A geometric approach to a new indirect fourier transform model.

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Here, a new model is deveoped, based on the projected electron density on a slice, which is then to be Fourier transformed. It is attempted to include all aspects in this electron density, such as the orientation distributions as well as the size distributions. The emphasis here, lies on avoiding a full 3D matrix that defines the volume and shape of the object. Instead, the electron density is projected onto a 2D plane. 3D is avoided because of its stringent requirements on memory and its large effect on the speed of the model. Thus, for each 3D operation, its effect on a projection is to be determined.

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THE INITIAL FUNCTION: THE SUPERELLIPS OF REVOLUTION

The superellipse

For making a shape of revolution (a lathe object), we need to start with a function capable of describing a cross-section of a scatterer. As a basic shape, the superellipse is a unique function. It describes shapes from cylindrical to ellipsoidal to diamond-shaped to hyperdiamond shaped cross-sections. Thus, it appears well suited to describe a wide range of rotationally symmetric scattering objects.

The superellipse is described by [1]:

$$1 = \left|\frac{x}{a}\right|^r + \left|\frac{y}{b}\right|^r \tag{1}$$

An example superellipse with $a = 1, b = 2$ and $r = 3$ is shown in Figure 1

revolving a shape

given a shape function in an xy plane, revolving around the y-axis gives us our lathe object. Being able to describe this revolution as a projection of the density of the object onto the xy plane would provide us with the density map, the fourier transform of which corresponds to the scattering pattern of the shape.

To rephrase, what is sought is the projected (electron) density of a 3D shape of constant density onto a 2D surface. The 3D shape is described by revolving a 2D function around one axis. Figure 5 shows graphically that which we are searching for (i.e. ρ).

In order to find $\rho(r_i, r_c)$ we have defined a few values as defined in figure 5. r_c is the length from the axis of revolution to the contour point on the image plane, r_i is the point for which the density is sought. This point is revolved around the rotation axis, and the density ρ is thus sought. It can be shown that

$$\frac{\rho(x, r_c)}{2} = r_c \sin(\zeta) \tag{2}$$

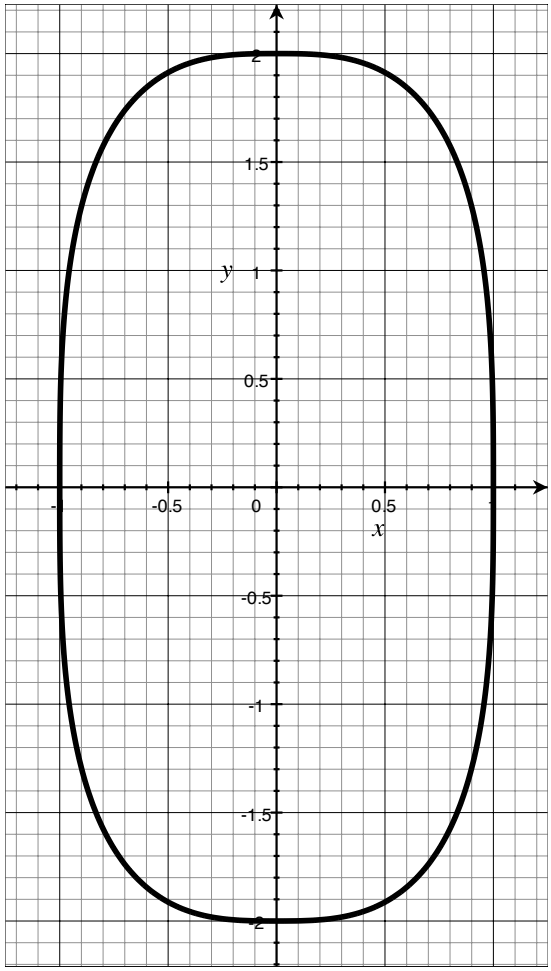

FIG. 1: Superellipse contour with $a = 1, b = 2$ and $r = 3$.

where ζ can be composed out of the ratio of r_c and r_i:

$$\zeta = \arccos\left(\frac{r_i}{r_c}\right) \tag{3}$$

Combination results in:

$$\rho(r_i, r_c) = 2r_c \sin\left(\arccos\left(\frac{r_i}{r_c}\right)\right) \tag{4}$$

This function then provides us with the ability to turn any arbitrary cross-section into a shape of revolution. The function is plotted in Figure 3 for $r_c = 1$.

implementation examples

This function has been implemented in Matlab.

IMPLEMENTING THE ORIENTATION DISTRIBUTION

Rotational smearing of the 2D scattering pattern around its centre poses little difficulty. However, rotation of the scattering pattern in the image plane does not take into account the full rotational freedom of the scattering elements in 3D (c.f. Figure 4), but instead only rotates the scatterers in real space in one plane.

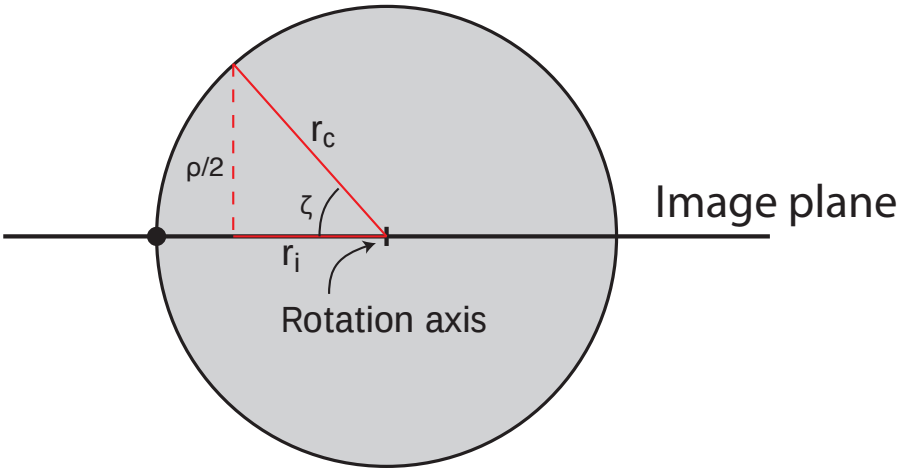

FIG. 2: Making the revolution. The image is a top view onto the (xy) plane, the dot has been revolved around the rotation axis to make the shape of revolution.

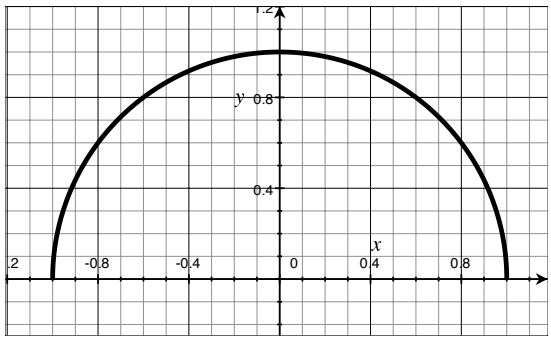

FIG. 3: Making the revolution; showing equation 4 for $r_c = 1$.

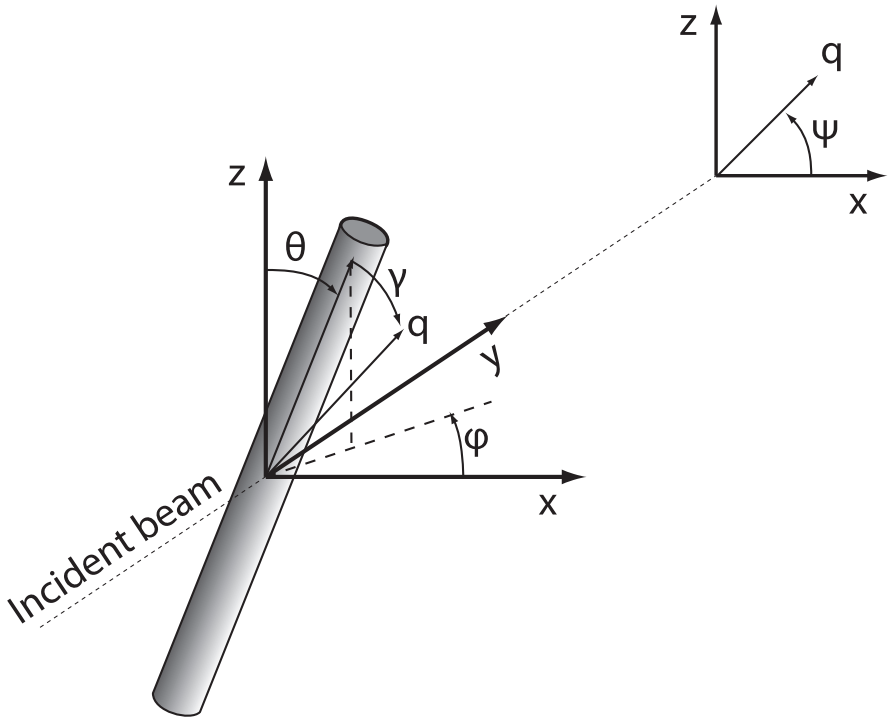

FIG. 4: Angles used in the model description and development.

In order to get around this issue, we will attempt to derive a mathematical method of smearing a 2D projection of the electron density (obtained in the previous step). This method will subsequently rotationally smear the projection in the image plane, after which a rotation step is applied around the y-axis. The thus obtained electron density map may be identical to that obtained by stepping through individual steps of a tilt of the pattern followed by a rotation around y. Thus it has to be shown, algebraically, that:

$$\sum_{step=1}^{step=n} p \times \mathrm{tiltofn/90degreesrotationaroundy-axis} = \mathrm{rotationaroundy-axis} \times \sum_{step=1}^{step=n} p \times \mathrm{tiltofn/90degrees} \tag{5}$$

where $p(n)$ is the probability of that tilt of that particular angle. Tilt smearing in this fashion, is relatively simple, and relatively fast. This method is already implemented, and does tilt smearing in one degree steps for 90 steps. This method has been described in a different paper.

The one step which is not straightforward is the computation of the rotational average, for computing the smeared intensity when rotating around the y-axis. For this, one needs to compute the projected density per point on the image during the rotation. The way this is done, is by computation of the "residence" time of the point during a full rotation around y. In other words, computing the speed of the projected point on the xy-plane during rotation (c.f. Figure 5).

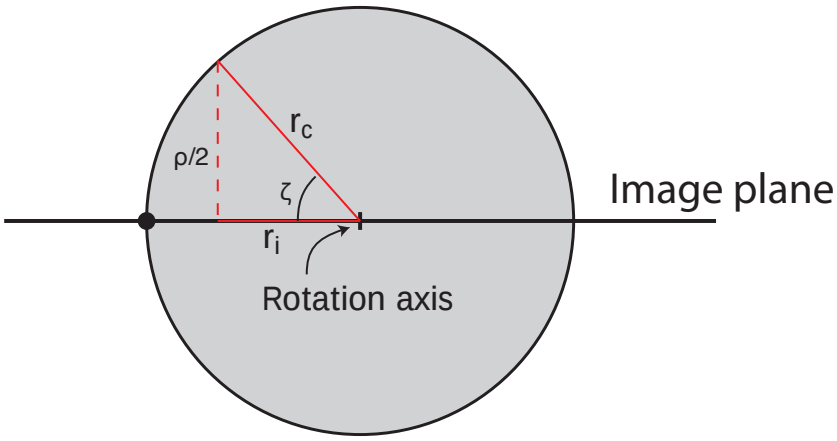

FIG. 5: Angles used in the rotational smearing model description and development.

The projection on the x-axis of the point during rotation with constant speed, is computed to be:

$$x = r_c \sin(t) \tag{6}$$

If we take t as going from $-\frac{\pi}{2}$ to $\frac{\pi}{2}$, then the position of the point is graphically shown in Figure 6.

inverting this function allows us to express the time as a function of position:

$$\arcsin\left(\frac{x}{r_c}\right) = t \tag{7}$$

and the derivative of this gives us a residence time, and thus the density of the projected point per pixel:

$$d_t = \frac{1}{\sqrt{1 + \frac{x}{r_c}^2}} \tag{8}$$

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[1] E. W. Weisstein, *"superellipse." from mathworld–a wolfram web resource.* (2008), URL http://mathworld.wolfram.com/Superellipse.html.

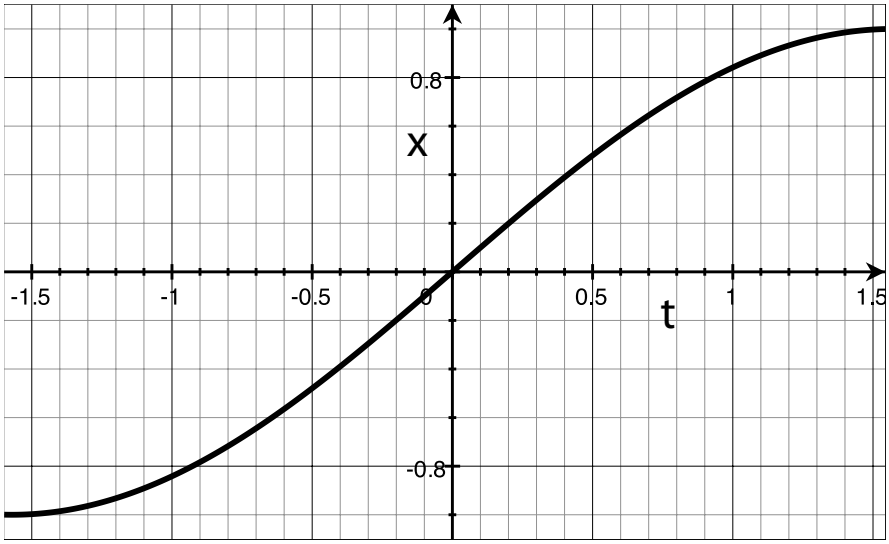

FIG. 6: The projection of a point on the x-axis (vertical) as it revolves around the y-axis with a constant speed t (horizontal axis).