

1. GENERAL RELATIONSHIPS AND TECHNIQUES

- (i)  $w_{\boldsymbol{\mu}} = \langle T_{\mathbf{x}}^0, \exp(-2\pi i \boldsymbol{\mu} \cdot \mathbf{x}) \rangle$
- (ii)  $T_{\mathbf{x}} = \sum_{\boldsymbol{\mu} \in \mathbb{Z}^n} w_{\boldsymbol{\mu}} \exp(+2\pi i \boldsymbol{\mu} \cdot \mathbf{x})$

are referred to as the *Fourier analysis* and the *Fourier synthesis* of  $T$ , respectively (there is a discrepancy between this terminology and the crystallographic one, see Section 1.3.4.2.1.1). In other words, any periodic distribution  $T \in \mathcal{S}'$  may be represented by a Fourier series (ii), whose coefficients are calculated by (i). The convergence of (ii) towards  $T$  in  $\mathcal{S}'$  will be investigated later (Section 1.3.2.6.10).

1.3.2.6.5. *The case of non-standard period lattices*

Let  $\Lambda$  denote the non-standard lattice consisting of all vectors of the form  $\sum_{j=1}^n m_j \mathbf{a}_j$ , where the  $m_j$  are rational integers and  $\mathbf{a}_1, \dots, \mathbf{a}_n$  are  $n$  linearly independent vectors in  $\mathbb{R}^n$ . Let  $R$  be the corresponding lattice distribution:  $R = \sum_{\mathbf{x} \in \Lambda} \delta_{(\mathbf{x})}$ .

Let  $\mathbf{A}$  be the non-singular  $n \times n$  matrix whose successive columns are the coordinates of vectors  $\mathbf{a}_1, \dots, \mathbf{a}_n$  in the standard basis of  $\mathbb{R}^n$ ;  $\mathbf{A}$  will be called the *period matrix* of  $\Lambda$ , and the mapping  $\mathbf{x} \mapsto \mathbf{A}\mathbf{x}$  will be denoted by  $A$ . According to Section 1.3.2.3.9.5 we have

$$\langle R, \varphi \rangle = \sum_{\mathbf{m} \in \mathbb{Z}^n} \varphi(\mathbf{A}\mathbf{m}) = \langle r, (\mathbf{A}^{-1})^{\#} \varphi \rangle = |\det \mathbf{A}|^{-1} \langle A^{\#} r, \varphi \rangle$$

for any  $\varphi \in \mathcal{S}$ , and hence  $R = |\det \mathbf{A}|^{-1} A^{\#} r$ . By Fourier transformation, according to Section 1.3.2.5.5,

$$\mathcal{F}[R] = |\det \mathbf{A}|^{-1} \mathcal{F}[A^{\#} r] = [(\mathbf{A}^{-1})^T]^{\#} \mathcal{F}[r] = [(\mathbf{A}^{-1})^T]^{\#} r,$$

which we write:

$$\mathcal{F}[R] = |\det \mathbf{A}|^{-1} R^*$$

with

$$R^* = |\det \mathbf{A}| [(\mathbf{A}^{-1})^T]^{\#} r.$$

$R^*$  is a lattice distribution:

$$R^* = \sum_{\boldsymbol{\mu} \in \mathbb{Z}^n} \delta_{[(\mathbf{A}^{-1})^T \boldsymbol{\mu}]} = \sum_{\boldsymbol{\xi} \in \Lambda^*} \delta_{(\boldsymbol{\xi})}$$

associated with the *reciprocal lattice*  $\Lambda^*$  whose basis vectors  $\mathbf{a}_1^*, \dots, \mathbf{a}_n^*$  are the columns of  $(\mathbf{A}^{-1})^T$ . Since the latter matrix is equal to the adjoint matrix (*i.e.* the matrix of co-factors) of  $\mathbf{A}$  divided by  $\det \mathbf{A}$ , the components of the reciprocal basis vectors can be written down explicitly (see Section 1.3.4.2.1.1 for the crystallographic case  $n = 3$ ).

A distribution  $T$  will be called  $\Lambda$ -periodic if  $\tau_{\boldsymbol{\xi}} T = T$  for all  $\boldsymbol{\xi} \in \Lambda$ ; as previously,  $T$  may be written  $R * T^0$  for some motif distribution  $T^0$  with compact support. By Fourier transformation,

$$\begin{aligned} \mathcal{F}[T] &= |\det \mathbf{A}|^{-1} R^* \cdot \mathcal{F}[T^0] \\ &= |\det \mathbf{A}|^{-1} \sum_{\boldsymbol{\xi} \in \Lambda^*} \mathcal{F}[T^0](\boldsymbol{\xi}) \delta_{(\boldsymbol{\xi})} \\ &= |\det \mathbf{A}|^{-1} \sum_{\boldsymbol{\mu} \in \mathbb{Z}^n} \mathcal{F}[T^0][(\mathbf{A}^{-1})^T \boldsymbol{\mu}] \delta_{[(\mathbf{A}^{-1})^T \boldsymbol{\mu}]} \end{aligned}$$

so that  $\mathcal{F}[T]$  is a weighted reciprocal-lattice distribution, the weight attached to node  $\boldsymbol{\xi} \in \Lambda^*$  being  $|\det \mathbf{A}|^{-1}$  times the value  $\mathcal{F}[T^0](\boldsymbol{\xi})$  of the Fourier transform of the motif  $T^0$ .

This result may be further simplified if  $T$  and its motif  $T^0$  are referred to the standard period lattice  $\mathbb{Z}^n$  by defining  $t$  and  $t^0$  so that  $T = A^{\#} t$ ,  $T^0 = A^{\#} t^0$ ,  $t = r * t^0$ . Then

$$\mathcal{F}[T^0](\boldsymbol{\xi}) = |\det \mathbf{A}| \mathcal{F}[t^0](\mathbf{A}^T \boldsymbol{\xi}),$$

hence

$$\mathcal{F}[T^0][(\mathbf{A}^{-1})^T \boldsymbol{\mu}] = |\det \mathbf{A}| \mathcal{F}[t^0](\boldsymbol{\mu}),$$

so that

$$\mathcal{F}[T] = \sum_{\boldsymbol{\mu} \in \mathbb{Z}^n} \mathcal{F}[t^0](\boldsymbol{\mu}) \delta_{[(\mathbf{A}^{-1})^T \boldsymbol{\mu}]}$$

in non-standard coordinates, while

$$\mathcal{F}[t] = \sum_{\boldsymbol{\mu} \in \mathbb{Z}^n} \mathcal{F}[t^0](\boldsymbol{\mu}) \delta_{(\boldsymbol{\mu})}$$

in standard coordinates.

The reciprocity theorem may then be written:

$$(iii) \quad W_{\boldsymbol{\xi}} = |\det \mathbf{A}|^{-1} \langle T_{\mathbf{x}}^0, \exp(-2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) \rangle, \quad \boldsymbol{\xi} \in \Lambda^*$$

$$(iv) \quad T_{\mathbf{x}} = \sum_{\boldsymbol{\xi} \in \Lambda^*} W_{\boldsymbol{\xi}} \exp(+2\pi i \boldsymbol{\xi} \cdot \mathbf{x})$$

in non-standard coordinates, or equivalently:

$$(v) \quad w_{\boldsymbol{\mu}} = \langle t_{\mathbf{x}}^0, \exp(-2\pi i \boldsymbol{\mu} \cdot \mathbf{x}) \rangle, \quad \boldsymbol{\mu} \in \mathbb{Z}^n$$

$$(vi) \quad t_{\mathbf{x}} = \sum_{\boldsymbol{\mu} \in \mathbb{Z}^n} w_{\boldsymbol{\mu}} \exp(+2\pi i \boldsymbol{\mu} \cdot \mathbf{x})$$

in standard coordinates. It gives an  $n$ -dimensional Fourier series representation for any periodic distribution over  $\mathbb{R}^n$ . The convergence of such series in  $\mathcal{S}'(\mathbb{R}^n)$  will be examined in Section 1.3.2.6.10.

1.3.2.6.6. *Duality between periodization and sampling*

Let  $T^0$  be a distribution with compact support (the ‘motif’). Its Fourier transform  $\mathcal{F}[T^0]$  is analytic (Section 1.3.2.5.4) and may thus be used as a multiplier.

We may rephrase the preceding results as follows:

(i) if  $T^0$  is ‘periodized by  $R$ ’ to give  $R * T^0$ , then  $\mathcal{F}[T^0]$  is ‘sampled by  $R^*$ ’ to give  $|\det \mathbf{A}|^{-1} R^* \cdot \mathcal{F}[T^0]$ ;

(ii) if  $\mathcal{F}[T^0]$  is ‘sampled by  $R^*$ ’ to give  $R^* \cdot \mathcal{F}[T^0]$ , then  $T^0$  is ‘periodized by  $R$ ’ to give  $|\det \mathbf{A}| R * T^0$ .

Thus the Fourier transformation establishes a duality between the periodization of a distribution by a period lattice  $\Lambda$  and the sampling of its transform at the nodes of lattice  $\Lambda^*$  reciprocal to  $\Lambda$ . This is a particular instance of the convolution theorem of Section 1.3.2.5.8.

At this point it is traditional to break the symmetry between  $\mathcal{F}$  and  $\mathcal{F}$  which distribution theory has enabled us to preserve even in the presence of periodicity, and to perform two distinct identifications:

(i) a  $\Lambda$ -periodic distribution  $T$  will be handled as a distribution  $\tilde{T}$  on  $\mathbb{R}^n/\Lambda$ , was done in Section 1.3.2.6.3;

(ii) a weighted lattice distribution  $W = \sum_{\boldsymbol{\mu} \in \mathbb{Z}^n} W_{\boldsymbol{\mu}} \delta_{[(\mathbf{A}^{-1})^T \boldsymbol{\mu}]}$  will be identified with the collection  $\{W_{\boldsymbol{\mu}} | \boldsymbol{\mu} \in \mathbb{Z}^n\}$  of its  $n$ -tuply indexed coefficients.

1.3.2.6.7. *The Poisson summation formula*

Let  $\varphi \in \mathcal{S}$ , so that  $\mathcal{F}[\varphi] \in \mathcal{S}$ . Let  $R$  be the lattice distribution associated to lattice  $\Lambda$ , with period matrix  $\mathbf{A}$ , and let  $R^*$  be associated to the reciprocal lattice  $\Lambda^*$ . Then we may write:

$$\begin{aligned} \langle R, \varphi \rangle &= \langle R, \mathcal{F}[\mathcal{F}[\varphi]] \rangle \\ &= \langle \mathcal{F}[R], \mathcal{F}[\varphi] \rangle \\ &= |\det \mathbf{A}|^{-1} \langle R^*, \mathcal{F}[\varphi] \rangle \end{aligned}$$

*i.e.*