Polynomials for crystal frameworks and the rigid unit mode spectrum

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To each discrete translationally periodic bar-joint framework $C$ in $\mathbb{R}^d$, we associate a matrix-valued function $\Phi_C(z)$ defined on the $d$-torus. The rigid unit mode (RUM) spectrum $\Omega(C)$ of $C$ is defined in terms of the multi-phases of phase-periodic infinitesimal flexes and is shown to correspond to the singular points of the function $z \rightarrow \text{rank} \Phi_C(z)$ and also to the set of wavevectors of harmonic excitations which have vanishing energy in the long wavelength limit. To a crystal framework in Maxwell counting equilibrium, which corresponds to $\Phi_C(z)$ being square, the determinant of $\Phi_C(z)$ gives rise to a unique multi-variable polynomial $p_C(z_1, \ldots, z_d)$. For ideal zeolites, the algebraic variety of zeros of $p_C(z)$ on the $d$-torus coincides with the RUM spectrum. The matrix function is related to other aspects of idealized framework rigidity and flexibility, and in particular leads to an explicit formula for the number of supercell-periodic floppy modes. In the case of certain zeolite frameworks in dimensions two and three, direct proofs are given to show the maximal floppy mode property (order $N$). In particular, this is the case for the cubic symmetry sodalite framework and some other idealized zeolites.

1. Introduction

Let $C$ be a mathematical crystal framework, by which we mean a connected structure in the Euclidean space $\mathbb{R}^d$ consisting of a set $C_e$ of framework edges, representing bars or bonds, with a corresponding set $C_v$ of framework points (vertices), representing joints or atoms, such that $C_e$ is periodic with respect to a discrete translation group $T$ of isometries of $\mathbb{R}^d$, with $T$ of full rank. We consider mainly the case $d = 2, 3$ together with the locally finite assumption that $C_e$ is generated by the translations of a finite set of edges. Such a geometric bar-joint framework...
can serve as a model for the essential geometry of the disposition of atoms and bonds in a material crystal $\mathcal{M}$. In this case, the vertices have atomic identifiers, such as H, He, Li, B, etc., and the chosen edges may correspond just to the strong bonds. The identification of strongly bonded molecular units, such as SiO$_4$ and TiO$_6$, implies a polyhedral net structure for $\mathcal{C}$ and in particular aluminosilicate crystals and zeolites provide in this way a fascinating diversity of tetrahedral nets in which every vertex is shared by two tetrahedra.

Material scientists are interested in the manifestation and explanation of various forms of low-energy oscillation and excitation modes. Of particular interest are the rigid unit modes (RUMs) in crystalline materials, the low-energy (long wavelength) modes of oscillation related to the relative motions of rigid units, such as the SiO$_4$ tetrahedral units in quartz. The wavevectors of these modes are observed in neutron-scattering experiments and have been shown to correlate closely with those for the modes observed in computer simulations with periodic networks of rigid units. In both the experimental measurements and the simulations, the background mathematical model is classical lattice dynamics, and the RUM wavevectors are observed where phonon dispersion curves display markedly low energy. There is now a considerable body of literature tabulating the RUM wavevectors of various crystals and it has become evident that the primary determinant in a material $\mathcal{M}$ is the geometric structure of an associated abstract framework $\mathcal{C}$. This was outlined in the seminal paper of Giddy et al. [1]. See also Swainson & Dove [2], Hammond et al. [3,4] and Dove et al. [5]. This experimental work shows that the wavevectors of RUMs often lie along lines and planes in reciprocal space. However, for many materials the wavevectors also lie on more mysterious curved surfaces. See also the recent computer-assisted analysis of Wegner [6].

In what follows, we develop a mathematical theory of RUMs in idealized crystal frameworks. As we shall demonstrate, this is essentially a linear first-order theory and one can side-step lattice dynamical formulations that relate to higher energy phonons and their dispersion curves. In fact in definition 5.2, we define the RUM spectrum $\Omega(\mathcal{C})$ of an idealized crystal framework $\mathcal{C}$, with given translation group, as the set of multi-phasex which there exists a nonzero phase-periodic infinitesimal flex. This form of the spectrum was first given in Owen & Power [7] as a by-product of the analysis of square-summable infinitesimal flexes. Mapping the $d$-torus to the unit cube in $\mathbb{R}^d$ by taking logarithms gives the usual wavevector parametrization space for RUMs used by crystallographers. The spectrum $\Omega(\mathcal{C})$ leads naturally to a definition of the RUM dimension $\text{dim}_{\text{RUM}} \mathcal{C}$, which takes integer values from 0 to $d$ and which gives a measure of the infinitesimal flexibility of $\mathcal{C}$. In the interesting special case of a crystal framework in Maxwell counting equilibrium (see definition 2.2), for example a tetrahedral net framework derived from an idealized zeolite, the spectrum $\Omega(\mathcal{C})$ is determined as the zero set of a multi-variable polynomial $p_C(z_1,\ldots,z_d)$ defined on the $d$-torus. This polynomial may vanish identically, which corresponds to the case $\text{dim}_{\text{RUM}} \mathcal{C} = d$, and for $d = 2, 3$ this is also known as ‘order N’. (See theorem 5.6.) This property occurs, for example, in the case of the cubic form sodalite framework $\mathcal{C}_{\text{SOD}}$, as we prove below in §7 by infinitesimal analysis. Interestingly, Kapko et al. [8] have recently conducted a simulation analysis to determine the extent of this property in idealized zeolites.

The infinitesimal flex perspective is useful for several reasons. Firstly, it brings into play the fairly well-established theory of infinitesimal rigidity for finite bar-joint frameworks and this is of significance for local flexibility. On the other hand, the consideration of general infinitesimal flexes in infinite bar-joint frameworks gives a route to understanding and predicting the appearance of linear components (lines, planes, hyperplanes, etc.) observed experimentally in RUM wavevector sets. In addition, the first-order infinitesimal flexibility properties of a crystal framework $\mathcal{C}$ are implicit in the infinite rigidity matrix $R(\mathcal{C})$ of $\mathcal{C}$, and for phase-periodic flexibility this simplifies to the consideration of a finite function matrix $\Phi_C(z)$ defined on the $d$-torus. This matrix function, which we also refer to as the symbol function of $\mathcal{C}$ (borrowing terminology from Hilbert space operator theory) also arises naturally from square-summable flex perspectives [7] and may be a useful tool more generally. When the matrix is square, the crystal polynomial $p_C(z)$ of $\mathcal{C}$ is defined as a natural normalization of its determinant.
In the development, we give definitions, theorems, proofs and illustrative examples all of which lie within a mathematical theory of infinite bar-joint frameworks. While the focus is on rigidity and flexibility properties related to the disposition of the bonds, rather than their strengths, the theory has the potential to relate to applied analysis and simulations.

In §§2 and 3, we give examples of crystal frameworks and various spaces of infinitesimal flexes. In §§4–6, we define the matrix function \( \Phi_C(z) \), the RUM spectrum \( \Omega(C) \) (definition 5.2), the RUM dimension (definition 5.3) and the crystal polynomial \( p_C(z) \). Also, we give connections between phase-periodic infinitesimal flexes, the so-called periodic floppy modes, and low-energy harmonic excitations. (For discussions of wavevectors, see Dove [9], the account of phonon modes in §6, and the remarks following definition 5.2 in §5 where we define the wavevector of a phase-periodic infinitesimal flex.) In particular, the matrix function \( \Phi_C(z) \) features in a counting formula for the periodic floppy modes in an \( n \)-fold supercell.

The final sections give determinations of \( \Omega(C) \) for a range of examples and some proofs. In particular, we give the novel example of a two-dimensional zeolite whose floppy modes are of order \( N \).

### 2. Crystal frameworks: terminology and examples

Let \( G = (V, E) \) be a simple graph, finite or countable, with vertices \( V = \{v_1, v_2, \ldots \} \) and \( E \subseteq V \times V \) a countable set of edges, and let \( p_1, p_2, \ldots \) be a sequence of points in the Euclidean space \( \mathbb{R}^d \), with \( p_i \neq p_j \) if \( (v_i, v_j) \) is an edge. Then the pair \((G,p)\), with \( p = (p_1, p_2, \ldots) \) is said to be a bar-joint framework in \( \mathbb{R}^d \) with framework points or joints, \( p_i \), and framework edges or bars, given by the line segments \([p_i, p_j]\) between \( p_i \) and \( p_j \) when \((v_i, v_j)\) is an edge in \( E \). In all our examples in fact, the framework points are distinct.

An isometry of \( \mathbb{R}^3 \) is a distance-preserving map \( T: \mathbb{R}^3 \to \mathbb{R}^3 \). A full-rank translation group \( T \) is a set of translation isometries \( \{T_k: k \in \mathbb{Z}^3\} \) with \( T_{k+l} = T_k + T_l \) for all \( k, l \), \( T_k \neq \text{Id} \) if \( k \neq 0 \) and such that the three period vectors

\[
a = T_{\gamma_1}0, \quad b = T_{\gamma_2}0 \quad \text{and} \quad c = T_{\gamma_3}0
\]

associated with the generators \( \gamma_1 = (1,0,0) \), \( \gamma_2 = (0,1,0) \) and \( \gamma_3 = (0,0,1) \) of \( \mathbb{Z}^3 \) are not coplanar. Full-rank translation groups in \( \mathbb{R}^d \) are similarly defined.

The following definition of a crystal framework \( C \) follows the formalism of Owen & Power [7] and pairs a bar-joint framework of crystallographic structure with a group \( T \) of its translation symmetries. The definition brings into play the periodic partitioning of the vertices and edges of \( C \) by the \( T \)-translates of a finite geometrical motif of framework vertices and edges.

**Definition 2.1.** A crystal framework \( C = (F_v, F_e, T) \) in \( \mathbb{R}^d \), with full-rank translation group \( T = \{T_k: k \in \mathbb{Z}^d\} \) and motif \( (F_v, F_e) \), is a countable bar-joint framework \((G,p)\) with framework vertices \( p_{\kappa,k} \), for \( 1 \leq \kappa \leq t, k \in \mathbb{Z}^d \), such that

(i) \( F_v \) is a finite set of framework vertices, \( \{p_{\kappa,0}: 1 \leq \kappa \leq t \} \) in \( \mathbb{R}^d \), and \( F_e \) is a finite set of framework edges,

(ii) for each \( \kappa \) and \( k \) the vertex \( p_{\kappa,k} \) is the translate \( T_k p_{\kappa,0} \),

(iii) the set \( C_v \) of framework vertices is the union of the disjoint sets \( T_k(F_v) \) for \( k \in \mathbb{Z}^d \), and

(iv) the set \( C_e \) of framework edges is the union of the disjoint sets \( T_k(F_e) \) for \( k \in \mathbb{Z}^d \).

This definition contains all the ingredients necessary for the definition of rigidity matrices and operators associated with the various forms of periodic infinitesimal flexes that we shall consider. We also refer to the framework vertices simply as the framework points. Natural choices for \( T \) are maximal translation subgroups of the crystallographic (spatial) symmetry group, subgroups respecting preferred symmetry directions and subgroups corresponding to supercell periodicity.

In figures 1 and 2, motif choices are shown for the kagome framework \( C_{\text{kag}} \) and the squares framework \( C_{\text{sq}} \), where the filled vertices indicate the points of \( F_v \) and where the translation group
is determined by the period vectors. Thus, $C_{kag}$ is the well-known framework of pairwise corner-connected congruent equilateral triangles in regular hexagonal arrangement, whereas $C_{sq}$ is a translationally periodic framework of corner-connected rigid square units.

One can similarly identify motifs for other well-known frameworks and translation groups, such as (i) the grid framework $C_{Z^d}$ in $\mathbb{R}^d$ with $C_v = \mathbb{Z}^d$ and $C_e$ equal to the set of line segments between the nearest neighbours, (ii) $C_{tri}$, the fully triangulated framework from the regular triangular tiling of the plane, and (iii) $C_{hex}$, the crystal framework in the plane associated with the regular hexagon tiling.

In the examples, we employ a mnemonic notational convenience with, typically, $C_{xyz}$ with all lower case letters indicating a planar framework, $C_{Xyx}$ with leading letter upper case indicating a three-dimensional framework, and $C_{XYZ}$ indicating a three-dimensional framework which derives in a well-defined way from the zeolite with name XYZ. For example, we write $C_{Oct}$ to denote the basic regular octahedron net framework in three dimensions formed by corner-connected congruent octahedra with maximal cubic symmetry. Also $C_{SOD}$, defined below, derives from the cubic form of the zeolite sodalite, whereas the companion framework $C_{RWY}$ derives from the sodalite RWY. These conventions can be useful, for example, when discussing subframeworks lying in vector subspaces (slices).

The following definition is convenient.

**Definition 2.2.** A crystal framework $C$ in $\mathbb{R}^d$ is said to be in *Maxwell counting equilibrium* if $d|F_v| = |F_e|$ for some, and hence every, motif. If $d|F_v| < |F_e|$, then $C$ is said to be *edge rich*, while if $d|F_v| > |F_e|$ then $C$ is said to be *edge sparse*.

We now define a number of illustrative crystal frameworks in dimensions two and three, and in §7 we compute their RUM spectra. Of particular interest with regard to rigidity and
flexibility are the 4-regular (4-coordinated) frameworks in two dimensions and the 6-regular frameworks in three dimensions, examples of which are provided by idealized zeolites in the sense of definition 2.3.

(a) Graphene and diamond bar-joint frameworks, \( C_{\text{gra}} \), \( C_{\text{Dia}} \), \( C_{\text{Dia}}^2 \)

The usual visualization of graphene is as a two-dimensional hexagonal bond–node network of carbon atoms with the geometry of \( C_{\text{hex}} \). However, \( C_{\text{hex}} \) is edge sparse and this image is not suggestive of the strength of the material. If we view the C–C–C angles as rigid, or, equivalently, if we also view second nearest neighbours as bonded, then this leads to the edge-rich crystal framework, \( C_{\text{hex}}^2 \) say, implied by figure 3. In the motif shown, we take two of the edges of one of the equilateral triangles to determine period vectors and a corresponding translation group \( T \).

This crystal framework is of interest in its own right and we also write it as \( C_{\text{gra}} \) when viewed as a bar-joint framework in \( \mathbb{R}^2 \). It may be assembled or decomposed in a number of ways to reveal substructure, and in particular it may be constructed as a fusion of two congruent crystal subframeworks as follows. Let \( C_{\text{tri}}^+ \) be obtained from the triangular framework \( C_{\text{tri}} \) by adding bars, in which alternate triangles have three extra short bars added, connecting the triangle joints to a new joint at the centroid of the triangle. Note that these added centroid joints are in natural one to one correspondence with the joints of \( C_{\text{tri}} \) by a small translation. Then, \( C_{\text{gra}} \) is congruent to the framework formed from the join of two copies of \( C_{\text{tri}}^+ \), one of which is rotated by \( \pi \), and where the copies are connected by identifying the centroids of one copy with the non-centroid joints of the other, together with identification of the resulting double edges.

Similarly, crystalline diamond is usually indicated pictorially by a face-centred unit cell, with 14 C atoms at face centres and corners, plus 4 internal C atoms, and the nearest neighbour connectivity. Again, the implied 4-coordinated edge sparse bar-joint framework, \( C_{\text{Dia}} \) say, does not of itself impart a sense of rigidity. It is natural for us to consider, once again, the derived first-and-second-nearest neighbour framework, and to take this as the definition of an associated bar-joint framework, which we denote \( C_{\text{Dia}}^2 \). This too may be understood, or defined, in various constructive ways. For one such construction, echoing the graphene framework decomposition, note that there is a bipartite red–blue colouring of the nodes of \( C_{\text{dia}} \) with face atoms red and internal atoms blue. The extra edges of \( C_{\text{Dia}}^2 \) are either blue–blue or red–red. The red–red determined subframework we refer to as the tetrahedron framework \( C_{\text{Tet}} \). Adding to this framework, the blue–red edges of \( C_{\text{Dia}} \) gives a framework we call \( C_{\text{Tet}}^+ \) (created by centroid addition). It follows that \( C_{\text{Dia}}^2 \) is a join of two copies of \( C_{\text{Tet}}^+ \) (with reflected orientation), the join being effected by centroid/non-centroid identification, as before.
The crystal framework $C_{\text{SOD}}$ in three dimensions is built from 4-rings of tetrahedra in a way which echoes the crystal structure of the cubic form of the zeolite sodalite (figure 4).

The following general definition is convenient.

**Definition 2.3.** An ideal (or mathematical) zeolite in two (resp. three) dimensions is a crystal framework $C$ in the plane (resp. $\mathbb{R}^3$) consisting of congruent triangles (resp. congruent tetrahedra), each pair of which intersects disjointly or at a common vertex and is such that every vertex is shared by two triangles (resp. tetrahedra).

We remark that in databases (such as http://www.iza-structure.org/databases/) material zeolite frameworks are most frequently indicated as a network of ‘T atoms’ corresponding to tetrahedral centres, each of which is 4-coordinated with neighbouring T atoms. This contrasts with the rigid unit view here of a tetrahedral net framework implied by the positions of O atoms as vertices.

The 4-ring building units of $C_{\text{SOD}}$ are oriented in the high-symmetry arrangement indicated in figure 4. Six such rings may be placed on (the outside of) the six faces of an imaginary cube so that the contact vertices sit on the midpoints of the edges of the cube. This gives a finite bar-joint framework consisting of six regular 4-rings connected together to form a finite bar-joint framework which we call the sodalite cage framework. With unit edge length for the tetrahedra the cube has side length $1 + \sqrt{2}$, while the three orthogonal period vectors (determining unit cell geometry) have length $2 + \sqrt{2}$.

A motif for the framework can be given using the set $F_e$ of edges in three pairwise-connected pairwise orthogonally oriented 4-rings of the sodalite cage. The images of the edges of $F_e$ under the action of the associated isometry group $T$ are essentially disjoint and generate the crystal framework $C_{\text{SOD}}$. For an appropriate set $F_v$, an examination of the positioning of $F_v$ in the sodalite cage shows that one must take the vertices of $F_e$ except for nine redundant exterior vertices.

The kagome net framework $C_{\text{Knet}}$

We give two specifications of the *kagome net* framework in three dimensions. Firstly, it may be constructed in a layered manner. Form upward tetrahedral rigid unit frameworks on alternate triangles of a two-dimensional kagome framework lying in the $xy$-plane. Similarly, form downward tetrahedra on the other triangles, and thereby create a layer framework of pairwise-connected tetrahedra. Parallel copies of such layers can be joined at their exposed joints together to fill space, creating, unambiguously, the crystal framework we denote as $C_{\text{Knet}}$.

Alternatively, $C_{\text{Knet}}$ is a translationally periodic bar-joint framework with period vectors formed by three edges of a regular parallelepiped, with pairwise angles of $\pi/3$. Each
parallelapiped contains two tetrahedral rigid units located at opposite ‘acute’ corners of the parallelapiped and with edge length half that of the parallelapiped edges. The planar slices of \( C_{\text{Knet}} \), determined by each pair of period vectors, give copies of \( C_{\text{kag}} \).

(d) The frameworks \( C_{\text{star}} \) and \( C_{\text{oct}} \)

The kagome framework can be viewed as arising from the connection of translates of a regular six-pointed star. There are analogous frameworks, \( C_{\text{star}} \) and \( C_{\text{oct}} \), arising from similar tilings using a regular four-pointed star and an eight-pointed star, respectively. Figure 6, in §7, indicates the (primitive) star template for \( C_{\text{star}} \), while figure 5 indicates tiling templates for four two-dimensional zeolite crystal frameworks. More precisely, a natural choice of translation group for each of the associated bar-joint frameworks is that which is generated by horizontal and vertical translation. One can note that the third framework (with exterior angle \( 8\pi/12 \)), viewed as simply a bar-joint framework, is also recognizable as a congruent (rotated) copy of the bar-joint framework of \( C_{\text{star}} \). One can also confirm similarly that the second and fourth frameworks are congruent by an isometry of \( \mathbb{R}^2 \). The fourth framework here, with translation isometry group, is what we define as the crystal framework \( C_{\text{oct}} \).

A motif \((F_v, F_e)\) for \( C_{\text{oct}} \) may be provided with \( F_v \) the set of four boundary vertices (indicated as solid vertices in the fourth template) plus the eight internal vertices (of the octagon), and with \( F_e \) the set of all 24 edges of the template. Evidently, there is a smooth periodic edge-length-preserving continuous motion (continuous or ‘finite’ flex in the terminology of bar-joint frameworks) which ‘connects’ these frameworks and which is parametrized by specification of the indicated exterior angle \( \alpha \) say. This continuous motion, or evolution, maintains the squareness of the unit cells indicated in figure 5 but evidently changes their edge lengths (and the period of translational periodicity). In §6, we give an indication of how the RUM spectrum evolves under this motion. The motion here may be viewed as an example of the idealization of displacive phase transitions in materials [9]. We remark that the derivative of this motion at any particular value of \( \alpha \) gives a particular infinitesimal flex of the bar-joint framework associated with the value \( \alpha \). Such infinitesimal flexes are of **affine type** or **flexible lattice type** and are not strictly periodic in the sense of definition 3.4. For more on such infinitesimal flexes, which are associated with infinitesimal affine motions of the ambient space, see Borcea Streinu [10], Power [11] and Ross et al. [12].
Further examples

Simple but informative examples of three-dimensional zeolite frameworks can be built from two-dimensional zeolite frameworks in various ways by layer constructions. With \( c_{\text{oct}} \), for example, embedded in the \( x,y \) plane of \( \mathbb{R}^3 \), we may add bars and joints to obtain alternately upward and downward pointing tetrahedral units, and so create a layer framework. These layers may be joined consecutively at their exposed points to fill \( \mathbb{R}^3 \) and thereby create an associated ideal zeolite framework \( \tilde{c}_{\text{oct}} \). Similarly, one can view \( c_{\text{Knet}} \) as the framework \( \tilde{c}_{\text{kag}} \).

We also note that interesting and diverse examples of mathematical crystal frameworks are implied by various tilings and periodic nets. For an account of three-periodic nets and connections with crystal chemistry, see Delgado Friedrichs et al. [13,14]. Such an (unlabelled) net, in any dimension, may be defined as a pair \((N,P)\), where \( N \) the union of the edges of a crystal framework whose framework edges only intersect at framework vertices and where \( P \) is the set of framework points.

3. Infinitesimal flexibility and rigidity

We now define various flexes which act on the entire infinite crystal framework in a locally infinitesimal manner. The definition is the same as that for a finite bar-joint framework.

Definition 3.1. An infinitesimal flex of a finite or countable bar-joint framework \((G,p)\) is a vector \( u = (u_i) \), with each component \( u_i \) a vector in \( \mathbb{R}^d \), such that for each edge \([p_i,p_j]\) \[
(p_i - p_j, u_i) = (p_i - p_j, u_j).
\]

Regarding the \( u_i \) as velocity vectors this asserts that for each edge the components of the endpoint velocities in the edge direction are in agreement. This is equivalent to the assertion that an infinitesimal flex is a velocity vector \( v = (v_i) \) for which the distance deviation

\[
|p_i - p_j| - |(p_i + tu_i) - (p_j + tu_j)|
\]

of each edge is of order \( t^2 \), as the time parameter \( t \) tends to zero.

We will not be concerned particularly with continuous flexes, which are also called finite flexes (or finite edge-length-preserving deformations). For such flexes, each framework point undergoes a continuous motion \( p_{\kappa,k}(t) \) such that edge lengths are preserved for all values of time \( t \) in some range. However, we note that, as for a finite framework, the derivative \( u = p'(0) = (p'_i(0)) \) of a continuous flex \( p(t) = (p_i(t)) \) with differentiable vertex trajectories provides an infinitesimal flex.

In the case of a crystal framework in \( \mathbb{R}^d \), a velocity vector is a doubly indexed sequence \( v \) of vectors \( v_{\kappa,k} \) in \( \mathbb{R}^d \) regarded as instantaneous velocities applied to the framework vertices \( p_{\kappa,k} \), and it is convenient to consider the vector space of all velocity sequences, written as a direct product, namely

\[
\mathcal{H}_{\text{atom}} = \prod_{\kappa,k} \mathbb{R}^d.
\]

Thus, a real infinitesimal flex \( u \) for the crystal framework \( C \) is a velocity vector \( u \) in \( \mathcal{H}_{\text{atom}} \) such that

\[
(p_{\kappa,k} - p_{\tau,l}, u_{\kappa,k} - u_{\tau,l}) = 0
\]

for each framework edge \([p_{\kappa,k},p_{\tau,l}]\). In particular, the set of all infinitesimal flexes forms a vector subspace, \( \mathcal{H}_{\text{fl}} \), say, of \( \mathcal{H}_{\text{atom}} \). Also, each non-trivial infinitesimal isometry of \( \mathbb{R}^d \) gives rise to a one-dimensional vector subspace of \( \mathcal{H}_{\text{fl}} \).

The rigidity matrix \( R(C) \) of \( C \) is a real infinite matrix defined as in the finite framework case.
**Definition 3.2.** The rigidity matrix \( R(C) \) of the crystal framework \( C \) in \( \mathbb{R}^3 \) has rows labelled by the edges \( e = [p_\kappa, p_\tau,j] \) and columns labelled by the framework point coordinate indices \((\kappa, x, k), (\kappa, y, k)\) and \((\kappa, z, k)\). The row for edge \( e \) takes the form

\[
[\cdots 0 (p_\kappa, k - p_\tau,j) 0 \cdots 0 (p_\tau,j - p_\kappa, k) 0 \cdots],
\]

where the vector entry \((p_\kappa, k - p_\tau,j)\) indicates that the three coordinates of this vector lie in the columns for \((\kappa, x, k), (\kappa, y, k)\) and \((\kappa, z, k)\).

The definition of \( R(C) \) for \( d = 2, 4, 5, \ldots \) and also for general countably infinite bar-joint frameworks [15] is essentially the same. We remark that one may take the view that \( R(C) \) has at the most \( 2d \) non-zero entries and the image \( R(u) \) is given by the well-defined matrix multiplication \( R(C)u \). As for finite frameworks, one has the following elementary proposition.

**Proposition 3.3.** The infinitesimal flexes of the crystal framework \( C \) are the velocity vectors in \( H_{\text{atom}} \) that lie in the nullspace of the linear transformation \( R(C) \).

Let us introduce notation for the natural basic sequences of \( H_{\text{atom}} \) and \( H_{\text{bond}} \). Write \( \xi_x, \xi_y, \xi_z \) for the standard coordinate basis of \( \mathbb{R}^3 \), \( \xi_z = (1, 0, 0) \) etc., and for \( \sigma \in \{x, y, z\} \) write \( \xi_{\kappa, \sigma, k} \) for the position indicator vector in \( H_{\text{atom}} \) with

\[
(\xi_{\kappa, \sigma, k})_{k', \sigma} = \delta_{\kappa, k'} \delta_{k, k} \xi_{\sigma},
\]

where \( \delta_{\kappa, k'} \) is the Kronecker delta. While \( H_{\text{atom}} \) does not have countable vector space dimension, its subspace of finitely non-zero sequences has the set \( \{\xi_{\kappa, \sigma, k}\} \) as a vector space basis. However, the set is a generalized product type basis for \( H_{\text{atom}} \) in the sense below. In particular, we may define the infinitesimal unit translation flex \( u_x \) in the \( x \)-direction as the well-defined infinite sum

\[
u_x = \sum_{\kappa, k} \xi_{\kappa, x, k}.
\]

Similarly, we may write \( \eta_{\kappa, k} \) for the basic sequence in \( H_{\text{bond}} \) which is zero but for the value 1 for the coordinate position \( e, k \).

Let \( (G, p) \) be a countably infinite bar-joint framework in \( \mathbb{R}^d \). A product type basis for a subspace \( M \) of the velocity space \( H_{\text{atom}} \) of \( (G, p) \) is a countable set \( S = \{w^1, w^2, \ldots \} \) of vectors in \( M \) such that,

(i) every vector \( u \) in \( M \) has a unique representation

\[
u = \sum_{n \in \mathbb{N}} \alpha_n w^n, \quad \alpha_n \in \mathbb{R},
\]

(ii) for each index \( k \) only a finitely many elements \( w^n \) of \( S \) have non-zero \( k \)th component \( w^k \).

The basic grid framework \( C_{2^d} \) has evident non-zero infinitesimal flexes \( u \) that act only on linear subframeworks (copies of \( C_2 \) in \( \mathbb{R}^2 \)). One can show that a set, \( S_d \) of representatives of all such flexes, is a product-type basis for \( H_{\ell_0} \). In fact, we show elsewhere that it is possible to identify
product-type bases for the vector space of all infinitesimal flexes for many other basic crystal frameworks. Two examples are $C_{kag}$ and the three-dimensional crystal framework $C_{Oct}$.

The following definition gives the context for the special classes of infinitesimal flexes of a crystal framework that concern us.

**Definition 3.4.** Let $C$ be a crystal framework with translation group $T$ as above.

(i) An infinitesimal flex (or velocity sequence) $u$ is **strictly periodic** if the following periodicity condition holds: $u_{\kappa,k} = u_{\kappa,0}$ for all $k \in \mathbb{Z}^d$.

(ii) An infinitesimal flex (or velocity sequence) $u$ is **supercell-periodic** if $u_{\kappa,k} = u_{\kappa,0,\alpha}$ for all $k$ in a subgroup $r_1\mathbb{Z} \times \cdots \times r_d\mathbb{Z}$ for some positive integers $r_1, \ldots, r_d$.

(iii) An infinitesimal flex $u$ is a **local infinitesimal flex** if $u_{\kappa,k} = 0$ for all but finitely many values of $\kappa, k$.

Note the elementary fact that if there exists a local infinitesimal flex for $C$ then this framework is rich in supercell-periodic flexes. Indeed, if $u$ is such a local infinitesimal flex and if $k \to \alpha_k$ is any supercell-periodic coefficient sequence then the sum

$$w = \sum_k \alpha_k T_k u$$

is a well-defined supercell-periodic infinitesimal flex.

In §5, we turn our attention to complex scalar infinitesimal flexes which are phase-periodic, the real and imaginary parts of which provide real infinitesimal flexes. It is such phase-periodic flexes that are closely allied to RUM wavevectors. They lead naturally to the formulation of a matrix-valued function associated with $C$ and $T$ and we describe this association in the next section.

The strictly periodic infinitesimal flexes are also referred to as fixed lattice flexes. We remark that there is an interesting class of infinitesimal flexes which lie outside our considerations here of (fixed lattice) RUM analysis, namely the affinely periodic infinitesimal flexes. Such ‘flexible lattice’ flexes allow, roughly speaking, an infinitesimal adjustment of the period vectors. (See also the comments on the frameworks in figure 5.) For this and discussions of associated finite motions see, for example, Borcea & Streinu [10], Malestein & Theran [16], Owen & Power [7], Power [11] and Ross et al. [12].

(a) **Infinitesimal rigidity**

If a connected bar-joint framework $(G,p)$, finite or infinite, has no infinitesimal flexes other than rigid motion flexes, then it is said to be **infinitesimally rigid**. The simplest way in which this occurs is when $(G,p)$ is **sequentially infinitesimally rigid** in the sense that it is the union of an increasing sequence of infinitesimally rigid finite frameworks. This is evidently the case for the edge-rich frameworks $C_{tri}$, $C_{gra}$, $C_{tet}$ and $C_{Dia}$. In particular, it follows from the definitions below that the primitive RUM spectrum of each of these frameworks is trivial. Indeed, the RUM spectrum of a crystal framework is trivial when there are no phase-periodic infinitesimal flexes other than the strictly periodic flexes for infinitesimal translation. For a sequentially rigid framework, all infinitesimal flexes are trivial in this sense. In fact in Kitson & Power [17] we give characterizations of infinitesimal rigidity and sequential infinitesimal rigidity for general countably infinite frameworks.

On the other hand, we remark that overconstrained frameworks such as these edge-rich crystal frameworks are rich in periodic infinitesimal self-stresses. Following terminology for finite frameworks, a **self-stress** $w = (w_e)_{e \in C_e}$ of a crystal framework $C$ is an assignment of scalars to edges such that for every framework point $p_{k,\kappa}$ the finite vector sum

$$\sum_{\tau, l : e = [p_{k,\kappa}, p_{\tau,l}]} w_e (p_{k,\kappa} - p_{\tau,l})$$

would be a well-defined self-stress. For a sequentially rigid framework, all self-stresses are trivial in this sense.
taken over all edges incident to \( p_{k,j} \) is equal to zero. This is a companion notion to that of an infinitesimal flex and indeed \( w \) is a self-stress if and only if \( w \) lies in the nullspace of the transpose of the rigidity matrix \( R(C)^T \). One may similarly consider subspaces of strictly periodic self-stresses and phase-periodic self-stresses in a manner following the definitions for flexes.

One may relax the notion of infinitesimal rigidity to various forms of rigidity which are associated with a (possibly normed) space \( S \) of velocity vectors. This is a viewpoint taken in Owen & Power \([7,15,18]\) leading to definitions of square-summable rigidity, summable rigidity, vanishing flex rigidity (\( c_0 \)-rigidity) and local flex rigidity (\( c_{00} \)-rigidity). It is an interesting issue to determine which classes of crystal frameworks are rigid in such a relative sense.

4. The matrix function \( \Phi_C(z) \)

A matrix-valued function, or symbol function, for \( C \) is determined by the periodicity group \( T \) and the given motif \( (F_v,F_e) \) as follows.

Write \( z = (z_1, \ldots, z_d) \), with \( z_i \in \mathbb{C} \), \( |z_i| = 1 \), to denote general points in the \( d \)-torus \( \mathbb{T}^d \). Also, write \( z^k \) for the monomial function \( z \rightarrow z^k \) from \( \mathbb{T}^d \) to \( \mathbb{C} \). As \( z_i^{-k} = z_i^k \) for points on the circle \( T \) we may think of general monomials \( z^k \) as products of the \( z_i \) or \( \bar{z}_i \) with just non-negative powers.

It is convenient to define the edge vector \( v_e \) of the directed edge \( e = [p_{k,j}, p_{\tau,j}] \) as \( v_e = p_{k,j} - p_{\tau,j} \) and to write \( v_{e,\sigma} \), for \( 1 \leq \sigma \leq d \), for the coordinates of \( v_e \).

**Definition 4.1.** Let \( C \) be a crystal framework in \( \mathbb{R}^d \) with motif sets

\[
F_v = \{ p_{k,\sigma} : 1 \leq k \leq |F_v| \} \quad \text{and} \quad F_e = \{ e_i : 1 \leq i \leq |F_e| \}.
\]

Then, \( \Phi_C(z) \) is the matrix-valued function on \( \mathbb{T}^d \) with rows labelled by the edges \( e = [p_{k,j}, p_{\tau,j}] \in F_e \) and with columns labelled by pairs \( k, \sigma \). As a matrix of scalar function, the entries are given by

\[
(\Phi_C(z))_{e,(k,\sigma)} = v_{e,\sigma} z^k
\]

and

\[
(\Phi_C(z))_{e,(\tau,\sigma)} = -v_{e,\sigma} \bar{z}^l,
\]

if \( k \neq \tau \), while for a reflexive edge, with \( k = \tau \),

\[
(\Phi_C(z))_{e,(k,\sigma)} = v_{e,\sigma} (z^k - \bar{z}^l).
\]

The other entries are equal to the zero function.

Different motifs for \( T \) give matrix functions that are equivalent in a natural way. Indeed, replacement of a motif edge (resp. vertex) by a \( T \)-equivalent one results in the multiplication of the appropriate row (resp. column) by a monomial. Thus, in general two motif matrix functions \( \Phi(z) \) and \( \Psi(z) \) satisfy the equation

\[
\Psi(z) = D_1(z) A \Phi(z) BD_2(z),
\]

where \( D_1(z) \) and \( D_2(z) \) are diagonal matrix functions with monomial functions on the diagonal and where \( A, B \) are permutation matrices, associated with edge and vertex relabelling.

The next two examples and those we consider later occur in two and three dimensions and in this case we simply write \( (z,w) \) and \( (z,w,u) \), respectively, for general points of \( \mathbb{T}^2 \) and \( \mathbb{T}^3 \).

**Example (a).** The motif for \( C_{\text{sq}} \) implied by \( \text{figure 2} \) has \( F_v \) equal to the ordered set \( \{(1/2,0),(0,1/2)\} \) and \( F_e = \{e_1, \ldots, e_5\} \). Here the period vectors, given by the sides of the parallelogram unit cell, are scaled with unit length. It follows that the matrix function for \( C_{\text{sq}} \) is

\[
\begin{bmatrix}
  1 & -1 & -1 & 1 \\
  -1 & -1 & \bar{z} & \bar{z} \\
  \bar{w} & \bar{w} & -1 & -1 \\
  -\bar{w} & \bar{w} & \bar{z} & -\bar{z} \\
  0 & 0 & -2 + 2\bar{z} & 0
\end{bmatrix}
\]
If the final row of $\Phi_{C_{sq}}(z, w)$ is deleted, then one has the matrix function for the realization of the square grid framework, $C_{Z^2}$, when rotated by $\pi/4$. This framework is in Maxwell counting equilibrium, and so the matrix function is square and we may compute

$$\det \Phi_{C_{Z^2}}(z, w) = 4(\bar{w} - \bar{z})(\bar{w}z - 1).$$

We consider further matrix function analysis for this example in §7, example (f).

Example (b). With a choice of labelling for the motif in figure 1, with period vectors of length one, the matrix function $\Phi_{kag}(z, w)$ of the kagome framework $C_{kag}$ takes the form given by

$$\Phi_{kag}(z, w) = \frac{1}{4} \begin{bmatrix}
-2 & 0 & 2 & 0 & 0 & 0 \\
0 & 0 & 1 & -\sqrt{3} & -1 & \sqrt{3} \\
-1 & -\sqrt{3} & 0 & 0 & 1 & \sqrt{3} \\
2 & 0 & -2z & 0 & 0 & 0 \\
0 & 0 & -1 & \sqrt{3} & \bar{z}w & -\sqrt{3}\bar{z}w \\
\bar{w} & \sqrt{3}\bar{w} & 0 & 0 & -1 & -\sqrt{3}
\end{bmatrix}.$$ 

In this case, the determinant is equal to a constant multiple of

$$\bar{z}\bar{w}(z - 1)(w - 1)(z - w).$$

For a different motif, for the given translation group, this determinant would change by a monomial factor.

(a) Polynomials for crystal frameworks

Let $C$ be a crystal framework in $\mathbb{R}^d$ with a given isometry group $T$. If $C$ is in Maxwell counting equilibrium, then we may form the polynomial $\det(\Phi_C(z))$ of the matrix function associated with a particular motif. This is a polynomial in the coordinate functions $z_i$ and their complex conjugates $\bar{z}_i$, and is possibly identically zero. In the non-zero case, we remove dependence on the motif and formally define the crystal polynomial $p_C(z_1, \ldots, z_d)$, associated with the pair $C, T$ and a lexicographic monomial ordering, as the product $\alpha z^\gamma \det(\Phi_C(z))$ where the multi-power $\gamma$ and the scalar $\alpha$ are chosen so that

(i) $p_C(z)$ is a linear combination of non-negative power monomials,

$$p_C(z) = \sum_{\alpha \in \mathbb{Z}_+^d} a_\alpha z^\alpha,$$

(ii) $p_C(z)$ has minimum total degree, and

(iii) $p_C(z)$ has leading monomial with coefficient 1.

It is natural to order monomials lexicographically, so that, for example, the monomial function $z_1^2z_2$ has higher multi-degree than $z_1z_2^3$. In this way, one defines the leading term of a multivariable polynomial. (See also the discussion in Cox et al. [19] for example.)

It follows that the crystal polynomial for the kagome framework and the (primitive case) translation group, as above, is

$$p_{kag}(z, w) = (z - 1)(w - 1)(z - w),$$

with lexicographic order $z > w$. Also, for the grid framework $C_{Z^2}$ and the non-axial translation group given above we see from the form of the determinant that

$$p_{Z^2}(z, w) = (z - w)(zw - 1).$$

For the grid frameworks $C_{Z^d}$, it is in fact more natural to take the standard axial translation group $T$ and a minimal motif which consists of a single vertex and $d$ edges, one for each axial direction.
For this pair \( C, T \), the crystal polynomial is simply
\[
(z_1 - 1)(z_2 - 1) \cdots (z_d - 1).
\]

5. Rigid unit modes and \( \Phi_C(z) \)

We first show how \( \Phi_C(z) \) arises as a family of matrices parametrized by points \( z \) in the \( d \)-torus where the matrix for \( z = \omega \) determines the possible existence of infinitesimal flexes which are periodic modulo the multi-phase \( \bar{\omega} \).

Let \( \mathcal{K}_{\text{atom}}, \mathcal{K}_{\text{bond}} \) be the complex scalar versions of the vector spaces \( \mathcal{H}_{\text{atom}}, \mathcal{H}_{\text{bond}} \). Write \( \mathcal{K}_{\alpha}^\omega \) for the complex vector space of complex velocity vectors \( v = (v_k, k) \) such that \( v_k, k = \omega^j v_k, 0 \) for \( k \in F_v, k \in \mathbb{Z}^d \). This is a finite-dimensional subspace of \( \mathcal{K}_{\text{atom}} \) of dimension \( d|F_v| \).

Similarly, let \( \mathcal{K}_{\beta}^\omega \subset \mathcal{K}_{\text{bond}} \) be the subspace of the bond vector space of complex sequences \( w = (w_k)e \in \mathcal{K}_{\text{bond}} \) which are phase-periodic in this way for the phase \( \omega \). Note that the rigidity matrix \( R(C) \) provides a linear transformation \( R^\omega : \mathcal{K}_{\alpha}^\omega \to \mathcal{K}_{\beta}^\omega \) by restriction. Indeed, with \( d = 3 \), let \( \gamma_i, 1 \leq i \leq 3 \), denote the usual generators for \( \mathbb{Z}^3 \) and let \( W_i \) and \( U_i \) be the shift transformations on \( \mathcal{K}_{\text{atom}} \) and \( \mathcal{K}_{\text{bond}} \), respectively, with
\[
W_i : \xi_{\kappa, \sigma, k} \to \xi_{\kappa, \sigma, k + \gamma_i}
\]
and
\[
U_i : \eta_{\epsilon, k} \to \eta_{\epsilon, k + \gamma_i}.
\]
Then, we have the commutation relations
\[
R(C)W_i = U_i R(C), \quad 1 \leq i \leq 3,
\]
and the identities \( W_i u = \overline{\omega_i} u \), for \( u \in \mathcal{K}_{\alpha}^\omega \), and \( U_i v = \overline{\omega_i} v \), for \( v \in \mathcal{K}_{\beta}^\omega \). Thus, for \( u \) in \( \mathcal{K}_{\alpha}^\omega \),
\[
U_i (R(C)u) = R(C)(W_i u) = R(C)(\overline{\omega_i} u) = \overline{\omega_i} R(C)u,
\]
and so \( R(C)u \in \mathcal{K}_{\beta}^\omega \).

Let \( \{ \xi_{\kappa, \sigma} : \kappa \in F_v, \sigma \in \{ x, y, z \} \} \) be the natural basis for the column vector space \( \mathbb{C}^{|F_v|} \). Write \( \xi_{\kappa, \sigma}^\omega \) for the displacement vectors in \( \mathcal{K}_{\alpha}^\omega \) which ‘extend’ the basis elements \( \xi_{\kappa, \sigma} \). Formally, in terms of Kronecker delta symbol, we have
\[
(\xi_{\kappa, \sigma}^\omega)_k \omega = \delta_{\kappa, \kappa'} \omega^k \xi_{\sigma, \sigma'}.
\]
Similarly, let \( \eta_{\epsilon, \epsilon} \in F_v \) be the standard basis for \( \mathbb{C}^{|F_v|} \) and write \( \eta_{\epsilon, \epsilon}^\omega \), \( \epsilon \in F_v \), for the natural associated basis for \( \mathcal{K}_{\beta}^\omega \), with
\[
(\eta_{\epsilon, \epsilon}^\omega)_\epsilon \omega = \delta_{\epsilon, \epsilon'} \omega^\epsilon \eta_{\epsilon, \epsilon'}.
\]

**Theorem 5.1.** Let \( C \) be a crystal framework in \( \mathbb{R}^d \) with matrix function \( \Phi_C(z) \) and let \( \omega \in \mathbb{T}^d \). Then, the scalar matrix \( \Phi_C(\bar{\omega}) \) is the representing matrix for the linear transformation \( R^\omega : \mathcal{K}_{\alpha}^\omega \to \mathcal{K}_{\beta}^\omega \) with respect to the natural bases \( \{ \xi_{\kappa, \sigma}^\omega \} \) and \( \{ \eta_{\epsilon, \epsilon}^\omega \} \).

**Proof.** Let \( \bar{u} \) be a velocity vector in \( \mathcal{K}_{\alpha}^\omega \) determined by \( u \in \mathbb{C}^{|F_v|} \) as above. Let \( e \in F_v \) be an edge of the form \( [p_{e, k}, p_{e, r}] \) and let \( \langle \cdot, \cdot \rangle \) denote the bilinear form on \( \mathbb{C}^d \). Then, from the definition of the rigidity matrix \( R(C) \), the \( (e, 0) \)th entry of \( R(C)u \in \mathcal{K}_{\beta}^\omega \) can be written as
\[
(R(C)\bar{u})_e = (v_e, u_{k, k}) + (-v_e, u_{k, r})
\]
\[
= (v_e, \omega^k u_k) + (-v_e, \omega^r u_r)
\]
\[
= (\omega^k v_e, u_k) + (-\omega^r v_e, u_r).
\]
This agrees with \( (\Phi_C(\bar{\omega})u)_e \), both in the case \( \kappa \neq \tau \) and in the reflexive case \( \kappa = \tau \) and the theorem follows. \( \blacksquare \)

In particular, the strictly periodic (one-cell-periodic) (real or complex) infinitesimal flexes are determined by the (real or complex) vectors in the nullspace of the real matrix \( \Phi(1, \ldots, 1) \). This
periodic rigidity matrix has rows carrying entries from the vectors \( v_\epsilon, -v_\epsilon \) in the case of non-reflexive edges of the motif (in the sense of definition 4.1), with reflexive edges contributing zero rows.

The terminology of the following definition is justified in the next section.

**Definition 5.2.** The RUM spectrum of the crystal framework \( \mathcal{C} \) in \( \mathbb{R}^d \), with translation group \( T \), is the set \( \Omega(\mathcal{C}) \) of points \( \omega = (\omega_1, \ldots, \omega_d) \) in \( \mathbb{T}^d \) for which there is a non-zero vector \( u \) in \( \mathcal{K}_u^\omega \), which is an infinitesimal flex for \( \mathcal{C} \).

We also define the RUMs themselves as the non-zero infinitesimal flexes that give rise to points in the RUM spectrum. The mode multiplicity function is the integer-valued function defined on \( \Omega(\mathcal{C}) \) by \( \mu(\omega) = \dim \ker R_\omega^\omega \).

Note that from the theorem we have

\[
\Omega(\mathcal{C}) = \{ \omega \in \mathbb{T}^d : \ker \Phi(\omega) \neq \{0\} \}.
\]

In particular, from a commutative algebra perspective this set can be viewed as a real or complex algebraic variety.

Evidently, the RUM spectrum is a construct of the crystal framework \( \mathcal{C} = (F_v, F_e, T) \) and the ordering of coordinates matches the ordering of the generators of the translation group \( T = \{ T_k : k \in \mathbb{Z}^d \} \). In the case of motif change, under a fixed translation group \( T = \{ T_k : k \in \mathbb{Z}^d \} \), one has two logically distinct crystal frameworks, \( \mathcal{C} = (F_v, F_e, T) \) and \( \mathcal{C}' = (F'_v, F'_e, T) \), with formally distinct symbol functions, \( \Phi(\zeta) \) and \( \Psi(\zeta) \) say. However, our earlier observation relating these functions shows that in this case \( \Omega(\mathcal{C}) \) and \( \Omega(\mathcal{C}') \) are identical subsets of the \( d \)-torus.

**Remarks.** In the next section, we make precise the connection between RUMs as we have defined them above and the low-energy phonon modes that are of interest to material scientists, and are referred to as RUMs. The convention in material science is to indicate the set of reduced wavevectors that arise with these modes, rather than indicating a set of multi-phases, as we are doing here for their mathematical infinitesimal flex counterparts, but the conventions are simply related.

If a material RUM has a wavevector \( \mathbf{k} = (k_1, k_2, k_3) \) then it has a multi-phase \( \omega = (\omega_1, \omega_2, \omega_3) \) in \( \mathbb{T}^3 \) obtained by exponentiating, with \( \omega_1 = \exp(2\pi i k_1) \). The reduced wavevector for the RUM is the reduction modulo 1 in each coordinate and is the point \( \mathbf{k}' = (k_1', k_2', k_3') \) in the unit cube \([0, 1)^3 \). It is obtained by taking the (principal) logarithms of each coordinate of the multi-phase.

For a simple crystal framework \( \mathcal{C} \) in two or three dimensions (see, for example, example (f) in §7) the set of RUM wavevectors often consists of the intersection of \([0, 1)^d \) with a union of a finite number of points, lines and planes (hyperplanes for \( d > 3 \)) which are determined by equations over \( \mathbb{Q} \). Also, in interesting cases the RUM wavevectors may fill all of \([0, 1)^d \), with \( \Omega(\mathcal{C}) = \mathbb{T}^d \). In these cases, we say that \( \Omega(\mathcal{C}) \) is a standard RUM spectrum. Otherwise, borrowing terminology from Dove et al. [5], we shall say that the RUM spectrum is exotic. This includes the case of curves or curved surfaces in the unit cube. (The author is not aware of examples of crystal frameworks whose RUM spectrum has isolated irrational points or ‘exposed’ irrational lines.)

**(a) The dimension \( \dim_{\text{rum}}(G, p) \)**

Returning to the RUM spectrum recall that \( \Omega(\mathcal{C}) \) is a well-defined set in \( \mathbb{T}^d \) determined by the underlying bar-joint framework \((G, p)\) and a translation group \( T = \{ T_k : k \in \mathbb{Z}^d \} \), and where generator permutations for \( T \) correspond to a coordinate permutation. We now define the RUM dimension of \((G, p)\), which takes an integer value between 0 and \( d \) inclusive.

We first define the primitive RUM spectrum \( \Omega_{\text{prim}}(G, p) \) of the crystallographic bar-joint framework \((G, p)\) as the RUM spectrum for the crystal framework \( \mathcal{C} \) associated with \((G, p)\) and a maximal translation group of isometric automorphisms of \((G, p)\). (The terminology borrows from the notion of a primitive unit cell for a crystallographic set in \( \mathbb{R}^d \).) To see that \( \Omega_{\text{prim}}(G, p) \) is well defined, up to permutation of the coordinates, we first recall the classical fact of Bieberbach that a
crystallographic group in any number of dimensions has a unique maximal normal free Abelian subgroup. In our setting, this entails that two maximal translation subgroups \( T = \{ T_k : k \in \mathbb{Z}^d \} \) and \( T' = \{ T'_k : k \in \mathbb{Z}^d \} \) of the isometric (spatial) automorphism subgroup are congruent by an isometry \( Z \) of \( \mathbb{R}^d \) which effects an automorphism \( Z \) of \((G, p)\). In this case, we have \( T'_k = ZT_k Z^{-1} \) for all \( k \). Moreover, in view of our earlier discussion we may assume that the motif \((F_v, F_e)\) for \( T' \) is given and that the motif \((F'_v, F'_e)\) for \( T' \) is chosen as the image of \((F_v, F_e)\) under \( Z \), with a corresponding labelling. It follows that the respective symbol functions \( \Phi(z) \) and \( \Phi(z)' \) are simply related. Indeed, let \( S \) be the linear isometry component of \( Z \). Then, in the notation for the symbol functions the new motif edge vector \( v'_e \) associated with framework edge \( Ze \) is given by \( Zv_e = Zp_e,k - Zp_e,j \) which, being a difference, is equal to \( Sv_e \). It follows from this that

\[
\Phi(z)' = \Phi(z)X,
\]

where \( X \) is an invertible block diagonal (scalar) matrix \( X \oplus \cdots \oplus X \) (with \(|F_v|\) summands). The well-definedness of the primitive RUM spectrum of \((G, p)\) now follows.

**Definition 5.3.** Let \((G, p)\) be the crystallographic bar-joint framework, that is, a bar-joint framework that underlies a crystal framework. Then the RUM dimension \( \text{dim}_{\text{rum}}(G, p) \) of \((G, p)\) is the real dimension of the real algebraic variety \( \Omega_{\text{prim}}(G, p) \).

The dimension here can be considered as the topological dimension of the manifold of non-singular points in case \( \Omega_{\text{prim}}(G, p) \) is irreducible. Otherwise, it is the maximal such dimension over irreducible components. In fact, we see in appendix A that the dimension of the RUM spectrum \( \Omega(C) \) of a crystal framework does not depend on the choice of translation group in view of a simple relationship between the RUM spectrum and the primitive RUM spectrum. Thus, we may view the RUM dimension of \( C \) as this common dimension.

In view of the determinations in §7 and our comments below, we shall see that

\[
\text{dim}_{\text{rum}}(C_{\text{sq}}) = 0, \quad \text{dim}_{\text{rum}}(C_{\text{star}}) = 1, \quad \text{dim}_{\text{rum}}(C_{\text{kag}}) = 1, \quad \text{dim}_{\text{rum}}(C_{\text{oct}}) = 1,
\]

in two dimensions, and in higher dimensions we have

\[
\text{dim}_{\text{rum}}(C_{\mathbb{Z}^d}) = d - 1, \quad \text{dim}_{\text{rum}}(C_{\text{Knet}}) = 2, \quad \text{dim}_{\text{rum}}(C_{\text{Oct}}) = 1, \quad \text{dim}_{\text{rum}}(C_{\text{SOD}}) = 3.
\]

For a framework in Maxwell counting equilibrium, the variety \( \Omega(C) \) is simply the zero set of \( p_C(z) \). For the kagome framework, for example, the polynomial is \((z - 1)(w - 1)(z - w)\) and we obtain the set which is the union of the three curves on \( \mathbb{T}^2 \) defined by \( z = 1, w = 1 \) and \( z = w \). In terms of wavevectors, this translates to the union of the three parametrized lines \((0, \alpha), (\alpha, 0)\) and \((\alpha, \alpha)\). Thus, the RUM dimension is 1.

When \( C \) is edge rich, with \(|F_e| > d|F_v|\), then one may instead form the finite family of polynomials of the \( d|F_v| \times d|F_v| \) submatrices of \( \Phi_C(z) \). Then the RUM spectrum will be a variety contained in the intersections of the zero sets of these polynomials on the \( d \)-torus.

We remark that the RUM spectrum will generally carry symmetries reflecting the point group symmetries of the crystal framework. Even so, the point group may be trivial and the following rather theoretical inverse problem may well have an affirmative answer.

**Problem.** Let \( q(z, w) \) be a polynomial with real coefficients with \( q(1, 1) = 0 \). Is there a crystal polynomial \( p(z, w) \) whose zero set on the 2-torus is the same as that for \( q(z, w) \)?

**(b) Floppy modes and their asymptotic order**

In applications, the term *floppy mode* often refers to rigid unit flexibility and oscillation within a large supercell and there is interest in the asymptotic order of the number of such modes as the supercell dimensions tend to infinity. In particular, a so-called *order N* crystal structure (to use terminology employed by material scientists) is one for which the asymptotic order agrees with the order of the number of atoms in the supercell, which is of order \( N = n^3 \) in an \( n \times n \times n \) supercell of a three-dimensional crystal. We now formalize this terminology in the direction of infinitesimal flexes and indicate connections with the RUM spectrum.
Definition 5.4. Let $C$ be a crystal framework in $\mathbb{R}^d$ with translation group $T = \{T_k : k \in \mathbb{Z}^d\}$.

(i) An $n$-fold periodic floppy mode of $C$ is a non-zero real vector $u = (u_k, k)$ in the nullspace (kernel) of the rigidity matrix $R(C)$ which is periodic for the subgroup $(n\mathbb{Z})^d$. That is, $u_k, k = u_k, 0$ for all $k \in (n\mathbb{Z})^d$.

(ii) $\nu_n$ is the dimension of the real linear space of real $n$-fold periodic floppy modes.

(iii) A crystal framework $C$ in $\mathbb{R}^3$ is of order $N\alpha$ for floppy modes, where $\alpha = 0, 1/3, 2/3$ or 1, if $\nu_n \geq Cn^{3\alpha}$ for all $n$ for some $C > 0$, while there is no such constant for the power $\alpha + 1/3$.

In particular, $C$ is said to be of order $N$ if $\nu_n \geq cn^3$ for some constant $c > 0$.

As the real and imaginary parts of a complex infinitesimal flex are real infinitesimal flexes, it follows that $\nu_n \leq \dim \ker R_n(C) \leq 2\nu_n$, where $R_n(C)$ is the rigidity matrix for $n$-fold periodicity viewed as a complex vector space linear transformation. Thus, in considerations of asymptotic order we may more conveniently consider the complex scalar case. The matrix $R_n(C)$ is the rigidity matrix for strict periodicity relative to the subgroup $T'$ of $T$ corresponding to the index subgroup $n\mathbb{Z} \times \cdots \times n\mathbb{Z}$. Accordingly, it is given as the periodic rigidity matrix associated with a motif for the $n$-fold supercell. Such a matrix can be taken simply as the union of $n^d$ translates of the given motif. More conveniently, it is possible to explicitly block diagonalize $R_n(C)$ (as a complex vector space transformation) as a direct sum (even an orthogonal direct sum for the natural inner product) of the matrices $\Phi(\omega)$ as $\omega$ ranges over the set of points, $T_n$ say, with coordinates $\omega_j$ of the form $e^{2\pi i k_j}/n$, where $0 \leq k_j < n$ are integers. This then gives the following counting formula for floppy modes:

$$\dim \ker R_n(C) = \sum_{0 \leq k_i, |< i \leq d} \dim \ker(\Phi_{C}(\omega^k)),$$

where $\omega^k = (e^{2\pi i k_1}/n, \ldots, e^{2\pi i k_d}/n)$. This formula resolves a question posed by Simon Guest. An elementary direct proof follows from the fact that non-zero vectors $u, v$ from distinct nullspaces $\ker \Phi_{C}(\omega^k)$ are linearly independent, on the one hand, and that, on the other hand, by the usual averaging arguments, any $n$-fold periodic flex may be decomposed as a sum of pure frequency $n$-fold periodic infinitesimal flexes. By ‘pure frequency’ we mean phase-periodic in each coordinate for some $n$th root of unity (depending on the coordinate). Details are given in appendix A.

It is of interest then to consider the rational subset of the RUM spectrum corresponding to periodic floppy modes, namely

$$\Omega_{\text{rat}}(C) := \bigcup_{n=1}^{\infty} (\Omega(C) \cap T_n^d)$$

and to ask: to what extent does the asymptotic order of the periodic floppy modes determine the RUM dimension?

In the case of crystal frameworks with a primitive RUM spectrum which is standard in the above sense, there is in fact a close connection. We make this clear below in the case of order $N$ (the maximal order). In the exotic case, one should expect examples where the rational points of the RUM spectrum are not dense. It would be of theoretical interest to identify, for example, a curved RUM spectrum containing only a finite number of rational points. Possibly, the regular octagon ring framework $C_{\text{oct}}$ has this property.

For the proof of theorem 5.6, we note the following lemma.

Lemma 5.5.

(i) Let $C$ be a $d$-dimensional crystal framework with motif set $(F_v, F_e)$ and RUM spectrum $\Omega(C) \subseteq T_n^d$. Then,

$$d - 1 + |\Omega(C) \cap T_n^d| \leq \dim \ker R_n(C) \leq d |F_v| |\Omega(C) \cap T_n^d|,$$

where $|F_v|$ is the number of vertices in the partition unit cell and where $T_n^d$ is the ‘discrete torus’ (in the $d$-torus $T_n^d$) determined by $n$th roots of unity.

(ii) If $\dim \ker R_n(C) \geq cn^\alpha$ for some $c > 0$, $\alpha > 0$, then $\dim(\Omega(C)) \geq \alpha$. 


Proof. (i) The counting formula implies the second inequality because \( \dim \ker(\Phi_C(\omega)) \leq d|F_v| \) for all \( \omega \). Also, if \( \omega^k \in \Omega(C) \cap \mathbb{T}_n^d \) then \( \dim \ker(\Phi_C(\omega^k)) \geq 1 \), while for wavevector \( k = (0,0,0) \) we have \( \dim \ker(\Phi_C(1,\ldots,1)) \geq d \), because there are certainly \( d \) linearly independent translation infinitesimal flexes. Thus, the first inequality follows.

(ii) follows from (i) because for any algebraic variety \( \Omega \), if the dimension is less than the integer \( \alpha \) then the cardinality of \( \Omega \cap \mathbb{T}_n^d \) is at most of order \( n^{\alpha-1} \).

It can be shown by direct linear algebra that if a crystal framework has order \( N \) then there exists a local infinitesimal flex.

**Theorem 5.6.** With the notation above, the following properties are equivalent for a crystal framework \( C \) in \( \mathbb{R}^d \).

(i) \( C \) has a local infinitesimal flex.

(ii) \( C \) is of order \( N \).

(iii) \( \dim_{\text{rum}}(C) = d \).

(iv) \( \Omega(C) = \mathbb{T}^d \).

Proof. To see that (i) implies (ii) note that if \( u \) is a non-zero local infinitesimal flex and \( \omega \) is any multi-phase in \( \mathbb{T}^d \), then the well-defined sum

\[
v = \sum_{k \in \mathbb{Z}^d} \omega^k T_k u
\]

is a phase-periodic infinitesimal flex. Also it is non-zero for almost every \( \omega \). Thus, (iv) holds, and hence (iii) and (ii).

If (ii) holds then (iii), and hence (iv), follows from the lemma and the fact that \( \Omega(C) \) is a real algebraic variety in \( \mathbb{T}^d \).

As (iv) implies (ii), it remains to show that (ii) implies (i) and this we do in appendix A.

### (c) Rigid unit mode spectrum versus primitive rigid unit mode spectrum

Note that if one doubles all the period vectors for \( C \) to obtain \( C' \) then it follows that the new RUM spectrum contains the range of the old spectrum under the argument doubling map, \( \pi : (w_1,w_2,w_3) \rightarrow (w_1^2,w_2^2,w_3^2) \). This follows immediately from the definition. The new symbol function, the number of rows and columns of which have increased \( 2^d \)-fold, is less useful at this point. In fact, the map \( \pi \), and its general form for arbitrary multiples of period vectors, gives a surjection \( \pi : \Omega(C) \rightarrow \Omega(C') \). (The details are given in appendix A.) In particular, while as a set \( \Omega(C') \) can be ‘smaller’ than \( \Omega(C) \) (for example, horizontal lines with rational intercepts in \( \Omega(C') \) may be coalesced in \( \Omega(C') \) under \( \pi \)) the dimension of the spectrum (as indicated above) remains the same.

### (d) Square-summable flexes

An infinitesimal flex being local represents the strongest form of rapid decay possible because it applies zero velocities to the framework points outside some bounded region. It is natural to enquire to what extent a crystal framework \( C \) might be resistant to flexes whose velocities diminish to zero at infinity. With this in mind, write \( \mathcal{K}_{\text{atom}}^2 \) and \( \mathcal{K}_{\text{bond}}^2 \) for the Hilbert spaces of square summable sequences in \( \mathcal{K}_{\text{atom}} \) and \( \mathcal{K}_{\text{bond}} \). Thus, \( u = (u_{k,j}) \in \mathcal{K}_{\text{atom}}^2 \) is such that the sum of the squares of the Euclidean norms \( |u_{k,j}| \) is finite. It is elementary to show that \( R(C) \) then determines a bounded Hilbert space operator from \( \mathcal{K}_{\text{atom}}^2 \) to \( \mathcal{K}_{\text{atom}}^2 \). For a given translation group \( T \), this operator intertwines the associated shift transformations, as before, although now these transformations are unitary operators on \( \mathcal{K}_{\text{atom}}^2 \) and \( \mathcal{K}_{\text{bond}}^2 \). Identifying square-summable sequences with square-integrable functions in a standard way one obtains unitary equivalences \( U_a \) and \( U_b \) between \( \mathcal{K}_{\text{atom}}^2 \) and \( L^2(\mathbb{T}^d) \otimes \mathbb{C}^{d|F_v|} \) and between \( \mathcal{K}_{\text{bond}}^2 \) and \( L^2(\mathbb{T}^d) \otimes \mathbb{C}^{d|F_v|} \), respectively. The corresponding unitary
transform $U_pR(\mathcal{C})U_p^*$ of the operator $R(\mathcal{C})$ is then a multiplication operator between these matrix-valued function spaces and the multiplying function is in fact the symbol function $\Phi_\mathcal{C}(z)$. In this way, the matrix function for $\mathcal{C}$ and its translation group appears naturally from the point of view of square-summable velocity sequences. For more details, see Owen & Power [7] where other operator-theoretic considerations are given.

More speculatively, it would be of interest to investigate other possible roles of the matrix function, particularly with regard to approximate flexes and quantitative issues. For example, for the three-dimensional framework $\mathcal{C}$ we may define the non-negative scalar function $\lambda$ on $\mathbb{T}^3$ with

$$\lambda: (z_1, z_2, z_3) \to \lambda_{\min}(\Phi_\mathcal{C}(z_1, z_2, z_3) \Phi_\mathcal{C}(z_1, z_2, z_3)),$$

where $\lambda_{\min}(A)$ denotes the smallest eigenvalue of the positive operator $A$. In particular, when the spectrum is trivial, that is, equal to the singleton set $\{(1, 1, 1)\}$, the function is non-vanishing except at this point, and so $\lambda$ could be viewed as a measure of RUM resistance.

6. Rigid unit modes and low-energy phonons

In the less idealized setting of traditional mathematical crystallography, mathematical models for crystalline dynamics assume that the atoms oscillate harmonically. The bond strengths are finite and a dynamical matrix embodying them governs the modes and wavevectors of phonon excitations. We show how the RUM spectrum $\Omega(\mathcal{C})$ arises as the set of wavevectors $\mathbf{k}$ of the harmonic excitations of $\mathcal{C}$ which induce vanishing bond distortion in their low-frequency (long-wavelength, low-energy) limits.

Suppose that $\mathcal{C}$ is a crystal framework in $\mathbb{R}^d$, with motif data $(F_v, F_e, T)$ and suppose that the vertices $p_{\kappa, \mathbf{k}}$ undergo a standard wave motion,

$$p_{\kappa, \mathbf{k}}(t) = p_{\kappa, \mathbf{k}} + u_{\kappa, \mathbf{k}}(t), \quad \kappa \in F_v, \mathbf{k} \in \mathbb{Z}^d,$$

where $u_{\kappa, \mathbf{k}}(t)$ represents the local oscillatory motion of atom $\kappa$ in the translated unit cell with label $k \in \mathbb{Z}^3$. Following standard formula-simplifying conventions, the framework point motions take values in $\mathbb{C}^d$, the case of real motion being recoverable from real and imaginary parts [9]. Thus, it is assumed that we have

$$u_{\kappa, \mathbf{k}}(t) = u_{\kappa} \exp(2\pi i \mathbf{k} \cdot \mathbf{k}) \exp(i\alpha t),$$

where $u = (u_\kappa)_{\kappa \in F_v}$ is a fixed vector in $\mathbb{C}^{|F_v|}$, where $\mathbf{k}$ is the wavevector and where $\alpha$ is the frequency.

Consider now the distortion $\Delta e(t)$ for the edge $e = [p_{\kappa, \mathbf{k}}, p_{\tau, \mathbf{k} + \delta(e)}]$ measured as the change in the square of the edge length. We have

$$\Delta e(t) := |p_{\kappa, \mathbf{k}}(t) - p_{\tau, \mathbf{k} + \delta(e)}(t)|^2 - |p_{\kappa, \mathbf{k}}(0) - p_{\tau, \mathbf{k} + \delta(e)}(0)|^2$$

$$= 2\text{Re}(p_{\kappa, \mathbf{k}} - p_{\tau, \mathbf{k} + \delta(e)}, u_{\kappa, \mathbf{k}}(t) - u_{\tau, \mathbf{k} + \delta(e)}(t))$$

$$+ 2\text{Re}(p_{\kappa, \mathbf{k}} - p_{\tau, \mathbf{k} + \delta(e)}, u_{\kappa, \mathbf{k}}(0) - u_{\tau, \mathbf{k} + \delta(e)}(0)) + \epsilon(u, \mathbf{k}, k, \alpha t),$$

where

$$\epsilon(u, \mathbf{k}, k, \alpha t) = |u_{\kappa, \mathbf{k}}(t) - u_{\kappa + \delta(e)}(t)|^2 - |u_{\kappa, \mathbf{k}}(0) - u_{\kappa + \delta(e)}(0)|^2.$$

First note that in any finite time period $[0, T]$ the difference quantities $\epsilon(u, \mathbf{k}, k, \alpha t)$ tend to zero uniformly, for all $t \in [0, T]$ and all $k$ in $\mathbb{Z}^3$, as the frequency $\alpha$ tends to zero. This follows readily from the fact that for any $\theta$ the quantity

$$|\sin(\alpha t + \theta) - \sin(\alpha t)|^2 - |\sin(\theta) - \sin(0)|^2$$

tends to zero uniformly for $t \in [0, T]$ as $\alpha$ tends to zero.
For the other terms for $\Delta_{\epsilon}(t)$ note that

$$2\text{Re}\langle p_{k,k} - p_{r,k+\delta(c)}, u_{k,k}(t) - u_{r,k+\delta(c)}(t) \rangle = 2\text{Re}[e^{-at-2\pi ik\cdot k}(p_{k,k} - p_{r,k+\delta(c)}, u_{k,k} - \omega^{\delta(c)} u_{r,k})]$$

$$= 2\text{Re}[e^{-at-2\pi ik\cdot k}(p_{k,k} - p_{r\delta(c)}, u_{k,k} - \omega^{\delta(c)} u_{r,k})]$$

which is zero, irrespective of $t$, if $(\omega^k u_k)$ is an infinitesimal flex of the framework.

It follows that we have proved the implication (i) implies (ii) in the following theorem and in fact the converse assertion follows from the same equations. The theorem underlies the correspondence of the points in $\Omega(C)$ with the wavevectors of RUM phonons that arise in simulations.

**Theorem 6.1.** Let $C$ be a crystal framework, with specified periodicity, and let $k$ be a wavevector with point $\omega \in \mathbb{T}^3$. Then, the following assertions are equivalent.

(i) $(\omega^k u_k)_{k,k}$ is a non-zero phase-periodic infinitesimal flex for $C$.

(ii) For the vertex wave motion

$$p_{k,k}(t) = p_{k,k} + u_k \exp(2\pi i k \cdot k) \exp(iat),$$

and a given time interval, $t \in [0, T]$, the bond length changes

$$\delta(t) = |p_{k,k}(t) - p_{r,k+\delta(c)}(t) - |p_{k,k}(0) - p_{r,k+\delta(c)}(0)|$$

tend to zero uniformly, in $t$ and $e$, as the wavelength $2\pi / \alpha$ tends to infinity.

In the past two decades, the RUM spectra of frameworks associated with specific material crystals have been derived by experiment and by simulation using lattice dynamics. Some of the results of this approach can be found in [1–5]. In particular, the program CRUSH has been used for this purpose and this method reflects principle (ii) in the theorem above. Indeed, in the simulations a double limiting process is used (the split atom method) in which each shared vertex (often an oxygen atom) is duplicated, for each rigid unit, and connected by bonds of zero length and increasing strength, tending to infinity. In this set-up, the RUM wavevectors coincide with those for which the long-wavelength limits have vanishing energy and through this connection they can be identified in simulation experiments and counted.

### 7. Determinations of rigid unit mode spectra

The RUM spectrum is now determined for a variety of basic crystal frameworks. Also, we emphasize an infinitesimal flex method for the identification of lines and planes of wavevectors. The spectrum is of standard type (in the sense given in the remarks in §5) for the frameworks $C_{2z^2}$, $C_{sq}$, $C_{star}$, $C_{kag}$, $C_{Knet}$, $C_{Oct}$ and $C_{SOD}$, while for the two-dimensional zeolite $C_{Oct}$ it is a union of four closed curves.

Consider once again the basic grid framework $C_{2z^2}$ in the plane with motif consisting of a single vertex, $F_v = \{p_k\}$, and two edges. Examining all edges, it becomes evident that there exists an infinitesimal flex $u$ supported on the $x$-axis, with $u_{k,(k_1,0)} = (1, 0)$ for all $k_1 \in \mathbb{Z}$. Using all the parallel translates $T(0,k_2)u$ of $u$, we may define a phase-periodic velocity vector $v$ in $\mathcal{K}_{atom}$,

$$v = \sum_{k_2 \in \mathbb{Z}} \omega^{k_2}_2 T(0,k_2)u,$$

where $\omega_2$ is a fixed point in $\mathbb{T}$. Note that $v$ is well defined and

$$R(C)v = R(C) \sum_{k_2 \in \mathbb{Z}} \omega^{k_2}_2 T(0,k_2)u = \sum_{k_2 \in \mathbb{Z}} \omega^{k_2}_2 R(C)T(0,k_2)u = \sum_{k_2 \in \mathbb{Z}} \omega^{k_2}_2 T(0,k_2)R(C)u = 0.$$
wavevectors \((0, \alpha)\). By symmetry, the line \((\alpha, 0)\) is also included. Similar arguments apply to the kagome lattice which also has linearly localized infinitesimal flexes. (See also [20,21] for example.)

More generally, suppose that a crystal framework \(C\) has a non-zero infinitesimal flex \(u\) which is

(a) band limited, in the sense of being supported by a set of framework vertices within a finite distance of a direction axis for \(T\) and

(b) periodic, or more generally, phase-periodic in the direction axis direction.

By (a) one can form a sum analogous to that above, using the complementary axis direction(s), to obtain a well-defined phase-periodic infinitesimal displacement which, by translational invariance and linearity, is an infinitesimal flex. If \(\omega_1\) is the phase in (b) then we deduce that \(\{\omega_1\} \times T^{d-1}\) is contained in \(\Omega(C)\).

Thus, for the grid framework \(C_{Z^3}\) in three dimensions, one deduces from the evident line-localized infinitesimal flexes that there are three surfaces, \(z = 1\), \(w = 1\) and \(u = 1\), in \(\Omega(C_{Z^3})\). In general, a line-localized flex of this type leads directly to a hyperplane of wavevectors in the RUM spectrum.

Similar observations hold for plane-localized flexes. In three dimensions, for example, such a flex, which is assumed to be ‘in-plane phase-periodic’, leads to a line of RUM wavevectors. This is the case for \(C_{Oct}\), considered below, and the RUM spectrum here is the union of these planes.

**Example (a): The regular 4-ring framework \(C_{\text{star}}\).** This two-dimensional zeolite is defined by translates of the regular 4-ring of equilateral triangles in figure 6. It is sufficiently simple that one can deduce its RUM spectrum and its crystal polynomial \(p_{\text{star}}(z, w)\) from infinitesimal arguments.

For a motif, we may take \(F_e\) to consist of the edges of the 12-edged star and take \(F_v\) to be the set of four vertices of the square together with the westward and southern vertex. The four edges in the motif incident to the external vertices (north and eastward) provide four rows of the 12 by 12 matrix \(\Phi_C(z, w)\) each of which carries simple monomials (either \(z\) or \(w\) or their conjugates). Thus, \(p_C(z, w)\) has total degree at most 4. One can identify band-limited infinitesimal flexes as indicated in figures 6 and 7. Here, the top and bottom vertices of each are fixed and there is horizontal periodic extension to a band-limited infinitesimal flex. In the former case, there is two-step horizontal periodicity while in the latter case there is strict horizontal periodicity although the band is two cells wide.

From the discussion above, the first band-limited flex shows that the phase \((-1, \omega_2)\) lies in \(\Omega(C)\) for all \(\omega_2 \in T\). By symmetry \((\omega_1, -1) \in \Omega(C)\) for all \(\omega_1 \in T\). The second band-limited flex shows that \(\{1\} \times T\) lies in \(\Omega(C_{\text{star}})\) and hence so too does \(T \times \{1\}\) by symmetry. Thus, \(\Omega(C)\) contains the set

\[\{(1) \times T\} \cup (T \times \{1\}) \cup ((-1) \times T) \cup (T \times \{-1\})\]

and so \(p_C(z, w)\) must be divisible by the irreducible factors \(z - 1, w - 1, z + 1, w + 1\). As \(p_C(z, w)\) has total degree at most 4 it follows that either \(p\) vanishes identically or

\[p_C(z, w) = (z - 1)(w - 1)(z + 1)(w + 1)\].

**Figure 6.** A 2-cell-periodic band-limited flex of \(C_{\text{star}}\).
In fact, the former case does not hold. One can see this, thematically, by demonstrating that there are no local flexes or one may compute $\det \Phi(1/3, 1/3) \neq 0$. Thus, the RUM spectrum is precisely the fourfold union above.

Example (b): The two-dimensional zeolite framework $C_{oct}$. There are no local or band-limited infinitesimal flexes evident for the regular octagon framework, and so the expectation is that the RUM spectrum is trivial or a union of proper curves.

Returning to the two-dimensional zeolites of figure 5, the third of these, with external angle $8\pi/12$, is equal to $C_{star}$, although with a different translation group, $T'$, for which the old period vectors are rotated by $\pi/4$ and scaled by the factor $\sqrt{2}$. In view of this rotation, it follows that

$$\Omega(C_{star}, T') = \{(w, w), (w, -w) : w \in \mathbb{T}\}.$$ 

In terms of reduced wavevectors, this corresponds to the subset of the unit square $[0, 1)^2$ given as the union of the two diagonals.

As we have noted earlier, the 4-pointed star framework is related to its 8-pointed star companion $C_{oct}$ by a continuous flex. It follows that the 24 by 24 symbol matrix function $\Phi_{star}(z_1, z_2)$ for the former (for $T'$) is naturally ‘continuously connected’ to the symbol function $\Phi_{oct}(z_1, z_2)$ by an explicit continuous path $t \rightarrow \Phi(t(z_1, z_2))$. This in turn provides a set-valued map which we refer to as the RUM spectrum evolution for this (periodicity-preserving) flex:

$$t \rightarrow \Omega(\Phi_t(z)).$$

When this is made explicit by computation the octagon framework has exotic (nonlinear) spectrum as indicated in figure 8 and evolves towards the cross-shaped spectrum of $C_{star}$ under the continuous flex.

In fact, one can obtain the RUM spectrum of the octagon framework completely analytically, although with some significant algebraic complexity, as follows.

Note first that a motif for $C_{oct}$ is formed by the 24 edges of the 8-ring for $F_e$ with $F_v$ obtained by omitting four boundary vertices as, for example, in figure 5. There are eight edges with external...
Figure 8. The curved wavevector spectrum of $C_{\text{oct}}$.

vertices and each contributes a row to $\Phi_{\text{oct}}$ with a simple monomial, and so it follows that $p_{\text{oct}}(z, w)$ has degree 8 at most. The $24 \times 24$ function matrix $\Phi_{\text{oct}}(z)$ is sparse and the (at most) four non-zero functions in each row may be conveniently normalized by dividing by the magnitude of the $x$-coordinate difference for that row. The magnitudes of the non-zero non-unit entries are then the tangents of the angles $k\pi/24$, for $k = 1, 3, 5, 7, 9, 11$, all of which lie in the field extension $\mathbb{Q}(\sqrt{2}, \sqrt{3})$.

The crystal polynomial can be computed and admits an explicit factorization as the product

$$p_{\text{oct}}(z, w) = p_1(z, w)p_2(z, w),$$

where

$$p_1(z, w) = z^2w - (\sqrt{3} + \sqrt{2})zw^2 + 2(\sqrt{3} + \sqrt{2} - 1)zw - (\sqrt{3} + \sqrt{2})z + w$$

and

$$p_2(z, w) = z^2w - (\sqrt{3} - \sqrt{2})zw^2 + 2(\sqrt{3} - \sqrt{2} - 1)zw - (\sqrt{3} - \sqrt{2})z + w.$$
finite framework which assigns zero velocities to the six boundary vertices and a non-zero vertical velocity to the central vertex. Thus, the entire framework has a local infinitesimal flex, and so the RUM spectrum is all of $T^2$.

We remark that in general it need not be the case that an order $N$ crystal framework has a local infinitesimal flex internal to a unit cell. For example, one could take a new motif and unit cell in which the central vertex is shifted to the boundary and in this case one has to consider a larger supercell before a local RUM appears.

**Example (d): The kagome net framework $C_{Knet}$ and its polynomial.** The RUM spectrum of the three-dimensional kagome net framework can be derived from that of the two-dimensional kagome framework. The spectrum of the latter is the zero set on the torus $T^2$ determined by the crystal polynomial, which an earlier computation showed was equal to $(z - 1)(w - 1)(z - w)$. One can derive this from infinitesimal flex analysis as follows. It is elementary to show that there is no local infinitesimal flex, and so $p_{kag}(z, w)$ is necessarily non-zero. There are line-supported infinitesimal flexes in the directions of the period vectors $a_1$ and $a_2$, so it follows from the discussion above that $(z - 1)$ and $(w - 1)$ are factors. Let $u$ be a (similar) infinitesimal flex supported on a line in the direction $a_1 - a_2$ and consider the infinitesimal flexes $v = \sum_{k \in \mathbb{Z}} \omega^k T_{(k,0)} u$ for $\omega \in T$. In view of the triangular symmetry of $C_{kag}$ in fact this flex is phase-periodic for the phase $(\omega_1, \omega_2)$ and it follows that $(z - w)$ is necessarily a factor of $p_{kag}(z, w)$. One can see, without calculation, that the total degree of this polynomial is at most three and so the derivation is complete.

Moving up a dimension, a phase-periodic flex of $C_{kag}$, with phase $(\omega_1, \omega_2)$ say, induces a ‘layer-limited’ infinitesimal flex of the kagome net framework $C_{Knet}$. Thus, for all $\omega \in T$ there is an infinitesimal flex of $C_{Knet}$ with phase $(\omega_1, \omega_2, \omega)$. Similar assertions hold for the other two translation group planes. The crystal polynomial $p_{Knet}(z, w, u)$ has total degree at most six and must vanish on the six planes $z - 1 = 0, w - 1 = 0, u - 1 = 0, z - w = 0, w - u = 0, z - u = 0$. It follows that

$$p_{Knet}(z, w, u) = (z - 1)(w - 1)(u - 1)(z - w)(w - u)(z - u),$$

for the monomial order with $z > w > u$.

The polynomial above was also obtained in Wegner [6] and Owen & Power [7] by direct calculation.

The kagome net framework and its various periodic positions or placements feature as the tetrahedral net frameworks for a range of materials and their phases. It is the framework for $\beta$-cristobalite, for example, while a particular placement gives the framework for tridymite. This was the first material for which curved surfaces of RUMs were observed [5].

**Example (e): Sodalite and $C_{SOD}$.** The framework $C_{SOD}$ has a symbol function with 72 rows and columns. Indeed, it is in Maxwell counting equilibrium, being a three-dimensional zeolite crystal framework, and the motif set $F_e$ consists of the edges of three 4-rings of tetrahedra. We prove that
\(C_{\text{SOD}}\) is of order \(N\). Specifically, we show, by infinitesimal flex geometry, that there is a non-zero infinitesimal flex \(v\) of the finite sodalite cage framework such that all the outer vertices are fixed by \(v\). That is, \(v_{x,y} = 0\) if \(p_{x,y}\) is any of the 24 outer vertices of the cage. The ‘outer fixed’ sodalite cage framework has 36 free vertices with 108 degrees of freedom while there are 144 constraining edges. Despite this considerable overconstraint, there is sufficient symmetry to allow in a proper infinitesimal flex.

We shall show that an individual 4-ring, \(R_1\) say, of the sodalite cage has an infinitesimal flex, \(v^{(1)}\) say, which fixes a coplanar quadruple of ‘outer’ vertices, such as the upper vertices of the 4-ring in figure 4, and flexes the other quadruples in their common plane. These four velocities have equal magnitudes and in figure 4 are directed towards two opposing corners of the imaginary cube. (See the flex arrows in figure 4.) Taking \(v^{(1)}\) so that these vectors have magnitude 1 it follows that \(v^{(1)}\) is determined up to sign and that this sign may be specified by labelling the cube corners ‘a’ and ‘r’ for their attracting and repelling sense. Note that one can label the eight corners of the imaginary cube in this manner so that no similar labels are adjacent. In this case, the individual flexes \(v^{(1)}, \ldots, v^{(6)}\) of the six 4-rings of the sodalite cage have equal displacement vectors at common vertices. This consistency shows that there is an infinitesimal flex of the entire sodalite cage in which the outer vertices are fixed, as required.

It remains to show that there is the stated flex of the 4-ring \(R_1\). To this end, let \(p_1, p_2\) be two non-opposite top vertices of \(R_1\) which are forced to have the same displacement and let \(p_1, p_3, p_4\) be the vertices of an inward facing face of a tetrahedron of \(R_1\) with vertices \(p_1, p_3, p_4, p_5\), so that the lower vertex \(p_5\) is a cube-edge midpoint. There is a unique ‘inward and upward’ displacement velocity \(u_3\) of the intermediate vertex \(p_3\) which has unit length and is such that \((u_1, u_2, u_3) = (0, 0, u_3)\) is a flex for the two edges \([p_1, p_3], [p_3, p_2]\). The displacement vector \(u_3\) induces a unique displacement vector \(u_5\) which is in the direction of the cube edge and is such that

\[
(u_5 - u_3, p_5 - p_3) = 0.
\]

The triple \(u_1 = 0, u_3\) and \(u_5\) now determine the infinitesimal motion of the tetrahedron, with flex vector \(u_4\) for \(p_4\). However, the reversal (sign change) of \(u_3\) induces the reversal of \(u_5\), so it is clear from the symmetric position of the tetrahedron that \(u_4\) must be the unique unit norm ‘outward and downward’ flex at \(p_4\). Continuing around the ring it follows that \(R_1\) has the desired infinitesimal flex.

One can apply similar constructive flex arguments to other zeolite frameworks and of course to any zeolite crystal framework which contains a sodalite cage as above, such as \(C_{\text{LTA}}\). Also we note (as do Kapko et al. [23]) that \(C_{\text{RWY}}\) is derived from \(C_{\text{SOD}}\) by replacing each tetrahedron by a rigid unit of four tetrahedra. Thus, the same infinitesimal flex geometry applies and \(C_{\text{RWY}}\) has order \(N\).

**Example (f): Perovskite, \(C_{\text{sq}}\) and \(C_{\text{Oct}}\).** Consider the integer translation group \(T\) and the determination of the framework through the primitive motif \((F_v, F_e)\), where

\[
F_v = \{0, \frac{1}{2}, \frac{1}{2}, (\frac{1}{2}, 0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}, 0)\} = \{p_{x,y} : 1 \leq x \leq 3\}
\]

and where \(F_e\) consists of the twelve framework edges between the centres of adjacent faces of the unit cube \([0, 1]^3\). Thus, the vertices of \(V(F_e) F_v\) have the form \(p_{i,y,z}\), where \(y_1 = (1, 0, 0), y_2 = (0, 1, 0)\) and \(y_3 = (0, 0, 1)\). The framework is therefore edge rich and the matrix function \(\Phi_{\text{Oct}}(z)\) is 12 by 9.

The framework \(C_{\text{Oct}}\) is a three-dimensional analogue of the two-dimensional squares framework \(C_{\text{sq}}\) and may be obtained from it by a layer construction and a discarding of redundant edges internal to the octahedra. Thus, infinitesimal flexes of the two-dimensional squares lattice imply plane-localized flexes for \(C_{\text{Oct}}\). This observation can be made the basis for an infinitesimal flex analysis determination of the RUM spectrum. A more algebraic approach is possible as follows.
Performing row operations on $\Phi_{C_{sq}}(z)$, as given in §2, we see that $(\bar{z}, \bar{w})$ is a point of the RUM spectrum if and only if the equivalent matrix

$$
\Psi(z, w) = \begin{bmatrix}
1 & -1 & -1 & 1 \\
0 & -2 & z - 1 & z + 1 \\
0 & 0 & 1 - wz & 1 - wz \\
0 & 0 & 0 & -2z + 2w \\
0 & 0 & -2 + 2z & 0
\end{bmatrix}
$$

has rank less than 4. This occurs if and only if

$$
\begin{bmatrix}
1 - wz & 1 - wz \\
0 & -2z + 2w \\
-2 + 2z & 0
\end{bmatrix}
$$

has rank equal to 0 or 1. The rank is 0 if and only if $z = w = 1$, corresponding to the two-dimensional space of rigid motions with phase $(1, 1)$, and the rank is 1 if and only if $z = w = -1$. Thus,

$$
\Omega(C_{sq}) = \{(1, 1), (-1, -1)\}.
$$

The infinitesimal flex for the phase $(-1, -1)$ is the one for which the rigid units, in this case squares with diagonals, rotate infinitesimally in alternating senses.

The alternating rotation flex of $C_{sq}$ induces a plane-localized flex of $C_{Oct}$ in each of the framework planes $x = 1/2, y = 1/2, z = 1/2$. It follows that $\Omega(C_{Oct})$ contains the three sets of phases

$$
\mathbb{T} \times \{-1\} \times \{-1\}, \quad \{-1\} \times \mathbb{T} \times \{-1\} \quad \text{and} \quad \{-1\} \times \{-1\} \times \mathbb{T}.
$$

That the spectrum is no more than the union of these sets and the singleton $(1, 1, 1)$ can be seen from a row analysis of the 12 by 9 function matrix $\Phi_{C_{oct}}(z)$ in the same style as the argument for $C_{sq}$. Thus, in wavevector formalism, the RUM spectrum of the octahedral net $C_{Oct}$ is the set of lines

$$
(\alpha, \frac{1}{2}, \frac{1}{2}), \quad (\frac{1}{2}, \alpha, \frac{1}{2}) \quad \text{and} \quad (\frac{1}{2}, \frac{1}{2}, \alpha)
$$

together with the wavevector $(0, 0, 0)$.

The corner-connected octahedron net crystal framework $C_{Oct}$ is associated with cubic perovskites, such as SiTO$_3$, and RUM distributions have been determined experimentally [1,5].

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Appendix A. The periodic floppy mode counting formula

For notational clarity, we assume that $d = 3$. Let $r = (r_1, r_2, r_3)$ and consider the finite-dimensional space $K^r_d$ of $r$-periodic complex velocity vectors.

Write $k \in r$ to denote $k = (k_1, k_2, k_3)$ with $0 \leq k_i < r_i$. For $\omega_l = e^{2\pi i/r_l}$ for $l = 1, 2, 3$, write $\mathbb{T}^3_r$ for ‘discrete torus’

$$
\mathbb{T}^3_r = \{\omega = (\omega_1^{k_1}, \omega_2^{k_2}, \omega_3^{k_3}) : k \in r\}.
$$

If $z = (z_1, z_2, z_3)$ is a point of the usual 3-torus $\mathbb{T}^3$ we write $z^k$ for the product $z_1^{k_1} z_2^{k_2} z_3^{k_3}$ in $\mathbb{T}^3$. Similarly, with $W_1, W_2, W_3$ defined as the shift transformations $T_{r_1}, T_{r_2}, T_{r_3}$ restricted to the space $K^r_d$ we write $W^k$ for the product $W_1^{k_1} W_2^{k_2} W_3^{k_3}$. In particular, $W^r = I$. 

Note that if $u$ is an $r$-fold periodic flex then the velocity vector
\[ u' = \sum_{k \in \mathbb{Z}} W^k u \]
is strictly periodic. As $R(C)$ commutes with the shifts the velocity vector $u'$ is a sum of infinitesimal flexes, and so is a strictly periodic infinitesimal flex.

Similarly, if $\omega \in \mathbb{T}^3$ then
\[ u_\omega = \sum_{k \in \mathbb{Z}} \omega^k W^k u \]
is an infinitesimal flex which is phase-periodic for $\tilde{\omega}$. As we have the recovery formula
\[ u = \frac{1}{r_1 r_2 r_3} \sum_{\omega \in \mathbb{T}^3} u_\omega \]
it follows that the space of $r$-fold periodic infinitesimal flexes is the direct sum of the space of $\omega$-phase periodic infinitesimal flexes. The counting formula now follows.

**Surjectivity of $\pi : \Omega(C) \to \Omega(C')$.** Similarly, let $T'$ be the subgroup of the translation group $T = \{T_k : k \in \mathbb{Z}^3\}$ for $C$ which is associated with $(r_1, r_2, r_3)$, let $C'$ be the associated crystal framework and suppose that $u$ is a non-zero phase-periodic infinitesimal flex of $C'$ with multi-phase $\eta$ in $\mathbb{T}^3$.

Let $\mathbb{T}_{r, n}$ be the set of points $(z_1, z_2, z_3)$ where $z_i$ ranges over the $r_i$ roots of $\eta_i$. If $\omega \in \mathbb{T}_{r, n}$, then the velocity vector
\[ u_\omega = \sum_{k \in \mathbb{Z}} \omega^k W^k u \]
is an infinitesimal flex for $C$ which is phase-periodic for $C'$, with multi-phase $\tilde{\omega}$. Also, we have the recovery formula
\[ (\eta_1 \eta_2 \eta_3)u = \frac{1}{r_1 r_2 r_3} \sum_{\omega \in \mathbb{T}^3} u_\omega. \]

It follows that at least one of the flexes $u_\omega$ is non-zero. That is, there is an $r$-fold root of $\eta$ in the RUM spectrum $\Omega(C)$ and the surjectivity of the map $\pi$ follows.

**The existence of local infinitesimal flexes.** We prove the following.

**Theorem A.1.** Let $C$ be a crystal framework in $\mathbb{R}^d$ which is of maximal order (‘order $N$’) for periodic floppy modes. Then, $C$ has a local infinitesimal flex.

**Proof.** Consider the vector space $\mathcal{V}_n$, say, of $n$-fold periodic real velocity vectors. This has dimension $|dF_v|n^d$ as $n$ goes to infinity. By assumption, the subspaces $\ker R_n(C)$ have dimensions of order $n^d$. Fix the motif $M = (F_v, F_\omega)$ for $C$ and consider the natural motifs $M_n$ for the $n$-fold translation group which are formed by translates of $M$ ($n^d$ translates in fact). (One could arrange $M_n \subseteq M_{n+1}$ but this is not necessary for the argument.) The motif $M_n$, which is a pair $(F_v(n), F_\omega(n))$, has boundary vertices by which we mean the vertices of edges in $F_\omega(n)$ which are not vertices in $F_v(n)$. Note that the cardinality of these sets gives a sequence of order $n^{d-1}$. Thus the vector subspace, $B_n$, say, of $n$-fold periodic real velocity vectors which assign zero velocities to the non-boundary vertices has dimension of order $n^{d-1}$.

Let $P_n : \mathcal{V}_n \to B_n$

be linear transformations that are projections. Then, in view of the order of dimension growth elementary linear algebra shows that there is a non-zero vector $u$ in $\ker R_n(C)$ for some large enough $n$ such that $P_n(u) = 0$.

Let $u'$ be the velocity vector which agrees with $u$ for components for the non-boundary framework points of $M_n$ and is defined to be zero for all other coordinates.

As the $n$-fold periodic flex $u$ ‘vanishes on the boundary of the $n$-fold supercell’ in the sense above, one can readily check that $u'$ is an infinitesimal flex of $C$. Also $u'$ is non-zero and finitely supported, as desired. ■
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