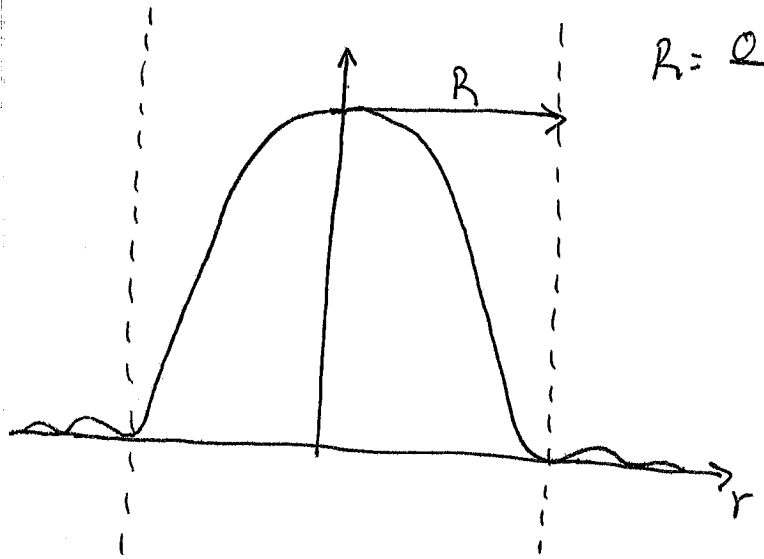
The Resolution Problem

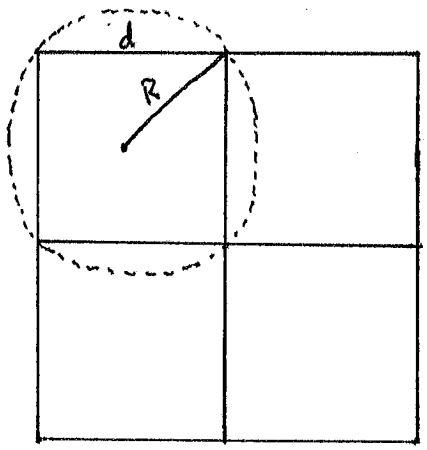
R = resolution = "res" in the code

Airy



$$R = \frac{0.61}{Q}$$

We approximate the cylindrical shape of the pixel in the experiment by a rectangle in the simulation (as shown below) so that every atom is counted once and only once.



where each pixel has side length d as a function of R:

$$\sqrt{d^2 + d^2} = 2R$$

$$\Rightarrow d = \sqrt{2}R$$

Therefore the side length of the model must be an integer multiple of $\sqrt{2}R$.

In the intensity function in the code, only atoms within $\frac{1}{2}d = \sqrt{0.5}R$ of the center of the pixel are used (in a square). Only x and y directions are considered. This correctly selects the atoms that are used in the intensity calculation.