A - FOURIER TRANSFORM

In $\mathbb{R}^n$ we usually write:

$$\langle \vec{x}, \vec{q} \rangle = \frac{1}{(2\pi)^{n/2}} e^{-i \vec{q} \cdot \vec{x}}$$

(1)

$$\int d^n x \ e^{i \vec{q} \cdot \vec{x}} \langle \vec{x}, \vec{q} \rangle = \int d^n \vec{q} \ e^{-i \vec{x} \cdot \vec{q}} = \delta(\vec{x})$$

(2)

$$\int d^n \vec{x} \ e^{-i \vec{q} \cdot \vec{x}} - \delta(\vec{q}) \vec{x} = \int d^n \vec{q} \ e^{i \vec{x} \cdot \vec{q}} \delta(\vec{x} - \vec{x}^\prime)$$

(3)

$$\int d^n \vec{x} \ e^{-i \vec{q} \cdot \vec{x}} = \delta(\vec{x} - \vec{x}^\prime), \quad \int d^n \vec{q} \ e^{i \vec{x} \cdot \vec{q}} = \delta(\vec{x} - \vec{x}^\prime)$$

(4)

$$\hat{f}(\vec{q}) = \frac{1}{(2\pi)^{n/2}} \int d^n x \ e^{-i \vec{q} \cdot \vec{x}} f(\vec{x}) , \quad \hat{f}(\vec{q}) = \frac{1}{(2\pi)^{n/2}} \int d^n \vec{q} \ e^{i \vec{x} \cdot \vec{q}} \hat{f}(\vec{q})$$

(5)

Now let us consider a perfect crystal, which consists of a space-filling array of periodically repeated identical copies of a single structural unit containing some distribution of mass and charge. The repeated structural unit is called a unit cell. The unit cell with the smallest possible volume is called a primitive unit cell. If the unit cell contains more than one atom, the position of the atoms relative to the center of the cell are called the basis.

Equivalent points in unit cells in a $n$-dimensional perfect crystal lie on a periodic lattice, called a Bravais lattice, consisting of a mathematical array of points. Any lattice point can be specified by an integral linear combination of independent primitive translation vectors

$$\vec{a}_1, \vec{a}_2, \ldots, \vec{a}_n$$

(6)

where $\vec{e} = (e_1, e_2, \ldots, e_n)$ is a $n$-dimensional vector with components $e_i$. $\vec{e}$ indexes a particular unit cell, $\vec{R}$ specifies its position in real space. The set of vectors $\vec{a}_1, \vec{a}_2, \ldots, \vec{a}_n$ completely define the mathematical lattice. A translation vector, or lattice vector,

$$\vec{T} = \vec{R} - \vec{R}_e$$

(7)

connects equivalent points in the lattice, for any $\vec{e}$ and $\vec{T}$, the lattice points
in Euclidean space is often called the direct lattice.

Associated with any periodic lattice is a set of parallel planes containing all lattice points. Each set of these planes can be defined by its normal vector \( \vec{e} \). Let a vector \( \vec{T} \) in a given plane perpendicular to \( \vec{e} \) satisfy \( \vec{e}, \vec{T} = 2\pi \). For this set of parallel planes, all lattice vectors \( \vec{x} \) in some plane when satisfies

\[ \vec{e} \cdot \vec{T} = 2\pi m \]

for some integer \( m \). The coefficient \( 2\pi \) is chosen by convention so that

\[ \vec{e} \cdot \vec{T} = 1 \]

Any point \( \vec{x}_m \) (not just a lattice point \( \vec{x} \)) in the \( m \)th plane associated with \( \vec{e} \) satisfies \( \vec{e} \cdot \vec{x}_m = 2\pi m \). The difference \( \vec{x}_m - \vec{x}_{m+1} \) between points in adjacent planes satisfies \( \vec{e} \cdot (\vec{x}_m - \vec{x}_{m+1}) = 2\pi \). The distance \( \ell \) between adjacent planes is the component of \( \vec{x}_m - \vec{x}_{m+1} \) parallel to \( \vec{e} \). Thus

\[ \ell = \frac{2\pi}{\vec{e} \cdot \vec{T}} \]

For any set of primitive translation vectors \( \vec{b}_1, \vec{b}_2, ..., \vec{b}_d \) it is always possible to construct a set of reciprocal vectors \( \vec{b}_1^*, \vec{b}_2^*, ..., \vec{b}_d^* \) satisfying

\[ \vec{b}_i \cdot \vec{b}_j^* = 2\pi \delta_{ij} \]

Any vector satisfying (1) can be written as

\[ \vec{e} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + ... + m_d \vec{b}_d \]

where \( m_i \) \((i = 1, 2, ..., d)\) are positive or negative integers or zero. The vectors \( \vec{e} \), therefore, form a periodic lattice, called the reciprocal lattice, with translation vectors \( \vec{b}_1^*, \vec{b}_2^*, ..., \vec{b}_d^* \). The Wigner-Seitz unit cell for the reciprocal lattice is called the first Brillouin zone.

Let us consider a function \( f(x) \) of a single variable \( x \in [-\frac{1}{2}, \frac{1}{2}] \). If \( f(x) \) satisfies some reasonable continuity and boundedness conditions, it can be expanded in a uniformly convergent Fourier series.
\[ f(x) = A \sum_q e^{iqx} \hat{f}(q) \]  

where \( A \) is a constant and \( \exp(iz) \) must satisfy the same boundary conditions as \( f(x) \). As it is well known for large system we can always choose as boundary conditions, periodic boundary conditions,

\[ f(x + L) = f(x) \]

and therefore the values of \( q \) appearing in \((1)\) are

\[ q = \frac{2\pi m}{L}, \quad m = 0, \pm 1, \pm 2, \ldots \]

Note that \( \exp(iz) \) satisfy the orthogonality relation

\[ \int_{-\frac{L}{2}}^{\frac{L}{2}} dx \ \exp(iz) = \begin{cases} 0, & z \neq 0 \\ L, & z = 0 \end{cases} \]

as well as the completeness relation

\[ \sum_q e^{-iqx} = \lim_{M \to \infty} \sum_{m = -M}^{M} e^{i(2\pi m/L)x} = \lim_{M \to \infty} e^{i(2\pi M/L)x} \frac{1 - e^{-i(2\pi/L)2M}}{1 - e^{-i(2\pi/L)}} \]

Then we have

\[ \int_{-\frac{L}{2}}^{\frac{L}{2}} dx \ \exp(iz) = L \delta_{z,0} \]

orthogonality relation

\[ \sum_q e^{-iqx} = L \delta(x) \]

completeness relation

Hence

\[ f(x) = A \sum_q e^{iqx} \hat{f}(q) \]

\[ \hat{f}(q) = \frac{1}{AL} \int_{-\frac{L}{2}}^{\frac{L}{2}} dx \ e^{-iqx} f(x) \]

when \( A \) is an arbitrary constant and \( q = \frac{2\pi m}{L}, \quad m = 0, \pm 1, \pm 2, \ldots \)
Let us now try to recover the continuum limit. Up to this end let us take \( L \to \infty \); in this case the discrete variable \( q \) turns out to be a continuous variable. Then (3.4) and (3.5) imply

\[
L \delta_{q, q'} \longrightarrow \frac{1}{2\pi} \delta(q - q')
\]

and (3.4) gives

\[
\langle \mathbf{r} \rangle = \frac{AL}{(2\pi)} \int_{-\frac{\pi}{AL}}^{\frac{\pi}{AL}} dq \ e^{-i q \mathbf{r}} \ \hat{f}(q)
\]

\[
\hat{f}(q) = \frac{i}{AL} \int_{-\frac{\pi}{AL}}^{\frac{\pi}{AL}} dx \ e^{-i q \mathbf{x}} \ f(x)
\]

and the usual result is obtained: namely

\[
AL = (2\pi)^{1/2}
\]

The generalization of these formulae to \( D \)-dimensions is straightforward. Let \( \{ \mathbf{r} \} \) be a function of a \( D \)-component vector \( \mathbf{r} = (x_1, x_2, \ldots, x_D) \), and impose periodic boundary conditions

\[
\{ (x_1, x_2, \ldots, x_M, \ldots, x_D) = \{ (x_1, x_2, \ldots, x_M + L, \ldots, x_D) \}
\]

Then we can expand \( \{ \mathbf{r} \} \) in a Fourier series similar to (3.1)

\[
\{ \mathbf{r} \} = A \sum_{\mathbf{q}} e^{i \mathbf{q} \cdot \mathbf{r}} \ \hat{f}(\mathbf{q})
\]

where

\[
\mathbf{q} = \left( \frac{2\pi}{L_1}, \frac{2\pi}{L_2}, \ldots, \frac{2\pi}{L_D} \right) \quad m_i = 0, \pm 1, \pm 2, \ldots \quad \forall i
\]

The orthogonality and completeness relations (3.4) and (3.5) are now

\[
\int dx_1 \ldots \int dx_D \ e^{i \mathbf{q} \cdot \mathbf{r}} \ \delta(\mathbf{q} - \mathbf{q'}) \ \mathbf{r} = V \delta_{\mathbf{q}, \mathbf{q'}}
\]

\[
\sum_{\mathbf{q}} e^{-i \mathbf{q} \cdot \mathbf{r}} = V \delta(\mathbf{r})
\]
\[(\mathbf{r}) = A \sum_{\xi} e^{i \xi \cdot \mathbf{r}} \mathbf{f}(\xi)\]

\[\mathbf{f}(\xi) = \frac{1}{AV} \int_{-L/2}^{L/2} \ldots \int_{-L/2}^{L/2} e^{-i \xi \cdot \mathbf{r}} d\mathbf{r} \]

Then the continuous limit is obtained \(L \to \infty\) and

\[V \delta_{\xi, \xi'} \to (2\pi)^{D} \delta(\xi - \xi')\]

\[\frac{1}{V} \sum_{\xi} \to \frac{1}{(2\pi)^{D}} \int d\xi\]

and the usual formula for the Fourier transform is obtained by

\[AV = (2\pi)^{D/2}\]

Often one is interested in functions that are defined only at points of a regular periodic lattice rather than at all points in space. Let us begin with a one-dimensional lattice. Let \(f\) be a function of the integer \(q\) indexing the lattice site located at position \(R_q = qa\) of a one-dimensional lattice with lattice spacing \(a\). The function \(f\) can be expanded in a discrete Fourier series

\[f(q) = A \sum_{q} e^{i \xi q R_e} \]

Again, we choose the periodic boundary condition

\[f_R = f_{R+N}\]

where \(N\) is an integer. The possible values of \(q\) are

\[q = \frac{2\pi}{Na}, m = 0, 1, 2, \ldots, n\text{ integer}\]

Because \(R_e\) is an integral multiple of the lattice spacing \(a\), the function

\[e^{i q (R_e + N a)}\]

in (14) is periodic in \(q\) as well as in \(R_e\)

\[e^{i q (R_e + N a)} = e^{i q R_e}, e^{i (q + 2\pi N/a) R_e} = e^{i q R_e}\]
Thus \( \exp(i \mathbf{q} \cdot \mathbf{R}_e) \) and \( \mathbf{I}_q \) are completely characterized by \( q \) in the interval \([-\frac{\pi}{a}, \frac{\pi}{a}]\), i.e. by \( q \) in the first Brillouin zone of the one-dimensional lattice.

\[
q = \frac{2\pi m}{Na}, \quad m = -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, \ldots, \frac{1}{2}, \frac{3}{2}
\]  

Now let us consider

\[
\sum_{l=0}^{N-1} e^{i (q - q') \cdot \mathbf{R}_e} = \sum_{l=0}^{N-1} e \cdot e^{i 2\pi (m-m') \cdot \mathbf{R}_e} = \sum_{l=0}^{N-1} e^{i 2\pi (m-m') \cdot \mathbf{R}_e} = \frac{1 - e^{i 2\pi (m-m')} \cdot N}{1 - e^{i 2\pi (m-m')} \cdot N}
\]

Furthermore

\[
\sum_{q \in \text{lattice}} e^{i q \cdot \mathbf{R}_e} = \sum_{m=-\frac{1}{2}}^{\frac{1}{2}} e^{i 2\pi m \mathbf{R}_e} = 1 - e^{i \frac{2\pi}{N} \cdot \mathbf{R}_e} = \frac{1 - e^{i 2\pi}}{1 - e^{i 2\pi}} = N \delta_{0,0}
\]

Then the orthogonality and completeness relations are

\[
\sum_{l=0}^{N-1} e^{i (q - q') \cdot \mathbf{R}_e} = N \delta_{q, q'}
\]

\[
\sum_{q \in \text{lattice}} e^{i q \cdot (\mathbf{R}_e - \mathbf{R}_e')} = N \delta_{q, q'}
\]

Then

\[
|e| = A \sum_{q \in \text{lattice}} e^{i q \cdot \mathbf{R}_e} \quad |q|
\]

\[
|q| = \frac{1}{NA} \sum_{l=0}^{N-1} e^{i q \cdot \mathbf{R}_e} |e|
\]
In the limit \( N \to \infty \) and \( Na = L = \text{const.} \), we recover from (6.4) and (6.5) 

\[
\sum_{n=0}^{N-1} \longrightarrow \frac{1}{a} \int_{-\frac{L}{2}}^{\frac{L}{2}} \delta(x-\xi) \, d\xi.
\]

If we wish to go directly from (6.4) and (6.5) to the continuous limit we take \( N \to \infty \) with \( Na = L = \text{const.} \), and then \( L \to \infty \).

\[
\sum_{n=0}^{\infty} \longrightarrow \frac{1}{a} \int_{-\infty}^{\infty} \delta(x-\xi) \, d\xi.
\]

Let \( \delta_q, q' \longrightarrow (2\pi) \delta(q-q') \) \quad \frac{1}{L} \sum_{q \in \mathbb{Z}} \rightarrow \frac{1}{2\pi} \int_{-\pi}^{\pi} \delta_q.

and hence we can obtain

\[
\int_{-\pi}^{\pi} \delta_{q-q'} \, e^{i(q-q')x} = (2\pi) \delta(q-q')
\]

\[
\int_{-\pi}^{\pi} a_{q} \, e^{-i(x-x')q} = (2\pi) \delta(q-q')
\]

\[
|\xi| = \frac{AL}{(2\pi)} \int_{-\pi}^{\pi} a_{q} \, e^{-i\xi q} \, \frac{1}{l(q)}
\]

\[
\frac{1}{l(q)} = \frac{1}{AL} \int_{-\pi}^{\pi} \delta(x) \, e^{-i\xi q} \, |\xi|
\]

which are the discrete formulae of

\[
AL = (2\pi)^{1/2}
\]

The generalization of the lattice Fourier transform to \( d \)-dimensional lattices is again straightforward. If \( \phi \) is a function of the lattice index \( \vec{\xi} \) satisfying periodic boundary conditions.

\[
\vec{\xi} = \vec{\xi} + \vec{a}
\]

where \( \vec{a} = (a_1, a_2, \ldots, a_d) \), then
\[\bar{e} = A \sum_{\bar{q}} e^{i \bar{q} \cdot \bar{r}_{\bar{e}} / \bar{q}} \]

with

\[\bar{q} = (\frac{2n_1}{m_1}, \frac{2n_2}{m_2}, \ldots, \frac{2n_n}{m_n})\]

being \(m_i\) integer numbers. Notice that since \(\bar{r}_{\bar{e}}\) are restricted to lattice points

\[e^{i \bar{q} \cdot \bar{r}_{\bar{e}}} = e^{i \bar{q} \cdot \bar{r}_0}\]

where \(\bar{q}\) is a reciprocal lattice vector. Thus, as in the one-dimensional case, only wave vectors \(\bar{q}\) in the first Brillouin zone need to be considered. The number of points in the first Brillouin zone is again equal to the number of points in the direct lattice \(N_1 N_2 N_3 \ldots N_n\). Then we obtain

\[\sum_{\bar{e}} e^{i (\bar{q} - \bar{q}_0) \cdot \bar{r}_{\bar{e}}} = N \delta_{\bar{q}_0, \bar{q}}\]

\[\sum_{\bar{q}} e^{-i \bar{q} \cdot (\bar{r}_{\bar{e}} - \bar{r}_0)} = N \delta_{\bar{q}, 0}\]

where the sum on \(\bar{e}\) are restricted to the \(N\) points of the direct lattice and the sum over \(\bar{q}\) on the \(N\) points of the first Brillouin zone. Also

\[\bar{e} = A \sum_{\bar{q}} e^{i \bar{q} \cdot \bar{r}_{\bar{e}} / \bar{q}} \]  \[\bar{q} = A \sum_{\bar{e}} e^{-i \bar{q} \cdot \bar{r}_{\bar{e}} / \bar{q}} \]

The minimum limit is obtained when \(N \to \infty\) and \(N V = V\), where \(V\) is the volume of the unit cell, and then \(V \to \infty\).

\[\sum_{\bar{e}} \to \frac{1}{N_0} \int d^3r \quad \sum_{\bar{q}} \to N_0 \delta(\bar{r} - \bar{r}_0) \]

\[\sum_{\bar{q}} \to (2\pi)^3 \delta(\bar{q} - \bar{q}_0) \quad \sum_{\bar{q}} \to \frac{1}{(2\pi)^3} \int d^3q \]

and to get the usual formulae

\[AV = (2\pi)^{3/2} \]