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Infinite geodesic paths and fibers, new topological invariants in periodic graphs

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Rings are well known invariants of nets. In this work, a generalization of the concepts of cycles and rings is introduced. Infinite paths in periodic graphs are defined as connected, acyclic, regular subgraphs of degree two; geodesics are defined as infinite paths such that the unique path between any pair of vertices is a geodesic path in the whole graph. An infinite path can be thought of as an infinite cycle and a geodesic as an infinite ring. In a further step, a geodesic fiber is defined as a minimal 1-periodic subgraph that contains all geodesic paths between any pair of its vertices. Geodesic fibers are topological invariants of periodic graphs whose labeled quotient graphs are subgraphs of the labeled quotient graph of the whole graph; the paper describes applications of geodesic fibers to the analysis of the automorphisms of minimal nets, crystallographic and non-crystallographic nets.

1. Introduction

The role of cycles and rings as topological invariants of nets has been stressed by many authors (see Goetzke & Klein, 1991, for example). The concept of cycle is the graph-theoretical analog to that of closed curves that are homeomorphic to the circle in Euclidean geometry. It is thus a surprise, in comparison, that no effort seems to have been devoted to adapt the concept of straight line or half-line to periodic graphs. This is the objective of this work. After the first section providing a brief survey of the graph-theoretical tools commonly used to describe crystallographic nets and their quotient graphs, the definitions of the new concepts of infinite path, infinite geodesic path, strong geodesic and geodesic fiber are given. Among geodesic fibers, an important role is played by T-fibers, which are invariant with respect to some automorphism from the translation subgroup T defining the periodic graph. It is shown that the labeled quotient graph of any geodesic T-fiber is isomorphic to some subgraph of the labeled quotient graph of the periodic graph with respect to the corresponding translation group, the labeling being conserved while taking the subgraph. Moreover, it is shown that any local automorphism of the periodic graph exchanges parallel T-fibers. This property turns geodesic fibers into nice topological tools for the study of periodic graphs. Illustrations are given through the analysis of local automorphisms in minimal nets, and crystallographic and non-crystallographic nets.

2. Graph theory in crystallography

The basic definitions of graph theory given hereafter have been adapted from Harary (1972). In short, we say that a graph G = (V, E, m) is a pair of vertex and edge sets, V and E, respectively, with an incidence map m: E $\mapsto$ V^2. If $m(e)$ = (u, v), we use the shorthand notation $e = uv$ and say that e runs from a *tail* u to an *end* v; u and v, collectively called the *endpoints* of the edge, are *adjacent* vertices and are *incident* to e. The *degree* of a vertex is the number of incident edges; a graph is regular if all its vertices have same degree. A *loop* is an edge that admits only one endpoint; the loop must be counted twice to obtain the degree of the corresponding vertex. The incidence map explicitly determines an orientation on the graph G, which enables us to define the reverse (negative) of the edge $e = uv$ as the same edge $e^- = vu$ traversed in the opposite direction. Each edge e has positive and negative orientations distinguished as e^+ (= e) and e^-. If more than one edge admits the same endpoints, we say that G has multiple edges. Notice that our definition of graph corresponds to what is usually called a pseudograph. A graph without loops or multiple edges is then called a *simple* graph. A graph G′ = (V′, E′, m') is a *subgraph* of G if V′ and E′ are subsets of V and E, respectively, and if the incidence function m' is a restriction of m. A *proper subgraph* of G is different from G and from the empty graph (the graph with no vertices). If G′ and G″ are two subgraphs of G such that G″ is a proper subgraph of G′, we also say that G′ is a proper *supergraph* of G″. A subgraph G′ of G is called a *maximal subgraph* (respectively: a *minimal subgraph*) with respect to some property P if P holds for G′ but does not hold for any proper supergraph (respectively: subgraph) of G′ in G. A *spanning subgraph* of G admits the same set V of vertices as the graph G. The *intersection* (respectively, *union*) *graph* G′ ∩ G″ (respectively, G′ ∪ G″) of two subgraphs G′ and G″ of G is the subgraph whose vertex and edge sets are defined as the intersections (respectively: unions) of the vertex and edge sets of G′ and G″ and whose incidence function is the restriction of the incidence function of G to its edge set.

A *walk* W between two vertices u_0 and u_n (the tail and end, together called the endpoints of the walk) is an alternate sequence of vertices and edges $u_0e_0 \ldots u_ie_iu_{i+1} \ldots u_n$, where each element of $V \cup E$ is incident to the following. As the vertices can be recovered from the only indication of the edges, they will not be indicated in the sequel. A graph is *connected* if there is a walk between any pair of vertices. A *component* of a graph is a maximal connected subgraph. The *length* $|W|$ of a walk W is the number of edges of the sequence. A *path* is a walk that does not run twice through the same vertex. A *geodesic path* is a path of minimum length between its two endpoints. The *distance* $d(u, v)$ between two vertices u and v is the length of a geodesic path between them. A *cycle* is a path with only one endpoint. However, since one comes back to the initial vertex after running along the cycle, the choice of the endpoint is rather arbitrary. If one does not need the reference to some particular origin (or *base*) vertex and analyzes the cycle as a whole, it is customary to characterize it by the absence of endpoint. It is worth mentioning that cycles are sometimes considered as finite connected regular subgraphs of degree 2. We shall say that a graph is c-*connected* if (*a*) it is connected and (*b*) there is at least one cycle or one loop traversing each vertex. A graph without cycle is called *acyclic*. A component of an acyclic graph is a *tree*. If a spanning tree is chosen in a graph, a *chord* is any edge that does not belong to the tree, so adding a chord to a tree will close exactly one cycle. The *cyclomatic* number is the number of independent cycles, equal to the number of chords of the graph.

In opposition to paths and cycles, walks can run several times through the same vertices and edges. It is then convenient to define a 1-*chain* as a formal (commutative) sum of edges affected with integer coefficients. By extension of the previous definitions, a 1-chain will be called a walk, a path or a cycle if it is possible to order the oriented edges of the sum into a sequence with the respective properties. We will then say that a walk W *decomposes* into a path P and some cycles C_i ($i = 1, \ldots, n$) if it is possible, by changing the order of the edges, to write down the corresponding 1-chain as the sum $W = P + \Sigma C_i$. The converse property is analyzed in Appendix *A*. It is worth noting that the decomposition may not be unique. The *support* of a 1-chain is the subgraph containing the edges with non-null coefficient together with the incident vertices.

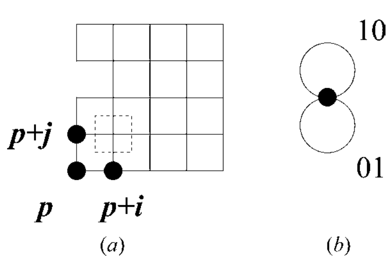

Figure 1
(*a*) The square net and (*b*) its labeled quotient graph.

An automorphism of a graph G is a pair (f_V, f_E) of bijective maps of V and E on themselves respecting the incidence map: $m[f_E(e)] = (f_V(u), f_V(v))$ for $e = uv$. Dropping all indices and using the shorthand notation, we get the simplified definition $f(uv) = f(u)f(v)$. An automorphism f is said to be a *local automorphism* if the distance between any vertex and its image by f is uniformly bounded by some constant called the norm of the automorphism, and denoted $|f|$. Thus, $d\{u, f(u)\} \leq |f|$ for all $u \in V$. An automorphism f of G is said to *act freely* on G if there is no fixed element, that is: $f(x) \neq x$ for all x of $V \cup E$. Following Delgado-Friedrichs (2004), we say that the pair (G, T) is an *n-periodic graph* if G is a simple graph admitting a free abelian group T of automorphisms of rank n acting freely on G and such that the number of (vertex and edge) orbits of G by T is finite. The elements of T are called the *translations* of the periodic graph. In the following, we always admit that T is a *maximal translation group* in the sense that the pair (G, T′) is not an n-periodic graph for any group extension T′ of T. *Crystallographic nets* are n-periodic graphs whose full automorphism group is isomorphic to some n-dimensional space group (Klee, 2004).

If (G, T) is a periodic graph, we denote by V/T and E/T the sets of vertex and edge orbits of G by T, also called vertex and edge *lattices*, respectively. We form the *quotient graph* $G/T \equiv (V/T, E/T, m_T)$, where the incidence function is defined by the relationship $m_T([uv]) = ([u], [v])$, where $[x]$ is the orbit of the element x of $V \cup E$ by T. The map q_T sending the element x on its orbit $[x]$, which is called the *natural projection* of (G, T) on its quotient G/T is a *homomorphism* of graphs satisfying $q_T(uv) = q_T(u)q_T(v)$. The *labeled quotient graph* (Chung *et al.*, 1984) is formed by attributing a *voltage*, *i.e.* an element from the translation group T, to each edge of the quotient graph. Labeled quotient graphs are therefore voltage graphs, following Gross & Tucker (2001). Since all vertices of a vertex lattice $[u]$ are equivalent by translation, one can choose an arbitrary vertex of $[u]$ as the origin, u_0, and index all other vertices of $[u]$ as u_t, where t is the translation mapping u_0 on $u_t = t(u_0)$. If the edge e_0 of (G, T) links vertex u_0 to vertex v_s, then we attribute the voltage s to the edge lattice $[e]$. Notice that we have for the translated edge:

$$e_t \cong t(e_0) = t(u_0v_s) = t(u_0)t(v_s) = u_tv_{s+t}.$$

If the edge e admits the voltage t, then the reverse edge e^- admits the opposite voltage $-t$ (we shall also use the multiplicative notation t^{-1}). The whole process can obviously be inverted. Given a voltage graph K with voltages from a free abelian group T of rank n, one can generate a unique n-periodic graph, called the *derived* graph.

Example 2.1. Consider the square net $N = (4^4)$ shown in Fig. 1(*a*). This is the infinite graph defined by $V = Z^2$ and $E = \{pq: (p, q) \in Z^2 \times Z^2$ and $q = p + i$ or $q = p + j\}$ with $i = (1, 0)$ and $j = (0, 1)$. Let us define the mapping f_t of (4^4) by $f_t(p) = p + t$ for each t and p of Z^2; clearly f_t is a graph automorphism and acts freely on (4^4). The automorphism group $T = \{f_t: t \in Z^2\}$ with the ordinary law of composition is isomorphic to the free group Z^2. Now, all the vertices of N are equivalent by T to the origin $a = (0, 0)$ and all the edges are equivalent to ai or to aj, so the square net with one vertex orbit and two edge orbits is a 2-periodic graph. The quotient graph N/T, which has then one vertex and two edges, is the *bouquet* of two loops represented in Fig. 1(b). One loop is the image by the natural projection of the edge ai and has voltage f_i (for which we use the conventional crystallographic notation **10**) since vertex i is the image of vertex a by the automorphism f_i. The same argument leads to attribute the voltage **01** to the second loop, image by the natural projection of the class of the edge aj.

The *net voltage* on a walk (respectively path and cycle) in the quotient graph G/T is the sum of all the voltages along the walk, with all edges oriented from the tail to the end of the walk. A cycle of null voltage in G/T is the natural projection of a cycle of G; otherwise we shall always consider oriented cycles since they can be traversed in both directions with opposite net voltages. Thus, an oriented cycle of net voltage t is the projection of a path between two vertices of G related by the translation t. A *ring* in a graph G is a cycle that does not admit any *short-cut*. This means that, for any pair of vertices of the cycle, the shortest path between them along the cycle is a geodesic path in the graph. A *strong ring* is a cycle that, as a 1-chain, cannot be written as a sum of shorter cycles. Rings and more particularly *strong rings* are important topological invariants in periodic graphs (Goetzke & Klein, 1991).

3. Geodesics and fibers in periodic graphs

This section introduces the concept of geodesic, which generalizes that of straight line in Euclidean geometry to periodic graphs. We start with the formal definitions of infinite path and infinite geodesic paths, which occur as natural extension of the geometric concept to graph theory. There are, however, two striking differences with geometry. In general, it is not possible to talk of *the* geodesic path between two vertices of a graph. Moreover, not every (finite) geodesic path can be prolonged into an infinite geodesic path: few directions

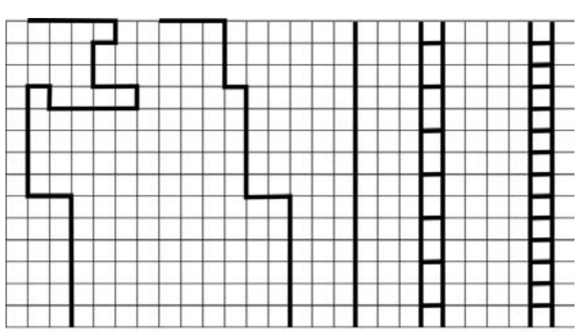

Figure 2
Infinite subgraphs of the square net (4^4): (a) an infinite path, (b) a geodesic, (c) a strong geodesic, (d) a 1-periodic ladder that is not geodesically complete, and (e) a 1-periodic ladder that is geodesically complete but not minimal.

in the graph appear to have this privilege. This motivates the definition of strong geodesics and fibers along some direction in a periodic graph. It is known that the geometry of a space, Euclidean or non-Euclidean, is associated to the nature of its geodesic curves, sometimes called intrinsic straight lines. Analogously, we will find that fibers are important topological invariants of periodic graphs.

Definition 3.1. An *infinite path* in a periodic graph (G, T) is a connected, acyclic, regular subgraph of degree 2.

Note that a path, in the sequel, always means a finite path as it is defined in §2; the use of the adjective *infinite* is then mandatory to specify the infinite path.

Definition 3.2. An *infinite geodesic path* or more simply a *geodesic* L in a periodic graph (G, T) is an infinite path such that the unique path in L between two of its vertices is a geodesic path in G.

Example 3.1. Figs. 2(a) and 2(b) illustrate Definitions 3.1 and 3.2 in the square net. Both subgraphs are infinite paths but only the latter, with no short-cut, is a geodesic.

The concepts of infinite path and geodesic generalize those of cycle and ring, respectively, in infinite graphs. Looking at the alternative definition of the cycle given in §2, an infinite path could also be called an infinite cycle; the definition of the geodesic can be rephrased from that of the ring by observing that a geodesic is an infinite path without short-cut.

An especially important kind of infinite path is obtained by *unwrapping* (or *lifting*) a cycle C of the quotient graph G/T. We will denote such an infinite path by $]C[$ and define it as a component of the preimage $q_T^{-1}(C)$. Only cycles that possess a shortest length among all those cycles (or loops) or combination of cycles with the same net voltage t can be lifted to a geodesic. In some periodic graphs, however, one can find different cycles, or closed walks, whose net voltages correspond to multiples of some translation t. The necessity of comparing the lengths of paths lifted from such closed walks motivates the next definition.

Definition 3.3. Let us denote by Ext(t) the maximal 1-periodic extension in T of the subgroup $\langle t \rangle$ generated by some translation $t \in$ T; Ext(t) is thus a subgroup of T. The *reduced length* of a closed walk, or combination of cycles, W of G/T with net voltage t is defined as the ratio $|W|/k$ where k is the index of $\langle t \rangle$ in Ext(t).

A necessary and sufficient condition for a cycle C with net voltage t to be lifted to a geodesic $]C[$ is that it has shortest reduced length among all those combinations of cycles with total net voltage in Ext(t). If a geodesic $]C[$ is interrupted at some vertex x, we will call each subgraph a *half geodesic*. If, on following the orientation induced in G by that of the cycle C, we find that the half geodesic runs outward from the terminal vertex x of degree 1, we will denote it by $[xC[$ or $[C[$ if the terminal vertex is not known; if it runs towards the terminal vertex, we use the complementary notations $]Cx]$ or $]C]$.

Definition 3.4. A *strong geodesic* is a geodesic such that any path between two of its vertices is the unique geodesic path between them in G.

Example 3.2. Fig. 2(*c*) shows a strong geodesic in the square net. Not all periodic graphs possess strong geodesics, as can be seen by examining the net (3^4.6) shown in Fig. 3. The following definitions allow a convenient generalization of the concept.

Definition 3.5. We say that a subgraph F of a graph G is *geodesically complete in* G if, for any pair of its vertices, it contains all geodesic paths between them in G.

Definition 3.6. (Fibers). A 1-periodic subgraph (F, S) of a periodic graph (G, T) is called a *geodesic fiber* or simply a fiber if (*a*) the translation group $S = \langle t \rangle$ can be generated by some local automorphism t of G, (*b*) the subgraph F is geodesically complete in G, and (*c*) F is minimal with respect to the conditions of periodicity (*a*) and completeness (*b*). We say that the fiber $(F, \langle t \rangle)$ runs along the *direction t*. We speak of a T-fiber when t is in T; two T-fibers $(F_1, \langle s \rangle)$ and $(F_2, \langle t \rangle)$ such that $\mathrm{Ext}(s) = \mathrm{Ext}(t)$ are said to be *parallel*.

As illustrated below, the 'minimum' criterion does endow T-fibers with nice properties; in particular, it will be seen that geodesic T-fibers reduce to strong geodesics when these exist.

Example 3.3. The three conditions (*a*), (*b*) and (*c*) of Definition 3.5 clearly hold for the strong geodesic of Fig. 2(*c*), which is then also a T-fiber along the direction **01** of the square net.

Example 3.4. The *ladder* of Fig. 2(*d*) is 1-periodic and admits the translation **02** of the square net as the generator of its translation group. However, it is not geodesically complete in (4^4) since the missing *rungs* are short-cuts to any path between their endpoints. Adding these *rungs* to the subgraph, one gets the ladder shown in Fig. 2(*e*), which is 1-periodic with translation **01**, geodesically complete in (4^4), but not minimal. Indeed, it admits as subgraphs the two *parallel* T-fibers, which are the replicas of the strong geodesic shown in Fig. 2(*c*).

Example 3.5. Fig. 3 exhibits two geodesic T-fibers of the net (3^4.6) along distinct crystallographic directions, evidencing the occurrence of fibers even when strong geodesics are absent.

Proposition 3.1. Through any vertex of a periodic graph, one cannot draw more than one T-fiber parallel to any direction.

Proof. Suppose that $(F_1, \langle s \rangle)$ and $(F_2, \langle t \rangle)$ are parallel T-fibers containing a common vertex. Then the intersection graph $F_1 \cap F_2$ is 1-periodic along some direction r with $\langle r \rangle = \langle s \rangle \cap \langle t \rangle$ and geodesically complete. Since both fibers F_1 and F_2 are minimal, their intersection cannot be a proper subgraph of any of them; since it is not empty, we must have $F_1 = F_2$. □

Automorphisms clearly respect geodesics, strong geodesics and fibers. In particular, the fiber $(F, \langle t \rangle)$ is mapped by any automorphism τ of the periodic graph (G, T) onto the fiber $(\tau F, \langle \tau . t . \tau^{-1} \rangle)$. This observation is quite general, but we will focus exclusively on T-fibers in the sequel, looking at their images, first by the translations of the periodic graph, then by arbitrary local automorphisms.

Proposition 3.2. T-fibers $(F, \langle t \rangle)$ of a periodic graph (G, T) are mapped on disjoint T-fibers, running along the same direction t, by translations that do not belong to their translation group $\langle t \rangle$.

Proof. Suppose that $(F, \langle t \rangle)$ is some T-fiber of (G, T) and let $s \in T$ be some translation of T; since T is abelian, the image sF of F by s is also a T-fiber along t. From Proposition 3.1, two situations can then arise:

(i) F and sF have a common vertex; then $F = sF$, which means that F is invariant by s and requires that $s \in \langle t \rangle$, or

(ii) $F \cap sF = \emptyset$, if $s \notin \langle t \rangle$. □

Example 3.6. Considering again the example of the square net, the ladder of Fig. 2(*e*) could not be a T-fiber since it has a non-empty intersection with its image by the translation **10**.

4. Quotient graph of a T-fiber

Consider the different mappings represented in the following diagram between a T-fiber $(F, \langle t \rangle)$, the periodic graph (G, T) and their respective quotient graphs $F/\langle t \rangle$ and G/T:

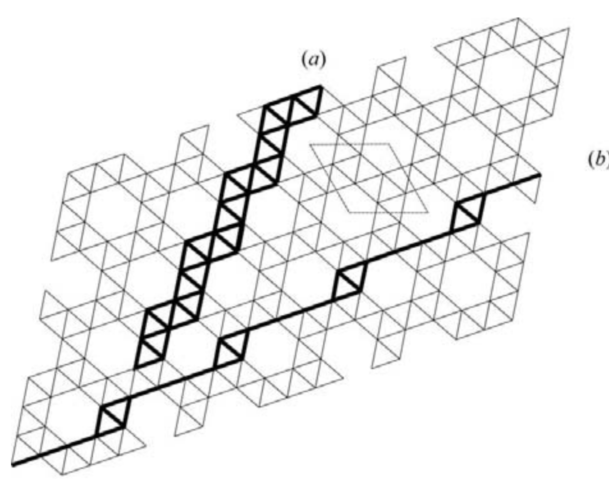

Figure 3
Two geodesic fibers of the net (3^4.6) along the directions (*a*) **11** and (*b*) **21**.

$$\begin{tikzcd} \mathrm{F} \arrow[r, "i"] \arrow[d, "q_{\langle t\rangle}"'] & \mathrm{G} \arrow[d, "q_{\mathrm{T}}"] \\ \mathrm{F}/\langle t\rangle \arrow[r, "\theta"] & \mathrm{G}/\mathrm{T} \end{tikzcd}$$

where the map i is the inclusion map; $q_{\langle t\rangle}$ and q_{T} are the natural projections of F and G on their respective quotient graphs. This diagram allows the definition of a map θ between both quotient graphs as follows; for $x \in \mathrm{F}$, we set $\theta[q_{\langle t\rangle}(x)] = q_{\mathrm{T}}[i(x)]$. It is easily verified that θ is well defined (*i.e.* the result does not depend on the choice of the vertex or edge x of F) and that it is a graph homomorphism.

Proposition 4.1. The quotient graph $\mathrm{F}/\langle t\rangle$ of a T-fiber in a periodic graph (G, T) is isomorphic to a subgraph of the quotient graph G/T.

Proof. We need only show that the graph homomorphism θ is injective. We prove it for the vertex set; a similar argument applies to the edge set of $\mathrm{F}/\langle t\rangle$. Suppose that A and B are two distinct vertices of $\mathrm{F}/\langle t\rangle$ with $\theta(A) = \theta(B)$. Then, there exist two vertices a and b of F, which we identify to their images by inclusion in G, such that: $A = q_{\langle t\rangle}(a) \neq q_{\langle t\rangle}(b) = B$ and $q_{\mathrm{T}}(a) = q_{\mathrm{T}}(b)$. This implies that the two vertices a and b of F are related by some translation s of T, so that $b = s(a) \in \mathrm{F} \cap s\mathrm{F}$ with $s \notin \langle t\rangle$, in contradiction with Proposition 3.2. □

Example 4.1. Trivially, in the case of the square net, the natural projection of the strong geodesic shown in Fig. 2(*c*) is the loop with voltage **01**.

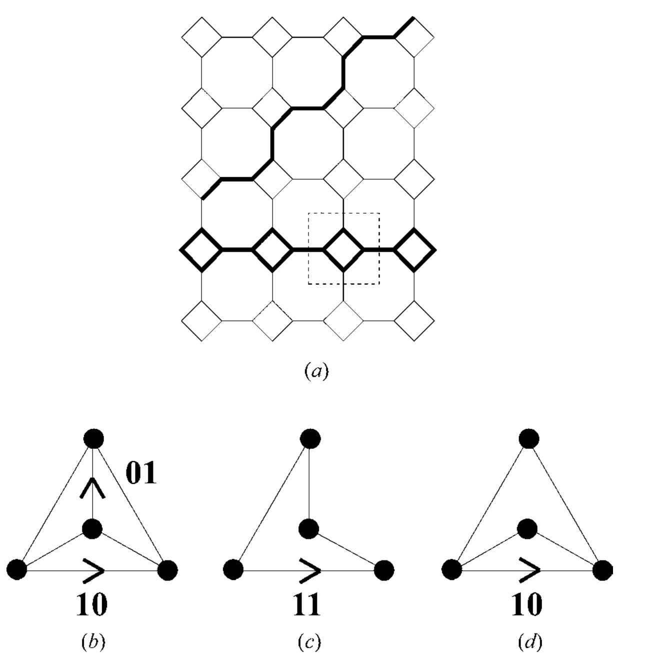

Figure 4
The net (4.8^2) and two geodesics fibers (*a*) along the directions **11** and **10**, with their quotient graphs (*b*), (*c*) and (*d*), respectively.

Example 4.2. Fig. 4(*a*) shows the net (4.8^2) and two geodesic T-fibers, one along the direction **11**, which is a strong geodesic, and the other along **10**. Their quotient graphs are drawn in Fig. 4(*b*) to Fig. 4(*d*), respectively.

Example 4.3. Fig. 5(*a*) shows the β-W net and two geodesic T-fibers; the first along the direction **11**, which is again a strong geodesic, and the second one along **01**. Their quotient graphs are drawn in Fig. 5(*b*) to Fig. 5(*d*), respectively.

In Examples 4.1 to 4.3, the quotient graph of the T-fiber is a subgraph of the quotient graph of the net, as expected. But it has also been possible to write the labeled quotient graph of the T-fiber by attributing to each common edge the same voltage in the quotient $\mathrm{F}/\langle t\rangle$ as in the quotient graph G/T of the net. Notice that the quotient graph of a strong geodesic is a cycle, so one can re-label the quotient by attributing the net voltage over the cycle to an arbitrary edge, as has been done in Fig. 4(*c*) and Fig. 5(*c*). These observations can now be generalized.

Theorem 4.1. The labeled quotient graph of a geodesic T-fiber $(\mathrm{F}, \langle t\rangle)$ in a periodic graph (G, T) is a labeled subgraph of the labeled quotient graph G/T.

Proof. Consider a T-fiber $(\mathrm{F}, \langle t\rangle)$ of a periodic graph (G, T) with labeled quotient graph G/T. An arbitrary cycle C of $\mathrm{F}/\langle t\rangle$ is the projection by $q_{\langle t\rangle}$ of a (maybe closed) walk between two vertices that are equivalent by $\langle t\rangle$. This walk projects by q_{T} on the cycle $\theta[C]$, which (following Proposition 4.1) we can identify to C by inclusion of $\mathrm{F}/\langle t\rangle$ in G/T. Since $\langle t\rangle$ is a subgroup of T, the net voltage over $\theta[C]$ in G/T belongs to the subgroup $\langle t\rangle$. It is then always possible to attribute the same voltage to the edges of the quotient graph $\mathrm{F}/\langle t\rangle$ as their images by θ in G/T. □

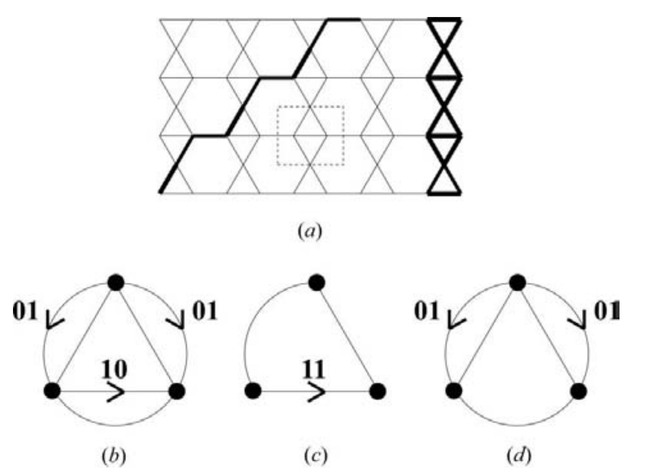

Figure 5
The β-W net and two geodesic fibers (*a*) along the directions **11** and **01**, with their quotient graphs (*b*), (*c*) and (*d*) respectively.

As was seen in the case of strong geodesics, commented on above, it can naturally happen that the voltages attributed to the edges of F/⟨t⟩ do not belong to the translation group ⟨t⟩. What really matters, however, is that the net voltage over any cycle of the quotient F/⟨t⟩ is a translation of ⟨t⟩. Relabeling can then be performed by using a spanning tree of F/⟨t⟩ and attributing the net voltage of the cycle to the corresponding chord.

Theorem 4.1 allows a procedure to be outlined to determine T-fibers directly from the labeled quotient graph G/T of their parent n-periodic graph. Initially, one must define the direction t of the fiber, based on the fact that the translation group ⟨t⟩ contains the net voltage of some cycle of G/T. One selects then a cycle C of G/T with shortest reduced length among all those cycles or combinations of cycles with net voltage in Ext(t). This ensures that]C[is a geodesic but does not ensure yet that it is a subgraph of some fiber. If there is some combination of cycles with (a) total net voltage in Ext(t) but individual net voltages not all in Ext(t), (b) the same reduced length as C, and (c) such that their union with C forms a connected graph, then the periodic graph has no fiber parallel to the corresponding direction. By completeness, all cycles within the combination should be included into the quotient graph of the fiber since they allow the construction of geodesic paths alternative to those obtained by lifting the chosen cycle in the periodic graph. But then, the derived graph would not be 1-periodic.

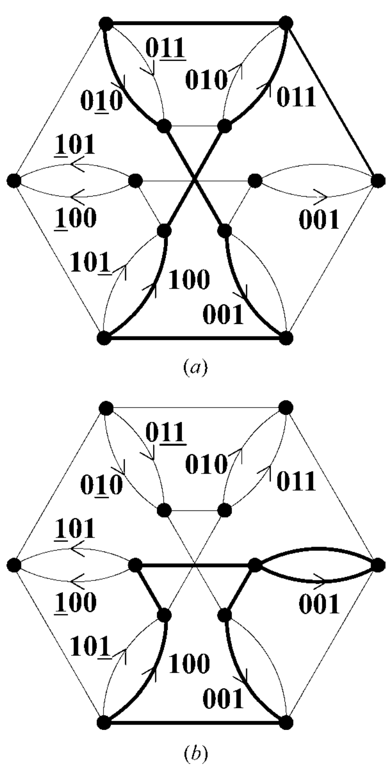

Figure 6
(a) A shorter cycle along **102** in the quotient graph of cancrinite and (b) two intersecting cycles along **101** and **001** with the same total length.

Example 4.4. Consider the cancrinite net whose labeled quotient graph is drawn in Fig. 6. The shortest cycle of net voltage **102** and length 8 has been thickened in Fig. 6(a) and two cycles with net voltages **101** and **001** and lengths 6 and 2, respectively, have been thickened in Fig. 6(b). Observe that the union of the three cycles forms a connected subgraph. Since a path obtained by lifting the latter two cycles together has equal length to a path constructed from the former, all three cycles must be included in the quotient graph of a maybe-fiber along **102** in order to satisfy to completeness. But then, the derived graph is two-dimensional since its quotient admits two cycles of independent voltages **101** and **001**. Thus, cancrinite has no fiber along direction **102** but it might have fibers along directions **101** and **001**. This example leads directly to the enunciation of Proposition 4.2.

Let us assume that it has been possible to choose a cycle C of net voltage t according to the aforementioned conditions. If another cycle C' of G/T with net voltage in Ext(t) and the same reduced length as C intersects it, its lift is another possible geodesic path between two equivalent vertices in G that project on a common vertex of C and C'. The corresponding geodesic]C'[must then also belong to F. This shows that the quotient graph F/S of the fiber contains all the cycles of G/T with net voltage in Ext(t) that have same reduced length and form a connected subgraph, say H, of G/T. On the other hand, F must contain all the geodesic paths existing (recursively) as 'transversal' paths between vertices of all the geodesics parallel to]C[. By natural projection on F/S, these 'transversal' paths together with segments of the cycles with non-null net voltage generate cycles with net voltage null. This shows that cycles of G/T with net voltage null must also be included in the quotient F/S if they provide short-cuts to paths in H. By construction, the generated subgraph of G/T does not contain any cycle with net voltage outside the subgroup Ext(t); then its derived graph is certainly a geodesic fiber, since it is 1-periodic, geodesically complete and minimal. For the sake of clarity, the previous conclusions are summarized in the following algorithm.

Algorithm 4.1. To get the quotient graph H = F/S of a T-fiber (F, S) along a direction in Ext(t) from the quotient G/T of a periodic graph (G, T):

1. List all cycles of G/T, computing their lengths and net voltages.
2. Choose a cycle (loop) C with net voltage in Ext(t) and shortest reduced length and check (a) that there is no combination of cycles (loops) with total net voltage in Ext(t) and shorter reduced length than C, and (b) that there is no combination of cycles (loops) with individual net voltages not all in Ext(t), but total net voltage in Ext(t), reduced length equal to C, and forming a connected subgraph with C.
3. Form the connected subgraph H of G/T of all the cycles with same reduced length as C and net voltage in Ext(t).
4. Add recursively to H all the cycles of G/T with net voltage null, if they provide short-cuts to paths already in H.

5. Get the translation group S of F as the subgroup generated by the net voltages of all cycles in H.

Proposition 4.2. Every n-periodic graph admits at least n T-fibers in n independent directions.

Proof. A strong obstacle for a cycle C of G/T with shortest reduced length to generate a T-fiber parallel to the corresponding direction is completeness. If there is a closed walk W obtained by combining cycles C_i with net voltages not all in Ext(t), but total net voltage in Ext(t), whose union with C forms a connected graph, and such that W has same reduced length as C, then all cycles C_i should belong to the quotient graph of the fiber. Indeed, the lift of W provides an alternative geodesic path to that of C. But then the fiber should contain the inverse image of the support of W and would be at least 2-periodic. In this case, the cycle C cannot generate any fiber; but instead, we can search for T-fibers parallel to the direction of the shorter cycles C_i, starting again Algorithm 4.1 from step 2. Since the total number of cycles of the quotient graph is finite, the search for shorter cycles satisfying step 2 of Algorithm 4.1 must end with at least n cycles in n independent directions for n-periodic graphs. □

Example 4.5. The quotient graph of the net (4.8^2) shown in Fig. 4 admits four 3-cycles, two with net voltage **10** and two with net voltage **01**, and three 4-cycles with net voltages **11**, **1−1** and **00**, respectively. The unique and shortest 4-cycle along **11** (respectively, **1−1**) is the quotient graph of a strong geodesic. Along direction **10** (respectively **01**), the two 3-cycles have a common edge; the union graph of both cycles, shown in Fig. 4(d), already contains the 4-cycle with net voltage null. It is thus the quotient graph of a fiber along **10**.

Example 4.6. The quotient graph of the β-W net shown in Fig. 5 admits three 2-cycles, one with net voltage **10** and two with net voltage **01**, and eight 3-cycles, two with net voltage **10**, two with net voltage **01**, one with net voltage **11**, one with net voltage **1−1** and two with net voltage **00**. The unique 3-cycle along **11** (respectively, **1−1**) is the quotient graph of a strong geodesic. The shortest cycles along **01** are 2-cycles with a common vertex. The union graph H of these two cycles shares two edges with both 3-cycles with net voltage null, so that the third edge is a short-cut and must be added to H to get the quotient graph of a fiber along **01**, as shown in Fig. 5(d). The shortest cycle along **10** is a 2-cycle with only one edge in common with 3-cycles of net voltage null; consequently, the 3-cycles do not provide any short-cut to paths in the 2-cycle, which is thus the quotient graph of a strong geodesic along **10**.

Example 4.7. In the bouquet B_2 of two loops, insert a new vertex on one loop and two vertices on the other. Attribute the voltages **2** and **3** in Z, respectively to these loops. Both have the same reduced length and a common vertex, so they generate a unique fiber by lifting. The translation group is $\langle \mathbf{2}, \mathbf{3} \rangle$ = Z; it is thus a fiber along Z = $\langle \mathbf{1} \rangle$, but its quotient graph has no cycle (or loop) with net voltage **1**.

Definition 4.1. A T-fiber (F, $\langle t \rangle$) is called *simple* if its quotient graph displays a cycle (or loop) with net voltage t.

Example 4.8. In the bouquet B_2, attribute the voltages **1** and **2** in Z to the loops. The loop with voltage **2** generates two disjoint parallel simple fibers, which are mapped to each other by the translation **1**; note that this result is in agreement with Proposition 3.2, since **1** is not in $\langle \mathbf{2} \rangle$.

5. Invariance of fibers

Let τ be a local automorphism of a periodic graph (G, T), not necessarily in T. This means that (G, T) may not be a crystallographic net. In this case, we know that τ need not respect vertex and edge lattices of (G, T). But what can we say about mappings of T-fibers? Another fundamental and correlated question is: what can we say in general about an arbitrary fiber (F, $\langle \tau \rangle$)? In fact, these questions cannot be dealt with separately since the image of a T-fiber (F, $\langle t \rangle$) is *a priori* an arbitrary fiber (τF, $\langle \tau.t.\tau^{-1} \rangle$). We shall begin this section by proving a more general property, namely that any infinite geodesically complete subgraph of a periodic graph contains at least one half geodesic. This result will enable us to show that any fiber is close enough to a half geodesic at infinity, which leads to Theorem 5.1, stating that any T-fiber of a periodic graph is mapped on a parallel T-fiber. We shall then be able to state Theorem 5.2, which establishes the identity between fibers and T-fibers.

Lemma 5.1. Given a vertex x of a fiber (F, $\langle \tau \rangle$), for any vertex y of F one can define an integer k such that $y \in B[\tau^k(x), \Delta]$, where $B[a, \Delta]$ is the ball of center a and radius Δ, called the *diameter* of the fiber.

Proof. Since a fiber is a 1-periodic graph, one can define the quotient graph F/$\langle \tau \rangle$. Choose a spanning tree of F/$\langle \tau \rangle$ of *diameter* Δ, defined as the maximum distance between two vertices of the spanning tree: Δ represents the size of the unit cell of F. □

Lemma 5.2. Given an infinite geodesically complete subgraph H of a periodic graph (G, T), any infinite sequence x_n of vertices of H induces at least one half-geodesic contained in H.

Proof. The argument is based on the construction of an adequate sequence of paths in H. We assume first that the sequence x_n has been ordered so that the distance $d(x_0, x_n)$ is an increasing function of n, and associate a sequence of geodesic paths $P_n = x_0x_n$ in H; note that the paths P_n are chosen arbitrarily but once and for all. Then, we project the paths P_n on G/T by the natural projection q_T; the mapped walks W_n, starting at $X = q_T(x_0)$, decompose into a path and a number of cycles of G/T. Since the total number of cycles of G/T is finite, and since the length of the geodesic path P_n can be made arbitrarily large, at least one cycle C of G/T (maybe a loop) will appear with unbounded coefficient in the decomposition of the walks W_n. Let us extract a subsequence of vertices y_m (possibly with repetitions) from the sequence x_n such that the projection of the corresponding geodesic path x_0y_m in G/T contains at least m copies of the cycle C. Orient this path from x_0 to y_m and call a_m the first vertex along the path x_0y_m whose projection A_m belongs to C, and b_m the last vertex along x_0y_m from the same vertex lattice A_m. Consider then the projection W of the geodesic path $x_0y_{m+1} = x_0a_{m+1}b_{m+1}y_{m+1}$, split into three parts by the vertices a_{m+1} and b_{m+1}. The first part x_0a_{m+1} projects on a walk W' from X to the vertex A_{m+1} of C, which cannot contain C in its decomposition; the projection K of the second part is a closed walk based on A_{m+1}, which contains at least $(m+1)$ copies of the cycle C, and a sum $\sum$ of cycles of G/T; the last part projects on another walk W'' from A_{m+1} to the projection of y_{m+1}. Observe that the sum of cycles $C + \sum$ is a 1-chain of G/T, which has the same support as the projection K of the walk $a_{m+1}b_{m+1}$; according to Proposition A.1 given in Appendix *A*, we can recombine the closed walk K by traversing first all (at least m) copies of C but one, followed by a closed walk derived from the sum $C + \sum$. This walk is lifted to another geodesic path between a_{m+1} and b_{m+1}, which belongs to H by hypothesis. In particular, the path lifted from the m copies of C and starting at the vertex a_{m+1} is contained in H.

The main body of the proof is by induction on the number of different cycles that appear with unbounded coefficient in the decomposition of the set of walks $q_T(x_0y_m)$ (which is a subset of the walks W_n). Suppose that a single cycle C of G/T appears with unbounded coefficient in this decomposition. Then, the number of possible walks W' is finite, and so is the set of vertices a_m in H; at least one of them is thus the endpoint of a half geodesic $[a_mC[$ contained in H. Suppose now that the lemma is true when at most p different cycles of G/T appear with unbounded coefficient in the decomposition of the walks W_n and consider the same construction as above in the case of $p + 1$ different cycles. It is again possible that the set of vertices a_m be finite, in which case the same conclusion as above can be drawn. If, on the contrary, the set of a_m is infinite, we apply the whole argument to this new set, in substitution to the set x_n, defining $a_0 = x_0$. Note that the geodesic path from a_0 to a_m necessarily corresponds to the first part of the path P_n already defined. Since the projection of the walk a_0a_m does not contain the cycle C, the induction hypothesis applies to the sequence of a_m, so that H also contains a half geodesic $[C[$ in the case p+1. □

Lemma 5.3. Any fiber $(F, \langle\tau\rangle)$ contains at least two half-geodesics $[C_+[$ and $[C_-[$ describing its behavior at infinity.

Proof. Pick an arbitrary vertex x of F and form the sequences $X^+ = \{\tau^n(x), n \in N\}$ and $X^- = \{\tau^{-n}(x), n \in N\}$. From Lemma 5.2, we can find two half-geodesics $[aC_+[$ and $[bC_-[$ contained in F induced by X^+ and X^-, respectively. Call t_+ and t_- the net voltages on the cycles C_+ and C_-.

From Lemma 5.1, any vertex of $[aC_+[$ is at less than a distance Δ from some vertex $\tau^k(x)$ in F. Conversely, the projection of $[aC_+[$ on the quotient graph $F/\langle\tau\rangle$ is a 1-chain, which, as the projection of a geodesic, must be consistent with the voltages, that is, it decomposes in cycles which have net voltages along a constant direction of $\langle\tau\rangle$. In other words, $[aC_+[$ crosses successively all unit cells of the 1-periodic graph F from its endpoint a in a direction consistent with one of the automorphisms τ or τ^{-1}. Consequently, every vertex of F on one 'side' of the vertex a is at less than a distance Δ from some vertex of $[aC_+[$. By construction, it is clear that $[aC_+[$ is associated with τ so that, more precisely, every vertex $\tau^k(x)$ for a sufficiently large (positive) value of k is at a distance less than $\Delta + |t_+|$ from some vertex $t_+^n(a)$. In the same way, every vertex of $[bC_-[$ is at less than a distance Δ from some vertex $\tau^k(x)$ with $k < 0$. □

Lemma 5.4. If τF is the image of a T-fiber $(F, \langle t\rangle)$ by a local automorphism τ, both half geodesics describing its behavior at infinity are parallel to F.

Proof. Let $s \in \{t_+, t_-\}$ be the net voltage on the cycle $C \in \{C_+, C_-\}$ defining the half geodesic $[aC[$ in τF. Consider now the sequence of translated vertices $s^n(a)$ in $[aC[$, standing at the increasing distance $n|C|$ from the initial vertex a. Following Lemma 5.1, their pre-images, which are at this same distance $n|C|$ from the vertex $y = \tau^{-1}a$ in F belong to the ball $B[t^k(y), \Delta]$ for some integer k. This can be written as follows:

$$d\{\tau^{-1}[s^n(a)], t^k(y)\} \leq \Delta.$$

Since τ, and thus τ^{-1}, are local automorphisms, we can also write

$$d\{s^n(a), \tau^{-1}[s^n(a)]\} \leq |\tau| \quad \text{and} \quad d\{t^k(\tau^{-1}a), t^k(a)\} \leq |\tau|,$$

so that:

$$d\{s^n(a), t^k(a)\} \leq \Delta + 2|\tau|.$$

Clearly, the last distance $d\{s^n(a), t^k(a)\}$ cannot remain bounded for arbitrarily large values of n unless $s \in \mathrm{Ext}(t)$ and the corresponding cycles have same reduced length. □

Lemma 5.5. Any geodesically complete subgraph of a periodic graph containing two parallel half geodesics $[C_+[$ and $]C_-]$ also contains the full geodesics $]C_+[$ and $]C_-[$.

Proof. We suppose here that a geodesically complete subgraph H of some periodic graph (G, T) contains two half geodesics $[aC_+[$ and $]C_-b]$, where the cycles C_+ and C_- of G/T may have different net voltages t^α and t^β but have the same reduced length, so that $\beta|C_+| = \alpha|C_-|$. We shall show that H also contains the translated half geodesic $]C_-t^{\alpha\beta}(b)]$, so that, by induction, it contains the whole geodesic $]C_-[$.

The situation is represented in Fig. 7 in the case $\alpha = \beta = 1$. We consider the sequence $u_n \equiv d\{b, t^{n\alpha}(a)\}$. It is clear that, for sufficiently large values of n, the sequence is an increasing function of n. Moreover, we can write:

$$\begin{aligned} u_{n+1} &= d\{b, t^{(n+1)\alpha}(a)\} \\ &\le d\{b, t^{n\alpha}(a)\} + d\{t^{n\alpha}(a), t^{(n+1)\alpha}(a)\} = u_n + |C_+| \end{aligned} \quad (1)$$

$$\begin{aligned} n|C_+| &= d\{a, t^{n\alpha}(a)\} \\ &\le d\{a, b\} + d\{b, t^{n\alpha}(a)\} = d\{a, b\} + u_n. \end{aligned} \quad (2)$$

Consider the set S of integers n for which $u_{n+1} - u_n < |C_+|$. This set is bounded, otherwise relation (2) could not hold for arbitrarily large values of n. Call then m the maximum value of S: for all $n > m$, we have $d\{b, t^{(n+1)\alpha\beta}(a)\} = d\{b, t^{n\alpha\beta}(a)\} + \beta|C_+|$. By completeness of the subgraph H, the path $bt^{n\alpha\beta}(a)t^{(n+1)\alpha\beta}(a)$, from b to $t^{n\alpha\beta}(a)$ and then to $t^{(n+1)\alpha\beta}(a)$ along $]C_+[$, which is a geodesic path, can be substituted by the alternative path from b to $t^{\alpha\beta}(b)$ along the geodesic $]C_-[$, of length $\alpha|C_-|$, followed by the image path $t^{\alpha\beta}\{bt^{n\alpha\beta}(a)\} = t^{\alpha\beta}(b)t^{(n+1)\alpha\beta}(a)$. This shows that the path $bt^{\alpha\beta}(b)$ along $]C_-[$ belongs to H and, thus, also the half geodesic $]C_-t^{\alpha\beta}(b)]$ up to vertex $t^{\alpha\beta}(b)$. □

Theorem 5.1. Local automorphisms in periodic graphs (G, T) map T-fibers on parallel T-fibers.

Proof. From Lemmas 5.4 and 5.5, the image τF of any T-fiber (F, $\langle t\rangle$) by a local automorphism τ in a periodic graph (G, T) contains a full geodesic $]C_-[$. From Algorithm 4.1, we conclude that τF must also contain the T-fiber generated by the cycle C_-, in order to satisfy to completeness. But then, according to the minimal criterion, τF is exactly the T-fiber of (G, T) determined by the cycle C_- and the vertex b. □

Theorem 5.2. Every fiber of a periodic graph (G, T) is also a T-fiber.

Proof. Consider a fiber (F, $\langle\tau\rangle$) and the half geodesics $[aC_+[$ and $[bC_-[$, defined as in Lemma 5.3. The natural projection of $[bC_-[$ on F/$\langle\tau\rangle$ is a walk, which traverses infinitely many times at least one vertex of this quotient graph. We can thus find two vertices, say u and v, of $[bC_-[$ that belong to the same vertex lattice of F/$\langle\tau\rangle$, so that $v = \tau^k(u) \in [bC_-[$ for some positive integer k. On the other hand, the full geodesics $]C_-[$ and $]C_+[$ certainly satisfy the criteria listed in Algorithm 4.1 for T-fibers, otherwise F could not be a fiber either. Let then (F′, $\langle s\rangle$) and (F″, $\langle t\rangle$) be the T-fibers generated by the geodesics $]C_-[$ and $]C_+[$, running through the vertices b and a, respectively. According to Theorem 5.1, the image τ^kF′ is also a T-fiber parallel to F′. But then, v is a common vertex to F′ and to its image τ^kF′, which means (following Proposition 3.1) that both T-fibers are identical: τ^kF′ = F′. That is: F′ is invariant by τ^k. Let us call Δ and Δ' the diameters of the fibers F and F′, respectively. According to Lemma 5.1, for any integer n we can find an integer m such that $\tau^{nk}(u)$, as a vertex of F′ belongs to the ball B[$s^m(b)$, Δ']. Now, for sufficiently large values of n we can send the image $\tau^{nk}(u)$, as a vertex of F, on the 'side' of the half geodesic $[aC_+[$; according to Lemma 5.3, it is thus possible to find an integer p so that this vertex belongs to the ball B[$t^p(a)$, Δ+|t |]. Clearly, this is not possible unless the T-fibers F′ and F″, and so the half geodesics $[C_+[$ and $]C_-]$, are parallel. Then, according to Lemma 5.5, the fiber F contains the full geodesic $]C_-[$ and so must be identical to F′. □

Theorems 5.1 and 5.2 have deep implications concerning the nature of local automorphisms of periodic graphs (G, T) that are not crystallographic nets. As recalled above, some local automorphisms that are not in T do not respect vertex and edge lattices of G, so that it is not possible to define a consistent action of the product $q_T \circ \tau \circ q_T^{-1}$ on the quotient graph G/T. For example, if we lift a cycle of G/T with non-null net voltage, map the resulting path in G by the local automorphism τ and finally get its image by the natural projection q_T, we do not obtain generally a cycle of G/T. However, Theorem 5.1 shows that the subgraphs of G/T corresponding to projections F/$\langle t\rangle$ of T-fibers are globally mapped on the subgraphs of parallel T-fibers by local automorphisms. Some applications are examined in the next sections.

6. Minimal nets

An important class of periodic graphs has maximal rank of the translation group T for the associated quotient graph. In this section, we consider finite c-connected graphs of cyclomatic number ν and attribute independent voltages from a translation group T of rank ν to the chords of a spanning tree. The derived ν-periodic graph is called a *minimal net* (Beukemann & Klee, 1992). We first analyze the nature of geodesic T-fibers in minimal nets, from which we deduce the important result expressed in Theorem 6.1.

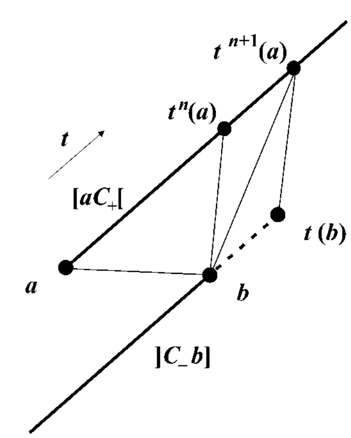

Figure 7
Two half geodesics $[aC_+[$ and $]C_-b]$ parallel to the same direction t (see text).

Proposition 6.1. Geodesic T-fibers in minimal nets are strong geodesics in 1–1 correspondence with the cycles or loops of the quotient graph.

Proof. No cycle of the quotient graph can have a net voltage null and no two cycles or loops can have the same net voltage. If some cycle is the combination of independent cycles of the quotient graph, then its length is shorter than the sum of the lengths of the combined cycles, since common edges are deleted in the addition process. It follows from Algorithm 4.1 that geodesic T-fibers in minimal nets are strong geodesics, in one-to-one relation with the cycles or loops of the quotient graph. □

Proposition 6.2. The group of local automorphisms of a minimal net derived from a *c*-connected graph acts freely on the net.

Proof. Consider a local automorphism f of the minimal net with a fixed vertex a and take an incident edge $e = ab$. If e belongs to some strong geodesic of the minimal net, then it is fixed by f, since the image of a geodesic is a parallel geodesic running through the same vertex a. Suppose, on the contrary, that no geodesic runs through the chosen edge and that b is mapped on another vertex c. Since the quotient graph is *c*-connected, at least one cycle or one loop runs through vertex B, the natural projection of b on the quotient graph, that is: at least one strong geodesic runs through vertex b in the minimal net. This geodesic maps a parallel geodesic running through vertex c, which can therefore be projected on a cycle or loop of the quotient graph with the same net voltage as the cycle or loop through vertex B. But no two cycles or loops of the quotient can have the same net voltage: it is thus the same cycle (it cannot be a loop) that runs through B and through the projection C of vertex c. Neither the edge AB, projection of the edge e on the quotient, nor the image AC of the mapped edge can belong to this cycle by hypothesis. However, running along this cycle from B to C, then back to B through the edges CA and AB, gives a new cycle of the quotient and thus a geodesic of the minimal net containing the edge e, a contradiction. We conclude that vertex b is also fixed by the automorphism f. This way, all vertices linked to a fixed vertex are also fixed vertices. By induction, the whole net must be fixed, since it is connected, and the unique local automorphism with a fixed vertex is the identity.

A similar argument shows that the unique local automorphism with a fixed edge is the identity. Suppose the edge $e = ab$ is mapped on the opposite edge ba. Then, a cycle C of G/T running through A is mapped on the same cycle running through B. Taking a path between A and B along C, which does not contain the edge AB and completing with this edge, we obtain a cycle of G/T running through AB. This means that e lies on a strong geodesic. A local automorphism, however, cannot reverse the orientation of a strong geodesic; otherwise it fails to be 'local'. The unique possibility to have a fixed edge while mapping the geodesic on itself is then to have two fixed vertices, a and b. □

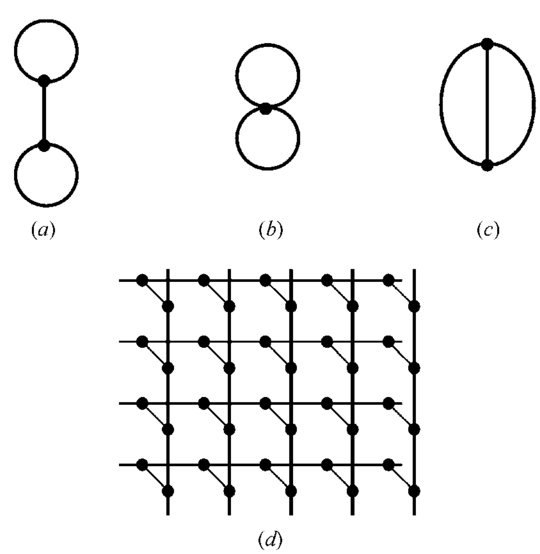

Figure 8
The quotient graphs of the two-dimensional minimal nets: (*a*) 2(3)2, (*b*) 1(4)1, (*c*) 2(3)1 and (*d*) the minimal net derived from 2(3)2. The nomenclature is the same as in Beukemann & Klee (1992).

Theorem 6.1. Minimal nets derived from *c*-connected graphs are crystallographic nets.

Proof. According to Eon (2005), it is sufficient to show that the group of local automorphism is equal to the translation group T. The argument is based on the structure of the quotient graph Q of the minimal net. If there is only one cycle in Q, the derived graph is the linear net and its local automorphism group is isomorphic to Z. Suppose there are at least two cycles in Q. For an arbitrary cycle C, we choose a *nearest cycle* C' (by nearest cycle, we mean that the smallest distance between two vertices x of C and y of C' is minimum; note that in a *c*-connected graph this distance is 0 or 1). Three distinct cases can arise:

(i) C and C' are disjoint; the union graph of the two cycles together with the unique edge linking them is a subgraph of Q homeomorphic to 2(3)2 (Fig. 8*a*);

(ii) C and C' share a single vertex; the union graph of the two cycles is a subgraph of Q homeomorphic to 1(4)1 (Fig. 8*b*);

(iii) C and C' share a common path; the union graph of the two cycles is a subgraph of Q homeomorphic to 2(3)1 (Fig. 8*c*).

Remarkably, the aforementioned subgraphs are the quotient graphs of the three two-dimensional minimal nets. The same argument applies in each case.

From Proposition 6.1, any cycle C of Q lifts to a strong geodesic $]C[$. From Theorem 5.1, a strong geodesic $]C[$ is mapped on a parallel geodesic by any local automorphism τ. Then, from Proposition 6.1 again, the image geodesic $\tau]C[$ must project on the same cycle C of Q. We can therefore interpret the action of the local automorphism on each strong geodesic, viewed in projection on the quotient graph, as a kind of rotation applied separately to the associated cycle of Q. In the three limit cases, however, the cycles C and C' cannot rotate freely since they are linked by an extra edge in (i), a common vertex in (ii) or a common path in (iii) that cannot follow the rotation in both cycles simultaneously: both cycles must be fixed. As a consequence, at least one vertex, say a, of the minimal net is mapped on a vertex of the same vertex–lattice, so that there is a translation t which acts the same way as τ on vertex a. Then, $t^{-1}\tau(a) = a$ and, from Proposition 6.2, $\tau = t$. □

Example 6.1. The 2-periodic net shown in Fig. 8(d) is the minimal net derived from the graph 2(3)2 of Fig. 8(a), after attributing voltages **10** and **01** to the loops. The net is a crystallographic net and its automorphism group is isomorphic to that of the square net.

7. Crystallographic and non-crystallographic nets

The 2-periodic graph shown as a planar embedding in Fig. 9(a) is not a crystallographic net, since it admits local automorphisms with fixed vertices, such as the permutation $\boldsymbol{\pi} = (a, b)$, which exchanges only the two vertices labeled a and b on the figure, together with the incident edges. The labeled quotient graph associated with this planar embedding is given in Fig. 9(b). The periodic graph presents a family of strong geodesics in the direction **10**, which project on the loop of the quotient graph and another family of geodesic fibers along **01**. These fibers project on the right part of the quotient graph, that is, the quotient graph of the fiber is obtained from that of the net by simply deleting the loop with voltage **10**. Now, we notice that there exists an automorphism of the quotient graph, which we shall denote by (A, B), that exchanges each edge CA with the edge CB of the same voltage, so that every cycle (or loop) of the graph maps a cycle (or loop) with the same net voltage. The vertex C, the edge AB and the loop on C are fixed elements of the automorphism (A, B), indicating that there are local automorphisms of the 2-periodic graph with fixed elements (Eon, 2005). We can choose among these automorphisms one that exchanges the vertices a and b, as does the automorphism $\boldsymbol{\pi}$, and holds fixed all geodesic fibers of the periodic graph. Informally, this automorphism can be interpreted as an extension by the translation group of the automorphism (a, b) to the whole 2-periodic graph.

It was implicitly assumed in Eon (2005) that the absence of automorphisms of the labeled quotient graph mapping cycles (loops) on cycles (loops) with the same net voltage should ensure that the derived periodic graph is a crystallographic net. It is possible to verify this assertion in particular cases by analyzing the images of geodesic T-fibers by local automorphisms. With Theorems 4.1 and 5.1, the analysis can be performed directly on the quotient of the periodic graph.

Example 7.1. The labeled quotient graph of the net (3^4.6), represented in Fig. 3, has been drawn in Fig. 10(a). The labeled quotient graphs of the geodesic fibers along directions **10** and **21** are shown in Figs. 10(b) and 10(c), respectively. Fig. 10 evidences the graph–subgraph relationship between the

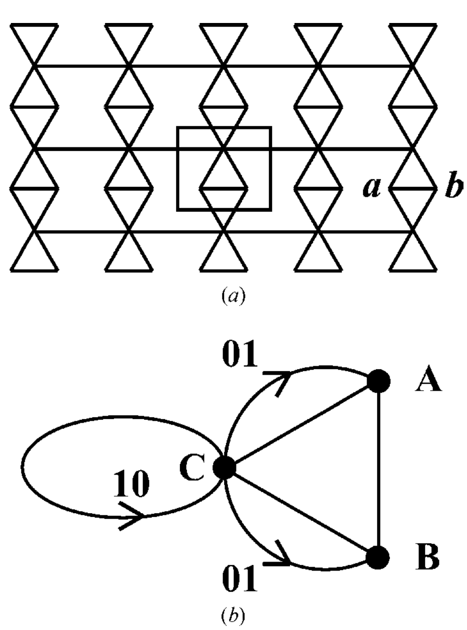

Figure 9
(a) A non-crystallographic net and (b) a possible quotient graph.

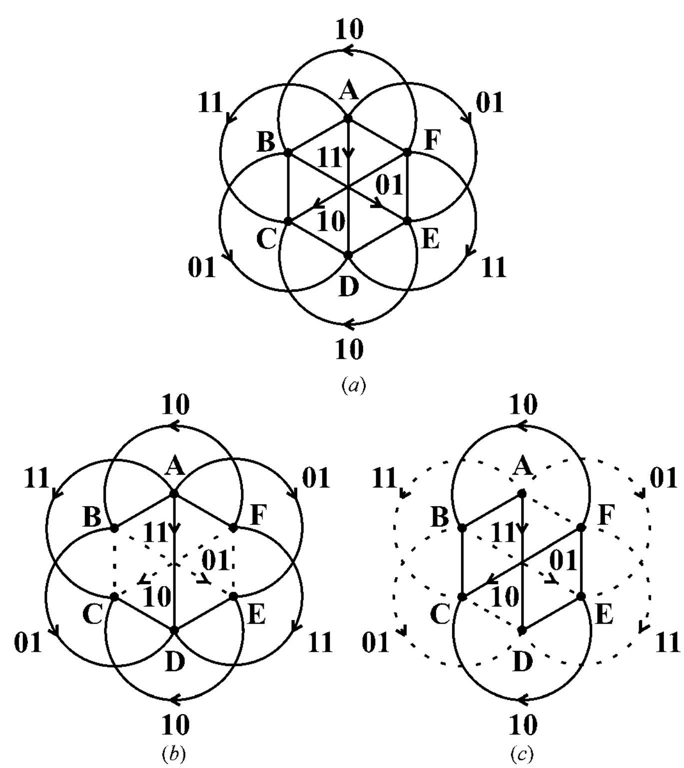

Figure 10
(a) Quotient graph of the net (3^4.6) with the quotient graphs of its two geodesic fibers along directions (b) **11** and (c) **21**.

labeled quotient graph of the net and those of its fibers. For the sake of clarity, however, the quotient graphs of the fibers have been re-drawn and re-labeled in Figs. 11(*a*) and 11(*b*), respectively. Both quotient graphs contain the six vertices of the quotient graph of the periodic net, so that (by Proposition 3.1) there is only one equivalence class of fiber by translation parallel to each direction, which (by Theorem 5.1) must be mapped onto itself by any local automorphism. To respect the structure of the fiber along the direction **21**, the path BADE must then be conserved, up to translation. This implies that the four vertex lattices B, A, D and E of the net are mapped on themselves by any local automorphism. But then some vertices from the vertex lattices C and F could exchange, which possibility appears to be excluded when looking at the fiber along direction **10** since vertices from B and E should then also exchange in order to respect adjacency relationships in this fiber. We conclude that all vertex lattices of the net (3^4.6) map on themselves by any local automorphism, and so that any local automorphism is a translation. Consequently, the net is a crystallographic net.

8. Order of fixed-vertex automorphisms

The only local automorphisms of strong geodesics, considered as 1-periodic graphs, are translations along the respective direction; this is clearly the fundamental reason why minimal nets derived from *c*-connected graphs are crystallographic nets. It is thus natural to analyze local automorphisms of geodesic T-fibers in general and more particularly local automorphisms with fixed vertices before we can decide about the order of local automorphisms in *n*-periodic graphs.

Lemma 8.1. Let f be an automorphism of an infinite graph G. If the cardinality of the orbits by f of the vertices of G is uniformly bounded, then f has finite order.

Proof. Let m be the superior bound of the cardinalities of the orbits by f; any vertex x of G has then order $q < m$. But then, for all vertices x, $f^{m!}(x) = x$. □

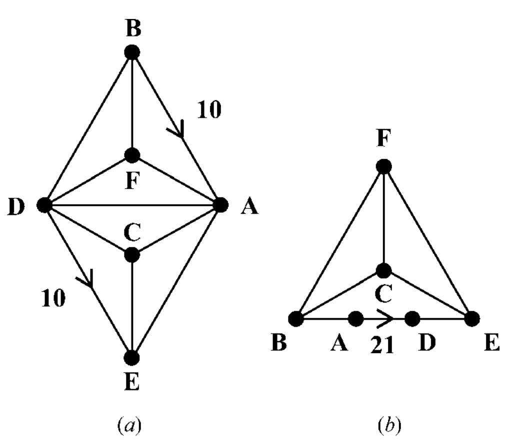

Figure 11
Re-labeling the quotient graphs of the geodesic fibers of the net (3^4.6) along directions (*a*) **11** and (*b*) **21**.

Corollary 8.1. Local automorphisms of 1-periodic graphs with a fixed vertex have finite order.

Proof. Let f be a local automorphism of a 1-periodic graph (G, T) with a fixed vertex v. In a 1-periodic graph, the number of vertices at some distance d from v is certainly bounded (in each orientation of the graph) by the number m of vertex lattices of the quotient graph G/T. Since local automorphisms conserve the distances as well as the orientation of the fiber, the orbit of each vertex contains at most m vertices. □

Theorem 8.1. Local automorphisms of n-periodic graphs with fixed vertices have finite order.

Proof. Let f be a local automorphism of an n-periodic graph (G, T) with a fixed vertex v. From Proposition 4.2, we can choose a set of n T-fibers F_i oriented along n independent directions of the periodic graph. Given any vertex x, we build a path $vx = \delta_0 p_1 \delta_1 \ldots p_n \delta_n$, where the path p_i belongs to a fiber parallel to F_i and the path δ_i is added when necessary to interlink the whole path between v and x through the sequence of fibers. It is always possible to choose the paths p_i (that is: the particular fiber parallel to F_i) so that the length of the paths δ_i is less than the diameter Δ of the quotient graph G/T. From Theorem 5.1, each fiber F_i is mapped by f to a parallel fiber, so that the path defining the image of vertex x has the same structure as the path vx: $vf(x) = f(vx) = f(\delta_0)f(p_1)f(\delta_1)\ldots f(p_n)f(\delta_n)$. The cardinality of the orbit of vertex x by f is then certainly bounded by the total number of paths with the same characteristics for the paths δ_i and p_i. This upper bound in turn is limited by two factors:

(i) the number of vertices one can find at a distance less than Δ from any vertex of the periodic graph G, which defines the maximum number of endpoints of the paths δ_i;

(ii) the number of vertex lattices on each fiber, which defines the maximum number of endpoints of the paths p_i.

The upper bound certainly does not depend on the lengths of the paths p_i, which turns the limit uniform for all vertices of the n-periodic graph. The result follows then from Lemma 8.1. □

9. Final considerations

The topology of most crystal structures is described by quotient graphs G with cyclomatic number larger than three. In this case, the derived 3-periodic graph P with translation group T is the *partial quotient* of the minimal net N associated to the quotient graph G with respect to some translation subgroup S of N. More specifically, if we denote by R the translation group of the minimal net, we can write G = P/T = N/R. The subgroup S of R is generated by the net voltages, in the labeled quotient graph N/R, of the closed walks that have a net voltage null in the labeled quotient graph P/T; we have then P = N/S. P is called a *partial quotient* because it is generated in the same way as the quotient graph N/R. But instead of using the full translation group R of the minimal net, we define the set of vertex and edge orbits of N by a subgroup S of lower rank so that T = R/S is again a translation group. Of course, this process is also a natural projection of the minimal net (Klee, 2004), but the partial quotient is an infinite graph. The subgroup S is called the kernel of the projection.

Example 9.1. The ladder of Fig. 2(*e*) admits the same quotient graph as the minimal net in Fig. 8(*d*), with relation to the subgroup ⟨**01**⟩ of the square net. The labeled quotient graph of the ladder is obtained from that shown in Fig. 8(*a*) by labeling both loops with the same voltage **01**. This indicates that the ladder is a partial quotient of the minimal net in Fig. 8(*d*). The kernel S of the natural projection is computed from the only non-trivial closed walk of net voltage null in the labeled quotient graph of the ladder. This walk follows one of the loops, crosses the bridge, follows the other loop and comes back through the bridge; it is in fact the image of a strong ring of the ladder. The same walk in the labeled quotient graph of the minimal net has net voltage **11** (or equivalently **1−1**); the ladder is thus the partial quotient of the minimal net in Fig. 8(*d*) by the translation subgroup S = ⟨**11**⟩. The minimal net admits two non-equivalent strong geodesics along directions **10** and **01**, while the ladder displays only one strong geodesic and one strong ring.

Although elementary, this example illustrates a quite general phenomenon. The minimal net derived from a *c*-connected graph is always, as we have seen, a crystallographic net. Upon natural projection to get partial quotients, however, one can obtain a non-crystallographic net. The descent in the rank of the translation group of the partial quotient upon projection is associated to two correlated changes in the topological invariants of the periodic graph. New rings describing the kernel of the projection (see Eon, 2006) are added; at the same time, strong geodesics are lost or give way to geodesic fibers. One can thus hope that the combined use of both kinds of invariants, strong rings and geodesic fibers, present in most periodic graphs, will be useful to the classification of non-crystallographic nets and of their automorphism groups, directly from their labeled quotient graph. This could be a precious tool for the synthetic chemist interested in preparing new compounds based on these certainly non-conventional topologies.

APPENDIX *A*

An elementary but important result needed for the proof of Lemma 5.2 is given by the following proposition.

Proposition A.1. Any 1-chain W of a graph G that can be written as a sum of cycles and has a connected support can be traversed as a closed walk.

Proof. One can construct a new graph S′ from the support S of W by substituting each oriented edge of S by a multiple edge with multiplicity equal to its coefficient in the chain, and equal orientation. Each cycle of the decomposition of the chain contributes with two edges at each vertex of S′: one incoming and one outgoing. In consequence, each vertex of S′ has equal incoming and outgoing degrees. It is well known that connected graphs with all vertices of equal incoming and outgoing degrees are Eulerian: such an Eulerian (oriented) circuit in S′ maps a closed walk in G after identifying again the edges of each multiple edge. □

On projecting geodesic paths of a periodic graph on its quotient graph and writing the associated 1-chains, it may happen that some edges cancel out. In this case, these edges correspond to the bridges between different components of the support and cannot be traversed more than once in each direction. However, Proposition A.1 can yet be applied if we substitute such an edge by a 2-cycle, that is: a pair of edges with opposite orientations, and agree to keep it as an effective cycle in the decomposition of the 1-chain, instead of canceling out. Since these 2-cycles appear in finite number in the decomposition of any 1-chain, their presence does not affect the argument developed in the proof of Lemma 5.2.

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