CHAPTER 9

# Plugin functions for SESANS

The depolarization of the neutron beam as a function of the spin-echo length $z$ is given by

$$\frac{P_n(z)}{P_{n0}} = \exp\left(\tilde{G}(z) - \tilde{G}(0)\right) \tag{9.1}$$

where the SESANS correlation function reads as

$$\tilde{G}(z) = \frac{1}{k_0^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}Q_y \, \mathrm{d}Q_z \frac{\mathrm{d}\Sigma(\mathbf{Q})}{\mathrm{d}\Omega} \frac{\cos(Q_z z)}{S} \tag{9.2}$$

$$= \frac{1}{k_0^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}Q_y \, \mathrm{d}Q_z \frac{\mathrm{d}\sigma(\mathbf{Q})}{\mathrm{d}\Omega} t \cos(Q_z z) \tag{9.3}$$

with $\mathbf{Q} = (0, Q_y, Q_z)^T$ and $\frac{\Sigma(\mathbf{Q})}{\mathrm{d}\Omega}$ being the macroscopic differential scattering cross section in units of $\mathrm{cm}^2$ and $\frac{\sigma(\mathbf{Q})}{\mathrm{d}\Omega} = \frac{1}{V}\frac{\Sigma(\mathbf{Q})}{\mathrm{d}\Omega}$ differential scattering cross section normalized on the sample volume $V = tS$ in units of $\mathrm{cm}^{-1}$. $t$ is the sample thickness and $S$ the aperture cross section defining the illuminated sample area. For isotropic scattering $\frac{\sigma(\mathbf{Q})}{\mathrm{d}\Omega} = \frac{\sigma(Q)}{\mathrm{d}\Omega}$, where the scattering only depends on the modulus of the scattering vector $Q = |\mathrm{Q}|$ the SESANS correlation function simplifies to a Hankel transform of the scattering intensity. To see this, one can change from the cartesian coordinate system $(0, Q_y, Q_z)$ to the polar coordinate system $Q(0, \sin\phi, \cos\phi)$ with $\mathrm{d}Q_y \mathrm{d}Q_z = Q\mathrm{d}Q\mathrm{d}\phi$. The integration over $\phi$ yield the cylindrical zeroth-order Bessel function

$$J_0(Qz) = \frac{1}{2\pi} \int_0^{2\pi} \cos\left(Q\cos(\phi)z\right) \mathrm{d}\phi \tag{9.4}$$

so that one finds

$$\tilde{G}(z) = \frac{2\pi t}{k_0^2} \int_0^{\infty} Q J_0(Q, z) \frac{\mathrm{d}\sigma(Q)}{\mathrm{d}\Omega} \mathrm{d}Q \tag{9.5}$$

$$= \frac{\lambda^2 t}{4\pi^2} \int_0^{\infty} 2\pi Q J_0(Q, z) \frac{\mathrm{d}\sigma(Q)}{\mathrm{d}\Omega} \mathrm{d}Q = \frac{\lambda^2 t}{4\pi^2} \mathcal{H}\left[\frac{\mathrm{d}\sigma(Q)}{\mathrm{d}\Omega}\right] \tag{9.6}$$

where $\mathcal{H}[\ldots]$ denotes the Hankel transform. The unnormalized SESANS correlation function is normally calculated via the Abel transform of the scattering length density autocorrelation function $\tilde{\gamma}(\mathbf{r}) = \int \rho(\mathbf{r}')\rho(\mathbf{r}' - \mathbf{r})\mathrm{d}\mathbf{r}'$.

$$\tilde{G}(z)\frac{4\pi^2}{\lambda^2 t} = 2\int_z^\infty \frac{\tilde{\gamma}(r)r}{\sqrt{r^2 - z^2}}\mathrm{d}r \tag{9.7}$$

The scattering intensity $I(Q)$ and $\tilde{\gamma}(r)$ are related by Fourier transform

$$I(Q) = \int_0^\infty \tilde{\gamma}(r)\frac{\sin Qr}{Qr}4\pi r^2 \mathrm{d}r \tag{9.8}$$

In literature the expressions for the scattering length density autocorrelation function are often normalized to to 1 for $r = 0$, i.e. the expressions $\gamma_0(r) = \tilde{\gamma}(r)/\tilde{\gamma}(0)$ are given.

## 9.1. Sphere

The scattering intensity for a single sphere is given by

$$I(Q) = \left(\frac{4}{3}\pi R^3 \Delta\eta\right)^2 \left(3\frac{\sin QR - QR\cos QR}{Q^3R^3}\right)^2 \tag{9.9}$$

The unnormalized autocorrelation function for this sphere is given by

$$\tilde{\gamma}(r) = \begin{cases} \Delta\eta^2 \frac{4}{3}\pi R^3 \left(1 - \frac{3}{4}\frac{r}{R} + \frac{1}{16}\left(\frac{r}{R}\right)^3\right) & \text{for } r \leq R \\ 0 & \text{for } r > R \end{cases} \tag{9.10}$$

and the unnormalized SESANS correlation function

$$\tilde{G}(z)\frac{4\pi^2}{\lambda^2 t} = \Delta\eta^2 \pi R^4 \left(\sqrt{1-\xi^2}(2+\xi^2) - \xi^2(\xi^2 - 4)\ln\left(\frac{\xi}{1+\sqrt{1-\xi^2}}\right)\right) \tag{9.11}$$

with $\xi = \frac{z}{2R}$.