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An algorithm for the arithmetic classification of multilattices

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A procedure for the construction and the classification of monoatomic multilattices in arbitrary dimension is developed. The algorithm allows one to determine the location of the points of all monoatomic multilattices with a given symmetry, or to determine whether two assigned multilattices are arithmetically equivalent. This approach is based on ideas from integral matrix theory, in particular the reduction to the Smith normal form, and can be coded to provide a classification software package.

1. Introduction

A monoatomic $(N+1)$-lattice is a set of points in $\mathbb{R}^n$ that is the union of $N+1$ identical Bravais lattices, and can be described by a reference (or skeletal) Bravais lattice and N shift vectors $(\mathbf{p}_\alpha)_{\alpha=1,\ldots,N}$, which represent the translations of the additional lattices with respect to the reference one. Equivalently, a monoatomic $(N+1)$-lattice can be described as a Bravais lattice with N additional identical points per unit cell (*cf. e.g.* Pitteri & Zanzotto, 2003).

The symmetry of a multilattice is determined by those point-group operations of the skeletal lattice that leave the multilattice invariant, *i.e.* that interchange the additional points modulo lattice translations (Pitteri & Zanzotto, 1998, 2000; Fadda & Zanzotto, 2000, 2001*a*). A symmetry operation of an $(N+1)$-lattice can be identified to a triple $\mathbf{R}$, (A_α^β), $(\mathbf{t}_\alpha)$ such that

$$\mathbf{R}\mathbf{p}_\alpha = \sum_{\beta=1}^{N} A_\alpha^\beta \mathbf{p}_\beta + \mathbf{t}_\alpha, \quad \alpha = 1, \ldots, N, \tag{1}$$

with $\mathbf{R}$ a point-group symmetry of the skeletal lattice, (A_α^β) an integral matrix that corresponds to the permutation action of $\mathbf{R}$ on the points of the multilattice, and $(\mathbf{t}_\alpha)$ are lattice vectors. Working in components in a skeletal lattice basis, we can equivalently rewrite equation (1) as

$$MP = PA + T, \tag{2}$$

with $M = (M_j^i)$ a unimodular integral matrix in the lattice group of the skeletal lattice, $A = (A_\alpha^\beta)$, $T = (T_\alpha^i)$ a matrix of integers representing a set of lattice translations, and $P = (P_\alpha^i)$ the matrix whose columns are the components of the shift vectors.

To each triple (M, A, T) an $(N+n)\times(N+n)$ matrix of the form

$$\begin{pmatrix} M & T \\ 0 & A \end{pmatrix} \tag{3}$$

can be associated, and it turns out that the set of all triples that satisfy equation (2) for a given set of shift vectors is a group under matrix multiplication, which is isomorphic to the space group of the multilattice, and which we refer to as the lattice group of the multilattice (Pitteri & Zanzotto, 1998).

We denote by $\Gamma_{n,N}$ the group of all matrices of the form (3) for arbitrary unimodular integral M, a linear representation of a permutation A, and an integral matrix T: two $(N+1)$-lattices are arithmetically equivalent if their lattice groups are conjugated in $\Gamma_{n,N}$. This notion of equivalence generalizes to multilattices the usual arithmetic classification of simple lattices in Bravais types (Schwarzenberger, 1972; Miller, 1972; Engel, 1986; Pitteri & Zanzotto, 1998).

We refer to (1) as the master equation of the multilattice. It can be used either to compute the shift vectors $(\mathbf{p}_\alpha)$, given the lattice group, or to compute the lattice group given the skeletal lattice and the shift vectors.

In this work we describe a procedure to solve the master equation for any given skeletal lattice. The procedure is based on ideas from integral matrix diagonalization (Smith, 1861; Newman, 1972; Gohberg *et al.*, 1982; Havas & Majewski, 1997; Dumas *et al.*, 2001; Jäger, 2005) and automatically yields a single representative for each arithmetical equivalence class of multilattices. The idea is as follows: rewriting equation (2) as a linear system of the form

$$L\widetilde{P} = 0 \bmod \mathbb{Z},$$

with L an integral matrix and $\widetilde{P}$ a suitable unknown vector, it is a well known result that L can be written in a canonical form D whose only nonzero entries are integers, are along the diagonal and are arranged in a sequence such that each element divides the next one. Using the canonical form of L, the system (2) decouples into a finite number of elementary equations with integral coefficients $D_i^i \in \mathbb{Z}$ and unknowns X_i:

$$D_i^i X_i = 0 \bmod \mathbb{Z}, \quad i = 1, \ldots, r,$$

whose solutions have the form

$$\left(\frac{k_1}{D_1^1},\ \frac{k_2}{D_2^2},\ldots,\frac{k_r}{D_r^r},\ t_{r+1},\ t_{r+2},\ldots,t_{nN}\right),$$

where $k_i \in \{0, 1, 2, \ldots, D_i^i - 1\}$ are integers and t_j are real numbers in $[0, 1)$ [*cf.* (14)]. Hence, the transformation to Smith canonical form allows all solutions of equation (2) to be constructed at the sole cost of computing the canonical form itself.

Further, as a side result, this approach yields a simple criterion for the arithmetic equivalence of two given monoatomic multilattices whose underlying skeletal lattices are arithmetically equivalent.

In conclusion, the procedure described in this paper provides a basis for an algorithm for the classification of multilattices with an arbitrary number of points, but also yields a simple method to determine regular sets of points in arbitrary dimensions. This sort of calculation is useful for instance when high-dimensional crystallography is used, *via* a projection approach, to study quasicrystals or sets of points with noncrystallographic symmetry (Indelicato, Cermelli *et al.*, 2012).

Also, arithmetic equivalence, which yields a finer classification than the classical classification according to affine equivalence classes of space groups, is an essential tool in characterizing and studying reconstructive phase transitions based on the notion of Bain strain, in which there is no symmetry reduction between the parent and product phases (for instance simple cubic and body- or face-centered cubic), but their lattice groups are not arithmetically equivalent (Indelicato, Cermelli *et al.*, 2012; Indelicato, Keef *et al.*, 2012).

In order to improve readability, we have collected all the proofs in Appendix *A*, and we have devoted the last section to a detailed discussion of two specific examples in three dimensions: the derivation of all inequivalent hexagonal 2-lattices (Fadda & Zanzotto, 2001*b*) and all inequivalent cubic 3-lattices (Hosoya, 1987). Such results could also be obtained using the Wyckoff positions of the relevant space groups, which can, in turn, be determined in any dimension (Fuksa & Engel, 1994; Eick & Souvignier, 2006), but our approach has the advantage of not requiring the computation of high-dimensional space groups, and taking into account arithmetical equivalence and site symmetry by design.

2. Multilattices and the master equation

2.1. Multilattices

$O(n)$ is the orthogonal group of $\mathbb{R}^n$, $GL(n,\mathbb{Z})$ is the group of integral $n\times n$ unimodular matrices, $\mathcal{M}(n\times N,\mathbb{R})$ and $\mathcal{M}(n\times N,\mathbb{Z})$ are the linear space and $\mathbb{Z}$-module of $n\times N$ real and integral matrices, respectively.

A *simple* (*Bravais*) *lattice* with basis $\{\mathbf{e}_i\}_{i=1,\ldots,n}\subset\mathbb{R}^n$ and origin $Q_0\in\mathbb{R}^n$ is the set of points in $\mathbb{R}^n$ defined by

$$\mathcal{L}=\mathcal{L}(Q_0,\{\mathbf{e}_i\}_{i=1,\ldots,n}):=\left\{Q_0+\sum_{i=1}^n m^i\mathbf{e}_i\in\mathbb{R}^n : m^i\in\mathbb{Z}\right\}.$$

The *point group* $\mathcal{P}$ of $\mathcal{L}$ is the group of orthogonal transformations that leave the lattice invariant:

$$\mathcal{P}=\left\{\mathbf{R}\in O(n) : \exists M=(M_i^j)\in GL(n,\mathbb{Z}) : \mathbf{R}\mathbf{e}_i=\sum_{j=1}^n M_i^j\mathbf{e}_j\right\}. \quad (4)$$

The *lattice group* $\mathcal{G}$ of $\mathcal{L}$ is the group of integral unimodular matrices M defined by (4). It follows from this definition that the lattice group is the matrix representation of the point group in the lattice basis.

Two lattices $\mathcal{L}$ and $\mathcal{L}'$ are *arithmetically equivalent* if the associated lattice groups $\mathcal{G}$ and $\mathcal{G}'$ are conjugated in $GL(n,\mathbb{Z})$, *i.e.* there exists $H\in GL(n,\mathbb{Z})$ such that

$$\mathcal{G}=H^{-1}\mathcal{G}'H.$$

Consider now a simple lattice $\mathcal{L}(Q_0,\{\mathbf{e}_i\}_{i=1,\ldots,n})$ and N points $Q_1,\ldots,Q_N$ not belonging to $\mathcal{L}$ and not pairwise equivalent modulo $\mathcal{L}$.

An $(N+1)$-lattice with basis $\{\mathbf{e}_i\}_{i=1,\ldots,n}$ is the union of $N+1$ simple lattices $\mathcal{L}(Q_\alpha,\{\mathbf{e}_i\}_{i=1,\ldots,n})$:

$$\mathcal{L}_{N+1}=\bigcup_{\alpha=0}^{N}\left\{Q_\alpha+\sum_{i=1}^n m^i\mathbf{e}_i : m^i\in\mathbb{Z}\right\}. \quad (5)$$

The position of the points $Q_1,\ldots,Q_N$ with respect to the origin of the lattice $\mathcal{L}$, called the skeletal lattice, is given by the shift vectors

$$\mathbf{p}_\alpha=Q_\alpha-Q_0,\quad \alpha=0,\ldots,N.$$

Notice that $\mathbf{p}_0=\mathbf{0}$.

The description (5) is one of many possible for a given $(N+1)$-lattice $\mathcal{L}_{N+1}$: in fact, in addition to changing the lattice basis, any relabeling of the points $(Q_0,\ldots,Q_N)$ of the form $(Q_{\sigma(0)},\ldots,Q_{\sigma(N)})$, with σ a permutation of $\{0,\ldots,N\}$, yields an equivalent description of the same point set. The shift vectors measured with respect to the new reference lattice $\mathcal{L}(Q_{\sigma(0)},\{\mathbf{e}_i\}_{i=1,\ldots,n})$ have the form

$$\hat{\mathbf{p}}_\alpha=Q_{\sigma(\alpha)}-Q_{\sigma(0)},$$

and are related to the original shift vectors by

$$\hat{\mathbf{p}}_\alpha=Q_{\sigma(\alpha)}-Q_0-(Q_{\sigma(0)}-Q_0)=\mathbf{p}_{\sigma(\alpha)}-\mathbf{p}_{\sigma(0)}.$$

2.2. Essential and non-essential description of a multilattice

The lattice vectors

$$\mathcal{T}=\left\{\sum_{i=1}^n m^i\mathbf{e}_i : m^i\in\mathbb{Z}\right\}$$

define a translation group that leaves the multilattice invariant, but this is not necessarily the maximal group of translational symmetries of (5). Consider a multilattice $\mathcal{L}_{N+1}$ as defined in (5), with lattice vectors $\mathcal{T}$: we say that the description (5) is essential if all translational symmetries of $\mathcal{L}_{N+1}$ belong to $\mathcal{T}$, *i.e.* if

$$\mathbf{t}\in\mathcal{T}\quad\Leftrightarrow\quad\mathcal{L}_{N+1}+\mathbf{t}=\mathcal{L}_{N+1}.$$

When this is not the case, the set (5) is an $(N'+1)$-lattice, with $N' < N$, and (5) is called a non-essential description of the $(N'+1)$-lattice.

A simple criterion to establish whether a description of a multilattice is non-essential is established by Parry (2004), who proved the following result:

Proposition 1. Assume that the representation (5) is non-essential. Then there exist $\mathbf{s} \in \mathbb{R}^n$ and a permutation σ of the set of $N+1$ integers $\{0, \ldots, N\}$ such that

$$\mathbf{p}_{\sigma(\alpha)} - \mathbf{p}_\alpha = \mathbf{s} \bmod \mathcal{T}, \quad \alpha = 0, \ldots, N. \tag{6}$$

When (6) holds, σ decomposes into cycles of equal length, q say, where $q \geq 2$ and $q\mathbf{s} = 0 \bmod \mathcal{T}$.

Conversely, when (6) holds for some permutation σ, the representation (5) is non-essential.

This criterion implies that, for instance, a 2-lattice with shift $\mathbf{p}$ is a simple lattice if and only if the shift is half a lattice vector of the skeletal lattice, as in the case of body-centered lattices.

2.3. The lattice group of a multilattice

Loosely speaking, the symmetry of a multilattice is described by those point-group operations of the skeletal lattice that interchange the additional points modulo lattice translations. In order to make this notion precise, we need to characterize how to express permutations of the points of a multilattice in terms of the shift vectors.

The symmetric group S_{N+1}, acting as a group of permutations on the $(N+1)$ points $Q_0, \ldots, Q_N$, also acts linearly on the $\mathbb{Z}$-module generated by the shift vectors $\{\mathbf{p}_1, \ldots, \mathbf{p}_N\}$ as follows:

$$\mathbf{p}_\alpha \longmapsto \mathbf{p}_{\sigma(\alpha)} - \mathbf{p}_{\sigma(0)}, \quad \alpha = 1, \ldots, N, \quad \sigma \in S_{N+1}.$$

We denote by $\mathcal{S}_{N+1}$ the group of matrices corresponding to this action,

$$\mathcal{S}_{N+1} = \Big\{ (A_\alpha^\beta) \in GL(N, \mathbb{Z}) : \exists \sigma \in S_{N+1} \text{ such that } \sum_{\beta=1}^{N} A_\alpha^\beta \mathbf{p}_\beta = \mathbf{p}_{\sigma(\alpha)} - \mathbf{p}_{\sigma(0)} \Big\},$$

which is isomorphic to the symmetric group S_{N+1} [*cf.* pp. 309–310 of Pitteri & Zanzotto (2003), and p. 366 of Pitteri & Zanzotto (1998)]. In general, given a finite group $\mathcal{G}$, we refer to a group morphism $\mathcal{G} \to S_{N+1}$ as a permutation representation (permrep) of $\mathcal{G}$, and to the associated map $\mathcal{G} \to \mathcal{S}_{N+1}$ as a linear permutation representation.

The symmetry of a multilattice $\mathcal{L}_{N+1}$ is described by the set of triples

$$(\mathbf{R}, (A_\alpha^\beta), (\mathbf{t}_\alpha)),$$

with $\mathbf{R} \in \mathcal{P}$ a point-group symmetry of the skeletal lattice, $(A_\alpha^\beta) \in \mathcal{S}_{N+1}$ and $\mathbf{t}_\alpha \in \mathcal{T}$ for $\alpha = 1, \ldots, N$, such that the action of the point-group operation $\mathbf{R}$ on the shift vectors corresponds to a permutation of the points $\{Q_0, \ldots, Q_N\}$ modulo translations of the lattice or, equivalently, to a change of descriptors of the multilattice. In short, $(\mathbf{R}, (A_\alpha^\beta), (\mathbf{t}_\alpha))$ is a symmetry operation of $\mathcal{L}_{N+1}$,

$$\mathbf{R}\mathbf{p}_\alpha = \sum_{\beta=1}^{N} A_\alpha^\beta \mathbf{p}_\beta + \mathbf{t}_\alpha, \quad \alpha = 1, \ldots, N. \tag{7}$$

Granted (4), and writing $\mathbf{p}_\alpha = \sum_{i=1}^n P_\alpha^i \mathbf{e}_i$ and $\mathbf{t}_\alpha = \sum_{i=1}^n T_\alpha^i \mathbf{e}_i$, with $(P_\alpha^i) \in \mathcal{M}(n \times N, \mathbb{R})$, $(T_\alpha^i) \in \mathcal{M}(n \times N, \mathbb{Z})$, we may rewrite equation (7) in the form

$$\sum_{j=1}^{n} M_j^i P_\alpha^j = \sum_{\beta=1}^{N} P_\beta^i A_\alpha^\beta + T_\alpha^i, \quad \alpha = 1, \ldots, N, \tag{8}$$

i.e. with $M = (M_j^i)$, $P = (P_\alpha^i)$, $A = (A_\alpha^\beta)$, $T = (T_\alpha^i)$,

$$MP = PA + T. \tag{9}$$

We refer to equations (8) or (9) as the *master equation*. The matrices M and A satisfying equation (9) form the symmetry group of the multilattice.

Proposition 2. Given an $(N+1)$-lattice with shifts $P \in \mathcal{M}(n \times N, \mathbb{R})$, let $\mathcal{H}$ be the subset of $GL(n, \mathbb{Z})$ of matrices M such that there exist $A \in \mathcal{S}_{N+1}$ and $T \in \mathcal{M}(n \times N, \mathbb{Z})$ that satisfy the master equation (9). Then

(i) $\mathcal{H}$ is a subgroup of the lattice group $\mathcal{G}$ of the skeletal lattice;

(ii) the map $\mathcal{H} \to \mathcal{S}_{N+1}$ mapping M to A in equation (9) defines a permutation representation of $\mathcal{H}$ on the set $\{Q_0, \ldots, Q_N\}$, such that $Q_{\sigma(\alpha)} - Q_{\sigma(0)} = \sum_{\beta=1}^N A_\alpha^\beta \mathbf{p}_\beta$.

We denote by $\Gamma_{n,N}$ the set of matrices in $GL(n+N, \mathbb{Z})$ defined by

$$\Gamma_{n,N} = \Big\{ \begin{pmatrix} H & E \\ O & B \end{pmatrix} \in GL(n+N, \mathbb{Z}) : H \in GL(n, \mathbb{Z}), E \in \mathcal{M}(n \times N, \mathbb{Z}),\ B \in \mathcal{S}_{N+1} \Big\}.$$

Proposition 2 motivates the definition of *lattice group of an* $(N+1)$*-lattice* with shift vectors P as the group of matrices $\mathcal{K} \subset \Gamma_{n,N}$ such that

$$\mathcal{K} = \Big\{ \begin{pmatrix} M & T \\ 0 & A \end{pmatrix} \in \Gamma_{n,N} : M \in \mathcal{H},\ MP = PA + T \Big\}. \tag{10}$$

The group $\mathcal{K}$ is isomorphic to the space group of the multilattice, as discussed in Pitteri & Zanzotto (1998).

Two $(N+1)$-lattices with lattice groups $\mathcal{K}$ and $\mathcal{K}'$ are *arithmetically equivalent* if $\mathcal{K}$ and $\mathcal{K}'$ are conjugated in $\Gamma_{n,N}$, *i.e.* if there exists a matrix $Q \in \Gamma_{n,N}$ such that

$$\mathcal{K}' = Q^{-1} \mathcal{K} Q.$$

Further, since $\mathcal{H}$ and $\mathcal{K}$ are finite, they admit a finite set of generators $(M^{(1)}, \ldots, M^{(K)})$ and $(G^{(1)}, \ldots, G^{(K)})$, with

$$G^{(k)} = \begin{pmatrix} M^{(k)} & T^{(k)} \\ 0 & A^{(k)} \end{pmatrix};$$

Proposition 2 allows one to conclude that if the master equation holds for each generator, then it holds for all elements of the group $\mathcal{K}$. Hence equation (9), which holds for every element of $\mathcal{K}$, can be replaced by

$$M^{(k)} P - P A^{(k)} = T^{(k)}, \quad k = 1, \ldots, K. \tag{11}$$

2.4. An example

We discuss here a two-dimensional example to show that the master equation (7) embodies the symmetries of a multilattice. Consider the monoatomic planar 3-lattice with space group $p4mm$ (Fig. 1) and square skeletal lattice: one description of this point set is obtained by letting $Q_0 = (0, 0)$, $Q_1 = (1/2, 0)$, $Q_2 = (0, 1/2)$, and choosing the shift vectors as

$$\mathbf{p}_1 = Q_1 - Q_0, \quad \mathbf{p}_2 = Q_2 - Q_0.$$

A different description arises by choosing $\hat{Q}_0 = (1/2, 0)$, $\hat{Q}_1 = (0, 0)$, $\hat{Q}_2 = (0, 1/2)$, with shift vectors

$$\hat{\mathbf{p}}_1 = \hat{Q}_1 - \hat{Q}_0 = -\mathbf{p}_{\sigma(0)}, \quad \hat{\mathbf{p}}_2 = \hat{Q}_2 - \hat{Q}_0 = \mathbf{p}_{\sigma(2)} - \mathbf{p}_{\sigma(0)},$$

with σ the transposition of 0 and 1 that fixes 2.

The point group of the planar square lattice is $4mm$, and we choose as generators of the lattice group the integral matrices

$$M^{(1)} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad M^{(2)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The generator $M^{(1)}$ fixes Q_0 and permutes Q_1 and Q_2 modulo the lattice, while the action of $M^{(2)}$ on the points Q_0, Q_1, Q_2 is lattice invariant:

$$M^{(1)}\mathbf{p}_1 = \mathbf{p}_2, \quad M^{(1)}\mathbf{p}_2 = -\mathbf{p}_1 = \mathbf{p}_1 - \mathbf{e}_1,$$

and

$$M^{(2)}\mathbf{p}_1 = \mathbf{p}_1, \quad M^{(2)}\mathbf{p}_2 = -\mathbf{p}_2 = \mathbf{p}_2 - \mathbf{e}_2,$$

where $\mathbf{e}_1 = (1, 0)$ and $\mathbf{e}_2 = (0, 1)$ are the basis vectors of the square lattice. Hence, the action of the point group of the skeletal lattice on the shifts can be written in the form (7), in terms of the matrices

$$A^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad A^{(2)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Alternatively, using the description of the multilattice in terms of the shift vectors $\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2$, we have

$$M^{(1)}\hat{\mathbf{p}}_1 = \hat{\mathbf{p}}_1 - \hat{\mathbf{p}}_2, \quad M^{(1)}\hat{\mathbf{p}}_2 = -\hat{\mathbf{p}}_2 - \mathbf{e}_1,$$

and

$$M^{(2)}\hat{\mathbf{p}}_1 = \hat{\mathbf{p}}_1, \quad M^{(2)}\hat{\mathbf{p}}_2 = \hat{\mathbf{p}}_2 - \mathbf{e}_2,$$

which now involves the matrices

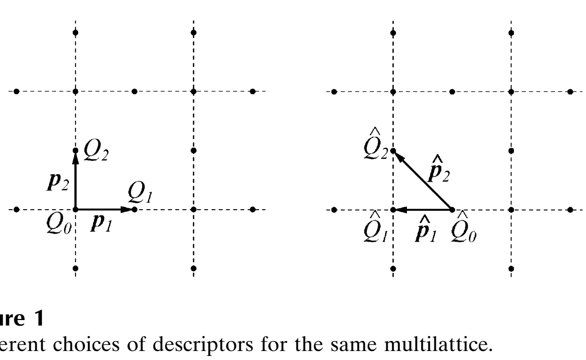

Figure 1
Different choices of descriptors for the same multilattice.

$$\hat{A}^{(1)} = \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix}, \quad \hat{A}^{(2)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

It turns out that these matrices are conjugated to $A^{(1)}$ and $A^{(2)}$ by the element of $\mathcal{S}_3$ associated with the permutation $\sigma = (01)(2)$: the two descriptions lead to different, but equivalent, forms of the master equation.

3. The master equation as a system of linear equations

The master equation is both a relation that uniquely characterizes the lattice group $\mathcal{K}$ of a multilattice, given the shift vectors $(\mathbf{p}_\alpha)$, and an equation in the unknowns $(\mathbf{p}_\alpha)$, that allows all the multilattices with a given lattice group $\mathcal{K}$ to be determined. In this section we take the latter point of view, and assume that $\mathcal{K}$, or rather $\mathcal{H}$, is given. Specifically, the problem we want to solve is:

(i) fix a simple lattice $\mathcal{L}(Q_0, \{\mathbf{e}_i\}_{i=1,\ldots,n})$ with point group $\mathcal{P}$ and lattice group $\mathcal{G}$;

(ii) choose the number N of (unknown) additional points $(Q_1, \ldots, Q_N)$ in the unit cell of the skeletal lattice;

(iii) fix a subgroup $\mathcal{H} \subset \mathcal{G}$;

(iv) choose a permutation representation $\mathcal{H} \to S_{N+1}$ that associates to each generator $M^{(k)} \in \mathcal{H}$, with $k = 1, \ldots, K$, a permutation of the points $(Q_0, \ldots, Q_N)$, and determine the resulting linear representation $\mathcal{H} \to \mathcal{S}_{N+1}$ in terms of the matrices $A^{(k)}$, recalling that the permutation representations of a finite group can be decomposed in terms of its action on the coset spaces by its maximal subgroups (Aschbacher, 2000);

(v) compute the shifts: solve the master equation (11) in the unknowns P for every $M^{(k)} \in \mathcal{H}$ and corresponding $A^{(k)} \in \mathcal{S}_{N+1}$, and for every possible $T^{(k)}$;

(vi) compare the solutions for different choices of $T^{(k)}$, and establish which are arithmetically equivalent;

(vii) decide whether the structures determined in the preceding steps are genuine $(N+1)$-lattices or non-essential descriptions of an $(N'+1)$-lattice, with $N' < N$, using the criterion in Proposition 1.

3.1. The solution procedure

The system of master equations (11), corresponding to the K generators of the lattice group $\mathcal{K}$, can be written in compact form as a linear system,

$$L\widetilde{P} = \widetilde{T}, \tag{12}$$

where the vectors $\widetilde{P} \in \mathbb{R}^{nN}$, $\widetilde{T} \in \mathbb{Z}^{nNK}$ have components obtained by ordering lexicographically the columns of P and $T^{(k)}$, and L is an integral matrix in $\mathcal{M}(nNK \times nN, \mathbb{Z})$, whose explicit form in terms of the generators of $\mathcal{K}$ is given in Appendix A2.

Consider first a diagonal system of linear equations with integral coefficients

$$DX = S, \tag{13}$$

with $D \in \mathcal{M}(l \times m, \mathbb{Z})$ $(l \geq m)$ and $D^J_i = 0$ for $J \neq i$, $X \in \mathbb{R}^m$ and $S \in \mathbb{Z}^l$, *i.e.*

$$\begin{cases} D_i^i X^i = S^i & \text{for } i \le r \\ 0 = S^i & \text{for } i > r \end{cases}$$

with[1] $r = \text{rank } D$ and D_i^i are integers. The set $\mathcal{X}$ of the m-tuples of the form

$$\mathcal{X} := \left\{ \left(\frac{k_1}{D_1^1}, \frac{k_2}{D_2^2}, \ldots, \frac{k_r}{D_r^r}, t_{r+1}, t_{r+2}, \ldots, t_m \right) \right\}, \qquad (14)$$

where $k_i \in \{0, 1, 2, \ldots, D_i^i - 1\}$ are integers and t_j are real numbers in $[0, 1)$, parametrizes all solutions of equation (13).

Proposition 3. The solutions X of equation (13) have the form $X = K + Y$, with $Y \in \mathcal{X}$ and $K \in \mathbb{Z}^m$, and, conversely, all vectors of this form are solutions.

Actually, in order to find a set of representatives of the solutions in $\mathcal{X}$, it is enough to solve equation (13) for S in the set

$$\{(S^1, \ldots, S^l) \in \mathbb{Z}^l : 0 \le S^i < D_i^i \quad \text{for} \quad i = 1, \ldots, r, \\ S^i = 0 \quad \text{for} \quad i = r+1, \ldots, l\}.$$

Consider now the full system of linear equations (12): instead of solving it for a fixed value of the right-hand side, we look for solutions for some integral vector $\widetilde{T}$, and rewrite equation (12) in the form

$$L\widetilde{P} = 0 \bmod \mathbb{Z}^{nNK}. \qquad (15)$$

Recall that L is a matrix with integral entries: it is a classical result that every such matrix can be reduced to a diagonal canonical form, the Smith canonical form (Newman, 1972; Gohberg *et al.*, 1982). Precisely, for every matrix $L \in \mathcal{M}(nNK \times nN, \mathbb{Z})$ there exist matrices $U \in GL(nNK, \mathbb{Z})$ and $V \in GL(nN, \mathbb{Z})$ such that

$$L = UDV, \quad D \in \mathcal{M}(nNK \times nN, \mathbb{Z}), \qquad (16)$$

with $D_a^I = 0$ for $I \neq a$, and D_i^i divides D_{i+1}^{i+1} if $D_{i+1}^{i+1} \neq 0$. The Smith canonical form D is unique, whereas the matrices U and V are not.

Notice that if $\widetilde{P}$ is a solution of equation (15) so also is $\widetilde{P} + \widetilde{W}$, with $\widetilde{W}$ an arbitrary integral vector. Hence, we may restrict to solutions in $[0, 1)^{nN}$ and introduce the set

$$\mathcal{Y} = \{\widetilde{P} \in [0, 1)^{nN} : \widetilde{P} = V^{-1}X - [V^{-1}X] \text{ for } X \in \mathcal{X}\}, \qquad (17)$$

where $\mathcal{X}$ is defined as in (14) with $m = nN$, V is defined in (16) and, for $W \in \mathbb{R}^{nN}$, $[W] \in \mathbb{Z}^{nN}$ is the vector whose components are the integer parts of the components of W. In other words, $\mathcal{Y}$ is the inverse image of $\mathcal{X}$ by V, translated into the unit cell of the skeletal lattice. Notice that since $\mathcal{X}$ is a set of solutions of (13), then trivially $\mathcal{Y}$ is a set of solutions of (15). It can be proved that the definition of $\mathcal{Y}$ is independent of the choice of the diagonalizing matrices U, V.

The following results characterize completely the solution set of the master equation (15).

Proposition 4. Let $L \in \mathcal{M}(nNK \times nN, \mathbb{Z})$, and D its Smith normal form, with $r = \text{rank}(D)$: then all solutions of equation (15) belong to $\mathcal{Y} \bmod \mathbb{Z}^{nN}$. More precisely, the system (15) admits $(D_1^1 D_2^2 \ldots D_r^r)$ solutions modulo $\mathbb{Z}^{nN}$, each depending on $nN - r$ real parameters, and these are given by

$$\widetilde{P} = V^{-1}X - \left[V^{-1}X\right], \; X = \left(\frac{k_1}{D_1^1}, \frac{k_2}{D_2^2}, \ldots, \frac{k_r}{D_r^r}, t_1, \ldots, t_{nN-r} \right),$$

with V such that $L = UDV$ [with $U \in GL(nNK, \mathbb{Z})$ and $V \in GL(nN, \mathbb{Z})$] and

$$k_i \in \{0, 1, \ldots, D_i^i - 1\}, \quad t_j \in [0, 1).$$

By construction, the matrix L only depends on the group $\mathcal{H}$ and its permutation representation $\mathcal{H} \to \mathcal{S}_{N+1}$. Every solution $\widetilde{P}$ of the master equation (15) defines a (possibly non-essential) $(N+1)$-lattice with lattice group $\mathcal{K}$, as defined in equation (10), where the translation matrix $\widetilde{T}$ is computed from $\widetilde{T} := L\widetilde{P}$.

The question arises naturally as to whether two solutions of the same master equation correspond to arithmetically equivalent multilattices. We shall discuss this topic in the following section.

4. Arithmetic equivalence

The main result in this section shows that two equivalent multilattices have the same Smith normal form, and provides a criterion to establish when two multilattices are equivalent.

Consider two equivalent $(N+1)$-lattices. By definition, their lattice groups $\mathcal{K}$ and $\mathcal{K}'$ are conjugated by some

$$Q = \begin{pmatrix} H & R \\ 0 & B \end{pmatrix} \in \Gamma_{n,N}. \qquad (18)$$

In particular, the associated subgroups $\mathcal{H}$ and $\mathcal{H}'$ of the lattice group of the skeletal lattice, as well as their permutation representations in $\mathcal{S}_{N+1}$, are conjugated by H and B, respectively. To simplify, we choose the generators

$$G^{(k)} = \begin{pmatrix} M^{(k)} & T^{(k)} \\ 0 & A^{(k)} \end{pmatrix}, \quad G'^{(k)} = \begin{pmatrix} M'^{(k)} & T'^{(k)} \\ 0 & A'^{(k)} \end{pmatrix}, \\ k = 1, \ldots, K,$$

of $\mathcal{K}$ and $\mathcal{K}'$ to be pairwise conjugate, which implies in turn that

$$M'^{(k)} = H^{-1}M^{(k)}H \text{ and } A'^{(k)} = B^{-1}A^{(k)}B \qquad (19)$$

for every $k = 1, \ldots, K$.

We write the master equations corresponding to each multilattice as in equation (12),

$$L\widetilde{P} = \widetilde{T}, \quad L'\widetilde{P}' = \widetilde{T}', \qquad (20)$$

with Smith canonical form

$$DX = S, \quad D'X' = S'. \qquad (21)$$

Finally, for a given square matrix $W \in \mathcal{M}(nN \times nN, \mathbb{Z})$, we denote by $W_K \in \mathcal{M}(nNK \times nNK, \mathbb{Z})$ the square matrix of the form

[1] $S^{r+1}, \ldots, S^l$ must be zero in order that equation (13) has solutions.

$$W_K = \left.\begin{pmatrix} W & 0 & \dots & 0 \\ 0 & W & \dots & 0 \\ 0 & \dots & \dots & 0 \\ 0 & 0 & \dots & W \end{pmatrix}\right\} K \text{ times.}$$

Proposition 5. For two equivalent $(N+1)$-lattices, L and L' satisfy the relation

$$L' = W_K^{-1} L W,$$

where $W \in GL(nN, \mathbb{Z})$ is the integral matrix associated with the conjugating matrices H and B in (19) through the relation (36) in Appendix A. As a consequence, the matrices L and L' in equation (20) have the same Smith normal form

$$D' = D. \qquad (22)$$

Further, the vectors $S, S' \in \mathbb{Z}^{nNK}$ in equation (21) are related through

$$S' = U'^{-1} W_K^{-1} U S + D' Z, \qquad (23)$$

with $U, U' \in GL(nNK, \mathbb{Z})$ are such that $L = UDV$ and $L' = U'D'V'$, and $Z \in \mathbb{Z}^{nN}$ is a vector of integers.

Conversely, given two non-necessarily equivalent $(N+1)$-lattices, assume that the groups $\mathcal{H}$ and $\mathcal{H}'$ defined in Proposition 2, as well as their permutation representations in $\mathcal{S}_{N+1}$, are conjugated, *i.e.* there exists $H \in GL(n, \mathbb{Z})$ and $B \in \mathcal{S}_{N+1}$ such that equation (19) holds for some set of generators, and therefore (22) holds. If there exists an integral vector $Z \in \mathbb{Z}^{nN}$ such that (23) holds, then the two multilattices are equivalent.

Notice that, as we will see below, there exist multilattices for which (23) is not true, that have the same associated Smith normal form but are not equivalent.

The above result allows one, among other things, to classify the inequivalent solutions of the master equation, as shown by the following corollary. Consider to this purpose a group $\mathcal{H} \subset GL(n, \mathbb{Z})$ with generators $\{M^{(1)}, \dots, M^{(K)}\}$, and a permutation representation $\mathcal{H} \to \mathcal{S}_{N+1}$, and write $\{A^{(1)}, \dots, A^{(K)}\}$ for the images of the generators of $\mathcal{H}$. Let L be the integral $nNK \times nN$ matrix associated with these generators, and let $D = U^{-1} L V^{-1}$ be its Smith normal form.

Corollary 1. Under the above hypotheses, consider two solutions X and X' of the master equation in diagonal form $DX = 0 \bmod \mathbb{Z}^{nN}$, and let $S = DX$, $S' = DX'$. Then the corresponding multilattices are arithmetically equivalent if and only if there exists an integral vector $Z \in \mathbb{Z}^{nNK}$ such that

$$S' = U^{-1} W_K^{-1} U S + DZ,$$

where $W_K \in GL(nNK, \mathbb{Z})$ is the integral matrix associated with the conjugating matrices H and B through the relation (36), with $H \in GL(n, \mathbb{Z})$, $B \in \mathcal{S}_{N+1}$ elements of the centralizers of $\mathcal{H}$ and its permutation representation, respectively, *i.e.*

$$H^{-1} M^{(i)} H = M^{(i)}, \quad B^{-1} A^{(i)} B = A^{(i)},$$

for every $i = 1, \dots K$.

The above criterion for arithmetic equivalence could also be formulated in terms of the integral matrices T and T', but we find it easier to use it in this form, as the subsequent examples show.

5. Applications: construction of all inequivalent multilattices with a given point group

The procedure discussed in the previous sections can help to solve a classical problem of the arithmetic classification of multilattices, namely how to generate all arithmetic equivalence classes of $(N+1)$-lattices with a given point group. Notice that the algorithm in §3 involves the lattice group of the skeletal lattice, instead of its point group: this is necessarily so since two skeletal lattices with the same point group could be arithmetically inequivalent, and have therefore lattice groups that are not conjugated in $GL(n, \mathbb{Z})$, as is the case for the three cubic lattices in three-dimensions (primitive, face centered and body centered).

5.1. First example: 2-lattices with hexagonal point group in three dimensions

We show how to obtain all inequivalent 2-lattices with hexagonal point group $6/mmm$ and space groups $P6_3/mmc$ and $P6/mmm$ (Nos. 194 and 191 in *International Tables for Crystallography* Volume A). These structures are listed as 6, 27 and 28 in Fadda & Zanzotto (2001*b*).

In this case $n = 3$, $N = 1$ and $K = 3$. The hexagonal Bravais lattice has the point group $\mathcal{P} = 6/mmm$: there is only a single arithmetic class in this case, and the corresponding lattice group $\mathcal{G}$ is the matrix representation of the point group in the lattice basis. Using the conventional choices for the lattice basis given in *International Tables for Crystallography* Volume A (Hahn, 2005), we choose as generators of $\mathcal{G}$ the integral matrices (Fadda & Zanzotto, 2001*b*)

$$M^{(1)} = \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad M^{(2)} = \begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

together with the inversion, denoted here as $M^{(3)}$. In this case, all possible representations of $6/mmm$ as a permutation group on 2 elements result by associating to each generator $M^{(i)}$ either the identity permutation or the transposition, corresponding to $A^{(i)} = 1$ or $A^{(i)} = -1$, respectively.

We describe below only the two cases that yield non-trivial results.

(i) $A^{(1)} = A^{(2)} = -A^{(3)} = 1$: the master equation is

$$M^{(1)} P = P + T^{(1)}, \quad M^{(2)} P = P + T^{(2)}, \quad M^{(3)} P = -P + T^{(3)},$$

and since $M^{(3)}$ is the inversion, the third equation is identically satisfied and can be neglected. The matrix L corresponding to the first two equations, and its Smith normal form are

$$L = \begin{pmatrix} -2 & 1 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & -2 \\ -2 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 6 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

with

$$V = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 3 & -2 \\ 0 & -1 & 1 \end{pmatrix}, \quad U = \begin{pmatrix} -2 & 3 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & -1 & 0 & 0 & 0 \\ -2 & 3 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

The diagonal system $DX = 0 \bmod \mathbb{Z}^6$ has five nontrivial distinct solutions

$$X_i = (0, 0, i/6), \quad i = 1, \ldots, 5,$$

and the corresponding shift vectors (components in the hexagonal basis) are

$$\mathbf{p}^1 = (2/3, 1/3, 1/2), \quad \mathbf{p}^2 = (1/3, 2/3, 0), \quad \mathbf{p}^3 = (0, 0, 1/2),$$
$$\mathbf{p}^4 = (2/3, 1/3, 0), \quad \mathbf{p}^5 = (1/3, 2/3, 1/2).$$

The translation vectors S_i are

$$S_i = (0, 0, i, 0, 0, 0), \quad i = 1, \ldots, 5.$$

To establish which of these solutions are mutually equivalent, we can now apply Corollary 1. The integral centralizers $H \in GL(3, \mathbb{Z})$ of the lattice group are defined by

$$M^{(1)}H = HM^{(1)}, \quad M^{(2)}H = HM^{(2)},$$

and those of its permreps are the integers B such that $BA^{(1)}B = A^{(1)}$ and $BA^{(2)}B = A^{(2)}$, *i.e.* $B = \pm 1$. A direct calculation shows that H must have the form

$$H = \pm \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \pm \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Now, S_1 and S_5 satisfy equation (23), *i.e.*

$$S_1 = U^{-1} \widetilde{W}_K^{-1} U S_5 + DZ,$$

with $B = -1$ and $H = I_3$ the identity in $\mathbb{R}^3$, which implies that $\widetilde{W}_K = -I_6$ is the inversion in $\mathbb{R}^6$. In fact, for this choice (23) reduces to

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = - \begin{pmatrix} 0 \\ 0 \\ 5 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 6 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \\ m_5 \\ m_6 \end{pmatrix}$$

with m_i integers, which is satisfied by $Z = (0, 0, 1, 0, 0, 0)$.

The same argument shows that

$$S_2 = U^{-1} \widetilde{W}_K^{-1} U S_4 + DZ,$$

with the same H, B and Z as before. It is possible to check that equation (23) cannot hold for other choices of the centralizers. Hence we conclude that the 2-lattices with shifts $\mathbf{p}^1$ and $\mathbf{p}^5$ are arithmetically equivalent, as are those with shifts $\mathbf{p}^2$ and $\mathbf{p}^4$. However, $\mathbf{p}^1$ and $\mathbf{p}^2$ are not equivalent.

Finally, we notice that the structure corresponding to the shift $\mathbf{p}^3$ is not a 2-lattice, but a non-essential description of the hexagonal Bravais lattice with half-vertical lattice parameter. This follows from Parry's criterion Proposition 1 applied to 2-lattices.

(ii) $-A^{(1)} = A^{(2)} = -A^{(3)} = 1$: the master equation is

$$M^{(1)}P = -P + T^{(1)}, \; M^{(2)}P = P + T^{(2)}, \; M^{(3)}P = -P + T^{(3)},$$

and, as before, the third equation is identically satisfied and can be neglected. The matrix L corresponding to the first two equations, and its Smith normal form are ($V = I_3$ and U are omitted here)

$$L = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The diagonal system $DX = 0 \bmod \mathbb{Z}^6$ has infinite nontrivial solutions

$$X = (0, 0, t), \quad t \in [0, 1),$$

and the corresponding shift vectors in the hexagonal basis are

$$\mathbf{p}^6 = (0, 0, t), \quad t \in [0, 1).$$

The 2-lattice corresponding to this shift vector is not arithmetically equivalent to those determined previously, because the permutation representations of the hexagonal point group are not equivalent. We conclude that the 2-lattices with shift vectors (components in the hexagonal basis)

$$\mathbf{p}^1 = (2/3, 1/3, 1/2), \quad \mathbf{p}^4 = (2/3, 1/3, 0),$$
$$\mathbf{p}^6 = (0, 0, t), \quad t \in [0, 1),$$

i.e. the structures 26, 27 and 28 in Fadda & Zanzotto (2001*b*), are the only inequivalent monoatomic 2-lattices with hexagonal skeletal lattice and point group the holohedry $6/mmm$.

These 2-lattices can also be found by placing points at equivalent Wyckoff positions of multiplicity 2 of the corresponding space groups. Consider first $P6/mmm$: it has three Wyckoff positions with multiplicity 2:

$$2c = \{Q_0 = (2/3, 1/3, 0), \; Q_1 = (1/3, 2/3, 0)\},$$
$$2d = \{Q_0 = (2/3, 1/3, 1/2), \; Q_1 = (1/3, 2/3, 1/2)\},$$
$$2e = \{Q_0 = (0, 0, -t), \; Q_1 = (0, 0, t)\}.$$

Letting $\mathbf{p} = Q_1 - Q_0$ modulo lattice translations, the corresponding shift vectors are

$$2c, 2d : \mathbf{p}^4 = (2/3, 1/3, 0), \quad 2e : \mathbf{p}^6 = (0, 0, t).$$

Notice that the Wyckoff positions $2c$ and $2d$ yield the same 2-lattice: this is because they are equivalent under the affine normalizer of $P6/mmm$, whose only non-trivial coset representative is a translation.

Consider now $P6_3/mmc$: it has four Wyckoff positions with multiplicity 2:

$$2a = \{Q_0 = (0, 0, 0), Q_1 = (0, 0, 1/2)\},$$
$$2b = \{Q_0 = (0, 0, 1/4), Q_1 = (0, 0, 3/4)\},$$
$$2c = \{Q_0 = (2/3, 1/3, 3/4), Q_1 = (1/3, 2/3, 1/4)\},$$
$$2d = \{Q_0 = (2/3, 1/3, 1/4), Q_1 = (1/3, 2/3, 3/4)\}.$$

The corresponding shift vectors are, with the same conventions as above

$$2a, 2b : \mathbf{p}^3 = (0, 0, 1/2), \quad 2c, 2d : \mathbf{p}^1 = (1/3, 2/3, 1/2),$$

which are exactly the same solutions found by our algorithm.

5.2. Second example: 3-lattices with cubic point group in three dimensions

We discuss here an application to 3-lattices, showing how to obtain the structures with three identical atoms per unit cell and cubic symmetry listed by Hosoya (1987), p. 16, corresponding to the space groups $Pm\overline{3}m$, $Fm\overline{3}m$ and $Im\overline{3}m$ (Nos. 221, 225 and 229, respectively, in *International Tables for Crystallography* Volume *A*). According to the classification of Hosoya, such structures belong to genus A_3 (three identical atoms per unit cell).

The work can be organized following the steps listed in §3, with $n = 3$ and $N = 2$: fix one of the three cubic lattices in $\mathbb{R}^3$, consider its lattice group, which is conjugate to the cubic point group O_h, determine all its permutation representations, write the master equation and solve it with the techniques described in the paper.

As a first step we compute all permutation representations of O_h, recalling that they can be determined in terms of its actions on the coset spaces O_h/H, with H a maximal subgroup (Aschbacher, 2000).

Since we are interested in permutation representations on sets of three objects, we only need to consider subgroups of O_h of index less or equal to three, namely D_{4h} (index 3), T_d (index 2), T_h (index 2) and O (index 2).

We use here a presentation of O_h in terms of five generators ($K = 5$):

$$M^{(1)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad M^{(2)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$
$$M^{(3)} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \qquad M^{(4)} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$
$$M^{(5)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The permutation representations corresponding to the maximal subgroups of O_h are

(*a*) D_{4h} (index 3): the permutations corresponding to $M^{(1)}$, $M^{(2)}$, $M^{(3)}$, $M^{(4)}$, $M^{(5)}$ are $\sigma_1 = \sigma_2 = \sigma_5 = (1)(2)(3)$, $\sigma_3 = (123)$, $\sigma_4 = (1)(23)$, with two-dimensional linear representations

$$A^{(1)} = A^{(2)} = A^{(5)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; A^{(3)} = \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix},$$
$$A^{(4)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

(*b*) T_h (index 2): the permutations on two objects corresponding to $M^{(1)}$, $M^{(2)}$, $M^{(3)}$, $M^{(4)}$, $M^{(5)}$ are $\tau_1 = \tau_2 = \tau_3 = \tau_5 = (1)(2)$, $\tau_4 = (12)$, which can be extended to permutations on three objects (modulo conjugation in S_3) as follows: $\sigma_1 = \sigma_2 = \sigma_3 = \sigma_5 = (1)(2)(3)$, $\sigma_4 = (1)(23)$, with two-dimensional linear representations

$$A^{(1)} = A^{(2)} = A^{(3)} = A^{(5)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A^{(4)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

(*c*) T_d (index 2): the permutations on two objects corresponding to $M^{(1)}$, $M^{(2)}$, $M^{(3)}$, $M^{(4)}$, $M^{(5)}$ are $\tau_1 = \tau_2 = \tau_3 = (1)(2)$, $\tau_4 = \tau_5 = (12)$, which can be extended to permutations on three objects (modulo conjugation in S_3) as follows: $\sigma_1 = \sigma_2 = \sigma_3 = (1)(2)(3)$, $\sigma_4 = \sigma_5 = (1)(23)$, with two-dimensional linear representations

$$A^{(1)} = A^{(2)} = A^{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A^{(4)} = A^{(5)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

(*d*) O (index 2): the permutations on two objects corresponding to $M^{(1)}$, $M^{(2)}$, $M^{(3)}$, $M^{(4)}$, $M^{(5)}$ are $\tau_1 = \tau_2 = \tau_3 = \tau_4 = (1)(2)$, $\tau_5 = (12)$, which can be extended to permutations on three objects (modulo conjugation in S_3) as follows: $\sigma_1 = \sigma_2 = \sigma_3 = \sigma_4 = (1)(2)(3)$, $\sigma_5 = (1)(23)$, with two-dimensional linear representations

$$A^{(1)} = A^{(2)} = A^{(3)} = A^{(4)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A^{(5)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

We now turn to the actual solution procedure.

(i) Consider first the primitive cubic lattice. According to the definition following (4), its lattice group is the matrix representation of the point group in the lattice basis, in this case the canonical basis. Its generators are therefore the matrices $M^{(1)}, \ldots, M^{(5)}$ above. Solving the master equation for each of the four permreps we find only one non-trivial solution corresponding to two shift vectors [permrep (*a*)]:

$$\mathbf{p}_1 = (1/2, 1/2, 0), \quad \mathbf{p}_2 = (1/2, 0, 1/2).$$

The corresponding 3-lattice is $\{\mathbb{Z}^3\} \cup \{\mathbf{p}_1 + \mathbb{Z}^3\} \cup \{\mathbf{p}_2 + \mathbb{Z}^3\}$, *i.e.*

$$\{(0, 0, 0) + \mathbb{Z}^3\} \cup \{(1/2, 1/2, 0) + \mathbb{Z}^3\} \cup \{(1/2, 0, 1/2) + \mathbb{Z}^3\}.$$

This coincides with the 3-lattice with space group $Pm\overline{3}m$ given by Hosoya (1987). In that work the positions of the three atoms in the conventional cubic unit cell are given in terms of the Wyckoff positions of $Pm\overline{3}m$ with multiplicity 3, in this case 3*c* and 3*d*, which are equivalent under the normalizer of $Pm\overline{3}m$. Since the only non-trivial coset representative of the normalizer is a translation, they correspond to the same multilattice. The points are located at the center of the faces of the conventional cubic unit cell, all other points of the structure being obtained by a translation of the simple cubic lattice. Using an orthogonal coordinate system such that the cubic lattice is $\mathbb{Z}^3$, this set of points has the representation

$$\{(0, 1/2, 1/2) + \mathbb{Z}^3\} \cup \{(1/2, 0, 1/2) + \mathbb{Z}^3\} \cup \{(1/2, 1/2, 0) + \mathbb{Z}^3\}.$$

This structure coincides with the one found by our procedure translated by the vector $(0, 1/2, 1/2)$.

(ii) Consider now the face-centered cubic (FCC) lattice. The generators of its lattice group are the integral matrices $B_{\rm FCC}^{-1}M^{(1)}B_{\rm FCC}, \ldots, B_{\rm FCC}^{-1}M^{(5)}B_{\rm FCC}$, with

$$B_{\rm FCC} = \begin{pmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1/2 & 1/2 \end{pmatrix}.$$

Solving the master equation for all possible permreps we find only one nontrivial solution [permrep (c)] with shift vectors, expressed in components in the standard cubic basis,

$$\mathbf{p}_1 = (1/4, 1/4, 1/4), \quad \mathbf{p}_2 = (3/4, 3/4, 3/4),$$

and the corresponding 3-lattice has the form

$$\{(0, 0, 0) + \mathcal{L}_{\rm FCC}\} \cup \{(1/4, 1/4, 1/4) + \mathcal{L}_{\rm FCC}\} \cup \{(3/4, 3/4, 3/4) + \mathcal{L}_{\rm FCC}\},$$

with

$$\mathcal{L}_{FCC} = \{m^1(1/2, 1/2, 0) + m^2(1/2, 0, 1/2) + m^3(0, 1/2, 1/2), (m^1, m^2, m^3) \in \mathbb{Z}^3\}.$$

This result coincides with the 3-lattice with space group $Fm\bar{3}m$ in Hosoya (1987). According to Hosoya, the atoms are located at the Wyckoff positions 4a and 8c, *i.e.* using as before an orthogonal coordinate system corresponding to the conventional cubic unit cell, one atom at the origin of the conventional unit cell (position 4a), and two atoms at $(1/4, 1/4, 1/4)$ and $(1/4, 1/4, 3/4)$ (positions 8c), all other atoms being obtained by translations of the FCC lattice. This structure has the representation

$$\{(0, 0, 0) + \mathcal{L}_{\rm FCC}\} \cup \{(1/4, 1/4, 1/4) + \mathcal{L}_{\rm FCC}\} \cup \{(1/4, 1/4, 3/4) + \mathcal{L}_{\rm FCC}\},$$

and is the same as ours.

(iii) Consider finally the body-centered cubic (BCC) lattice. The generators of its lattice group are the integral matrices $B_{\rm BCC}^{-1}M^{(1)}B_{\rm BCC}, \ldots, B_{\rm BCC}^{-1}M^{(5)}B_{\rm BCC}$, with

$$B_{\rm BCC} = \begin{pmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{pmatrix}.$$

Solving the master equation for all possible permreps we find only one nontrivial solution [permrep (a)] with shifts, expressed in components in the standard cubic basis,

$$\mathbf{p}_1 = (0, 1/2, 0), \quad \mathbf{p}_2 = (1/2, 0, 0).$$

The resulting 3-lattice has the representation

$$\{(0, 0, 0) + \mathcal{L}_{\rm BCC}\} \cup \{(1/2, 0, 0) + \mathcal{L}_{\rm BCC}\} \cup \{(0, 1/2, 0) + \mathcal{L}_{\rm BCC}\},$$

with

$$\mathcal{L}_{\rm BCC} = \{m^1(1/2, 1/2, 1/2) + m^2(-1/2, 1/2, 1/2) + m^3(1/2, 1/2, -1/2), (m^1, m^2, m^3) \in \mathbb{Z}^3\}.$$

This result coincides with the 3-lattice with space group $Im\bar{3}m$ in Hosoya (1987). According to this work, the atoms are located at the Wyckoff positions 6b, *i.e.* at the face centers of the conventional unit cell, all other points being obtained by translation of the BCC lattice. This structure has the representation

$$\{(1/2, 1/2, 0) + \mathcal{L}_{\rm BCC}\} \cup \{(1/2, 0, 1/2) + \mathcal{L}_{\rm BCC}\} \cup \{(0, 1/2, 1/2) + \mathcal{L}_{\rm BCC}\}.$$

To see that this and our structure are equivalent, it is enough to apply the translation $(0, 0, 1/2)$.

6. Conclusions

Monoatomic multilattices are periodic structures that generalize simple lattices in any dimension. Their study is important not only for materials science, but also to provide a general description of those quasiperiodic structures that can be obtained by projection of regular sets of points from high- to low-dimensional spaces, *via*, for instance, the well known cut-and-project scheme for quasicrystals.

A first fundamental problem is to establish whether two multilattices are equivalent in some sense, as well as to determine all multilattices that belong to a given equivalence class. In this context, it has been proved that, in analogy to simple lattices, arithmetic equivalence is strictly finer than affine equivalence (Pitteri & Zanzotto, 1998). Hence, we focus here on arithmetic equivalence.

We approach the problem *via* the so-called master equation (1), that either characterizes all monoatomic multilattices with a given symmetry or can be used to establish the symmetry group of a given multilattice. By reducing the master equation to a suitable normal form, *i.e.* the Smith normal form, it is possible to enumerate all solutions, and determine easily which of these solutions are arithmetically equivalent using the criterion in Proposition 1, which only involves the characterization of the centralizer of a finite crystallographic group. Since the centralizers of the crystallographic groups in any dimension are finite or finitely generated, this procedure yields an algorithm which, in principle, can be coded and yields a solution to the arithmetic classification problem for multilattices.

In order to elucidate the basic features of our method, we discuss two examples from the literature, recovering in a few steps some relevant cubic and hexagonal 2- and 3-lattices in three dimensions.

APPENDIX *A*
Proofs

A1. Proof of Proposition 2

By hypothesis, if $M, H \in \mathcal{H}$, there exist $A_M, A_H \in \mathcal{S}_{N+1}$ and T_M, T_H integral matrices such that

$$MP = PA_M + T_M, \quad HP = PA_H + T_H.$$

Hence

$$(MH)P = M(PA_H + T_H) = (PA_M + T_M)A_H + MT_H \\ = P(A_M A_H) + (T_M A_H + MT_H).$$

Further, by multiplying $MP = PA_M + T_M$ to the left by M^{-1} and to the right by A_M^{-1}, we find

$$M^{-1}P = PA_M^{-1} - M^{-1}T_M A_M^{-1}.$$

Hence, since $T_M A_H + MT_H$ and $M^{-1}T_M A_M^{-1}$ are matrices of integers, MH and M^{-1} satisfy the master equation, and $\mathcal{H}$ is a group. Further, the mapping $M \longmapsto A_M \in \mathcal{S}_{N+1}$ is single-valued. In fact, noting first that it is implicit in the hypothesis that the shift vectors P provide an essential description of the multilattice, assume that there exists $A \neq I_N$ such that $P = PA + T$, *i.e.* $I_n \longmapsto A \neq I_N$, where I_n and I_N are the identity in $GL(n, \mathbb{Z})$ and $GL(N, \mathbb{Z})$, respectively. Explicitly, this means that

$$\mathbf{p}_{\sigma(\alpha)} - \mathbf{p}_\alpha = \mathbf{p}_{\sigma(0)} \bmod \mathcal{T}, \quad \alpha = 1, \ldots, N,$$

with σ the permutation corresponding to A, and this, by Proposition 1, implies that the description is non-essential, which is a contradiction. Hence, the map $M \longmapsto A_M \in \mathcal{S}_{N+1}$ is a group morphism, and $A_{MH} = A_M A_H$. Finally, the above argument shows that the map

$$M \longmapsto \begin{pmatrix} M & T_M \\ 0 & A_M \end{pmatrix} \in \Gamma_{n,N}$$

is also a group morphism, so that $\mathcal{K}$ is also a group.

A2. The master equation as a linear system: §3.1

The master equation (8) for a fixed element

$$G = \begin{pmatrix} M & T \\ 0 & A \end{pmatrix} \in \mathcal{K}$$

can be rewritten as a conventional system of linear equations. To do so, given $\alpha \in \{1, \ldots, N\}$ and $i \in \{1, \ldots, n\}$, define

$$a = i + (\alpha - 1)n, \tag{24}$$

so that a takes values in $\{1, \ldots, nN\}$. Conversely, let $a = 1, \ldots, nN$ and define α and i through the identities

$$\alpha = \left[\frac{a-1}{n}\right] + 1, \quad i = a - (\alpha - 1)n, \tag{25}$$

where $[\cdot]$ denotes the integer part of its argument. As a varies in $\{1, \ldots, nN\}$, then α and i take values in $\{1, \ldots, N\}$ and $\{1, \ldots, n\}$, respectively, and the relation between a and the pair (α, i) is bijective. Let

$$L_b^a := \delta_\alpha^\beta M_j^i - \delta_j^i A_\alpha^\beta,$$

i.e.

$$L = \left.\begin{pmatrix} M - A_1^1 I_n & \ldots & \ldots & -A_1^N I_n \\ -A_2^1 I_n & \ldots & \ldots & -A_2^1 I_n \\ \ldots & \ldots & \ldots & \ldots \\ -A_N^1 I_n & \ldots & \ldots & M - A_N^N I_n \end{pmatrix}\right\} Nn$$

with I_n the identity matrix in $\mathbb{R}^n$, and

$$\widetilde{P}^b := P_\beta^j, \quad \widetilde{T}^a := T_\alpha^i, \tag{26}$$

where α, i are defined as in equation (25) and, for $b \in \{1, \ldots, nN\}$

$$\beta = \left[\frac{b-1}{n}\right] + 1, \quad j = b - (\beta - 1)n, \tag{27}$$

with δ_α^β and δ_j^i Kronecker deltas. The nN-dimensional vector $(\widetilde{P}^b)$ has components that are obtained by ordering the vectors $\mathbf{p}_\alpha$.

In terms of the vectors $\widetilde{P}$ and $\widetilde{T}$ and the matrix L, the master equation (8) takes the form

$$\sum_{b=1}^{nN} L_b^a \widetilde{P}^b = \widetilde{T}^a. \tag{28}$$

The above assertion follows from a simple argument: let $\widetilde{Y}^b := Y_\beta^j$ and $\widetilde{Z}_b := Z_j^\beta$, with $b = 1, \ldots, nN$, $j = 1, \ldots, n$ and $\beta = 1, \ldots, N$ consistent with the indexing rule (27). Then

$$\begin{aligned} \sum_{b=1}^{nN} \widetilde{Y}^b \widetilde{Z}_b &= \widetilde{Y}^1 \widetilde{Z}_1 + \ldots + \widetilde{Y}^n \widetilde{Z}_n + \widetilde{Y}^{1+(2-1)n} \widetilde{Z}_{1+(2-1)n} \\ &\quad + \ldots + \widetilde{Y}^{n+(2-1)n} \widetilde{Z}_{n+(2-1)n} + \ldots \\ &\quad + \widetilde{Y}^{1+(N-1)n} \widetilde{Z}_{1+(N-1)n} + \ldots + \widetilde{Y}^{n+(N-1)n} \widetilde{Z}_{n+(N-1)n} \\ &= Y_1^1 Z_1^1 + \ldots + Y_1^n Z_n^1 + Y_2^1 Z_1^2 + \ldots + Y_2^n Z_n^2 + \ldots \\ &\quad + Y_N^1 Z_1^N + \ldots + Y_N^n Z_n^N \\ &= \sum_{\beta=1}^{N} \sum_{j=1}^{n} Y_\beta^j Z_j^\beta. \end{aligned}$$

Hence

$$\sum_{j=1}^{n} M_j^i P_\alpha^j - \sum_{\beta=1}^{N} P_\beta^i A_\alpha^\beta = \sum_{\beta=1}^{N} \sum_{j=1}^{n} (M_j^i \delta_\alpha^\beta - \delta_j^i A_\alpha^\beta) P_\beta^j = \sum_{b=1}^{nN} L_b^a \widetilde{P}^b.$$

Consider now the system of master equations (11) for the full set of generators of $\mathcal{K}$, *i.e.*

$$\sum_{j=1}^{n} M_j^{(k)i} P_\alpha^j - \sum_{\beta=1}^{N} P_\beta^i A_\alpha^{(k)\beta} = T_\alpha^{(k)i}, \quad k = 1, \ldots, K,$$

with K the number of generators of $\mathcal{K}$. The associated system of linear equations (28) is now replaced by a system of the form

$$\sum_{b=1}^{nN} L_b^J \widetilde{P}^b = \widetilde{T}^J, \tag{29}$$

with

$$L_b^J := \delta_\alpha^\beta M_j^{(k)i} - \delta_j^i A_\alpha^{(k)\beta}, \quad \widetilde{P}^b = P_\beta^j, \quad \widetilde{T}^J = T_\alpha^{(k)i}, \tag{30}$$

with $J = 1, \ldots, nNK$ given by

$$J = i + (k-1)nN + (\alpha - 1)n, \tag{31}$$

with inverse

$$\begin{cases} k = \left[\dfrac{J-1}{nN}\right] + 1, \\ \alpha = \left[\dfrac{J-(k-1)nN-1}{n}\right] + 1, \\ i = J - (k-1)nN - (\alpha-1)n, \end{cases}$$

and the relations between b, β and j are as in equation (27).

A3. Proof of Proposition 3

Given $S \in \mathbb{Z}^r \times \{0\}^{l-r}$, then for all $i = 1, \ldots, r$ there exist $K_i \in \mathbb{Z}$ and $C^i \in \{0, 1, \ldots, D^i_i - 1\}$ such that

$$S^i = D^i_i K_i + C^i.$$

Then $D^i_i X^i = D^i_i K_i + C^i$ and, as a consequence, $X^i = K^i + Y^i$ with $Y^i = C^i/D^i$, for $i = 1, \ldots, r$, and the statement is proved.

A4. Proof of Proposition 4

The general procedure to solve equation (15) is as follows: let

$$X^a = \sum_{b=1}^{nN} V^a_b \widetilde{P}^b,$$

so that, since $(U^I_J) \in GL(nNK, \mathbb{Z})$, the system (15) can be written in the form

$$\sum_{a=1}^{nN} D^J_a X^a = 0 \operatorname{mod} \mathbb{Z}^{nNK}, \tag{32}$$

i.e.

$$\begin{cases} D^1_1 X^1 = 0 \operatorname{mod} \mathbb{Z}, \\ D^2_2 X^2 = 0 \operatorname{mod} \mathbb{Z}, \\ \ldots \\ D^r_r X^r = 0 \operatorname{mod} \mathbb{Z}, \end{cases} \tag{33}$$

where $r = \operatorname{rank}(D^J_a)$. By Proposition 3, it is sufficient to solve equation (33) in the set $\mathcal{X}$: we obtain

$$\begin{cases} X^1 = 0, \dfrac{1}{D^1_1}, \dfrac{2}{D^1_1}, \ldots, \dfrac{D^1_1 - 1}{D^1_1} \\ X^2 = 0, \dfrac{1}{D^2_2}, \dfrac{2}{D^2_2}, \ldots, \dfrac{D^2_2 - 1}{D^2_2} \\ \ldots \\ X^r = 0, \dfrac{1}{D^r_r}, \dfrac{2}{D^r_r}, \ldots, \dfrac{D^r_r - 1}{D^r_r} \\ X^{r+1} = t_1 \in [0, 1), \\ \ldots \\ X^{nN} = t_{nN-r} \in [0, 1), \end{cases}$$

with t_i real parameters.

Once the X^a and the corresponding $\widetilde{P}^b$ are computed, the right-hand sides of the master equation (29) are determined, and $(30)_{2,3}$ yield the solution in terms of the (P^i_α) and $(T^{(k)i}_\alpha)$.

A5. Tensor form of the master equation

The relation between the master equation and the matrix L can be rewritten in more compact form as follows. For $M \in GL(n, \mathbb{Z})$ and $A \in GL(N, \mathbb{Z})$, consider the fourth-order tensor

$$M \otimes A^\top, \tag{34}$$

with components $(M \otimes A^\top)^{i\alpha}_{j\beta} = M^i_j A^\beta_\alpha$, and where $A^\top$ is the transpose of the matrix A. The set of tensors of the form (34) is a group with the product

$$(M \otimes A^\top) * (H \otimes B^\top) := MH \otimes A^\top B^\top, \tag{35}$$

and the indexing rules (24) and (25) define a morphism between the group of such tensors and the group of invertible $nN \times nN$ matrices.

Proposition 6. For $i, j = 1, \ldots, n$, $\alpha, \beta = 1, \ldots, N$, let

$$a = i + (\alpha - 1)n, \quad b = j + (\beta - 1)n,$$

then the rule

$$W^a_b := M^i_j A^\beta_\alpha \tag{36}$$

defines a map $M \otimes A^\top \longmapsto W$ between $GL(n, \mathbb{R}) \otimes GL(N, \mathbb{R})$, with product $*$, and $GL(nN, \mathbb{R})$ which is a group morphism.

Proof. Notice first that if M and A are invertible, then W is invertible, with inverse W^{-1} associated with the tensor $M^{-1} \otimes A^{-\top}$, with $A^{-\top} = (A^{-1})^\top$. Now let $R^a_b := H^i_j B^\beta_\alpha$: then

$$\begin{aligned} \sum_{c=1}^{nN} W^a_c R^c_b &= \sum_{h=1}^{n} \sum_{\gamma=1}^{N} W^{i+(\alpha-1)n}_{h+(\gamma-1)n} R^{h+(\gamma-1)n}_{j+(\beta-1)n} = \sum_{h=1}^{n} \sum_{\gamma=1}^{N} M^i_h A^\gamma_\alpha H^h_j B^\beta_\gamma \\ &= (MH)^i_j (BA)^\beta_\alpha = (MH \otimes (BA)^\top)^{i\alpha}_{j\beta} \\ &= [(M \otimes A^\top) * (H \otimes B^\top)]^{i\alpha}_{j\beta}, \end{aligned}$$

which proves the assertion. □

Further, the tensors of the form (34) act linearly on the space of real matrices $\mathcal{M}(n \times N, \mathbb{R})$ as follows:

$$(M \otimes A^\top) : P \longmapsto MPA, \quad P \in \mathcal{M}(n \times N, \mathbb{R}). \tag{37}$$

Letting $\widetilde{P} \in \mathbb{R}^{nN}$ be given by equation (26), the above action corresponds to the linear action of $GL(nN, \mathbb{R})$ on $\mathbb{R}^{nN}$. In fact

$$\begin{aligned} \sum_{b=1}^{nN} W^a_b \widetilde{P}^b &= \sum_{j=1}^{n} \sum_{\beta=1}^{N} W^{i+(\alpha-1)n}_{j+(\beta-1)n} \widetilde{P}^{j+(\beta-1)n} \\ &= \sum_{j=1}^{n} \sum_{\beta=1}^{N} M^i_j A^\beta_\alpha P^j_\beta = (MPA)^i_\alpha. \end{aligned}$$

The tensor form of the master equation (9) then follows in the form

$$(M \otimes I_N + I_n \otimes A^\top)P = T,$$

with I_N and I_n the N-dimensional and n-dimensional identity matrices, respectively.

A6. Proof of Proposition 5

Consider two mutually conjugated generators of $\mathcal{K}$ and $\mathcal{K}'$,

$$G^{(k)} = \begin{pmatrix} M^{(k)} & T^{(k)} \\ 0 & A^{(k)} \end{pmatrix}, \quad G'^{(k)} = \begin{pmatrix} M'^{(k)} & T'^{(k)} \\ 0 & A'^{(k)} \end{pmatrix};$$

by hypothesis

$$G'^{(k)} = Q^{-1} G^{(k)} Q, \tag{38}$$

with Q given by (18), so that, in particular, $M'^{(k)} = H^{-1} M^{(k)} H$ and $A'^{(k)} = B^{-1} A^{(k)} B$. Letting

$$\begin{aligned} \widetilde{L}^{(k)} &= M^{(k)} \otimes I_N - I_n \otimes (A^{(k)})^\top, \\ \widetilde{L}'^{(k)} &= M'^{(k)} \otimes I_N - I_n \otimes (A'^{(k)})^\top, \\ \widetilde{W} &= H \otimes B^{-\top}, \end{aligned}$$

then

$$\widetilde{L}'^{(k)} = \widetilde{W}^{-1} * \widetilde{L}^{(k)} * \widetilde{W}, \quad k = 1, \ldots, K. \tag{39}$$

In fact, by equation (35)

$$\begin{aligned} (H^{-1} \otimes B^\top) * (M^{(k)} \otimes I_N - I_n \otimes (A^{(k)})^\top) * (H \otimes B^{-\top}) \\ = H^{-1} M^{(k)} H \otimes B^\top I_N B^{-\top} \\ - H^{-1} I_n H \otimes B^\top (A^{(k)})^\top B^{-\top} \\ = M'^{(k)} \otimes I_N - I_n \otimes (A'^{(k)})^\top. \end{aligned}$$

The first assertion of the thesis then follows by letting W be the matrix in $GL(nN, \mathbb{Z})$ associated with $\widetilde{W}$ through the rule (36), and using equation (39) and the definition (30) of L.

Further, for each k, equations (37) and (38) imply that

$$T'^{(k)} = H^{-1} T^{(k)} B + (M'^{(k)} \otimes I_N - I_n \otimes (A'^{(k)})^\top) H^{-1} R,$$

which in turn means that

$$\widetilde{T}' = W_K^{-1} \widetilde{T} + L' J,$$

with $J \in \mathbb{Z}^{nN}$ the integral vector associated with the matrix $H^{-1}R$ through the relation $(30)_2$ [notice that $H \in GL(n, \mathbb{Z})$ and $R \in \mathcal{M}(n \times N, \mathbb{Z})$]. Finally, we obtain equation (23) by multiplying the above identity by U'^{-1}.

A7. Proof of Corollary 1

We first need an auxiliary result.

Proposition 7. Given two $(N+1)$-lattices as above, assume that $\mathcal{H}$ and $\mathcal{H}'$, subgroups of the lattice group of the skeletal lattices, as well as their permutation representations in $\mathcal{S}_{N+1}$, are conjugated, *i.e.* there exist $H \in GL(n, \mathbb{Z})$ and $B \in \mathcal{S}_{N+1}$ such that writing

$$G^{(k)} = \begin{pmatrix} M^{(k)} & T^{(k)} \\ 0 & A^{(k)} \end{pmatrix}, \quad G'^{(k)} = \begin{pmatrix} M'^{(k)} & T'^{(k)} \\ 0 & A'^{(k)} \end{pmatrix},$$

for the generators of $\mathcal{K}$ and $\mathcal{K}'$, respectively, then

$$M'^{(k)} = H^{-1} M^{(k)} H \quad \text{and} \quad A'^{(k)} = B^{-1} A^{(k)} B, \tag{40}$$

for each $k = 1, \ldots, K$. If there exists an integral vector $Z \in \mathbb{Z}^{nN}$ such that

$$S' = U'^{-1} W_K^{-1} U S + D' Z, \tag{41}$$

with the same notations of Proposition 5, the two multilattices are equivalent.

Proof. Clearly, (23) implies that there exists $R \in \mathcal{M}(n \times N, \mathbb{Z})$ such that

$$\widetilde{T}' = W_K^{-1} \widetilde{T} + L' J,$$

with $J \in \mathbb{Z}^{nN}$ the integral vector associated with the matrix $H^{-1}R$ through the relation $(30)_2$. This, together with equation (19), implies in turn that

$$G'^{(k)} = Q^{-1} G^{(k)} Q$$

holds for each k, with Q given by equation (18). □

In order to prove Corollary 1, it is enough to apply Proposition 7, with $M'^{(k)} = M^{(k)}$ and $A'^{(k)} = A^{(k)}$. In this case, the conjugants H and B are just operations that fix $(M^{(1)}, \ldots, M^{(K)})$ and $(A^{(1)}, \ldots, A^{(K)})$, respectively, *i.e.*, elements of the centralizers.

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