Frameworks with crystallographic symmetry

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Periodic frameworks with crystallographic symmetry are investigated from the perspective of a general deformation theory of periodic bar-and-joint structures in Euclidean spaces of arbitrary dimension. It is shown that natural parametrizations provide affine section descriptions for families of frameworks with a specified graph and symmetry. A simple geometrical setting for displacive phase transitions is obtained. Upper bounds are derived for the number of realizations of minimally rigid periodic graphs.

1. Introduction

The notions of periodic graph and periodic framework emerged as abstractions of crystal structures. Enquiries about lattice sphere packings sprang from the same source.

We show that a classical setting, used in the theory of positive definite quadratic forms and lattice sphere packings, leads to natural parametrizations for placements of periodic graphs. In this description, all placements with a specified crystallographic symmetry correspond with a certain affine section. As a result, the deformation theory for periodic frameworks presented in our papers \cite{1,2} is adapted in a natural way so as to encompass all cases of higher crystallographic symmetry.

We shall assume a certain level of familiarity with the motivations, background and theoretical foundations offered in \cite{1} and comment here mostly on the rapport of the earlier perspective, with its focus on the periodicity group $\Gamma$ corresponding to translational symmetries, and the current perspective, which allows for infinite framework graphs $G$ with arbitrary crystallographic symmetry group $\Sigma$.

The new stance complements the earlier one also with respect to factoring out framework equivalence under Euclidean isometries. In this sense, it may be seen as a
periodic version of the approach used in [3] for finite linkages. For finite configurations, equivalence under isometries may be factored out by passing to ‘Cayley–Menger coordinates’ based on mutual squared distances. For periodic configurations, this amounts to recording the metric through the Gram matrix of an independent set of generators for the periodicity lattice.

In a succinct formulation, the passage from the Abelian lattice case \((G, \Gamma)\) to the more general crystallographic case \((G, \Sigma)\) is mediated by a switch from the perspective of a fixed metric and a moving lattice to that of a moving metric and a fixed lattice. As mentioned, this alternative is traditional lore in the theory of positive definite quadratic forms and lattice sphere packings [4–6]. One may add here the remark that the classical notion of perfect form [7] is equivalently characterized through the rigidity of the periodic (one orbit) contact graph for the associated lattice sphere packing.

The current approach offers geometrical models for displacive phase transitions in minerals, when the related phases have commensurate crystallographic symmetry groups [8]. Other problems in chemistry or structural engineering, such as periodic framework realizations with higher symmetry [9,10], may also be addressed with our methods.

2. Symmetries of a periodic framework

We adopt here definitions introduced in [1]. Let \((G, \Gamma)\) be a \(d\)-periodic graph. The infinite graph \(G = (V, E)\) is assumed connected and, when given a periodic placement \((p, \pi)\) in \(R^d\), the corresponding periodic framework is denoted \((G, \Gamma, p, \pi)\). Recall that \(\Gamma \subset Aut(G)\) is a free Abelian group of rank \(d\) and \(\pi\) is a faithful representation of \(\Gamma\) by a lattice of translations of rank \(d\). Moreover,

\[
p : V \to R^d \quad \text{and} \quad \pi : \Gamma \to T(R^d)
\]

are related by

\[
p \circ \gamma = \pi(\gamma) \circ p \quad \text{for all} \quad \gamma \in \Gamma.
\]

Relation (2.2) shows that \(\pi\) may be inferred from \(p\), but most considerations about framework deformations and symmetries benefit from observing both functions. The quotient multi-graph \(G/\Gamma\) is assumed to be finite and we put

\[
n = |V/\Gamma| \quad \text{and} \quad m = |E/\Gamma|.
\]

Periodic frameworks are abstract, idealized versions of crystalline materials and, like them, may possess other symmetries, besides those expressing periodicity under \(\Gamma\). Thus, there might be a larger group of automorphisms \(\Gamma' \subset \Sigma \subset Aut(G)\) and an extension of \(\pi\) to a faithful representation of \(\Sigma\) by a crystallographic group \(\pi(\Sigma) \subset E(d)\), such that relation (2.2) would hold for all \(\sigma \in \Sigma\).

Considering that \(Aut(G, \Gamma)\) is the normalizer of \(\Gamma\) in \(Aut(G)\), a natural assumption for investigating this set-up will be that \(\Gamma\) is normal in \(\Sigma\), that is, \(\Gamma \subset \Sigma \subset Aut(G, \Gamma)\). If all translational symmetries of the framework \((G, \Gamma, p, \pi)\) are in \(\pi(\Gamma)\), then this is necessarily the case, because the subgroup of translations in a crystallographic group is normal. In general, the normality assumption would hold after replacing the initial periodicity group \(\Gamma\) by an appropriate subgroup of finite index \(\tilde{\Gamma} \subset \Gamma\). Alternatively, instead of relaxing, one may refine the periodicity group by adopting all translational symmetries of the given framework.

For these reasons, we proceed below with the study of framework symmetries that correspond to graph automorphisms in the normalizer \(N(\Gamma)\) of \(\Gamma\) in \(Aut(G)\). Note that the quotient group \(N(\Gamma)/\Gamma\) acts naturally on the quotient graph \(G/\Gamma\). It follows that \(N(\Gamma)/\Gamma\) is finite, because \(G/\Gamma\) is finite and \(G\) connected.
**Definition 2.1.** We say that \( \sigma \in N(\Gamma) = Aut(G, \Gamma) \) is a symmetry of the \( d \)-periodic framework \((G, \Gamma, p, \pi)\) when the result of acting by \( \sigma \) on the framework is the same as the result of acting by an isometry \( s \in E(d) \), that is,

\[
s \circ p = p \circ \sigma. \tag{2.4}
\]

In other words, we have a commutative diagram

\[
\begin{array}{ccc}
V & \xrightarrow{p} & R^d \\
\downarrow \sigma & & \downarrow s \\
V & \xrightarrow{p} & R^d.
\end{array}
\tag{2.5}
\]

As remarked above, it is convenient to keep \( p \) and \( \pi \) on an equal footing. Then, (2.4) becomes the equivalent but more revealing condition

\[
s \circ p = p \circ \sigma \quad \text{and} \quad C_s \circ \pi = \pi \circ C_{\sigma}, \tag{2.6}
\]

where \( C_s \) denotes the restriction to the group of translations \( T(R^d) \) of the conjugation by \( s \) in \( E(d) \) and \( C_{\sigma} \) denotes the restriction to \( \Gamma \) of the conjugation by \( \sigma \) in \( Aut(G) \).

With \((p, \pi)\) given, it follows from (2.6) that \( s \) is uniquely determined by \( \sigma \). Indeed, assuming the origin in \( R^d \) to be the image by \( p \) of a particular vertex \( v_0 \in G \), we have

\[
s(x) = Sx + t, \tag{2.7}
\]

and

\[
\text{with } S = C_s \text{ when } R^d \equiv T(R^d) \quad \text{and} \quad t = s(0) = p(\sigma v_0). \tag{2.8}
\]

Note that \( s \) is a translation if and only if \( C_s \) is the identity, that is, if and only if \( \sigma \) belongs to the centralizer \( C(\Gamma) \) of \( \Gamma \) in \( N(\Gamma) \)

\[
C(\Gamma) = \{ \delta \in N(\Gamma) \mid \delta \gamma = \gamma \delta \text{ for all } \gamma \in \Gamma \}.
\]

Thus, the set of all symmetries of \((G, \Gamma, p, \pi)\) becomes a group under composition. This is the symmetry group of the framework and will be denoted by \( \Sigma = \Sigma(G, \Gamma, p, \pi) \subset N(\Gamma) \subset Aut(G) \). The periodicity group \( \Gamma \) is a normal subgroup of \( \Sigma \), and the injective homomorphism \( \sigma \mapsto s \) is an extension of \( \pi : \Gamma \rightarrow T(R^d) \) to \( \Sigma \rightarrow E(d) \). For the sake of simplicity, this extension is also denoted by \( \pi \). Because \( \pi(\Sigma) \) is a crystallographic group, we may refer to the framework \((G, \Gamma, p, \pi)\) as having crystallographic symmetry \( \Sigma \).

### 3. Symmetry constraints

For a given \( \sigma \in N(\Gamma) \), we may identify all periodic placements \((p, \pi)\) for which \( \sigma \) is a symmetry of the framework \((G, \Gamma, p, \pi)\). It will be convenient to give this description in terms of parameters based on the following choices: a complete set of representatives \( v_0, v_1, \ldots, v_{n-1} \) for the vertex orbits of \( \Gamma \) on \( V \) and an isomorphism \( \mathbb{Z}^d \approx \Gamma \). Later on, a complete set of edge representatives of the form \( e_{ij} = (v_i, v_j + \gamma_j) \) for the orbits of \( \Gamma \) on \( E \) will be implicated in obtaining equations for the length preservation of edges under deformation.

Note that we allow the additive notation \( \gamma v = v + \gamma \) for the action of \( \gamma \in \Gamma \) on a vertex of the graph, which will facilitate writing the corresponding translation in a placement \((p, \pi)\) as \( \pi(\gamma)p(v) = p(v) + \lambda \), when the translation \( \pi(\gamma) \in T(R^d) \) has the formula \( \pi(\gamma)(x) = x + \lambda \) and is identified with the translation vector \( \lambda \in R^d \).

Besides the frequent identification \( T(R^d) \equiv R^d \), which induces an inner product on the group of translations, other routine conventions and notations will be the following. With the chosen
isomorphism $Z^d \approx \Gamma$, the automorphisms of the free Abelian group $\Gamma$ are given by $d \times d$ matrices with integer entries and determinant $\pm 1$, that is, $\text{Aut}(\Gamma)$ is identified with the unimodular group $GL(d, Z)$. Moreover, by turning the free module $Z^d$ into the $d$-dimensional vector space,

$$R^d = Z^d \otimes Z R \approx \Gamma \otimes Z R,$$

unimodular transformations will be conceived as linear transformations. In particular, conjugation by $\sigma \in N(\Gamma)$ gives an automorphism $C_\sigma \in \text{Aut}(\Gamma)$, and thereby a unimodular transformation that we denote by the same symbol $C_\sigma \in GL(d, Z)$. Thus, we have a representation $N(\Gamma) \rightarrow GL(d, Z)$ with kernel $C(\Gamma)$.

When given a periodic placement $(p, \pi)$ of $(G, \Gamma)$, $\pi$ gives an isomorphism

$$R^d \approx \Gamma \otimes Z R \rightarrow T(R^d) \equiv R^d.$$

Thus, two bases are at play: the fixed Cartesian standard basis of $R^d \equiv T(R^d)$ and the lattice basis which depends on $\pi: Z^d \approx \Gamma \rightarrow T(R^d)$, Sometimes, the coordinates based on the Cartesian basis are called geometrical and those based on the periodicity lattice are called arithmetic.

We have seen above that a necessary condition for $\sigma \in N(\Gamma)$ to be a symmetry of the framework $(G, \Gamma, p, \pi)$ is that $C_\sigma \in GL(d, Z)$ should become orthogonal, when expressed in Cartesian coordinates. The remaining conditions refer to the translation part $t$ in (2.7), namely

$$t = p(\sigma(v_i)) - S(p(v_i)),$$

which must be the same for all $i = 0, 1, \ldots, n - 1$. It will be useful to express this in arithmetic coordinates. Let us assume that $\sigma$ acts on the vertex representatives $v_0, v_1, \ldots, v_{n-1}$ according to the formulae

$$\sigma(v_i) = v_{\sigma(i)} + \gamma_i,$$

where $\sigma(i)$ is the index corresponding to the permutation effect of $\sigma$ on $V/\Gamma$ and $\gamma_i \in \Gamma$. Recall that the arithmetic or lattice coordinates are introduced through $\pi: \Gamma \rightarrow T(R^d)$ and the chosen identification $Z^d \approx \Gamma$. Note that each period $\lambda_i \in \Gamma$ in (3.3) will correspond with $n_i \in Z^d$, and these vectors with integer entries depend only on $\sigma$ and the lattice identification $Z^d \approx \Gamma$. We allow here the same symbol $C_\sigma$ for the conjugation given by $\sigma$ on $\Gamma$, its expression as an automorphism of $Z^d$ and its extension to $Z^d \otimes Z R$.

With $e_k$, $1 \leq k \leq d$ the standard basis in $Z^d$, we let $A_\pi = \Lambda \in GL(d, R)$ denote the matrix with columns given by the lattice basis $\pi(e_k)$. We define vector parameters $t_i$ by

$$p(v_i) = A_t t_i$$

and obtain from (3.2) and (3.3) the following conditions:

$$t_{\sigma(i)} + n_i - C_\sigma t_i = t_{\sigma(j)} + n_j - C_\sigma t_j \quad \text{for} \ 0 \leq i, j \leq n - 1.$$

Let us put $\omega_\pi = \omega = \Lambda^t A$ for the Gram matrix of the period lattice basis. Then, the geometrical orthogonality condition for $C_\sigma \in GL(d, Z)$ becomes

$$C_\sigma^t \omega C_\sigma = \omega.$$

In summary, we have

**Proposition 3.1.** A graph automorphism $\sigma \in N(\Gamma) = \text{Aut}(G, \Gamma)$ is a symmetry of the $d$-periodic framework $(G, \Gamma, p, \pi)$ if and only if conditions (3.5) and (3.6) are satisfied.

Recall that the placement information $(p, \pi)$ enters in these equations through the parameters $t_i$, $0 \leq i \leq n - 1$ and $\omega$, as described above. In subsequent sections, we shall elaborate on their role in describing symmetric periodic placements and symmetry-preserving deformations.

4. **Parametrizations**

The deformation theory developed in [1] for periodic bar-and-joint frameworks in $R^d$ emphasized the analogy with the traditional theory of finite linkages. In particular, equivalent realizations
resulting from isometries applied to any given framework were not immediately factored out. However, enumerative purposes or other concerns require the quotient operation. In the finite case [3], Cayley–Menger matrices or, equivalently, Gram matrices serve the purpose. In the periodic case, crystallography and lattice theory have proved long ago the importance of the identification of the quotient $O(d,R)\backslash GL(d,R)$ with the space of positive definite quadratic forms in $d$ variables, itself represented by the open cone $\Omega(d)$ of symmetric $d \times d$ matrices with positive eigenvalues [4–6,11,12].

The parametrization used in the previous section follows this classical perspective. All the information about the lattice of periods $\pi(\Gamma)$, up to orthogonal transformations, is contained in the symmetric matrix $\omega = \Lambda^t \Lambda \in \Omega(d)$, whereas the ‘shift vectors’ $t_i$ indicate (relative to the lattice basis) the placement of the vertex representatives $v_i$. By requesting that $t_0 = 0$, equivalence under translation is eliminated as well. This yields

**Proposition 4.1.** Let $(G, \Gamma)$ be a $d$-periodic graph. Then, all periodic placements in $\mathbb{R}^d$, up to equivalence under the group of Euclidean isometries $E(d)$, are parametrized by $(\mathbb{R}^d)^{n-1} \times \Omega(d)$, which is an open set of $\mathbb{R}^{dn + \binom{d}{2}}$.

**Remark 4.2.** The vertex image sets of periodic placements are multi-lattices, and this type of configuration has been considered in different contexts. While not implicating an edge structure, the study of multi-lattices envisaged in [13,14] is related to the kinematics of phase transitions in crystalline materials. When approached from the point of view of periodic sphere packings, as in [6,15], multi-lattices do acquire an edge structure from contacts between spheres. The resulting “packing frameworks” are a very particular class of periodic frameworks. A study of homogeneous sphere packings in three dimensions has been undertaken by Fischer and co-workers [16] in a series of papers. The planar homogeneous case goes back to Niggl [17,18] and see also [19,20].

The bar-and-joint understanding of a framework brings in the (squared) length function for edges and the notion of deformations [1]. For a given $d$-periodic framework $(G, \Gamma, p, \pi)$, vertices become joints, and edges become straight rigid bars between them. It is enough to register the representatives $v_i$. When isometries are factored out, we obtain, as stated above in proposition 4.1, the result of all isometric replicas of all frameworks. Hence, the fibres of the left vertical arrow are

\[
(R^d)^n \times GL(d, R) \quad \text{q.e.d.} \quad (R^d)^n \times GL(d, R)
\]

where $(R^d)^n \times GL(d, R)$ is the parametrization used in [1] for periodic placements which include all isometric replicas of all frameworks. Hence, the fibres of the left vertical arrow are realization spaces for weighted periodic graphs $(G, \Gamma, \ell)$, that is, periodic graphs with prescribed lengths for their edges. When isometries are factored out, we obtain, as stated above in proposition 4.1, the parameter space $(R^d)^{n-1} \times \Omega(d)$ with the bottom map (4.2). With explicit formulae, we have the following description.
\((R^d)^n \times GL(d, R)\) parametrizes periodic placements \((p, \pi)\) by recording the positions of the \(n\) vertex representatives and the basis of the lattice of periods \(\pi(\Gamma)\), that is, \((p(v_0), \ldots, p(v_{n-1}), \Lambda)\). The left action of the isometry group \(E(d)\) on these parameters is given by

\[
u(p(v_0), \ldots, p(v_{n-1}), \Lambda) = (u \circ p(v_0), \ldots, u \circ p(v_{n-1}), u\Lambda)\]  

(4.4)

for an isometry \(u(x) = Ux + t\), with \(U \in O(d, R)\) and \(t \in R^d\). The quotient map \(q\) works by the formula

\[
q(p(v_0), \ldots, p(v_{n-1}), \Lambda) = (t_1, \ldots, t_{n-1}, \omega) \\
= (\Lambda^{-1}(p(v_1) - p(v_0)), \ldots, \Lambda^{-1}(p(v_{n-1}) - p(v_0)), \Lambda^t \Lambda).
\]  

(4.5)

The left vertical arrow is the composition \(f \circ q\).

A direct enumerative consequence of the current presentation will be an upper bound for the number of distinct possible configurations of a minimally rigid periodic graph with generic edge length prescriptions. Recall from [1,2] that minimally rigid periodic graphs have \(m\) number of distinct possible configurations of a minimally rigid periodic graph. The left action of the isometry group \(E\) must be equivalent under the action of \(\Gamma\). Hence, in parameters \((t_1, \ldots, t_{n-1}, \omega)\) has at most \(3^m\) non-congruent configurations in \(R^d\) for a generic prescription of edge lengths.

\textbf{Proposition 4.3.} Let \((G, \Gamma)\) be a minimally rigid \(d\)-periodic graph with \(n = |V/\Gamma|\) and \(m = |E/\Gamma| = nd + \binom{d}{2}\). Let \(\mu\) be the number of cubic edge constraints \((i \neq j)\) in (4.2). Then, \(dn - d \leq \mu \leq m\) and \((G, \Gamma)\) has at most \(3^m\) non-congruent configurations in \(R^d\) for a generic prescription of edge lengths.

\textbf{Remark 4.4.} This upper bound result is analogous to the one obtained in [3] for finite minimally rigid graphs. The main similarity of the two scenarios resides in recognizing that factoring out the action of Euclidean motions leads, over the complex field, to identifiable varieties: determinantal in the finite case and affine here. Edge-length constraints are then expressed as intersections with low-degree hypersurfaces. For instance, in (4.2), for \(i \neq j\), the total degree in the variables \((t_1, \ldots, t_{n-1}, \omega)\) is explicitly three.

5. Actions and representations

We may now return to symmetry considerations and elaborate on the affine nature of the symmetry constraints obtained in proposition 3.1 in terms of placement parameters \((t_1, \ldots, t_{n-1}, \omega)\).

Let us recall that, by definition, \(\sigma \in \text{Aut}(G, \Gamma)\) becomes a symmetry of a placement \((p, \pi)\) when the effect of \(\sigma\) on the periodic graph \((G, \Gamma)\) is \textit{reproduced} by the effect of an isometry \(s \in E(d)\) on the image of the graph determined by \(p(V)\). In other words, the placements \((p, \pi)\) and \((p \circ \sigma, \pi \circ \sigma)\) must be equivalent under the action of \(E(d)\). Hence, in parameters \((t_1, \ldots, t_{n-1}, \omega)\), we must have one and the same point. By proposition 3.1, the fixed point locus of such an action by \(\sigma\) is given by an affine linear subvariety, and this fact leads to the obvious expectation that the action itself is expressed by an affine map in the parameters \((t_1, \ldots, t_{n-1}, \omega)\).

This is indeed the case, as ensuing computations will confirm. In order to discuss the action of \(\text{Aut}(G, \Gamma)\) on placements and the quotient parameter space \((R^d)^{n-1} \times \Omega(d) \subset R^{dn+\binom{d}{2}}\) as a left action, we adopt the following convention.

\textbf{Definition 5.1.} Let \(\sigma \in \text{Aut}(G, \Gamma)\) be an automorphism of a \(d\)-periodic graph \((G, \Gamma)\). The left action of \(\text{Aut}(G, \Gamma)\) on periodic placements in \(R^d\) is defined by the formula

\[
\sigma(p, \pi) = (p \circ \sigma^{-1}, \pi \circ C_\sigma^{-1}).
\]  

(5.1)
Theorem 5.2. When expressed in parameters \((t_1, \ldots, t_{n-1}, \omega)\), action (5.1) corresponds with an affine representation

\[ A : Aut(G, \Gamma) \to Aff \left( dn + \left( \frac{d}{2} \right) \right), \] (5.2)

which factors through \(Aut(G, \Gamma)/\Gamma = Aut(G/\Gamma)\).

For any subgroup \(\Gamma \subset \Sigma \subset Aut(G, \Gamma)\), the periodic placements of \((G, \Gamma)\) with crystallographic symmetry \(\Sigma\) are parametrized by the fixed locus of \(A(\Sigma)\) in \((\mathbb{R}^d)^{n-1} \times \Omega(d)\), that is,

\[ \mathcal{F}(\Sigma) = \{ x \in (\mathbb{R}^d)^{n-1} \times \Omega(d) : A(\sigma)x = x, \text{ for all } \sigma \in \Sigma \}. \] (5.3)

The locus with full symmetry \(\mathcal{F}(Aut(G, \Gamma))\) is not empty.

Proof. For the computation in coordinates \((t_1, \ldots, t_{n-1}, \omega)\), let us put

\[ \sigma(t_1, \ldots, t_{n-1}, \omega) = (\tilde{t}_1, \ldots, \tilde{t}_{n-1}, \tilde{\omega}) \]

and recall that \(t_0 = \tilde{t}_0 = 0\). We have \(\tilde{\omega} = \tilde{\Lambda}^j \tilde{\Lambda}, \text{ with } \tilde{\Lambda} = \Lambda C_{\sigma^{-1}}\), hence

\[ \tilde{\omega} = (C_{\sigma^{-1}})^j \omega C_{\sigma^{-1}}. \] (5.4)

Recall also that \(\sigma^{-1}\) induces a permutation on \(\{0, \ldots, n-1\}\) by its effect on \(V/\Gamma\). By (3.3) and (4.5), we find \(\sigma^{-1}(v_j) = v_{\sigma^{-1}(j)} - C_{\sigma^{-1}}v_{\sigma^{-1}(j)}, \text{ and then } \)

\[ \tilde{t}_j = C_{\sigma}(t_{\sigma^{-1}(j)} - t_{\sigma^{-1}(j)}) + (n_{\sigma^{-1}(j)} - n_{\sigma^{-1}(j)}). \] (5.5)

Formulae (5.4) and (5.5) give the explicit form of the action of \(\sigma\), which is linear in the components of \(\omega\) and affine in the components of \(t_j, j = 1, \ldots, n-1\).

Resulting homomorphism (5.2) is obviously trivial on \(\Gamma\). Because \(Aut(G, \Gamma)/\Gamma = Aut(G/\Gamma)\) is finite, the image group must have at least one fixed point (the barycentre of an orbit). \(\square\)

Corollary 5.3. There is an inclusion reversing correspondence \(\Sigma \mapsto F(\Sigma)\) between subgroups \(\Gamma \subset \Sigma \subset Aut(G, \Gamma)\) and a finite system of non-empty affine linear sections of \((R^d)^{n-1} \times \Omega(d)\) which parametrize periodic placements with a specified crystallographic symmetry.

It may be observed that this approach obtains periodic placements for \((G, \Gamma)\) with full symmetry \(Aut(G, \Gamma)\) realized by corresponding crystallographic groups, without recourse to a minimizing principle. Other methods for proving the existence of placements with higher symmetry rely explicitly on some ‘energy functional’ minimization technique for finding ‘barycentric placements’ [21] or a harmonic ‘standard placement’ [22]; see also [23]. For deformation problems, it is important to identify, as we do, all placements with specified crystallographic symmetry.

6. Relaxing or refining symmetry

Up to this point, our considerations have focused on a given \(d\)-periodic graph \((G, \Gamma)\) with framework placements \((G, \Gamma, p, \pi)\) in \(\mathbb{R}^d\). However, various problems may require a relaxation \(\hat{\Gamma} \subset \Gamma\) or a refinement \(\Gamma \subset \hat{\Gamma}\) of the periodicity group. As emphasized in [1] and illustrated in [24], changing the periodicity group may have considerable impact on deformation or rigidity properties. For similar issues related to notions of jamming for sphere packings or rigidity of spherical codes, we refer to [25,26].

With the perspective gained in the preceding sections, we introduce the following definition.

Definition 6.1. Let \(G = (V, E)\) be an infinite graph and let \(\Gamma_1, \Gamma_2 \subset Aut(G)\) be free Abelian groups of rank \(d\) such that the corresponding \(d\)-periodic graphs \((G, \Gamma_i)\) admit periodic presentations in \(\mathbb{R}^d\). Then, \(\Gamma_1\) and \(\Gamma_2\) are called commensurate when \(\Gamma_1 \cap \Gamma_2\) is of finite index in both groups \(\Gamma_1\) and \(\Gamma_2\).
Let us observe the effect of relaxing periodicity from $\Gamma$ to a subgroup $\tilde{\Gamma} \subset \Gamma$ of index $k$. We select a complete set of representatives $v_0 = 0, v_1, \ldots, v_{k-1}$ for $\Gamma/\tilde{\Gamma}$. Then, representatives for $V/\tilde{\Gamma}$ are given by $v_i + v_j$ with $0 \leq i \leq n - 1$ and $0 \leq j \leq k - 1$.

When each periodicity group is identified with $\mathbb{Z}^d$, the inclusion of $\tilde{\Gamma}$ in $\Gamma$ corresponds to an invertible matrix $M$ with $\det(M) = k$. Of course, the $\Gamma$-periodic placements of $(G, \Gamma)$ are contained in the $\tilde{\Gamma}$-periodic placements of $(G, \tilde{\Gamma})$, and for a placement $(p, \pi)$ this inclusion takes the form

$$(t_i), \omega) \mapsto (\tilde{t}_i, \tilde{\omega}), \quad \text{with } t_0 = 0 = \tilde{t}_{00}. \quad (6.1)$$

With $\pi(v_j) = m_j$ as translation vectors, we have $p(v_i + v_j) = p(v_i) + m_j$. By (4.5) and its counterpart for $\tilde{\Gamma}$, we find

$$\tilde{\Lambda} = \Lambda M, \quad \text{hence } \tilde{\omega} = \tilde{\Lambda}^t \Lambda = M^t \omega M \quad (6.2)$$

and

$$\tilde{t}_{ij} = M^{-1}t_i + M^{-1}A^{-1}m_j. \quad (6.3)$$

We already know that, from the perspective of $(G, \tilde{\Gamma})$, the placements with ‘higher’ symmetry $\Gamma$ are parametrized by an affine linear section, and the above computation confirms the expected fact that we have an affine inclusion map which identifies the parameter space for periodic placements of $(G, \Gamma)$ with this affine linear section. It follows that the affine and convexity structure of the parameter space $(\mathbb{R}^d)^{n-1} \times \Omega(d) \subset \mathbb{R}^{dn+k(d)}$ for periodic placements of $(G, \Gamma)$ is preserved when relaxing the lattice.

Recall that a crystallographic group in dimension $d$ is a discrete subgroup of isometries $K \subset E(d)$, with a compact quotient $E(d)/K$. Bieberbach [27–29] showed that the subgroup of translations in $K$, that is, $L = K \cap T(\mathbb{R}^d)$, must be a lattice of rank $d$ and is uniquely determined as the maximal free Abelian normal subgroup of $K$. Moreover, $K/L$ is a finite group. Thus, if $\Sigma \subset \text{Aut}(G)$ is isomorphic with a crystallographic group $K \subset E(d)$, we may refer to the free Abelian normal subgroup $\Gamma \subset \Sigma$ corresponding to $L \subset K$, and form the $d$-periodic graph $(G, \Gamma)$.

We have seen above that, when $(G, \Gamma)$ allows periodic placements in $\mathbb{R}^d$, some of them, namely those parametrized by $\mathcal{F}(\Sigma)$, will have Euclidean symmetries given by some crystallographic group isomorphic with $\Sigma$ and $K$ (which must be, according to another Bieberbach theorem [29], an affine conjugate of $K$).

Under these circumstances, we may refer to $\Sigma \subset \text{Aut}(G)$ as a crystallographic subgroup of $\text{Aut}(G)$ and use the pair notation $(G, \Sigma)$ for the graph $G$ with the specified crystallographic symmetry $\Sigma$. It is also understood that, up to Euclidean isometry, the placements of $(G, \Sigma)$ are those parametrized by $\mathcal{F}(\Sigma)$. We note that $\mathcal{F}(\Sigma)$ can be determined in the placement parameter space of any periodic graph $(G, \tilde{\Gamma})$ with $\tilde{\Gamma} \subset \Gamma$ of finite index and stable under conjugation by $\Sigma$. This determination amounts to solving a linear system of equations with integer coefficients of the form (3.5) and (3.6), corresponding to a finite set of transformations $\sigma \in \Sigma$ which provide generators for $\Sigma/\tilde{\Gamma}$. Verifications entirely similar to those performed above show that the affine and convexity structure of $\mathcal{F}(\Sigma)$ is the same for all choices of $\tilde{\Gamma}$.

The commensurability equivalence relation extends as follows.

**Definition 6.2.** Two crystallographic subgroups $\Sigma_1, \Sigma_2 \subset \text{Aut}(G)$ are called commensurate when $\Sigma_1 \cap \Sigma_2$ is of finite index in both $\Sigma_1$ and $\Sigma_2$.

**Remark 6.3.** It would be enough to assume $\Sigma_1 \cap \Sigma_2$ of finite index in one of the groups, but we prefer the symmetric formulation. Clearly, in this case, the intersection $\Sigma_1 \cap \Sigma_2$ is itself a crystallographic subgroup of $\text{Aut}(G)$. Subgroups of finite index in crystallographic groups can be found by simple procedures [30].

Relaxing or refining the symmetry of a framework is associated with certain variations within the framework’s commensurability equivalence class. This language seems favourable for addressing geometrical aspects of displacive phase transitions in crystalline materials [8,31]. The vertices of the infinite graph $G$ may serve as labels for a subfamily or all of the atoms in some idealized crystal, with edges marking bonds. Under variations of temperature or pressure, the same material...
may have phases with different crystallographic symmetry. Displacive phase transitions involve no bond rupture, hence the graph remains the same. When two phases have commensurate symmetry groups $\Sigma_1, \Sigma_2$, our approach gives the simplest geometrical common ground for a passage, namely $\mathcal{F}(\Sigma_1 \cap \Sigma_2)$, which contains both $\mathcal{F}(\Sigma_1)$ and $\mathcal{F}(\Sigma_2)$ as affine linear sections.

Of course, as a guiding scenario, this has been formulated long ago. The new insight, at least at the geometrical level, is that the symmetry-preserving loci have a simple affine structure and description. However, nonlinearity resurfaces when bonds are assumed to maintain their length. This is considered in §7.

7. Symmetry-preserving deformations

When returning to edge-squared length function (4.2), a first simple remark is that $f$ is $\text{Aut}(G, \Gamma)$ equivariant. To see this, it is convenient to write $R^E$ as the space $R^E/\Gamma$ of real-valued functions on $E/\Gamma$. Then, the left action of $\text{Aut}(G, \Gamma)$ is simply defined as

$$\sigma(\phi) = \phi \circ \sigma^{-1}, \quad \text{for } \phi \in R^E/\Gamma$$

(7.1)

with the action on $E$ and on $E/\Gamma$ denoted by the same symbol. Then, one easily verifies that

$$f(\sigma(p, \pi)) = \sigma(f(p, \pi)).$$

(7.2)

When given a framework $(G, \Gamma, p, \pi)$ with crystallographic symmetry $\Sigma \subset N(\Gamma) = \text{Aut}(G, \Gamma)$ and we want to consider only deformations that preserve this symmetry (and all edge lengths), we have to restrict $f$ to $\mathcal{F}(\Sigma)$ and consider the fibre of $f(p, \pi)$. Because $\Sigma$ acts trivially on $\mathcal{F}(\Sigma)$, the image by $f$ must consist of points invariant under $\Sigma$, that is, $f$ factors through $R^E/\Sigma$.

**Remark 7.1.** Strictly speaking, we should write $\Sigma \setminus E$ for the quotient by an action on the left. Expecting no harm, we continue with $E/\Sigma$ and note that $E/\Gamma \to E/\Sigma$ induces $R^E/\Sigma \to R^E/\Gamma$.

It follows that the edge length control for frameworks with crystallographic symmetry $\Sigma$ is given by a map which we allow to be denoted by the same symbol

$$f : \mathcal{F}(\Sigma) \to R^E/\Sigma.$$  

(7.3)

Thus, we obtain a setting entirely analogous to the basic case $\Sigma = \Gamma$.

8. An example: the tridymite framework

Tridymite is a polymorph of silicon dioxide [32,33]. The periodic graph $(G, \Gamma)$ to be considered here is that of the ideal framework or *aristotype*, made of regular tetrahedra and illustrated in figure 1. The periodicity group $\Gamma$ is represented by all translational symmetries.

The aristotype structure may be conceived as an alternation of layers, with reflected successive layers. Each layer is constructed from a planar Kagome pattern made of bases of tetrahedra with apices alternating above and below this plane.

In order to describe the normalizer $N(\Gamma)$ of $\Gamma$ in $\text{Aut}(G)$, we refer to figure 2, which depicts a six-ring of tetrahedra in a layer. The symmetry group of the six-ring is generated by the reflection $r$ in the plane $P$ cutting through opposite tetrahedra and the order two rotation $\rho$ around the axis $a$, which is a nearby diagonal of the basic hexagon. When restricted to the plane of the basic hexagon, the two transformations generate the *dihedral group* $D_6$ of the regular hexagon. Thus, the group $\langle \rho, r \rangle$ generated by $\rho$ and $r$ is isomorphic with $D_6$.

Let us denote by $s$ the reflection in the plane of the apices of the upward-pointing tetrahedra. Then, $N(\Gamma)$ can be described as the group $\langle \Gamma, \rho, r, s \rangle$ generated by the periodicity group $\Gamma$ and the
**Figure 1.** A fragment of the ideal tridymite framework (aristotype). Three generators for the periodicity lattice are indicated by arrows. (Online version in colour.)

**Figure 2.** A six-ring of the ideal tridymite framework, with symmetries generated by reflecting in the plane $P$ and rotating with $\pi$ around the axis $a$. (Online version in colour.)

Graph automorphisms represented by $\rho, r$ and $s$. After factorization by $\Gamma$, $s$ commutes with $\rho$ and $r$ in the quotient, which is also called the ‘point group’ of $N(\Gamma)$,

$$N(\Gamma) = \langle \Gamma, \rho, r, s \rangle, \quad \text{with } N(\Gamma)/\Gamma \approx Z_2 \times D_6.$$  

(8.1)

The action of the point group $N(\Gamma)/\Gamma$ on the quotient graph $G/\Gamma$ can be observed in figure 3. Some of the induced quotient graph automorphisms may be conveniently visualized on the
Figure 3. The quotient multi-graph has \( n = 8 \) vertices and \( m = 24 \) edges. For suggestive purposes, the nearby rendering shows the eight vertices as the vertices of a cube. (Online version in colour.)

proposed cubic rendering. For instance, with a natural labelling, the action of \( r \) corresponds with reflecting in one of the three diagonal planes.

For the unimodular representation \( N(\Gamma)/\Gamma \to \text{GL}(3, \mathbb{Z}) \) described in §3, we may use the two generators of \( \Gamma \) illustrated in figure 2 and a third generator orthogonal to them. We find

\[
\rho \mapsto \begin{pmatrix} 1 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad r \mapsto \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad s \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{8.2}
\]

The crystallographic groups \( \Sigma \) between \( \Gamma \) and \( N(\Gamma) = \text{Aut}(G, \Gamma) \) are in one-to-one correspondence with the subgroups of \( N(\Gamma)/\Gamma \approx \mathbb{Z}_2 \times D_6 \). The arrangement of affine sections follows suit according to corollary 5.3.

For the nonlinear aspects related to the deformation space where all edges have unit length, we refer to [34].

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