

# Delta Function

Defined as:

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

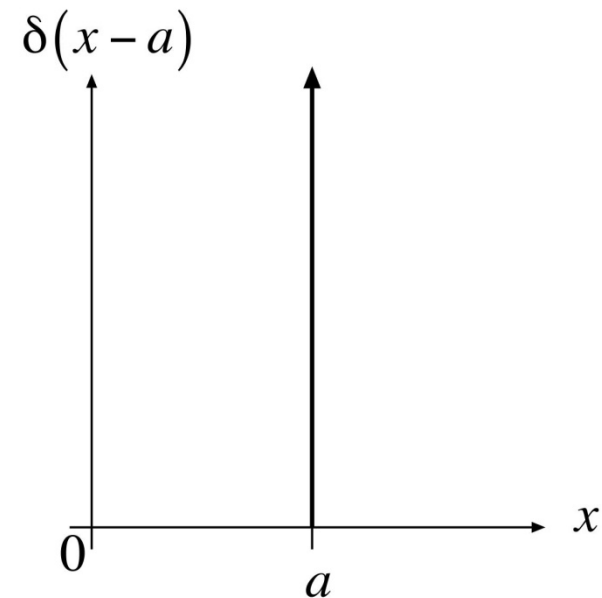
This is called the “sampling property” of the delta function.

Notice that:

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

It might be more appropriate to write:

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



Note: delta functions are sometimes called “unit impulse functions”

# Fourier transform

$$f(k) = \int_{x=-\infty}^{\infty} f(x) e^{-2\pi i k x} dx = \mathfrak{F}[f(x)] \text{ //Fourier transform}$$

$$f(x) = \int_{k=-\infty}^{\infty} f(k) e^{2\pi i k x} dk = \mathfrak{F}^{-1}[f(k)] \text{ //inverse Fourier transform}$$

Example, delta function:

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

Notice that the delta function can be written as:

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

Another example, two delta functions:

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

# 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:

$$f_1(k) = \mathfrak{F}\{f_1(x)\}$$

$$f_2(k) = \mathfrak{F}\{f_2(x)\}$$

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

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

## Three-dimensional versions

In 3-D, the Fourier transform is:

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

and the inverse Fourier transform is:

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

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The delta function is:

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

and has the property:

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

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The convolution is evaluated as:

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

and the convolution theorem is:

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

# 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:

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

In 3-D:

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

Another form:

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

# Proof of Convolution Theorem

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

$$\begin{aligned} g(k) &= \mathfrak{T}\{g(x)\} = \int_x dx g(x) e^{-2\pi i k x} \\ &= \int_x dx \left[ \int_{x'} dx' f(x') h(x - x') \right] e^{-2\pi i k x} \\ &= \int_x dx \int_{x'} dx' \left[ \int_{k'} dk' f(k') e^{2\pi i k' x'} \right] \left[ \int_{k''} dk'' h(k'') e^{2\pi i k''(x - x')} \right] e^{-2\pi i k x} \\ &= \int_{k'} dk' \int_{k''} dk'' f(k') h(k'') \int_{x'} dx' e^{-2\pi i(k'' - k')x'} \int_x dx e^{-2\pi i(k - k'')x} \\ &= \int_{k'} dk' \int_{k''} dk'' f(k') h(k'') \Delta(k'' - k') \Delta(k - k'') \\ &= \int_{k''} dk'' f(k'') h(k'') \Delta(k - k'') \\ g(k) &= f(k) \cdot h(k) \end{aligned}$$

# Fourier components

Let's define a normalized Fourier transform:

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

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

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

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

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

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

The only non-vanishing Fourier components are the RLVs.



# Fourier components of crystal potential

The crystal potential can be written as:

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

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

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

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

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

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

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

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

If the crystal is centrosymmetric:

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

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

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

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

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

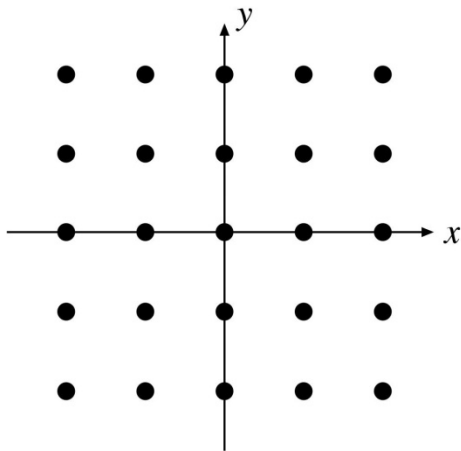
# Evaluating the crystal potential by convolution

$$X(\mathbf{r}) = \sum_n \delta(\mathbf{r} - \mathbf{r}_n)$$

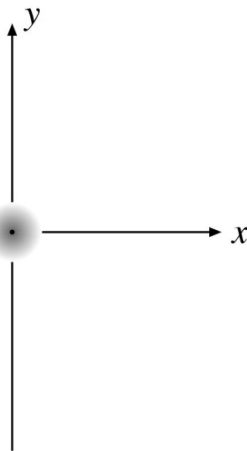
$$\phi(\mathbf{r})$$

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

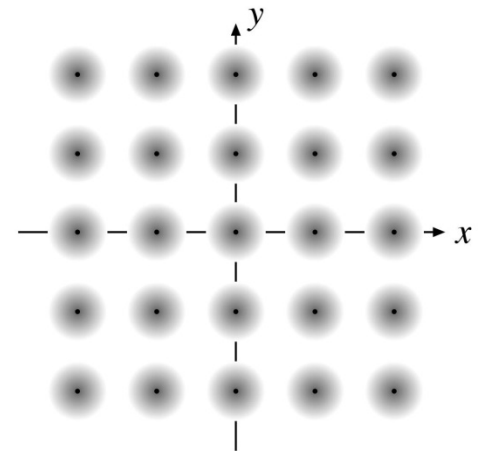
*array of delta functions*



*atomic potential(s)*



*crystal potential*



In direct space:

$$\Rightarrow \Phi(\mathbf{r}) = \sum_n \phi(\mathbf{r} - \mathbf{r}_n)$$

In reciprocal space:

$$\Rightarrow \mathfrak{T}\{\Phi(\mathbf{r})\} = \mathfrak{T}\{\phi(\mathbf{r})\} \cdot \mathfrak{T}\{X(\mathbf{r})\}$$

# Crystal Function (Lattice Sum)

For an infinite crystal:

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

The Fourier components are:

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

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

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

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

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:

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

The unit-cell potential is:

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

For individual atoms:

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

$$s = g/2$$

$$4\pi sr = 2\pi gr$$

Convention uses  
opposite sign

The Fourier transform of the unit-cell potential is:

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



## Evaluating the Fourier Components of $\Phi(\mathbf{r})$

Recall that  $\Phi(\mathbf{r})$  is the convolution:

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

So:

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