FANCY BACKGROUND SUBTRACTION, A DERIVATION

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1. Why

For strongly absorbing scattering, it is important to accurately extract the sample scattering contribution, from the contributions of the upstream and downstream sample container wall. Furthermore, the attenuation of the unscattered and scattered radiation needs to be considered.

2. Base definitions

2.1. System definitions. The scattering system is considered to consist of a three-component, sandwich-like structure (Figure 1): An upstream sample container wall, followed by the sample, followed by the downstream sample container wall. All components are considered to be plate-like in shape, with the plate normal parallel to the direct beam. Furthermore, the distance between the sample and the detector is considered to be much larger than the thickness of the sample.

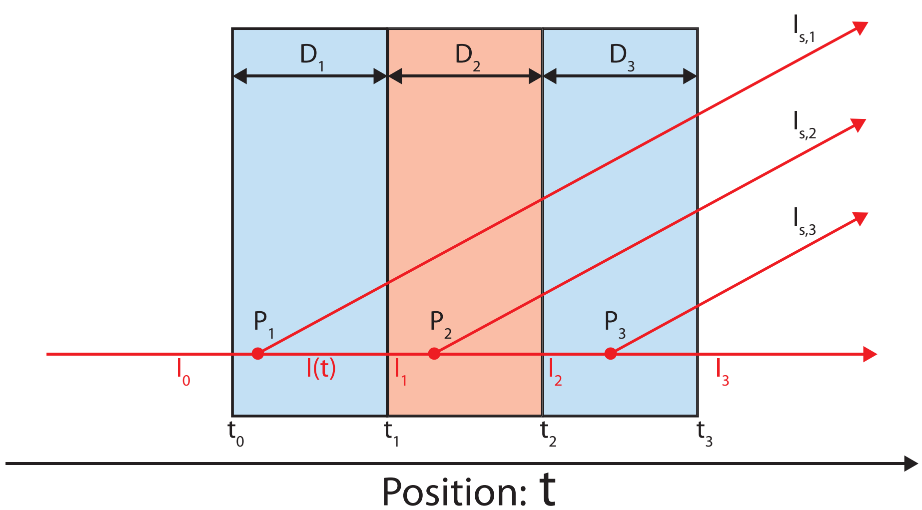

Figure 1. Schematic drawing of the scattering and absorbing elements in the X-ray beam.

2.2. **Geometric definitions.** The upstream sample wall is denoted by the subscript $_1$, the sample by $_2$, and the downstream container wall by $_3$. The following definitions are made:

- D: The thickness of a phase
- t: The running variable of distance travelled through a phase
- t_0: position at the start of the upstream sample container component
- t_1: position at the start of the sample component (end of the upstream sample container component)
- t_2: position at the start of the downstream sample container component (end of sample component)
- t_3: position at the end of the downstream sample container component
- $SA(2\theta)$: The self-absorption correction for scattering occurring within a component
- $P(2\theta)$: The scattering probability
- $I(t)$: The primary beam intensity at position t
- $I_s(t)$: The scattered intensity at position t
- I_0: The primary beam intensity
- I_1: The primary beam intensity entering the sample phase
- I_2: The primary beam intensity entering the downstream sample container component
- I_3: The primary beam intensity after absorption through all of the components
- α: The linear absorption coefficient
- 2θ: The angle of the scattered radiation

2.3. **Absorption of the unscattered beam.** The unscattered beam absorption is defined as:

$$I_0(t) = I_0 \exp(-\alpha t) \tag{1}$$

The beam intensities entering the various phases therefore work out as:

$$\begin{aligned} I_1 = &\quad I_0 \exp(-\alpha_1 D_1) \\ I_2 = &\quad I_0 \exp(-(\alpha_1 D_1 + \alpha_2 D_2) \\ I_3 = &\quad I_0 \exp(-(\alpha_1 D_1 + \alpha_2 D_2 + \alpha_3 D_3) \end{aligned} \tag{2}$$

2.4. **Absorption of scattered beam by subsequent components.** Components in place after a scattered photon will absorb the scattered radiation with an absorption length slightly larger than the unscattered beam. The length of travel of the photon though subsequent materials is defined as:

$$l(2\theta, t) = \frac{D - t}{\cos(2\theta)} \tag{3}$$

The absorption factor ζ of scattered radiation through subsequent phases therefore is:

$$\zeta_n(2\theta) = \frac{I_{s,n}}{I_{s,n-1}} = \exp(-\alpha_n l(2\theta)) \tag{4}$$

2.5. **Intensity scattered from the total.** The total scattered intensity is the sum of the scattering from all three components in the beam, attenuated by their subsequent phases.

$$I_s = I_{s,1}\zeta_2(2\theta)\zeta_3(2\theta) + I_{s,2}\zeta_3(2\theta) + I_{s,3} \tag{5}$$

The scattered intensities of the individual components are defined as follows:

$$I_{s,n} = I_n \int_{t_n}^{t_{n+1}} \exp(-\alpha_n t) P_n(2\theta) \exp\left(-\alpha_n \frac{D-t}{\cos(2\theta)}\right) \mathrm{d}t \tag{6}$$

And since the scattering probability P_n is independent of the location t in the phase:

$$I_{s,n} = I_n P_n(2\theta) \int\limits_{t_n}^{t_{n+1}} \exp\left(-\alpha_n \left[t + \frac{D-t}{\cos(2\theta)}\right]\right) \mathrm{d}t \tag{7}$$

2.6. **Extracting the bit we are after.** We can extract the scattering probability of the second component (the bit we are after) through rearrangement of equations 5 and 7:

$$P_2(2\theta) = \frac{I_s - I_{s,3} - I_{s,1}\zeta_2(2\theta)\zeta_3(2\theta)}{\zeta_3(2\theta) I_2 \int\limits_{t_n}^{t_{n+1}} \exp\left(-\alpha_n \left[t + \frac{D-t}{\cos(2\theta)}\right]\right) \mathrm{d}t} \tag{8}$$