research papers

Acta Crystallographica Section A Foundations of Crystallography

ISSN 0108-7673

Received 1 November 2010 Accepted 18 February 2011

Non-crystallographic nets with freely acting, non-abelian local automorphism groups

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Non-crystallographic (NC) nets are defined as periodic nets whose automorphism groups are not isomorphic to any isometry group in Euclidean space. This work focuses on a simple class of NC nets, restricted to nets with nonabelian, freely acting local automorphism groups. A general method is presented to derive such NC nets from crystallographic nets and some non-trivial examples are explored. It is shown that the labelled quotient graph of these nets does not necessarily possess non-trivial automorphisms which exchange cycles having the same net voltage. However, barycentric representations of these nets systematically display vertex collisions.

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1. Introduction

(a)

(b)

Periodic nets may be used to represent the topology of crystal structures (Wells, 1977; O'Keeffe & Hyde, 1980). Additionally, the space group of the crystal is isomorphic to a subgroup of the automorphism group of the associated net. *p*-Periodic nets whose automorphism group is isomorphic to some *p*-dimensional space group are called crystallographic nets (Klee, 2004). Here, we define a *non-crystallographic net* as a periodic net whose automorphism group is not isomorphic to

lic net whose automorphism group is not isomorphic to B_{00} A_{01} A_{01}

Figure 1

(a) A 2-periodic net and (b) its labelled quotient graph with voltages in \mathbb{Z}^2 .

any isometry group in Euclidean space (of any dimension). It may be noticed that the topology of many ideal crystal structures is represented by a crystallographic net, although no physical reason has ever been invoked to explain this observation. As a matter of fact, examples of noncrystallographic (NC) nets are still quite rare (Chung *et al.*, 1984; Delgado-Friedrichs, 2005).

Periodic nets are infinite graphs, so their labelled quotient graphs, which are finite graphs, are more convenient to handle (Chung *et al.*, 1984). In particular, generation of *p*-periodic nets can be done routinely by assigning different vector labels from the translation group \mathbb{Z}^p to the edges of any finite graph with at least *p* independent cycles (Bader *et al.*, 1997). Although the net is uniquely determined by its labelled quotient graph, it is by no means clear whether one can determine the whole automorphism group of the net from the sole examination of its labelled quotient graph. Let us consider an example.

The 2-periodic net N drawn in Fig. 1(a) admits the automorphism $\varphi_N = (B_{00}, C_{00})$ which exchanges the two vertices B_{00} and C_{00} and fixes every other vertex. It is a kind of reflection symmetry which acts locally, on a single unit cell. This 2-periodic net is thus an NC net. Now, on examining its labelled quotient graph G in Fig. 1(b), one can see that there is an automorphism, say ϕ_G , which exchanges the two vertices B and C as well as the edges AB and AC with the same vector labels. However, ϕ_G induces the automorphism of the net which exchanges every pair of vertices B_{ij} and C_{ij} , while fixing vertex lattice A; this automorphism is readily seen to commute with the translation group of the net. However, the existence of φ_N is not implied by that of ϕ_G .

The existence in a labelled quotient graph of non-trivial automorphisms which exchange cycles having the same *net voltage* (*i.e.* the same sum of vector labels over their edges following the orientation of the cycle) may nonetheless reveal the non-crystallographic nature of the derived net (Eon, 2005). One of the objectives of this paper is to display an infinite family of NC nets whose labelled quotient graph does not even possess such automorphisms.

Why should we study NC nets? Clearly, in a systematic derivation of nets performed by assigning every possible vector label in \mathbb{Z}^p to the edges of some finite graph, it should be of great help to be able to tell apart crystallographic nets from NC nets by direct examination of their quotient. Besides, crystals whose topology is represented by an NC net might well exhibit unforeseen properties owing to some flexibility in the structure. For instance, profiting by the 2-periodic net in Fig. 1, one may fancy applying to information storage any compound which realizes this topology, where each unit cell provides one bit. In other words, the search and synthesis of such materials might become in itself a (challenging) goal to the chemist.

In this paper, we study specifically NC nets with nonabelian, freely acting local automorphism groups. We show how to construct an infinite family of NC nets such that their quotient graphs admit no automorphisms that exchange cycles having the same net voltage. But we also show that any barycentric representation of these nets displays collisions.

§2 gives a short account of the principal mathematical tools from graph and group theory that are needed to follow the paper. The fundamental results of this work are stated in §3, where it will be shown in particular that any barycentric representation of an NC net with non-abelian, freely acting local automorphism group admits vertex collisions. §4 presents a general two-step procedure to generate an infinite family of such nets. This procedure and non-trivial examples are explored in §§5–7. It is shown that the local automorphism group may be inserted in a direct product $\mathcal{H} \times \mathbb{Z}^n$ where \mathcal{H} is a finite non-abelian group. §8 generalizes this result and develops a direct (one-step) method for generating NC nets from crystallographic ones.

2. Mathematical tools

Most of the following definitions are in accordance with Harary (1972). A graph G = (V, E, m) is a pair of vertex set V and edge set E with an incidence mapping $m: E \longrightarrow V^2$. If m(e) = (A, B), we use the notation e = AB and say that e runs from the source A to the end B. Although this definition does not apply to loops, it is easily extended to cover this case (Eon, 2011). The *edge space* of G is formally defined as the vector space on \mathbb{R} admitting the edges of G as basis vectors. A coboundary of a subset U of vertices is defined (Harary, 1972) as the combination of edges joining the vertices of U to the vertices that are not in U. The co-cycle space is defined as the subspace of the edge space containing all the linear combinations of co-boundaries; this space may be generated by the set of co-boundaries of single vertices. A cycle of G is a combination of edges inducing a connected subgraph of degree 2. The cycle space is the subspace of the edge space containing all the linear combinations of cycles. The cyclo*matic number* of the graph is the dimension of its cycle space and is given by c = |E| - |V| + 1 where |E| and |V| are the cardinality of the edge and vertex set, respectively. It is known that the edge space is the direct sum of the cycle and co-cycle spaces of the graph (Godsil & Royle, 2004).

An *automorphism* of *G* is a pair (f_V, f_E) of bijective mappings of *V* and *E* on themselves respecting the incidence mapping: $f_E(e) = f_V(A)f_V(B)$ for e = AB. It is a *local automorphism* if the distance between any vertex and its image by *f* is uniformly bounded by some constant. An automorphism *f* is said to *act freely* on *G* if there is no fixed element, that is: $f(X) \neq X$ for every $X \in V \cup E$. The automorphism group of *N* is denoted Aut(*N*).

A net is a simple 3-connected graph which is locally finite (i.e. vertex degrees are finite). 3-Connectedness is not so restrictive a condition as it might seem. For instance, the topology of some crystal structures with 2-coordinated atoms such as oxygen in zeolites is strictly represented by a 2-connected graph. By convention, the graph is then contracted, that is: every link A-O-B where O has degree 2 is substituted by a single edge AB. The resulting graph is 3-connected and no topological information has been lost. We say that the pair (N, T) is a *p*-periodic net if N is a net and $T < \operatorname{Aut}(N)$ is a free abelian group 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. Crystallographic nets are p-periodic nets whose automorphism group is isomorphic to some *p*-dimensional space group (Klee, 2004). We shall say that a periodic net is non-crystallographic if its automorphism group is not isomorphic to any isometry group in Euclidean space. In particular, the automorphism group of an NC net cannot be isomorphic to a subperiodic (layer or rod) group. If (N, T) is a periodic net, we denote, respectively, by V/T and E/T the sets of vertex and edge orbits (or lattices) of N by T, and q_T the mapping which sends an *element* (vertex or edge) X to its orbit [X]. The quotient graph is the graph $N/T \equiv (V/T, E/T, m_T)$, where m_T is given by $m_T([e]) = ([A], [B])$ for an edge $e = AB \in E$. The mapping q_T is called the *natural projection* of (N, T) to its quotient graph N/T. If an origin A_0 is chosen in every vertex lattice [A] of the net and every vertex indexed by the translation t which maps to it the origin of the respective lattice, one may assign to every edge [e] = [A][B] of the quotient graph the index t of the edge $A_0 B_t \in [e]$. The correspondence between the periodic net and the labelled quotient graph is one-to-one, up to the choice of lattice basis and origins. For example, the square net, pcu, is a 2-periodic net with one vertex and two translationally nonequivalent edges per unit cell. Since every edge joins two vertices from the same vertex lattice, the quotient graph of pcu by its translation group is the graph with one vertex and two loops at this vertex, called the *bouquet* B_2 . Because any edge of **pcu** links a vertex U to the translated vertex t(U), where t is the translation 01 or 10, we assign one of these translations to each loop of B_2 . With this assignment, B_2 unequivocally represents the square net.

Labelled quotient graphs are a special case of *voltage* graphs. Following Gross & Tucker (2001), a voltage graph

 (G, α) is given by a graph G with an orientation and an assignment $\alpha: E \to \mathcal{A}$ from the edge set of G to an arbitrary, possibly non-abelian group A such that $\alpha(e)\alpha(-e) = 1$, where 1 is the identity of the group. The net voltage on an oriented walk $w = e_1 e_2 \dots e_n$ is the product of the voltages along the oriented edges of w in the same order: $\alpha(e_1)\alpha(e_2)\ldots\alpha(e_n)$. From any voltage graph, one generates a unique graph, called the *derived* graph G^{α} . The derived graph is an oriented graph with vertex set $V \times A$, edge set $E \times A$ and incidence relation (e, a) = (u, a)(v, ab) for any $a \in \mathcal{A}$ if e = uv has voltage b. We often use the shorthand notation $(u, a) = u_a$ so that the incidence relationship reads $e_a = u_a v_{ab}$. G is called the *base* graph of G^{α} . The group \mathcal{A} acts freely on the derived graph G^{α} if the action of $f \in \mathcal{A}$ on the vertex (or edge) $x_a \in G^{\alpha}$ is given by $f(x_a) = x_{fa}$. This property ensures that the natural projection mapping $x_a \in G^{\alpha}$ to $x \in G$ is a *covering* projection [*i.e.* for every vertex, the set of outgoing (respectively, ingoing) edges is mapped one-to-one to the set of outgoing (respectively, ingoing) edges at its image]. Notice the left action of f on the voltage a in the definition of the automorphism compared to the right action of the voltage b in the definition of the incidence mapping. As a simple example of a voltage graph, we may take the bouquet B_2 with vertex U where the two loops l and l' are now assigned voltages 0 and 1, respectively, in $\mathbb{Z}/3\mathbb{Z}$ (the additive group $\{0, 1, 2\}$ satisfying 1 + 2 = 0). The derived graph thus has three vertices U_i , $i \in \mathbb{Z}/3\mathbb{Z}$ and six edges l_i and l'_i , $i \in \mathbb{Z}/3\mathbb{Z}$. Edge l_i runs from U_i to $U_{i+0} = U_i$ and is thus a loop at U_i ; edge l'_i runs from U_i to U_{i+1} so that the three edges derived from the loop l' form a triangle.

Definitions and properties of geodesic paths and fibres can be found in Eon (2007). We just mention that a *geodesic fibre* in a periodic net is a minimal 1-periodic subgraph containing all *geodesic* (*i.e.* shortest) paths in the net between any pair of its vertices. Geodesic fibres are topological invariants whose main property is that local automorphisms in periodic nets (N, T) map fibres onto parallel fibres. Only the special case of *strong geodesic lines*, or strong geodesics, is needed in this work: a strong geodesic in a periodic net is defined as a twoway infinite path which contains the unique geodesic path in the net between any pair of its vertices. A strong geodesic in the periodic net (N, T) projects onto a shortest cycle of the quotient graph N/T and is mapped on a parallel strong geodesic by any local automorphism.

A linear representation ρ of a graph in 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. A representation presents vertex collision if different vertices are mapped on the same Euclidean point. A barycentric representation of a periodic net is a periodic, linear representation of the net where every point is located at the centre of gravity of its first neighbours. 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 barycentric representation of the derived net with the given lattice, up to translation (Delgado-Friedrichs, 2005). Let *m* and *n* be, respectively, the number of edges and vertices of the quotient N/T of a *p*-periodic net (N, T). Let (e_i) be the $m \times 1$ matrix associated with the basis of the edge space of N/T, and let (C_i) be the $m \times 1$ matrix associated with the *cycle-co-cycle basis*, where the sets $\{C_i : 1 \le i \le m - n + 1\}$ and $\{C_i : m - n + 1 < i \le m\}$ form, respectively, a basis of the cycle space and a basis of the co-cycle space of N/T. Let $[\alpha(C_i)]$ be the $m \times p$ voltage matrix associated with its cycle-co-cycle basis: the first m - n + 1 rows of $[\alpha(C_i)]$ give the net voltages on the cycles in the cycle basis of N/T, and the remaining n - 1 rows, which give the projection of the co-cycle basis, are the zero vector for a barycentric representation. If K is the $m \times m$ matrix whose rows give the expression of the cycle and co-cycle basis vectors with relation to the edge vectors, then $(C_i) = K(e_i)$, or $(e_i) = K^{-1}(C_i)$ and the edges of N/T are mapped in the barycentric representation (Eon, 2011) to the rows of the matrix

$$[\rho(e_i)] = \mathsf{K}^{-1}[\alpha(C_i)]. \tag{1}$$

3. Freely acting local automorphism groups

The objective of this section is to show that any barycentric representation of an NC net which admits a non-abelian, freely acting local automorphism group presents vertex collisions. Observe that this would be more easily proved if we could find, for every automorphism of the net, a representative automorphism acting on its quotient graph. Let (N, T) be a periodic net with translation group T, and let L be the local automorphism group of the net. In general, a local automorphism φ of (N, T), not contained in T, does not respect the vertex and edge lattices of (N, T). This implies that it is not possible to define a consistent action, induced by φ , on the quotient graph N/T. But we might circumvent the difficulty by working with a special subgroup S of T that commutes with φ ; S should then belong to the centre of L. We show here that such a subgroup of T does exist and that it has finite index in L and T.

Lemma 3.1. Suppose that L, the local automorphism group of the periodic net (N, T), acts freely on the net. Let $\varphi \in L$ and $t \in T$; then there exists a translation in $\langle t \rangle$ which commutes with φ .

Proof. Denote by $|\varphi|$ the maximum distance in N between a vertex and its image by φ . Consider an arbitrary vertex V of N and the set of images $\{V_n = t^{-n}\varphi t^n(V) : n \in \mathbb{N}\}$. We have then $d(V, V_n) = d[t^n(V), \varphi t^n(V)] \le |\varphi|$. Since the net is locally finite, $V_m = V_n$ for at least two different integers m and n. Let p = m - n > 0; then $t^p \varphi(V) = \varphi t^p(V)$ and since the only local automorphism with a fixed vertex is the identity, we conclude that $t^p \varphi = \varphi t^p$.

Theorem 3.1. If the local automorphism group L of a periodic net (N, T) acts freely on the net, then L is finitely generated and its centre contains a subgroup $S \le T$ of finite index in L.

Proof. Since L acts freely on the net, it is possible to define the quotient graphs $G_T = N/T$ and $G_L = N/L$ together with the respective quotient maps q_T and q_L (see Fig. 2). Notice

that G_L is finite, since $T \leq L$. Let λ and τ be voltage assignments for G_L and G_T in L and T, respectively, such that the derived graphs G_L^{λ} and G_T^{τ} are isomorphic to N. [According to Gross & Tucker (2001), such assignments always exist.] That L is finitely generated is readily seen, since N is connected and the voltages of G_L form a set of generators. Since both L and T are finitely generated, we may apply Lemma 3.1 to every pair of generators (α , t) $\in L \times T$ and hence find a subgroup $S \leq T$ of finite index in T which commutes with any local automorphism of N, and so belongs to the centre of L.

Note that N/S is a finite graph since *S* has finite index in *T*. Fig. 2 depicts the whole set of relations between the net and its three quotients, *i.e.* the natural projection q_S of the net to its quotient N/S and the covering projections θ_{TL} , θ_{SL} and θ_{ST} . For instance, we define θ_{TL} , the projection from G_T to G_L , by $\theta_{TL}[q_T(x)] = q_L(x)$, for $x \in N$. With these definitions, the diagram shown in Fig. 2 is commutative.

We can now prove the result that was anticipated at the beginning of this section.

Corollary 3.1. If the local automorphism group L of a periodic net (N, T) is non-abelian and acts freely on the net, then any barycentric representation of the net presents collisions.

Proof. According to Delgado-Friedrichs (2005), a local automorphism $\varphi \in L$ is a *periodic automorphism* of the periodic net (N, S) since it commutes with any translation of S. Hence, following Corollary 9 of this reference, φ acts as a translation on any barycentric representation of (N, S). But clearly, for a given origin and lattice basis, (N, S) and (N, T) admit the same barycentric representation. If L is non-abelian, we can find two local automorphisms φ and ψ and a vertex U in the net such that $\varphi \psi(U) \neq \psi \varphi(U)$. However, φ and ψ act as (commuting) translations on the barycentric representation of the net, so that the two vertices $\varphi \psi(U)$ and $\psi \varphi(U)$ are represented by the same Euclidean point. In other words, any barycentric representation of the net shows vertex collisions.

More generally, the whole local automorphism group L acts as a translation group \mathcal{T} on any barycentric representation of the net N. As a consequence, there is a graph homomorphism from the quotient N/L onto the quotient $\rho(N)/\mathcal{T}$ of the barycentric representation $\rho(N)$ by \mathcal{T} .

4. Generation of NC nets

This section describes a procedure for generating NC nets with non-abelian, freely acting local automorphism groups. The key is the construction of the voltage graph N/S. Because any automorphism $\varphi \in L$ commutes with S, it preserves vertex and edge lattices by S as well as incidence relationships between them; hence it induces an automorphism of N/S (the graph of the lattices). Because φ is a local automorphism of N, the induced automorphism of N/S maps cycles to cycles having the same net voltage (Eon, 2005). The group \mathcal{H} of these automorphisms induced in N/S should also act freely on N/Sand be non-abelian. It is clear from Fig. 2 that the quotient of N/S by \mathcal{H} is isomorphic to the quotient N/L. This means that we may derive N/S from N/L by voltage assignment in \mathcal{H} . We thus start our procedure with a finite graph P to which we assign as voltages the elements of a set of generators of a finite, non-abelian group \mathcal{H} . We know then that \mathcal{H} acts freely on the derived graph D (Gross & Tucker, 2001). It remains to assign voltages in \mathbb{Z}^n to D in such a way that cycles which are in the same orbit by \mathcal{H} obtain the same net voltage. A periodic net Nmay then be derived, which admits a non-trivial local automorphism group L.

The next section details every step of the construction applied to a simple example. We analyse the properties of the net and those of its local automorphism group L. In particular, we determine its maximal translation groups T, together with the respective labelled quotient graphs N/T. We find the quotient N/L, write it as a voltage graph with assignments in Land analyse the relation with the barycentric representation of the net.

5. The graph B_2 with voltages (1,2) and (1,2,3) in S_3

We consider here the simplest possible case, when the base graph P is the bouquet B_2 assigning as voltages to the loops the transposition (1, 2) and the cyclic permutation (1, 2, 3), taken as generators of S_3 , the group of the permutations of the three elements in the set $\{1, 2, 3\}$. For the sake of simplification, we shall write 12 and 123 instead of using the full cyclic notations (1, 2) and (1, 2, 3), respectively. The base graph and its derived graph D are shown in Fig. 3, where the labels of vertices and edges of D were obtained as explained in §2. The voltage group has order six and the base graph contains one vertex and two edges; hence the derived graph contains $6 \times 1 = 6$ vertices and $6 \times 2 = 12$ edges. As in the base graph, each vertex U_p of the derived graph is the source of two edges a_p and b_p for $p \in S_3$ (and the end point of two edges). For instance, edge a_{12} runs from vertex U_{12} to vertex $U_{12,12} = U_e$ and edge b_{12} runs from vertex U_{12} to vertex $U_{12.123} = U_{23}$ (permutations in a product are applied from right to left).

We know that the voltage group S_3 acts freely on the derived graph D. To avoid confusion, let us call \mathcal{H} the subgroup of Aut(D) that is isomorphic to S_3 . Let us denote by ϕ_p the automorphism of D in correspondence with $p \in S_3$. The action of the two generators ϕ_{12} and ϕ_{123} of \mathcal{H} is given by the



Figure 2 Projections between a periodic net *N* and its different quotient graphs.

following permutations of the elements x_p (vertices or edges) of *D*:

$$\phi_{12} = (x_e, x_{12})(x_{13}, x_{132})(x_{123}, x_{23}), \qquad (2)$$

$$\phi_{123} = (x_e, x_{123}, x_{132})(x_{13}, x_{23}, x_{12}). \tag{3}$$

[Remember the left action of the voltage. For instance: $\phi_{12}(x_{13}) = x_{12,13} = x_{132}$.]

We look now for possible voltages on D in order to generate a periodic net N. These voltages are chosen in a translation group in such a way that every automorphism of \mathcal{H} sends cycles to cycles of the same net voltage. D has cyclomatic number 7; we may choose as independent cycles for a cycle basis the three 2-cycles, the internal 3-cycle and the three 4-cycles limiting the regions of the plane in Fig. 3, all with clockwise orientation. It is apparent that the three 2-cycles are equivalent by \mathcal{H} and so must obtain the same net voltage, as is also the case for the three 4-cycles. The internal and external 3-cycles are also exchanged by ϕ_{12} , but with reversal of their orientation. Let us call $\alpha(C_n)$ the net voltage on the *n*-cycle (n = 2, 3, 4) in the cycle basis; the net voltage on the external 3-cycle must then be $-\alpha(C_3)$. On the other hand, the external 3-cycle is the sum of all the cycles of the basis, which gives then the following relation between net voltages:

$$3\alpha(C_2) + 3\alpha(C_4) + \alpha(C_3) = -\alpha(C_3).$$
 (4)

Because of the existence of this relation between the net voltages of the three (remaining) independent cycles, the periodicity of the derived net will be at most 2. This equation may be parameterized as

$$\begin{cases} \alpha(C_3) = -3t, \\ \alpha(C_2) + \alpha(C_4) = 2t. \end{cases}$$
(5)







The graph D of §5 with voltages in \mathbb{Z}^2 . Edge labels are given in parentheses.

A possible choice of voltage assignment, corresponding to t = 10 and $\alpha(C_2) = 01$, is shown in Fig. 4. In fact, any other assignment such that $\alpha(C_2)$ and $\alpha(C_4)$ are linearly independent generates an isomorphic 2-periodic net.

Owing to a great number of crossings, representations of NC nets may be highly confusing. The representation of the 2-periodic net N derived from D, which is displayed in Fig. 5, has been drawn as a distortion of a barycentric representation of the net; for the sake of clarity, and quite informally, we shall refer to such a representation as a *pseudo-barycentric* representation. Using edge labels shown in Fig. 4, seven cycles were chosen to form the basis of the cycle space: (1,8,5,4), (2,3,10,11), (2,4), (6,8), (10,12), (3,9,5) and (1,7,11). Five co-



Figure 5

A representation of the NC net derived from the voltage graph given in Fig. 4. Vertices that collide in barycentric representations of the net have been segregated within black circles and form two classes: $\{A, B, C\}$ and $\{D, E, F\}$.

cycles were chosen to form the basis of the co-cycle space: (1,2,-4,-11), (7,8,-1,-6), (11,12,-7,-10), (3,4,-2,-5) and (5,6,-8,-9). The matrices associated with the cycle-co-cycle basis K, and the lines in any barycentric representation are, respectively,

The 12 × 2 matrix multiplying K^{-1} is, according to equation (1), the voltage matrix $[\alpha(C_i)]$ associated with the cycle– co-cycle matrix K. For instance, the first row of K corresponds to cycle (2,4) with net voltage 01; the last five rows of K correspond to vectors from the co-cycle basis which are mapped to the zero vector in barycentric representations. As expected, the 12 edges of the quotient graph *D* are represented by only two vectors in \mathbb{R}^2 : the edges with odd labels, pre-images of the edge *b* of the base graph *P*, are represented by (1, 0), and the edges with even labels, pre-images of the edge *a* of *P*, are represented by (0, 1/2).

The representation of some edges of the net as vectors of the unit cell implies the occurrence of collisions. For instance, vertex A_{ij} is linked to B_{i+1j} by an edge represented by the vector (1, 0), meaning that the representative points satisfy $\rho(B_{i+1j}) = \rho(A_{ij}) + (1, 0) = \rho(A_{i+1j})$. This observation extends to every pair of vertices linked by edges that belong to the preimage of edge *b* in the base graph *P*, whence we obtain a collision of all vertices in the net by triples:

$$\begin{cases} \rho(A_{ij}) = \rho(B_{ij}) = \rho(C_{ij}) = \rho(A_{00}) + (i, j) = (i, j), \\ \rho(D_{ij}) = \rho(E_{ij}) = \rho(F_{ij}) = \rho(D_{00}) + (i, j) = (i, j - 1/2). \end{cases}$$
(8)

Notice that the barycentric representation of the net is the square lattice, in agreement with the observation ending §3. This can be seen from Fig. 5 by allowing the three vertices

inside every black circle to collapse into a single vertex and thereafter substituting each generated set of multiple edges by a single edge.

We now look for a complete description of the local automorphism group L of the net. The first motivation is to check that L acts freely on the net, in order to validate our construction. But it is also instructive to determine a maximal translation subgroup $T \ge S$ and to analyse the automorphisms of the respective labelled quotient graph N/T.

By construction, we know that \mathcal{H} acts freely and (vertex-) transitively on *N/S*. Since \mathcal{H} also preserves the net voltages on cycles of *N/S*, we can derive at least one local automorphism sending vertex A_{00} to an arbitrary vertex X_{ij} ($X = A, B, \ldots F$) of the net and respecting the vertex lattices by *S*.

Observe now that, among all cycles in N/S, the 2-cycles with voltage 01 and the 3-cycles with voltage 30 have the shortest reduced length (see Eon, 2007). Hence, their pre-images in N are strong geodesic lines. Through any vertex of the net there runs exactly one strong geodesic parallel to 10 and one parallel to 01. Moreover, the whole net is connected through these geodesic lines: every edge of N belongs to some geodesic line from one or the other family. (These properties permitted us to represent the two families of geodesics as horizontal and vertical lines, respectively, in Fig. 5, drawn with different colours to distinguish crossing geodesics). Since local automorphisms map strong geodesic lines to parallel strong geodesic lines (Eon, 2007), it follows that there is a single automorphism mapping A_{00} to X_{ij} and thence that L acts freely on N.

Let α and β denote the local automorphisms lifted from ϕ_{12} and ϕ_{123} which send A_{00} to its first neighbours D_{01} and B_{10} , respectively. With the help of Fig. 5, the definition of the two automorphisms may be completed as follows:

$$\alpha : \begin{cases} A_{ij} \to D_{ij+1} \to A_{ij+1} \\ B_{ij} \to F_{ij+1} \to B_{ij+1} \\ C_{ij} \to E_{ij+1} \to C_{ij+1} \end{cases}$$
(9)

$$\beta: \begin{cases} A_{ij} \to B_{i+1j} \to C_{i+2j} \to A_{i+3j} \\ D_{ij} \to F_{i+1j} \to E_{i+2j} \to D_{i+3j} \end{cases}.$$
 (10)

The previous results showed that L acts freely and (vertex-) transitively on the net. Hence, the quotient graph N/L is well defined and is isomorphic to the bouquet B_2 . Of course, α and β may be taken as the voltages in N/L of the loops a and b, respectively (see Fig. 3). As a consequence, α and β are two generators of L. It is worth noting that the two automorphisms α and β act as translations along 01 and 10, respectively, on the barycentric representation of the net (Fig. 5).

The fact that every automorphism in L is uniquely associated with (i) an automorphism in \mathcal{H} and (ii) a translation of the barycentric embedding suggests inserting L into the direct product $S_3 \times \mathbb{Z}^2$ by using the following correspondence:

$$\begin{cases}
A_{ij} \to [e; (i, 2j)] \\
B_{ij} \to [123; (i, 2j)] \\
C_{ij} \to [132; (i, 2j)] \\
D_{ij} \to [12; (i, 2j-1)] \\
E_{ij} \to [23; (i, 2j-1)] \\
F_{ij} \to [13; (i, 2j-1)].
\end{cases}$$
(11)

On the left-hand side, vertices X_{ij} (X = A, B, ..., F) in N have been labelled as derived from N/S with voltage in \mathbb{Z}^2 . On the right-hand side appears the pair $(p; t) \in S_3 \times \mathbb{Z}^2$ where $\phi_p \in \mathcal{H}$ maps A to X and $t \in \mathbb{Z}^2$ is the translation mapping $\rho(A_{00})$ to $\rho(X_{ij})$ in the barycentric embedding. Note the factor 2 in the second component of the translation coordinate which takes into account the fractional coordinates in the barycentric embedding. We obtain the desired insertion by noting that each vertex of the net may be derived directly from B_2 with voltages in L, and labelled as U_{φ} with single index $\varphi \in L$, hence given on the right-hand side in the above display. In particular, the translation group S of N is the subgroup $\{[e; (i, 2j)] : (i, j) \in \mathbb{Z}^2\}$. As usual, the group operation in $S_3 \times \mathbb{Z}^2$ is defined by

$$(p_1; t_1)(p_2; t_2) = (p_1 p_2; t_1 + t_2),$$
(12)

which is consistent with the action of L on the net given by $\varphi_1 U_{\varphi_2} = U_{\varphi_1 \varphi_2}$ [the two components p and t of $\varphi = (p, t)$ act separately on N/S and on the barycentric embedding of N, respectively]. L is clearly a non-trivial subgroup of $S_3 \times \mathbb{Z}^2$. It is in fact a *subdirect product* of S_3 and \mathbb{Z}^2 (*i.e.* the projections defined by the first and second coordinates p and t are surjective mappings over S_3 and \mathbb{Z}^2 , respectively). The two generators of L may be identified as

$$\alpha = [12; (0, 1)]; \quad \beta = [123; (1, 0)]. \tag{13}$$

We look now for maximal extensions of *S*, that is: maximal translation subgroups of the net. It is readily seen that α extends *S*, yielding a free abelian subgroup *T* of *L*. Adding to *S* any other automorphism with a transposition 12, 13 or 23 as the first coordinate would also work. On the other hand, cyclic permutations of order 3 cannot be used. Let us add, for instance, [123; (i, 2j)] to *S*; then the extension also contains $\varphi = [123; (0, 0)]$, which verifies $\varphi^3 = e$, and so is not a free group. This means that *T* itself cannot be extended by another automorphism with a transposition 13 or 23 as its first coordinate, since then it would also contain an automorphism with



Figure 6

The quotient N/T of the net represented in Fig. 5, with vertex classes $[A] = \{A, D\}, [B] = \{B, E\}$ and $[C] = \{C, F\}$. Note that the translation vector along 01 in T is half that in S in the same direction; translation vectors along 10 are equal in both groups.

the permutation 123 as the first coordinate. Hence, there are exactly three isomorphic maximal extensions of S. Fig. 6 shows the quotient graph N/T.

Before leaving this section, we stress that, although the derived net is not a crystallographic net, there are no non-trivial automorphisms of N/T that preserve the net voltage on the cycles.

6. The graph B_2 with voltages (1,2) and (1,3) in S_3

Suppose now that the base graph P is the graph B_2 with voltages 12 and 13. The derived graph D is described in Fig. 7.

Using the same notations as in §5, the action of the two generators ϕ_{12} and ϕ_{13} of \mathcal{H} is given by the following permutations of the elements x_p (vertices or edges) of D:

$$\phi_{12} = (x_e, x_{12})(x_{13}, x_{132})(x_{123}, x_{23}), \tag{14}$$

$$\phi_{13} = (x_e, x_{13})(x_{12}, x_{123})(x_{132}, x_{23}). \tag{15}$$

Reasoning as above, it can be seen that there is a unique twodimensional net, up to isomorphism, admitting D as its quotient graph and such that the action of ϕ_{12} and ϕ_{13} maps cycles to cycles with the same net voltage. The corresponding labelled quotient graph is shown in Fig. 8 and the derived net in Fig. 9.

Again, it may be checked that the 12 edges of N/S are represented by only two vectors in barycentric representations: the edges 1, 2, 5, 6, 9, 10 by (1, 1/2) and the edges 3, 4, 7, 8, 11, 12 by (0, 1/2) (see Fig. 8 for edge labels). It results that the three vertex lattices A, C and E collide, as well as the three



Figure 7 The base graph P of §6 and the derived graph D.

vertex lattices B, D and F. Again, the barycentric representation of the net N is the square lattice, as may be seen in Fig. 9 after allowing vertices inside the black circles to collide.

The different coordinates are as follows:

$$\begin{cases} \rho(A_{ij}) = \rho(C_{ij}) = \rho(E_{ij}) = \rho(A_{00}) + (i, j) = (i, j), \\ \rho(B_{ij}) = \rho(D_{ij}) = \rho(F_{ij}) = \rho(F_{00}) + (i, j) = (i, j + 1/2). \end{cases}$$
(16)

The pre-image of every 2-cycle of the quotient graph N/S is again a strong geodesic line and, as above, it may be seen that the local automorphism group L acts freely and transitively on the net. Therefore, the quotient graph N/L is once again isomorphic to the bouquet B_2 and only two generators are needed. We may also embed L in the direct product $S_3 \times \mathbb{Z}^2$ with the following correspondence between a vertex in the net and the pair of group elements mapping A_{00} to this vertex (as above),

$$\begin{cases}
A_{ij} \to [e; (i, 2j)] \\
B_{ij} \to [12; (i, 2j+1)] \\
C_{ij} \to [132; (i, 2j)] \\
D_{ij} \to [23; (i, 2j+1)] \\
E_{ij} \to [123; (i, 2j)] \\
F_{ij} \to [13; (i, 2j+1)].
\end{cases}$$
(17)

The two generators of L may now be identified as

$$\alpha = [12; (1, 1)]; \quad \beta = [13; (0, 1)]. \tag{18}$$

The translation group *S* of *N* is the same subgroup $\{[e; (i, 2j)] : (i, j) \in \mathbb{Z}^2\}$. Again, three isomorphic extensions of *S* are possible by adding any automorphism with a transposition as its first coordinate. The labelled quotient graph is shown in Fig. 10, where it is apparent that there are no automorphisms that preserve the voltage of the cycles in N/T.

The two nets represented in Figs. 5 and 9 appear to have so many similarities that it is legitimate to ask whether they are isomorphic. They are not, as shown by the analysis of linked pairs of parallel strong geodesic lines. Consider two linked parallel geodesic lines -A-B-C- and -D-E-F- in the first net, drawn as orange lines in Fig. 5. They are only linked by edges



Figure 8

The graph D of §6 with voltages in \mathbb{Z}^2 . Edge labels are given in parentheses.





A pseudo-barycentric representation of the NC net derived from the voltage graph given in Fig. 8. Vertices that collide in barycentric representations of the net have been segregated within black circles and form two classes: $\{A, C, E\}$ and $\{B, D, F\}$.

AD, that is: the induced (infinite) subgraph is a ladder with two vertices of degree 2 between two rungs. There is no such subgraph in the second net, where every linked pair of strong geodesic lines shows one vertex of degree 2 alternating with a rung. Notice that the argument on the net possesses a (less clear) counterpart on the quotient graphs (N/S). The ladder in the first net projects on the subgraph of the quotient graph in Fig. 4 containing the two 3-cycles and the edge AD with label 4. Linked pairs of geodesics in the second net project on 2-cycles linked by a single edge.

7. The graph $K_2^{(3)}$ with voltages *e*, (1,2) and (1,3) in S_3

The bouquet with its two loops is a very particular case. Less trivial is the example of the graph $K_2^{(3)}$ with voltages 12 and 13 in S_3 . The derived graph *D* is displayed in Fig. 11 and a choice of voltage assignment in Fig. 12.



Figure 10

The quotient N/T of the net represented in Fig. 9, with vertex classes $[A] = \{A, B\}, [C] = \{C, F\}$ and $[D] = \{D, E\}$. Note that the translation vector along 01 in T is half that in S in the same direction; translation vectors along 10 are equal in both groups.



Figure 11 The base graph P of §7 and the derived graph D.

The pseudo-barycentric representation of the derived net is drawn in Fig. 13. The barycentric representation of N is the honeycomb, in agreement with the observation ending §3. We may embed L in the direct product $S_3 \times \mathbb{Z}^2$ with the following correspondence:

$$\begin{cases}
A_{ij} \rightarrow [132; (i, 2j)] \\
C_{ij} \rightarrow [123; (i, 2j)] \\
E_{ij} \rightarrow [e; (i, 2j)] \\
H_{ij} \rightarrow [12; (i, 2j - 1)] \\
J_{ij} \rightarrow [13; (i, 2j - 1)] \\
L_{ii} \rightarrow [23; (i, 2j - 1)].
\end{cases}$$
(19)

The two generators of L may now be identified as

$$\alpha = [12; (1, 1)]; \quad \beta = [13; (0, 1)]. \tag{20}$$

The translation group *S* of *N* is the same subgroup $\{[e; (i, 2j)] : (i, j) \in \mathbb{Z}^2\}$. Again, three isomorphic extensions of *S* are possible by adding any automorphism with a transposition as its first coordinate. The labelled quotient graph is shown in Fig. 14, where it is apparent that there are no automorphisms that preserve the voltage of the cycles in N/T.

Interestingly, the net that may be derived from $K_2^{(3)}$ with voltages *e*, 12 and 123 in S_3 is isomorphic to the net we have just described. In fact, the finite derived graph *D* is already isomorphic to that described in Fig. 11, which may be seen as follows. Let us use the same symbol for the elements of $K_2^{(3)}$ with both voltage assignments, just adding primes for the graph with voltages 12 and 123. It may be observed that right



Figure 12 The graph *D* of §7 with voltages in \mathbb{Z}^2 .

multiplication by 12 of the voltages e, 12 and 13 of the first assignment yields the voltages 12, e and 123 of the second assignment, with exchange of the voltages of the first two edges. This suggests defining a mapping θ between the respective derived graphs as follows:



Figure 13

A pseudo-barycentric representation of the NC net derived from the voltage graph given in Fig. 12. Vertices that collide in barycentric representations of the net have been segregated within black circles and form four classes: $\{A, C, E\}, \{B, D, F\}, \{G, I, K\}$ and $\{H, J, L\}$.



Figure 14

The quotient N/T of the net represented in Fig. 13, with vertex classes $[A] = \{A, J\}, [B] = \{B, K\}, [C] = \{C, L\}, [D] = \{D, G\}, [E] = \{H, E\}$ and $[I] = \{I, F\}$. Note that the translation vector along 01 in *T* is half that in *S* in the same direction; translation vectors along 10 are equal in both groups.

$$\theta: \quad \begin{cases} U_p \longmapsto U'_p \\ V_p \longmapsto V'_{p,12} \end{cases}, \quad \begin{cases} a_p \longmapsto b'_p \\ b_p \longmapsto a'_p \\ c_p \longmapsto c'_p \end{cases}$$
(21)

It is readily verified that θ is a graph isomorphism.

8. Direct generation of NC nets

The procedure used above for indexing the elements of the freely acting local automorphism group L may be extended for directly generating *n*-periodic NC nets. Suppose ϕ is an automorphism in L mapping vertex A_0 , chosen as origin, to vertex B_s ; ϕ may be written as $(p, t) \in \mathcal{H} \times \mathbb{Z}^n$, where p is the permutation of \mathcal{H} mapping vertex A to vertex B in N/S, and t



Figure 15

The graph $K_2^{(4)}$ with voltages in $S_3 \times \mathbb{Z}^3$ and a pseudo-barycentric (diamond-like) representation of the derived net.

is the translation mapping $\rho(A_0)$ to $\rho(B_s)$ in the barycentric representation of the net. It is readily verified that the mapping $\phi \mapsto (p, t)$ is a monomorphism (*i.e.* an injective group homomorphism). We will show that, conversely, it is possible to derive directly an NC net N by assigning voltages (h_i, t_i) $(i \in I)$ from $\mathcal{H} \times \mathbb{Z}^n$ to the chords of a spanning tree in a finite graph P. From Gross & Tucker (2001), we know that the group \mathcal{G} generated by the pairs (h_i, t_i) acts freely on the derived infinite graph. (Assigning voltages to the chords of P ensures that the whole group \mathcal{G} , and not a subgroup, acts on the derived graph.) If (i) all vertices have degree at least 3 in P and (ii) different voltages are assigned to the edges in multiple edges, the derived graph is a net. We will now show that this net is a periodic net and that \mathcal{G} is a subgroup of the local automorphism group L of this net.

Proposition 8.1. Consider a finite graph P as above, with voltage assignment in the direct product $\mathcal{H} \times \mathbb{Z}^n$, where \mathcal{H} is any non-abelian finite group. Then, the derived graph is an NC *n*-periodic net on which the non-abelian group \mathcal{G} , generated by the voltages, acts freely. In general \mathcal{G} is a subgroup of the local automorphism group of the derived net.

Proof. To any *relator* $r = \prod_k h_{\theta_k}^{\varepsilon_k}$ of \mathcal{H} with $\theta_k \in I$ and $\varepsilon_k \in \{-1, 1\}$ (*i.e.* any string, or formal expression, of the h_i 's and their inverses whose product is actually equal to the identity e of \mathcal{H} and such that no sub-string is itself equal to e), let us associate the translation $s(r) = \sum_k \varepsilon_k t_{\theta_k}$. Let S be the subgroup of \mathbb{Z}^n generated by the translations s(r). By construction, we have

$$\prod_{k} (h_{\theta_k}, t_{\theta_k})^{\varepsilon_k} = [e, s(r)],$$
(22)

so that S may be identified with a translation subgroup of the net. Clearly, S belongs to the centre of \mathcal{G} . Since \mathcal{H} is a finite group, every element h_i has finite order; hence S has finite index in \mathcal{G} , showing that the derived net is a periodic net. On the other hand, the quotient N/S may also be derived from P by considering as voltages the first coordinates h_i instead of the pairs (h_i, t_i) . Voltages in S for the edges of N/S may be obtained after lifting the closed walks with net voltage r in P: these provide cycles of N/S with net voltage s(r). Now, because an arbitrary automorphism $(h, t) \in \mathcal{G}$ commutes with S, it is associated with an automorphism of N/S: this automorphism is given by the action of the first coordinate h on this graph. Since N/S is derived from P with voltages in \mathcal{H} , any cycle of N/S and its image by h project on the same closed walk in P, and so have the same net voltage in S. This shows that (h, t) is a local automorphism of N. If h has order w in \mathcal{H} , we have $(h, t)^w = (e, wt) = (e, s) \in S$; hence (h, t) acts as the translation t = s/w on the barycentric representation of the net. \Box

According to Proposition 8.1 we may produce an NC net with a non-abelian, freely acting local automorphism group from any crystallographic net by simply adding the first permutation coordinate to the voltages in \mathbb{Z}^n of its labelled quotient graph. Both nets, the crystallographic one and the derived NC net, admit the same barycentric representation.

Fig. 15 for instance shows the NC net derived from the diamond net by inserting voltages 12 and 13 from the substitution group S_3 as first coordinates for two of the four edges of $K_2^{(4)}$. The remaining edges were assigned the identity of S_3 as the first coordinate. This group was chosen for the sake of clarity since the number of colliding points is determined by the order and the structure of the permutation group.

We finally observe that no limitation exists to the order of the permutation group. Since S_n can be generated from only two permutations, say a and b, two edges in a graph with voltages (a, s) and (b, t) in $\mathcal{S}_n \times \mathbb{Z}^p$ are enough to produce an NC net with a local automorphism group that is a subdirect product of $S_n \times \mathbb{Z}^p$ (it being assumed that *p*-periodicity is provided by the whole set of second coordinates). Thus, for any integer n, we may assign the two voltages [12, (10)] and [12...n, (01)] in $S_n \times \mathbb{Z}^2$ to the loops of B_2 and derive a labelled quotient graph with n! vertices and $2 \times n!$ edges, since 12 and 12...*n* generate the whole group S_n . Fig. 16 displays the labelled quotient graph derived from the bouquet B_2 with voltages [12,(10)] and [1234,(01)] in $\mathcal{S}_4 \times \mathbb{Z}^2$. Colliding points in the barycentric representation are given by applying automorphisms of the form (h, 0) $(h \neq e)$, with the zero vector as the second coordinate, since these are non-trivial local automorphisms of the net associated with the null translation of its barycentric representation. When independent vectors define the second coordinate of the voltages in $\mathcal{S}_n \times \mathbb{Z}^p$, it is readily verified that collisions are associated with permutations hin the commutator subgroup $[S_n, S_n] = A_n$, the alternating subgroup (Kargapolov & Merzljakov, 1979) with $|\mathcal{A}_n| = n!/2$. This observation justifies the occurrence of triple collisions in the diamond-like NC net, and shows that we should expect 12 colliding points in the barycentric representation of the net derived from B_2 with voltages in $S_4 \times \mathbb{Z}^2$.

9. Final considerations

According to the previous results, there are infinitely many NC nets of any periodicity with a freely acting non-abelian local automorphism group. The above construction shows that the quotient graph N/T of every such net N with respect to a maximal translation group T has no automorphisms that preserve the net voltages over its cycles, which may make the direct identification of an NC net from its labelled quotient graph less easy. From the above examples, it is apparent that such nets should be quite commonly generated in a systematic search for new nets from their labelled quotient graph. Indeed, the three quotient graphs given in Figs. 6, 10 and 14 have been listed by Beukemann & Klee (1992) as the quotient graphs 3(4)2, 3(4)4 and 6(3)5 of 4-periodic minimal nets. It is thus of importance to examine available tools for recognizing such nets from their labelled quotient graph. Fortunately, we know from §3 that barycentric representations of these nets always display collisions. This is not a sufficient criterion, however, for some crystallographic nets are known to be unstable. Further progress can be made by the analysis of geodesic fibres.

Let us consider the case of the labelled quotient graph given in Fig. 6 from this point of view. To begin with, it is easily



Figure 16

The labelled quotient graph of the NC net obtained by assigning voltages [12,(10)] and [1234,(01)] in $S_4 \times \mathbb{Z}^2$ to the loops of the bouquet B_2 . Vertices are labelled by permutations in S_4 . For the sake of clarity, edges are coloured according to their voltages in \mathbb{Z}^2 . Note that the unit cell of the barycentric representation is centred in relation to the primitive cell of the net.

verified that the barycentric representation has collisions. Inspection of the quotient N/T reveals the existence of a single strong geodesic line projecting on the triangle *ABC* with net voltage 30 and two strong geodesic lines parallel to direction 01, projecting, respectively, on the loop at vertex *A* and on the 2-cycle *BC* with net voltage 02. Since geodesic lines are mapped on parallel geodesic lines by any local automorphism, we ought to discover whether these two different lines along 01 are equivalent in the net. Now, such an equivalence cannot be shown by analysing the quotient unless both lines project on cycles with equal lengths. So we are led to double the unit cell in this direction. Duplication yields here the quotient shown in Fig. 4, which as we have seen generates an NC net.

More generally, expanded cells should be used in order to enable the comparison of geodesic fibres in every direction. If the net admits a freely acting, non-trivial local automorphism group, be it abelian or not, there should be an automorphism of the expanded quotient graph that preserves the net voltage over equivalent cycles.

Finally, we observe that the results exposed here also apply to nets admitting local automorphisms with fixed elements. It should only be true that the full local automorphism group admits a non-trivial subgroup (*i.e.* a subgroup that is not isomorphic to a free abelian subgroup) which acts freely on the net.

J.-G. Eon thanks CNPq, Conselho Nacional de Desenvolvimento e Pesquisa of Brazil, for support during the preparation of this work.

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