots}{a-b}=1-\dfrac{1}{2}(a+b)+\dfrac{1}{6}(a^2+ab+b^2)+\ldots \\ \dfrac{\pi}{2}<|\psi|<\pi & \dfrac{1-\exp[-(a-b)]}{a-b}=\dfrac{1-1+(a-b)-\frac{1}{2}(a-b)^2+\frac{1}{6}(a-b)^3\ldots}{a-b}=1-\dfrac{1}{2}(a-b)+\dfrac{1}{6}(a-b)^2+\ldots \end{cases}$$

and

$$\mathrm{SAF}=\begin{cases} |\psi|\le\dfrac{\pi}{2} & \dfrac{1}{2}\{\exp(-a)+\exp(-b)\}\approx\dfrac{1}{2}\left(1-a+\dfrac{1}{2}a^2+1-b+\dfrac{1}{2}b^2+\ldots\right)=1-\dfrac{1}{2}(a+b)+\dfrac{1}{4}(a^2+b^2)+\ldots \\ \dfrac{\pi}{2}<|\psi|<\pi & \dfrac{1}{2}\{1+\exp(-(a-b))\}\approx\dfrac{1}{2}\left(1+1-(a-b)+\dfrac{1}{2}(a-b)^2+\ldots\right)=1-\dfrac{1}{2}(a-b)+\dfrac{1}{4}(a-b)^2+\ldots \end{cases}$$

Hence $\boxed{\mathrm{SSF}(\psi)\approx\mathrm{SAF}(\psi)}$.