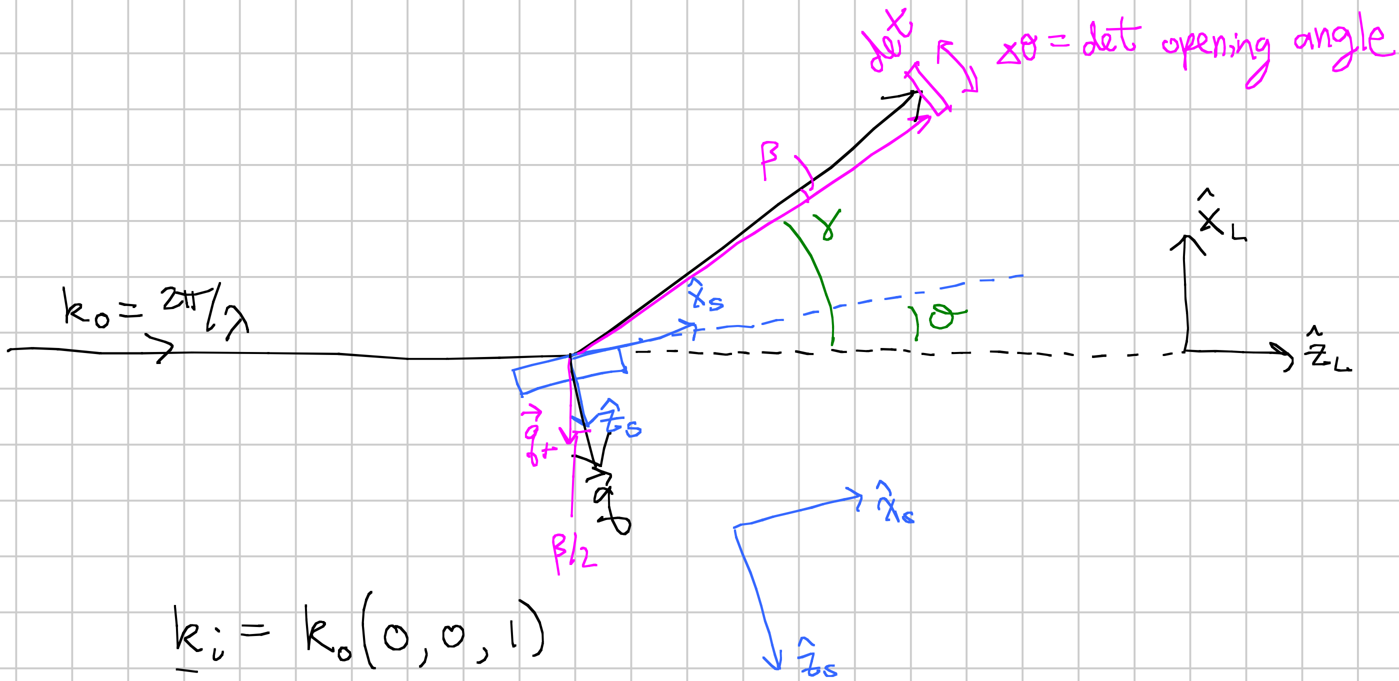
Q Resolution Journal Club

Collimated beam, finite detector



$$\underline{k}_i = k_0(0, 0, 1)$$

$$\underline{k}_s = k_0(\sin\gamma, 0, \cos\gamma)$$

Momentum transferred to sample, in lab coordinates.

$$\underline{q} = \underline{k}_i - \underline{k}_s = k_0(-\sin\gamma, 0, 1-\cos\gamma)$$

$$\vec{q} = 2k_0 \sin\frac{\gamma}{2}\left(-\cos\frac{\gamma}{2}, 0, -\sin\frac{\gamma}{2}\right)$$

Transform to sample coordinates w/ unitary rotation matrix

$$U = \begin{pmatrix} \cos\theta+\frac{\pi}{2} & 0 & +\sin\theta+\frac{\pi}{2} \\ & 1 & \\ -\sin\theta+\frac{\pi}{2} & 0 & \cos\theta+\frac{\pi}{2} \end{pmatrix}$$

$$q_s = 2k_0\sin\frac{\gamma}{2}\left(\sin\left(\theta-\frac{\gamma}{2}\right),\ 0,\ \cos\left(\theta-\frac{\gamma}{2}\right)\right)$$

Sample reflects when $q_s = Q_0 = (0, 0, |Q_0|)$
sample coordinates

Suppose beam has finite bandwidth Δk, ie $k_0 - \frac{\Delta k}{2} < k < k_0 + \frac{\Delta k}{2}$.
Detector finite w/ opening angle $\Delta\theta$.
β denotes a position on finite detector $-\Delta\theta/2 < \beta < \Delta\theta/2$ with $\beta = 0$ being detector center.

$$\vec{q}_s(\beta,k) = 2k\sin\left(\frac{\gamma}{2}-\frac{\beta}{2}\right)\left[-\sin\left(\theta-\frac{\gamma}{2}+\frac{\beta}{2}\right),\ 0,\ \cos\left(\theta-\frac{\gamma}{2}+\beta/2\right)\right]$$

Expand and linearize in β:

$$\sin\left(\frac{\gamma}{2}-\frac{\beta}{2}\right) = \sin\frac{\gamma}{2}\cos\frac{\beta}{2} - \cos\frac{\gamma}{2}\sin\frac{\beta}{2} \approx \sin\frac{\gamma}{2} - \frac{\beta}{2}\cos\frac{\gamma}{2}$$

$$\sin\left(\theta-\frac{\gamma}{2}+\frac{\beta}{2}\right) = \sin\left(\theta-\frac{\gamma}{2}\right)\cos\frac{\beta}{2} + \cos\left(\theta-\frac{\gamma}{2}\right)\sin\frac{\beta}{2} \approx \sin\left(\theta-\frac{\gamma}{2}\right) + \frac{\beta}{2}\cos\left(\theta-\frac{\gamma}{2}\right)$$

$$\cos\left(\theta-\frac{\gamma}{2}+\frac{\beta}{2}\right) = \cos\left(\theta-\frac{\gamma}{2}\right)\cos\frac{\beta}{2} - \sin\left(\theta-\frac{\gamma}{2}\right)\sin\beta/2 \approx \cos\left(\theta-\frac{\gamma}{2}\right) - \frac{\beta}{2}\sin\left(\theta-\frac{\gamma}{2}\right)$$

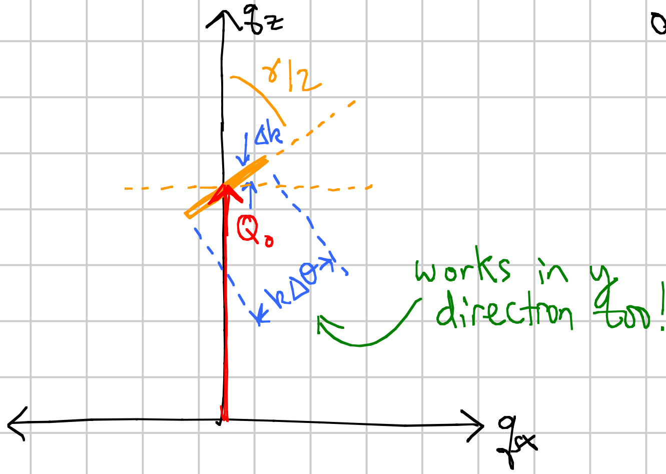
$$\vec{q}_s(\beta,k) = 2k\left(\sin\frac{\gamma}{2} - \frac{\beta}{2}\cos\frac{\gamma}{2}\right)\left[-\sin\left(\theta-\frac{\gamma}{2}\right) - \frac{\beta}{2}\cos\left(\theta-\frac{\gamma}{2}\right),\ 0,\ \cos\left(\theta-\frac{\gamma}{2}\right) - \frac{\beta}{2}\sin\left(\theta-\frac{\gamma}{2}\right)\right]$$

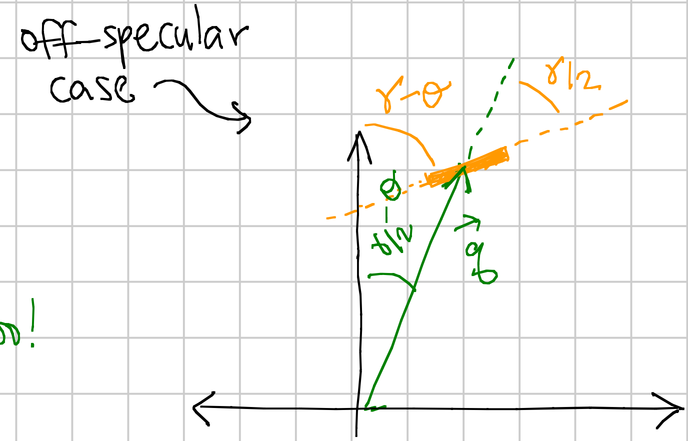
Suppose we're on the Bragg condition, ie $\theta = \frac{\gamma}{2} = \theta_B$

$$q_s(\beta,k) = \left(2k\sin\frac{\gamma}{2} - \frac{\beta}{2}\cos\frac{\gamma}{2}\right)\left(-\frac{\beta}{2},\ 0,\ 1\right)$$

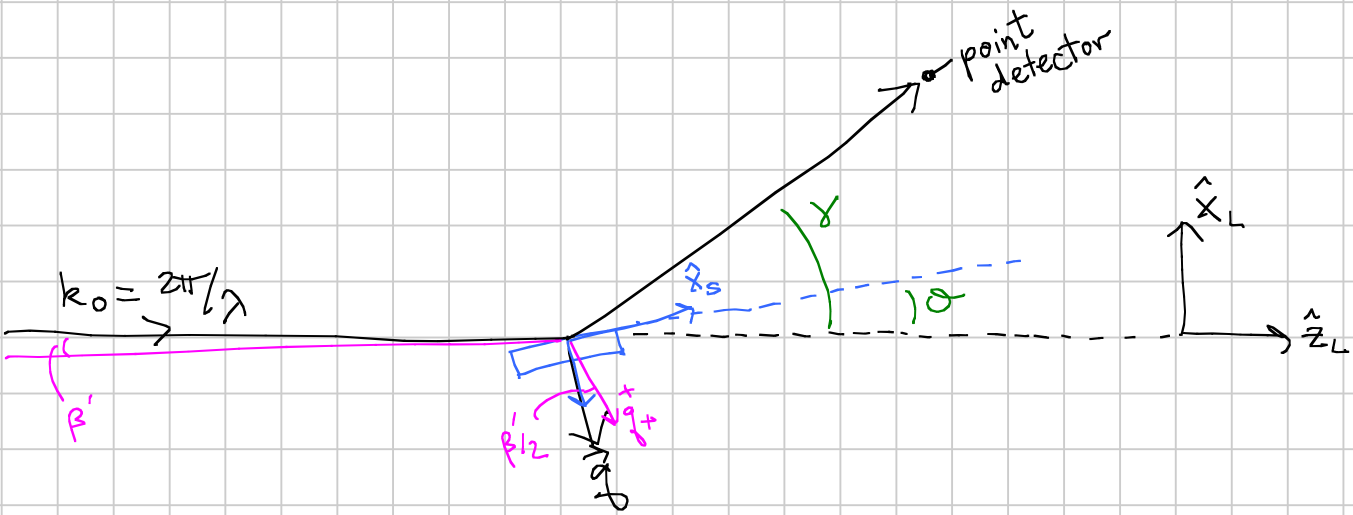
$$\boxed{q_s(\beta,k) = 2k\sin\frac{\gamma}{2}\left(-\frac{\beta}{2},\ 0,\ 1-\frac{\beta}{2}\cot\frac{\gamma}{2}\right)} + O(\beta^2)$$

Traces out trapezoid in momentum space.





Before proceeding, consider what would happen if, instead, the detector were infinitesimal, and beam were <u>diverging</u>.



x componant has the <u>opposite</u> sign:

tips the other way!

$$\vec{q}_s(\beta',k) = 2k\sin\left(\frac{\gamma}{2}-\frac{\beta'}{2}\right)\left[+\sin\left(\theta-\frac{\gamma}{2}+\frac{\beta'}{2}\right),\ 0,\ \cos\left(\theta-\frac{\gamma}{2}+\frac{\beta'}{2}\right)\right]$$

Conclusion: Which way the "pancake" tilts depends on whether resolution is set by detector or beam.

Resolution detector-limited at...

1. X1B
2. APS Sector 9

Bandwidth-limited at

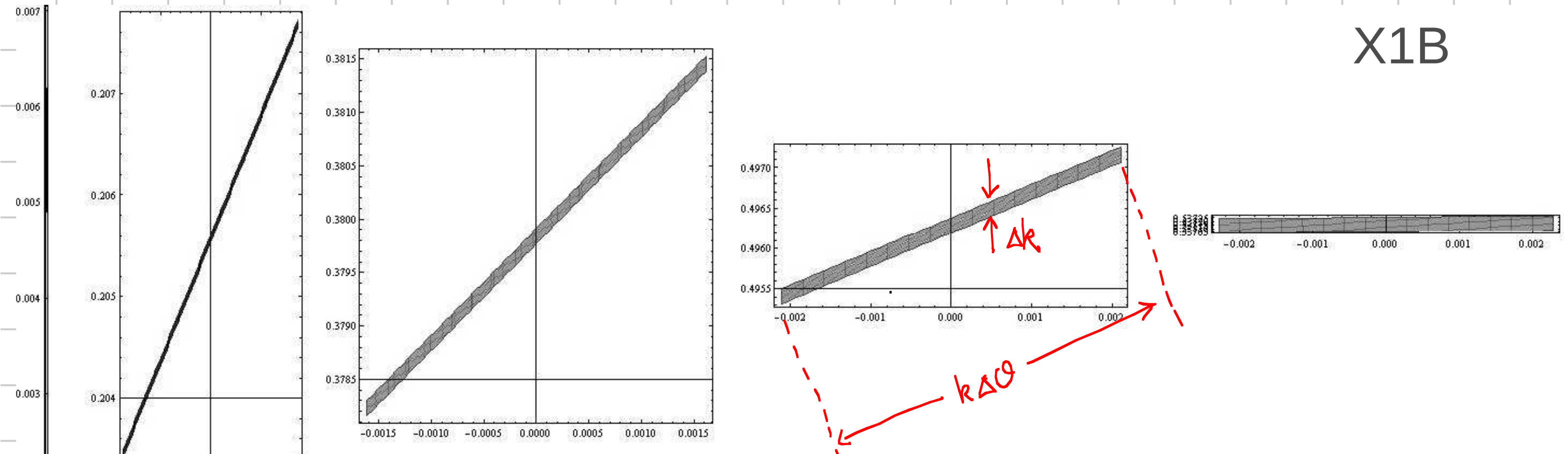
1. Rigaku (?)

Specific case: X1B

$E = 530$ eV, $\Delta E = 0.2$ eV, $\Delta\theta = \frac{7mm}{0.4m} = 17$ mrad

$\Delta k_{angular} = k\Delta\theta = 0.004566\ Å^{-1}$

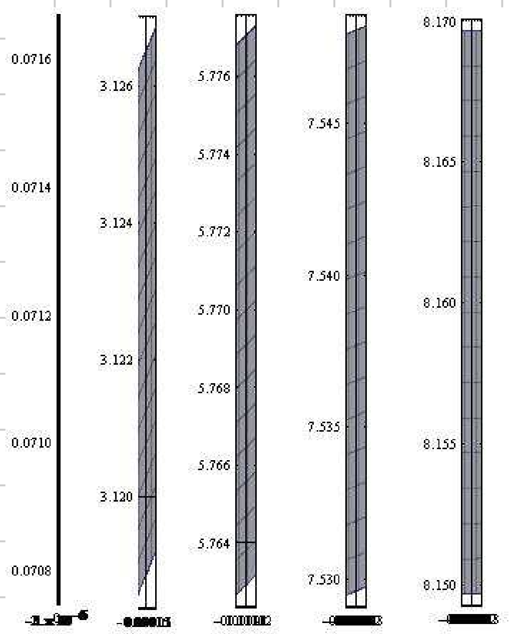
$\Delta k_{bandwidth} = k_0 \cdot \frac{\Delta E}{E} = 0.000101\ Å^{-1}$



1°　45°　90°　135°　179° $= \gamma$

Specific case: Rigaku (?)

$\lambda = 1.54\ Å$, $\Delta\theta = 0.01°$, $\Delta E = 20$ eV (?)



$\gamma =$ 1°　45°　90°　135°　179°