ON EFFECTIVE AND OPTICAL RESOLUTIONS OF DIFFRACTION DATA SETS

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Supplementary Material

Reminder A: the three-dimensional interference function

In order to calculate the integral

$$\rho(r) = \rho(|\mathbf{r}|) = \int\limits_{|\mathbf{s}| \le D} e^{-2\pi i(\mathbf{rs})} d\mathbf{s} \qquad \text{(A1)}$$

one may use the spherical symmetry of the resulted function and calculate its value along the axis **OZ**. In the polar coordinates,

$$(\mathbf{rs}) = zs\cos\theta \qquad \text{(A2)}$$

where θ is the angle between **OZ** and the vector $\mathbf{s}$ of the length *s*. Therefore,

$$\rho(z) = \int_0^D \int_0^\pi \int_0^{2\pi} s^2 \sin\theta e^{-2\pi i z s\cos\theta} d\varphi d\theta ds = 2\pi \int_0^D \int_0^\pi s^2 \sin\theta e^{-2\pi i z s\cos\theta} d\theta ds =$$

$$= -2\pi \int_0^D \int_0^\pi s^2 e^{-2\pi i z s\cos\theta} d(\cos\theta) ds = 2\pi \int_0^D \int_{-1}^1 s^2 e^{-2\pi i z s t} dt ds = 2\pi \int_0^D s^2 \frac{1}{2\pi i z s}\left(e^{2\pi i z s} - e^{-2\pi i z s}\right) ds =$$

$$= \frac{2}{z}\int_0^D s\sin(2\pi z s) ds = \frac{2}{z}\left[-\frac{s\cos(2\pi z s)}{2\pi z}\Bigg|_0^D + \frac{1}{2\pi z}\int_0^D \cos(2\pi z s) ds \right] =$$

$$= \frac{1}{\pi z^2}\left[-D\cos(2\pi z D) + \frac{1}{2\pi z}\sin 2\pi z s\Bigg|_0^D \right] = \frac{1}{2\pi^2 z^3}\left[-2\pi z D\cos(2\pi z D) + \sin 2\pi z D \right] =$$

$$= \frac{4\pi D^3}{3}\left[3\frac{\sin 2\pi z D - 2\pi z D\cos(2\pi z D)}{(2\pi z D)^3} \right] \tag{A3}$$

With $d = D^{-1}$ and the interference function (Fig. 1a of the main text)

$$G_3(t) = 3\frac{\sin(t) - t\cos(t)}{t^3} \tag{A4}$$

we obtain

$$\rho(r) = \frac{4\pi d^{-3}}{3} G_3(2\pi r / d) \tag{A5}$$

Obviously, derivatives of this function can be calculated analytically as well.

Reminder B: some features of the interference function

Various characteristics of the interference function $G_3(t) = G_3(2\pi r d^{-1})$ are known.

a) Its first zero is $t \approx 4.49$ corresponding to the distance $r/d \approx 0.715$, and the first minimum is at $r/d \approx 0.917$. In crystallographic literature this was indicated, for example by James (1948) and Stenkamp & Jensen (1984).

b) Its development in the Taylor series in the origin

$$G_3(t) \approx \frac{3}{t^3}\left[\left(t - \frac{t^3}{3!} + \frac{t^5}{5!} - \frac{t^7}{7!} + \right) - t\left(1 - \frac{t^2}{2!} + \frac{t^4}{4!} - \frac{t^6}{6!}\right)\right] =$$

$$= \frac{3}{t^3}\left[-\frac{t^3}{3!} + \frac{t^5}{5!} - \frac{t^7}{7!} + \frac{t^3}{2!} - \frac{t^5}{4!} + \frac{t^7}{6!}\right] = \tag{B1}$$

$$= 3\left[-\frac{1}{3!} + \frac{t^2}{5!} - \frac{t^4}{7!} + \frac{1}{2!} - \frac{t^2}{4!} + \frac{t^4}{6!}\right] = 1 - \frac{t^2}{10} + \frac{t^4}{280}$$

proves that $G_3(0) = 1$ and gives also an approximation

$$G_3(t) \approx \exp\left(-\frac{t^2}{2\sigma_t^2}\right) \text{, with } \sigma_t = \sqrt{5} \tag{B2}$$

or

$$\rho(x) \approx \exp\left(-\frac{(2\pi x)^2}{2\sigma_\tau^2}\right) = \exp\left(-\frac{x^2}{2\sigma_x^2}\right) , \tag{B3}$$

with

$$\sigma_x = \frac{\sqrt{5}}{2\pi} \approx 0.356 \tag{B4}$$

used by Vaguine *et al.* (1999).

c) The inflection point of the Taylor expansion (B1) is defined by its second derivative

$$-\frac{2}{10}+\frac{12t^2}{280}=0 \tag{B5}$$

giving

$$t=\sqrt{\frac{70}{15}}\approx 2.160 \tag{B6}$$

Converting this to x gives

$$x=\frac{t}{2\pi}\approx 0.344 \tag{B7}$$

However, a direct calculation of the inflection point as a root of

$$\begin{aligned} G_3''(t) &= \frac{d}{dt}\left\{3\left[\frac{\cos(t)}{t^3}-\frac{3\sin(t)}{t^4}+\frac{2\cos(t)}{t^3}+\frac{\sin(t)}{t^2}\right]\right\}= \\ &=3\frac{d}{dt}\left[-\frac{3\sin(t)}{t^4}+\frac{3\cos(t)}{t^3}+\frac{\sin(t)}{t^2}\right]= \\ &=3\left[\frac{12\sin(t)}{t^5}-\frac{3\cos(t)}{t^4}-\frac{9\cos(t)}{t^4}-\frac{3\sin(t)}{t^3}-\frac{2\sin(t)}{t^3}+\frac{\cos(t)}{t^2}\right]= \\ &=\frac{3}{t^5}\left[12\sin(t)-12t\cos(t)-5t^2\sin(t)+t^3\cos(t)\right] \end{aligned} \tag{B8}$$

gives $t\approx 2.507$ and $x\approx 0.399$ different from (B6) and (B7), respectively, as well as from (B4).

d) One may note also that for the inflection point

$$G_3(2.507)\approx 0.4991\approx 0.5=0.5G_3(0) \tag{B9}$$

Reminder C: separation of two equal Gaussian peaks

It is known that a Gaussian peak

$$g(r) = e^{-\frac{r^2}{2\sigma^2}} \tag{C1}$$

has its inflection point at the distance σ because

$$\frac{d^2 g(r)}{dr^2} = \frac{d}{dr}\left(-\frac{r}{\sigma^2} e^{-\frac{r^2}{2\sigma^2}}\right) = \frac{d}{dr}\left(-\frac{1}{\sigma^2} + \frac{r^2}{\sigma^4}\right) e^{-\frac{r^2}{2\sigma^2}} = 0 \tag{C2}$$

for $r = \sigma$. This means that two Gaussian peaks defined as

$$\rho_{G,0}(r) = \left(\frac{4\pi}{B}\right)^{3/2} e^{-\frac{1}{B}(2\pi\, r)^2} \tag{C3}$$

are seen separately when the distance between them is larger than the limit value 2σ, *i.e.*

$$d_{opt} = \sqrt{\frac{B}{2\pi^2}} \tag{C4}$$