These spaces play a fundamental role in the theory of partial differential equations, and in the mathematical theory of tomographic reconstruction – a subject not unrelated to the crystallographic phase problem (Natterer, 1986).

1.3.2.6. Periodic distributions and Fourier series

1.3.2.6.1. Terminology

Let $\mathbb{Z}^n$ be the subset of $\mathbb{R}^n$ consisting of those points with (signed) integer coordinates; it is an n-dimensional *lattice*, *i.e.* a free Abelian group on n generators. A particularly simple set of n generators is given by the standard basis of $\mathbb{R}^n$, and hence $\mathbb{Z}^n$ will be called the *standard lattice in* $\mathbb{R}^n$. Any other 'nonstandard' n-dimensional lattice Λ in $\mathbb{R}^n$ is the image of this standard lattice by a general linear transformation.

If we identify any two points in $\mathbb{R}^n$ whose coordinates are congruent modulo $\mathbb{Z}^n$, *i.e.* differ by a vector in $\mathbb{Z}^n$, we obtain the *standard n-torus* $\mathbb{R}^n/\mathbb{Z}^n$. The latter may be viewed as $(\mathbb{R}/\mathbb{Z})^n$, *i.e.* as the Cartesian product of n circles. The same identification may be carried out modulo a nonstandard lattice Λ, yielding a *nonstandard n-torus* $\mathbb{R}^n/\Lambda$. The correspondence to crystallographic terminology is that 'standard' coordinates over the standard 3-torus $\mathbb{R}^3/\mathbb{Z}^3$ are called 'fractional' coordinates over the unit cell; while Cartesian coordinates, *e.g.* in ångströms, constitute a set of nonstandard coordinates.

Finally, we will denote by I the unit cube $[0, 1]^n$ and by C_ε the subset

$$C_\varepsilon = \{\mathbf{x} \in \mathbb{R}^n \| x_j| < \varepsilon \text{ for all } j = 1, \ldots, n\}.$$

1.3.2.6.2. $\mathbb{Z}^n$-periodic distributions in $\mathbb{R}^n$

A distribution $T \in \mathcal{D}'(\mathbb{R}^n)$ is called *periodic with period lattice* $\mathbb{Z}^n$ (or $\mathbb{Z}^n$-periodic) if $\tau_{\mathbf{m}} T = T$ for all $\mathbf{m} \in \mathbb{Z}^n$ (in crystallography the period lattice is the *direct* lattice).

Given a distribution with compact support $T^0 \in \mathcal{E}'(\mathbb{R}^n)$, then $T = \sum_{\mathbf{m}\in\mathbb{Z}^n} \tau_{\mathbf{m}} T^0$ is a $\mathbb{Z}^n$-periodic distribution. Note that we may write $T = r * T^0$, where $r = \sum_{\mathbf{m}\in\mathbb{Z}^n} \delta_{(\mathbf{m})}$ consists of Dirac δ's at all nodes of the period lattice $\mathbb{Z}^n$.

Conversely, any $\mathbb{Z}^n$-periodic distribution T may be written as $r * T^0$ for some $T^0 \in \mathcal{E}'$. To retrieve such a 'motif' T^0 from T, a function ψ will be constructed in such a way that $\psi \in \mathcal{D}$ (hence has compact support) and $r * \psi = 1$; then $T^0 = \psi T$. Indicator functions (Section 1.3.2.2) such as χ_1 or $\chi_{C_{1/2}}$ cannot be used directly, since they are discontinuous; but regularized versions of them may be constructed by convolution (see Section 1.3.2.3.9.7) as $\psi_0 = \chi_{C_\varepsilon} * \theta_\eta$, with ε and η such that $\psi_0(\mathbf{x}) = 1$ on $C_{1/2}$ and $\psi_0(\mathbf{x}) = 0$ outside $C_{3/4}$. Then the function

$$\psi = \frac{\psi_0}{\sum_{\mathbf{m}\in\mathbb{Z}^n} \tau_{\mathbf{m}} \psi_0}$$

has the desired property. The sum in the denominator contains at most 2^n nonzero terms at any given point $\mathbf{x}$ and acts as a smoothly varying 'multiplicity correction'.

1.3.2.6.3. Identification with distributions over $\mathbb{R}^n/\mathbb{Z}^n$

Throughout this section, 'periodic' will mean '$\mathbb{Z}^n$-periodic'.

Let $s \in \mathbb{R}$, and let $[s]$ denote the largest integer $\leq s$. For $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, let $\tilde{\mathbf{x}}$ be the unique vector $(\tilde{x}_1, \ldots, \tilde{x}_n)$ with $\tilde{x}_j = x_j - [x_j]$. If $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, then $\tilde{\mathbf{x}} = \tilde{\mathbf{y}}$ if and only if $\mathbf{x} - \mathbf{y} \in \mathbb{Z}^n$. The image of the map $\mathbf{x} \longmapsto \tilde{\mathbf{x}}$ is thus $\mathbb{R}^n$ modulo $\mathbb{Z}^n$, or $\mathbb{R}^n/\mathbb{Z}^n$.

If f is a periodic function over $\mathbb{R}^n$, then $\tilde{\mathbf{x}} = \tilde{\mathbf{y}}$ implies $f(\mathbf{x}) = f(\mathbf{y})$; we may thus define a function $\tilde{f}$ over $\mathbb{R}^n/\mathbb{Z}^n$ by putting $\tilde{f}(\tilde{\mathbf{x}}) = f(\mathbf{x})$ for any $\mathbf{x} \in \mathbb{R}^n$ such that $\mathbf{x} - \tilde{\mathbf{x}} \in \mathbb{Z}^n$. Conversely, if $\tilde{f}$ is a function over $\mathbb{R}^n/\mathbb{Z}^n$, then we may define a function f over $\mathbb{R}^n$ by putting $f(\mathbf{x}) = \tilde{f}(\tilde{\mathbf{x}})$, and f will be periodic. Periodic functions over $\mathbb{R}^n$ may thus be identified with functions over $\mathbb{R}^n/\mathbb{Z}^n$, and this identification preserves the notions of convergence, local summability and differentiability.

Given $\varphi^0 \in \mathcal{D}(\mathbb{R}^n)$, we may define

$$\varphi(\mathbf{x}) = \sum_{\mathbf{m}\in\mathbb{Z}^n} (\tau_{\mathbf{m}}\varphi^0)(\mathbf{x})$$

since the sum only contains finitely many nonzero terms; φ is periodic, and $\tilde{\varphi} \in \mathcal{D}(\mathbb{R}^n/\mathbb{Z}^n)$. Conversely, if $\tilde{\varphi} \in \mathcal{D}(\mathbb{R}^n/\mathbb{Z}^n)$ we may define $\varphi \in \mathcal{E}(\mathbb{R}^n)$ periodic by $\varphi(\mathbf{x}) = \tilde{\varphi}(\tilde{\mathbf{x}})$, and $\varphi^0 \in \mathcal{D}(\mathbb{R}^n)$ by putting $\varphi^0 = \psi\varphi$ with ψ constructed as above.

By transposition, a distribution $\tilde{T} \in \mathcal{D}'(\mathbb{R}^n/\mathbb{Z}^n)$ defines a unique periodic distribution $T \in \mathcal{D}'(\mathbb{R}^n)$ by $\langle T, \varphi^0\rangle = \langle\tilde{T}, \tilde{\varphi}\rangle$; conversely, $T \in \mathcal{D}'(\mathbb{R}^n)$ periodic defines uniquely $\tilde{T} \in \mathcal{D}'(\mathbb{R}^n/\mathbb{Z}^n)$ by $\langle\tilde{T}, \tilde{\varphi}\rangle = \langle T, \varphi^0\rangle$.

We may therefore identify $\mathbb{Z}^n$-periodic distributions over $\mathbb{R}^n$ with distributions over $\mathbb{R}^n/\mathbb{Z}^n$. We will, however, use mostly the former presentation, as it is more closely related to the crystallographer's perception of periodicity (see Section 1.3.4.1).

1.3.2.6.4. Fourier transforms of periodic distributions

The content of this section is perhaps the central result in the relation between Fourier theory and crystallography (Section 1.3.4.2.1.1).

Let $T = r * T^0$ with r defined as in Section 1.3.2.6.2. Then $r \in \mathcal{S}'$, $T^0 \in \mathcal{E}'$ hence $T^0 \in \mathcal{O}'_C$, so that $T \in \mathcal{S}'$: $\mathbb{Z}^n$-periodic distributions are tempered, hence have a Fourier transform. The convolution theorem (Section 1.3.2.5.8) is applicable, giving:

$$\mathcal{F}[T] = \mathcal{F}[r] \times \mathcal{F}[T^0]$$

and similarly for $\bar{\mathcal{F}}$.

Since $\mathcal{F}[\delta_{(\mathbf{m})}](\xi) = \exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{m})$, formally

$$\mathcal{F}[r]_\xi = \sum_{\mathbf{m}\in\mathbb{Z}^n} \exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{m}) = Q,$$

say.

It is readily shown that Q is tempered and periodic, so that $Q = \sum_{\mu\in\mathbb{Z}^n} \tau_\mu(\psi Q)$, while the periodicity of r implies that

$$[\exp(-2\pi i\xi_j) - 1]\psi Q = 0, \quad j = 1, \ldots, n.$$

Since the first factors have single isolated zeros at $\xi_j = 0$ in $C_{3/4}$, $\psi Q = c\delta$ (see Section 1.3.2.3.9.4) and hence by periodicity $Q = cr$; convoluting with χ_{C_1} shows that $c = 1$. Thus we have the fundamental result:

$$\boxed{\mathcal{F}[r] = r}$$

so that

$$\mathcal{F}[T] = r \times \mathcal{F}[T^0];$$

i.e., according to Section 1.3.2.3.9.3,

$$\mathcal{F}[T]_\xi = \sum_{\mu\in\mathbb{Z}^n} \mathcal{F}[T^0](\boldsymbol{\mu}) \times \delta_{(\boldsymbol{\mu})}.$$

The right-hand side is a *weighted* lattice distribution, whose nodes $\boldsymbol{\mu} \in \mathbb{Z}^n$ are weighted by the *sample values* $\mathcal{F}[T^0](\boldsymbol{\mu})$ of the transform of the motif T^0 at those nodes. Since $T^0 \in \mathcal{E}'$, the latter values may be written