THE FIRST-ORDER FLEXIBILITY OF A CRYSTALLOGRAPHIC FRAMEWORK

E. KASTIS AND S.C. POWER

Abstract. Four sets of necessary and sufficient conditions are obtained for the first-order rigidity of a periodic bond-node framework $\mathcal{C}$ in $\mathbb{R}^d$ which is of crystallographic type. In particular, an extremal rank characterisation is obtained which incorporates a multi-variable matrix-valued transfer function $\Psi_{\mathcal{C}}(z)$ defined on the product space $\mathbb{C}_*^d = (\mathbb{C}\backslash\{0\})^d$. In general the first-order flex space is the closed linear span of polynomially weighted geometric velocity fields whose geometric multi-factors in $\mathbb{C}_*^d$ lie in a finite set. It is also shown that, paradoxically, a first-order rigid crystal framework may possess a nontrivial continuous motion. Examples of this phenomenon are given which are associated with aperiodic displacive phase transitions between periodic states.

1. Introduction

Let $\mathcal{C}$ be a periodic bar-joint framework in $\mathbb{R}^d$, where $d \geq 2$, which is of crystallographic type. The vector space $\mathcal{F}(\mathcal{C};\mathbb{R})$ of real infinitesimal flexes, or first-order flexes, is the space of $\mathbb{R}^d$-valued velocity fields on the joints of $\mathcal{C}$ which satisfy the first-order flex condition for every bar. This space contains the finite-dimensional vector space $\mathcal{F}_{\rm rig}(\mathcal{C};\mathbb{R})$ for rigid body motions and, as in the theory of finite bar-joint frameworks ([3], [15]), the crystal framework $\mathcal{C}$ is said to be *infinitesimally rigid*, or *first-order rigid*, if $\mathcal{F}(\mathcal{C};\mathbb{R}) = \mathcal{F}_{\rm rig}(\mathcal{C};\mathbb{R})$. See Owen and Power [24], for example. There have been a number of recent theoretical accounts of flexibility and rigidity in infinite periodic structures, such as [10], [21], [23], [30]. Also, in materials science, over a much longer period, there have been extensive studies of flexibility, stability and phonon modes, such as [9], [12], [13], [16], [32]. However these accounts generally assume some form of periodic boundary conditions for the admissible velocity fields and so far there has been no characterisation given for first-order rigidity per se. In what follows we make no such assumptions and in Theorem 3.4 obtain four sets of necessary and sufficient conditions.

Our analysis is based on spectral synthesis for the flex space $\mathcal{F}(\mathcal{C};\mathbb{C})$ in terms of the *geometric spectrum* $\Gamma(\mathcal{C})$ (associated with a periodic structure). This spectrum was introduced in Badri, Kitson and Power [6] as a subset of $\mathbb{C}_*^d = (\mathbb{C}\backslash\{0\})^d$ which generalises the *rigid unit mode spectrum*, or RUM spectrum, $\Omega(\mathcal{C})$. Recall that $\Omega(\mathcal{C})$ is the subset of the d-torus $\mathbb{T}^d$ which underlies the analysis of low energy phonon modes (mechanical modes) and almost periodic flexes. In analogy with the Bohr spectrum of an almost periodic function it records the unimodular multiphases that are possible in the Bloch theory for these modes [5], [24], [25], [32]. The geometric spectrum contains the RUM spectrum together with points $\omega = (\omega_1,\dots,\omega_d)$ in $\mathbb{C}_*^d$ associated with unbounded flexes which are similarly periodic modulo the multiplicative factor ω. We refer to a factor in $\mathbb{C}_*^d\backslash\mathbb{T}^d$, as a nonunimodular factor. The infinitesimal rigidity of a crystal framework $\mathcal{C}$ implies that the geometric spectrum is trivial in the sense of reducing to the point $\underline{1} = (1,\dots,1)$. Additionally, the space of periodic flexes with respect to a choice of lattice of

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translations, and taken in the flexible lattice sense, must coincide with the space of rigid motion flexes. We show that these two conditions, stated in condition (iii) of Theorem 3.4, are sufficient as well as necessary.

We approach the rigidity analysis by viewing the geometric flex spectrum in two other ways. Firstly, in difference equation terms, it is the set of solutions of the characteristic equations of a set of linear difference equations, for vector-valued $\mathbb{Z}^d$-indexed sequences (referred to as multi-sequences), that arises from a choice of periodic structure for $\mathcal{C}$. These solutions are the points of rank degeneracy of a matrix-valued *transfer function* $\Psi_{\mathcal{C}}(z)$ on $\mathbb{C}_*^d$. In fact $\Psi_{\mathcal{C}}(z)$ is the extension of the symbol function $\Phi_{\mathcal{C}}(z)$, with domain $\mathbb{T}^d$, associated with rigid unit modes. Secondly, in commutative algebra terms, the geometric flex spectrum and the flex space $\mathcal{F}(\mathcal{C};\mathbb{C})$ are related by a natural duality to the $\mathbb{C}[z_1,\dots,z_d]$-module generated by the rows of the transfer function.

At the centre of the proof is Theorem 4.1, from Kastis and Power [17], which is a generalisation of a classical algebraic spectral synthesis result of M. Lefranc [19] for shift-invariant subspaces of $C(\mathbb{Z}^d)$. This leads to the fact that $\mathcal{F}(\mathcal{C};\mathbb{C})$ is the closed linear span of flexes which are vector-valued polynomially weighted geometric multi-sequences. Moreover, as stated in Theorem 3.6, there is a dense linear span of first-order flexes of this type where the associated geometric multi-factors $\omega \in \mathbb{C}_*^d$ of the velocity fields are finite in number. This finiteness derives from the Lasker-Noether decomposition of a $\mathbb{C}[z_1,\dots,z_d]$-module for $\mathcal{C}$. We also see that the first-order flex space $\mathcal{F}(\mathcal{C};\mathbb{C})$ is finite-dimensional if and only if the geometric spectrum is a finite set.

Finally, using only direct geometric arguments, we show that, paradoxically, a crystallographic bar-joint framework may be continuously flexible even when it is first-order rigid. Our examples in Section 5 are associated with aperiodic displacive phase transitions between periodic states.

2. Preliminaries

A *crystal framework* $\mathcal{C}$ in $\mathbb{R}^d$ is defined to be a bar-joint framework (G,p) where $G=(V,E)$ is a countable simple graph and $p: V \to \mathbb{R}^d$ is an injective translationally periodic placement of the vertices as joints $p(v)$. It is assumed here, moreover, that the periodicity is determined by a basis of d linearly independent vectors and that the corresponding translation classes for the joints and bars are finite in number. The assumption that $p: V \to \mathbb{R}^d$ is injective is not essential although with this relaxation one should assume that each bar $p(v)p(w)$ has positive length $\|p(v)-p(w)\|$.

The complex infinitesimal flex space $\mathcal{F}(\mathcal{C};\mathbb{C})$ is the vector space of $\mathbb{C}^d$-valued functions u on the set of joints satisfying the first-order flex conditions

$$(u(p(v)) - u(p(w))) \cdot (p(v) - p(w)) = 0, \quad vw \in E.$$

Coordinates for this vector space and the space $\mathcal{V}(\mathcal{C};\mathbb{C})$ of all velocity fields may be introduced, first, by making a (possibly different) choice of d linearly independent periodicity vectors for $\mathcal{C}$, which we shall denote as

$$\underline{a} = \{a_1,\dots,a_d\},$$

and, second, by choosing finite sets, F_v and F_e respectively, for the corresponding translation classes of the joints and the bars. We refer to the basis choice $\underline{a}$ as a choice of *periodic structure basis* for $\mathcal{C}$ while the pair $\{F_v, F_e\}$ represents a choice of *motif* for this periodic structure [24], [25].

2.1. **Transfer functions and $\mathbb{C}(z)$-modules.** Let $\mathbb{C}[z]=\mathbb{C}[z_1,\dots,z_d]$ be the ring of polynomials in the commuting variable $z_1,\dots,z_d$ over the field $\mathbb{C}$. Identify this with the algebra of multi-variable complex polynomials defined on $\mathbb{C}_*^d$ and write $\mathbb{C}(z)$ for the containing ring of functions on $\mathbb{C}_*^d$ generated by the coordinate functions $z_1,\dots,z_d$ and their inverses $z_1^{-1},\dots,z_d^{-1}$. We refer to this as the the *Laurent polynomial ring.*

Let $n = |F_v|$ and $m = |F_e|$. Borrowing terminology from the theory of difference equations we now define the *transfer function* $\Psi_{\mathcal{C}}(z)$ of $\mathcal{C}$, an $m \times dn$ matrix of functions in $\mathbb{C}(z)$ determined by the pair $\{F_v, F_e\}$. We label the vertices in V, and hence the joints $p(v)$ of $\mathcal{C}$, by pairs (v, k) where $p(v, 0) = p(v) \in F_v$ and $p(v, k)$, for $k = (k_1, \dots, k_d) \in \mathbb{Z}^d$, is the joint $p(v, 0) + k_1 a_1 + \dots + k_d a_d$. Also, using multinomial notation, we write z^{-k} for the product $z_1^{-k_1} z_2^{-k_2} \dots z_d^{-k_d}$.

We remark that, henceforth the notation k (resp. z) always denotes the d-tuple $(k_1, \dots, k_d)$ in $\mathbb{Z}^d$ (resp. $(z_1, \dots, z_d)$ in $\mathbb{C}^d$), and z^k always denotes the product $z_1^{k_1} \dots z_d^{k_d}$.

Definition 2.1. Let $\mathcal{C}$ be a crystal framework in $\mathbb{R}^d$ with motif $\{F_v, F_e\}$ and let $p(e) = p(v, k) - p(w, l)$ be the vector for the bar $p(v, k)p(w, l)$ in F_e associated with the edge $e = (v, k)(w, l)$.

(i) The *transfer function* $\Psi_{\mathcal{C}}(z)$ is the $m \times dn$ matrix over the Laurent polynomial ring whose rows are labelled by the edges e for the bars of F_e and whose columns are labelled by the vertices v for the joints of F_v and coordinate indices in $\{1, \dots, d\}$. The row for an edge $e = (v, k)(w, l)$ with $v \neq w$ takes the form

$$\begin{matrix} & & & & v & & & & w & & & \\ e & [\,0 & \cdots & 0 & p(e)z^{-k} & 0 & \cdots & 0 & -p(e)z^{-l} & 0 & \cdots & 0\,] \end{matrix}$$

while if $v = w$ it takes the form

$$\begin{matrix} & & & & v & & & \\ e & [\,0 & \cdots & 0 & p(e)(z^{-k} - z^{-l}) & 0 & \cdots & 0\,] \end{matrix}$$

(ii) The $\mathbb{C}(z)$-module of $\mathcal{C}$, associated with the motif $\{F_v, F_e\}$, is the submodule

$$M(\mathcal{C}) = \mathbb{C}(z)p_1(z) + \dots + \mathbb{C}(z)p_m(z)$$

of the $\mathbb{C}(z)$-module $\mathbb{C}(z) \otimes \mathbb{C}^{dn}$, where $p_1(z), \dots, p_m(z)$ are the $\mathbb{C}^{dn}$-valued multi-variable functions given by the rows of the transfer function.

Figure 1 indicates choices of periodicity bases and motifs $\{F_v, F_e\}$ for two simple examples, $\mathcal{C}_{\mathbb{Z}^2}$ and $\mathcal{C}_{\text{kite}}$, which in fact may be defined by this data. The periodicity bases are both equal to $\underline{a} = \{a_1, a_2\} = \{(1, 0), (0, 1)\}$.

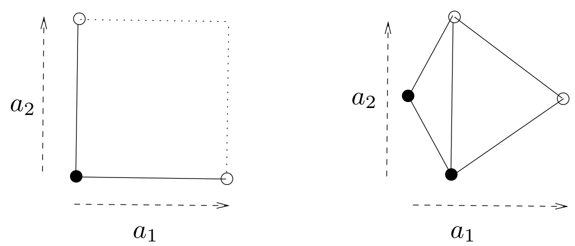

FIGURE 1. A motif for the grid framework $\mathcal{C}_{\mathbb{Z}^2}$, with $|F_v| = 1, |F_e| = 2$, and the kite framework $\mathcal{C}_{\text{kite}}$, with $|F_v| = 2, |F_e| = 5$.

For $\mathcal{C}_{\mathbb{Z}^2}$ the set F_v is the singleton joint set $\{(0, 0)\}$ and F_e is the set of bars $\{p_1p_2, p_1p_3\}$ where $p_1 = (0, 0), p_2 = (1, 0), p_3 = (0, 1)$. However, in our notation we have $p_1 = p(v_1, (0, 0)), p_2 = p(v_1, (1, 0)), p_3 = p(v_1, (0, 1))$, according to the labelling of joints by vertices $v_1, \dots, v_n$ and indices $k \in \mathbb{Z}^2$. The transfer function $\Psi(\mathcal{C}_{\mathbb{Z}^2})(z_1, z_2)$ is a 2×2 matrix with first row, for bar p_1p_2 say, equal to $(-1, 0)(1 - z_1^{-1})$, which is $(-1 + z_1^{-1}, 0)$. In this way we obtain

$$\Psi(\mathcal{C}_{\mathbb{Z}^2})(z_1, z_2) = \begin{bmatrix} -1 + z_1^{-1} & 0 \\ 0 & -1 + z_2^{-1} \end{bmatrix}, \qquad \text{for } z_1, z_2 \in \mathbb{C}\backslash\{0\}.$$

In the case of $\mathcal{C}_{\text{kite}}$ we have $F_v = \{p_1, p_2\}$ where $p_1 = (0,0), p_2 = (-0.25, 0.5)$. The set F_e has 5 bars involving the 4 joints $p_1 = p(v_1,(0,0)), p_2 = p(v_2,(0,0)), p_3 = p(v_1,(0,1)), p_4 = p(v_2,(1,0))$. Thus the row of the transfer function for the bar p_1p_4, for example, requires $p(e) = p_1 - p_4 = (-0.75, -0.5)$ and takes the form $(p(e)z^{(0,0)}, -p(e)z^{-(0,1)})$ which is

$$\tfrac{1}{4}[-3 \quad -2 \quad 3z_1^{-1} \quad 2z_1^{-1}]$$

Returning to the general discussion, for a given periodic structure basis one may rechoose the set F_v, through an appropriate translation into the positive cone of $\mathbb{R}^d$, so that the multi-variable vector-valued polynomials $p_i(z)$ are replaced by vector-valued polynomials $z^k p_i(z)$, in $\mathbb{C}[z] \otimes \mathbb{C}^{dn}$, for some fixed $k \in \mathbb{Z}^d$. Henceforth we assume that this choice has been made. We may therefore define a $\mathbb{C}[z]$-module, which we denote as $M(\mathcal{C})^*$, as the submodule of the left $\mathbb{C}[z]$-module $\mathbb{C}[z] \otimes \mathbb{C}^{dn}$ generated by the vector-valued multi-variable polynomials $p_1(z), \ldots, p_m(z)$. In particular we have

$$M(\mathcal{C})^* = M(\mathcal{C}) \cap (\mathbb{C}[z] \otimes \mathbb{C}^{dn}).$$

We remark that the superscript asterisk notation here is consistent with the usage in Lefranc [19] and Kastis and Power [17] and will only be used in this sense.

Different choices of F_e for the same periodic structure basis give transfer functions that are equivalent in a natural way. Specifically, the replacement of a motif edge by an alternative representative results in the multiplication of the appropriate row by a monomial. Also any relabelling of the motif joints and bars corresponds to column and row permutations. It follows that any two transfer functions, $\Psi_1(z)$ and $\Psi_2(z)$, for a given periodic structure basis satisfy the equation $\Psi_2(z) = D_1(z)A\Psi_1(z)BD_2(z)$, where $D_1(z)$ and $D_2(z)$ are diagonal monomial matrices and A, B are permutation matrices.

The values $z = \omega$ for which the rank of $\Psi_{\mathcal{C}}(\omega)$ is less than dn correspond to finite-dimensional spaces of complex infinitesimal flexes which are periodic up to the multiplicative factor $\omega = (\omega_1, \ldots, \omega_d)$. Such flexes are referred to here as *factor-periodic flexes* since they are characterised by a set of equations of the form

$$u_k = \omega^k u_0 = \omega_1^{k_1} \cdots \omega_d^{k_d} u_0,$$

which relate the (complex) velocity u_0 of a joint $p(v,(0,0))$ in F_v to the velocity u_k of the joint $p(v,k)$ for $k \in \mathbb{Z}^d$. See also [5], [6].

Definition 2.2. Let $\mathcal{C}$ be a crystal framework in $\mathbb{R}^d$ with a choice of periodic structure basis, labelled motif and associated transfer function $\Psi_{\mathcal{C}}(z)$.

(i) The *geometric flex spectrum* of $\mathcal{C}$ is the set

$$\Gamma(\mathcal{C}) = \{\omega \in \mathbb{C}_*^d = (\mathbb{C}\backslash\{0\})^d : \ker \Psi_{\mathcal{C}}(\omega^{-1}) \neq \{0\}\}.$$

(ii) The *rigid unit mode spectrum* or RUM spectrum of $\mathcal{C}$ is the subset $\Omega(\mathcal{C}) = \Gamma(\mathcal{C}) \cap \mathbb{T}^d$.

The geometric flex spectrum was introduced in Badri, Kitson and Power [6] in connection with the existence and nonexistence of bases of localised flexes which generate the entire space of infinitesimal flexes. From our earlier remarks it follows that the sets $\Gamma(\mathcal{C}), \Omega(\mathcal{C})$ depend only on the choice of periodic structure basis. For the grid framework with its standard periodicity basis, as indicated in Figure 1, the determinant of the 2×2 transfer function is $z_1^{-1}z_2^{-1}(z_1 - 1)(z_2 - 1)$ and so

$$\Gamma(\mathcal{C}_{\mathbb{Z}^2}) = \{1\} \times \mathbb{C}_* \cup \mathbb{C}_* \times \{1\}, \qquad \Omega(\mathcal{C}_{\mathbb{Z}^2}) = \{1\} \times \mathbb{T} \cup \mathbb{T} \times \{1\}.$$

On the other hand it can be shown that $\Gamma(\mathcal{C}_{\text{kite}})$ consists of $(1,1)$ and one other point, $\omega = (-2, -1)$. This point corresponds to an ω-periodic flex $e_{\omega,h}$ for which the 4-jointed kite subframeworks rotate infinitesimally in an alternating fashion and for which the velocity magnitudes for the joints $p(v_2,k), p(v_4,k)$ increase geometrically in the positive x-direction and are of constant magnitude in the y-direction.

2.2. **Velocity fields and forms of rigidity.** All variants of infinitesimal rigidity depend on a choice of vector space of preferred velocity fields. In this section we define such vector spaces and the resulting forms of periodic and aperiodic infinitesimal rigidity. We first describe a space of *exponential velocity fields* which plays a key role in our main results.

Let a be a vector in $\mathbb{C}^{dn}$ which is in the nullspace of $\Psi_{\mathcal{C}}(\omega^{-1})$. Then the function

$$u : \mathbb{Z}^d \to \mathbb{C}^{dn}, \quad k \to \omega^k a$$

defines a factor-periodic velocity field which is an infinitesimal flex [5], [25]. In this coordinate formalism a complex velocity field for the framework $\mathcal{C}$ is given by a function (or vector-valued multi-sequence) u in $C(\mathbb{Z}^d;\mathbb{C}^{nd})$ where $u(k)$ is a combined velocity vector for the n joints which are the translates of the motif joints by the vector $a(k) = k_1a_1 + \cdots + k_da_d$. Explicitly, with $F_v = \{v_1,\dots,v_n\}$, we have

$$u(k) = (u(p(v_1,k)),\dots,u(p(v_n,k)))$$

where $u(p(v_i,k))$ is the velocity vector at the joint $p(v_i,k) = p(v_i) + a(k)$, and where we have introduced notation (v_i,k) for the vertices of the underlying graph G.

We now introduce terminology for factor-periodic velocity fields and related velocity fields. Let $\omega \in \mathbb{C}_*^d$ and write $e_\omega \in C(\mathbb{Z}^d)$ for the *geometric multi-sequence* given by $e_\omega(k) = \omega^k$, for $k \in \mathbb{Z}^d$. More generally, a *polynomially weighted geometric multi-sequence*, or *pg-sequence*, is a multi-sequence in $C(\mathbb{Z}^d)$ of the form $e_{\omega,q} : k \to q(k)\omega^k$, where $q(z)$ is a polynomial in $\mathbb{C}[z]$. Define $\mathcal{V}_{\exp}(\mathcal{C};\mathbb{C})$, the space of *exponential velocity fields*, to be the subspace of $\mathcal{V}(\mathcal{C};\mathbb{C})$ formed by the linear span of the velocity fields $e_{\omega,q}\otimes a$, for all ω in $\mathbb{C}_*^d$, all polynomials $q(z)$ in $\mathbb{C}[z]$ and all vectors a in $\mathbb{C}^{dn}$. By a standard roots of unity argument it can be shown that this space does not depend on a choice of periodic structure basis. However, we do not need this fact.

An infinitesimal flex in $\mathcal{V}_{\exp}(\mathcal{C};\mathbb{C})$ is referred to as an *exponential flex* and these vectors determine a subspace, denoted $\mathcal{F}_{\exp}(\mathcal{C};\mathbb{C})$. That is,

$$\mathcal{F}_{\exp}(\mathcal{C};\mathbb{C}) = \mathcal{V}_{\exp}(\mathcal{C};\mathbb{C}) \cap \mathcal{F}(\mathcal{C};\mathbb{C}).$$

We say that $\mathcal{C}$ is $\mathcal{V}_{\exp}$-rigid, or *exponentially rigid* if $\mathcal{F}_{\exp}(\mathcal{C};\mathbb{C}) = \mathcal{F}_{\mathrm{rig}}(\mathcal{C};\mathbb{C})$.

We next recall various forms of periodic rigidity, each of which is associated with a subspace of $\mathcal{V}_{\exp}(\mathcal{C};\mathbb{C})$.

Given a choice of periodic structure basis for $\mathcal{C}$ define $\mathcal{V}_{\mathrm{per}}(\mathcal{C};\mathbb{C})$ to be the associated vector space of periodic velocity fields and write $\mathcal{F}_{\mathrm{per}}(\mathcal{C};\mathbb{C})$ for the subspace of periodic first-order flexes. When there is a possibility of confusion these flexes are also referred to as *strictly* periodic flexes, with the periodic structure understood. The periodic flexes are the factor-periodic flexes for the multi-factor $\omega = \underline{1} = (1,\dots,1)$. The framework $\mathcal{C}$ is said to be *periodically rigid*, or $\mathcal{V}_{\mathrm{per}}$-rigid, if $\mathcal{F}_{\mathrm{per}}(\mathcal{C};\mathbb{C}) \subseteq \mathcal{F}_{\mathrm{rig}}(\mathcal{C};\mathbb{C})$. The inclusion here is proper since infinitesimal rotations are not periodic infinitesimal flexes. The terms *fixed lattice rigid*, *fixed torus rigid*, *strictly periodically rigid* and *forced symmetry rigid* (for translation symmetries) are also used for this notion of rigidity.

A weaker form of periodic rigidity, known as *flexible lattice periodic rigidity* (and also termed *flexible torus rigidity* or simply *periodic rigidity*) is associated with a larger space of velocity fields $u \in C(\mathbb{Z}^d;\mathbb{C}^{nd})$ which have the form

$$u(k) = u(0) + (Xk,\dots,Xk), \quad \text{where} \quad X \in M_d(\mathbb{C}),$$

and $M_d(\mathbb{C})$ is the space of $d \times d$ complex matrices. These velocity fields form an $(nd+d^2)$-dimensional space of velocity fields which are periodic modulo an affine correction in which the

n joints in the k^{th}-cell each receive an additional velocity Xk. We write this space as $\mathcal{V}_{\rm fper}(\mathcal{C};\mathbb{C})$. In fact we have a direct sum

$$\mathcal{V}_{\rm fper}(\mathcal{C};\mathbb{C}) := \mathcal{V}_{\rm per}(\mathcal{C};\mathbb{C}) \oplus \mathcal{V}_{\rm axial}(\mathcal{C};\mathbb{C})$$

where $\mathcal{V}_{\rm axial}(\mathcal{C};\mathbb{C})$ is the space of the *axial velocity fields*, $u : k \to (Xk, \dots, Xk)$.

An infinitesimal rotation flex of a crystal framework is an exponential velocity field. To see this for the framework $\mathcal{C}_{\mathbb{Z}^2}$ with the simple periodicity basis of Figure 1, consider $\omega = \underline{1} = (1,1) \in \mathbb{T}^2$ and $h_1(z_1,z_2) = z_2$, $h_2(z_1,z_2) = z_1$. Then the velocity field u given by

$$u = e_{\omega,h_1} \otimes (1,0) + e_{\omega,h_2} \otimes (0,-1) : k \to (h_1(k), -h_2(k)) = (k_2, -k_1),$$

is an infinitesimal rotation flex.

Lemma 2.3. *Let $\mathcal{C}$ be a crystal framework. Then $\mathcal{V}_{\rm rig}(\mathcal{C};\mathbb{C}) \subseteq \mathcal{V}_{\rm fper}(\mathcal{C};\mathbb{C}) \subseteq \mathcal{V}_{\rm exp}(\mathcal{C};\mathbb{C})$.*

Proof. A translational infinitesimal flex $u : k \to \mathbb{C}^{nd}$, associated with the velocity $b \in \mathbb{C}^d$, has the form $e_{\underline{1},q} \otimes (b, \dots, b)$ with $q(z)$ identically equal to 1. In particular it is strictly periodic. On the other hand let u be the rotational infinitesimal flex associated with the matrix B in $M_d(\mathbb{R})$, let $(p_1, \dots, p_n)$ be the vector of joints from a motif for the periodic structure basis $\underline{a}$, and let $A : k \to k_1a_1 + \cdots + k_da_d$. Then $u(0) = (B(p_1), \dots, B(p_n)) = (b_1, \dots, b_n)$ and

$$u(k) = (B(p_1 + A(k)), \dots, B(p_n + A(k))) = (b_1 + BA(k), \dots, b_n + BA(k)).$$

The right hand expression is linear in $k_1, \dots k_d$ and so u may be written in the form

$$\sum_{|j|\le 1} q_j(k)c_j = \sum_{|j|\le 1} e_{\underline{1},q_j} \otimes c_j$$

where $c_j \in \mathbb{C}^{nd}$ and $q_j(z)$ is the linear polynomial z^j with total degree $|j| \le 1$. From these observations the inclusions follow. $\square$

Let $\mathcal{F}_{\rm fper}(\mathcal{C};\mathbb{C}) = \mathcal{F}(\mathcal{C};\mathbb{C}) \cap \mathcal{V}_{\rm fper}(\mathcal{C};\mathbb{C})$. This is the space of flexible lattice periodic flexes for the given periodic structure basis. It is also referred to as the space of affinely periodic infinitesimal flexes [10], [26].

Definition 2.4. A crystal framework $\mathcal{C}$ is said to be *flexible lattice periodically rigid*, or $\mathcal{V}_{\rm fper}$-rigid, if $\mathcal{F}_{\rm fper}(\mathcal{C};\mathbb{C}) = \mathcal{F}_{\rm rig}(\mathcal{C};\mathbb{C})$.

For a simple illustration let us note that the grid framework $\mathcal{C}_{\mathbb{Z}^2}$, with the periodicity basis given in Figure 1, is periodically rigid, since every periodic velocity field is an infinitesimal translation. However it is not flexible lattice periodically rigid since the shearing velocity field

$$u(k) = (k_2, 0), \quad k = (k_1, k_2) \in \mathbb{Z}^2,$$

is in $\mathcal{V}_{\rm fper}(\mathcal{C}_{\mathbb{Z}^2})$ and is an infinitesimal flex.

Let $\underline{1}$ be the point $(1, \dots, 1)$ in $\Gamma(\mathcal{C})$. A necessary and sufficient condition for periodic rigidity is that the scalar $m \times dn$ rigidity matrix $R_{\rm per}(\mathcal{C}) = \Psi(\underline{1})$ has rank $dn - d$. Borcea and Streinu [8] have obtained an analogous necessary and sufficient condition for flexible lattice periodic rigidity. Another derivation of this characterisation is in Power [26]. The rigidity condition requires the maximality of the rank of a matrix, which we write here as $R_{\rm fper}(\mathcal{C})$, which is an augmentation of $R_{\rm per}(\mathcal{C})$ by d^2 columns associated with the entries of the variable matrix X. The maximal rank condition is then

$$\operatorname{rank} R_{\rm fper}(\mathcal{C}) = dn + d(d-1)/2.$$

Although we do not need the form of this scalar matrix in subsequent proofs, for completeness we include the following definition.

Definition 2.5. Let $\mathcal{C}$ be a crystal framework in $\mathbb{R}^d$ with motif $\{F_v, F_e\}$ and let $p(e) = p(v,k) - p(w,l)$ be the vectors associated with the bars in F_e corresponding to edges $e = (v,k)(w,l)$. The flexible lattice periodic rigidity matrix $R_{\text{fper}}(\mathcal{C})$ is the $m \times (dn + d^2)$ matrix whose rows, labelled by the edges e with $v \neq w$, have the form

$$e \begin{bmatrix} 0 & \cdots & 0 & \overset{v}{p(e)} & 0 & \cdots & 0 & \overset{w}{-p(e)} & 0 & \cdots & (l_1 - k_1)p(e) & \cdots & (l_d - k_d)p(e) \end{bmatrix},$$

while the rows for $v = w$ take the form

$$\begin{bmatrix} 0 & \cdots & 0 & (l_1 - k_1)p(e) & \cdots & (l_d - k_d)p(e) \end{bmatrix}.$$

3. The main results

We first recall the elementary duality between $\mathbb{C}(z)$-modules and invariant subspaces, where $\mathbb{C}(z)$ is the (multi-variable) Laurent polynomial ring.

3.1. **$\mathbb{C}(z)$-modules and invariant subspaces.** Let $r \geq 1$ and let $C(\mathbb{Z}^d; \mathbb{C}^r)$ be the topological vector space of vector-valued functions $u : \mathbb{Z}^d \to \mathbb{C}^r$ with the topology of coordinatewise convergence. Also we write $C(\mathbb{Z}^d)$ for $C(\mathbb{Z}^d; \mathbb{C})$. Let $e_1, \dots, e_d$ be the generators of $\mathbb{Z}^d$ and let $W_i, 1 \leq i \leq d$, be the forward shift operators on the space $C(\mathbb{Z}^d; \mathbb{C}^r)$, so that $(W_i u)(k) = u(k - e_i)$, for all k and each i. A subspace A of $C(\mathbb{Z}^d; \mathbb{C}^r)$ is said to be an *invariant subspace* if it is invariant for the shift operators and their inverses, or equivalently if $W_i A = A$ for each i.

There is a bilinear pairing $\langle p, u\rangle : \mathbb{C}(z) \times C(\mathbb{Z}^d) \to \mathbb{C}$ such that, for $p(z) = \sum_k a_k z^k$ in $\mathbb{C}(z)$ and $u = (u_k)_{k \in \mathbb{Z}^d}$ in $C(\mathbb{Z}^d)$, $\langle p, u\rangle = \sum_k a_k u_k$. Similarly, considering $C(\mathbb{Z}^d; \mathbb{C}^r)$ as the space $C(\mathbb{Z}^d) \otimes \mathbb{C}^r$, for $p = (p_i) \in \mathbb{C}(z) \otimes \mathbb{C}^r$ and $u = (u_i) \in C(\mathbb{Z}^d) \otimes \mathbb{C}^r$ we have the corresponding pairing $\langle p, u\rangle : \mathbb{C}(z) \otimes \mathbb{C}^r \times C(\mathbb{Z}^d) \otimes \mathbb{C}^r \to \mathbb{C}$, where

$$\langle p, u\rangle = \langle (p_i), (u_i)\rangle = \sum_{i=1}^{r} \langle p_i, u_i\rangle.$$

With this pairing the vector space dual of $C(\mathbb{Z}^d) \otimes \mathbb{C}^r$ can be identified with $\mathbb{C}(z) \otimes \mathbb{C}^r$. Also, with the same pairing, the dual space of $\mathbb{C}(z) \otimes \mathbb{C}^r$ may be identified with $C(\mathbb{Z}^d) \otimes \mathbb{C}^r$. Thus both spaces are reflexive, that is, equal to their double dual in the category of vector spaces. These dual space identifications also hold in the category of linear topological spaces when each is endowed with the topology of coordinatewise convergence, simply because all linear functionals are automatically continuous with these topologies.

For a subspace A of $C(\mathbb{Z}^d) \otimes \mathbb{C}^r$ we write $B = A^\perp$ for the annihilator in $\mathbb{C}(z) \otimes \mathbb{C}^r$ with respect to the pairing. Thus

$$B = \{p \in \mathbb{C}(z) \otimes \mathbb{C}^r : \langle p, u\rangle = 0, \text{ for all } u \in A\}.$$

Similarly for a subspace B of $\mathbb{C}(z) \otimes \mathbb{C}^r$ we write $B^\perp$ for the annihilator in $C(\mathbb{Z}^d) \otimes \mathbb{C}^r$ with respect to the same pairing.

The following lemmas provide a route for the analysis of shift-invariant subspaces A in terms of the structure of their uniquely associated $\mathbb{C}(z)$-modules $B = A^\perp$. Note that it follows from the Noetherian property that $\mathbb{C}(z)$-modules in $\mathbb{C}(\mathbb{Z}^d) \otimes \mathbb{C}^r$ are necessarily closed.

Lemma 3.1. *Let A be a closed subspace of $C(\mathbb{Z}^d) \otimes \mathbb{C}^r$ and let M be a closed subspace of $\mathbb{C}(z) \otimes \mathbb{C}^r$. Then $A = (A^\perp)^\perp$ and $M = (M^\perp)^\perp$.*

Proof. This follows from the dual space identifications and from the Hahn-Banach theorem for topological vector spaces ([11], IV. 3.15). □

Lemma 3.2. *A closed subspace A in $C(\mathbb{Z}^d) \otimes \mathbb{C}^r$ is an invariant subspace if and only if $A^\perp$ is a $\mathbb{C}(z)$-submodule of the module $\mathbb{C}(z) \otimes \mathbb{C}^r$.*

Proof. For all $a \in A$, $b \in B = A^\perp$ and $1 \leq i \leq d$ we have $\langle W_i a, b\rangle = \langle a, z_i b\rangle$ and the lemma follows. □

3.2. **The main results.** We may now consider this duality in the context of the first-order flex space $\mathcal{F}(\mathcal{C};\mathbb{C})$ of a crystal framework $\mathcal{C}$, and we use notation from the previous section.

Definition 3.3. The $\mathbb{C}(z)$-*rigidity module* $M_{\text{rig}}(\mathcal{C})$, associated with a periodic structure basis for $\mathcal{C}$, is the annihilator of $\mathcal{F}_{\text{rig}}(\mathcal{C};\mathbb{C})$ in $\mathbb{C}(z) \otimes \mathbb{C}^{dn}$.

We say that a transfer function $\Psi_\mathcal{C}(z)$ is *rank extremal* if $\operatorname{rank} \Psi_\mathcal{C}(z) = dn$ for all $z \in \mathbb{C}^d_* \backslash \{\underline{1}\}$ and the rank of $\Psi_\mathcal{C}(\underline{1})$ is $dn - d$. Also we say that $R_{\text{fper}}(\mathcal{C})$ is *rank extremal* if its rank is $dn + d(d-1)/2$.

Theorem 3.4. *The following statements are equivalent for a crystal framework $\mathcal{C}$ in $\mathbb{R}^d$.*

(i) $\mathcal{C}$ is first-order rigid.

(ii) $\mathcal{C}$ is exponentially rigid.

(iii) For a given periodic structure basis, there are no nontrivial factor-periodic flexes or nontrivial flexible lattice periodic flexes.

(iv) For a given periodic structure basis and motif, the transfer function $\Psi_\mathcal{C}(z)$ and the matrix $R_{\text{fper}}(\mathcal{C})$ are rank extremal.

(v) For a given periodic structure basis, the $\mathbb{C}(z)$-module $M(\mathcal{C})$ agrees with the rigidity module $M_{\text{rig}}(\mathcal{C})$.

Definition 3.5. Let $\mathcal{C}$ be a crystal framework in $\mathbb{R}^d$ with a periodic structure basis with n translation classes of joints. A *vectorial pg-sequence* for $\mathcal{C}$, for this periodic structure basis, with *geometric index* $\omega \in \mathbb{C}^d_*$, is a velocity field $u_{\omega,h} : \mathbb{Z}^d \to \mathbb{C}^{nd}$ of the form

$$u_{\omega,h} : k \to \omega^k h(k)$$

where $h(z)$ is a vector-valued polynomial in $\mathbb{C}[z] \otimes \mathbb{C}^{dn}$.

The term *root sequence* for some $\mathbb{C}[z]$-module $\mathcal{M}$ refers to a choice of roots for a set of distinct prime ideals $P_1, \dots, P_s$ in $\mathbb{C}[z]$ with respect to which $\mathcal{M}$ has a P-primary decomposition. We give the formal details of this in Section 4.1. The term appears in our context in the next theorem. Recall that $M(\mathcal{C})^*$ is the module for the polynomial ring $\mathbb{C}[z]$ obtained from $M(\mathcal{C})$ by intersection. Also the term *closed* refers to the topology for coordinate-wise convergence or, more precisely, the topology of pointwise convergence in the space of velocity fields.

Theorem 3.6. *Let $\mathcal{C}$ be a crystal framework in $\mathbb{R}^d$ with a given periodic structure basis and associated $\mathbb{C}[z]$-module $M(\mathcal{C})^*$. Then $\mathcal{F}(\mathcal{C};\mathbb{C})$ is the closed linear span of pg-sequences $u_{\omega,h}$ in $\mathcal{F}(\mathcal{C};\mathbb{C})$ associated with the periodic structure basis. Moreover, if $\omega(1), \dots, \omega(s)$ is a root sequence for the Lasker-Noether decomposition of $M(\mathcal{C})^*$ then $\mathcal{F}(\mathcal{C};\mathbb{C})$ is the closed linear span of the pg-sequences $u_{\omega,h}$ in $\mathcal{F}(\mathcal{C};\mathbb{C})$ with geometric indices $\omega(1), \dots, \omega(s)$.*

It is possible, although unusual, for a crystal framework to have a finite-dimensional first-order flex space which is strictly larger than the finite-dimensional space of rigid motion flexes, and we give some examples below. The finiteness of the geometric spectrum is a simple necessary condition for this phenomenon and we shall show, from the primary decomposition structure of $M(\mathcal{C})^*$, that it is also a sufficient condition.

Theorem 3.7. *Let $\mathcal{C}$ be a crystal framework in $\mathbb{R}^d$ with a given periodic structure basis and associated geometric flex spectrum $\Gamma(\mathcal{C})$. Then the following statements are equivalent.*
(i) $\mathcal{F}(\mathcal{C};\mathbb{C})$ is finite-dimensional.
(ii) $\Gamma(\mathcal{C})$ is a finite set.

Remark 3.8. In view of the unbounded nature of a *pg*-flex with nonunimodular geometric multi-factor it might appear that these results have little relevance to materials science. This is definitely not the case however since *surface modes*, associated with a hyperplane boundary wall for example, arise as bounded restrictions of unbounded flexes of the bulk crystal. See for example Lubensky et al [20], Power [27], Rocklin et al [28] and Sun et al [31]. Thus the geometric spectrum in effect identifies free surfaces where one may find bounded surface modes which have geometric decay directions into the bulk.

The commutative algebra viewpoint also usefully extends the conceptual analysis of crystal frameworks which, for example, may now be described as *primary* or *properly decomposable* according to whether these properties hold for the $\mathbb{C}[z]$-module $M(\mathcal{C})^*$ associated with a primitive periodic structure basis.

3.3. **Examples.** (i) We show that for $\mathcal{C}_{\mathbb{Z}^2}$ there is a set of vectorial *pg*-sequences with dense span in the infinitesimal flex space. This is a universal property, assured by the first part of Theorem 3.6, but we may obtain it for this simple crystal framework by direct module arguments.

Assuming the usual periodicity basis $\underline{a}$ we may make choose a (translated) motif so that the transfer function $\Psi(z)$ has 2 row vector functions, $p_1(z_1,z_2)=(1-z_1,0), p_2(z_1,z_2)=(0,1-z_2)$. The corresponding $\mathbb{C}[z]$-module in $\mathbb{C}[z]\otimes\mathbb{C}^2$ is

$$M^*=\mathbb{C}[z]p_1(z)+\mathbb{C}[z]p_2(z)=(\mathbb{C}[z](1-z_1),\mathbb{C}[z](1-z_2)).$$

Let $Q_1^*=(\mathbb{C}[z](1-z_1),\mathbb{C}[z])$ and $Q_2^*=(\mathbb{C}[z],\mathbb{C}[z](1-z_2))$. Then $M^*=Q_1^*\cap Q_2^*$. Moreover M^* is a submodule of $N=\mathbb{C}[z]\otimes\mathbb{C}^2$ and N/Q_1^* is module-isomorphic to $\mathbb{C}[z]/(1-z_1)\mathbb{C}[z]$. Thus, for $p(z)\in\mathbb{C}[z]$ the map λ_p (see Definition 4.4) is injective if $(1-z_1)$ is not a factor of $p(z)$ and is zero otherwise. Thus Q_1^*, and similarly Q_2^*, are primary submodules of N. Also the ideals $P_1^*=(1-z_1)\mathbb{C}[z]$ and $P_2^*=(1-z_2)\mathbb{C}[z])$ are prime ideals in $\mathbb{C}[z]$, and in fact they are associated prime ideals in $\mathbb{C}[z]$ for Q_1^* and Q_2^*, respectively, and each Q_i^* is P_i^*-primary.

We now see that a root sequence $\{\omega(1),\dots,\omega(s)\}$, for M^*, can be any pair $\{(1,\xi_2),(\xi_1,1)\}$ with ξ_1,ξ_2 in $\mathbb{C}_*$. Let us take $\omega(1)=(1,1),\omega(2)=(1,1)$. Theorem 3.6 predicts that there is a set of infinitesimal flexes of the form

$$k\to(h_1(k),h_2(k)),\quad h_1(z),h_2(z)\in\mathbb{C}[z],$$

whose closed linear span is $\mathcal{F}(\mathcal{C}_{\mathbb{Z}^2};\mathbb{R})$. To see, independently, that this is true consider first the polynomials $h_1(z)$ of the form $h_1(z_1,z_2)=h(z_2)$, with $h(z)$ a single variable polynomial. The velocity field

$$u:k\to(h_1(k),0)$$

is a velocity field which gives a constant horizontal velocity to the joints on each horizontal line. These are infinitesimal flexes. Moreover it is straightforward to show by direct arguments that the closed span of these flexes give the space of *all* infinitesimal flexes with this horizontal constancy property, including, in particular, the localised translational flexes which are supported on a single horizontal line of joints. We remark that these localised translational flexes are evidently not in the (unclosed) linear span of vectorial *pg*-sequences.

Exchanging the roles of the variables it follows similarly that there are vectorial *pg*-flexes whose closed linear span contains the vertically localised flexes. The closed span of the vertically localised flexes and the horizontally localised flexes is the space of all flexes, since one can show that every infinitesimal flex is an *infinite* linear sum of the line-localised flexes. Thus the conclusion of the first assertion of Theorem 3.6 is confirmed for $\mathcal{C}_{\mathbb{Z}^2}$.

(ii) Another favoured crystal framework example in $\mathbb{R}^2$ is the *kagome framework*, $\mathcal{C}_{\rm kag}$, which is associated with the semiregular tiling of the plane by hexagons and triangles. There are 3 joints and 6 bars in a (minimal, primitive) motif and the $\mathbb{C}[z]$-module $M(\mathcal{C}_{\rm kag})^*$ is a submodule of $\mathbb{C}[z] \otimes \mathbb{C}^6$. A direct verification of the density of *pg*-flexes may be obtained, as above, by exploiting the fact that the line-localised flexes form a generalised basis for the flex space [6].

(iii) A simple 2-dimensional crystal framework which illustrates Theorem 3.7 may be obtained from $\mathcal{C}_{\mathbb{Z}^2}$ by adding the diagonal bars $(n,m)(n+1,m+1)$, for $n+m$ even. This well-known structure, which can be viewed as a kite framework where the kite subframeworks are square, is Example 3 from the gallery of examples in Badri, Kitson and Power [5], and it appears in 2D slices of cubic perovskites [13]. An explicit primitive motif consists of 2 joints and 5 bars and the RUM spectrum and the geometric spectrum are equal to the set $\{(1,1),(-1,1)\}$. One can verify directly that the first-order flex space is 4-dimensional and is spanned by a basis for the rigid motion flexes together with a single geometric flex, with $\omega = (-1,1)$, that restricts to alternating rotational flexes of each diagonalised square subframework.

(iv) For a 3-dimensional illustration of Theorem 3.7, with $\Gamma(\mathcal{C}) = \{\underline{1}\}$, one may take an infinitesimally rigid crystal framework and attach a parallel copy (with the same period vectors) by means of parallel bars between corresponding joints. In this case the first-order flex space has dimension 8.

Remark 3.9. While the geometric flexes alone need not have dense span in the flex space they may nevertheless be sufficient for restricted classes of first-order flexes with respect to other closure topologies. This is so for uniformly almost periodic flexes [5]. It would be of interest to develop further such analytic spectral synthesis and to find spectral integral representations for other classes of flex spaces.

Remark 3.10. The existence of generalised bases of localised geometric flexes for a crystal framework is considered in Badri, Kitson and Power [6]. It seems, as in the case of the kagome framework for example, that such bases give the best way of understanding the first-order flex space and rigid unit modes in that every such flex is an infinite linear combination of basis elements. However such crystal flex bases need not exist and the considerations in [6] suggest that this is typical unless the geometric spectrum has sufficient linear structure.

Remark 3.11. One can also consider forms of rigidity, which one might call persistent rigidity, with respect to *all* periodic structures, both in the strict (fixed lattice) case and the flexible lattice case. The latter form is known as *ultrarigidity* (see Malestein and Theran [22]) while the former form we refer to as *persistent periodic rigidity.* Each may be defined in terms of the vector space of velocity fields which is the union over all periodic structures of the appropriate spaces of periodic velocity fields. These rigidity notions are weaker than strict periodic infinitesimal rigidity but stronger than first-order rigidity.

For a periodic structure basis for $\mathcal{C}$ define the *rational RUM spectrum* $\Omega_{\rm rat}(\mathcal{C})$ to be the intersection of $\Omega(\mathcal{C})$ with the points in $\mathbb{T}^d$ whose arguments are rational multiples of 2π. Then it can be shown that a crystal framework $\mathcal{C}$ is persistently periodically rigid if and only if the matrix values of the transfer function on the subset $\Omega_{\rm rat}(\mathcal{C})$ have extremal rank. The analogous characterisation for ultrarigidity, together with detailed algorithmic considerations, is given in [22].

We also remark that for generic crystallographic frameworks, that is, those for which the joints in a motif are generically placed, there are combinatorial characterisations of various forms of periodic rigidity. See for example the survey of Schulze and Whiteley in [14] and the recent characterisation of Bernstein [7] for flexible lattice periodicity.

4. The proofs of Theorem 3.4, Theorem 3.6 and Theorem 3.7

The next theorem is the main result from [17] characterising closed shift-invariant subspaces in the sense of Section 3.1. It provides a key step in the proofs.

Theorem 4.1. *Let A be a closed invariant subspace of $C(\mathbb{Z}^d) \otimes \mathbb{C}^r$. Then there is a finite set of geometric indices such that A is the closed linear span of the vectorial pg-sequences in A with geometric indices in this set.*

The following degree reduction lemmas will be used in the proof of Theorem 3.4. The degree of a multi-variable polynomial $p(z)$ is the maximum, denoted $\deg p$, of the total degrees $|k| = |k_1 + \cdots + k_d|$ of the terms $a_k z^k$ that appear in a reduced sum representation of $p(z)$. The leading term of $p(z)$ is defined to be the term $a_k z^k$ of highest total degree where k is first in lexicographic order on $\mathbb{Z}^d_+$. For a vector-valued polynomial $p(z)$, its degree is defined to be the maximum of $\deg p_i$ over the coordinate functions.

Lemma 4.2. *Let $u_{\omega,p} : k \to \omega^k p(k)$ be a vectorial pg-sequence in $\mathbb{C}[z] \otimes \mathbb{C}^d$ with degree $\delta > 1$. Also, let $k = (k_1, \ldots, k_d)$ be the leading term monomial multi-index with $|k| = \delta$ and let k_j be the first nonzero entry of k. Then $u_{\omega,p} - W_j u_{\omega,p}$ is a nonzero pg-sequence $u_{\omega,g}$ with $\deg g = \deg p - 1$.*

Proof. We have $u_{\omega,p} - W_j u_{\omega,p} = u_{\omega,p-S_j p}$ where S_j is the shift operator given by the substitution $z_j \to z_j - 1$ in each coordinate function of $p(z) = (p_1(z), \ldots, p_d(z))$. Note that each function $p_i - S_j p_i$ has no terms of total degree δ. Also for the pg-sequence $u_{\omega,g} = u_{\omega,p} - W_j u_{\omega,p}$ we have $\deg g = \deg p - 1$. □

The next degree reduction lemma is needed in conjunction with the previous lemma to deduce the existence of a *nontrivial flexible lattice periodic first-order flex* from a higher degree (nonlinear) pg-flex $u_{\underline{1},h}$.

Let $p(x)$ be a quadratic vector-valued polynomial in the variables $x_1, \ldots, x_d$ which takes values in $\mathbb{R}^d$ and is given by

$$p(x_1, \ldots, x_d) = \sum_{l=1}^{d} \left(\sum_{i=1}^{d} a_{ii}^{(l)} x_i^2 + \sum_{i<j} a_{ij}^{(l)} x_i x_j + \sum_{i=1}^{d} a_i^{(l)} x_i + a_0^{(l)} \right) e_l,$$

where $\{e_l\}_{l=1}^n$ is the standard basis for $\mathbb{R}^d$. Also, for $i > j$, define

$$a_{ij}^{(l)} = a_{ji}^{(l)} \tag{1}$$

for $l \in \{1, \ldots, d\}$. Let $q_i = p - W_i p$, where W_i is the forward shift operator on the i-th coordinate. Then

$$q_i(x_1, \ldots, x_d) = \sum_{l=1}^{d} \left((2a_{ii}^{(l)} x_i - a_{ii}^{(l)}) + \sum_{j \neq i} a_{ij}^{(l)} x_j + a_i^{(l)} \right) e_l. \tag{2}$$

Consider the linear polynomial $q_{R,b}$ given by

$$q_{R,\underline{b}}(x_1, \ldots, x_d) = R \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} + \begin{bmatrix} b_1 \\ \vdots \\ b_d \end{bmatrix}$$

where R is a skew symmetric real matrix and $b_i \in \mathbb{R}$ for each i. This polynomial can be viewed as a real-valued velocity field on $\mathbb{R}^d$ which is an infinitesimal rigid body motion. Also the set of restrictions of these velocity fields to the joints of a crystal framework $\mathcal{C}$ in $\mathbb{R}^d$ gives the vector space $\mathcal{F}_{\text{rig}}(\mathcal{C}; \mathbb{R})$.

Lemma 4.3. *Let $p(x)$ be a quadratic polynomial in $x_1, \dots, x_d$ taking values in $\mathbb{R}^d$. Then for some i in $\{1, \dots, d\}$ the linear polynomial $q_i = p - S_i p$ does not have the form $q_{R,\underline{b}}$.*

Proof. We have seen that q_i has the form

$$q_i(x_1, \dots, x_d) = \sum_{l=1}^{d} \left(2a_{ii}^{(l)} x_i + \sum_{j \neq i} a_{ij}^{(l)} x_j \right) e_l + \underline{d}(i) \tag{3}$$

where $\underline{d}(i) = \sum_{l=1}^{d} (-a_{ii}^{(l)} + a_i^{(l)}) e_l$. Suppose that for each i the function q_i is of the form $q_{R,\underline{b}}$ with $R = R_i$. Then for each i we have

$$R_i \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} = \begin{bmatrix} 0 + r_{12}^{(i)} x_2 + \cdots + r_{1d}^{(i)} x_d \\ -r_{12}^{(i)} x_1 + \ 0 \ + \cdots + r_{2d}^{(i)} x_d \\ \vdots \\ -r_{1d}^{(i)} x_1 - r_{2d}^{(i)} x_d + \cdots + \ 0 \end{bmatrix}.$$

Since the i^{th} coordinate function of q_i has no dependence on x_i it follows from equation (3) that $a_{ii}^{(i)} = 0$ for each i. Also, since the l^{th} coordinate function of q_i for any $l \neq i$ has no dependence on x_l it follows from (3), that $a_{il}^{(l)} = 0$ for all l. In view of the skew symmetry of the matrix R_i we have $a_{ij}^{(l)} = -a_{il}^{(j)}$. Also, by equation (1) the element $a_{ij}^{(l)}$ is both the lj entry in the q_i matrix and the li entry in the q_j matrix. Thus, for every i, j, l we have

$$a_{ij}^{(l)} = -a_{il}^{(j)} = -a_{li}^{(j)} = a_{lj}^{(i)} = a_{jl}^{(i)} = -a_{ji}^{(l)} = -a_{ij}^{(l)}$$

and therefore $a_{ij}^{(l)} = 0$. This implies that the polynomial $p(x_1, \dots, x_d)$ is linear, a contradiction which completes the proof. □

Proof of Theorem 3.4. Note that (v) is equivalent to (i) by the duality assertions of Lemma 3.1. Also (i) evidently implies (ii). To see that (ii) implies (i) we must show that if there is a first-order flex which is not a rigid motion flex then in fact there exists an exponential flex which is a nonrigid motion flex. This conclusion follows immediately from Theorem 4.1 which shows that in fact there must exist a nonrigid motion flex $u_{\omega,\underline{h}}$.

Assertions (iii) and (iv) are equivalent, by the discussion preceding Definition 2.4, and they are implied by (i).

It remains to show that (iii) implies (i). Assume that (i) does not hold. We show that (iii) fails, that is, there exists a nontrivial factor-periodic flex or there exists a nontrivial flexible lattice periodic flex. Since $\mathcal{C}$ is infinitesimally flexible, by Theorem 4.1 there exists a nonrigid motion infinitesimal flex of the form $u = u_{\omega,\underline{h}}$, for some ω. If $\omega \neq \underline{1}$, then applying Lemma 4.2 a number of times we obtain a nonzero geometric flex $u_{\omega,g}$ with g a constant polynomial. This is a factor periodic infinitesimal flex, with ω in the geometric spectrum, and so (iii) does not hold.

On the other hand, if $\omega = \underline{1}$ then we must be more careful since a similar full degree reduction to $u = u_{\underline{1},g}$ leaves the possibility that this is a nonzero translation flex and so a negation of (iii) is not obtained.

Suppose first that $\deg h = 1$, so that the nontrivial flex u has the form

$$u(k) = u_{\underline{1},h}(k) = (h_1(0) + X_1 k, \dots, h_n(0) + X_n k) \quad k \in \mathbb{Z}^d,$$

where $X_1, \dots, X_n$ are linear transformations which are not all zero. If $X_i = X_j$ for all i, j then u is a nontrivial infinitesimal flex in $\mathcal{V}_{\mathrm{fper}}(\mathcal{C})$, contradicting (iii). We may assume then that $X_s \neq X_t$, for some $1 \leq s, t \leq n$, with $X_s e_j \neq X_t e_j$ for some standard basis element e_j of $\mathbb{Z}^d$. Performing degree reduction with the W_j shift gives the infinitesimal flex $u_{\underline{1},f}$ with $f(z)$ the constant (degree 0) polynomial $f(z) = -(X_1e_j, \dots, X_ne_j)$. This is a periodic flex which is not a translation, contradicting (iii).

Finally, suppose that $\deg h \geq 2$. By Lemma 4.2 we may assume that $\deg h = 2$ so that for some $1 \leq s \leq n$ the function $p = h_s$ has degree 2. It follows from Lemma 4.3 there is a degree reduction to an infinitesimal flex, $u_{\underline{1},h'}$ say, which is of degree 1 and is not a rigid motion flex. Thus we may argue as in the previous paragraph to obtain the desired contradiction. □

4.1. ***P*-primary decompositions.** We recall the formal definitions of a root sequence for a $\mathbb{C}[z]$-module and a P-primary decomposition. The Lasker-Noether theorem states that every submodule of a finitely generated module M over a Noetherian ring is a finite intersection of primary submodules. However, a stronger form asserts that M has a decomposition as given in Definition 4.5, which is known as a *P-primary decomposition.* Moreover any such decomposition leads to a *reduced* P-primary decomposition with distinct primes ideals P_i, and this set of prime ideals is uniquely determined by M. For more details and discussion see Ash [2], as well as Atiyah and MacDonald [4], Krull [18] and Rotman [29].

Definition 4.4. Let R be a Noetherian ring, let L be a submodule of an R-module N, and for $p \in R$, let $\lambda_p : N/L \to N/L$ be multiplication by p. Then L is a *primary submodule* of N if L is proper and for every p the map λ_p is either injective or nilpotent. If $P = \{p \in R : \lambda_p \text{ is nilpotent}\}$ then P is a prime ideal and L is said to be a *P-primary submodule* of N.

Definition 4.5. Let $M = Q_1 \cap \cdots \cap Q_s$ be a primary decomposition of the $\mathbb{C}[z]$-module M where Q_i is P_i-primary for distinct primes $P_i, 1 \leq i \leq s$. A *root sequence* for M is a set $\omega(1), \dots, \omega(s)$ of points in $\mathbb{C}^d$ where for each $1 \leq i \leq s$ the point $\omega(i)$ is a *root* of P_i in the sense that $p(\omega(i)) = 0$ for all $p(z)$ in P_i.

Proof of Theorem 3.6. The first assertion follows from Theorem 4.1. The second assertion recounts the detail in [17] that the finite set of geometric indices is a set of roots, in the sense of Definition 4.5. □

Proof of Theorem 3.7. If $\Gamma(\mathcal{C})$ is infinite then the flex space is infinite-dimensional since a finite set of geometric flexes with distinct periodicity factors is linearly independent. On the other hand if $\Gamma(\mathcal{C})$ is the finite set $\omega(1), \dots, \omega(s)$ then the $\mathbb{C}[z]$-module $M(\mathcal{C})^*$, in $\mathbb{C}[z] \otimes \mathbb{C}^{dn}$, has a P-primary decomposition of length s in terms of P_i^*-primary modules Q_i^* in $\mathbb{C}[z] \otimes \mathbb{C}^{dn}$ with unique root $\omega(i)$, for $1 \leq i \leq s$. (We remark that the starred notation P_i^* and Q_i^* can be viewed purely formally in the rest of the proof. However the notation is natural since $P_i^* = P_i \cap \mathbb{C}[z]$ and $Q_i^* = Q_i \cap (\mathbb{C}[z] \otimes \mathbb{C}^{dn})$ for some associated prime P_i in $\mathbb{C}(z)$ and associated module Q_i which is P_i-primary in $\mathbb{C}(z) \otimes \mathbb{C}^{dn}$.) Since P_i^* is prime and has a unique root it is a maximal ideal.

We have
$$P_i^* = \{a : \lambda_a : \mathbb{C}[z] \otimes \mathbb{C}^r/Q_i^* \to \mathbb{C}[z] \otimes \mathbb{C}^r/Q_i^* \text{ is nilpotent}\},$$
where $r = dn$. Fix a value of i. Then for each $a \in P_i^*$ there exists n such that $a^n(\mathbb{C}[z] \otimes \mathbb{C}^r) \subseteq Q_i^*$. In particular since $z_l - \omega(i)_l$ is in P_i^* for each $1 \leq l \leq d$, there are powers n_l such that
$$(z_l - \omega(i)_l)^{n_l}(\mathbb{C}[z] \otimes \mathbb{C}^r) \subseteq Q_i^*.$$
For each vector e of $\mathbb{C}^r$ the module Q_i^* contains the submodule $J \otimes e_i$ where J is the ideal generated by the powers $(z_l - \omega(i)_l)^{n_l}$, for $1 \leq l \leq d$. Since J has finite codimension it follows that Q_i^* has finite dimensional annihilator.

Finally, the annihilator of the module $M(\mathcal{C})^*$ is the closed span of the annihilators of $Q_1^*, \dots, Q_s^*$ and so is also finite-dimensional. By Theorem 3.6 this annihilator is equal to the first-order flex space of $\mathcal{C}$ and so the proof is complete. □

5. First-order rigid and yet continuously flexible

We now consider direct geometric arguments to show that a crystallographic bar-joint framework may be continuously flexible even when it is first-order rigid. This phenomenon is not possible for finite bar-joint frameworks (Asimow and Roth [3]) since one may use the algebraic variety structure of the configuration space to show that the existence of a continuous flex implies the existence of a differentiable flex.

Consider first the semi-infinite periodic strip framework $\mathcal{Q}_{\text{right}}$ suggested by Figure 2 where the triples of joints $\{A, X, Q\}, \{B, Y, S\}, \dots$ are collinear. We claim that this is first-order rigid.

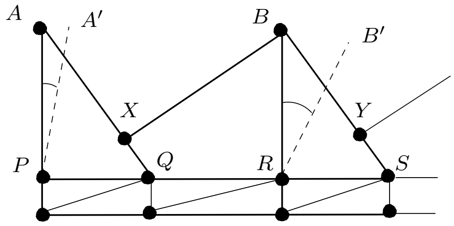

Figure 2. The semi-infinite strip framework $\mathcal{Q}_{\text{right}}$. The angle t at APA' determines the angle $\theta(t)$ at BRB'.

To see this suppose, by way of contradiction, that there exists an infinitesimal flex which is not of trivial (rigid motion) type. Since the strip subframework determined by the joints lying on and below the line through $PQRS$ is infinitesimally rigid we may assume, by subtracting a trivial infinitesimal flex, that u assigns the zero velocity to these joints. Let $u_X, u_Y, u_Z, \dots$ be the velocities of u assigned to the joints $X, Y, Z, \dots$. One of these velocities must be nonzero and without loss of generality we assume that $u_X \neq 0$. Thus $u_B \neq 0$, and we note from the collinearity of B, Y, S that it must be in the direction of the positive x-axis. However, $u_S = 0$ and by this same collinearity we have a contradiction since there is no finite velocity u_Y such that u_B, u_Y, u_S satisfy the flex conditions for the edges BY and YS.

We claim that for a suitable choice of geometry the framework $\mathcal{Q}_{\text{right}}$ is continuously flexible. We do this by showing that each finite stretch of the framework, from AP to another vertical bar, has a unique continuous flex parametrised by the angle t for the inclination angle of the bar AP, where the parameter t ranges over a fixed finite interval. The important point here is that the finite interval does not depend on the stretch.

Assume that $|XQ| < |QR|$ and $|QB| > |XB| > |RB|$ and consider the finite subframework, $\mathcal{G}$ say, supported by the labelled vertices and the four vertices below P, Q, R, S. Consider the joints P, Q, R, S as fixed and note that there is a continuous flex of $\mathcal{G}$ in which AP rotates at constant speed through a clockwise angle parameter $t > 0$. In this motion the bar XQ rotates continuously clockwise to achieve a horizontal position corresponding to final parameter value $t = t_1$ say. The induced angular positions $\theta(t)$ of BR in this motion increases first to a local maximum, θ_{max}, when QX and XB are collinear, and then decreases through positive values to a final value $\theta_{fin} = \theta(t_1)$. Assume next that,

$$|XB| \geq \sqrt{|BR|^2 + (|RQ| - |RX|)^2}$$

so that $\theta_{fin} > 0$. Then the range of the continuous function $\theta : t \to \theta(t)$, for $0 \leq t \leq t_1$, is included in the range of its argument t. Thus, the continuous flex $\pi(t)$ of $\mathcal{G}$, with flex parameter $0 \leq t \leq t_1$, is uniquely extendible to a continuous flex $t \to p(t), 0 \leq t \leq t_1$, of any finite stretch, and so defines a nontrivial continuous flex the semi-infinite framework $\mathcal{Q}_{\text{right}}$, as desired. We remark that the inverse function $s \to \theta^{-1}(s)$ is defined on a suitable interval $[0, \delta]$. Since it is right differentiable at 0, with derivative 0, we may view the continuous flex as having infinite initial velocity at the joint B.

Let $\mathcal{Q}$ be the two-sided periodic strip associated with $\mathcal{Q}_{\rm right}$. The continuous flex $p(t)$, with full parameter range $0 \leq t \leq t_1$, does not extend to a continuous flex of $\mathcal{Q}$. Indeed the maximum possible positive angular deviation of the bar BR, is limited by the colinearity position of bars QX and XB. However, we claim that $\mathcal{Q}$ is continuously flexible, with the angular motions of all the vertical bars taking place within the range $[0, \theta_{max}]$.

To see this consider again the angle propagation function $\theta : t \to \theta(t)$. Let $t = t_{\rm fix}$ be the positive solution of $\theta(t) = t$ and note that $t_{\rm fix} < t_{max}$. (We remark that the angular motion of the n-th vertical bar of $\mathcal{Q}_{\rm right}$ is governed by the iterates of θ and it follows that as t tends to $t_{\rm fix}$ the inclination of each vertical bar converges to t_{fix}.) We claim that the continuous motion of $\mathcal{G}$, parametrised by $0 \leq t \leq t_{fix}$, can be extended to the left strip of $\mathcal{Q}$, and so defines a nontrivial continuous flex of $\mathcal{Q}$.

To see this consider once more the subframework $\mathcal{G}$ linking AP and BR, but with BR providing the driving angular displacement, with angular parameter $s \geq 0$. The leftward angle propagation function is the inverse function $s \to \theta^{-1}(s)$. This is a smooth decreasing function which is well-defined for the range $0 < s \leq \theta_{max}$, with derivative 0 at $s = 0$. It follows by simple iteration, that this continuous flex of $\mathcal{G}$ extends to the left hand side of $\mathcal{Q}$ and so the claim follows.

It is now straightforward to construct a crystal framework in $\mathbb{R}^2$, which is continuously flexible and first-order rigid, by taking parallel copies of the strip framework $\mathcal{Q}$ and rigidly connecting their rigid base subframeworks in a periodic manner.

5.1. **Aperiodic phase transitions.** The continuous flex $t \to p(t)$ of the two-way periodic strip framework $\mathcal{Q}$ adopts aperiodic positions for each intermediate value of t, with $0 < t < t_{\rm fix}$, while the terminal position, for $t = t_{\rm fix}$, is a periodic strip framework which we denote as $\mathcal{Q}_1$. Thus $\mathcal{Q}_1$ is a tilted placement of $\mathcal{Q}$ and we can view the motion as an *aperiodic phase transition* between 2 periodic states. By varying the initial geometry, so that in the initial periodic position A, X, Q are not collinear, one can also construct strip frameworks with aperiodic phase transitions which are smooth paths. By embedding strip frameworks such as these in higher dimensional constructions one can obtain 3D periodic frameworks with similar aperiodic phase transitions between crystal states. It would be interesting to discover if such locally chaotic transitions between periodic states could serve as a model for abrupt transitions in material crystals, such as martensitic changes of state. (See Anwar et al [1] for example for such a transition.)

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Dept. Math. Stats., Lancaster University, Lancaster LA1 4YF, U.K.
E-mail address: `l.kastis@lancaster.ac.uk`
E-mail address: `s.power@lancaster.ac.uk`