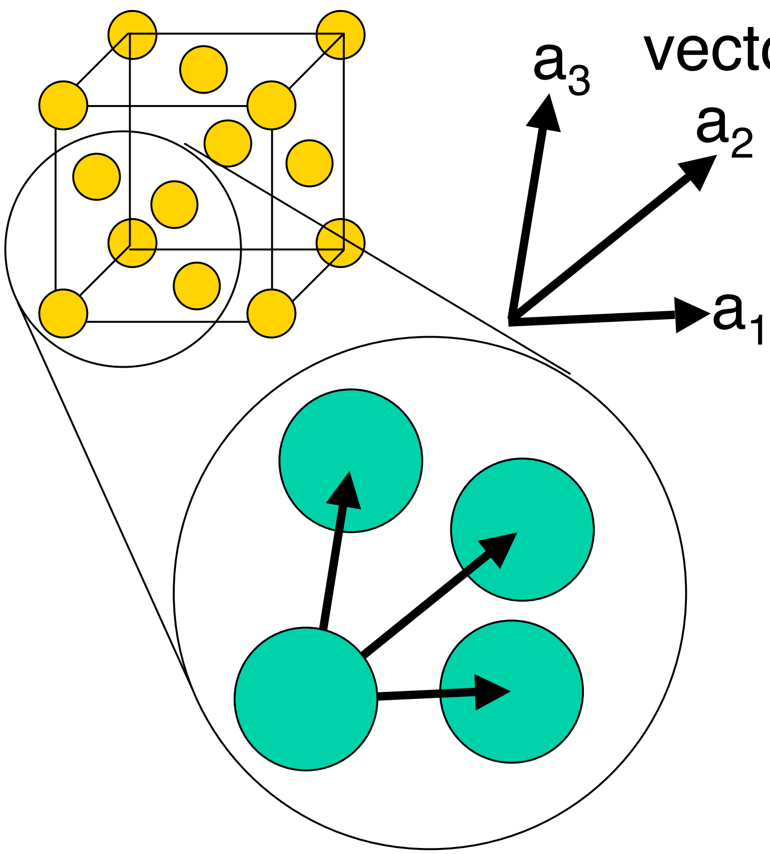
The Reciprocal Lattice

Defined as follows:

Real space lattice:

Basis vectors:



Reciprocal lattice:

$\mathbf{b}_1 = (\mathbf{a}_2 \text{ x } \mathbf{a}_3)/(\mathbf{a}_1 \cdot \mathbf{a}_2 \text{x} \mathbf{a}_3)$
$\mathbf{b}_2 = (\mathbf{a}_3 \text{ x } \mathbf{a}_1)/(\mathbf{a}_1 \cdot \mathbf{a}_2 \text{x} \mathbf{a}_3)$
$\mathbf{b}_3 = (\mathbf{a}_1 \text{ x } \mathbf{a}_2)/(\mathbf{a}_1 \cdot \mathbf{a}_2 \text{x} \mathbf{a}_3)$

by definition.

Unit volume $V = \mathbf{a}_1 \cdot \mathbf{a}_2 \text{x} \mathbf{a}_3$

Note: magnitude of the b's is inversely related to the magnitudes of the a's.

The Reciprocal Lattice

Real space lattice planes and reciprocal lattice vectors

A plane (hkl) has a **spacing** d in a cubic lattice given by:

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

This is also the **length** of the reciprocal lattice vector:

$$\mathbf{b}_{hkl} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

The direction of the reciprocal lattice vector is perpendicular to the lattice plane.

$$\mathbf{b}_{100} \cdot \mathbf{a}_{100} = ab = 1$$
$$\mathbf{b}_{110} \cdot \mathbf{a}_{001} = 0$$

Arbitrary directions are perpendicular when:

$$(u\mathbf{a}_1+v\mathbf{a}_2+w\mathbf{a}_3)\cdot(h\mathbf{b}_1+k\mathbf{b}_2+l\mathbf{b}_3) = 0$$

The Reciprocal Lattice

Constructing a reciprocal lattice for a fcc crystal:

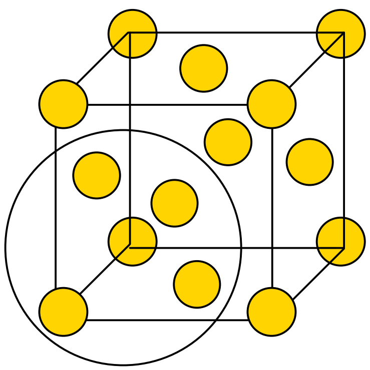
Recall:

$$\mathbf{b}_3 = (\mathbf{a}_1 \times \mathbf{a}_2)/(\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3)$$

$$\mathbf{b}_3 = \frac{\sqrt{2}}{a}(110) \times (101)$$

$$\mathbf{b}_3 = \frac{\sqrt{2}}{a}(1\bar{1}\bar{1})$$

Real space fcc lattice:

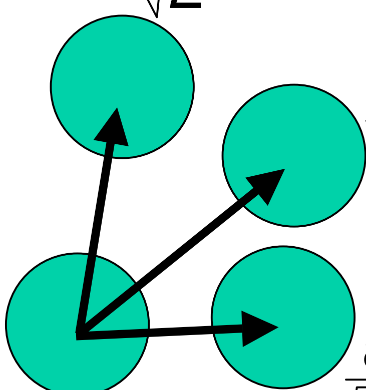


Basis vectors:

$$\frac{a}{\sqrt{2}}(011)$$

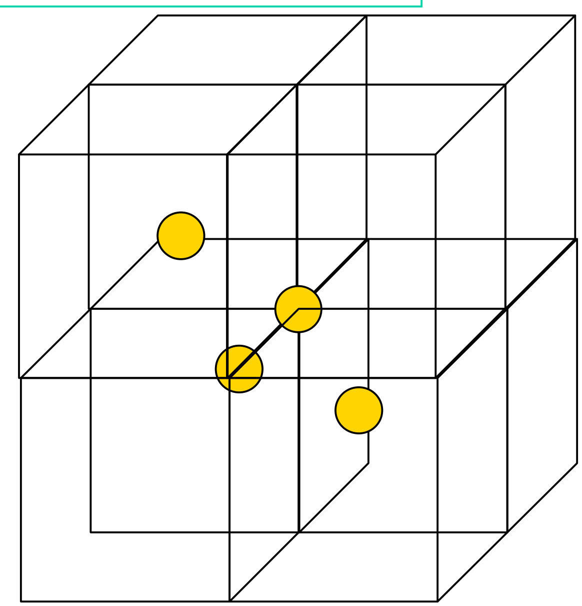
$$\frac{a}{\sqrt{2}}(101)$$

$$\frac{a}{\sqrt{2}}(110)$$

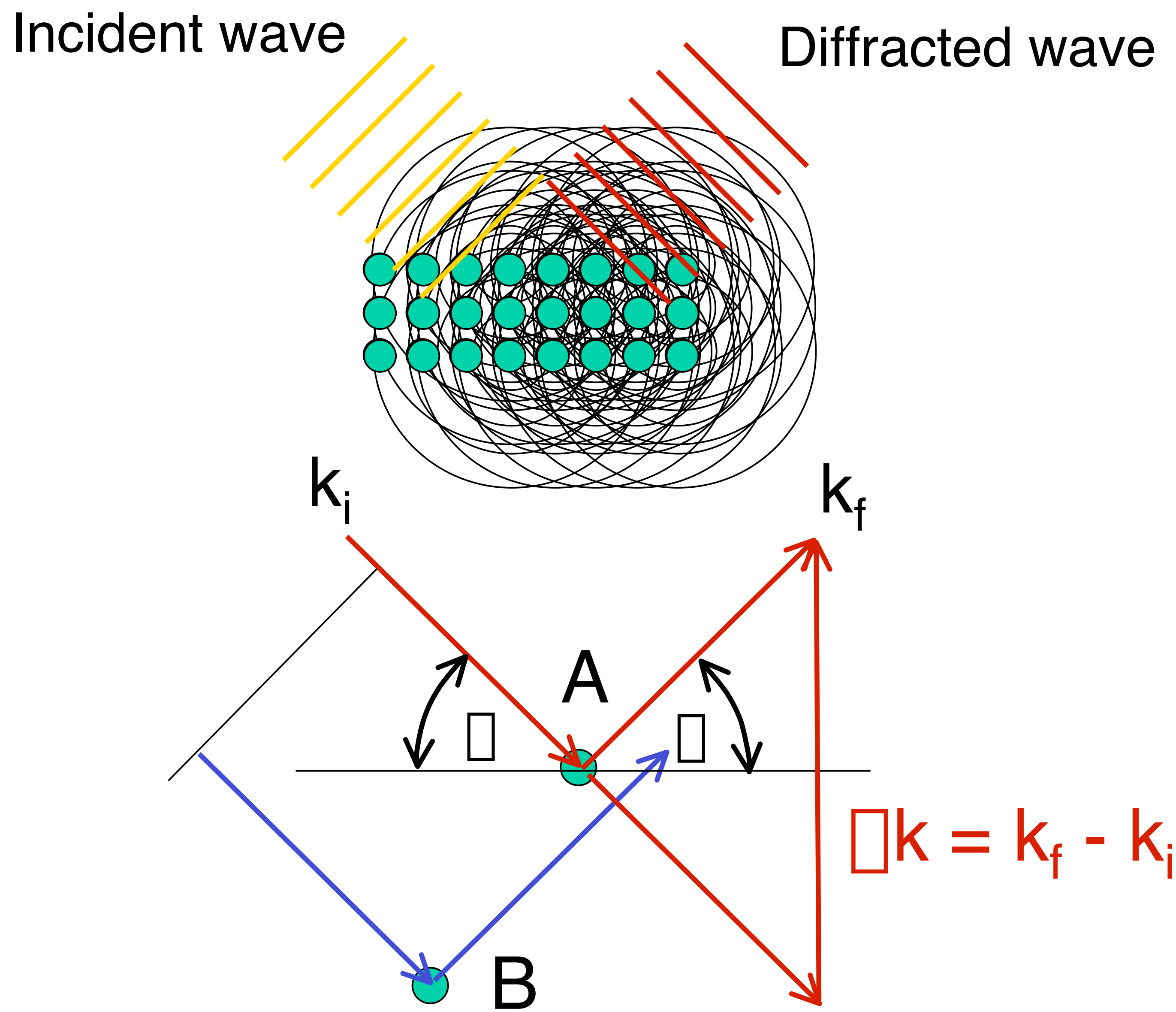


$$\mathbf{b}_1 = \frac{\sqrt{2}}{a}(\bar{1}\bar{1}1)$$

$$\mathbf{b}_2 = \frac{\sqrt{2}}{a}(\bar{1}1\bar{1})$$

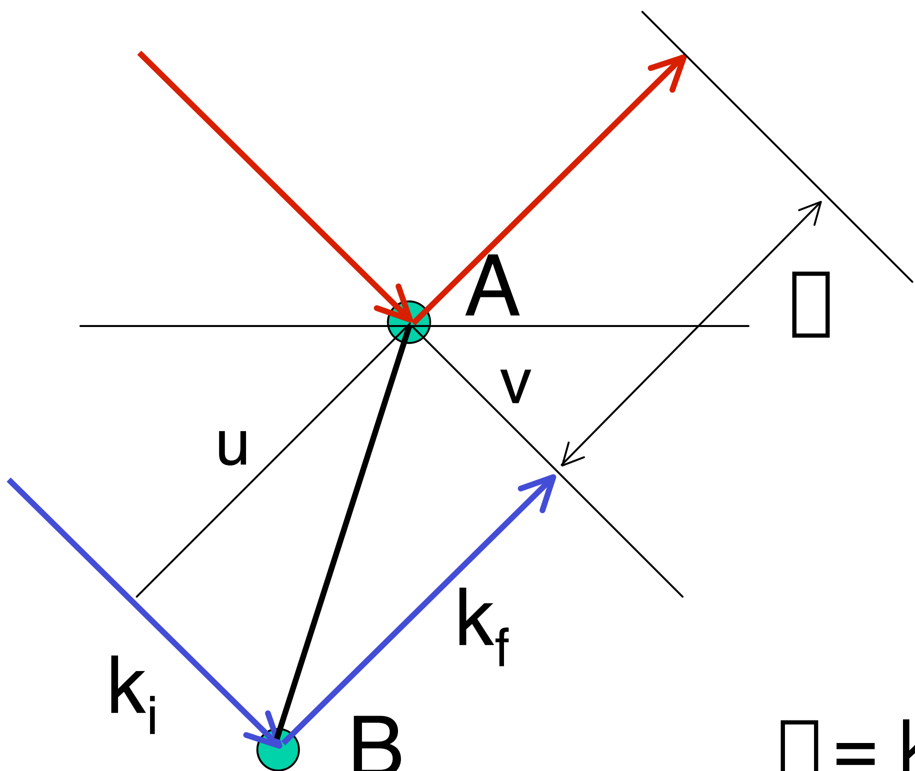


Diffraction



Diffraction

Scattering Geometry



Length difference □:

$□ = u + v$

But u and v can be projected onto k_i and k_f:

$v = k_i \cdot AB$
$u = k_f \cdot (-AB)$

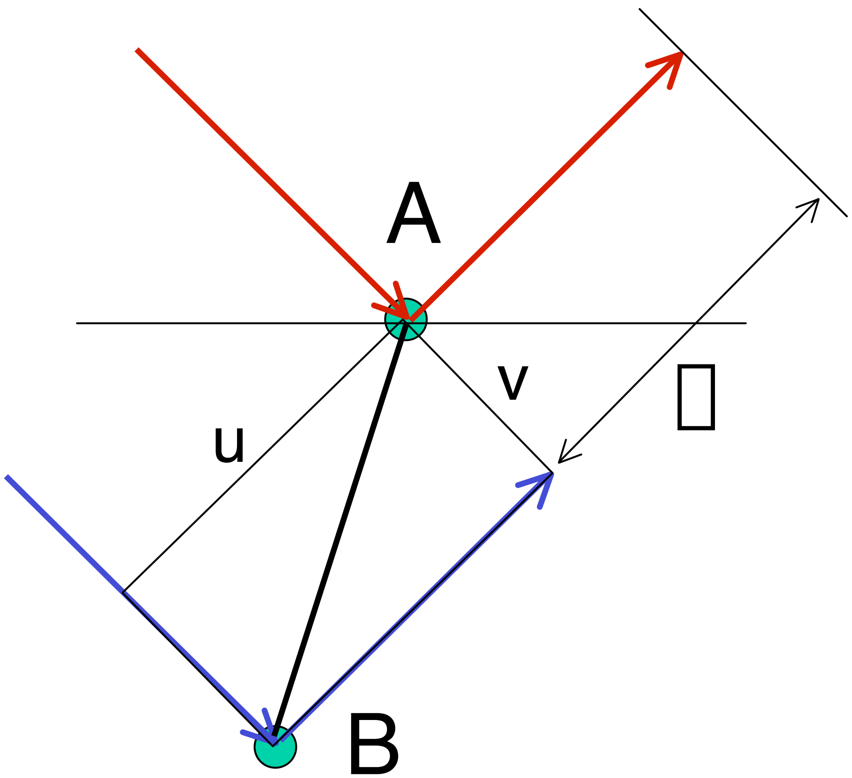
So

$□ = k_i \cdot AB - k_f \cdot AB = □k \cdot AB$

Diffraction

Phase difference: □ = -2□□

□ = -2□ $(k_f - k_i) \cdot \overline{AB}$



Let $\overline{AB} = u\mathbf{a}_1 + v\mathbf{a}_2 + w\mathbf{a}_3$
As it is a real-space translation
u,v,w: integers (it's a lattice)

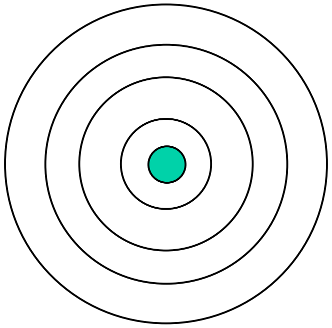
Let □$\mathbf{k} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$
As it is a reciprocal-space vector

□$\mathbf{k} \cdot AB = uh + vk + wl$

Diffraction occurs when this is an integer. ie: when h,k,l are integers!

ie: when □$\mathbf{k} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$
is a reciprocal lattice vector!

Fourier Transforms



1 wave: $e^{i\,\mathbf{k}\cdot\mathbf{r}}$

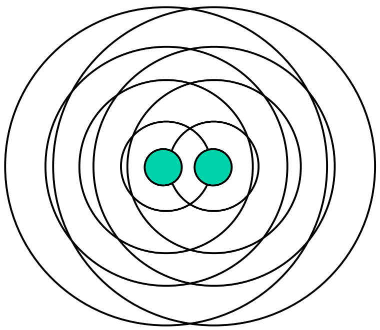
(fully radially symmetric)

Definition:

$f(r) = \square\ f(k)\ e^{i\,\mathbf{k}\cdot\mathbf{r}}$

f(k) = strength of wave k

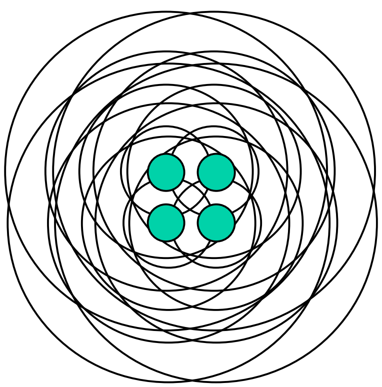
(can you think of an example?)



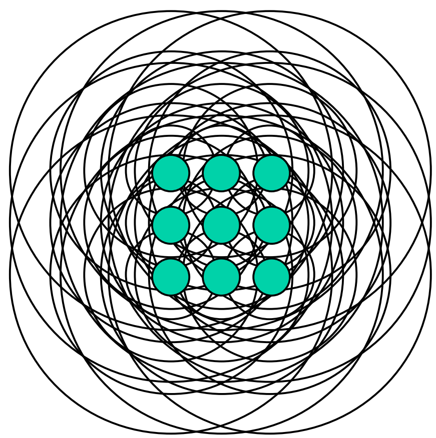
2 waves: $e^{i\,\mathbf{k}\cdot\mathbf{r}} + e^{i\,\mathbf{k}\cdot(\mathbf{r}+\mathbf{R})}$

(R is a lattice translation vector)

Notice how the blackest regions are beginning to define squares and wave fronts.



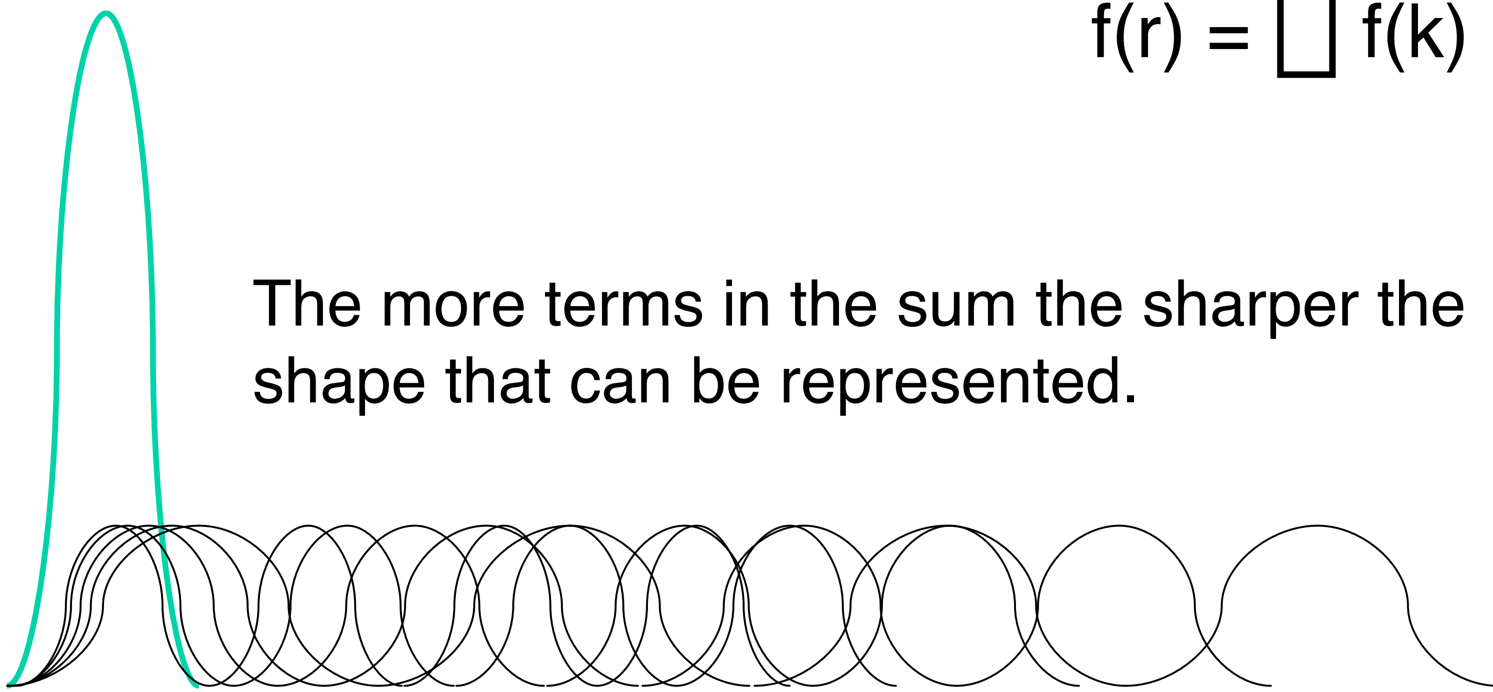
4 waves



9 waves

Fourier Transforms

$$f(r) = \sum f(k)\, e^{i\, \mathbf{k} \cdot \mathbf{r}}$$



The more terms in the sum the sharper the shape that can be represented.

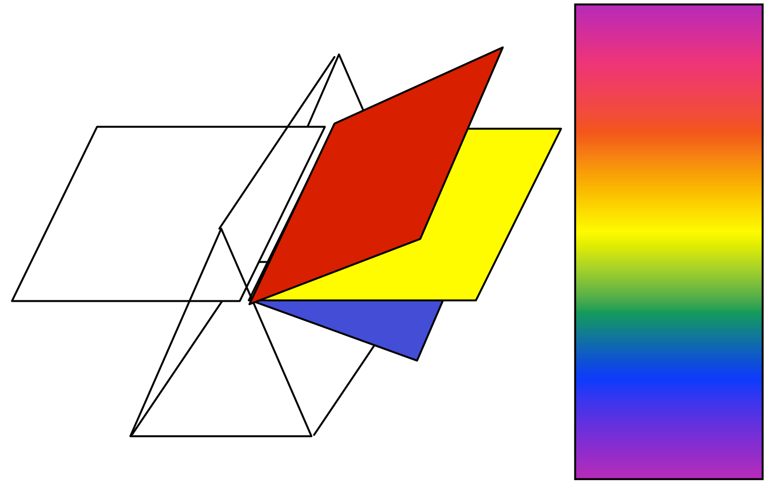
Example: a square wave of amplitude h

$$f(x) = h/2 + 2h/\pi \sum_{n} \frac{\sin(nx)}{n}$$

Fourier Transforms

Determining the coefficients:

$$f(k) = \int_0^{2\pi} f(r)\, \frac{e^{i\,\mathbf{k}\cdot\mathbf{r}}}{2\pi}\, dr$$



In other words, how much intensity is there in a wave of wave vector k anywhere in the space interval 0 to 2π.

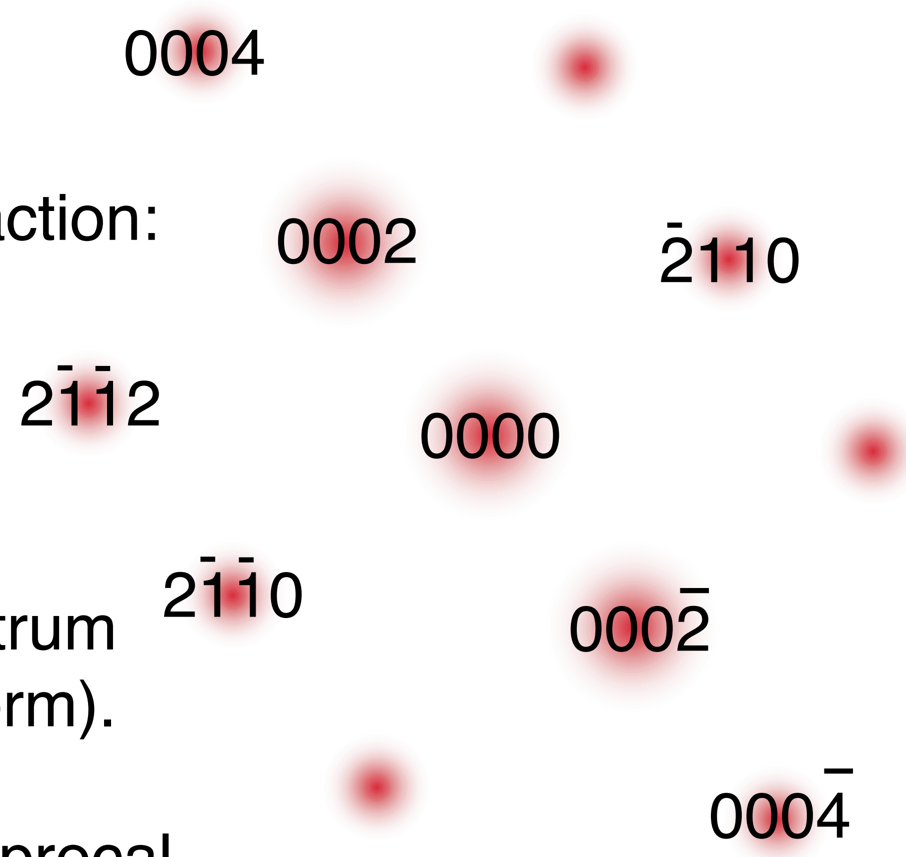
A musical analogy:

If a random noise passes over the strings of a harp the amount each string vibrates is the coefficient of that string's frequency.

The brightness of different colors in a rainbow is f(k), a Fourier transform of sunlight.

Fourier Transforms

The reciprocal lattice and diffraction:



The reciprocal lattice is a spectrum of real space (a Fourier transform).

The sharpness of points in reciprocal space determines the regularity of real space.

Sharper points indicate fewer waves present and hence more order.