Fourier transforming by hand: the sinc function

Brian R. Pauw

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1 Introduction

Those who read the older SAXS literature will note liberal use of Fourier transformation to calculate the scattering behaviour of odd-shaped particles. Likewise, the effects of smearing due to (for example) beam shape (think "blurring" of the scattering pattern) can be easily determined using such transforms. It is useful to get a feel for the methods for derivation of such Fourier transforms, so I decided it was time to refresh my rusty Fourier transform skills.

This document describes one Fourier transformation in excessive detail, with (hopefully) easy to follow steps.

2 Fourier transform definitions

We use the definition of the Fourier transform applied to scattering from Ruland [1964], thus defining $F(\mathbf{q})$ as our form factor:

$$F(\mathbf{q}) = \int_v \rho(\mathbf{r}) \exp^{-i\mathbf{qr}} \mathrm{d}v \tag{1}$$

where ρ is the electron density distribution, r is the real-space vector, and the magnitude of the reciprocal space vector $\mid \mathbf{q} \mid= q$ defined as $q = 4\pi/\lambda \sin\theta$. We can choose which volume space coordinate system makes our Fourier Transform-life easiest for us, depending on the description of ρ. Typical choices are the cartesian coordinate system (i.e. where $\mathbf{r}$ is described in orthogonal coordinates x, y, z), for which the volume integral is:

$$F(\mathbf{q}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \rho(\mathbf{r}) \exp^{-i\mathbf{qr}} \mathrm{d}x\mathrm{d}y\mathrm{d}z \tag{2}$$

the cylindrical coordinate system, with $\mathbf{r}$ described in coordinates of radius r, height z and azimuthal angle θ (sorry for reusing theta there):

$$F(\mathbf{q}) = \int_{-\infty}^{\infty}\int_{0}^{\pi}\int_{0}^{\infty} \rho(\mathbf{r}) \exp^{-i\mathbf{qr}} r\mathrm{d}r\mathrm{d}\theta\mathrm{d}z \tag{3}$$

and the spherical coordinate system, with $\mathbf{r}$ described in coordinates of radius r, polar angle θ and azimuthal angle ϕ:

$$F(\mathbf{q}) = \int_{0}^{2\pi}\int_{0}^{\pi}\int_{0}^{\infty} \rho(\mathbf{r}) \exp^{-i\mathbf{qr}} r^2 \sin\theta \mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi \tag{4}$$

3 Definition of $\rho(\mathbf{r})$

For our simplest system, we consider two slit edges, separated over a distance $2R$. We therefore define:

$$\rho(\mathbf{r}) = \rho(x) \begin{cases} \frac{1}{2R} & \text{, for } -R \leq x \leq R \\ 0 & \text{, for } x < -R, x > R \end{cases} \tag{5}$$

This is a handy definition, as is zero outside the limits $x \leq -R, x \geq R$.

4 Additional useful equivalencies

We will be able to use the following equivalencies: for the complex numbers z:

$$z = x + iy = \mid z \mid (\cos\theta + i \sin\theta) = \mid z \mid \exp^{i\theta} \tag{6}$$

and some trigonometric identities:

$$\begin{aligned} \cos(-x) &= \cos x \\ \sin(-x) &= -\sin(x) \end{aligned} \tag{7}$$

5 Derivation

Since we are considering one direction x only, and we consider the scattering in the direction perpendicular to the edge only, the Fourier transform becomes:

$$F(q) = \int_{-R}^{R} \rho(x) \exp^{-iqx} \, \mathrm{d}x \tag{8}$$

substituting $\rho(x)$:

$$F(q) = \frac{1}{2R} \int_{-R}^{R} \exp^{-iqx} \, \mathrm{d}x \tag{9}$$

integrating:

$$F(q) = \frac{-1}{2iqR} \left[\exp^{-iqR} - \exp^{iqR} \right] \tag{10}$$

Changing the representation of the complex numbers using the equivalency listed in Equation 6:

$$F(q) = \frac{-1}{2iqR} \left[\cos(-qR) + i \sin(-qR) - \cos(qR) - i \sin(qR) \right] \tag{11}$$

Substituting the equivalencies in Equation 7:

$$F(q) = \frac{-1}{2iqR} \left[2i \sin(-qR) \right] \tag{12}$$

Which simplifies to:

$$F(q) = \frac{-1}{qR} \sin(-qR) \tag{13}$$

and we get the end result as:

$$F(q) = \frac{\sin(qR)}{qR} \tag{14}$$

6 Applications

The resulting function, known as the "sinc" function, can be found in many equations in scattering. For example, it is found in the full scattering equation for a cylinder and cuboids, as summarised by Pedersen [1997]. It is also found in many smearing and smoothing functions summarised by Koberstein et al. [1980].

References

Koberstein J T, Morra B and Stein R S 1980 *J. Appl. Cryst.* **13**, 34–45.

Pedersen J S 1997 *Adv. Coll. Interf. Sci.* **70**, 171–210.

Ruland W 1964 *Acta Cryst.* **17**, 138–142.