PSD + Q-buffer $\Rightarrow$ (ΔE, h, k, l) mapping.

prerequisites: data header contains E_{fo}
data block contains h_o, k_o, l_o, ΔE_o
data header contains $a, b, c, \alpha, \beta, \gamma$
data header contains u, v, or assigned by user
ka is chosen by user (default = 1.87325 for PG 002)

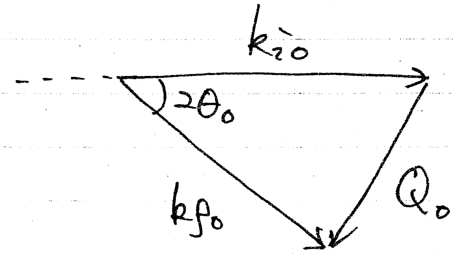
step 1) Energy transfer (ΔE_p) mapping.

- read E_{fo} from data header
- read E_{fp} from calibration file
- ~~E_i~~
- read ΔE_o from the data point
- $E_{io} = E_{fo} + \Delta E_o$ (common for all pixels)
- $\Delta E_p = E_{io} - E_{fp}$

step 2) Q_p mapping

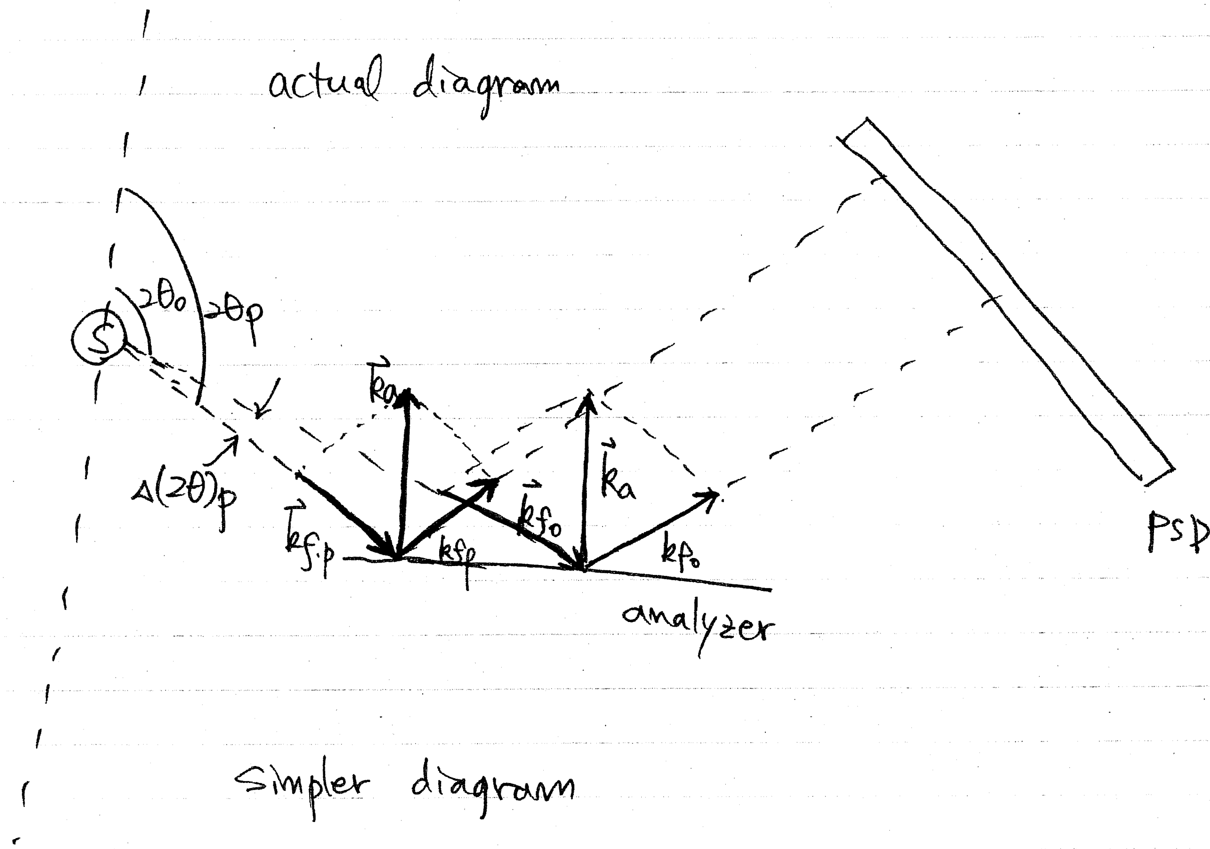
- read (h_o, k_o, l_o) from data point
- convert to Q_o using the lattice parameters
- $2\theta_o = \cos^{-1}\left[\dfrac{k_{io}^2 + k_{fo}^2 - Q_o^2}{2k_{io}k_{fo}}\right]$

$$= \cos^{-1}\left[\frac{E_{io} + E_{fo} - 2.0717\,Q_o^2}{2\sqrt{E_{io}E_{fo}}}\right]$$

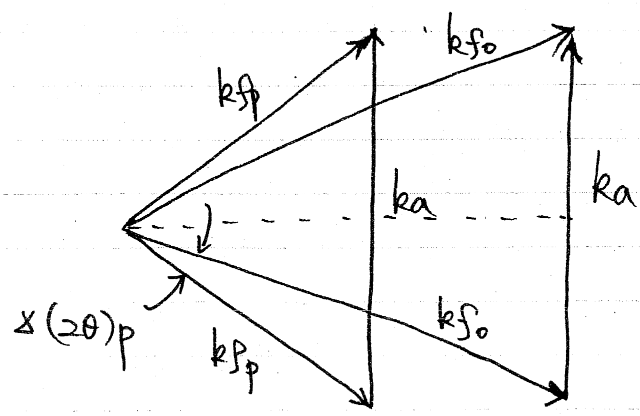


- find the spread in 2θ, that is $\Delta(2\theta)_p$
assuming that $\vec{k}_a$ is constant for all the pixels

actual diagram



simpler diagram



$$\Delta(2\theta)_p = \sin^{-1}\left[\frac{k_a/2}{k_{fp}}\right] - \sin^{-1}\left[\frac{k_a/2}{k_{fo}}\right]$$

then $2\theta_p = 2\theta_o + \Delta(2\theta)_p$

- calculate Q_p using $2\theta_p$ and E_{fp}

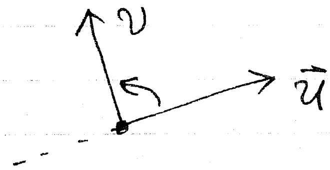
$$Q_p = \sqrt{k_{io}^2 + k_{fp}^2 - 2k_{io}k_{fp}\cos(2\theta_p)}$$

$$= \sqrt{(E_{io} + E_{fp} - 2\sqrt{E_{io}E_{fp}}\cos(2\theta_p))/2.0717}$$

step 3) (h_p. k_p. l_p) mapping.

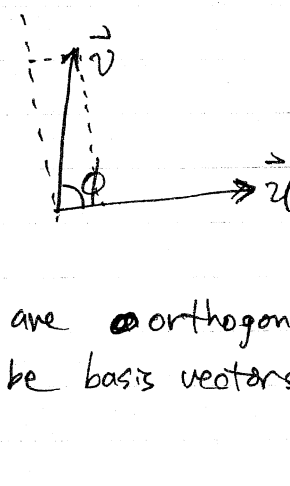
- read $\vec{u}$ & $\vec{v}$, which are two orientation vectors in the scattering plane. $\vec{v}$ is always less than $180°$ away from $\vec{u}$ in the counterclockwise rotation

We want to find a new vector, which is ① perpendicular to $\vec{u}$, ② same length as $\vec{u}$, and ③ in the same scattering plane. We will call it $\vec{\omega}$.



$$\vec{\omega} \parallel \vec{v} - |\vec{v}|\cos\phi \frac{\vec{u}}{|\vec{u}|}$$

then adjust the length to match $|\vec{\omega}| = |\vec{u}|$



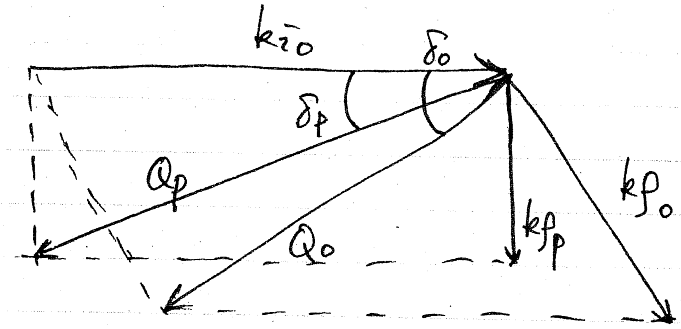
- Now we have $\vec{u}$ & $\vec{\omega}$, which are orthogonal and equal in length. They can be basis vectors on our scattering plane.

- $(h_o, k_o, l_o) = a_o\vec{u} + b_o\vec{\omega} + 0\,\vec{u}\times\vec{\omega}$

$$= (a_o, b_o, 0)\begin{pmatrix} u_h & u_k & u_l \\ \omega_h & \omega_k & \omega_l \\ (u\times\omega)_h & (u\times\omega)_k & (u\times\omega)_l \end{pmatrix}$$

$$\Rightarrow \quad (a_0, b_0, 0) = (h_0, k_0, l_0) \begin{pmatrix} u_h & u_k & u_l \\ \omega_h & \omega_k & \omega_l \\ (u\times\omega)_h & (u\times\omega)_k & (u\times\omega)_l \end{pmatrix}^{-1}$$

Then, (a_0, b_0) can be rotated by rotational matrix to find the spread in (a_p, b_p) IF we know the angularspread of Q_p.



$$kf_0^2 = k_{i0}^2 + Q_0^2 - 2k_{i0} Q_0 \cos\delta_0$$
$$kf_p^2 = k_{i0}^2 + Q_p^2 - 2k_{i0} Q_p \cos\delta_p$$

$$\Delta\delta_p = \delta_p - \delta_0 = \cos^{-1}\left[\frac{k_{i0}^2 + Q_p^2 - kf_p^2}{2k_{i0}Q_p}\right] - \cos^{-1}\left[\frac{k_{i0}^2 + Q_0^2 - k\ldots}{2k_{i0}Q_0}\right.$$

Here $\Delta\delta_p > 0$ correspond to counterclockwise rotation

$$\begin{pmatrix} a_p \\ b_p \end{pmatrix} = \begin{pmatrix} \cos(\Delta\delta_p) & -\sin(\Delta\delta_p) \\ \sin(\Delta\delta_p) & \cos(\Delta\delta_p) \end{pmatrix} \begin{pmatrix} a_0 \\ b_0 \end{pmatrix}$$

$$(h_p\ k_p\ l_p) \parallel a_p \vec{u} + b_p \vec{\omega}$$

then adjust the length of the vector to match $|Q_p|$