Relationships between various correlation functions and the scattering profiles

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Here, we outline the relationships between various frequently used functions defining structure and their scattering corollaries. Common variables used here are scattering power for a scatterer, f_i, scalar distance between two scatterers (j and k), r_{jk}, total number of scatterers in a sample, N, number density of scatterers, ρ_0. Note that although scattering power inherently has a q dependence, in the small angle region scattering power may be considered constant[**?**].

1.1 Structural correlation functions definitions

Radial distribution function, $R(r)$:

$$R(r) = \frac{1}{\langle f \rangle} \sum_j \sum_k f_j^* f_k \delta(r - r_{jk}). \tag{1}$$

Real space pair density, $\rho(r)$:

$$\rho(r) = \frac{1}{4\pi r^2 N \langle f \rangle^2} \sum_{j \neq k} f_j f_k \delta(r - r_{jk}). \tag{2}$$

Atomic pair distribution function (PDF), $g(r)$:

$$g(r) = 4\pi r \left[\rho(r) - \rho_0\right] = \frac{1}{rN \langle f \rangle^2} \sum_{j \neq k} f_j f_k \delta(r - r_{jk}) - 4\pi r \rho_0. \tag{3}$$

Reduced pair distribution function, $G(r)$:

$$G(r) = 4\pi r \rho_0 \left[g(r) - 1\right]. \tag{4}$$

1.2 Scattering profile function definitions

The full scattering, $I(q)$:

$$I(q) = I_{coh}(q) + I_{incoh}(q), \tag{5}$$

where the incoherent scattering, I_{incoh}, is defined as:

$$I_{incho} = \sum_{j} f_j^* f_j = N \left\langle f^2 \right\rangle , \tag{6}$$

and the coherent scattering, I_{coh} is:

$$I_{coh} = \sum_{j,k} f_j^* f_k \, \exp\left(\mathrm{i}\,\vec{q} \cdot \vec{r}_{jk}\right). \tag{7}$$

The discrete scattering, I_d, which is the coherent component minus the incoherent, may be defined:

$$I_d = I_{coh} - I_{incho} = \sum_{i \neq j} f_j^* f_k \, \exp\left(\mathrm{i}\,\vec{q} \cdot \vec{r}_{jk}\right). \tag{8}$$

The total scattering structure function, $S(q)$, is defined as:

$$S(q) = \frac{I_{coh}}{N \left\langle f \right\rangle^2} - \frac{\left\langle \left(f - \left\langle f \right\rangle\right)^2 \right\rangle}{\left\langle f \right\rangle^2} \tag{9}$$

which if we take into account angle-averaging, may be written as:

$$S(q) - 1 = \frac{1}{N \left\langle f \right\rangle^2} \sum_{j \neq k} f_j^* f_k \, \exp\left(\mathrm{i}\,\vec{q} \cdot \vec{r}_{jk}\right). \tag{10}$$

The reduced total scattering structure function, $F(q)$, being $[S(q) - 1]$ rescaled by q and averaged over all angles, may be written:

$$F(q) = q\,[S(q) - 1] = \frac{1}{N \left\langle f \right\rangle^2} \sum_{j \neq k} f_j^* f_k \, \frac{\sin\left(q\, r_{jk}\right)}{r_{jk}}. \tag{11}$$

The sine-transform of $F(q)$ generates a function, $h(r)$, which is defined:

$$\begin{aligned} h(r) &= \frac{2}{\pi} \int_0^\infty \frac{1}{N \left\langle f \right\rangle^2} \sum_{j \neq k} f_j^* f_k \, \frac{\sin\left(q\, r_{jk}\right)}{r_{jk}} \sin(qr) \mathrm{d}q \\ &= \frac{1}{rN \left\langle f \right\rangle^2} \sum_{j \neq k} f_j^* f_k \left[\delta(r - r_{jk}) - \delta(r + r_{jk})\right] \end{aligned}$$

limiting the calculation to values of $r > 0$ only, one finds:

$$h(r) = \frac{1}{rN \left\langle f \right\rangle^2} \sum_{j \neq k} f_j^* f_k \delta(r - r_{jk}). \tag{12}$$

1.3 Relations between various scattering and correlation functions

The relationships between the total scattering structure function $S(q)$, total scattering intensity $I(q)$, reduced total scattering structure function $F(q)$, and the coherent scattering intensity $I_{coh}(q)$:

$$S(q) = \frac{I(q)}{\left\langle f \right\rangle^2} = \frac{F(q)}{q} + 1 = \frac{I_{coh}}{N \left\langle f \right\rangle^2} - \frac{\left\langle (f - \left\langle f \right\rangle)^2 \right\rangle}{\left\langle f \right\rangle^2}. \tag{13}$$

The relationships between the real space pair density, $\rho(r)$, the radial distribution function $R(r)$, and Fourier transform of the reduced total scattering structure function, $k(r)$, the atomic pair distribution function, $g(r)$, and the reduced pair distribution function $G(r)$, are:

$$\rho(r) = \frac{k(r)}{4\pi r} = \frac{R(r)}{4\pi r^2} = \frac{g(r)}{4\pi r} + \rho_0 = \frac{G(r) + 4\pi r \rho_0 \left(1 + 4\pi r \rho_0\right)}{16\pi^2 r^2 \rho_0} \tag{14}$$

The weighted pair density function, $w(r)$ (defined in equation **??**), asymptotically approaches a rescaled $\rho(r)$ as:

$$\lim_{N_p \to \text{all}} [w(r)] = 4\pi r^2 N \left\langle f \right\rangle^2 \rho(r). \tag{15}$$

As we have defined $I^a(q)$, it's closest corollary is the coherent scattering, $I_{coh}(q)$, which has been angle averaged over the scattering interaction $\mathbf{q} \cdot \mathbf{r}_{jk}$, though as one can see in equation 13, this quantity is closely related to many others. Note that $I^a(q)$ represents the scattering from a finite ensemble of scatters. If the ensemble represents a subsample of a larger volume, the amplitude may be scaled such that the approximative scattering from the full volume, $I^a_f(q)$, is defined:

$$I^a_f(q) = \frac{nV_{tot}}{N} I^a(q) \tag{16}$$

where n is the number density of scatterers, V_{tot} is the total volume scattering occurs over (not just the ensemble), and N is the number of scatterers in the subsample ensemble.