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Non-crystallographic nets with finite blocks of imprimitivity for bounded automorphisms

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Periodic nets are commonly used to represent the topology of crystal structures. Non-crystallographic (NC) nets are *p*-periodic nets whose automorphism groups are not isomorphic to any isometry group in the Euclidean space. This work deals with the special class of NC nets possessing non-trivial finite blocks of imprimitivity for bounded automorphisms. It is shown that periodic, barycentric representations of NC nets with this property display vertex collisions, every block being represented as a single point. As a consequence, the labelled quotient graph of these nets shows an equitable partition that also respects the voltages over the edges, introduced as an *equivoltage* partition. Possible motions within linked blocks of imprimitivity are characterized as *correlation groups*. Some non-trivial examples of NC nets that have bounded automorphism groups with and without fixed points are explored from the viewpoint of equivoltage partitions and correlation groups, and a general algorithm is proposed to this end. It is shown that the group of bounded automorphisms of these nets can be described using wreath products of finite permutation groups by translation groups.

1. Introduction

Non-crystallographic (NC) nets are periodic nets whose automorphism group is not isomorphic to any isometry group in the Euclidean space (Moreira de Oliveira Jr & Eon, 2011). Freedom degrees associated to non-rigid motions in a geometric realisation of NC nets may be specific of a wide variety of periodic nets that have not yet been explored. In this paper, we are mainly concerned with the automorphisms that do not respect the periodicity of the net, in contrast with such deformation theories as that formulated by Borcea & Streinu (2010). For most NC nets, the complexity of the automorphism (symmetry) group resulting from such freedom degrees requires the introduction of new mathematical tools. Consider for instance the infinite 1-periodic graph of Fig. 1. The automorphism (B_1, C_1) acts locally on the two vertices B_1 and C_1 while fixing all other vertices of the graph, but we may take as an automorphism of this graph any combination of exchanges $\phi_I = \prod_{i\in I}(B_i, C_i)$, where I is any finite or infinite subset of integers. As a result, the automorphism group of this graph is uncountable and certainly not finitely generated. We will show that such automorphism groups are naturally embedded in the *wreath product* of a finite permutation group by a translation group.

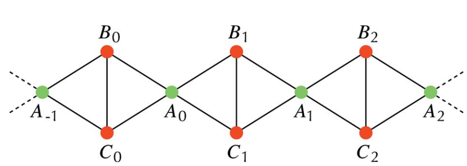

Figure 1
A 1-periodic graph with an uncountable automorphism group.

Because NC nets do not display a unique maximal translation subgroup, as already pointed out by Chung *et al.* (1984), the concept of translation is substituted by that of bounded (local) automorphism (Eon, 2005). It is generally sufficient to analyse the normal subgroup of bounded automorphisms to characterize an NC net. A special class of NC nets with freely acting (*i.e.* with no fixed vertices) bounded automorphisms was analysed in the above-mentioned paper (Moreira de Oliveira Jr & Eon, 2011). We show here that the main results of the latter paper can be extended to periodic nets with a system of finite blocks of imprimitivity (*i.e.* a partition of the vertex set into finite subsets that is stable under the action of bounded automorphisms). It is shown in particular that periodic, barycentric representations of NC nets with a non-trivial system of finite blocks of imprimitivity for bounded automorphisms display vertex collisions, every cell of the partition, or block, being represented as a single point. As a consequence, it is possible to find an equitable partition of the labelled quotient graph of the net which is consistent with the voltages over its edges. These observations lead to the introduction of the concepts of *equivoltage partitions* and *correlation groups*, from which the structure of the group of bounded automorphisms can be recovered directly from the labelled quotient graph, with no need to analyse automorphisms in the net.

A more detailed overview of the methodology is presented in §2. Some basic concepts from graph theory are briefly reviewed in §3. The group-theoretic notion of imprimitivity in periodic nets is studied in §4. Linear representations of periodic nets are analysed in §5 and the main results concerning barycentric representations of NC nets are exposed in §6. Equivoltage partitions are introduced in §7 and correlation groups in §8. Various examples of NC nets admitting a system of imprimitivity for bounded automorphisms are described in §7 and analysed in §8 from the point of view of their labelled quotient graphs. An algorithm for analysing the group of bounded automorphisms of such periodic nets from an arbitrary labelled quotient graph is described in §9 and applied to three orthorhombic sphere packings with collisions in §10.

In the second part of the paper, we draw the consequences of this result with respect to the structure of the labelled quotient graphs of such NC nets. We show that to a system of imprimitivity in the periodic net there corresponds an equitable partition of the vertices in the quotient. By properly setting the origin in every vertex lattice, this partition can also be made to respect the edge voltages (label vectors). It is then possible to take the respective quotient by the partition: the new labelled quotient graph turns out to correspond to the periodic graph associated to the barycentric representation of the NC net. Analysis of the relations between the two labelled quotient graphs enables the study of those automorphisms that stabilize finite blocks of imprimitivity. That is: one may get precise information concerning the group structure of these automorphisms in the NC net directly from its finite labelled quotient graphs. A few examples are treated to show the applicability of the method.

We emphasize that the whole analysis can be performed on the labelled quotient graph of the net. Even the first step, *i.e.* the characterization of blocks of imprimitivity, which proceeds through the determination of vertex collisions in a periodic, barycentric representation of the net, does not demand the construction of the net. This step only requires writing down and inverting the matrix whose entries are the coefficients of cycles and cocycles of the quotient graph expressed as linear combinations of the (oriented) edges of this graph; this inverse matrix should then be right-multiplied by a matrix giving the vector labels (voltages) over the corresponding cycles and cocycles. The method was extensively discussed in Eon (2011) and may be routinely performed on a computer.

2. An overview

Our analysis follows from the observation that periodic, barycentric representations of some non-crystallographic nets display collisions between vertices that are equivalent under a special class of automorphisms. More exactly, vertices segregate into periodic colliding subsets called *blocks*, which are stable under the action of bounded automorphisms. For instance, vertices B_i and C_i collide for all i in a periodic, barycentric representation of the periodic graph shown in Fig. 1. These vertices are equivalent under the class of automorphisms ϕ_I described above, giving rise to a partition into finite blocks $\Delta_i = \{B_i, C_i\}$ which is stable under the action of the family of ϕ_I. Such blocks are also called blocks of imprimitivity in group theory, which motivates our short introduction to related concepts in §4. However, systems of imprimitivity are generally defined in transitive spaces, which is not the normal case for periodic nets. We thus follow the general group-theoretic definitions and then extend the concept to spaces with a finite number of orbits.

Systematic vertex collisions within blocks for periodic, barycentric representations of NC nets have striking implications. Consider again the graph in Fig. 1. If T is a maximal translation group, any conjugate group $\phi_I T \phi_I^{-1}$ is again a maximal translation group and defines another periodic structure for this graph. But, given a geometric lattice in Euclidian space, all corresponding periodic, barycentric representations of this graph overlap whatever its periodic structure. In other words, and generalizing the observation to other periodic nets, any bounded automorphism of an NC net appears to act as a translation on a periodic, barycentric representation. To understand these properties, we widen the notion of barycentric representation, analysing also bounded and line-bounded barycentric representations. Applying these concepts, we achieve the first result of the paper, showing that periodic nets which have automorphisms that stabilize finite blocks of imprimitivity will indeed display vertex collisions in periodic, barycentric representations.

3. Basic concepts

A graph $G = (\mathcal{V}, \mathcal{E}, i)$ is defined on two disjoint sets $\mathcal{V} = \mathcal{V}(G)$ and $\mathcal{E} = \mathcal{E}(G)$, called the vertex and edge sets of G when an incidence mapping $i : \mathcal{E} \longrightarrow \mathcal{P}$ is given from the edge set $\mathcal{E}$ to the set $\mathcal{P}$ of 2-element subsets (unordered pairs) of $\mathcal{V}$. The notation $e = AB$ is used for $i(e) = \{A, B\}$; e is *incident* to A and B, also called the end vertices of e, and these two vertices are said to be *adjacent*. Two edges are *adjacent* if they are incident to a common vertex. Vertices or edges that are not adjacent are also called *independent*. The *degree* of a vertex A, denoted by deg(A), is the number of edges incident at A. (We shall not be concerned with the degree of vertices with loops in this work.) A graph is *locally finite* if all vertices have finite degree and *regular* if all its vertices have same degree. An element of the union set $\mathcal{V} \cup \mathcal{E}$ will be called an *element* of G. A subgraph of G is a graph whose vertex and edge sets are subsets of $\mathcal{V}$ and $\mathcal{E}$, such that the incidence mapping is a restriction of i. An important subgraph in a graph G is the *star* centred at a vertex $A \in G$, defined as the subgraph containing A, all the adjacent vertices together with the edges incident at A. The subgraph *induced* by a subset $\mathcal{V}' \subset \mathcal{V}$ is the subgraph of G containing $\mathcal{V}'$ and all the edges in $\mathcal{E}$ with both end vertices in $\mathcal{V}'$. The subgraph *induced* by a subset $\mathcal{E}' \subset \mathcal{E}$ is the subgraph of G containing $\mathcal{E}'$ and all the end vertices of edges in $\mathcal{E}'$.

A *path* $p = UV$ between vertices U and V in a graph G is a subgraph such that U and V have degree one and all remaining vertices have degree two. The *length* of the path is the cardinality of its edge set. A graph G is *connected* if there is a path between any pair of its vertices. More generally, a graph is *n-connected* if one needs to delete at least n vertices to disconnect it. In a connected graph, one defines the *distance* $d(U, V)$ between two vertices U and V as the length of a shortest path $p = UV$. A *cycle* in a graph G is a finite regular connected subgraph of degree 2. The number of edges is called the *length* of the cycle. The *sum* of two cycles with edge sets $\mathcal{E}_1$ and $\mathcal{E}_2$ is the subgraph induced by the symmetric difference $\mathcal{E}_1 \Delta \mathcal{E}_2$. The sum of an arbitrary number of cycles is defined by associativity. A *strong ring* is a cycle that cannot be written as the sum of shorter cycles (Goetzke & Klein, 1991).

Let $G = (\mathcal{V}, \mathcal{E}, i)$ be a graph with $\mathcal{V} = \{V_1, \ldots, V_n\}$ and $\mathcal{E} = \{e_1, \ldots, e_m\}$; the *adjacency* matrix $A(G) = (a_{ij})_{n\times n}$ of G is defined by $a_{ij} = 1$ if $V_iV_j \in \mathcal{E}$ and $a_{ij} = 0$ otherwise. The *degree* matrix $D(G) = (d_{ij})_{n\times n}$ is defined by $d_{ij} = \deg(V_i)$ if $i = j$ and $d_{ij} = 0$ otherwise. Finally, the *Laplacian* matrix $L(G) = (l_{ij})_{n\times n}$ is defined as $L(G) = D(G) - A(G)$. These definitions are trivially extended to infinite graphs with countable elements.

In a graph $G = (\mathcal{V}, \mathcal{E}, i)$, an orientation is given to an edge e when one of its incident vertices is chosen as an *initial* vertex [see Gross & Tucker (2001) or Godsil & Royle (2004)]. Each edge has thus two possible orientations; if A is chosen as the initial vertex for the edge e such that $i(e) = \{A, B\}$, we write $e^+ = AB$ and $e^- = BA$. The graph is *oriented* when every edge e has been given a positive and a negative orientation, e^+ and e^-, respectively. We emphasize that oriented graphs are not to be confused with directed graphs. Arcs in directed graphs are one-way while edges in oriented graphs are two-way; the notation keeps track of the chosen way. The case of loops may be dealt with in a similar fashion (see Eon, 2011). There is generally no need to attribute an orientation to periodic nets. It is, however, necessary to give an orientation to their quotient graphs, as explained further on. An orientation of the net is then induced by that of its quotient.

An *automorphism* f of a graph $G = (\mathcal{V}, \mathcal{E}, i)$ is a permutation of vertices and edges that preserves incidence relations, and can be formally defined as a pair $f = (f_V, f_E)$ of bijective mappings of $\mathcal{V}$ and $\mathcal{E}$ on themselves respecting the incidence mapping: $f_E(e) = f_V(A)f_V(B)$ for $e = AB$. Notice that introducing the edge mapping f_E is necessary to work on graphs with loops or multiple edges, as are quotient graphs of periodic nets. f is a *bounded automorphism* if the set of distances $\{d[f(U), U] | U \in \mathcal{V}(G)\}$ is uniformly bounded by some constant. [Bounded automorphisms were first mentioned by Trofimov (1983) and rediscovered by Eon (2005), where they were called local automorphisms.] For example, the image $\phi_I(V)$ of a vertex V by every automorphism ϕ_I of the periodic graph in Fig. 1, as defined above, is at a distance at most one of V. An automorphism f is said to *act freely* on G if there is no fixed element, that is: $f(X) \neq X$ for all $X \in \mathcal{V} \cup \mathcal{E}$. The automorphism group of G is denoted $\mathrm{Aut}(G)$; the subset $B(G)$ of bounded automorphisms is a normal subgroup of $\mathrm{Aut}(G)$.

A *simple* graph is a graph without loops or multiple edges. A *net* is a locally finite simple 3-connected graph. A *p-periodic net* is defined as a pair (N, T) composed of a net N and a free abelian group $T \leq \mathrm{Aut}(N)$ of rank p, such that the number of vertex and edge orbits by T in N is finite. T is called the translation group of (N, T) and acts freely on the net N. In some examples we shall also consider periodic graphs, using a locally finite simple graph instead of a net. Those p-periodic nets whose full automorphism group is isomorphic to some p-dimensional space group are called *crystallographic nets* (Klee, 2004). Periodic nets whose automorphism group is not isomorphic to any isometry group in the Euclidean space are called *non-crystallographic nets*. Note that the only bounded automorphisms in crystallographic nets are translations: $B(N, T) = T$ (Eon, 2005). If (N, T) is a periodic net, $\mathcal{V}/T$ and $\mathcal{E}/T$ are, respectively, the sets of vertex and edge *lattices* (or *orbits*) of N by T. The mapping q_T sends an element X to its lattice $[X]$. The *quotient graph* is the graph $N/T \equiv (\mathcal{V}/T, \mathcal{E}/T, i_T)$, where i_T is given by $i_T([e]) = ([A], [B])$ for an edge $e = AB \in \mathcal{E}$. In the *labelled quotient graph* the edges of this graph are assigned a vector label (also called *voltage*) indicating the difference between the unit cells of its two end vertices. This clearly presupposes that the quotient graph has been given an orientation. By convention, edges with zero voltage are not labelled.

4. Imprimitivity in periodic nets

Let G be a finite or infinite graph and $\Gamma \leq \mathrm{Aut}(G)$. G is said to be Γ-transitive if, given any two vertices U and V in $\mathcal{V}(G)$, one can always find an automorphism $g \in \Gamma$ such that $V = g(U)$. In a Γ-transitive graph G, a partition of the vertex set $\mathcal{V}(G)$ into subsets, called *blocks*, is said to be a *system of imprimitivity* for Γ if Γ preserves the partition, *i.e.* if any automorphism $g \in \Gamma$ maps the block Δ to a block $g(\Delta)$ (Bhattacharjee *et al.*, 1998). If the blocks consist solely of single vertices, or if the whole vertex set is a block, the system of imprimitivity is said to be *trivial*. If all the systems of imprimitivity of a group Γ are trivial, then the action of Γ is *primitive*. Notice that a system of imprimitivity is completely described by providing a single block.

For the analysis of periodic nets (N, T), we shall consider the subgroup $\Gamma = B(N)$ of all bounded automorphisms. Observe, however, that p-periodic nets are imprimitive for translation groups. For instance, in the case of the square net we may take as a block the infinite subset $\Delta = \{t^n(O) | n \in \mathbb{Z}\}$, where O is some vertex of the net and t is any non-trivial translation. On the other hand, the existence of finite blocks of imprimitivity is not a trivial property for periodic nets. We will say that the action of $B(N)$ on the graph N is *finitely primitive* if there is no finite, non-trivial block of imprimitivity.

Periodic nets (N, T) are not generally $B(N)$-transitive; however, the number of $B(N)$-orbits is finite and the above definitions may be applied to each orbit separately. In particular, a system of imprimitivity for the net is completely described by providing one block per $B(N)$-orbit. The result is that the action of $B(N)$ on a net (N, T) is finitely primitive whenever it is so on every $B(N)$-orbit. In this case we use a different colour for each $B(N)$-orbit, which helps to detach the blocks of imprimitivity. The graph in Fig. 1, for example, has two $B(N)$-orbits shown in green and red, respectively. The action of $B(N)$ on the green one is finitely primitive since the only finite block contains a single vertex; the red orbit admits the set $\{B_0, C_0\}$ as a block of imprimitivity so that the action of $B(N)$ on this subset is not finitely primitive. Note that the action of $B(N) = T$ on a crystallographic net (N, T) is finitely primitive.

5. Linear representations of periodic nets

A *linear representation*, or simply a *representation* ρ of a graph in the Euclidean space is a mapping of vertices and edges to points and line segments, respectively, such that $\rho(e) = \rho(U)\rho(V)$ for $e = UV$. We may also use the word 'representation' when referring to the image of the mapping ρ in the Euclidean space. A bounded set in the Euclidean space, or simply a bounded set, is a set whose elements are located inside a closed ball centred at the origin for a sufficiently large radius. We will say that the representation ρ is *bounded* if $\rho(N)$ is a bounded set and that it is *line bounded* if there is a maximal length l for the image of every edge: $\forall e, \|\rho(e)\| \le l$. In a *barycentric representation* of a graph every point $\rho(U)$ is located at the centre of gravity of the points $\rho(V)$ representing the neighbours V of U. When not explicitly stated, all vertices are affected by equal weights. A representation presents *vertex collisions* if different vertices are mapped on the same Euclidean point. Note that the whole graph collapses to a single point in a barycentric representation of a finite graph. Nevertheless, infinite graphs do display non-trivial bounded barycentric representations, as shown in Fig. 2 for the infinite tree derived from the graph $K_2^{(3)}$ using as voltages two free generators.

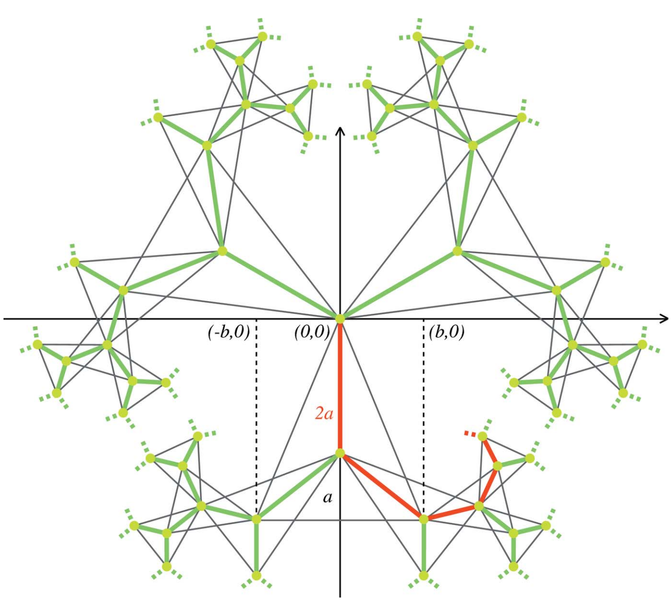

Figure 2
An example of a non-trivial bounded barycentric representation of the infinite regular tree of degree 3. The tree was built starting at the origin with a symmetric star, generating three branches. At each step of the construction two new vertices are added on every branch in order to complete the neighbourhood of the vertices of degree 1 (the *leaves*). For this, similar isosceles triangles with parameter θ are drawn such that each leaf is at the barycentre and its neighbours are at the vertices of one of these triangles. If $2a$ represents the length of the terminal edge, the basis $2b$ of the triangle is given by $b = a\theta$. Note that if $\theta = 3^{1/2}$, then (i) a and b are constant at every step and (ii) the hexagonal net **hxl** is obtained.

Bounded and line-bounded barycentric representations of periodic nets have nice properties.

Lemma 5.1. Let ρ be a bounded, barycentric representation of a periodic net (N, T) such that every vertex in some vertex lattice is mapped onto the same point P; then $\rho(N) = P$.

Proof. Suppose that in the barycentric representation ρ of (N, T) the vertex lattice $[A]$ collides at a point P. We consider an orthogonal projection π of ρ on some axis containing P; clearly π is also a bounded, barycentric representation of N. Suppose π covers an open interval $]U, V[$. Since the boundary V is an accumulation point of π we may choose a vertex X_1 such that $\pi(X_1)$ is at a distance less than ε from V (see Fig. 3). Observe now that every vertex in the net is at a maximum (graph-theoretical) distance d from some vertex in $[A]$, where d is the diameter of the quotient graph N/T (the maximum distance between two vertices in N/T). It is then possible to choose a shortest path $p = X_1X_2\ldots X_n$ with $X_n \in [A]$ and $n \le d$. Denote by r the maximum degree of vertices in the net. Because $\pi(X_1)$ is the barycentre of its neighbours, among which is $\pi(X_2)$, this point is at a distance less than $r\varepsilon$ from the boundary V. Repeating the procedure shows that $\pi(X_n) = P$ is at a distance less that $r^d\varepsilon$ from V for any value of ε, a contradiction. If, on the other hand, there is some vertex X verifying $\pi(X) = V$, then all neighbours of X must collide at V and, by induction, the whole net is mapped on $V = P$. □

A representation ρ of a periodic net (N, T) is *periodic* if some translation group T^* of rank p in the Euclidean space may be isomorphically associated to T through a mapping $* : t \mapsto t^*$ such that $\rho[t(U)] = t^*[\rho(U)]$ for any $t \in T$ and $U \in \mathcal{V}(N)$. For a labelled quotient graph with voltages in $\mathbb{Z}^p$ and a lattice basis $\mathcal{B}_p$ of $\mathbb{R}^p$, there is a unique periodic barycentric representation of the derived net with the given lattice, up to translation (Delgado-Friedrichs, 2005).

Consider a representation ρ of a periodic net (N, T); since the vertex set $\mathcal{V}(N)$ is a countable set, it is possible to define an infinite sequence $V_\rho = (\rho(V_1), \rho(V_2), \ldots)$ containing all the points in $\rho(N)$. We call such a sequence a *representation vector*: V_ρ is uniquely determined by the representation ρ and conversely V_ρ defines a representation of the net. If L is the Laplacian matrix of a periodic net (N, T), then the product

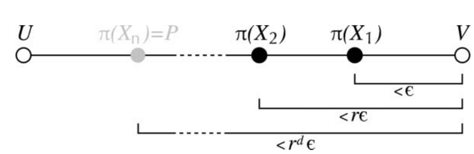

Figure 3
A finite sequence of points starting at $\pi(X_1)$, close to an accumulation point, to $P = \pi(X_n)$.

LV_ρ is null for a barycentric representation ρ, since the rows of this product define exactly the barycentric equations for all points of $\rho(N)$.

Example 5.1. We build the representation vector $(P_1, P_2, P_3, \ldots)$ of the square net according to the spiral order as shown in Fig. 4. The infinite Laplacian matrix L respecting the same vertex order is given below. The first row of the Laplacian matrix, for instance, provides the barycentric equation for vertex P_1: $4P_1 = P_2 + P_4 + P_6 + P_8$.

$$L = \begin{pmatrix} 4 & \bar{1} & 0 & \bar{1} & 0 & \bar{1} & 0 & \bar{1} & 0 & 0 & 0 & \cdots \\ \bar{1} & 4 & \bar{1} & 0 & 0 & 0 & 0 & 0 & \bar{1} & 0 & \bar{1} & \cdots \\ 0 & \bar{1} & 4 & \bar{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \bar{1} & 0 & \bar{1} & 4 & \bar{1} & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \bar{1} & 4 & \bar{1} & 0 & 0 & 0 & 0 & 0 & \cdots \\ \bar{1} & 0 & 0 & 0 & \bar{1} & 4 & \bar{1} & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \bar{1} & 4 & \bar{1} & 0 & 0 & 0 & \cdots \\ \bar{1} & 0 & 0 & 0 & 0 & 0 & \bar{1} & 4 & \bar{1} & 0 & 0 & \cdots \\ 0 & \bar{1} & 0 & 0 & 0 & 0 & 0 & \bar{1} & 4 & \bar{1} & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{1} & 4 & \bar{1} & \cdots \\ 0 & \bar{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{1} & 4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

We note that, given a periodic net (N, T) and two barycentric representations with representation vectors V_{ρ_1} and V_{ρ_2}, the difference vector $V_{\rho_1} - V_{\rho_2}$ describes another barycentric representation, since the order of the points is unchanged and $L(V_{\rho_1} - V_{\rho_2}) = LV_{\rho_1} - LV_{\rho_2} = 0$.

The next theorem strengthens previous results obtained by Delgado-Friedrichs (2005) and Eon (2011).

Theorem 5.1. There is one, and only one, barycentric, line-bounded representation of a periodic net which maps a given vertex lattice onto some pre-defined point lattice in Euclidean space.

Proof. The existence of a periodic barycentric representation with a given lattice basis is already known. Let ρ_1 and ρ_2 be two (not necessarily periodic) barycentric representations of (N, T) mapping a given vertex lattice $[X]$ to some pre-defined point lattice in Euclidean space. Since both representations are barycentric and line-bounded, the difference vector $R = V_{\rho_1} - V_{\rho_2}$ defines a bounded barycentric representation of (N, T) which maps the vertex lattice $[X]$ to the origin of the space. According to Lemma 5.1, this representation collapses to the origin so that $V_{\rho_1} = V_{\rho_2}$. □

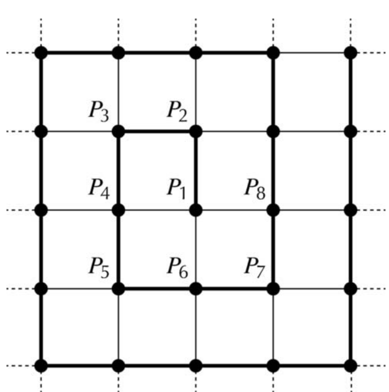

Figure 4
A barycentric representation of the square net in the plane. The representation vector can be defined as the sequence $(P_1, P_2, P_3, \ldots)$, obeying a spiral pattern.

6. Bounded automorphism groups and systems of imprimitivity

We consider now non-crystallographic nets for which there is a non-trivial automorphism fixing a vertex lattice. For example, in the 1-periodic graph of Fig. 1 vertex lattice $[A]$ is (pointwise) fixed by ϕ_I. It may be verified that periodic barycentric representations of this graph display collisions: vertices B_i and C_i collide for any $i \in \mathbb{N}$. This result is an immediate consequence of Theorem 5.1.

Corollary 6.1. Suppose there is a non-trivial automorphism f of a periodic net (N, T) that fixes every vertex in some vertex lattice $[X]$. Then any periodic, barycentric representation of the net in Euclidean space presents vertex collisions. In particular, every vertex in (N, T) is mapped on the same point as its image by f.

Proof. Let ρ be a periodic, barycentric representation of (N, T). Then, the mapping ρ': $U \mapsto \rho[f(U)]$ is also a barycentric representation of (N, T) and it is clearly line-bounded. Moreover, for any vertex $U \in [X]$, we have $\rho'(U) = \rho[f(U)] = \rho(U)$ so that both representations map vertex lattice $[X]$ to the same point lattice. Hence, according to Theorem 5.1, $\rho' = \rho$. Now, since f is not the trivial automorphism, there is some vertex V with $f(V) \neq V$; for this vertex we have $\rho[f(V)] = \rho'(V) = \rho(V)$, showing that V and its image $f(V)$ collide in the representation ρ. □

The existence of non-trivial automorphisms fixing one or more vertex lattices in non-crystallographic nets is not the rule, but fortunately the result may be extended to periodic nets which have automorphisms that stabilize finite blocks of imprimitivity.

Corollary 6.2. Let (N, T) be a periodic net with a non-trivial system σ of finite blocks of imprimitivity for the subgroup of bounded automorphisms $B(N)$. Denote by $B(N)_\sigma$ the subgroup of $B(N)$ which stabilizes every block in σ and suppose that $B(N)_\sigma$ is transitive on each block. Then, any barycentric representation in Euclidean space of (N, T) displays vertex collisions, every block being represented by a single point.

Proof. Notice that σ is periodic since $T \subset B(N)$. Let us denote by $\sigma(X)$ the block containing vertex X. We define an auxiliary abstract periodic net N_σ with vertex set $\mathcal{V}(N_\sigma) = \mathcal{V}(N) \cup \sigma$ and edge set $\mathcal{E}(N_\sigma) = \mathcal{E}(N) \cup \{X\sigma(X), X \in \mathcal{V}(N)\}$. So, blocks are abstractly considered as new elements of the vertex set and linked to their constituting vertices. It is clear that N_σ admits T as a translation group, so that we may consider the periodic net (N_σ, T). We now define $g_\sigma \in B(N_\sigma)$ by extension of $g \in B(N)_\sigma$ as follows. For every $X \in \mathcal{V}(N)$, we set $g_\sigma(X) = g(X)$ and $g_\sigma[\sigma(X)] = \sigma(X)$. According to Corollary 6.1, all vertices in a block collide in a periodic, barycentric representation of (N_σ, T). The added vertex $\sigma(X)$, being at the barycentre of vertices mapped on a single point, is also mapped on this point, which means that the given periodic, barycentric representation of (N_σ, T) is also a periodic, barycentric representation of (N, T), but possibly with different weights. The weight of a given block is indeed equal to the number of edges linking this block to the central one. □

An example of a barycentric representation with unequal weights is given in §7.3. It is also worth noting that several non-equivalent blocks may collapse into a single point of the barycentric representation, as shown in §7.1.

7. Equivoltage partitions

A vertex partition of a graph into subsets B_i, called *cells*, is *equitable* if the number of neighbours in B_j of a vertex U in B_i is a constant b_{ij}, *i.e.* it is independent of the chosen vertex U (Godsil & Royle, 2004). Clearly, orbits by some automorphism group form an equitable partition. Accordingly, a system of finite blocks of imprimitivity for the subgroup of bounded automorphisms forms an equitable partition σ of an NC net whenever their setwise stabilizer is transitive on every block. Since σ is also periodic, this partition projects on an equitable partition of the quotient graph N/T. Moreover, all edges linking two given blocks are represented by the same line segment in a periodic, barycentric representation of the net: it is thus possible to attribute the same label vector to all the representative edges in the labelled quotient graph. This observation leads us to introduce the next concept.

Definition 7.1. A vertex partition of a voltage graph is *equivoltage* if (i) it is equitable and (ii) there is a bijective mapping between the stars of any two vertices of the same cell, which respects both voltages and partition. That is: given a cell B_j and a vertex $U \in B_i$, the list of b_{ij} voltages of edges UV for $V \in B_j$ does not depend on the chosen vertex U. A loop in a star must be counted as two edges, one outgoing and the other ingoing, both with the same voltage.

Hence, labelled quotient graphs of non-crystallographic nets admitting a stable, transitive system of finite blocks of imprimitivity will present an equivoltage partition of their vertex set if the origin is suitably chosen in each vertex lattice. Fig. 5 illustrates the importance of this setting; if the origins of equivalent vertex lattices are not chosen in the same block of imprimitivity, then the labelled quotient graph fails to show an equivoltage partition.

The following examples show that all non-crystallographic nets that are known so far can be mapped on a labelled quotient graph with an equivoltage partition. These examples illustrate different relationships between non-crystallographic nets and their periodic, barycentric representations interpreted through the prism of an equivoltage partition of their labelled quotient graphs.

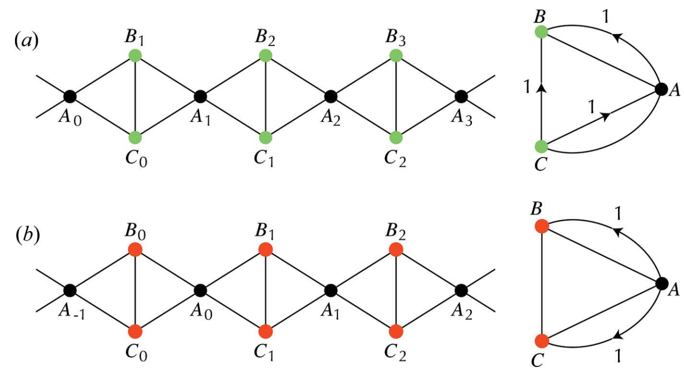

Figure 5
A 1-periodic graph with a system of finite blocks of imprimitivity and two labelled quotient graphs: (*a*) without and (*b*) with an equivoltage partition.

The most important property is schematized in Fig. 6. For the periodic net (N, T) with system of imprimitivity σ, we can construct the quotient N/σ whose vertices are the blocks $\sigma(X)$ for $X \in \mathcal{V}(N)$. Because both nets, N and N/σ, admit the same translation group T, we can also build their labelled quotient graphs with voltages in T. The diagram may now be completed by a homomorphism θ mapping N/T to its quotient Q by the equivoltage partition and defined by $\theta([X]_T) = [\sigma(X)]_T$; notice that θ preserves voltages in the sense that it maps edges of N/T on edges of Q with the same voltage in T. As a consequence, edges in N between vertices in the same block are mapped onto a loop with zero voltage in Q: such loops must be deleted. We emphasize that the quotient Q can be obtained directly from N/T and brings immediate information concerning the barycentric representation of N with collisions, as the following example of the *double ladder* shows.

7.1. The double ladder

Fig. 7 displays the 1-periodic net of the double ladder with three vertex lattices: $[A]$, $[B]$ and $[C]$. There are two non-equivalent blocks of imprimitivity, namely $\{A_0, C_0\}$ and $\{B_0\}$, hence according to Corollary 6.2, we expect the collision of vertex lattices $[A]$ and $[C]$ in the barycentric representation. In fact, the three vertex lattices collide into a single point lattice $[F]$ because the net N/σ itself is a non-crystallographic net (the ladder) with a stable, transitive system of finite blocks of imprimitivity, $\{D_i, E_i\}$. Quotient graphs provide a clear understanding of these facts. The quotient graph of the double

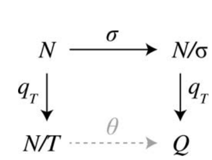

Figure 6
Schematic definition of the quotient by an equivoltage partition of the quotient graph of a periodic net.

ladder presents an equivoltage partition with two cells, $\{A, C\}$ and $\{B\}$; the respective quotient Q is precisely the labelled quotient graph of the (simple) ladder. In turn this also presents an equivoltage partition with a single cell $\{D, E\}$ whose quotient is a loop.

7.2. The NC nets uld and uld-z

Fig. 8 shows the labelled quotient graphs of the two cubic sphere packings initially classified as $4/3/c25$ and $4/3/c26$ by Fischer (1974) and today codified as **uld** and **uld-z** in the Reticular Chemistry Structure Resource (RCSR) database of crystal nets (O'Keeffe *et al.*, 2008).

We first observe that both labelled quotient graphs present the same automorphism $\varphi = \prod_{k=1,\ldots,12}(U_{2k-1}, U_{2k})$, acting as a mirror on each trigonal prism. In both cases, φ preserves voltages on the cycles of the graph and fixes the edges of the prisms, indicating the existence in the net of a bounded automorphism, say $\phi = \prod_{t\in T,k=1,\ldots,12}(tU_{2k-1}, tU_{2k})$, which commutes with the respective translation groups. Hence, both nets are non-crystallographic nets and, as such, they have more than one maximal translation group. Let us write as i, j and k the three generators of the translation group of **uld**; the three automorphisms $i\phi$, $j\phi$ and $k\phi$ form the generators of an isomorphic translation group for this net. It may be verified that the labelled quotient graph of **uld** relative to this new translation group is isomorphic to that of **uld-z**. Hence, **uld** and **uld-z** are isomorphic nets but with a different periodic structure. This explains why all topological invariants of **uld** and **uld-z** are identical, although they display non-ambiently isotopic embeddings.

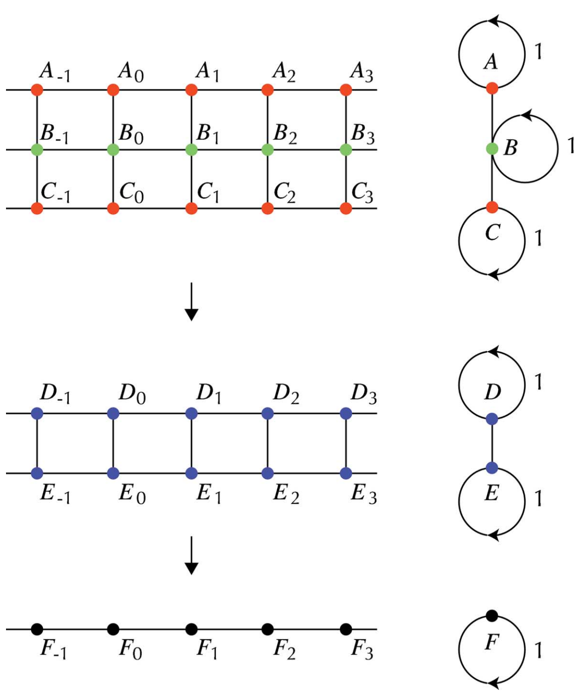

Figure 7
From (top) the double ladder with two non-equivalent finite blocks of imprimitivity shown in green and red and its quotient graph to (bottom) its barycentric representation (the infinite path).

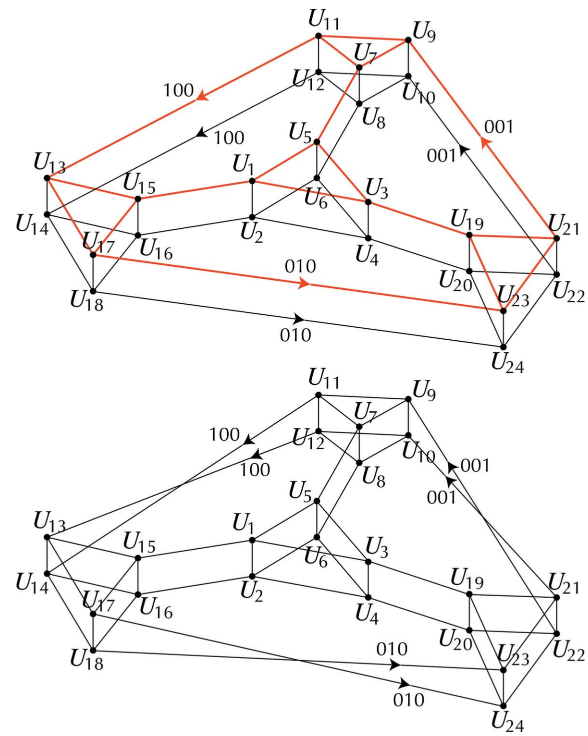

Figure 8
The labelled quotient graphs of (top) **uld-z** and (bottom) **uld** with the equivoltage partition $\theta = \{\{U_1, U_2\}, \{U_3, U_4\}, \ldots, \{U_{23}, U_{24}\}\}$. The quotient by θ drawn as the red subgraph of the quotient of **uld-z** is isomorphic to the labelled quotient graph of the crystallographic net **srs-a**.

The partition $\sigma = \{\{tU_{2k-1}, tU_{2k}\} : t \in T, k = 1, \ldots, 12\}$ forms a system of finite blocks of imprimitivity for each net which is setwise stabilized by the transitive subgroup $B(N)_\sigma = \{1, \phi\}$. Accordingly, both labelled quotient graphs display an equivoltage partition formed by the edges of the trigonal prisms; the quotient is given in Fig. 8 as the red subgraph of the quotient of **uld-z**. This is isomorphic to the labelled quotient graph of **srs-a**, the crystallographic net obtained from **srs** by decoration. It was verified that the three nets **uld**, **uld-z** and **srs-a** have the same periodic barycentric representation where, in agreement with Corollary 6.2, all the edges of the trigonal prisms collapse.

7.3. A double hxl

It is worth illustrating the existence of unequal weights in the periodic, barycentric representations of the nets (N_σ, T) and (N, T) (in the notations of the proof of Corollary 6.2).

To this end, Fig. 9 shows a non-crystallographic net obtained by duplication of **hxl** and its labelled quotient graph with an equivoltage partition, the quotient by this partition being $K_2^{(3)}$, as expected. Every block of imprimitivity contains two vertices; these may be exchanged by bounded automorphisms which act as a kind of local reflection on the net. Now, every block is linked by double edges to two other blocks while it is linked by a quadruple edge to the third block. As a result, the three edges have weights 1, 1 and 2, respectively, in the periodic barycentric representation of the quotient N/σ, as shown in Fig. 10.

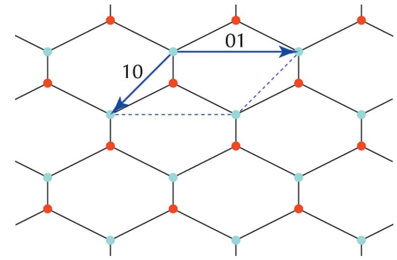

Figure 10
A periodic, barycentric representation of the 'double' **hxl**; the vertical (shorter) edge has weight 2.

7.4. A triple sqr

In the last example of this section, we consider the non-crystallographic net shown in Fig. 11, already studied in detail by Moreira de Oliveira Jr & Eon (2011). In contrast with the double ladder and **uld** or **uld-z**, the subgroup of bounded automorphisms of this net acts freely on the net. However, we will see that this net also presents a system of finite blocks of imprimitivity: $\sigma = \{\{A_{ij}, B_{ij}, C_{ij}\}, \{D_{ij}, E_{ij}, F_{ij}\} : i, j \in \mathbb{Z}\}$.

It was shown in the above-mentioned paper that the group of bounded automorphisms of the net is a subdirect product of $\mathcal{S}_3$ and $\mathbb{Z}^2$ with generators $(12; (0, 1))$ and $(123; (1, 0))$. Moreover, because this group is transitive and acts freely on the net, any vertex can be indexed by the automorphism that takes the origin to it, providing the following correspondence, where e is the identity permutation in $\mathcal{S}_3$.

$$\begin{cases} A_{ij} & \rightarrow & (e; (i, 2j)) \\ B_{ij} & \rightarrow & (123; (i, 2j)) \\ C_{ij} & \rightarrow & (132; (i, 2j)) \\ D_{ij} & \rightarrow & (12; (i, 2j - 1)) \\ E_{ij} & \rightarrow & (23; (i, 2j - 1)) \\ F_{ij} & \rightarrow & (13; (i, 2j - 1)). \end{cases}$$

The representative automorphisms of the first family of blocks $\Delta_{ij} = \{A_{ij}, B_{ij}, C_{ij}\}$ have even permutations as first coordinates, while in the other family, $\Delta'_{ij} = \{D_{ij}, E_{ij}, F_{ij}\}$, they admit odd permutations as first coordinates. To check that σ is a system of imprimitivity, we observe that the action of an arbitrary bounded automorphism (p, t) on a block, that is, the result by left multiplication of the three representative automorphisms by (p, t), only depends on the parity of the permutation p. An even permutation p stabilizes the two families while an odd permutation exchanges them. On the other hand, the second (translational) coordinates being identical for the three vertices in a block remains so after multiplication by (p, t). Hence any bounded automorphism maps a block to another block; in particular the subgroup of order three generated by $(123, (0, 0))$ transitively stabilizes every block.

As expected, the labelled quotient graph presents an equivoltage partition with three vertices per cell. The respective quotient by this partition is the graph $K_2^{(2)}$ with a loop at each vertex, from which one may derive the net **sqr** with double cell. In agreement with Corollary 6.2, the periodic barycentric representation of the NC net displays collisions. Because there are only triple edges between two linked blocks of imprimitivity, it is isomorphic to the barycentric representation of **sqr**.

It is worth noting that the labelled quotient graph of the net presents an automorphism, say φ_1, in which both the internal and external 3-cycles slide along themselves, and which preserves the voltages over its cycles. The quotient by φ_1 and the quotient by the equivoltage partition are isomorphic. It is not possible, however, to attribute voltages in $\mathbb{Z}^2$ to the loops of the quotient by the automorphism, since this voltage, say α, should verify $\alpha^3 = 30$ with $\alpha \neq 10$. We emphasize that the quotient by an equivoltage partition does not describe the net, but a net associated to its barycentric representation. That the respective net is isomorphic to the square net with double cell is implied by the existence of the automorphism φ_3, exchan-

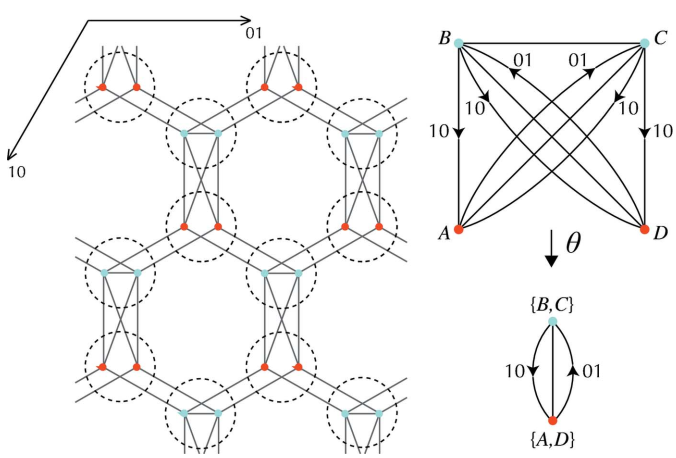

Figure 9
A periodic net with a system of imprimitivity, its labelled quotient graph and the quotient by an equivoltage partition.

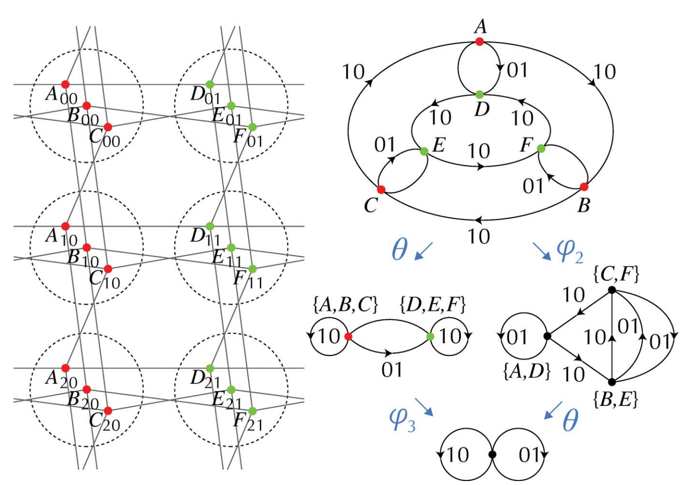

Figure 11
An NC net with a system of imprimitivity, but with a freely acting bounded automorphism group, its labelled quotient graph and different quotients. θ indicates the quotient by an equivoltage partition, φ the quotient by an automorphism group.

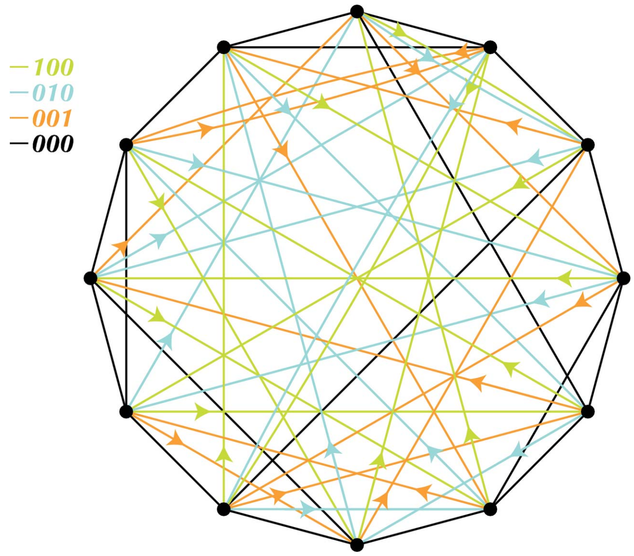

Figure 12
A labelled quotient graph based on the Frucht graph (in black); the colour of an edge symbolizes the respective voltage.

ging the two vertices and mapping cycles to cycles with the same voltages. Moreover, equivoltage partitions may exist even in the absence of an automorphism of the labelled quotient graph, as may also be seen on this same example. There is indeed another automorphism of the labelled quotient graph of the net, say φ_2, which exchanges the internal and external 3-cycles and preserves voltages over every cycle. This quotient by φ_2 may be labelled, as shown in Fig. 11, and is indeed the labelled quotient graph of the net associated to a maximal translation group. This graph admits no automorphism that preserves voltages over its cycles, but there is an equivoltage partition; the three vertices belong to the same cell and the quotient by this partition is the bouquet B_2 with voltages 10 and 01.

7.5. A periodic net based on the Frucht graph

Before leaving this section, we want to call the attention of the reader to the fact that the existence of an equivoltage partition in a labelled quotient graph is not enough to ensure that the derived net is non-crystallographic. Fig. 12 shows a labelled quotient graph constructed from the Frucht graph (Frucht, 1939). This graph is the smallest cubic graph on twelve vertices with trivial automorphism group; it is drawn in black in the figure and the respective edges were attributed voltage 000. For each of the three voltages 100, 010 and 001 were added twelve edges in such a way that at every vertex one edge of each voltage comes in and another goes out. The resulting labelled quotient graph is thus regular of degree 9 and admits an equivoltage partition with a single cell. The quotient by this partition is the bouquet of three loops with voltages 100, 010 and 001; accordingly, the barycentric representation of the derived net is isomorphic to that of **pcu**, as we have indeed checked.

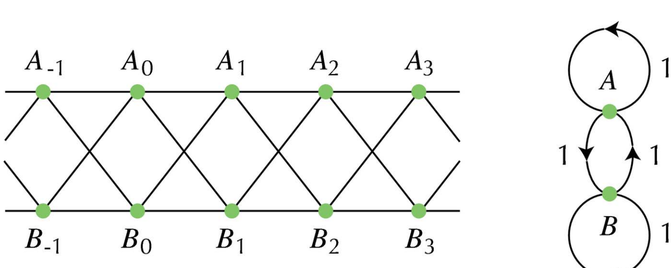

Figure 13
An NC transitive net with a system of imprimitivity and its labelled quotient graph.

Through every vertex of the labelled quotient graph run exactly three cycles of voltages $p00$, $0q0$ and $00r$, respectively, where p, q and r are the lengths of the respective cycles. This means that each of these cycles is the projection of a strong geodesic line of the derived periodic net (Eon, 2007). Moreover, every edge of non-zero voltage belongs to exactly one of these cycles. These properties may be lifted to the derived periodic net. The edges with zero voltage induce in every unit cell of the net a Frucht graph; coloured edges lift to strong geodesic lines which join the unit 'Frucht cells' in the three directions 100, 010 and 001. Since bounded automorphisms map strong geodesic lines to strong geodesic lines in the same direction, the unit Frucht cells should map on themselves. Of course, a Frucht graph can only map identically on another Frucht graph, and because there is exactly one strong geodesic line through each vertex of the net in each of the three directions, any bounded automorphism must be a translation, hence the derived net is a crystallographic net. We conclude that the existence of a non-trivial system of finite blocks of imprimitivity is linked to that of non-trivial automorphisms in the subgraph induced by the block.

8. Correlation groups

It is known that groups with an imprimitive action can be embedded in a *wreath product* (see for instance, Bhattacharjee *et al.*, 1998). Before we give a more formal introduction to this purely group-theoretical concept, we analyse a simple application to the study of NC nets.

Fig. 13 shows a 1-periodic graph with a system of finite blocks of imprimitivity $\Delta_i = \{A_i, B_i\}$. This graph admits as bounded automorphism any combination of exchanges $\phi_I = \prod_{i\in I}(A_i, B_i)$, where I is any finite or infinite subset of integers. Notice that for each block Δ_i the two vertices may be permuted or left invariant hence, relative to a given block, ϕ_I acts as a permutation of the symmetric group $\mathcal{S}_2$. This automorphism can then be written as a mapping $f:\mathbb{Z}\to\mathcal{S}_2$ which attributes to every block Δ_i the respective permutation. An arbitrary bounded automorphism is the combination of such ϕ_I with a translation t and can be written as (t, f) where $t\in\mathbb{Z}$ and $f\in(\mathcal{S}_2)^{\mathbb{Z}}$ are any translation in $\mathbb{Z}$ and any mapping from $\mathbb{Z}$ to $\mathcal{S}_2$, respectively. The multiplication law is given by

$$\begin{cases}(t_2, f_2)(t_1, f_1) = (t_2 + t_1, f_2^{-t_1} f_1),\\ f^{-t}(n) = f(n+t).\end{cases}$$

Note that $(\mathcal{S}_2)^{\mathbb{Z}}$ is provided a group structure with the *pointwise* product $(fg)(n) = f(n)g(n) \in \mathcal{S}_2$. The new group is called the *wreath product* of $\mathbb{Z}$ by $\mathcal{S}_2$ and is in fact the semi-direct product of $\mathbb{Z}$ and $(\mathcal{S}_2)^{\mathbb{Z}}$; this group is denoted $\mathbb{Z}$ Wr $\mathcal{S}_2$.

Although the definition of the wreath product shows no such restriction, we will only need the products $\mathbb{Z}^p$ Wr $\mathcal{S}_n$ to embed the group of bounded automorphisms of a transitive p-periodic net admitting a system of blocks of imprimitivity with n vertices per block. In this case, the formal definition is as above: the elements of the wreath product are written (t, f) where $t \in \mathbb{Z}^p$ and $f \in (\mathcal{S}_n)^{\mathbb{Z}^p}$ are any translation in $\mathbb{Z}^p$ and any mapping from $\mathbb{Z}^p$ to $\mathcal{S}_n$, respectively. The multiplication law is given by the same formula as above.

However, not every periodic net is transitive. In this case, one has to consider separately the action of bounded automorphisms on each orbit, generating the respective embedding in some wreath product and then construct the whole group as a subdirect product of these wreath products. Some periodic graphs are easily dealt with; the periodic graph in Fig. 1, for instance, presents two kinds of blocks of imprimitivity but mappings from $\mathbb{Z}$ to $\mathcal{S}_1$ associated to the blocks $\{A_i\}$ are trivial, so that the group of bounded automorphisms is isomorphic to the wreath product $\mathbb{Z}$ Wr $\mathcal{S}_2$ describing the behaviour of the only blocks $\{B_i, C_i\}$. Other groups are surprisingly much simpler; only three mappings $f \in (\mathcal{S}_3)^{\mathbb{Z}^2}$ are needed to describe the group of bounded automorphisms of the triple **hxl**. These mappings are called *constant* mappings and take any translation in $\mathbb{Z}^2$ to a given permutation in the group generated by the 3-cycle (1, 2, 3). In order to understand the origin of this diversity of groups of bounded automorphisms, we introduce the concept of *correlation groups*, which are built from the quotient Q of the labelled quotient graph N/T by the equivoltage partition.

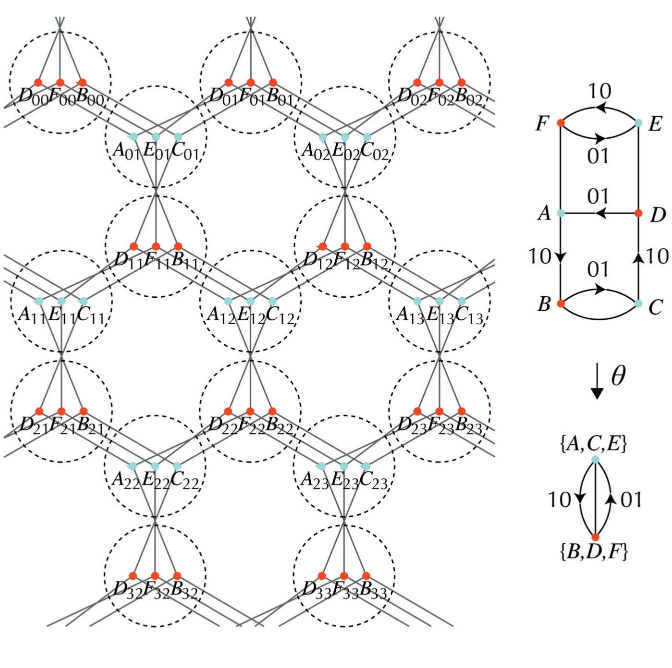

Figure 14
Pseudo-hexagonal representation of the triple **hxl**, an NC net with a system of imprimitivity admitting a freely acting group of bounded automorphisms, its labelled quotient graph and the quotient by an equivoltage partition.

A whole family of correlation groups Γ_t^e for $t \in T$ is associated to every edge e of Q as follows. Let $e = UV$ be an edge of Q with voltage r; U and V represent two – not necessarily different – cells of the equivoltage partition in N/T which are linked by all the edges in the pre-image of e with the same voltage r. Lifting up these cells to the periodic net, we have two blocks of imprimitivity, say U_t and V_{t+r}, for every $t \in T$ which are linked by edges in the pre-image of e. We consider then the subgraph of N induced by the union of the vertices in the blocks U_t and V_{t+r}, that is, the edge set contains all edges in the pre-image of e as well as in the pre-images of the edges with zero voltage inside cells U and V, respectively. The latter clearly link vertices within the same block U_t or V_{t+r}. Among the automorphisms of this graph, we consider only those that stabilize the two blocks, forming the correlation group Γ_t^e, and write them as (p_U, p_V), since they can be embedded in the direct product of the two automorphisms groups Γ_U and Γ_V of the graphs obtained from the cells U and V in N/T by inclusion of edges with zero voltage. We consider now three applications of correlation groups.

8.1. A triple hxl

Fig. 14 shows a triple **hxl**, another NC net already described by Moreira de Oliveira Jr & Eon (2011). By construction, the group of bounded automorphisms acts freely on the net. The labelled quotient graph displays an equivoltage partition whose quotient Q is isomorphic to $K_2^{(3)}$.

Because the quotient Q has three edges, there are three families of correlation groups. We obtain the correlation groups associated to the edge with voltage 10 by deleting in N/T all the edges with voltages 01 and 00, since the latter link vertices in different cells of the partition, and by taking then the automorphisms which preserve the two cells. In this case, the induced subgraph in the periodic net contains the three edges A_tB_{t+10}, C_tD_{t+10} and E_tF_{t+10}, hence for every permutation in the vertex subset $\{A_t, C_t, E_t\}$ there is exactly one permutation in the vertex subset $\{B_{t+10}, D_{t+10}, F_{t+10}\}$. Since the two permutation groups $\mathcal{S}_{\{A_t,C_t,E_t\}}$ and $\mathcal{S}_{\{B_{t+10},D_{t+10},F_{t+10}\}}$ are isomorphic, the correlation group is the *diagonal* subgroup of $\mathcal{S}_{\{A_t,C_t,E_t\}} \times \mathcal{S}_{\{B_{t+10},D_{t+10},F_{t+10}\}}$ containing only permutations $(p, \theta.p.\theta^{-1})$ for any $p \in \mathcal{S}_{\{A_t,C_t,E_t\}}$ where θ is the mapping induced by the edges:

$$\begin{cases} \theta(A_t) = B_{t+10} \\ \theta(C_t) = D_{t+10} \\ \theta(E_t) = F_{t+10}. \end{cases}$$

The same argument is valid for the other two edges of Q, from which we conclude that there is a strong correlation between possible permutations within linked blocks of imprimitivity. Indeed, if the vertex set is permuted in any block by p, the same permutation, up to the respective isomorphism, must occur in every block. This sets to six an upper bound for the order of the stabilizing subgroup $B(N)_\sigma$.

It is, however, necessary to check for the consistency of these correlations in the whole net. Given an initial permutation in some block, the permutation induced in any block should not depend on the path chosen to reach it. Equivalently, correlations should be consistent over strong rings in the net associated to the barycentric representation. In this case, p is the permutation in the block chosen as the origin of the ring and is induced by the sequence of edges along this ring, that is, we correlate the permutation in a block to itself through the equation $p = \theta.p.\theta^{-1}$. For the triple **hxl**, the only strong ring is lifted from the 6-cycle in Q running successively across the edges with voltages 10, 01, 00, $\bar{1}0$, $0\bar{1}$ and 00. It may be verified that the corresponding mapping is given by

$$\begin{cases} \theta(A_t) = E_t \\ \theta(E_t) = C_t \\ \theta(C_t) = A_t \end{cases}$$

and the only permutations that are self-conjugate by θ are those in the cyclic group generated by the permutation (A_t, E_t, C_t).

8.2. Linear graphs with no correlations

The 1-periodic graph shown in Fig. 5 presents two kinds of blocks of imprimitivity containing 1 and 2 vertices, respectively; the 1-periodic graph in Fig. 13 has a single kind of block with 2 vertices. The subgraphs induced in the periodic graphs by an edge in their quotient Q (a single loop with voltage 1) are, respectively, isomorphic to $K_{1,2}$ and $K_{2,2}$, and the associated correlation groups are isomorphic to the full direct products $\mathcal{S}_1 \times \mathcal{S}_2$ and $\mathcal{S}_2 \times \mathcal{S}_2$, respectively, indicating the absence of correlations: blocks are completely independent of their neighbours and the groups of bounded automorphisms are isomorphic to wreath products.

8.3. The double hxl

The examples in the two previous paragraphs correspond to extreme situations. An intermediate case is provided by the double **hxl**. There are two blocks of imprimitivity, one with the edge BC, the other with two independent vertices A and D. There are also two non-isomorphic subgraphs induced in the periodic net by an edge in the quotient Q. The subgraphs induced by the edges with voltages 00 and 01 contain two independent edges, namely AC and BD, whereas that induced by the edge with voltage 10 contains $K_{2,2}$. Hence there are strong correlations for the former and no correlations for the latter. As a result, a permutation in any block will necessarily propagate along the direction 01. In this case, the group of bounded automorphisms is given by the semidirect product of $\mathbb{Z}^2$ and $(\mathcal{S}_2)^{\mathbb{Z}}$.

9. Algorithm

The previous considerations lead us to propose an algorithm to analyse the nature of the subgroup $B(N)_\sigma$, and from it the bounded automorphism group $B(N)$, directly from the labelled quotient graph N/T. This algorithm should be applied when there is some suspicion that a periodic net might be non-crystallographic, for instance when the *Systre* program (Delgado-Friedrichs & O'Keeffe, 2003) crashes.

(*a*) Given a periodic net N defined through a labelled quotient graph, one should determine its barycentric embedding using the cycle–cocycle matrix method (Eon, 2011).

(*b*) If necessary, a common origin should be chosen for all colliding vertex lattices and the labelled quotient graph N/T redrawn, showing an equivoltage partition.

(*c*) Correlation groups should then be analysed for every edge in the quotient Q of N/T by the equivoltage partition, leading to the structure of the group of bounded automorphisms.

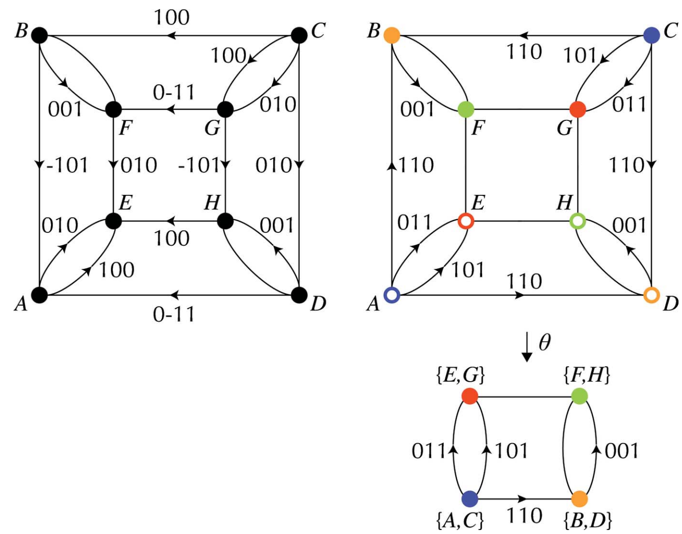

Figure 15
(Top left) the labelled quotient graph of 4/4/o19 (see text), (top right) the labelled quotient graph obtained after changes of origin in vertex lattices evidencing an equivoltage partition and (bottom) the respective quotient.

10. Application: three orthorhombic sphere packings

In a recent paper, Sowa (2012) listed newly found sphere packings with orthorhombic symmetry. Among the associated periodic nets, three display collisions and cannot be studied by *Systre*; these are 4/4/o18, 4/4/o19 and 5/3/o6. We look in thorough detail at the second one.

10.1. 4/4/o19

Fig. 15 displays the labelled quotient graph of the periodic net associated to sphere packing 4/4/o19, as extracted by the program *TOPOS* (Blatov, 2006) from Sowa's data. On applying the cycle–cocycle matrix method to get a barycentric embedding of this net, it is verified that vertex lattices collide by pairs: $\{A, C\}$, $\{B, D\}$, $\{E, G\}$ and $\{F, H\}$. Two vertices in the same pair have been marked with the same colour on the right quotient in this figure, one as an open circle and the other as a full disc. Changes of the origin in the different vertex lattices are necessary to get a common origin for vertices in the same block and yield the labelled quotient graph as displayed. This

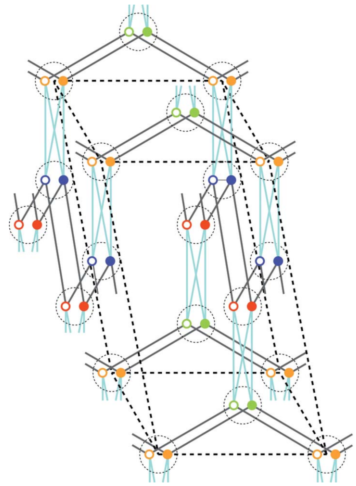

Figure 16
Representation of the net 4/4/*o*19 as a double **ths**; note that a primitive unit cell is described. Vertices are gathered in blocks using the same colours as in the quotient graph; edges lifted from the simple edges in Q and forming a subgraph isomorphic to $K_{2,2}$ are shown in blue, showing lack of correlations between linked 1-periodic lines.

graph clearly has an equivoltage partition with quotient given in the lower part of the figure. This quotient is known as the quotient graph of the minimal net **ths** (Beukemann & Klee, 1992), which allows the representation of the net as a double **ths**, as shown in Fig. 16.

As in the case of the double **hxl**, there are two non-isomorphic subgraphs induced in the periodic net by an edge in the quotient Q. The subgraphs induced by the double edges contain two independent edges, whereas those induced by the two simple edges contain $K_{2,2}$. Hence there are strong correlations for the former and no correlations for the latter. Thus permutations of two vertices in a block should only propagate along the 1-periodic subgraph running in the direction associated with the respective double edge in Q. Since permutations in the orthogonal directions associated with the two double edges in Q behave independently, the group of bounded automorphisms is isomorphic to the semidirect product of $\mathbb{Z}^3$ and $(\mathcal{S}_2)^{\mathbb{Z}^2} \times (\mathcal{S}_2)^{\mathbb{Z}^2}$, which can be embedded in the wreath product $\mathbb{Z}^3$ Wr $(\mathcal{S}_2 \times \mathcal{S}_2)$.

10.2. 4/4/*o*18 and 5/3/*o*6

The analysis of these two nets is similar to the previous one, so that we only present the respective quotient graphs in Fig. 17. The two labelled quotient graphs display an equivoltage partition with two vertices per cell and, strikingly, the quotient by this partition is again isomorphic to the quotient graph of **ths**, hence the two nets may also be drawn as a double **ths**. It appears, however, that all correlations are strong in the case of 4/4/*o*18 so that the stabilizing subgroup $B(N)_\sigma$ is isomorphic to $\mathcal{S}_2$ and the group of bounded automorphisms is isomorphic to the direct product $\mathbb{Z}^3 \times \mathcal{S}_2$. The case of 5/3/*o*6 is identical to that of 4/4/*o*19 with the small difference that vertices in the same block are linked one to the other.

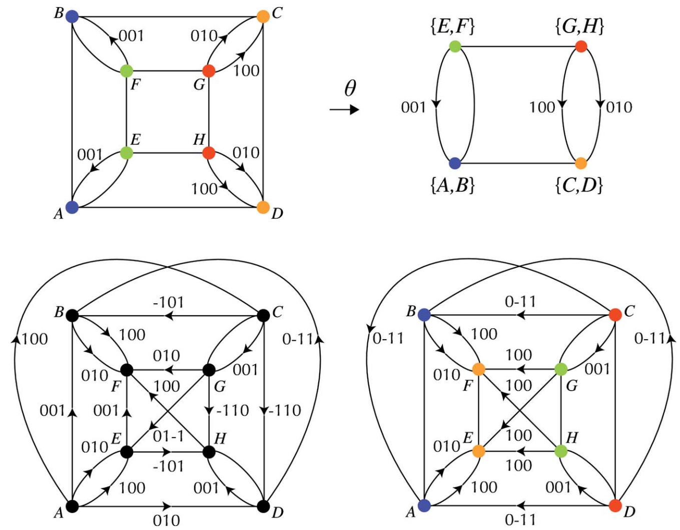

Figure 17
(Top) The labelled quotient graph of 4/4/*o*18 already displays an equivoltage partition with quotient isomorphic to the quotient of **ths**; (bottom) the labelled quotient graph of 5/3/*o*6 must be rewritten with change of origins to yield a graph with an equivoltage partition.

Hence, the three sphere packings are associated to non-crystallographic nets.

11. Final considerations

Non-crystallographic nets are still relatively unknown, but all the examples the authors are aware of display finite blocks of imprimitivity for the subgroup of bounded automorphisms. It should be remembered that some crystallographic nets do display vertex collisions. In this case, it is expected that the labelled quotient graph will have no equivoltage partition after the first step of the algorithm, or when it does, that correlation groups are trivially reduced to the identity, as was seen in the case of the net derived from the Frucht graph.

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