Delta Function

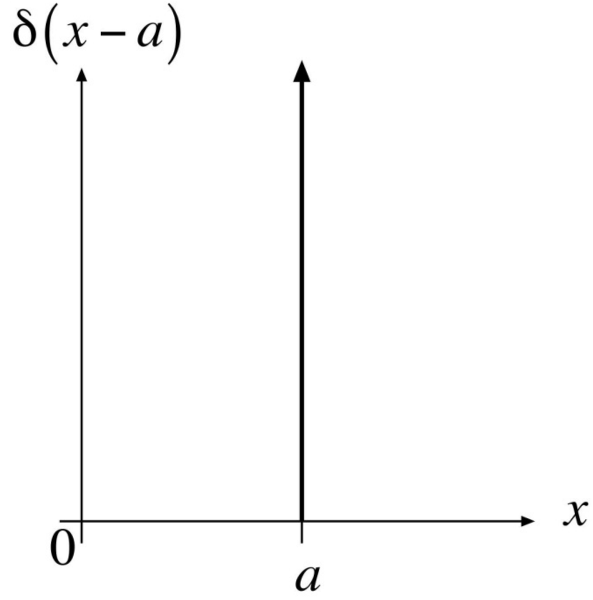
Defined as:

$$f(0) = \int_{x=-\infty}^{\infty} f(x) \cdot \delta(x) \cdot dx$$

This is called the "sampling property" of the delta function.

Notice that:

$$1 = \int_{x=-\infty}^{\infty} \delta(x)\, dx$$



It might be more appropriate to write:

$$\int_{x=-\infty}^{\infty} \quad \rightarrow \quad \lim_{L \to \infty} \int_{x=-L}^{L}$$

Note: delta functions are sometimes called "unit impulse functions"

Fourier transform

$$f(k) = \int_{x=-\infty}^{\infty} f(x)\mathrm{e}^{-2\pi ikx}dx = \mathfrak{I}\left[f(x)\right]$$ //Fourier transform

$$f(x) = \int_{k=-\infty}^{\infty} f(k)\mathrm{e}^{2\pi ikx}dk = \mathfrak{I}^{-1}\left[f(k)\right]$$ //inverse Fourier transform

Example, delta function:

$$f(x) = \delta(x-a) \Rightarrow f(k) = \mathrm{e}^{-2\pi ika}$$

Notice that the delta function can be written as:

$$\delta(x) = \mathfrak{I}^{-1}(1) = \int_{k=-\infty}^{\infty} \mathrm{e}^{2\pi ikx}dk$$

Another example, two delta functions:

$$f(x) = \frac{1}{2}\left[\delta(x-a) + \delta(x+a)\right] \Rightarrow f(k) = \cos(2\pi ka)$$

Convolution theorem

The convolution of two functions is given by:

$$f_1(x) * f_2(x) = \int_{x'=-\infty}^{\infty} f_1(x') f_2(x-x')\, dx'$$

If we know the Fourier transform the each function:

$$f_1(k) = \Im\{ f_1(x) \}$$

$$f_2(k) = \Im\{ f_2(x) \}$$

Then the Fourier transform of the convolution is just the product of the Fourier transforms:

$$\Im\{ f_1(x) * f_2(x) \} = f_1(k) \cdot f_2(k)$$

Three-dimensional versions

In 3-D, the Fourier transform is:

$$f(\mathbf{k}) = \lim_{V \to \infty} \int_{\mathbf{r}}^{V} f(\mathbf{r}) \mathrm{e}^{-2\pi i \mathbf{k}\cdot\mathbf{r}} d^3 r$$

and the inverse Fourier transform is:

$$f(\mathbf{r}) = \lim_{\Omega \to \infty} \int_{\mathbf{k}}^{\Omega} f(\mathbf{k}) \mathrm{e}^{2\pi i \mathbf{k}\cdot\mathbf{r}} d^3 k$$

The delta function is:

$$\delta(\mathbf{r}) = \lim_{\Omega \to \infty} \int_{\mathbf{k}}^{\Omega} \mathrm{e}^{2\pi i \mathbf{k}\cdot\mathbf{r}} d^3 k$$

and has the property:

$$f(\mathbf{r}_0) = \lim_{V \to \infty} \int_{\mathbf{r}}^{V} f(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}_0) d^3 r$$

The convolution is evaluated as:

$$f_1(\mathbf{r}) * f_2(\mathbf{r}) = \lim_{V \to \infty} \int_{\mathbf{r}'}^{V} f_1(\mathbf{r}') f_2(\mathbf{r} - \mathbf{r}') d^3 r'$$

and the convolution theorem is:

$$\Im\{ f_1(\mathbf{r}) * f_2(\mathbf{r}) \} = f_1(\mathbf{k}) \cdot f_2(\mathbf{k})$$

Periodic Function

Consider a function represented by the Fourier series:

$$f(\mathbf{r}) = \sum_{hkl} f_{hkl} e^{2\pi i \mathbf{g}_{hkl} \cdot \mathbf{r}}$$

The function is periodic, with translational symmetry, i.e.:

$$\begin{aligned} f(\mathbf{r} + \mathbf{r}_{uvw}) &= \sum_{hkl} f_{hkl} e^{2\pi i \mathbf{g}_{hkl} \cdot (\mathbf{r} + \mathbf{r}_{uvw})} \\ &= \sum_{hkl} f_{hkl} e^{2\pi i \mathbf{g}_{hkl} \cdot \mathbf{r}} \cdot e^{2\pi i \mathbf{g}_{hkl} \cdot \mathbf{r}_{uvw}} \\ &= \sum_{hkl} f_{hkl} e^{2\pi i \mathbf{g}_{hkl} \cdot \mathbf{r}} \cdot (1) \\ f(\mathbf{r} + \mathbf{r}_{uvw}) &= f(\mathbf{r}) \end{aligned}$$

We can adopt a shorthand notation:

$$f(\mathbf{r}) = \sum_{hkl} f_{hkl} e^{2\pi i \mathbf{g}_{hkl} \cdot \mathbf{r}} = \sum_{\mathbf{g}} f_{\mathbf{g}} e^{2\pi i \mathbf{g} \cdot \mathbf{r}}$$

where the sum is over the RLVs $\{\mathbf{g}\}$, i.e.: $\sum_{hkl} \rightarrow \sum_{\mathbf{g}}$

Another delta function

This one is a reciprocal-space function:

$$\Delta(k) \equiv \lim_{L\to\infty}\left(\int_x^L e^{-2\pi ikx}dx\right) = \begin{cases}\infty, & k=0\\ 0, & \text{otherwise}\end{cases}$$

In 3-D:

$$\Delta(\mathbf{k}) \equiv \lim_{V\to\infty}\left(\int_{\mathbf{r}}^V e^{-2\pi i\mathbf{k}\cdot\mathbf{r}}d^3r\right) = \begin{cases}\infty, & \mathbf{k}=\mathbf{0}\\ 0, & \text{otherwise}\end{cases}$$

Another form:

$$\Delta_{\mathbf{k}} \equiv \lim_{V\to\infty}\left(\frac{1}{V}\int_{\mathbf{r}}^V e^{-2\pi i\mathbf{k}\cdot\mathbf{r}}d^3r\right) = \begin{cases}1, & \mathbf{k}=\mathbf{0}\\ 0, & \text{otherwise}\end{cases}$$

Proof of Convolution Theorem

$$g(x) = f(x) * h(x) = \int_{x'} dx'\, f(x')\, h(x - x')$$

$$g(k) = \Im\{g(x)\} = \int_{x} dx\, g(x)\, \mathrm{e}^{-2\pi ikx}$$

$$= \int_{x} dx \left[\int_{x'} dx'\, f(x')\, h(x - x') \right] \mathrm{e}^{-2\pi ikx}$$

$$= \int_{x} dx \int_{x'} dx' \left[\int_{k'} dk'\, f(k')\, \mathrm{e}^{2\pi ik'x'} \right] \left[\int_{k''} dk''\, h(k'')\, \mathrm{e}^{2\pi ik''(x - x')} \right] \mathrm{e}^{-2\pi ikx}$$

$$= \int_{k'} dk' \int_{k''} dk''\, f(k')\, h(k'') \int_{x'} dx'\, \mathrm{e}^{-2\pi i(k'' - k')x'} \int_{x} dx\, \mathrm{e}^{-2\pi i(k - k'')x}$$

$$= \int_{k'} dk' \int_{k''} dk''\, f(k')\, h(k'')\, \Delta(k'' - k')\, \Delta(k - k'')$$

$$= \int_{k''} dk''\, f(k'')\, h(k'')\, \Delta(k - k'')$$

$$g(k) = f(k) \cdot h(k)$$

Fourier components

Let's define a normalized Fourier transform:

$$f_{\mathbf{k}} = \lim_{V \to \infty} \left\{ \frac{1}{V} \int_{\mathbf{r}}^{V} f(\mathbf{r}) e^{-2\pi i \mathbf{k}\cdot\mathbf{r}} d^3 r \right\}$$

Assume $f(\mathbf{r})$ is periodic:

$$f(\mathbf{r}) = \sum_{\mathbf{g}} f_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}}$$

$$f_{\mathbf{k}} = \lim_{V \to \infty} \left[\frac{1}{V} \int_{\mathbf{r}}^{V} \left(\sum_{\mathbf{g}} f_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}} \right) e^{-2\pi i \mathbf{k}\cdot\mathbf{r}} d^3 r \right]$$

$$= \sum_{\mathbf{g}} f_{\mathbf{g}} \left\{ \lim_{V \to \infty} \left[\frac{1}{V} \int_{\mathbf{r}}^{V} e^{2\pi i (\mathbf{g}-\mathbf{k})\cdot\mathbf{r}} d^3 r \right] \right\}$$

$$f_{\mathbf{k}} = \sum_{\mathbf{g}} f_{\mathbf{g}} \cdot \Delta_{\mathbf{g}-\mathbf{k}}$$

The only non-vanishing Fourier components are the RLVs.

Fourier components of crystal potential

The crystal potential can be written as:

$$\Phi(\mathbf{r}) = \sum_{\mathbf{g}} \Phi_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}}$$

$$\left[\Phi(\mathbf{r})\right]^* = \sum_{\mathbf{g}} \left(\Phi_{\mathbf{g}}\right)^* e^{-2\pi i \mathbf{g}\cdot\mathbf{r}}$$

If $\Phi(\mathbf{r})$ is real:

$$\Phi(\mathbf{r}) = \left[\Phi(\mathbf{r})\right]^*$$

$$\sum_{\mathbf{g}} \Phi_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}} = \sum_{\mathbf{g}} \left(\Phi_{\mathbf{g}}\right)^* e^{2\pi i(-\mathbf{g})\cdot\mathbf{r}}$$

$$\sum_{\mathbf{g}} \Phi_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}} = \sum_{\mathbf{g}} \left(\Phi_{-\mathbf{g}}\right)^* e^{2\pi i \mathbf{g}\cdot\mathbf{r}}$$

$$\rightarrow \qquad \left(\Phi_{\mathbf{g}}\right)^* = \Phi_{-\mathbf{g}}$$

$$\Phi(-\mathbf{r}) = \sum_{\mathbf{g}} \Phi_{\mathbf{g}} e^{-2\pi i \mathbf{g}\cdot\mathbf{r}}$$

If the crystal is centrosymmetric:

$$\Phi(\mathbf{r}) = \Phi(-\mathbf{r})$$

$$\sum_{\mathbf{g}} \Phi_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}} = \sum_{\mathbf{g}} \Phi_{\mathbf{g}} e^{-2\pi i \mathbf{g}\cdot\mathbf{r}}$$

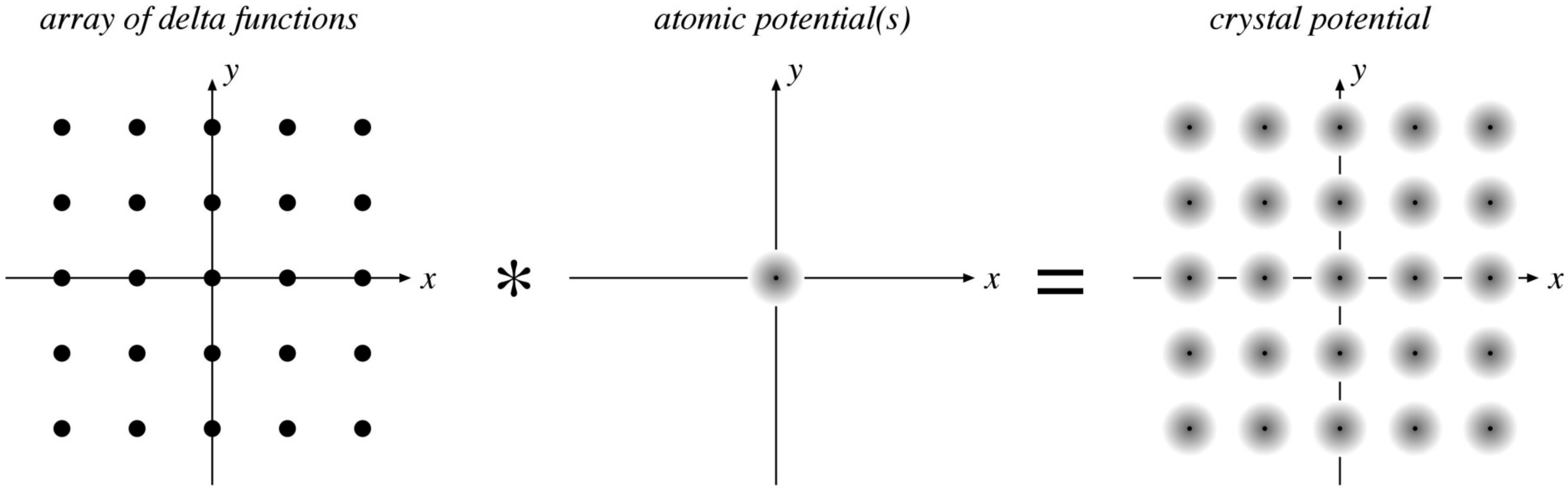
$$\sum_{\mathbf{g}} \Phi_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}} = \sum_{\mathbf{g}} \Phi_{-\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}}$$

$$\rightarrow \qquad \Phi_{\mathbf{g}} = \Phi_{-\mathbf{g}}$$

real *and* centrosymmetric: $\Phi_{\mathbf{g}} = \Phi_{-\mathbf{g}} = \left(\Phi_{\mathbf{g}}\right)^* = real$

Evaluating the crystal potential by convolution

$X(\mathbf{r}) = \sum_n \delta(\mathbf{r} - \mathbf{r}_n)$ $\qquad \phi(\mathbf{r})$ $\qquad \Phi(\mathbf{r}) = \phi(\mathbf{r}) * X(\mathbf{r})$



In direct space: $\Rightarrow \Phi(\mathbf{r}) = \sum_n \phi(\mathbf{r} - \mathbf{r}_n)$

In reciprocal space: $\Rightarrow \Im\{\Phi(\mathbf{r})\} = \Im\{\phi(\mathbf{r})\} \cdot \Im\{X(\mathbf{r})\}$

Crystal Function (Lattice Sum)

For an infinite crystal:

$$X(\mathbf{r}) = \lim_{N \to \infty}\left[\sum_{n=1}^{N} \delta(\mathbf{r} - \mathbf{r}_n)\right]$$

The Fourier components are:

$$X_{\mathbf{k}} = \lim_{V \to \infty}\left\{\frac{1}{V}\int_{\mathbf{r}}^{V} \lim_{N \to \infty}\left[\sum_{n=1}^{N} \delta(\mathbf{r} - \mathbf{r}_n)\right] e^{-2\pi i \mathbf{k}\cdot\mathbf{r}} d^3r\right\}$$

$$X_{\mathbf{k}} = \lim_{V \to \infty}\left\{\frac{1}{V} \lim_{N \to \infty}\left[\sum_{n=1}^{N} e^{-2\pi i \mathbf{k}\cdot\mathbf{r}_n}\right]\right\}$$

Substituting $V = Nv$, where v is the unit-cell volume:

$$X_{\mathbf{k}} = \lim_{N \to \infty}\left(\frac{1}{Nv}\sum_{n=1}^{N} e^{-2\pi i \mathbf{k}\cdot\mathbf{r}_n}\right) = \begin{cases} \frac{1}{v}, & \mathbf{k} = \text{an RLV} \\ 0, & \mathbf{k} = \text{otherwise} \end{cases}$$

In other words,

$$X(\mathbf{r}) = \sum_{\mathbf{g}} X_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}} = \left(\frac{1}{v}\right)\sum_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}}$$

Unit-cell potentials

The total potential is a sum over unit cells:

$$\Phi(\mathbf{r}) = \lim_{N \to \infty} \left[\sum_{n=1}^{N} \phi(\mathbf{r} - \mathbf{r}_n) \right]$$

The unit-cell potential is:

$$\phi(\mathbf{r}) = \sum_{m \text{ atoms}} \phi^{(m)}\left(\mathbf{r} - \mathbf{d}^{(m)}\right)$$

For individual atoms:

$$s = g/2$$

$$4\pi s r = 2\pi g r$$

$$\phi^{(m)}(g) = 4\pi \int_{r=0}^{\infty} r^2 \phi^{(m)}(r) \frac{\sin(2\pi g r)}{2\pi g r} dr$$

Convention uses opposite sign

The Fourier transform of the unit-cell potential is:

$$\phi(\mathbf{g}) = \lim_{V \to \infty} \left\{ \int_{\mathbf{r}}^{V} \left[\sum_{m \text{ atoms}} \phi^{(m)}\left(\mathbf{r} - \mathbf{d}^{(m)}\right) \right] \mathrm{e}^{-2\pi i \mathbf{g} \cdot \mathbf{r}} d^3 r \right\} = \sum_{m \text{ atoms}} \phi^{(m)}(g)\, \mathrm{e}^{-2\pi i \mathbf{g} \cdot \mathbf{d}^{(m)}}$$

Evaluating the Fourier Components of Φ(**r**)

Recall that Φ(**r**) is the convolution:

$$\Phi(\mathbf{r}) = \phi(\mathbf{r}) * X(\mathbf{r})$$

So:

$$\Phi_{\mathbf{g}} = \phi(\mathbf{g}) \cdot X_{\mathbf{g}}$$

Total Wave Function

Wave function above sample is a plane wave:

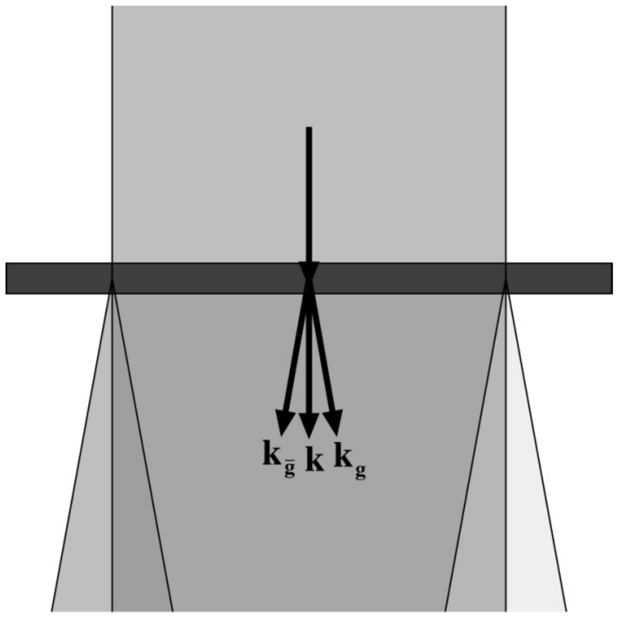
$$\psi(\mathbf{r}) = e^{2\pi i \mathbf{k}\cdot\mathbf{r}}$$ //incident beam

Wave function below sample is a collection of diffracted beams (and **0**):

$$\psi(\mathbf{r}) = \sum_{\mathbf{g}} \Psi_{\mathbf{g}} e^{2\pi i \mathbf{k}_{\mathbf{g}}\cdot\mathbf{r}}$$ //transmitted beams

$$\mathbf{k}_{\mathbf{g}} = \mathbf{k} + \mathbf{g} + \mathbf{s}_{\mathbf{g}}$$

We need to know the values of the $\Psi_{\mathbf{g}}$.



Intensities:

$$I_{\mathbf{g}} = \left|\Psi_{\mathbf{g}}\right|^2$$