What is the momentum resolution in x-ray scattering?

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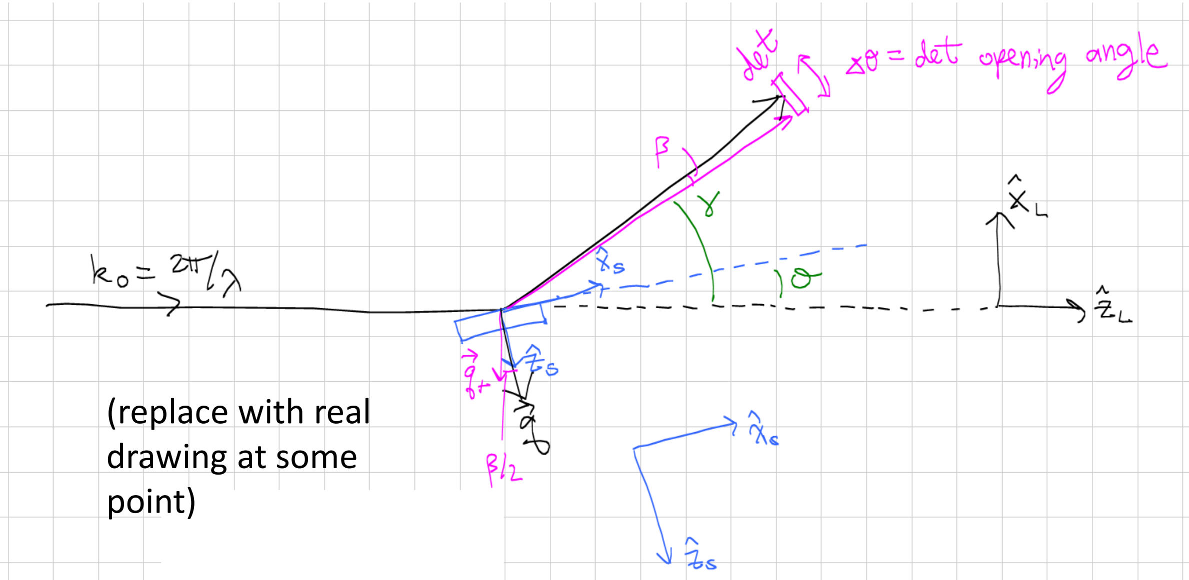
Case 1: Finite detector

Let's start with the case in which the incident beam is perfectly monochromatic and collimated and everything is limited by the detector.



(replace with real drawing at some point)

Incident beam in lab coordinates:

$$k_i = k(0,0,1)$$

Scattered beam

$$k_s = k(\sin\gamma, 0, \cos\gamma)$$

Momentum transferred *to the sample*:

$$q = k_i - k_s = k(-\sin\gamma, 0, 1-\cos\gamma)$$

This unitary rotation takes you from lab to sample coordinates:

$$U = \begin{pmatrix} \sin\theta & 0 & \cos\theta \\ 0 & 1 & 0 \\ -\cos\theta & 0 & \sin\theta \end{pmatrix}$$

For example, suppose γ = 2θ:

$$Uq = k\begin{pmatrix} \sin\theta & 0 & \cos\theta \\ 0 & 1 & 0 \\ -\cos\theta & 0 & \sin\theta \end{pmatrix}\begin{pmatrix} -\sin 2\theta \\ - \\ 1-\cos 2\theta \end{pmatrix}$$

$$= k\begin{pmatrix} -\sin\theta\sin 2\theta + \cos\theta - \cos\theta\cos 2\theta \\ 0 \\ \cos\theta\sin 2\theta + \sin\theta - \sin\theta\cos 2\theta \end{pmatrix} = k\begin{pmatrix} -\sin^2\theta\cos\theta + \cos\theta - \cos^3\theta \\ 0 \\ \sin\theta\cos^2\theta + \sin\theta + \sin^3\theta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 2k\sin\theta \end{pmatrix}$$

Case 1: Finite detector, cont.

Suppose your detector has a finite size given by $\Delta\theta = d/L$, where *d* is the detector size and *L* is the sample-detector distance. The measurement will integrate over a line segment of rays bounded by the following two points:

$$q^{+} = k\left(-\sin\left(\gamma + \Delta\theta/2\right), 0, 1 - \cos\left(\gamma + \Delta\theta/2\right)\right)$$

$$q^{-} = k\left(-\sin\left(\gamma - \Delta\theta/2\right), 0, 1 - \cos\left(\gamma - \Delta\theta/2\right)\right)$$

The detector is small, so

$$\sin\left(\gamma + \Delta\theta/2\right) = \sin\gamma\cos\Delta\theta/2 + \cos\gamma\sin\Delta\theta/2 \approx \sin\gamma + \cos\gamma\cdot\left(\Delta\theta/2\right)$$

$$\cos\left(\gamma + \Delta\theta/2\right) = \cos\gamma\cos\Delta\theta/2 - \sin\gamma\sin\Delta\theta/2 \approx \cos\gamma - \sin\gamma\cdot\left(\Delta\theta/2\right)$$

$$\sin\left(\gamma - \Delta\theta/2\right) = \sin\gamma\cos\Delta\theta/2 - \cos\gamma\sin\Delta\theta/2 \approx \sin\gamma - \cos\gamma\cdot\left(\Delta\theta/2\right)$$

$$\cos\left(\gamma - \Delta\theta/2\right) = \cos\gamma\cos\Delta\theta/2 + \sin\gamma\sin\Delta\theta/2 \approx \cos\gamma + \sin\gamma\cdot\left(\Delta\theta/2\right)$$

Therefore

$$q^{+} = k\left(-\sin\gamma - \cos\gamma\cdot\left(\Delta\theta/2\right), 0, 1 - \cos\gamma + \sin\gamma\cdot\left(\Delta\theta/2\right)\right) = q + k\left(-\cos\gamma, 0, \sin\gamma\right)\frac{\Delta\theta}{2}$$

$$q^{-} = k\left(-\sin\gamma + \cos\gamma\cdot\left(\Delta\theta/2\right), 0, 1 - \cos\gamma - \sin\gamma\cdot\left(\Delta\theta/2\right)\right) = q + k\left(\cos\gamma, 0, -\sin\gamma\right)\frac{\Delta\theta}{2}$$

Evidently we integrate over a range of momentum space from $q - \Delta q/2$ to $q + \Delta q/2$ where

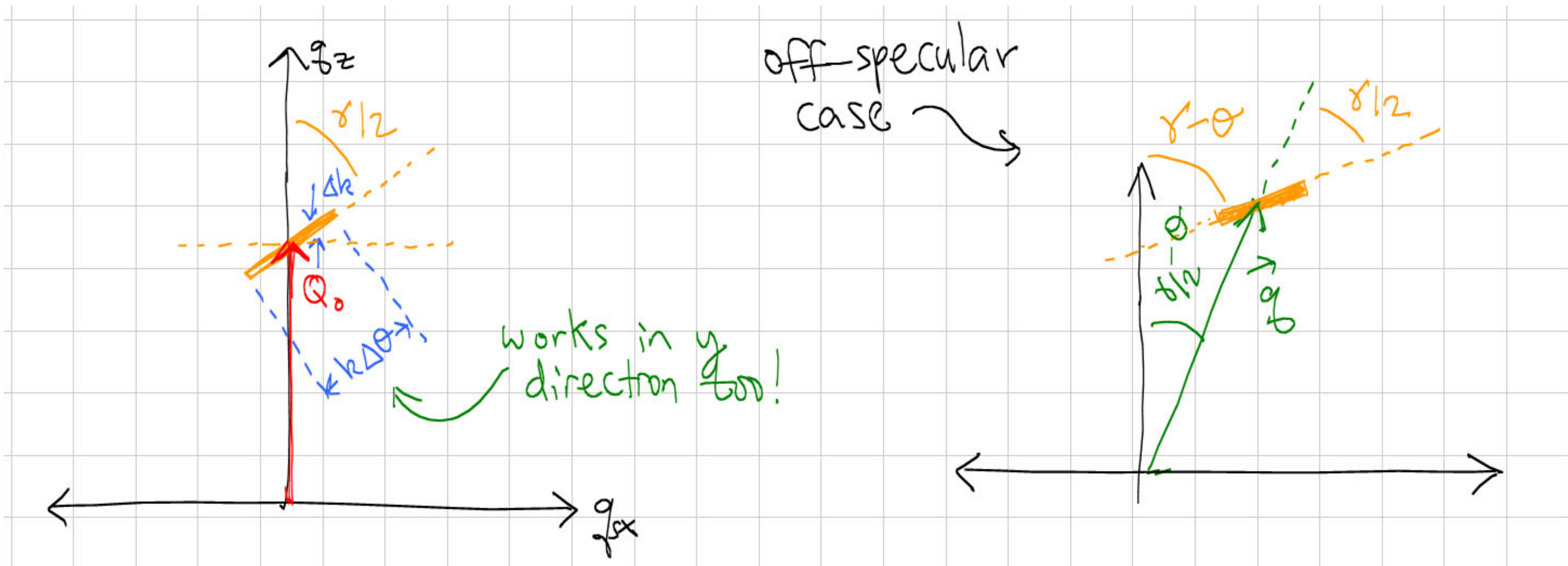
$$\Delta q = k\left(-\cos\gamma, 0, \sin\gamma\right)\Delta\theta$$

Case 1: Finite detector, cont.

We'd like to get a physical picture of where we are integrating in sample coordinates. This of course depends on the direction of *q*. Without loss of generality, let's assume *q* points along the *z* direction of the sample, i.e., $\gamma = 2\theta$, and write everything in sample coordinates. We already got *q* in this case (see page 1). Let's also get Δq:

$$U\Delta q = k\Delta\theta \begin{pmatrix} \sin\theta & 0 & \cos\theta \\ 0 & 1 & 0 \\ -\cos\theta & 0 & \sin\theta \end{pmatrix} \begin{pmatrix} -\cos\gamma \\ 0 \\ \sin\gamma \end{pmatrix} = k\Delta\theta \begin{pmatrix} \sin\gamma\cos\theta - \cos\gamma\sin\theta \\ 0 \\ \cos\theta\cos\gamma + \sin\theta\sin\gamma \end{pmatrix} = k\Delta\theta \begin{pmatrix} \sin(\gamma-\theta) \\ 0 \\ \cos(\gamma-\theta) \end{pmatrix} = k\Delta\theta \begin{pmatrix} \sin\theta \\ 0 \\ \cos\theta \end{pmatrix}$$

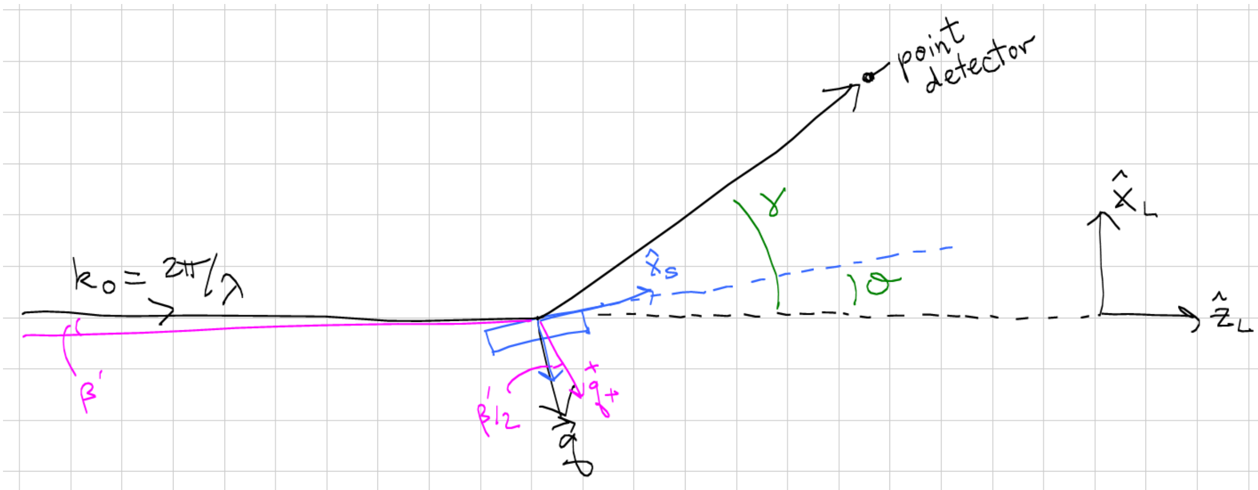
This is consistent with what is in my old notes:



Before proceeding it is easy to see what is the effect of having a finite bandwidth, Δk. Here the biggest effect is on *q* itself. In this geometry, in sample coordinates, *q* = (0,0,2 *k* sinθ). So a finite bandwidth just smears our line segment in the (longitudinal) z direction, making a trapezoid as shown.

Case 2: Finite beam divergence

OK, so let's now look at the situation in which the detector is infinitely small but the beam has a finite divergence.



Now the scattered beam is well-defined:

$$k_s = k(\sin\gamma, 0, \cos\gamma)$$

However there is a whole range of possible incident beams bounded by the following two momenta (lab coordinates):

$$k_i^+ = k\left(\sin(\Delta\theta/2), 0, \cos(\Delta\theta/2)\right) \qquad k_i^- = k\left(-\sin(\Delta\theta/2), 0, \cos(\Delta\theta/2)\right)$$

These define two momentum transfers, still in lab coordinates:

$$q^\pm = k_i^\pm - k_s = k\left(\pm\sin(\Delta\theta/2), 0, \cos(\Delta\theta/2)\right) - k(\sin\gamma, 0, \cos\gamma)$$

$$= k\left(\pm\sin(\Delta\theta/2) - \sin\gamma, 0, \cos(\Delta\theta/2) - \cos\gamma\right)$$

We'd like to find the vector Δq that has the following property:

$$q^\pm = q \pm \frac{\Delta q}{2} \qquad \text{where} \qquad q = k(-\sin\gamma, 0, 1-\cos\gamma)$$

Evidently

$$\Delta q = \pm 2\left(q^\pm - q\right)$$

Case 2: Finite beam divergence, cont.

Fair enough, let's use the positive sign:

$$\Delta q = 2\left(q^{+} - q\right) = 2k\left[\left(\sin\left(\Delta\theta/2\right) - \sin\gamma, 0, \cos\left(\Delta\theta/2\right) - \cos\gamma\right) - (-\sin\gamma, 0, 1 - \cos\gamma)\right]$$

$$= 2k\left(\sin\left(\Delta\theta/2\right), 0, \cos\left(\Delta\theta/2\right) - 1\right)$$

I guess this is a good time to do small angles:

$$\Delta q = 2k\left(\sin\left(\Delta\theta/2\right), 0, \cos\left(\Delta\theta/2\right) - 1\right) \approx 2k\left(\Delta\theta/2, 0, 0\right) = k\Delta\theta\left(1, 0, 0\right)$$

So, the resolution broadening in lab coordinates is always in the direction perpendicular to the beam, independent of the scattering angle. Again, let's look at this in sample coordinates for the case $\theta = \gamma/2$:

$$U\Delta q = k\Delta\theta \begin{pmatrix} \sin\theta & 0 & \cos\theta \\ 0 & 1 & 0 \\ -\cos\theta & 0 & \sin\theta \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = k\Delta\theta \begin{pmatrix} \sin\theta \\ 0 \\ -\cos\theta \end{pmatrix} = k\Delta\theta \begin{pmatrix} \sin\gamma/2 \\ 0 \\ -\cos\gamma/2 \end{pmatrix}$$

This is the same as the result for the finite-detector case, except the resolution broadening tips the opposite direction.

Final result

If all three effects are happening simultaneously, diverging beam, nonzero bandwidth, finite detector, the overall momentum resolution will be a convolution of the three. So you get this generic picture: