Two-beam intensity

We defined an effective excitation error for beam g:

$$s_{eff} \equiv \sqrt{s^2 + \frac{1}{\xi^2}}$$

The general two-beam result for **g** is:

$$\Psi_{\mathbf{g}}(T) = i\frac{\sin(\pi s_{eff} T)}{s_{eff}\xi} e^{-\pi i s T}$$

The two-beam intensity is:

$$I_{\mathbf{g}} = |\psi_{\mathbf{g}}(T)|^2 = \frac{\sin^2(\pi s_{eff} T)}{(s_{eff}\xi)^2} = \frac{\sin^2\left[\pi \cdot (T/\xi) \cdot \sqrt{1+w^2}\right]}{1+w^2} \qquad w \equiv s\xi$$

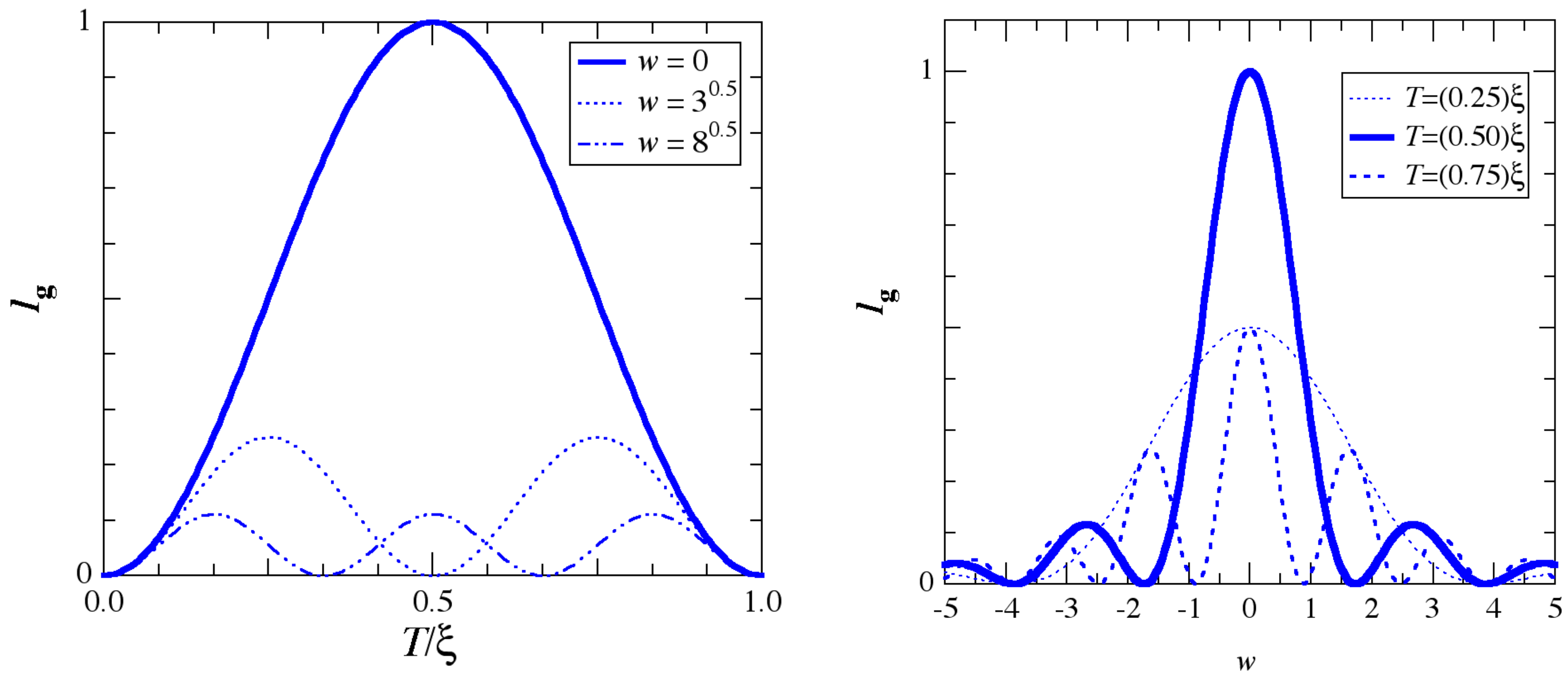
Alternative form

Alternatively, we could write the two-beam result for **g** as:

$$\psi_{\mathbf{g}}(T) = i\left(\frac{\pi T}{\xi}\right)\mathrm{sinc}\left(\pi s_{eff} T\right)\mathrm{e}^{-\pi i s T}$$

$$I_{\mathbf{g}} = \left|\psi_{\mathbf{g}}(T)\right|^2 = \left(\frac{\pi T}{\xi}\right)^2 \mathrm{sinc}^2\left(\pi s_{eff} T\right) = \left(\frac{\pi T}{\xi}\right)^2 \mathrm{sinc}^2\left(\frac{\pi\sqrt{1+w^2}\,T}{\xi}\right)$$

Variation with thickness/excitation error



pendellosung oscillations

Kinematical approximation

Assume coupling only to the (undiminished) **0** beam, the H-W equations give:

$$\frac{d\Psi_{\mathbf{g}}}{dz} \approx \left(\frac{i\pi}{\xi_{\mathbf{g}}}\right)\cdot(1)\cdot \mathrm{e}^{-2\pi i s_{\mathbf{g}} z} \qquad \left(\Psi_{\mathbf{0}} = 1\right)$$

Integrate over thickness:

$$\Psi_{\mathbf{g}} = \left(\frac{i\pi}{\xi}\right)\cdot \int_{z=0}^{T} \mathrm{e}^{-2\pi i s z} dz = \left(\frac{\mathrm{e}^{\pi i s T} - \mathrm{e}^{-\pi i s T}}{2s\xi}\right)\cdot \mathrm{e}^{-\pi i s T} = i\left(\frac{\pi T}{\xi}\right)\mathrm{sinc}\left(\pi s T\right)\mathrm{e}^{-\pi i s T}$$

Kinematic diffracted intensity:

$$I_{\mathbf{g}} = \left|\psi_{\mathbf{g}}\right|^2 = \left(\frac{\pi T}{\xi}\right)^2 \cdot \mathrm{sinc}^2\left(\pi s T\right) = \left(\frac{\pi T}{\xi}\right)^2 \cdot \mathrm{sinc}^2\left(\frac{\pi w T}{\xi}\right)$$

This is essentially the substitution: $s_{eff} \to s$ $\qquad \sqrt{1+w^2} \to w$

Applicable if $s \gg \dfrac{1}{\xi}$

Interpretation

$$\int_{z=0}^{T} \mathrm{e}^{-2\pi isz}\,dz = \int_{z=0}^{T} (1)\cdot \mathrm{e}^{-2\pi isz}\,dz = \Im\{L(z)\}$$

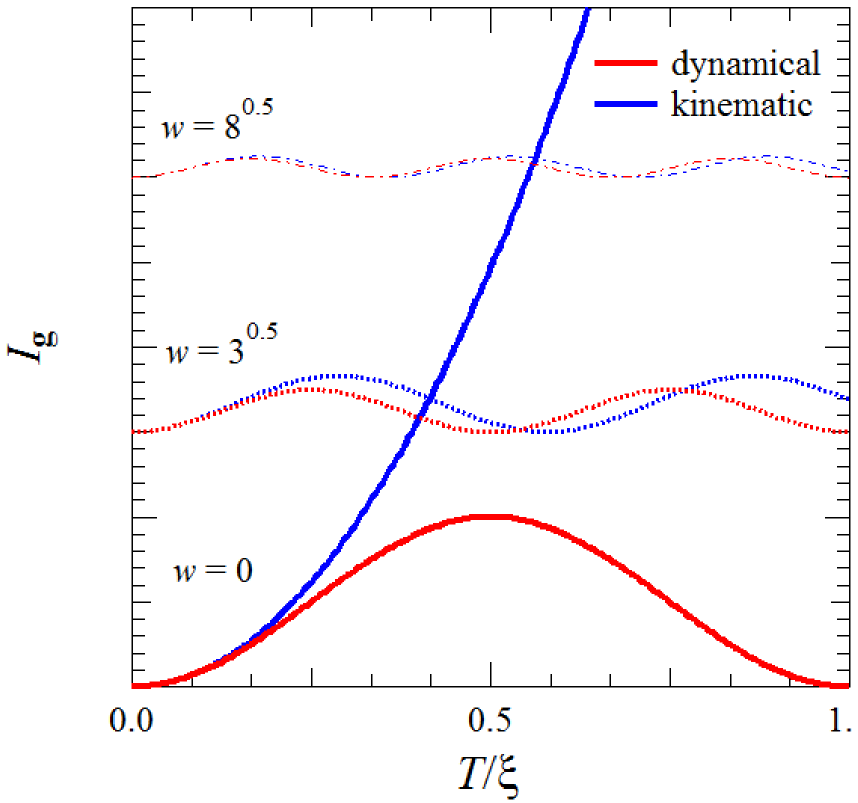
$$L(z) = \begin{cases} 1, & 0 \le z \le T \\ 0, & \text{otherwise} \end{cases}$$ //shape function

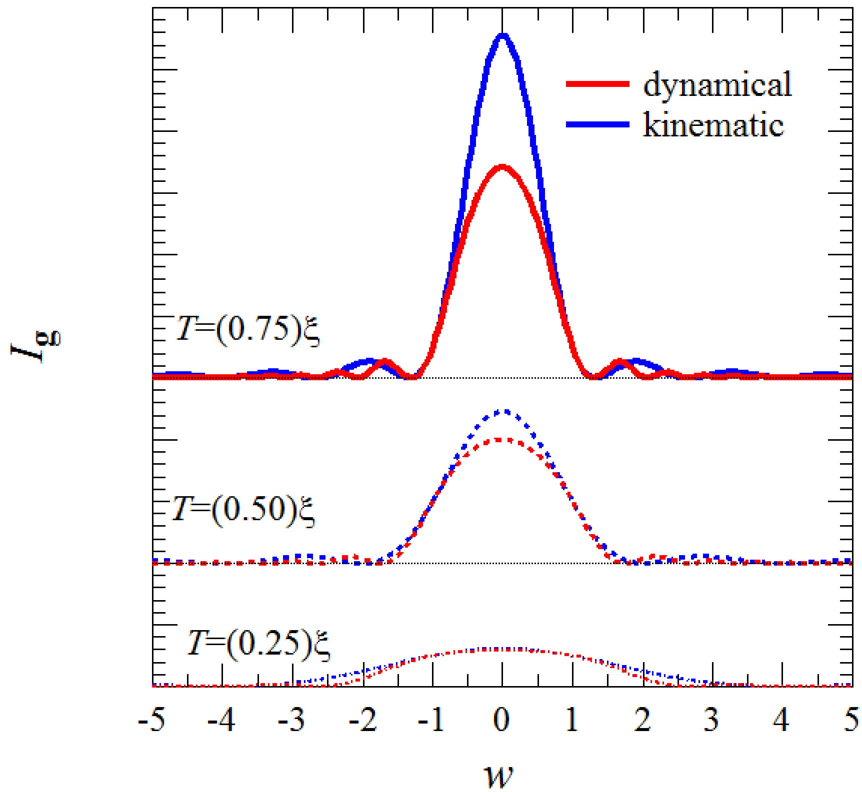
$$L(s) = T\cdot \mathrm{sinc}(\pi sT)\cdot \mathrm{e}^{-\pi isT}$$

$$\Psi_{\mathbf{g}} = \frac{i\pi}{\xi}\cdot L(s) = \frac{i\lambda\cdot F_{\mathbf{g}}}{v}\cdot L(s)$$

For small crystals, diffraction spots are broadened by the Fourier transform of the shape function

Dynamical vs. Kinematic





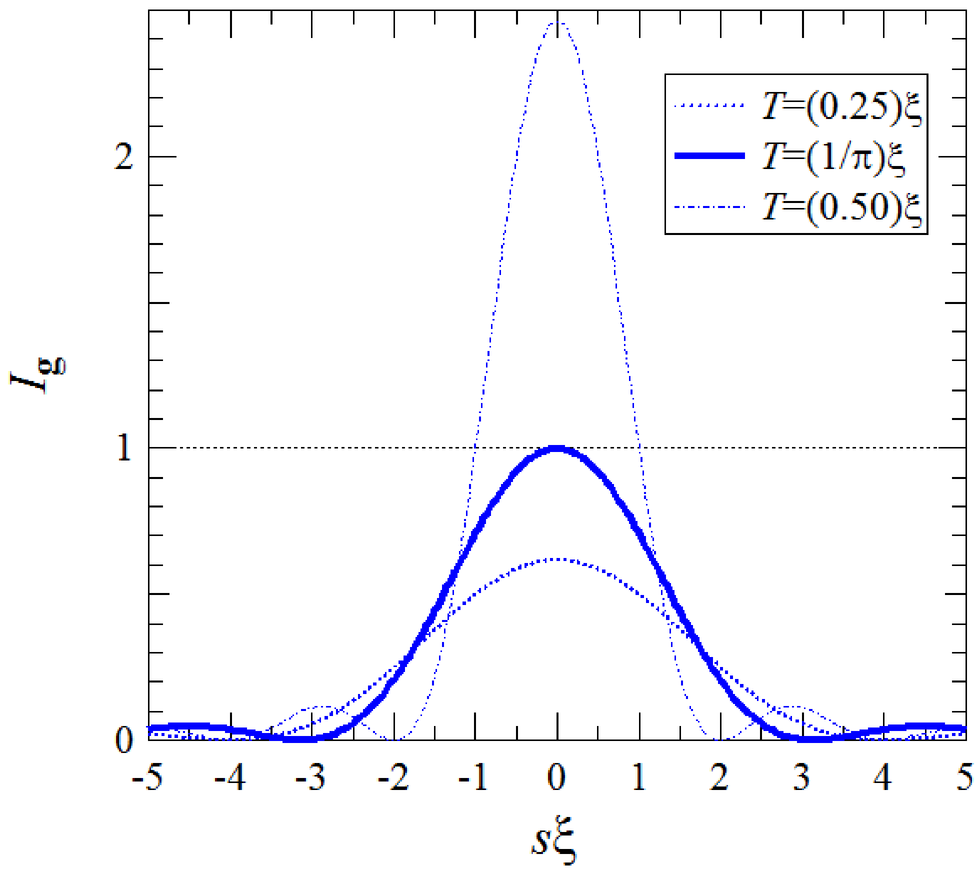
Limitations of kinematic theory

$$I_g\left(s=0\right)=\left(\frac{\pi T}{\xi}\right)^2$$

Intensity has an upper limit of unity: $I_g < 1$

Kinematic theory is only valid if:

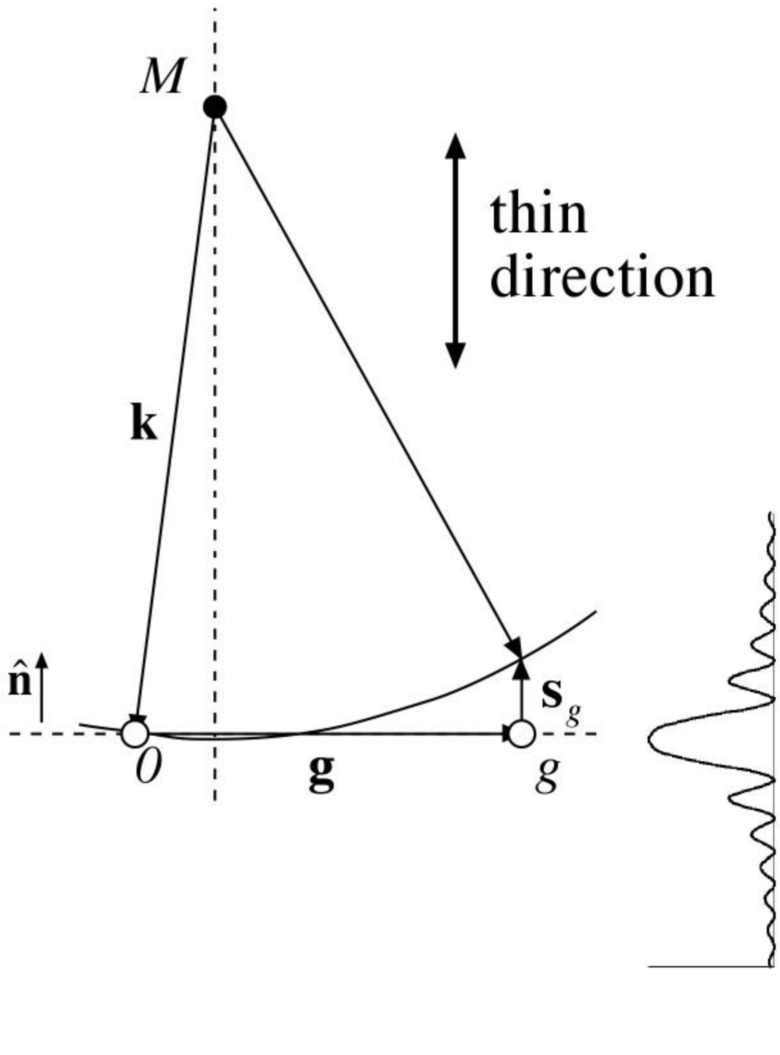
$$\Rightarrow \quad T < \frac{\xi}{\pi}$$



Kinematic Theory works best far from the Bragg condition.

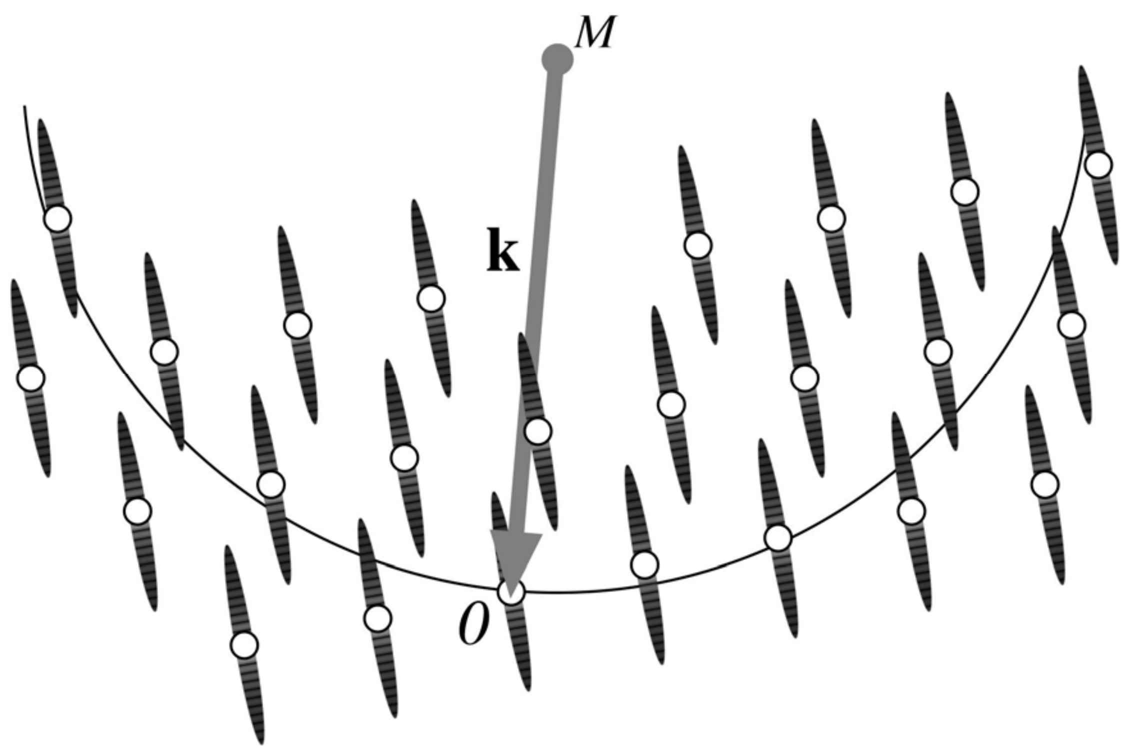
Relrods

Reciprocal-lattice rods extend normal to thin-foil plane



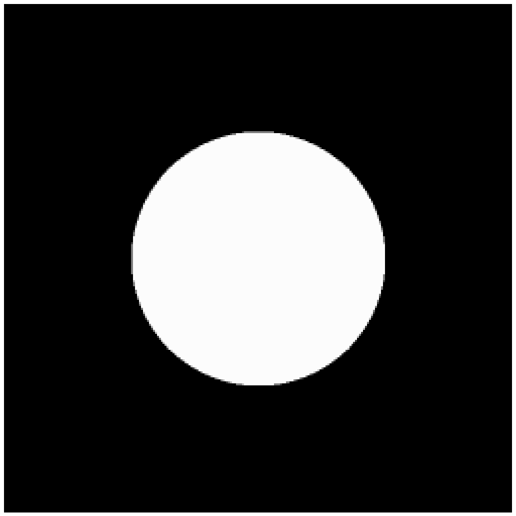
Diffraction from thin crystals

Intersection of relrod with Ewald sphere gives intensity



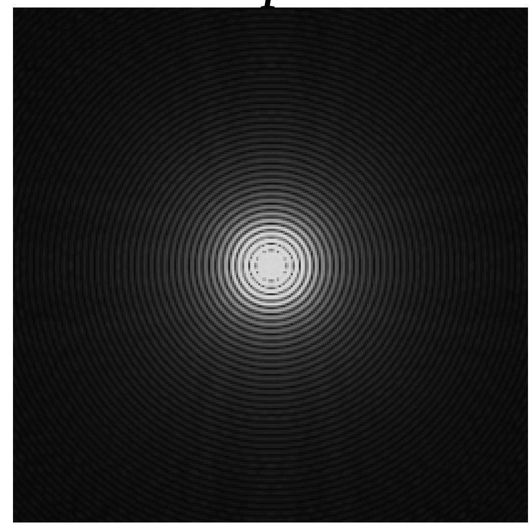
Shape function: circle

direct

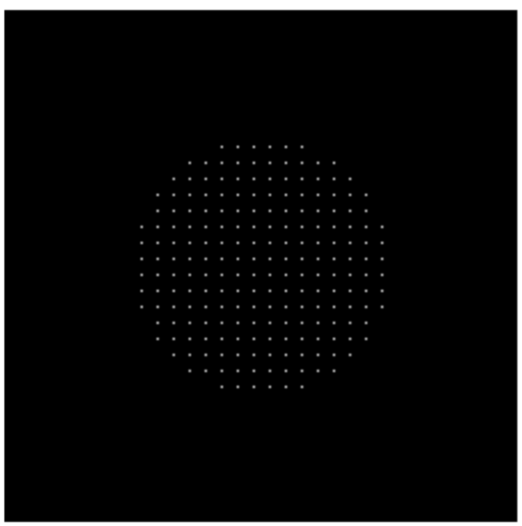


FFT

reciprocal

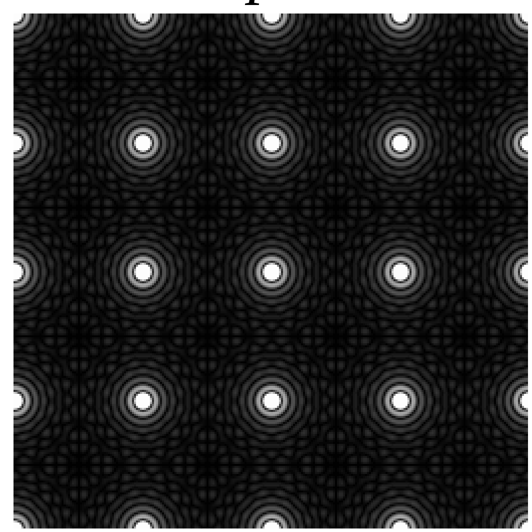


direct



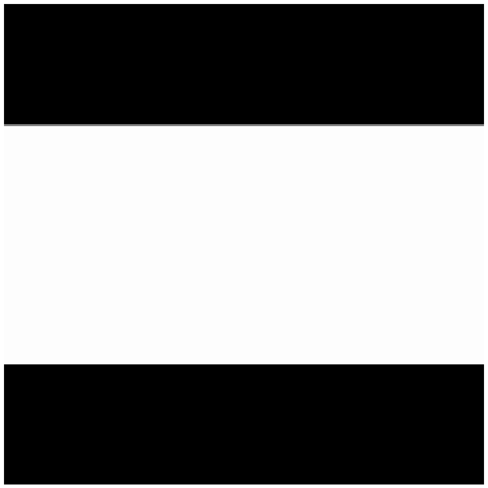
FFT

reciprocal



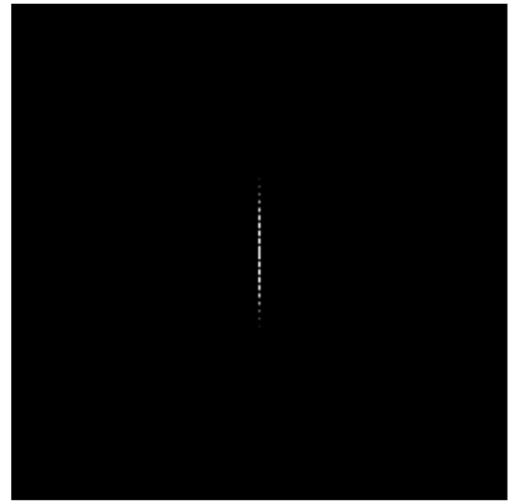
Shape function: thin foil

direct

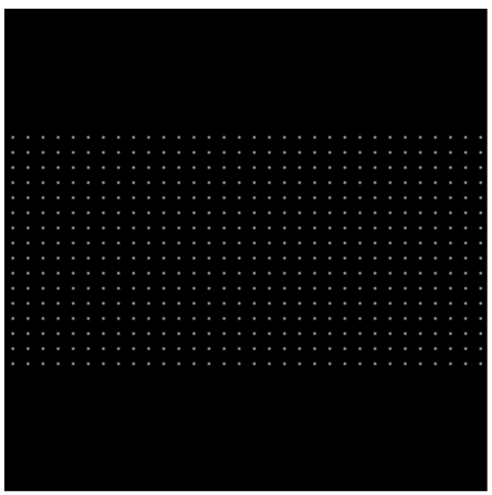


FFT

reciprocal

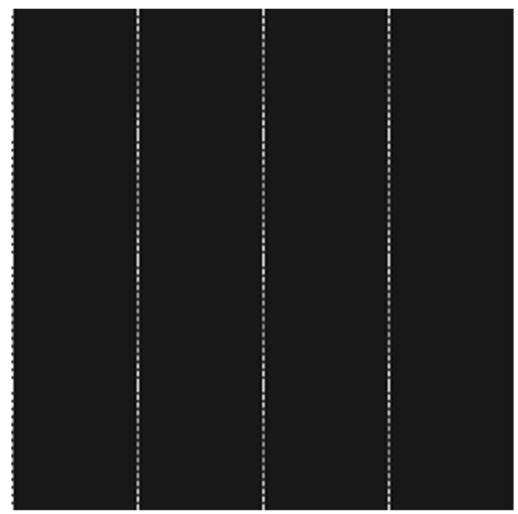


direct



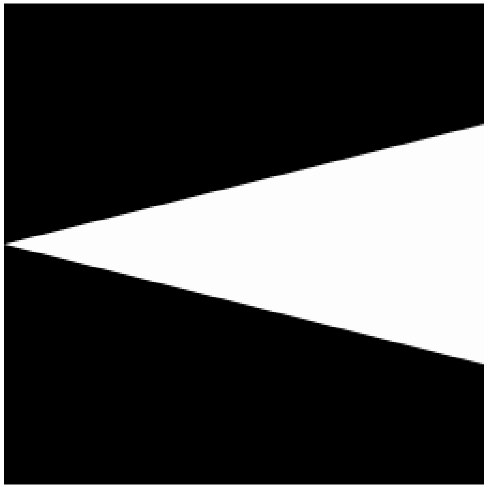
FFT

reciprocal



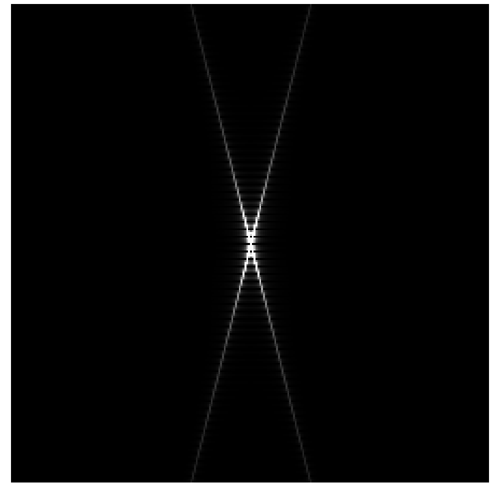
Shape function: wedge

direct

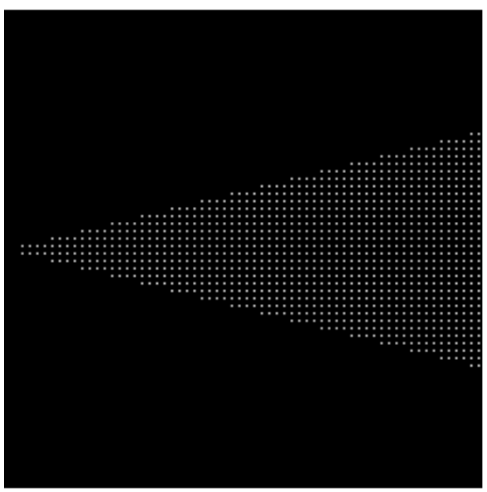


FFT

reciprocal

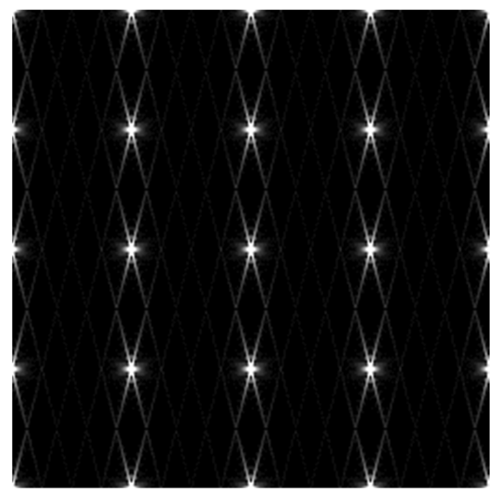


direct

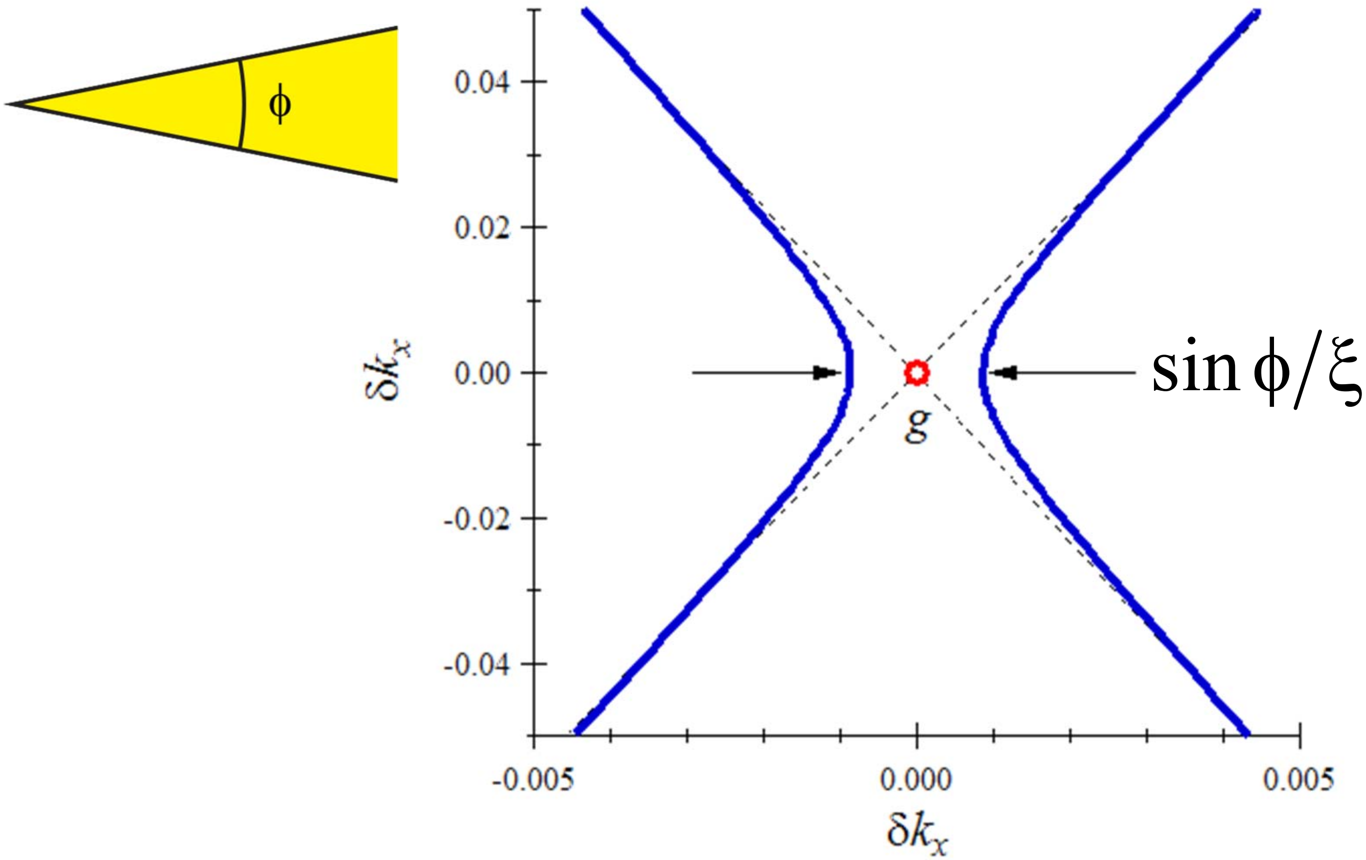


FFT

reciprocal



Dynamical theory: wedge



Dynamical theory predicts spot splitting at the Bragg condition, too.