A - FOURIER TRANSFORM

In R^D we usually write

$$\langle \vec{x} \mid \vec{q} \rangle = \frac{1}{(2\pi)^{D/2}} e^{i\vec{q}.\vec{x}} \tag{1}$$

$$\int d^D x \, |\vec{x}\rangle\langle\vec{x}| = \int d^D q \, |\vec{q}\rangle\langle\vec{q}| = I \tag{2}$$

$$\frac{1}{(2\pi)^D} \int d^D x \, e^{-i(\vec{q}-\vec{q}').\vec{x}} = \delta(\vec{q}-\vec{q}') \quad , \quad \frac{1}{(2\pi)^D} \int d^D q \, e^{i(\vec{x}-\vec{x}').\vec{q}} = \delta(\vec{x}-\vec{x}') \tag{3}$$

$$\langle \vec{x} \mid \vec{x}' \rangle = \delta(\vec{x}-\vec{x}') \quad , \quad \langle \vec{q} \mid \vec{q}' \rangle = \delta(\vec{q}-\vec{q}') \tag{4}$$

$$\hat{f}(\vec{q}) = \frac{1}{(2\pi)^{D/2}} \int d^D x \, e^{-i\vec{q}.\vec{x}} f(\vec{x}) \quad , \quad f(\vec{x}) = \frac{1}{(2\pi)^{D/2}} \int d^D q \, e^{+i\vec{q}.\vec{x}} \hat{f}(\vec{q}) \tag{5}$$

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 <u>unit cell</u>. The unit cell with the smallest possible volume is called a <u>primitive unit cell</u>. If the unit cell contains more that one atom, the position of the atoms relative to the center of the cell are called the <u>basis</u>. Equivalent points in unit cells in a D-dimensional perfect crystal lie on a <u>periodic lattice</u>, called a <u>Bravais lattice</u>, consisting of a mathematical array of points. Any lattice point can be specified by an integral linear combination of <u>independent primitive translation vectors</u> $\vec{a}_1, \vec{a}_2, \dots, \vec{a}_D$:

$$\vec{R}_{\vec{\ell}} = \ell_1 \vec{a}_1 + \ell_2 \vec{a}_2 + \dots + \ell_D \vec{a}_D \tag{6}$$

where $\vec{\ell} \equiv (\ell_1, \ell_2, \dots, \ell_D)$ is a D-dimensional vector with components ℓ_i. $\vec{\ell}$ indexes a particular unit cell, $\vec{R}_{\vec{\ell}}$ specifies its position in real space. The set of vectors $\vec{a}_1, \vec{a}_2, \dots, \vec{a}_D$ completely define the mathematical lattice. A translation vector, or <u>lattice vector</u>,

$$\vec{T} = \vec{R}_{\ell} - \vec{R}_{\ell'} \tag{7}$$

connects equivalent points in the lattice, for any $\vec{\ell}$ and $\vec{\ell}'$. The lattice points in the coordinate space is often called the direct lattice

Associated with any periodic lattice is a set of equispaced parallel planes containing all lattice points. Each set of those planes can be defined by its normal vector $\vec{G}$. Lattice vectors $\vec{T}$ in a given plane perpendicular to $\vec{G}$ satisfy $\vec{G}.\vec{T}$ = cte. For this set of parallel planes all lattice vectors lie in some plane which satisfies

$$\vec{G}.\vec{T} = 2\pi m \tag{1}$$

for some integer m. The coefficient 2π is choosen by convention so that

$$e^{i\vec{G}.\vec{T}} = 1 \tag{2}$$

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

$$\ell = \frac{2\pi}{|\vec{G}|} \tag{3}$$

For any set of primitive translation vectors $\vec{a}_1, \vec{a}_2, \ldots, \vec{a}_D$ it is always possible to construct a set of reciprocal vectors $\vec{b}_1, \vec{b}_2, \ldots, \vec{b}_D$ satisfying

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\, \delta_{ij} \qquad i,j = 1, 2, \ldots, D \tag{4}$$

Any vector satisfying (1) can be written as

$$\vec{G} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + \ldots + m_D \vec{b}_D \tag{5}$$

where m_i $(i = 1, 2, \ldots, D)$ are positive or negative integers or zero. The vectors $\vec{G}$, therefore form a periodic lattice, called the reciprocal lattice with translation vectors $\vec{b}_1, \vec{b}_2, \ldots, \vec{b}_D$. 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 $x \in [-L/2, L/2]$. If $f(x)$ satisfies some reasonable continuity and boundedness conditions, it can be expanded in a uniformly convergent Fourier series:

$$f(x) = A \sum_q e^{iqx} \hat{f}(q) \tag{1}$$

where A is a constant and exp(iqx) 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

$$f(x+L) = f(x) \tag{2}$$

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

$$q = \frac{2\pi}{L} m \quad , \quad m = 0, \pm 1, \pm 2, \dots \tag{3}$$

Notice that exp(iqx) satisfy the orthogonality relation

$$\int_{-L/2}^{+L/2} dx\, e^{i(q-q')x} = \frac{\sin[(q-q')L/2]}{[(q-q')/2]} = L \frac{\sin \pi(m-m')}{\pi(m-m')} = L\delta_{m,m'} = L\delta_{q,q'}$$

as well as the completeness condition

$$\sum_q e^{-iq.x} = \lim_{N\to\infty} \sum_{m=-N}^{N} e^{-i(2\pi m/L)x} = \lim_{N\to\infty} \frac{e^{i(2\pi x/L)N}\left[1 - e^{-i(2\pi x/L)(2N+1)}\right]}{1 - e^{-i(2\pi x/L)}}$$

$$= \lim_{N\to\infty} \frac{\sin[2\pi(N+1/2)x/L]}{\sin[\pi x/L]} = L\delta(x)$$

Then we have

$$\int_{-L/2}^{L/2} dx\, e^{i(q-q')x} = L\delta_{q,q'} \qquad \text{Orthogonality relation} \tag{4}$$

$$\sum_q e^{-iqx} = L\delta(x) \qquad \text{Completeness relation} \tag{5}$$

Hence

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

$$\hat{f}(q) = \frac{1}{AL} \int_{-L/2}^{+L/2} dx\, e^{-iqx} f(x) \tag{6}$$

where A is an arbitrary constant and $q = 2\pi m/L$, $m = 0, \pm 1, \pm 2, \dots$

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

$$L\, \delta_{q,q'} \longleftrightarrow (2\pi)\, \delta(q-q')$$ (1)

$$\frac{1}{L} \sum_{q} \longleftrightarrow \frac{1}{2\pi} \int_{-\infty}^{+\infty} dq$$

and (3.6) gives

$$f(x) = \frac{AL}{(2\pi)} \int_{-\infty}^{+\infty} dq\, e^{+iq.x}\, \hat{f}(q)$$ (2)

$$\hat{f}(q) = \frac{1}{AL} \int_{-\infty}^{+\infty} dx\, e^{-iq.x}\, f(x)$$

and the usual result is obtained assuming

$$AL = (2\pi)^{1/2}$$ (3)

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

$$f(x_1, x_2, \dots, x_i, \dots x_D) = f(x_1, x_2, \dots, x_i + L_i, \dots x_D)$$ (4)

Then we can expand $f(\vec{x})$ in a Fourier series similar to (3.1)

$$f(\vec{x}) = A \sum_{\vec{q}} e^{i\vec{q}.\vec{x}}\, \hat{f}(\vec{q})$$ (5)

where

$$\vec{q} = \left(\frac{2\pi}{L_1} m_1 , \frac{2\pi}{L_2} m_2 , \dots , \frac{2\pi}{L_D} m_D \right) \qquad m_i = 0, \pm 1, \pm 2, \dots \quad \forall i$$ (6)

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

$$\int_{-L_1/2}^{L_1/2} dx_1 \dots \int_{-L_D/2}^{L_D/2} dx_D\, e^{i(\vec{q}-\vec{q}').\vec{x}} = V\, \delta_{\vec{q},\vec{q}'} \qquad V \equiv L_1 L_2 \dots L_D$$ (7)

$$\sum_{\vec{q}} e^{-i\vec{q}.\vec{x}} = V\, \delta(\vec{x})$$

Hence

$$f(\bar{x}) = A \sum_{\bar{q}} e^{i\bar{q}.\bar{x}} \hat{f}(\bar{q})$$

$$\hat{f}(\bar{q}) = \frac{1}{AV} \int_{-L_1/2}^{L_1/2} dx_1 \cdots \int_{-L_D/2}^{L_D/2} dx_D \; e^{-i\bar{q}.\bar{x}} f(\bar{x}) \qquad (1)$$

Then the continuous limit is obtained $L_i \to \infty \ \forall i$ and

$$V \delta_{\bar{q},\bar{q}'} \longleftrightarrow (2\pi)^D \delta(\bar{q} - \bar{q}')$$

$$\frac{1}{V} \sum_{\bar{q}} \longleftrightarrow \frac{1}{(2\pi)^D} \int d\bar{q} \qquad (2)$$

and the usual formulae for the Fourier transform are obtained if

$$AV = (2\pi)^{D/2} \qquad (3)$$

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_ℓ be a function of the integer ℓ indexing the lattice site located at position $R_\ell = \ell a$ of a one-dimensional lattice with lattice spacing a. The function f_ℓ can be expanded in a discrete Fourier series

$$f_\ell = A \sum_q e^{iqR_\ell} \hat{f}_q \qquad (4)$$

Again, we choose the periodic boundary condition

$$f_\ell = f_{\ell+N} \qquad (5)$$

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

$$q = \frac{2\pi}{Na} m \qquad m = \text{integer} \qquad (6)$$

Because R_ℓ is an integral multiple of the lattice spacing a, the function $\exp(iqR_\ell)$ in (4) is periodic in q as well as in ℓ

$$e^{iq(R_\ell + Na)} = e^{iqR_\ell} \quad , \quad e^{i(q + 2\pi/a)R_\ell} = e^{iqR_\ell} \qquad (7)$$

Thus $\exp(iqR_\ell)$ and $\hat{f}_q$ are completely characterized by q in the interval $[-\pi/a, +\pi/a]$, i.e. by q in the first Brillouin zone of the one-dimensional lattice

$$q = \frac{2\pi}{Na} m \quad , \quad m = -N/2+1, -N/2+2, \ldots, N/2-1, N/2 \tag{1}$$

Now let us consider

$$\sum_{\ell=0}^{N-1} e^{i(q-q')R_\ell} = \sum_{\ell=0}^{N-1} e^{i(q-q')a\ell} = \sum_{\ell=0}^{N-1} e^{i2\pi(m-m')\ell/N} =$$

$$= \frac{1 - e^{i2\pi(m-m')}}{1 - e^{i2\pi(m-m')/N}} = \exp\left\{ i\pi(m-m')\frac{N-1}{N} \right\} \frac{\sin\pi(m-m')}{\sin\pi(m-m')/N} = N\delta_{mm'} \Rightarrow$$

$$\sum_{\ell=0}^{N-1} e^{i(q-q')R_\ell} = N\delta_{qq'} \tag{2}$$

Furthermore

$$\sum_{q\in 1st\,BZ} e^{-iqR_\ell} = \sum_{m=-N/2+1}^{N/2} e^{-i2\pi m\ell/N} = e^{-i2\pi\ell(-N/2+1)/N} \frac{1 - e^{-i2\pi\ell}}{1 - e^{-i2\pi\ell/N}} = N\delta_{\ell,0} \Rightarrow$$

$$\sum_{q\in 1st\,BZ} e^{-iqR_\ell} = N\delta_{\ell,0} \tag{3}$$

Then the orthogonality and completeness relation are

$$\sum_{\ell=0}^{N-1} e^{i(q-q')R_\ell} = N\delta_{q,q'}$$

$$\sum_{q\in 1st\,BZ} e^{-iq(R_\ell - R_{\ell'})} = N\delta_{\ell\ell'} \tag{4}$$

Then

$$f_\ell = A\sum_{q\in 1st\,BZ} e^{iqR_\ell}\hat{f}_q \tag{5}$$

$$\hat{f}_q = \frac{1}{NA}\sum_{\ell=0}^{N-1} e^{-iqR_\ell} f_\ell$$

In the limit $N \to \infty$ and $Na = L = \text{cont.}$ we recover from (6.4) and (6.5) those on pag 3 if

$$\sum_{\ell=0}^{N-1} \longleftrightarrow \frac{1}{a}\int_{-L/2}^{+L/2} dx \qquad (1)$$

$$\delta_{\ell,\ell'} \longleftrightarrow a\,\delta(x-x')$$

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

$$\sum_{\ell=0}^{N-1} \longleftrightarrow \frac{1}{a}\int_{-\infty}^{+\infty} dx \quad , \quad \delta_{\ell,\ell'} \longleftrightarrow a\,\delta(x-x') \qquad (2)$$

$$L\,\delta_{q,q'} \longleftrightarrow (2\pi)\,\delta(q-q') \quad , \quad \frac{1}{L}\sum_{q\in 1\text{sBZ}} \longleftrightarrow \frac{1}{2\pi}\int_{-\infty}^{+\infty} dq$$

and hence we can obtain

$$\int_{-\infty}^{+\infty} dx\; e^{i(q-q')x} = (2\pi)\,\delta(q-q')$$

$$\int_{-\infty}^{+\infty} dq\; e^{-i(x-x')q} = (2\pi)\,\delta(q-q') \qquad (3)$$

$$f(x) = \frac{AL}{(2\pi)}\int_{-\infty}^{+\infty} dq\; e^{iqx}\,\hat{f}(q)$$

$$\hat{f}(q) = \frac{1}{AL}\int_{-\infty}^{+\infty} dx\; e^{-iqx}\,f(x)$$

which are the desired formulae if

$$AL = (2\pi)^{1/2} \qquad (4)$$

The generalization of the lattice Fourier transform to D-dimensional lattices is again straightforward. If $f_{\vec{\ell}}$ is a function of the lattice index $\vec{\ell}$ satysfying periodic boundary conditions

$$f_{\vec{\ell}} = f_{\vec{\ell}+\vec{N}} \qquad (5)$$

where $\vec{N} = (N_1, N_2, \dots, N_D)$, then

$$f_{\vec{\ell}} = A \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{R}_{\vec{\ell}}} \hat{f}_{\vec{q}} \tag{1}$$

with

$$\vec{q} = \left(\frac{2\pi}{N_1 a_1} m_1 , \frac{2\pi}{N_2 a_2} m_2 , \ldots , \frac{2\pi}{N_D a_D} m_D \right) \tag{2}$$

being m_i integer numbers. Notice that since $\vec{R}_{\vec{\ell}}$ are restricted to lattice points

$$e^{i(\vec{q}+\vec{G})\cdot\vec{R}_{\vec{\ell}}} = e^{i\vec{q}\cdot\vec{R}_{\vec{\ell}}} \tag{3}$$

where $\vec{G}$ is a reciprocal lattice vector. Thus, as in the one dimensional case, only wave vectors $\vec{q}$ in the first Brillouin zone need to be considered. The number of point in the first Brillouin zone is again equal to the number of points in the direct lattice $N = N_1 N_2 \ldots N_D$. Then we obtain

$$\sum_{\vec{\ell}} e^{i(\vec{q}-\vec{q}\,')\cdot\vec{R}_{\vec{\ell}}} = N \delta_{\vec{q},\vec{q}\,'} \tag{4}$$

$$\sum_{\vec{q}} e^{-i\vec{q}\cdot(\vec{R}_{\vec{\ell}} - \vec{R}_{\vec{\ell}\,'})} = N \delta_{\vec{\ell},\vec{\ell}\,'} \tag{5}$$

where the sum on $\vec{\ell}$ are restricted the N points of the direct lattice and the sum over $\vec{q}$ on the N points in the first Brillouin zone. Also

$$f_{\vec{\ell}} = A \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{R}_{\ell}} \hat{f}_{\vec{q}} \tag{6}$$

$$\hat{f}_{\vec{q}} = \frac{1}{NA} \sum_{\vec{\ell}} e^{-i\vec{q}\cdot\vec{R}_{\ell}} f_{\vec{\ell}} \tag{7}$$

The continuum limit is obtained when $N \to \infty$ and $N v_0 = V$, where v_0 is the volume of the unit cell, and then $V \to \infty$.

$$\sum_{\vec{\ell}} \longleftrightarrow \frac{1}{v_0} \int d^D x \qquad \delta_{\vec{\ell},\vec{\ell}\,'} \longleftrightarrow v_0\, \delta(\vec{x}-\vec{x}\,') \tag{8}$$

$$V \delta_{\vec{q},\vec{q}\,'} \longleftrightarrow (2\pi)^D \delta(\vec{q}-\vec{q}\,') , \qquad \frac{1}{V}\sum_{\vec{q}} \longleftrightarrow \frac{1}{(2\pi)^D} \int d^D q$$

and to get the usual formulae

$$A V = (2\pi)^{D/2} \tag{9}$$